TITLE: TOWARDS CANCER-CELL SELECTIVE, NEAR-INFRARED-ABSORBING BIMETALLIC PHOTOSENSITIZERS FOR PHOTODYNAMIC THERAPY IN HYPOXIA

Topic number : ***2023_002***

Field : Chemistry, Physical chemistry and Chemical Engineering, ,

Subfield:

ParisTech School: Chimie ParisTech - PSL
Research team: Laboratory for Inorganic Chemical Biology
http://www.gassergroup.com
Research lab: I-CLEHS - Institute of chemistry for life and health
Lab location: Paris
Lab website:http://www.gassergroup.com

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Gasser Gilles gilles.gasser@chimieparistech.psl.eu
Advisor 2: Cariou Kevin kevin.cariou@chimieparistech.psl.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Photodynamic Therapy (PDT) is an approved medical technique to treat certain types of cancer. However, cancer cells have a lower amount of oxygen than healthy ones, limiting the success of PDT treatments since oxygen is one of the three required components with the presence of a photosensitizer and light. In this context, our group has recently demonstrated that some metal complexes could work under hypoxic conditions and under near-IR irradiation. However, such compounds are not selective for cancer cells. In this project, we envision to target some cancer-cell overexpressed enzymes such carbonic anhydrase to increase the selectivity of our compounds. In order to have a theranostic compound, bimetallic compounds will be prepared allowing for both therapy and imaging. At this end of this project, we hope to have unveiled a compound that work not only on cancer cells but also on mice tumor models.

Required background of the student: The applicant should have a sound knowledge (theoretical and practical) in both inorganic and organic synthetic chemistry and be proficient with analytical techniques

such as NMR and MS. The applicant must be fluent in English since it is the language spoken in the Gasser group. Practical knowledge in biology would be an asset.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. J. Karges, S. Kuang, F. Maschietto, O. Blacque, I. Ciofini, H. Chao,* and G. Gasser,* Nature Commun., 2020, 11, 3262.

2. J. Karges, F. Heinemann, M. Jakubaszek, F. Maschietto, C. Subecz, M. Dotou, R. Vinck, O. Blacque, M. Tharaud, B. Goud, E. Viñuelas Zahínos, B. Spingler,* I. Ciofini,* and G. Gasser,* J. Am. Chem. Soc., 2020, 142, 6578-6587.

3. A. Mani, T. Feng, A. Gandioso, R. Vinck, A. Notaro, L. Gourdon, P. Burckel, B. Saubaméa, O. Blacque, K. Cariou, J.-E. Belgaied, H. Chao,* and G. Gasser,* Angew. Chem. Int. Ed., 2023, 62, e202218347.

4. G. Vigueras and G. Gasser,* Nature Chem., 2023, 15, 896-898.

5. E. Ortega-Forte, A. Rovira, M. López Corrales, A Hernández García, F.J. Ballester, E. Izquierdo-García, M. Jordà-Redondo, M. Bosch, S. Nonell, M. Dolores Santana, J. Ruiz,* V. Marchán* and G. Gasser,* Chem. Sci., 2023, 14, 7170-7184.

Illustrations :

TITLE: ENGINEERING OF MULTIMODAL MAGNETIC RESONANCE AND OPTICAL IMAGING USING ACTIVABLE THERANOSTIC NANOPARTICLES FOR PDT AND PTT AGAINST CANCER IN PRECLINICS

Topic number : ***2023_003***

Field : Life and Health Science and Technology, Chemistry, Physical chemistry and Chemical Engineering,

Subfield: Nanotheranostics

ParisTech School: Chimie ParisTech - PSL
Research team: SEISAD https://iclehs.fr/research/seisad/
Research lab: I-CLEHS - Institute of chemistry for life and health
Lab location: Paris
Lab website:https://www.chimieparistech.psl.eu/recherche/les-laboratoires/i-clehs/

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Doan Bich-Thuy bich-thuy.doan@chimieparistech.psl.eu
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Cancer is a major public health problem worldwide. Clinical cancerology therefore needs the development of both: i) sensitive and efficient diagnostic methods such as bioimaging and ii) effective but better tolerated new therapies. In this context, the research in theranostics for innovative and efficient systems to effectively diagnose and treat cancers is highly active: design of multi-functional chemical objects composed of nanoparticles (NP) with bioimaging features. These objects are probes able to target tumoral tissues, to encapsulate medicine for therapeutical purpose, and more importantly to be activable by light to spatio temporally control their therapeutic activation. In particular, photodynamic PDT and photothermal PTT therapies will be investigated. We propose to develop quantitative multimodal and multiscale molecular bioimaging methods based on MRI and optical imaging to codevelop innovative nanomedecine based on various nanoparticles : luminescent and magnetic nanoparticles synthesized in collaboration with chemists team at the Université PSL and Sorbonne Université. The task is to gather multiparametric imaging data (molecular, functional, anatomic, …) to create new diagnostic

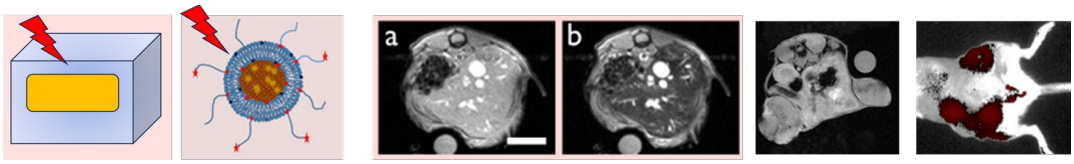
imaging biomarkers applied to the study of cancer on tumor murine models, and innovative activable photosensitizers nanoplatforms for photodynamic therapy PDT and photothermal therapy PTT.
The different tasks will be : participation in the formulation, physicochemical and imaging characterization of the theranostic probes in vitro, MRI and optical bioimaging developments adapted to the probes for antitumor therapy in preclinics, PDT aand PTT assays in vitro to in vivo

Required background of the student: Biophysics, Imaging, Chemistry, Biology

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Ramniceanu G., Doan BT., Vezignol C., Graillot A., Loubat C., Mignet N. and Berret J.-F. Delayed hepatic uptake of multi-phosphonic acid poly(ethylene glycol) coated iron oxide measured by real-time Magnetic Resonance Imaging, RSC Adv., 2016,6, 63788
2. Thébault CJ, Ramniceanu G, Boumati S, Michel A, Seguin J, Larrat B, Mignet N, Ménager C, Doan BT. Theranostic MRI liposomes for magnetic targeting and ultrasound triggered release of the antivascular CA4P. J Control Release. 2020 4;322:137-148. doi: https://doi.org/10.1016/j.jconrel.2020.03.003
3. Do HD, Couillaud BM, Doan BT, Corvis Y, Mignet N Advances on non-invasive physically triggered nucleic acid delivery from nanocarriers. Adv Drug Deliv Rev. 2019;138:3-17. doi: 10.1016/j.addr.2018.10.006
4. Boumati S. Gasser G., Doan BT. phD 2021. U PSL. Engineering of Multimodal Magnetic Resonance and optical Imaging using targeted theranostic nanoparticles for diagnosis and therapeutic studies against cancer in preclinics
5. Zhang Y, Doan BT, Gasser G. ACS rev. 2023 Zhang Y, Doan BT, Gasser G. Metal-Based Photosensitizers as Inducers of Regulated Cell Death Mechanisms. Chem Rev. 2023;123(16):10135-10155. doi: 10.1021/acs.chemrev.3c00161

Illustrations :


a
b

ParisTech

Arts et Métiers Sciences et Technologies

TITLE: REINFORCEMENT LEARNING-BASED TOPOLOGY-PRESERVING NON-RIGID DEFORMATION OF CAD MODELS FROM POINT CLOUDS FOR FIRST-TIME-RIGHT PRODUCTION IN SMART MANUFACTURING

Topic number : ***2023_007***

Field : Design, Industrialization, Information and Communication Science and Technology, Mathematics and their applications

Subfield: Artificial Intelligence

ParisTech School: Arts et Métiers
Research team:
Research lab: LISPEN - Laboratoire d'ingénierie des systèmes physiques et numériques
Lab location: Aix-en-Provence
Lab website:https://lispen.ensam.eu

Contact point for this topic: Arts et Métiers

Advisor 1: PERNOT Jean-Philippe jean-philippe.pernot@ensam.eu
Advisor 2: POLETTE Arnaud arnaud.polette@ensam.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: This PhD program addresses the way CAD models can be adapted and deformed to capture the manufacturing defaults and thus maintain the coherence between the digital model and its physical and manufactured counterpart. This is particularly useful to optimize tool paths and manufacturing parameters. New deformation operators will be developed to simulate and reproduce various state-of-the-art manufacturing behaviors and deviations, including free-form and non-rigid deformations. Those operators will be applied until the deviation between the CAD model and the acquired point cloud of the manufactured counterpart is minimized. During the deformation process, the topology of the CAD models will be preserved, to be able to maintain the whole coherency and possibly available semantic information. Based on these newly defined capabilities, it will also be possible to deform CAD models a priori, i.e. without any point cloud to serve as a reference and prior to the start of the manufacturing process or before a new manufacturing step, in order to compensate for future deviations and allow for first-time-right production. This will be made possible thanks to the use of a

reinforcement learning strategy, wherein an autonomous agent will learn how to define the deformation sequence to be applied to compensate the coming shape deviations between the theoretical model and its manufactured counterpart. Following this strategy, it will therefore be possible to mix both known rules coming from existing machine fault modeling theories, as well as unknown rules to be learned from experience. The proposed framework will be implemented and validated on academic as well as industrial examples.

Required background of the student: Ideally, a background in computer science, geometric modeling and computer-aided design.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Surleraux A., Lepert R., Pernot J-P., Kerfriden P., Bigot S., Machine Learning-based reverse model-ling approach for rapid tool shape optimization in die-sinking micro-Electro Discharge Machining, Journal of Computing and Information Science in Engineering, vol. 20(3), pp. 031002-1 to 11, 2020.
2. Shah G. A., Polette A., Pernot J-P., Giannini F., Monti M., Simulated annealing-based fitting of CAD models to point clouds of mechanical parts' assemblies, Engineering with Computers, vol. 37(4), pp. 2891-2909, 2021.
3. Peuzin-Jubert M., Polette A., Nozais D., Mari J-L., Pernot J-P., Survey on the View Planning Problem for reverse engineering and automated control applications, Computer-Aided Design, vol. 141, 103094, 2021
4. Hu S., Polette A., Pernot J-P., SMA-Net: Deep learning-based identification and fitting of CAD models from point clouds, Engineering with Computers, vol. 38, pp. 5467-5488, 2022
5. Zhang C., Pinquié R., Polette A., Carasi G., De Charnace H., Pernot J-P., Automatic 3D CAD models reconstruction from 2D orthographic drawings, Computers & Graphics, vol. 114, pp. 179-189, 2023

Illustrations :

Research Topic for the ParisTech/CSC PhD Program

Fields: Design & Industrialization, Information and Communication Sciences and Technologies, Mathematics and their applications.

ParisTech School : Arts et Métiers Sciences and Technologies – Laboratory LISPEN Campus of Aix-en-Provence

Title : **Reinforcement learning-based topology-preserving non-rigid deformation of CAD models from point clouds for first-time-right production in smart manufacturing**

Advisor(s):
Prof. Dr. Jean-Philippe PERNOT / jean-philippe.pernot@ensam.eu / https://lispen.ensam.eu
Dr. Arnaud POLETTE / arnaud.polette@ensam.eu / https://lispen.ensam.eu

Short description of possible research topics for a PhD :
This PhD program addresses the way CAD models can be adapted and deformed to capture the manufacturing defaults and thus maintain the coherence between the digital model and its physical and manufactured counterpart. This is particularly useful to optimize tool paths and manufacturing parameters. New deformation operators will be developed to simulate and reproduce various state-of-the-art manufacturing behaviors and deviations, including free-form and non-rigid deformations. Those operators will be applied until the deviation between the CAD model and the acquired point cloud of the manufactured counterpart is minimized. During the deformation process, the topology of the CAD models will be preserved, to be able to maintain the whole coherency and possibly available semantic information. Based on these newly defined capabilities, it will also be possible to deform CAD models a priori, i.e. without any point cloud to serve as a reference and prior to the start of the manufacturing process or before a new manufacturing step, in order to compensate for future deviations and allow for first-time-right production. This will be made possible thanks to the use of a reinforcement learning strategy, wherein an autonomous agent will learn how to define the deformation sequence to be applied to compensate the coming shape deviations between the theoretical model and its manufactured counterpart. Following this strategy, it will therefore be possible to mix both known rules coming from existing machine fault modeling theories, as well as unknown rules to be learned from experience. The proposed framework will be implemented and validated on academic as well as industrial examples.

Required background: Computer science, geometric modeling, computer-aided design.

A list of 5 (max.) representative publications of the group:

Surleraux A., Pernot J-P., Elkaseer A., Bigot S., Iterative surface warping to shape craters in micro-EDM simulation, Engineering with Computers, vol. 32(3), pp. 517-531, 2016.
Surleraux A., Lepert R., Pernot J-P., Kerfriden P., Bigot S., Machine Learning-based reverse model-ling approach for rapid tool shape optimization in die-sinking micro-Electro Discharge Machining, Journal of Computing and Information Science in Engineering, vol. 20(3), pp. 031002-1 to 11, 2020.
Shah G. A., Polette A., Pernot J-P., Giannini F., Monti M., Simulated annealing-based fitting of CAD models to point clouds of mechanical parts' assemblies, Engineering with Computers, vol. 37(4), pp. 2891-2909, 2021.
Peuzin-Jubert M., Polette A., Nozais D., Mari J-L., Pernot J-P., Survey on the View Planning Problem for reverse engineering and automated control applications, Computer-Aided Design, vol. 141, 103094, 2021.
Hu S., Polette A., Pernot J-P., SMA-Net: Deep learning-based identification and fitting of CAD models from point clouds, Engineering with Computers, vol. 38, pp. 5467-5488, 2022.
Zhang C., Pinquié R., Polette A., Carasi G., De Charnace H., Pernot J-P., Automatic 3D CAD models reconstruction from 2D orthographic drawings, Computers & Graphics, vol. 114, pp. 179-189, 2023.

TITLE: REINFORCEMENT LEARNING-BASED 3D RECONSTRUCTION OF CAD MODELS FROM DEAD MODELS FOR SMART MANUFACTURING APPLICATIONS

Topic number : ***2023_008***

Field : Design, Industrialization, Information and Communication Science and Technology, Mathematics and their applications

Subfield:

ParisTech School: Arts et Métiers
Research team:
Research lab: LISPEN - Laboratoire d'ingénierie des systèmes physiques et numériques
Lab location: Aix-en-Provence
Lab website:https://lispen.ensam.eu

Contact point for this topic: Arts et Métiers

Advisor 1: PERNOT Jean-Philippe jean-philippe.pernot@ensam.eu
Advisor 2: POLETTE Arnaud arnaud.polette@ensam.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: This PhD program addresses the way dead CAD models (as defined in STEP files) can be reverse engineered to discover the possible building trees from which they may originate, and more precisely the ones adapted for smart manufacturing applications. Such an approach is particularly interesting to define the bill of operations adapted to a given manufacturing process, but also to automatically generate the set of CAD models associated to the manufacturing steps. Indeed, being able to compare the CAD model at a given step to its manufactured and digitized counterpart is of major interest for control purposes and process optimization in the context of the Industry 4.0. The main idea relies in the use of reinforcement learning able to learn how to perform those complex tasks in a very efficient way, and without requiring large databases. Starting from state-of-the-art and known geometric and manufacturing rules to be established with the environment, an autonomous agent will learn the different actions to be applied at the feature level to move towards the next steps, with a known final objective that is the dead CAD model used as input of the algorithm. This singularity will be exploited to define the reward function to be

optimized step after step. The proposed framework will be implemented and validated on academic as well as industrial examples

Required background of the student: Ideally, computer science, geometric modeling and computer-aided design.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Lupinetti K., Pernot J-P., Monti M., Giannini F., Content-based CAD assembly model retrieval: Survey and future challenges, Computer-Aided Design, vol. 113, pp. 62-81, 2019
2. Surleraux A., Lepert R., Pernot J-P., Kerfriden P., Bigot S., Machine Learning-based reverse modelling approach for rapid tool shape optimization in die-sinking micro Electro Discharge Machining, Journal of Computing and Information Science in Engineering, vol. 20(3), pp. 031002-1 à 11, 2020.
3. Peuzin-Jubert M., Polette A., Nozais D., Mari J-L., Pernot J-P., Survey on the View Planning Problem for reverse engineering and automated control applications, Computer-Aided Design, vol. 141, 103094, 2021
4. Hu S., Polette A., Pernot J-P., SMA-Net: Deep learning-based identification and fitting of CAD models from point clouds, Engineering with Computers, vol. 38, pp. 5467-5488, 2022
5. Zhang C., Pinquié R., Polette A., Carasi G., De Charnace H., Pernot J-P., Automatic 3D CAD models reconstruction from 2D orthographic drawings, Computers & Graphics, vol. 114, pp. 179-189, 2023

Illustrations :

Research Topic for the ParisTech/CSC PhD Program

Fields: Design & Industrialization, Information and Communication Sciences and Technologies, Mathematics and their applications.

ParisTech School : Arts et Métiers Sciences and Technologies – Laboratory LISPEN Campus of Aix-en-Provence

Title : **Reinforcement learning-based 3D reconstruction of CAD models from dead models for smart manufacturing applications**

Advisor(s):
Prof. Dr. Jean-Philippe PERNOT / jean-philippe.pernot@ensam.eu / https://lispen.ensam.eu
Dr. Arnaud POLETTE / arnaud.polette@ensam.eu / https://lispen.ensam.eu

Short description of possible research topics for a PhD :
This PhD program addresses the way dead CAD models (as defined in STEP files) can be reverse engineered to discover the possible building trees from which they may originate, and more precisely the ones adapted for smart manufacturing applications. Such an approach is particularly interesting to define the bill of operations adapted to a given manufacturing process, but also to automatically generate the set of CAD models associated to the manufacturing steps. Indeed, being able to compare the CAD model at a given step to its manufactured and digitized counterpart is of major interest for control purposes and process optimization in the context of the Industry 4.0. The main idea relies in the use of reinforcement learning able to learn how to perform those complex tasks in a very efficient way, and without requiring large databases. Starting from state-of-the-art and known geometric and manufacturing rules to be established with the environment, an autonomous agent will learn the different actions to be applied at the feature level to move towards the next steps, with a known final objective that is the dead CAD model used as input of the algorithm. This singularity will be exploited to define the reward function to be optimized step after step. The proposed framework will be implemented and validated on academic as well as industrial examples.

Required background: Computer science, geometric modeling, computer-aided design.

A list of 5 (max.) representative publications of the group:
Mikchevitch A., Pernot J-P., Methodology for automatic recovering of 3D partitions from unstitched faces of non-manifold CAD models, Engineering with Computers, vol. 31(1), pp. 73-84, 2015.
Lupinetti K., Pernot J-P., Monti M., Giannini F., Content-based CAD assembly model retrieval: Survey and future challenges, Computer-Aided Design, vol. 113, pp. 62-81, 2019.
Surleraux A., Lepert R., Pernot J-P., Kerfriden P., Bigot S., Machine Learning-based reverse modelling approach for rapid tool shape optimization in die-sinking micro Electro Discharge Machining, Journal of Computing and Information Science in Engineering, vol. 20(3), pp. 031002-1 à 11, 2020.
Peuzin-Jubert M., Polette A., Nozais D., Mari J-L., Pernot J-P., Survey on the View Planning Problem for reverse engineering and automated control applications, Computer-Aided Design, vol. 141, 103094, 2021.
Hu S., Polette A., Pernot J-P., SMA-Net: Deep learning-based identification and fitting of CAD models from point clouds, Engineering with Computers, vol. 38, pp. 5467-5488, 2022.
Zhang C., Pinquié R., Polette A., Carasi G., De Charnace H., Pernot J-P., Automatic 3D CAD models reconstruction from 2D orthographic drawings, Computers & Graphics, vol. 114, pp. 179-189, 2023.

TITLE: VIRTUAL ARCHEOLOGICAL ARTEFACTS ASSEMBLY THROUGH GEOMETRICAL FEATURES

Topic number : ***2023_009***

Field : Information and Communication Science and Technology, ,

Subfield: Computer graphics, Geometry modelling, Virtual reality, Archeology

ParisTech School: Arts et Métiers
Research team: XR team https://institutchalon.ensam.eu/accueil-institut-de-chalon-sur-saone-102266.kjsp
Research lab: LISPEN - Laboratoire d'ingénierie des systèmes physiques et numériques
Lab location: Chalon-sur-Saône
Lab website:http://lispen.ensam.eu/

Contact point for this topic: Arts et Métiers

Advisor 1: Mérienne Frédéic frederic.merienne@ensam.eu
Advisor 2: Raffin Romain romain.raffin@u-bourgogne.fr
Advisor 3: Lou Ruding ruding.lou@ensam.eu
Advisor 4:

Short description of possible research topics for a PhD: Archaeology is a fascinating field that involves the study of human history and prehistory through the excavation and analysis of material remains such as artifacts. Archaeology today often employs an interdisciplinary approach, for more comprehensive and precise analysis of archaeological finds. It covers Geographic Information Systems, databases and ontologies, geometries, points clouds or images processing, big data and machine learning.
High-resolution 3D scanning and photogrammetry techniques have become standard tools in archaeology to create detailed 3D models of excavation sites, artifacts, and architectural structures. The analyze of geometrical features in 3D models of archaeological assemblies can provide valuable insights into the construction techniques, design, and organization of ancient structures or artifacts . An international contest, “Forma Urbis Romae” project is still active, pushing the scientists to the limits, to be able to reassemble a complete map of Ancient Rome, based on digitized fragments .
Another usage of these 3D models are Virtual Reality (VR) and

Augmented Reality (AR). There can be a powerful tool for the reconstruction and presentation of cultural heritage. It allows people to explore and experience historical sites, artifacts, and cultural contexts, in an immersive and interactive manner. Archaeologists can also use VR/AR to overview and analyze archaeological sites before physical excavation. This helps in planning excavations, understanding site layouts, and identifying potential research areas .
In this PhD thesis an innovative digital tool based on VR/AR will be designed and prototyped to allow archeologists exploring the different geometrical features of 3D artefacts and assembling them in order to reconstruct historical heritage; The research questions are: what is the best computer – human interface for the archeologists in virtual artefacts assembly tasks, and how to let them to perceive and interact with the geometrical features. The project is a collaboration between LISPEN (for AR/VR) and LIB (geometry processing).
References:
Le Tien, M., Tan, K. N., & Raffin, R. Matching correspondence between images and 3D model in a reconstruction process. Journal of Science and Technology, 2(1), 64-69. 2016.

Le Tien, M., Tan, K. N., & Raffin, R. Analysis of geometrical features of 3D model based on the surface curvature of a set of point cloud. In ICFNDS 2021.
Qi-Xing Huang, Simon Flöry, Natasha Gelfand, Michael Hofer, and Helmut Pottmann. 2006. Reassembling fractured objects by geometric matching. ACM Trans. Graph. 25, 3 (July 2006), 569–578.
https://formaurbis.stanford.edu/
Emmanuel Durand, Frederic Merienne, Christian Pere, and Patrick Callet. Ray-on, an On-Site Photometric Augmented Reality Device. J. Comput. Cult. Herit. 7, 2, Article 7, 2014.
LANDRIEU J., Père C., Rollier J., Castandet S. and SCHOTTÉ G. Digital Rebirth of the Greatest Church of Cluny maior Ecclesia: From Optronic Surveys to Real Time Use of the Digital Model. ISPRS, 2012.

Required background of the student: Computer science, General engineering, Computer aided design, Virtual reality

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Le Tien, M., Tan, K. N., Raffin, R. Matching correspondence between images and 3D model in a reconstruction process. Journal of Science and Technology, 2(1), 64-69. 2016.

2. Le Tien, M., Tan, K. N., Raffin, R. Analysis of geometrical features of 3D model based on the surface curvature of a set of point cloud. In ICFNDS 2021.

3. Le Tien, M., Tan, K. N., Raffin, R. Analysis of geometrical features of 3D model based on the surface curvature of a set of point cloud. In ICFNDS 2021.
4.
5.

Illustrations :

ParisTech

Arts et Métiers Sciences et Technologies

PHD RESEARCH TOPIC FOR APPLYING THE CSC SCHOLARSHIP

Field: ***Information and Communication Sciences and Technologies***

Subfield: Computer graphics, Virtual Reality.

Title: Virtual archeological artefacts assembly through geometrical features

Doctoral college: Arts et Métiers Sciences et Technologies

Advisors (Name, Email, Lab, Lab website, Lab Location):

Prof. Frédéric Mérienne,
frederic.merienne@ensam.eu,
LISPEN
http://lispen.ensam.eu/
Chalon-sur-Saône

Prof. Romain Raffin,
romain.raffin@u-bourgogne.fr
LIB
https://lib.u-bourgogne.fr/
Dijon

Dr. Ruding Lou
ruding.lou@ensam.eu
LISPEN
http://lispen.ensam.eu/
Chalon-sur-Saône

Short description of possible research topics for a PhD:

Archaeology is a fascinating field that involves the study of human history and prehistory through the excavation and analysis of material remains such as artifacts. Archaeology today often employs an interdisciplinary approach, for more comprehensive and precise analysis of archaeological finds. It covers Geographic Information Systems, databases and ontologies, geometries, points clouds or images processing, big data and machine learning.

High-resolution 3D scanning and photogrammetry techniques have become standard tools in archaeology to create detailed 3D models of excavation sites, artifacts, and architectural structures. The analyze of geometrical features in 3D models of archaeological assemblies can provide valuable insights into the construction techniques, design, and organization of ancient structures or artifacts [1-3]. An international contest, "Forma Urbis Romae" project is still active, pushing the scientists to the limits, to be able to reassemble a complete map of Ancient Rome, based on digitized fragments [4].

Another usage of these 3D models are Virtual Reality (VR) and Augmented Reality (AR). There can be a powerful tool for the reconstruction and presentation of cultural heritage. It allows people to explore and experience historical sites, artifacts, and cultural contexts, in an immersive and interactive manner. Archaeologists can also use VR/AR to overview and analyze archaeological sites before physical excavation. This helps in planning excavations, understanding site layouts, and identifying potential research areas [5-6].

In this PhD thesis an innovative digital tool based on VR/AR will be designed and prototyped to allow archeologists exploring the different geometrical features of 3D artefacts and assembling them in order to reconstruct historical heritage; The research questions are: what is the best computer – human interface for the archeologists in virtual artefacts assembly tasks, and how to let them to perceive and interact with the geometrical features. The project is a collaboration between LISPEN (for AR/VR) and LIB (geometry processing).

References:

[1] Le Tien, M., Tan, K. N., & **Raffin, R**. Matching correspondence between images and 3D model in a reconstruction process. Journal of Science and Technology, 2(1), 64-69. 2016.

[2] Le Tien, M., Tan, K. N., & **Raffin, R**. Analysis of geometrical features of 3D model based on the surface curvature of a set of point cloud. In ICFNDS 2021.

[3] Qi-Xing Huang, Simon Flöry, Natasha Gelfand, Michael Hofer, and Helmut Pottmann. 2006. Reassembling fractured objects by geometric matching. ACM Trans. Graph. 25, 3 (July 2006), 569–578.

[4] https://formaurbis.stanford.edu/

[5] Emmanuel Durand, **Frederic Merienne**, Christian Pere, and Patrick Callet. Ray-on, an On-Site Photometric Augmented Reality Device. J. Comput. Cult. Herit. 7, 2, Article 7, 2014.

[6] LANDRIEU J., Père C., Rollier J., Castandet S. and SCHOTTÉ G. Digital Rebirth of the Greatest Church of Cluny maior Ecclesia: From Optronic Surveys to Real Time Use of the Digital Model. ISPRS, 2012.

TITLE: FUNCTIONAL POLYMER NANOPARTICLES BY RING-OPENING POLYMERIZATION-INDUCED SELF-ASSEMBLY (ROPISA) FOR PHOTOBIOCATALYST AND ANTICANCER PHOTOTHERAPY

Topic number : ***2023_010***

Field : Chemistry, Physical chemistry and Chemical Engineering, ,

Subfield:

ParisTech School: Chimie ParisTech - PSL
Research team: Materials, interfaces and soft matter (MIM2)
http://www.ircp.cnrs.fr/la-recherche/equipe-mim2/
Research lab: IRCP - Institut de Recherche de Chimie de Paris
Lab location: Paris
Lab website:https://www.ircp.cnrs.fr/

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Li Min-Hui min-hui.li@chimieparistech.psl.eu
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Polymerization-induced self-assembly (PISA) is a powerful tool to prepare block copolymer nanoparticles with various morphologies, like spherical micelles, cylindrical micelles, vesicles and cubosomes, in-situ in the polymerization medium. PISA is based on the chain extension of a first soluble polymer with a monomer that forms an insoluble second polymer block. By controlling the chain length of this second block relative to that of the first block, the block copolymers self-assemble in situ into various polymer nanoparticles. PISA is now considered as one of the most important strategies in macromolecular nanotechnology, since it can produce a wide range of nanoparticles at high concentrations and on a large scale.
Reversible-deactivation radical polymerization (RDRP) was traditionally used to carry out PISA that afforded however nonbiodegradable polymers and nanoparticles. Recently, PISA with biodegradable and biocompatible product has been achieved by very few research groups using ring-opening polymerization (ROP) of N-carboxyanhydride (NCA)-induced self-assembly (NCA-ROPISA). In this PhD project, we propose to develop a

new system of ring-opening polymerization-induced self-assembly (ROPISA) using N-thiocarboxyanhydride (NTA) (NTA-ROPISA) where NTA monomers bear N-substituted functional groups like photocatalysts or photosensitizers. In the end of this PhD project, we hope to shed light on the way to perform NTA-ROPISA and obtain a series of polymer nanoparticles for both photobiocatalysis and anticancer phototherapy.

Required background of the student: The applicant should have a sound knowledge in both organic and polymer chemistry and be skilled in analytical techniques such as NMR, SEC, DLS and TEM. He/She must be fluent in English that is the working language in the laboratory. Experience in biology and biotechnology would be appreciated.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. (1) Zhang, N., Trépout, S., Chen, H., & Li, M. H. AIE Polymer Micelle/Vesicle Photocatalysts Combined with Native Enzymes for Aerobic Photobiocatalysis. Journal of the American Chemical Society 2023, 145, 288–299. https://doi.org/10.1021/jacs.2c09933
2. (2) Zhang, Z., Chen, H., Wang, Y., Zhang, N., Trépout, S., Tang, B. Z., Gasser, G. & Li, M. H. Polymersomes with Red/Near-Infrared Emission and Reactive Oxygen Species Generation. Macromolecular Rapid Communications, 2023, 44, 2200716. https://doi.org/10.1002/marc.202200716
3. (3) H Chen, Y Fan, N Zhang, S Trépout, P Bergam, A Brûlet, BZ Tang, MH Li, Fluorescent polymer cubosomes and hexosomes with aggregation-induced emission. Chemical Science, 2021, 12, 5495 – 5504. DOI: 10.1039/D1SC00270H
4. (4) Deng Y. W., Chen H., Tao X. F., Trépout S., Ling J., Li M.-H., “Synthesis and self-assembly of poly(ethylene glycol)-block-poly(N-3-(methylthio)propyl glycine) and their oxidation-sensitive polymersomes”, Chinese Chemical Letters 2020, 31, 1931-1935. https://doi.org/10.1016/j.cclet.2019.12.026
5. (5) Tao, X.; Chen, H.; Trépout, S.; Cen, J.; Ling, J.; Li, M-H. “Polymersomes with Aggregation-Induced Emission Based on Amphiphilic Block Copolypeptoids”, Chem. Commun. 2019, 55, 13530 – 13533. DOI: 10.1039/C9CC07501A

Illustrations :

ParisTech

Arts et Métiers Sciences et Technologies

TITLE: ADDITIVE MANUFACTURING OF HIGH-PERFORMANCE AL MATRIX COMPOSITE WITH MULTI-FUNCTIONAL REINFORCEMENTS

Topic number : ***2023_011***

Field : Material science, Mechanics and Fluids, Energy, Processes,

Subfield:

ParisTech School: Arts et Métiers
Research team:
Research lab: MSMP - Laboratoire Mécanique, Surface, Matériaux et Procédés
Lab location: Châlons-en-Champagne
Lab website:msmp.eu

Contact point for this topic: Arts et Métiers

Advisor 1: El Mansori Mohamed mohamed.elmansori@ensam.eu
Advisor 2: WANG Pei wangpei@hnas.ac.cn
Advisor 3: KANG Nan nan.kang@ensam.eu
Advisor 4:

Short description of possible research topics for a PhD: For meeting the requirements in complexity and lightweight design of components in next-generation aircraft, the development of the novel multi-functional Al with low cost for additive manufacturing will bring new opportunities to the materials design and intelligent manufacturing fields. Based on the above, from the intrinsic features of AM processed sample with special solidification and multi-scales heterogeneous structure, this work aims to obtain the design strategy for AM multi-functional Al matrix composite with high-performance (mechanical properties, tribological properties and thermal properties) by manufacturing the stable and metastable phases reinforced micro/nano-composite structure. Focusing on the formation and controlling mechanism of heterogeneous structure and corresponding multi-functional properties, the composite will be firstly designed using a high throughput method. Then, the relationship between alloy composition-process parameters-structure-properties of AM processed Al matrix composite will be established for guiding the realization of materials-structure-function AM of multi-scales reinforced Al matrix composites.

Required background of the student:

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. P. Wang, et. al, Transactions of Nonferrous Metals Society of China 30 (2020) 2001-2034.

2. P. Wang, et. al, Composites Part B: Engineering 147 (2018) 162-168.

3. N. KANG et al. Composites Part B: Engineering 155 (2018) 382-390.

4.

5.

Illustrations :

ParisTech

Arts et Métiers Sciences et Technologies

TITLE: SEISMIC CYCLE CHARACTERISTICS AND DEPENDENCE ON ROCK RHEOLOGY AND FRICTION

Topic number : ***2023_012***

Field : Material science, Mechanics and Fluids, Environment Science and Technology, Sustainable Development, Geosciences, Physics, Optics

Subfield:

ParisTech School: Arts et Métiers
Research team: Equipe DIPPE https://lampa.ensam.eu/equipe-dippe-134463.kjsp?RH=1415871394252
Research lab: LAMPA - Laboratoire angevin de mécanique, procédés et innovation
Lab location: Angers
Lab website:https://lampa.ensam.eu/

Contact point for this topic: Arts et Métiers

Advisor 1: AMMAR Amine amine.Ammar@ensam.eu
Advisor 2: EL AREM Saber saber.elarem@ensam.eu
Advisor 3: Latour Soumaya soumaya.latour@irap.omp.eu
Advisor 4:

Short description of possible research topics for a PhD:
Understanding how earthquakes initiate on active faults and whether this initiation could be detected is an issue of foremost importance in seismology. However, because the physical process of co-seismic rupture corresponds to the development of an instability, its physics is highly non-linear, and involves many scale-dependent processes. This leads to fundamental challenges in studying rupture initiation and propagation whether it be theoretically, numerically or experimentally. An experimental setup has allowed interesting observations of rupture nucleation, in this study we aim to reproduce numerically the experimental results. Nucleation on a heterogeneous interface with a periodic friction heterogeneity has been considered. It was shown experimentally that a large scale globally accelerating nucleation process can develop on a heterogeneous fault, while the details of the rupture propagation are controlled at smaller scale by the friction heterogeneity. The numerical model will help in better understanding of the rupture process by comparing with the experimental results and discussing their relevance with respect to recent theoretical developments and to

earthquakes preparatory processes. We want to derive a reliable friction law to be used in numerical exploration of seismic cycle characteristics and dependence on rock rheology and friction.

Required background of the student: Solid Mechanics, Applied physics, geophysics

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Gounon, A., Latour, S., Letort, J., & El Arem, S. (2022). Rupture nucleation on a periodically heterogeneous interface. Geophysical Research Letters, 49,e2021GL096816. https://doi.org/10.1029/2021GL096816

2. Latour, S., Schubnel, A., Nielsen, S., Madariaga, R., & Vinciguerra, S. (2013). Characterization of nucleation during laboratory earthquakes.Geophysical Research Letters,40440(19), 5064–5069.

3. The Corinth Rift Laboratory, Greece (CRL): A Multidisciplinary Near Fault Observatory (NFO) on a Fast Rifting System
P Bernard, H Lyon-Caen, A Deschamps, P Briole… - AGU Fall Meeting Abstracts, 2014

4. Influence of rheological and frictional slip properties on fault mechanics, deformation rates and localization phenomena: the Corinth Rift case
S El Arem, H Lyon-Caen, P Bernard, JD Garaud… - EGU General Assembly Conference Abstracts, 2013

5.

Illustrations :

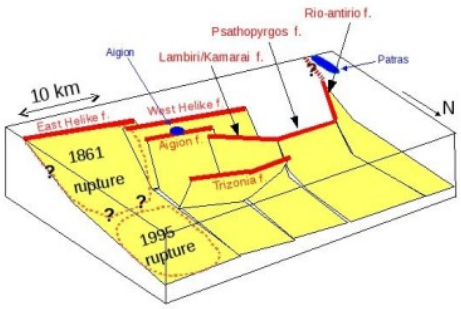


Figure 1: sketch of the major active faults of the CRL area. *Surface scarps in red. Trizonia fault is the only south dipping fault. The 1995 may have occurred on the Helike fault (uncertain dip and connectivity)*

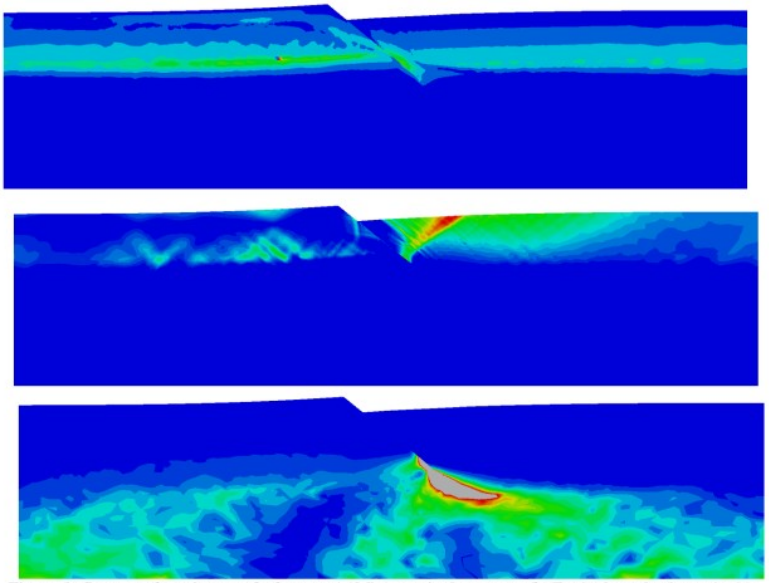
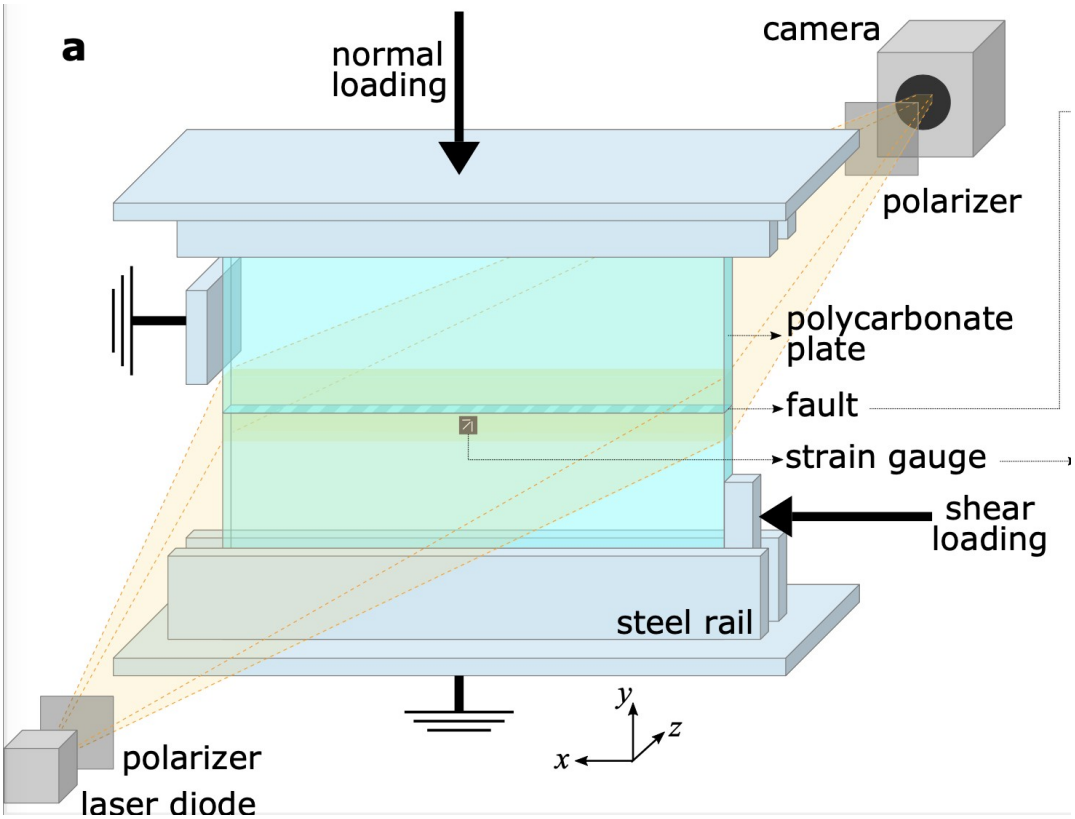
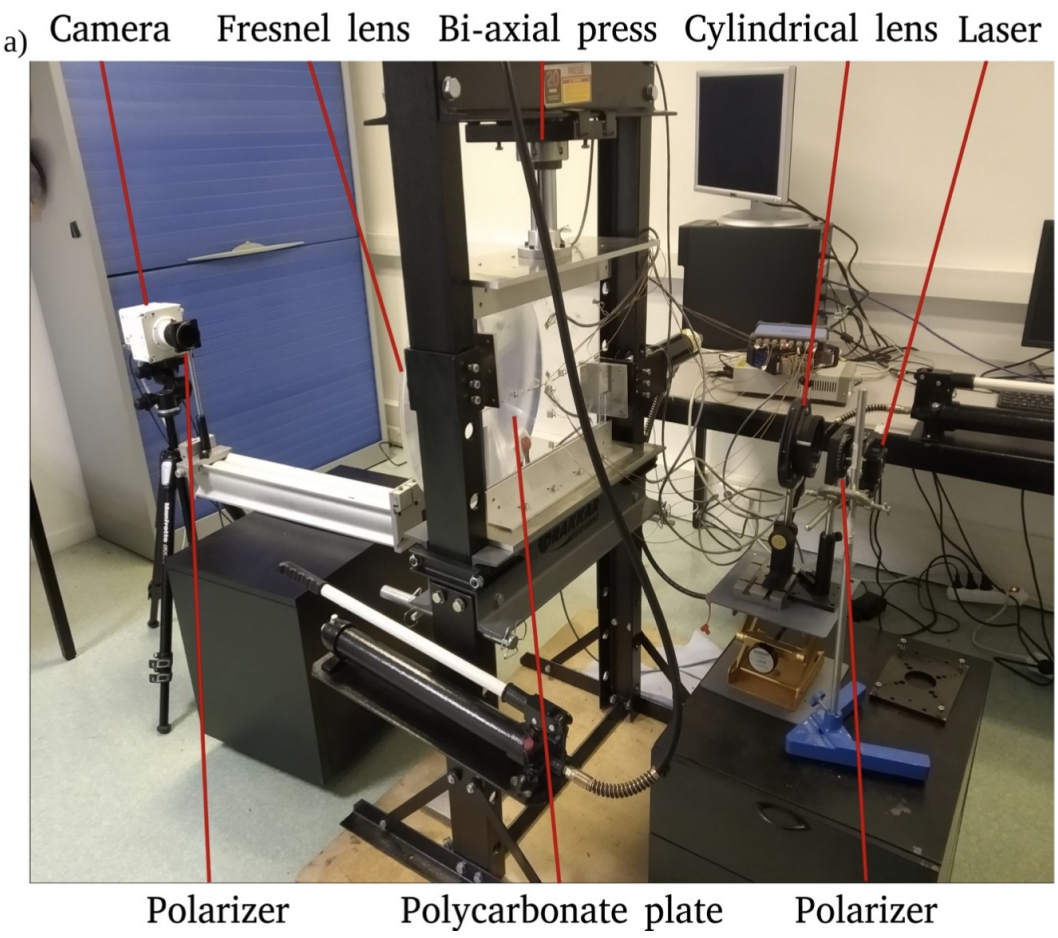


Figure 1: Stress and strain near fault zone. (a)Mises equivalent stress ***(b)*** Equivalent plastic strain ***(c)*** Equivalent creep strain.


a
normal loading
camera
polarizer
polycarbonate plate
fault
strain gauge
shear loading
steel rail
y
z
x
polarizer
laser diode


a) Camera Fresnel lens Bi-axial press Cylindrical lens Laser
Polarizer
Polycarbonate plate
Polarizer

ParisTech

Arts et Métiers Sciences et Technologies

TITLE: FAILURE MODELING OF CEMENTITIOUS COMPOSITES IN THE FRAMEWORK OF GRADIENT DAMAGE APPROACH

Topic number : ***2023_013***

Field : Material science, Mechanics and Fluids, Mathematics and their applications, Physics, Optics

Subfield:

ParisTech School: Arts et Métiers
Research team: Equipe DIPPE https://lampa.ensam.eu/equipe-dippe-134463.kjsp?RH=1415871394252
Research lab: LAMPA - Laboratoire angevin de mécanique, procédés et innovation
Lab location: Angers
Lab website:https://lampa.ensam.eu/accueil-lampa-100748.kjsp

Contact point for this topic: Arts et Métiers

Advisor 1: Ammar Amine amine.Ammar@ensam.eu
Advisor 2: EL AREM Saber saber.elarem@ensam.eu
Advisor 3: Miled karim karim.miled@enit.utm.tn
Advisor 4:

Short description of possible research topics for a PhD: The degradation of quasi-brittle materials such as concrete and cementitious composites are generally brittle at the microscopic scale and ductile at the macroscopic scale (damage). Moreover, this quasi-brittleness is depending on the heterogeneous microstructure of the material (volume fraction, shape and size of the inclusions as well as their nature and the contrast in rigidity between the cementitious matrix and the inclusions), which often generates a different failure modes. This often results in a transition from a brittle failure mode to a more ductile mode or vice versa, and generates a size effect on the compressive strength of cementitious materials whose apprehension and modeling are complex. Indeed, several types of inclusions with different physical and mechanical properties can be incorporated into a cementitious matrix depending on the desired application. In ordinary concrete of common density, these inclusions are natural aggregates of sand and gravel which are more rigid than hardened cement paste. On the other hand, in a light concrete, the inclusions are very flexible light aggregates or even air bubbles assimilated to pores. Furthermore, these inclusions can have different

shapes and sizes and can be regularly or randomly distributed in the cementitious matrix. Despite the abundance of scientific literature on the subject of compressive failure of quasi-brittle cementitious materials, this subject remains topical. In fact, there are several ways to model it. Some are purely empirical since they are based on tests on real materials in which the microstructure is varied. This approach is costly because it requires a very large number of tests to be able to correctly understand the failure mechanisms and predict all the effects of the microstructure of the material studied on its compressive strength. Other approaches are purely numerical and are based first on the modeling of the real or idealized microstructure of these materials and then on the adoption of a nonlinear constitutive law modeling the behavior of the cementitious matrix placed between the inclusions which are generally assumed to be elastic or perfectly rigid. This approach is efficient but costly in terms of numerical implementation and computation time. Moreover, certain local numerical models exhibit problems of pathological localization of the damage or concentration of the stresses in points of the cracks leading to problems of nonconvergence of computation or mesh dependence of the results. Recently, alternative methods for the numerical simulation of brittle fracture phenomena have appeared and where discontinuities are not explicitly introduced into the solid. The major advantage of using a phase field is that the evolution of the fracture surfaces stems from the resolution of a coupled system of PDE. It is not necessary to explicitly follow the topology of the crack nor to constrain its path a priori. Thus, this approach will be adopted in the PhD proposal to simulate the complete failure process of cementitious composites containing different types of inclusions.

Required background of the student: solid mechanics

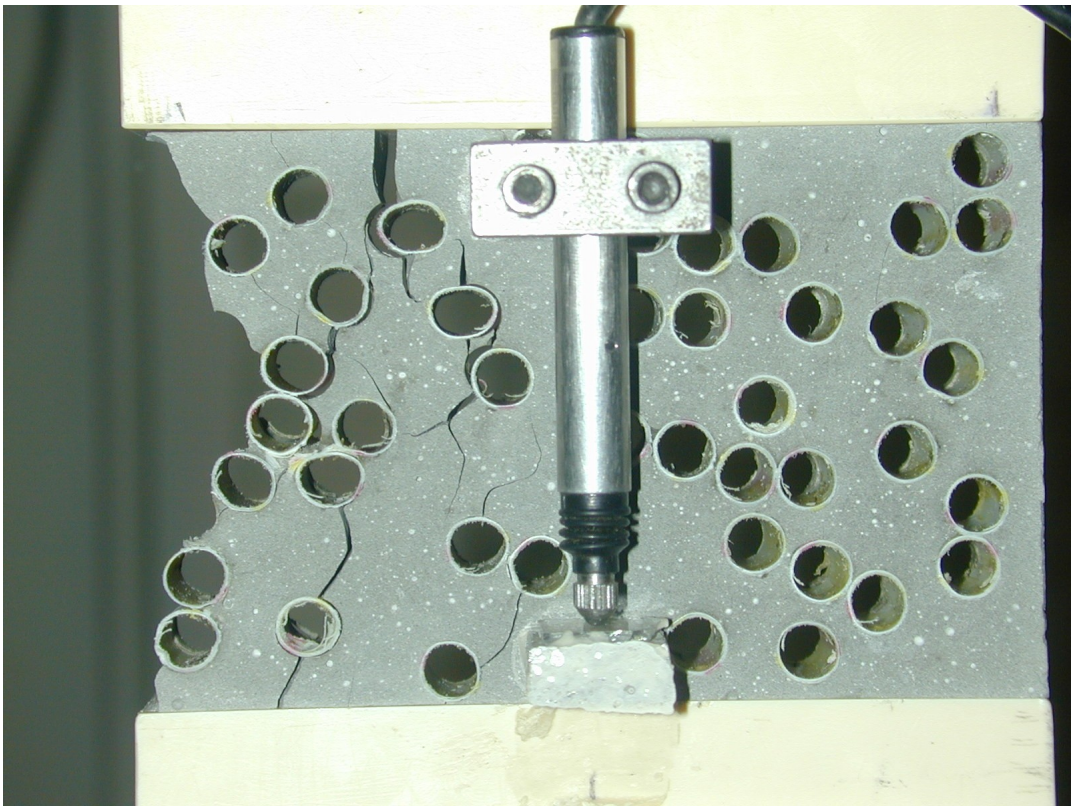
A list of 5 (max.) representative publications of the group: (Related to the research topic)

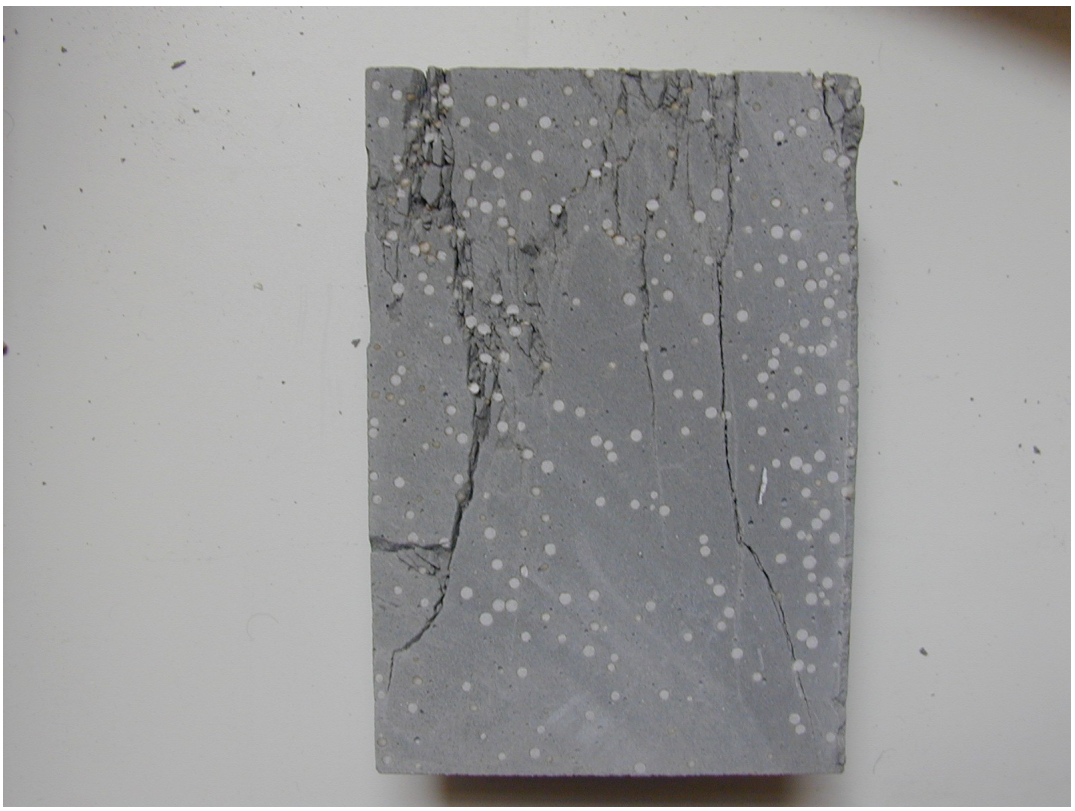
1. Ben Youssef M., Lavergne F., Sab, K., Miled K., Néji J., 2018. Upscaling the elastic stiffness of foam
concrete as a three-phase material. Cement and Concrete Research, vol. 110, pp. 13-23. DOI:
10.1016/j.cemconres.2018.04.02

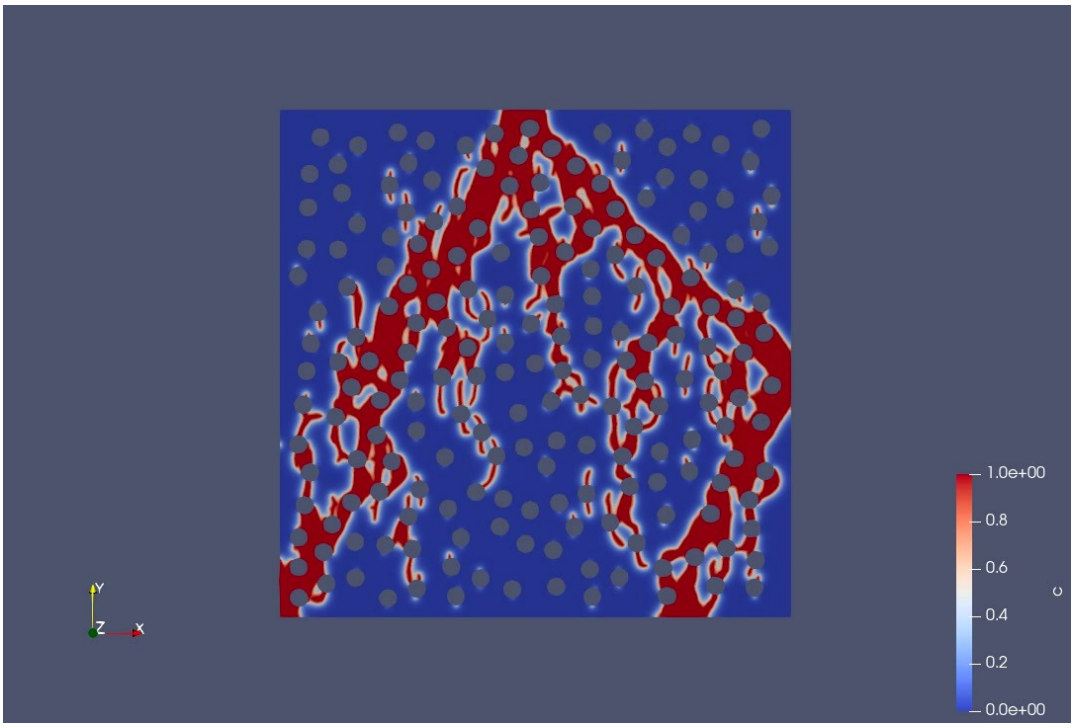
2. Naija A., Hassen G., Limam O., Miled K., 2020. Numerical study of the biaxial compressive strength of
high strength concrete based on a yield design micromechanical approach. International Journal for
Numerical and Analytical Methods in Geomechanics. DOI:
10.1002/nag.303.

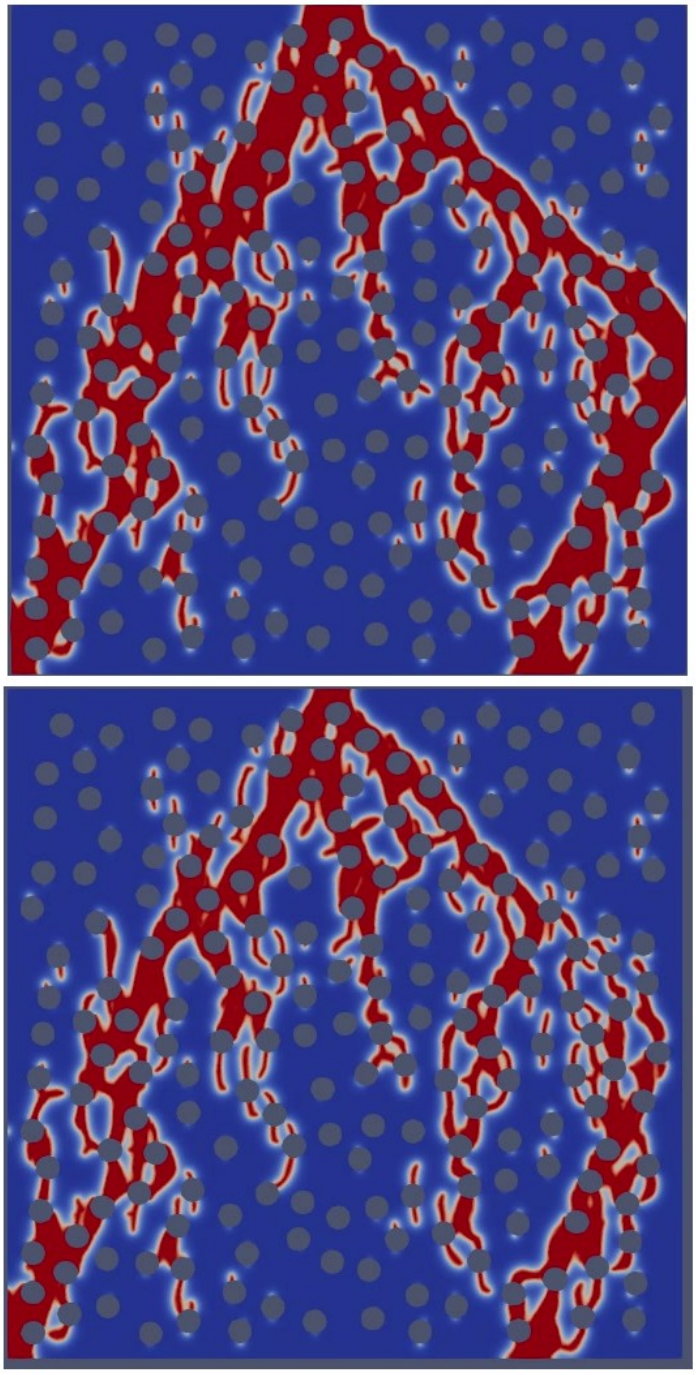
3. A phase-field model for brittle fracture of anisotropic materials
H Gmati, C Mareau, A Ammar, S El Arem - International Journal for Numerical Methods in …, 2020
4. Ben Youssef M., Miled K., Néji J., 2017. Mechanical properties of non-autoclaved foam concrete:
analytical models vs. experimental data, European Journal of Environmental and Civil Engineering,
Vol.24 (4), pp. 472-480, DOI:10.1080/19648189.2017.1398108.
5.

Illustrations :






1.0e+00
0.8
0.6
0.4
0.2
0.0e+00
c
Y
Z
X



Damage of the plate with holes under compression test.
Phase field approach to fracture by S. EL AREM

ParisTech

Arts et Métiers Sciences et Technologies

TITLE: CO-DESIGN OF RECONFIGURABLE MANUFACTURING AND MONITORING SYSTEMS

Topic number : ***2023_014***

Field : Design, Industrialization, Information and Communication Science and Technology, Mathematics and their applications

Subfield:

ParisTech School: Arts et Métiers
Research team: Design axis
Research lab: LCFC - Laboratoire de conception, fabrication, commande
Lab location: Metz
Lab website:lcfc.ensam.eu

Contact point for this topic: Arts et Métiers

Advisor 1: DANTAN Jean-Yves jean-yves.dantan@ensam.eu
Advisor 2: STIEF Paul paul.stief@ensam.eu
Advisor 3: SAVA Alexandre alexandre.sava@univ-lorraine.fr
Advisor 4:

Short description of possible research topics for a PhD: Industry 4.0 emerged during the last decade as new generation of manufacturing technology aimed to provide dramatic improvements in the performance of manufacturing systems. Smart manufacturing is a new manufacturing technology aiming to support Industry 4.0. It consists on a complete integration of all aspects of manufacturing using data and information exchange to respond in real time to changes in the factory, in the supply network and in customers' needs. Therefore, data quality is one of the pillars of smart manufacturing. In this context, data collection and data analytics play an important role for monitoring and data-driven decision making to continuously improve the overall system performance and enhance the adaptability and the agility of modern manufacturing systems to face product variety and demand variability. To collect relevant data, several research works elaborated approaches for the optimal design of sensor networks using criteria such the information gain through sensor placement and the cost of data collection. These works are application oriented and consider a specific configuration of an existing process. They do not consider the impact of sensor placement on the performance of the process neither the impact of the process on the monitoring system. Moreover, the reconfiguration brings new challenges

to the monitoring system design as different configuration may need specific data requirements for monitoring and decision-making. The aim of this thesis proposal is to elaborate a framework to co-design a reconfigurable manufacturing system and its monitoring system in the context of Industry 4.0, where reconfigurability and, in particularity, scalability of the global system are important challenges.

Required background of the student: Industrial Engineering / Mechanical Engineering / Mechatronics ; interest for smart manufacturing and manufacturing systems will be appreciated

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. L. D. Xu, E. L. Xu, and L. Li, ‘Industry 4.0: state of the art and future trends’, Int. J. Prod. Res., vol. 56, no. 8, pp. 2941–2962, Apr. 2018, doi: 10.1080/00207543.2018.1444806.
2. Y. Koren, X. Gu, and W. Guo, ‘Reconfigurable manufacturing systems: Principles, design, and future trends’, Front. Mech. Eng., vol. 13, no. 2, pp. 121–136, Jan. 2018, doi: 10.1007/s11465-018-0483-0.
3. U. Awasthi and G. M. Bollas, ‘Sensor network design for smart manufacturing – Application on precision machining’, IFACPapersOnLine, vol. 53, no. 2, pp. 11440–11445, 2020, doi: 10.1016/j.ifacol.2020.12.581.
4. P. Stief, JY. Dantan et al., ‘Product design improvement by a new similarity-index-based approach in the context of reconf. assembly processes’, J. Eng. Des., vol. 31, no. 6, 2020, doi: 10.1080/09544828.2020.1748181
5. R. Laref, E. Losson, A. Sava et al., ‘Support Vector Machine Regression for Calibration Transfer between Electronic Noses Dedicated to Air Pollution Monitoring’, Sensors, vol. 18, no. 11, p. 3716, 2018, doi: 10.3390/s18113716

Illustrations :

Co-Design of Reconfigurable Manufacturing and Monitoring Systems

Context: Industry 4.0 emerged during the last decade as new generation of manufacturing technology [1]. It relies on enabling technologies such as Cyber Physical Systems (CPPS) and the Internet of Things to integrate the physical space to the virtual one and enable manufacturing assets to share real-time data on their condition, the product quality and the evolution in stakeholders' expectations. In this context, smart manufacturing is a new manufacturing technology. It consists on a complete integration of all aspects of manufacturing using data and information exchange to respond in real time to changes in the factory, in the supply network and in customers' needs [2]. Data is therefore one of the pillars of smart manufacturing [3]. In consequence, data collection and data analytics play an important role for monitoring and data-driven decision making to continuously improve the overall system performance and enhance the adaptability and the agility of modern manufacturing systems. To collect relevant data, several approaches have been elaborated for the optimal design of sensor networks using criteria such the information gain through sensor placement and the cost of data collection [5]. These works do not consider the impact of sensor placement on the performance of the process such as delays due to the measurement or the impact of the process on the monitoring system. Moreover, the reconfiguration brings new challenges to the monitoring system design as different configuration may need specific data requirements for monitoring and decision-making.

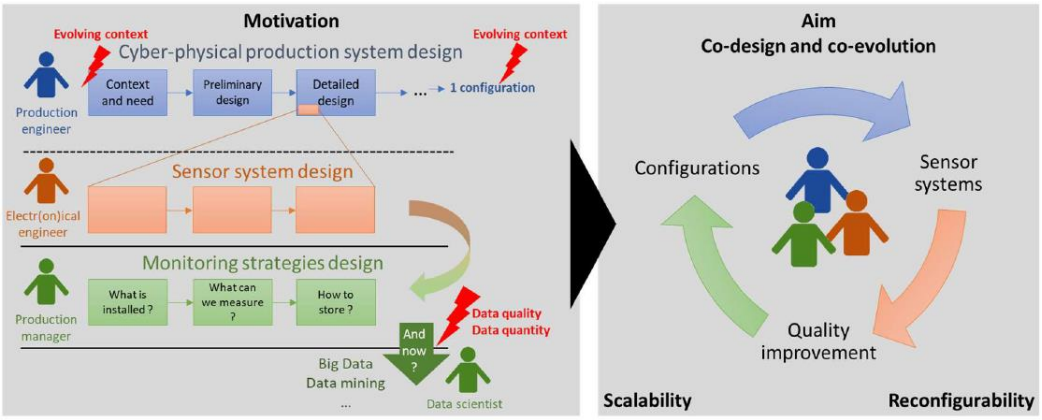


Figure 1. Motivation and scientific issue of the proposal

Scientific issue: The aim of this thesis proposal is to elaborate a framework to co-design a reconfigurable manufacturing system and its monitoring system in the context of Industry 4.0, where reconfigurability and, in particularity, scalability of the global system are important challenges. The project main question, illustrated in the right-hand side of figure 1, is: How to integrate the design of the monitoring systems in the design of a reconfigurable manufacturing system (RMS)?

Significant research work was conducted on:

- Industry 4.0 technology and its impact on modern manufacturing systems [1]
- Smart manufacturing [2,3]
- Data quality impact on diagnostics and prognostics [4] and Sensor networks design [5]
- RMS [6,7] and co-evolution product-process-manufacturing systems [8]
- Scalability in manufacturing systems [9]

Research questions (thesis perimeter to refine with the candidate):

- How to model jointly a production system with its monitoring system?
- How to evaluate the performance of a given configuration?
- How to evaluate the impact of the monitoring system on the production system?
- How to adapt the (re)configuration of the global system (monitoring and production)?

[1] L. D. Xu, E. L. Xu, and L. Li, 'Industry 4.0: state of the art and future trends', Int. J. Prod. Res., vol. 56, no. 8, pp. 2941–2962, Apr. 2018, doi: 10.1080/00207543.2018.1444806.
[2] S. Sahoo and C. Y. Lo, 'Smart manufacturing powered by recent technological advancements: A review', Journal of Manufacturing Systems, vol. 64, pp. 236–250, Jul. 2022, doi: 10.1016/j.jmsy.2022.06.008.
[3] A. Kusiak, 'Smart manufacturing', Int. J. Prod. Res., vol. 56, no. 1–2, pp. 508–517, Jan. 2018, doi:10.1080/00207543.2017.1351644.
[4] N. Omri et al., 'Towards an adapted PHM approach: Data quality requirements methodology for fault detection applications', Computers in Industry, vol. 127, p. 103414, May 2021, doi: 10.1016/j.compind.2021.103414.
[5] U. Awasthi and G. M. Bollas, 'Sensor network design for smart manufacturing – Application on precision machining', IFACPapersOnLine, vol. 53, no. 2, pp. 11440–11445, 2020, doi: 10.1016/j.ifacol.2020.12.581.
[6] Y. Koren, X. Gu, and W. Guo, 'Reconfigurable manufacturing systems: Principles, design, and future trends', Front. Mech. Eng., vol. 13, no. 2, pp. 121–136, Jan. 2018, doi: 10.1007/s11465-018-0483-0.
[7] M. Bortolini, F. G. Galizia, and C. Mora, 'Reconfigurable manufacturing systems: Literature review and research trend',Journal of Manufacturing Systems, vol. 49, pp. 93–106, Jan. 2018, doi: 10.1016/j.jmsy.2018.09.005.
[8] T. Tolio et al., 'SPECIES—Co-evolution of products, processes and production systems', CIRP Annals, vol. 59, no. 2, pp. 672–693, Jan. 2010, doi: 10.1016/j.cirp.2010.05.008.
[9] G. Putnik et al., 'Scalability in manufacturing systems design and operation: State-of-the-art and future developments roadmap', CIRP Annals, vol. 62, no. 2, pp. 751–774, 2013, doi: 10.1016/j.cirp.2013.05.002.

Contacts:
Dr. Paul STIEF paul.stief@ensam.eu ; Dr. Alexandre SAVA alexandre.sava@univ-lorraine.fr ; Prof. Jean-Yves DANTAN jean-yves.dantan@ensam.eu --- LCFC Arts et Métiers Metz, 4 Rue Augustin Fresnel, 57078 METZ

ParisTech

TITLE: STUDYING AMORPHOUS SOLIDS AND LIQUIDS THROUGH MACHINE-LEARNED POTENTIALS BASED ON AB INITIO DATA

Topic number : ***2023_016***

Field : Chemistry, Physical chemistry and Chemical Engineering, Material science, Mechanics and Fluids,

Subfield:

ParisTech School: Chimie ParisTech - PSL
Research team: COCP https://www.coudert.name
Research lab: IRCP - Institut de Recherche de Chimie de Paris
Lab location: Paris
Lab website:https://www.ircp.cnrs.fr

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Coudert François-Xavier fx.coudert@chimieparistech.psl.eu
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: In order to combine the chemical accuracy of ab initio methods, and the much lower computational cost of classical force field-based MD, we aim to develop a new machine learning potentials (MLP) for simulating disordered phases of condensed matter. This rapidly developing new generation of force field (representation of the interatomic interactions in the system) have several key advantages: they are not fixed to specific functional forms; they are inherently reactive, i.e. can describe chemical events like bond breaking and formation; they can be optimized based on data obtained at higher computational level, like DFT. Our group already has significant experience in the development of these MLPs, and data-based machine learning methods in chemistry in general. In this project, we apply these methods to two different categories of systems: (1) borosilicate glasses and their formation mechanism; (2) molten carbonates, their solvation of CO2, and the transient species generated by CO2 chemistry in carbonates.

Required background of the student: computational chemistry, physical chemistry

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. “Best practices in machine learning for chemistry”, N. Artrith, K. T. Butler, F.-X. Coudert, S. Han, O. Isayev, A. Jain and A. Walsh, Nature Chem., 2021, 13 (6), 505–508. https://doi.org/10.1038/s41557-021-00716-z

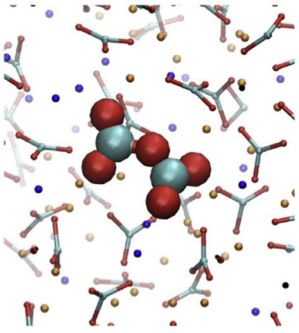
2. “Defective Nature of CdSe Quantum Dots Embedded in Inorganic Matrices”, W. Li, K. Li, X. Zhao, C. Liu and F.-X. Coudert, J. Am. Chem. Soc., 2022, 144 (25), 11296–11305. https://doi.org/10.1021/jacs.2c03039

3. “Liquid metal-organic frameworks”, R. Gaillac, P. Pullumbi, K. A. Beyer, K. W. Chapman, D. A. Keen, T. D. Bennett and F.-X. Coudert, Nature Mater., 2017, 16 (11), 1149–1154. https://doi.org/10.1038/nmat4998

4. “Pressure promoted low-temperature melting of metal–organic frameworks”, R. N. Widmer, G. I. Lampronti, S. Anzellini, R. Gaillac, S. Farsang, C. Zhou, A. M. Belenguer, C. Wilson, H. Palmer, A. K. Kleppe, M. T. Wharmby, X. Yu, S. M. Cohen, S. G. Telfer, S. A. T. Redfern, F.-X. Coudert, S. G. MacLeod and T. D. Bennett, Nature Mater., 2019, 18 (4), 370–376. https://doi.org/10.1038/s41563-019-0317-4

5. “Carbon dioxide transport in molten calcium carbonate occurs through an oxo-Grotthuss mechanism via a pyrocarbonate anion”, D. Corradini, F.-X. Coudert and R. Vuilleumier, Nature Chem., 2016, 8 (5), 454–460. https://doi.org/10.1038/nchem.2450

Illustrations :



Pyrocarbonate ion ($C_2O_5^{2-}$) in eutectic $LiKCO_3$, formed by the reaction of CO_2 with CO_3^{2-}.

ParisTech

TITLE: MODEL ORDER REDUCTION FOR ELECTRONIC STRUCTURE CALCULATIONS WITH QUANTUM OPTIMAL TRANSPORT

Topic number : ***2023_017***

Field : Mathematics and their applications, Chemistry, Physical chemistry and Chemical Engineering, Material science, Mechanics and Fluids

Subfield:

ParisTech School: Ecole des Ponts ParisTech
Research team: Modelisation, Analysis and Simulation
Research lab: CERMICS - Centre d'enseignement et de recherche en Mathématiques et calcul scientifique
Lab location: Champs-sur-Marne
Lab website:https://cermics-lab.enpc.fr/

Contact point for this topic: Ecole des Ponts ParisTech

Advisor 1: Ehrlacher Virginie virginie.ehrlacher@enpc.fr
Advisor 2: Dusson Geneviève genevieve.dusson@math.cnrs.fr
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: The objective of this PhD is to propose novel numerical methods for constructing new reduced-order models in order to accelerate the simulation of parametrized electronic structure calculations. In particular, we would like to focus on reduced-order modeling techniques in order to efficiently compute approximations of the so-called density matrix of the electronic system, which is a self-adjoint trace-class operator. To this aim, we wish to use quantum optimal transport theory, in particular the notion of quantum Wasserstein barycenters, which is an extension of classical Wasserstein barycenters. Indeed, Wasserstein barycenters are common tools nowadays in order to compute interpolations between probability measures, and quantum Wasserstein barycenters will be used in this PhD to build interpolations between self-adjoint trace-class operators. The aim of the PhD is to analyze from a theoretical viewpoint this new methodology and propose new efficient algorithms which will be used in practice to accelerate simulations of real molecules. The topic of the PhD thus lies at the

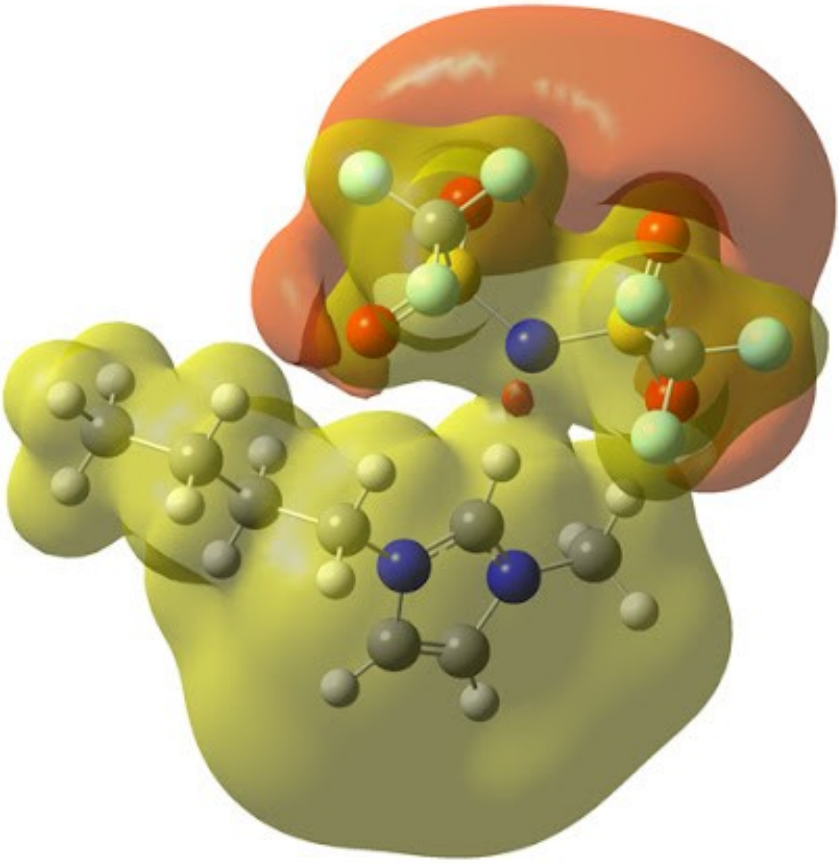
interface between spectral theory, optimal transport and quantum chemistry.

Required background of the student: M2 level in applied mathematics, preferably PDE and numerical analysis

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. GOLSE François, MOUHOT Clément, PAUL Thierry. On the mean field and classical limits of quantum
mechanics. Communications in Mathematical Physics, 2016, vol. 343, p. 165-205.
2. AGUEH Martial, CARLIER Guillaume. Barycenters in the Wasserstein space. SIAM Journal on Mathematical
Analysis, 2011, vol. 43, no 2, p. 904-924.
3. DALERY, Maxime, DUSSON Geneviève, EHRLACHER Virginie, LOZINSKI Alexeï. Nonlinear reduced basis
using mixture Wasserstein barycenters: application to an eigenvalue problem inspired from quantum chemistry,
https://arxiv.org/abs/2307.15423
4.
5.

Illustrations :



ParisTech

TITLE: ANALYSIS OF PATIENT LANGUAGE, HETEROGENEOUS DATA USING AUTOMATED ARTIFICIAL INTELLIGENCE METHODS FOR QUALITY OF LIFE IN ONCOLOGY

Topic number : ***2023_018***

Field : Life and Health Science and Technology, Mathematics and their applications,

Subfield:

ParisTech School: Chimie ParisTech - PSL
Research team: SEISAD https://iclehs.fr/research/seisad/
Research lab: I-CLEHS - Institute of chemistry for life and health
Lab location: Paris
Lab website:https://www.chimieparistech.psl.eu/recherche/les-laboratoires/i-clehs/

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Doan Bich-Thuy bich-thuy.doan@chimieparistech.psl.eu
Advisor 2: Doan Bich-Lien bich-lien.doan@centralesupelec.fr
Advisor 3: Buvet Pierre André
Advisor 4: no

Short description of possible research topics for a PhD: In the hospital environment, in the case of cancer treatment, it is important for doctors to have access to as much diagnostic data as possible, so that they can assess the progress of the pathology in real time. Numerous digital artificial intelligence tools have been developed.
It is also essential to have information from the patient's point of view, in terms of how they feel and their level of information, so that they are as well informed as possible about the side effects and additional support resources offered by the hospital, so that they can play an active role in their well-being and therefore in their recovery.
The general objective is to structure the patient's experience by identifying biomarkers present in the patient's language and to enrich a clinical assessment to help the clinician and the patient to orient themselves towards the supportive care offered by the hospital.
To do this, we propose to develop an automated computer science tool using AI methods, leading to recommendations for the patient's well-being.
- Our aim is to identify and develop automated digital tools using AI and

Deep Learning to classify patients according to their level of well-being, in order to recommend referral to a doctor or to supportive care.
This project will be performed in collaboration with 3 partners including an AI ML team from Lisn Paris Saclay University, Language Text Numerical Theories AI team from Sorbonne Paris Nord, and a team of clinicians from Paris Hospital.

Required background of the student: Engineering sciences, Mathematics, Artificial Intelligence, Machine Learning, Biophysics

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Thebault CJ. ... Menager C., Doan BT. Theranostic MRI liposomes for magnetic targeting and ultrasound triggered release of the antivascular CA4P. J Control Release. 2020 322, 137.
2. Galofaro F., Toffano Z. , Doan BL. A quantum-based semiotic model for textual semantics 2018/2/7, Kybernetes, 47, 2, 307-320
3. Bouramoul A., Kholladi M., Doan BL. How ontology can be used to improve semantic information retrieval: the AnimSe finder tool, 2011/5, International Journal of Computer Applications, 21, 9, 48-54
4. Fadel W., Bouchentouf T., Buvet PA, Bourja O.: Adapting Off-the-Shelf Speech Recognition Systems for Novel Words. Inf. 14(3): 179 (2023)
5. Buvet PA, Fache B., Fadel W., A Rouam: A. How Does a Social Robot Analyze Emotions? FTC (3) 2022: 463-477

Illustrations :



ParisTech

ESPCI PARIS PSL

TITLE: SYNTHESIS OF FUNCTIONALIZED MACROCYCLES USING A RING-EXPANSION STRATEGY

Topic number : ***2023_019***

Field : Chemistry, Physical chemistry and Chemical Engineering, ,

Subfield:

ParisTech School: ESPCI Paris - PSL
Research team: Benjamin Laroche https://www.cmc.espci.fr/Dr-Benjamin-Laroche
Research lab: C3M - Chimie Moléculaire, Macromoléculaire, et Matériaux
Lab location: Paris
Lab website:https://www.cmc.espci.fr/-Home-

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Laroche Benjamin benjamin.laroche@espci.fr
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Macrocycles are ubiquitous scaffolds in bioactive natural products, but only a very few synthetic macrocyclic compounds have found applications in medicinal chemistry. Along with the deviation from Lipinski's rule of five, the difficulty in the synthesis of macrocycle limits their potential to become successful drug candidates. In general, macrocycles are obtained by intramolecular cyclization, which requires high energy to overcome the activation barrier. To circumvent this limitation, our group designed a strategy to access functionalized macrocycles through a two-step fused-ring formation and ring-opening macrocyclization sequence. This break-it-to-make-it strategy will thus be harnessed to obtain highly functionalized N-macrocycles with high potential for medicinal applications. If possible, this two-step protocol will be applied to continuous-flow reactors to highlight the scalability of the process.

Required background of the student: Organic synthesis

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. J. Mallinson, I. Collins, Future Medicinal Chemistry 2012, 4 (11) 1409.
2. C. A. Lipinski, F. Lombardo, B. W. Dominy, P. J. Feeney, Adv. Drug Deliv. Rev. 1997, 23, 3.
3. K. T. Mortensen, T. J. Osberger, T. A. King, H. F. Sore, D. R. Spring, Chem. Rev. 2019, 17, 10288.
4.
5.

Illustrations :

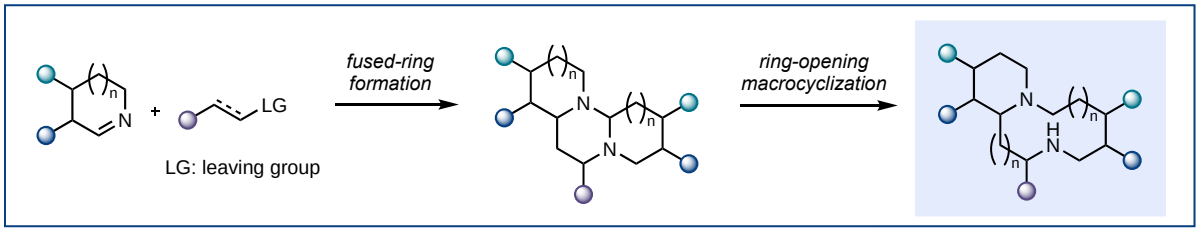
PhD in organic chemistry

Institution and supervisor:
Host Institution : ESPCI-Paris/PSL University
Host Team : Molecular Chemistry and Catalysis (CMC, C3M Unit)
Supervisor *:* Dr. Benjamin Laroche
E-mail : benjamin.laroche@espci.fr
Webpage : www.cmc.espci.fr/Dr-Benjamin-Laroche

Position :
In the framework of the PhD-ParisTech-CSC 2023/2024, we are looking for a PhD student for a period of 4 years motivated in ***organic synthesis*** to work on the ***synthesis of functionalized macrocycles*** using a ***ring-expansion strategy***. The work will be supervised by Dr. Benjamin Laroche at the prestigious ESPCI-Paris/PSL University (www.espci.psl.eu/en).

Project:
Synthesis of functionalized macrocycles using a ring-expansion strategy

Macrocycles are ubiquitous scaffolds in bioactive natural products, but only a very few synthetic macrocyclic compounds have found applications in medicinal chemistry.[1] Along with the deviation from Lipinski's rule of five,[2] the difficulty in the synthesis of macrocycle limits their potential to become successful drug candidates. In general, macrocycles are obtained by intramolecular cyclization, which requires high energy to overcome the activation barrier.[3] To overcome and circumvent this limitation, our group designed a strategy to access functionalized macrocycles through a two-step fused-ring formation and ring-opening macrocyclization sequence (Scheme 1).



Scheme 1. General strategy for the synthesis of nitrogen-containing macrocycles

Preliminary results showed that the fused-rings scaffold (**1**) can be obtained by mixing cyclic imines **2** with compound **3** in a one-pot fashion. Then, nitrogen-containing macrocycles **4** can be obtained by a selective C—N bond breaking. This break-it-to-make-it strategy will thus be harnessed to obtain highly functionalized *N*-macrocycles with high potential for medicinal applications. If possible, this two-step protocol will be applied to ***continuous-flow reactors*** to highlight the scalability of the process.

Required skills:
The student will focus on the synthesis of new macrocycles through a multi-step sequence. In this sense, ***very good theoretical and working knowledge in organic synthesis*** is expected (Master level is required). The student should also ***be comfortable with classical analytical techniques in organic chemistry*** such as NMR, MS, IR spectroscopy. The research work will take place in an international environment including several research groups, so he/she will be expected to have very good communication skills (**fluent English is mandatory**) and a good

team spirit. In addition, we expect the student to be motivated and well-organized to allow him/her to progress smoothly in his research work.

Specific skills developed during the PhD and perspectives:

The student will get a PhD degree from ESPCI/PSL-University, a world-leading research institution. He/she will face various synthetic challenges during their PhD and will thereby become an expert in multistep organic synthesis. In addition, the student will develop great communication and dissemination skills by presenting the advancement of his/her works on a regular basis. Finally, he/she will develop a know-how in flow chemistry, a real asset for his/her future career either in academia or industry.

References:

[1] J. Mallinson, I. Collins, *Future Medicinal Chemistry* **2012**, 4 (11) 1409.
[2] C. A. Lipinski, F. Lombardo, B. W. Dominy, P. J. Feeney, *Adv. Drug Deliv. Rev.* **1997**, *23*, 3.
[3] K. T. Mortensen, T. J. Osberger, T. A. King, H. F. Sore, D. R. Spring, *Chem. Rev.* **2019**, *17*, 10288.

ParisTech

TITLE: FOLLOWING EXCITED STATES EVOLUTION USING DENSITY BASED METHODS

Topic number : ***2023_020***

Field : Chemistry, Physical chemistry and Chemical Engineering, ,

Subfield:

ParisTech School: Chimie ParisTech - PSL
Research team: Theoretical Chemistry and Modelling Team (TCM) https://www.quanthic.fr/
Research lab: I-CLEHS - Institute of chemistry for life and health
Lab location: Paris
Lab website:https://iclehs.fr/

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Ciofini Ilaria ilaria.ciofini@chimieparistech.psl.eu
Advisor 2: Labat Frederic frederic.labat@chimieparistech.psl.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Density Functional Theory (DFT) and Time-dependent DFT (TD-DFT) are nowadays one of the quantum methods more largely applied to study the reactivity and properties of complex chemical systems at the ground and the excited states, respectively. Various literature contributions have nonetheless assessed their limitations especially for the description of excited states. In this thesis we want to develop and apply novel physically motivated corrections to current DFT approaches to improve their description of excited states, with a special emphasis on methods enabling to more efficiently describe excited states relaxation. This methods will be applied to two classes of compounds : 1) metal containing complexes developed for photodynamic therapy and 2) luminescent molecules in condensed phases (crystalline or amorphous). The applications will benefit from ongoing collaborations with experimental groups.

Required background of the student: physical chemistry, theoretical chemistry, computational Chemistry

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. A. Savin et al DFT Exchange: Sharing Perspectives on the Workhorse of Quantum Chemistry and Materials Science PCCP (2022) 24, 28700-28781 doi.org/10.1039/D2CP02827A
2. M. Turelli, I. Ciofini, Q. Wang, A. Ottochian, F. Labat, C. Adamo Organic compounds for solid state luminescence enhancement/aggregation induced emission: a theoretical perspective Phys. Chem. Chem. Phys., (2023) 25, 17769-17786
3. F. A. Korsaye, A. de la Lande, I. Ciofini Following the Density evolution using Real Time Density Functional Theory and Density Based indexes: application to model push-pull molecules JCC (2022) 43, 1464-1473
4. F. Maschietto, M. Campetella, J. Sanz-García, C. Adamo, I. Ciofini Chasing unphysical TD-DFT excited states in transition metal complexes with a simple diagnostic tool J Chem Phys. 154 (2021) 204102
5. J. Karges, S. Kuang, F. Maschietto, O. Blacque, I. Ciofini, H. Chao and G. Gasser Ruthenium Complexes for 1- and 2-Photon Photodynamic Therapy: From In Silico Prediction to In Vivo Applications Nature Comm 11 (2020) 3262.

Illustrations :

TITLE: DEVELOPING SERIOUS GAMES FOR TEACHING SMART AND CONNECTED PRODUCT DESIGN

Topic number : ***2023_021***

Field : Design, Industrialization, ,

Subfield:

ParisTech School: Arts et Métiers
Research team:
Research lab: LCPI - Laboratoire conception de produits et innovation
Lab location: Paris
Lab website:https://lcpi.ensam.eu/

Contact point for this topic: Arts et Métiers

Advisor 1: JEAN Camille camille.jean@ensam.eu
Advisor 2: LOU Ruding ruding.lou@ensam.eu
Advisor 3: SEGONDS Frédéric frederic.segonds@ensam.eu
Advisor 4:

Short description of possible research topics for a PhD: Design and innovation are necessary for companies to succeed in a globalized and competitive world. With the rapid development of digital technologies, forecasts on product development predict that smart and connected products will keep on growing fast (ISAKSSON et al., 2020; BRIARD et al., 2021). One of the key issues for companies lies in employing engineers and designers that understand the full technique of design and innovation of those product as well as continuously train those already hired.
Serious games are one solution to develop skills and teach product design in a ludic way (MA et al., 2019). Their usage is frequent as they can improve enjoyment, passionate involvement, structure, and social interaction while the learning takes place.
However, very few serious games tackle the subject of smart and connected product design. This thesis aims at proposing a method to develop serious games for teaching smart and connected product design.

Required background of the student:

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. BRIARD, T., JEAN, C., AOUSSAT, A., VERON, P., LE CARDINAL, J. & WARTZACK, S. (2021). Data-driven design challenges in the early stages of the product development process. Proceedings of the Design Society, 1, 851-860. https://doi:10.1017/pds.2021.85
2. LI, B., SEGONDS, F., MATEEV, C., LOU, R., MERIENNE, F. (2018). Design in context of use: An experiment with a multi-view and multi-representation system for collaborative design, Computers in Industry, 103: 28 - 37, 2018. https://doi.org/10.1016/j.compind.2018.09.006
3. MA, Y., VALLET, F., CLUZEL, F., & YANNOU, B. (2019). Analyzing the Relevance of Serious Game Elements for Effectively Teaching Innovation Processes. Proceedings of the Design Society: International Conference on Engineering Design, 1(1), 439-448. https://doi:10.1017/dsi.2019.47
4. PHAM VAN, L., JEAN, C., MEYRUEIS, V., GAZO, C., MANTELET, F., GUEGUAN, J., BUISINE, S. & SEGONDS, F. 2022 IdeAM Running Quiz: A Digital Learning Game to Enhance Additive Manufacturing Opportunities Discovery. International Journal of Emerging Technologies in Learning (iJET), 17(10), pp. 32–50. https://doi.org/10.3991/ijet.v17i10.25695
5. ISAKSSON, O., ECKERT, C., (2020). Product Development 2040. The Design Society.
https://doi.org/10.35199/report.pd2040

Illustrations :


Texture
Temperature
Location
Hue
Form
Light
Speed
Size
Orientation
Brightness
Elevation

CSC PhD Scholarships

Developing serious games for teaching smart and connected product design

Keywords: Innovation, Design Science, Serious Game, smart and connected Product, IOT

Design and innovation are necessary for companies to succeed in a globalized and competitive world. With the rapid development of digital technologies, forecasts on product development predict that **smart and connected products** will keep on growing fast (ISAKSSON et al., 2020; BRIARD et al., 2021). One of the key issues for companies lies in employing engineers and designers that understand the full technique of design and innovation of those product as well as continuously train those already hired.

Serious games are one solution to develop skills and teach product design in a ludic way (MA et al., 2019). Their usage is frequent as they can improve enjoyment, passionate involvement, structure, and social interaction while the learning takes place.

However, very few serious games tackle the subject of smart and connected product design.

This thesis aims at **proposing a method to develop serious games for teaching smart and connected product design.**

Application of this method will lead to the creation of one or more physical or digital serious games for teaching smart and connected product design. The last technologies of Virtual and Augmented Reality could be used (LI et al., 2018; PHAM VAN et al., 2022). The learning competences of the serious games created have to integrate the themes of smart and connected product design, data collection, sensors integration and user experience. A robust evaluation of the serious games created will have to be carried out to validate the principles, heuristics and recommendations formulated.

The research will be divided into three main phases:

- **State of the art**: The first year will be devoted to the development of a state of the art on the existing methodologies for the design of smart and connected product and serious games. Following this work, specifications will be formulated, and hypotheses of resolutions proposed. At the end of this first year, a detailed schedule of experiments will be defined
- **Proposal of a tooled methodology and experiments:** The second and third year will be devoted to experiments. The objective is to test, but above all to strengthen and validate the proposals. The methodology, tools and recommendations will be perfected by iteration, as experiments and conclusions can be drawn.
- **Formalization of research advances**: The last year will aim to synthesize all the work carried out to get an optimal proposition adapted to the context of the thesis.

References:

- BRIARD, T., JEAN, C., AOUSSAT, A., VERON, P., LE CARDINAL, J. & WARTZACK, S. (2021). Data-driven design challenges in the early stages of the product development process. *Proceedings of the Design Society*, *1*, 851-860. https://doi:10.1017/pds.2021.85
- LI, B., SEGONDS, F., MATEEV, C., LOU, R., MERIENNE, F. (2018). Design in context of use: An experiment with a multi-view and multi-representation system for collaborative design, Computers in Industry, 103: 28 - 37, 2018. https://doi.org/10.1016/j.compind.2018.09.006
- MA, Y., VALLET, F., CLUZEL, F., & YANNOU, B. (2019). Analyzing the Relevance of Serious Game Elements for Effectively Teaching Innovation Processes. *Proceedings of the Design Society: International Conference on Engineering Design, 1*(1), 439-448. https://doi:10.1017/dsi.2019.47
- PHAM VAN, L., JEAN, C., MEYRUEIS, V., GAZO, C., MANTELET, F., GUEGUAN, J., BUISINE, S. & SEGONDS, F. 2022 IdeAM Running Quiz: A Digital Learning Game to Enhance Additive Manufacturing Opportunities Discovery. *International Journal of Emerging Technologies in Learning (iJET),* 17(10), pp. 32–50. https://doi.org/10.3991/ijet.v17i10.25695
- ISAKSSON, O., ECKERT, C., (2020). Product Development 2040. The Design Society. https://doi.org/10.35199/report.pd2040

TITLE: INNOVATIVE DESIGN FOR ADDITIVE MANUFACTURING THROUGH KNOWLEDGE MANAGEMENT AND ARTIFICIAL INTELLIGENCE

Topic number : ***2023_022***

Field : Design, Industrialization, Information and Communication Science and Technology, Mathematics and their applications

Subfield:

ParisTech School: Arts et Métiers
Research team:
Research lab: LCFC - Laboratoire de conception, fabrication, commande
Lab location: Metz
Lab website:https://lcfc.ensam.eu/lcfc-accueil-119817.kjsp

Contact point for this topic: Arts et Métiers

Advisor 1: Siadat Ali ali.siadat@ensam.eu
Advisor 2: Hassan Alaa alaa.hassan@univ-lorraine.fr
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Additive manufacturing (AM) offers significant opportunities for product innovation in many fields . The Design for Additive Manufacturing (DfAM) approach could be considered as a guideline for the design team in the early phase of the product development process . However, AM is becoming a data-intensive activity and the design of a new product can be facilitated by using previous knowledge from successful projects and the literature. This relevant knowledge is not easy to find or reuse. In this context, Artificial Intelligence (AI) is increasingly involved in the decision-makings throughout the stages of AM product development . AI techniques like Machine Learning (ML) is able to assist practitioners in product design, pre-manufacturing planning, and product quality assessment and control . The theory of inventive problem solving methodology (TRIZ) is a well-established accelerator to support problem solving by linking specific engineering problems and solutions to general patterns and laws . TRIZ method can be coupled with a well-structured knowledge base (KB) and ML algorithms in order to build a DfAM support system that helps the engineers in finding the most suitable rules and constraint-solving principles to fully exploit the potential of AM.
The main objectives of the proposal are:

1. Development of a KB system in order to capture and structure the DfAM principles and knowledge. Web Ontology Language (OWL) or System Modelling Language (SysML) could be used.
2. Integrating the TRIZ inventive principles into the KB system supported by ML algorithms in order to build DfAM support system. AI could be used to map the problem space to the solution space and to retrieve the relevant information.

Required background of the student: The candidate must have a master degree in industrial, systems or informatics engineering. Skills in programming and Artificial Intelligence will be appreciated.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. T. J. Hagedorn, S. Krishnamurty, and I. R. Grosse, “A Knowledge-Based Method for Innovative Design for Additive Manufacturing Supported by Modular Ontologies,” J. Comput. Inf. Sci. Eng., vol. 18, no. 2, pp. 1–12, 2018.
2. S. Kadkhoda-Ahmadi, A. Hassan, and E. Asadollahi-Yazdi, “Process and resource selection methodology in design for additive manufacturing,” Int. J. Adv. Manuf. Technol., vol. 104, no. 5–8, pp. 2013–2029, 2019.
3. C. Liu, W. Tian, and C. Kan, “When AI meets additive manufacturing: Challenges and emerging opportunities for human-centered products development,” J. Manuf. Syst., vol. 64, no. May, pp. 648–656, 2022.
4. C. Wang, X. P. Tan, S. B. Tor, and C. S. Lim, “Machine learning in additive manufacturing: State-of-the-art and perspectives,” Addit. Manuf., vol. 36, no. January, p. 101538, 2020.
5. N. Kretzschmar and S. Chekurov, “The applicability of the 40 TRIZ principles in design for additive manufacturing,” Ann. DAAAM Proc. Int. DAAAM Symp., vol. 29, no. 1, pp. 888–893, 2018.

Illustrations :

Research Topic for the ParisTech/CSC PhD Program

Subfield: Industrial Engineering, Information Engineering

ParisTech School: Arts et Métiers ParisTech campus de Metz

Title: Innovative Design for Additive Manufacturing through Knowledge Management and Artificial Intelligence

Advisors: Pr. Ali SIADAT ali.siadat@ensam.eu
Dr. Alaa HASSAN alaa.hassan@univ-lorraine.fr

Short description of possible research topics for a PhD:

Additive manufacturing (AM) offers significant opportunities for product innovation in many fields [1]. The Design for Additive Manufacturing (DfAM) approach could be considered as a guideline for the design team in the early phase of the product development process [2]. However, AM is becoming a data-intensive activity and the design of a new product can be facilitated by using previous knowledge from successful projects and the literature. This relevant knowledge is not easy to find or reuse. In this context, Artificial Intelligence (AI) is increasingly involved in the decision-makings throughout the stages of AM product development [3]. AI techniques like Machine Learning (ML) is able to assist practitioners in product design, pre-manufacturing planning, and product quality assessment and control [4]. The theory of inventive problem solving methodology (TRIZ) is a well-established accelerator to support problem solving by linking specific engineering problems and solutions to general patterns and laws [5]. TRIZ method can be coupled with a well-structured knowledge base (KB) and ML algorithms in order to build a DfAM support system that helps the engineers in finding the most suitable rules and constraint-solving principles to fully exploit the potential of AM.
The main objectives of the proposal are:

1. Development of a KB system in order to capture and structure the DfAM principles and knowledge. Web Ontology Language (OWL) or System Modelling Language (SysML) could be used.
2. Integrating the TRIZ inventive principles into the KB system supported by ML algorithms in order to build DfAM support system. AI could be used to map the problem space to the solution space and to retrieve the relevant information.

Required background of the student:

The candidate must have a master degree in industrial, systems or informatics engineering. Skills in programming and Artificial Intelligence will be appreciated.

A list of 5 (max.) representative publications of the group:

[1] T. J. Hagedorn, S. Krishnamurty, and I. R. Grosse, “A Knowledge-Based Method for Innovative Design for Additive Manufacturing Supported by Modular Ontologies,” J. Comput. Inf. Sci. Eng., vol. 18, no. 2, pp. 1–12, 2018.
[2] S. Kadkhoda-Ahmadi, A. Hassan, and E. Asadollahi-Yazdi, “Process and resource selection methodology in design for additive manufacturing,” Int. J. Adv. Manuf. Technol., vol. 104, no. 5–8, pp. 2013–2029, 2019.
[3] C. Liu, W. Tian, and C. Kan, “When AI meets additive manufacturing: Challenges and emerging opportunities for human-centered products development,” J. Manuf. Syst., vol. 64, no. May, pp. 648–656, 2022.
[4] C. Wang, X. P. Tan, S. B. Tor, and C. S. Lim, “Machine learning in additive manufacturing: State-of-the-art and perspectives,” Addit. Manuf., vol. 36, no. January, p. 101538, 2020.
[5] N. Kretzschmar and S. Chekurov, “The applicability of the 40 TRIZ principles in design for additive manufacturing,” Ann. DAAAM Proc. Int. DAAAM Symp., vol. 29, no. 1, pp. 888–893, 2018.

ParisTech

Arts et Métiers Sciences et Technologies

TITLE: DEVELOPMENT OF A DIGITAL TWIN FOR QUALIFICATION OF ADDITIVE MANUFACTURING PARTS

Topic number : ***2023_023***

Field : Design, Industrialization, Information and Communication Science and Technology, Mathematics and their applications

Subfield:

ParisTech School: Arts et Métiers
Research team:
Research lab: LCFC - Laboratoire de conception, fabrication, commande
Lab location: Metz
Lab website:https://lcfc.ensam.eu/lcfc-accueil-119817.kjsp

Contact point for this topic: Arts et Métiers

Advisor 1: Siadat Ali ali.siadat@ensam.eu
Advisor 2: Hassan Alaa alaa.hassan@univ-lorraine.fr
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: The quality of the part fabricated by additive manufacturing (AM) process remains one of the main challenges for the industry. AM processes are typically optimized utilizing offline modelling and monitoring tools and parts are inspected at the end of the process . Various experimental approaches have been proposed to control part quality by establishing its links with process parameters such as speed, temperature and layer thickness . Some research works combine experimental, numerical and statistical approaches in order to predict the part quality . While feedback on some AM process parameters is available (e.g. directed energy deposition) , other processes, such as Fused Filament Fabrication (FFF), are not equipped with sensors to provide this information. To address this problem, the digital twin concept is a promising holistic approach for digitalizing the AM process chain like FFF. Its advantages include reducing time-to-market, minimizing expensive trial and error optimization with physical parts, detecting defects and shortening the path for product qualification .
The main objectives of the proposal are:
1. Modification of an FFF 3D printer by integrating heat and speed sensors.

2. Design and implementation of a digital twin approach that combines physics-based models (analytical models, computational models) and data-driven models (empirical data extracted from sensors to observations).
3. Providing a platform for the monitoring and detection of AM part faults by combining theoretical predictions with real-time sensor data, thereby providing a basis for model-based feedforward control in AM.

Required background of the student: The candidate must have a master degree in industrial, mechatronics or informatics engineering. Skills in Data Analysis and Artificial Intelligence will be appreciated.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. P. Stavropoulos, A. Papacharalampoloulos, and K. Tzimanis, “Design and Implementation of a Digital Twin Platform for AM processes,” Procedia CIRP, vol. 104, no. March, pp. 1722–1727, 2021.
2. Y. Tu, J. A. Arrieta-Escobar, A. Hassan, U. K. uz Zaman, A. Siadat, and G. Yang, “Optimizing Process Parameters of Direct Ink Writing for Dimensional Accuracy of Printed Layers,” 3D Print. Addit. Manuf., Dec. 2021.
3. Z. Huang, J. Y. Dantan, A. Etienne, M. Rivette, and N. Bonnet, “Geometrical deviation identification and prediction method for additive manufacturing,” Rapid Prototyp. J., 2018.
4. A. Gaikwad, R. Yavari, M. Montazeri, K. Cole, L. Bian, and P. Rao, “Toward the digital twin of additive manufacturing: Integrating thermal simulations, sensing, and analytics to detect process faults,” IISE Trans., vol. 52, no. 11, pp. 1204–1217, 2020.
5. P. Stavropoulos, A. Papacharalampoloulos, and K. Tzimanis, “Design and Implementation of a Digital Twin Platform for AM processes,” Procedia CIRP, vol. 104, no. March, pp. 1722–1727, 2021.
Y. Tu, J. A. Arrieta-Escobar, A. Hassan, U. K. uz Zaman, A. Siadat, and G. Yang, “Optimizing Process Parameters of Direct Ink Writing for Dimensional Accuracy of Printed Layers,” 3D Print. Addit. Manuf., Dec. 2021.
Z. Huang, J. Y. Dantan, A. Etienne, M. Rivette, and N. Bonnet, “Geometrical deviation identification and prediction method for additive

manufacturing,” Rapid Prototyp. J., 2018.
A. Gaikwad, R. Yavari, M. Montazeri, K. Cole, L. Bian, and P. Rao, “Toward the digital twin of additive manufacturing: Integrating thermal simulations, sensing, and analytics to detect process faults,” IISE Trans., vol. 52, no. 11, pp. 1204–1217, 2020.
S. Krückemeier and R. Anderl, “Concept for Digital Twin Based Virtual Part Inspection for Additive Manufacturing,” Procedia CIRP, vol. 107, no. March, pp. 458–462, 2022.

Illustrations :

Research Topic for the ParisTech/CSC PhD Program

Subfield: Industrial Engineering, Information Engineering

ParisTech School: Arts et Métiers ParisTech campus de Metz

Title: Development of a digital twin for qualification of additive manufacturing parts

Advisors: Pr. Ali SIADAT ali.siadat@ensam.eu
Dr. Alaa HASSAN alaa.hassan@univ-lorraine.fr

Short description of possible research topics for a PhD:

The quality of the part fabricated by additive manufacturing (AM) process remains one of the main challenges for the industry. AM processes are typically optimized utilizing offline modelling and monitoring tools and parts are inspected at the end of the process [1]. Various experimental approaches have been proposed to control part quality by establishing its links with process parameters such as speed, temperature and layer thickness [2]. Some research works combine experimental, numerical and statistical approaches in order to predict the part quality [3]. While feedback on some AM process parameters is available (e.g. directed energy deposition) [4], other processes, such as Fused Filament Fabrication (FFF), are not equipped with sensors to provide this information. To address this problem, the digital twin concept is a promising holistic approach for digitalizing the AM process chain like FFF. Its advantages include reducing time-to-market, minimizing expensive trial and error optimization with physical parts, detecting defects and shortening the path for product qualification [5].

The main objectives of the proposal are:

1. Modification of an FFF 3D printer by integrating heat and speed sensors.
2. Design and implementation of a digital twin approach that combines physics-based models (analytical models, computational models) and data-driven models (empirical data extracted from sensors to observations).
3. Providing a platform for the monitoring and detection of AM part faults by combining theoretical predictions with real-time sensor data, thereby providing a basis for model-based feedforward control in AM.

Required background of the student:

The candidate must have a master degree in industrial, mechatronics or informatics engineering. Skills in Data Analysis and Artificial Intelligence will be appreciated.

A list of 5 (max.) representative publications of the group:

[1] P. Stavropoulos, A. Papacharalampoloulos, and K. Tzimanis, “Design and Implementation of a Digital Twin Platform for AM processes,” *Procedia CIRP*, vol. 104, no. March, pp. 1722–1727, 2021.

[2] Y. Tu, J. A. Arrieta-Escobar, A. Hassan, U. K. uz Zaman, A. Siadat, and G. Yang, “Optimizing Process Parameters of Direct Ink Writing for Dimensional Accuracy of Printed Layers,” *3D Print. Addit. Manuf.*, Dec. 2021.

[3] Z. Huang, J. Y. Dantan, A. Etienne, M. Rivette, and N. Bonnet, “Geometrical deviation identification and prediction method for additive manufacturing,” *Rapid Prototyp. J.*, 2018.

[4] A. Gaikwad, R. Yavari, M. Montazeri, K. Cole, L. Bian, and P. Rao, “Toward the digital twin of additive manufacturing: Integrating thermal simulations, sensing, and analytics to detect process faults,” *IISE Trans.*, vol. 52, no. 11, pp. 1204–1217, 2020.

[5] S. Krückemeier and R. Anderl, “Concept for Digital Twin Based Virtual Part Inspection for Additive Manufacturing,” *Procedia CIRP*, vol. 107, no. March, pp. 458–462, 2022.

TITLE: TIME REVERSAL MIRROR FOR RADIOFREQUENCY SIGNALS

Topic number : ***2023_024***

Field : Physics, Optics, Information and Communication Science and Technology,

Subfield:

ParisTech School: ESPCI Paris - PSL
Research team: Atomic processors https://www.institut-langevin.espci.fr/processeurs_atomiques_pour_le_traitement_du_signal159?lang=en
Research lab: Institut Langevin
Lab location: Paris
Lab website:https://www.institut-langevin.espci.fr/home

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Louchet-Chauvet Anne anne.louchet-chauvet@espci.fr
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Time reversal is a technique based on the invariance of the wave propagation equation in an inhomogeneous medium. It ensures spatial and temporal refocusing of a wave in such a medium, after having recorded the transmission channel signature. When the propagation medium is non-stationary, the transmission channel characteristics keep changing. The time-reversed signal must be sent as quickly as possible, otherwise the refocusing will not be effective. It is therefore crucial to minimize the latency time between the measurement of the impulse response and the emission of the time-reversed impulse response. In the first demonstrations of time-reversal with RF waves, analog-to-digital converters (ADC) were used, limiting the processing bandwidth. In the aim of reaching the GHz regime, the latency time becomes problematic because of the limited sampling rate of ADCs. Conversely, a fully analog solution has the advantage of avoiding this conversion step.

At Institut Langevin we design original analog architectures for the optically-carried radiofrequency signal processing. These architectures rely on light-matter interaction in rare-earth ion-doped crystals cooled

down to a few K. In these crystals, one can make the atomic medium emit a light pulse with a controlled temporal shape by using the photon echo process. We recently proposed a modified version of this photon echo sequence that allows the analog generation of the time-reversed copy of an arbitrary waveform. While the first results are encouraging, a lot remains to be done to validate its potential for broadband wave refocusing in a non-stationary medium.

The goal of this internship/thesis will be to work on improving the performance of this original time-reversal architecture. In particular, the time reversal fidelity, its robustness to phase modulation, the processing bandwidth and the latency time are the figures of merit that will be studied and optimized, in relation to the rare-earth ion-doped crystal spectroscopic properties. A demonstration of time-reversal with real RF signals propagating in a reverberating cavity will be an interesting way to assess the potential of our approach, via the quality of the spatial and/or temporal refocusing.

Required background of the student: atomic physics, optics, light-matter interaction

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Analog time-reversal of optically-carried RF signals with a rare earth ion-doped processor with broadband potential,

A. Louchet-Chauvet

IEEE Microwave Photonics (2018)

https://doi.org/10.1109/MWP.2018.8552903

2. Time Reversal of Electromagnetic Waves

G. Lerosey, J. de Rosny, A. Tourin, A. Derode, G. Montaldo, and M. Fink

Phys. Rev. Lett. 92, 193904 (2004)

https://doi.org/10.1103/PhysRevLett.92.193904

3. RF Spectrum Analyzer for Pulsed Signals: Ultra-Wide Instantaneous Bandwidth, High Sensitivity, and High Time-Resolution

Perrine Berger, Yoann Attal, Muriel Schwarz, Stéphanie Molin, Anne Louchet-Chauvet, Thierry Chanelière, Jean-Louis Le Gouët, Daniel Dolfi, and Loïc Morvan

Journal of Lightwave Technology Vol. 34, Issue 20, pp. 4658-4663 (2016)

4.

5.

Illustrations :

ParisTech

ESPCI PARIS PSL

TITLE: NON-LOCAL INTELLIGENT METASURFACES FOR MICROWAVE APPLICATIONS

Topic number : ***2023_025***

Field : Physics, Optics, Information and Communication Science and Technology,

Subfield:

ParisTech School: ESPCI Paris - PSL
Research team:
Research lab: Institut Langevin
Lab location: Paris
Lab website:https://www.institut-langevin.espci.fr/home

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Ourir Abdelwaheb a.ourir@espci.fr
Advisor 2: de Rosny Julien julien.derosny@espci.fr
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: The growth of interest in metasurfaces has led to novel and interesting possibilities for imaging and telecommunication applications. Metasurfaces have unique abilities for blocking, absorbing, concentrating, dispersing, or guiding waves, from microwave through visible frequencies. Our team has realized theoretical and experimental research in this domain that spreads from fundamental explorations of physics to actual device design . Recently, optical analog signal processing using non-local metasurfaces has been gaining significant attention as a way to overcome the speed and energy limitations of digital techniques . Most fabricated metasurfaces are passive, meaning that they cannot be tuned post fabrication. In contrast, reconfigurable intelligent surfaces (RIS) allow the dynamic control of its properties under external incidence (See figure 1). They could be useful in applications ranging from free space optical communications to holographic displays, and depth sensing. Here, we propose to study the behavior of non-local RISs in the microwave regime. The investigation will include the design, the modeling and the characterization of such structures. The aim is to propose original non-local RISs concepts for novel application systems.

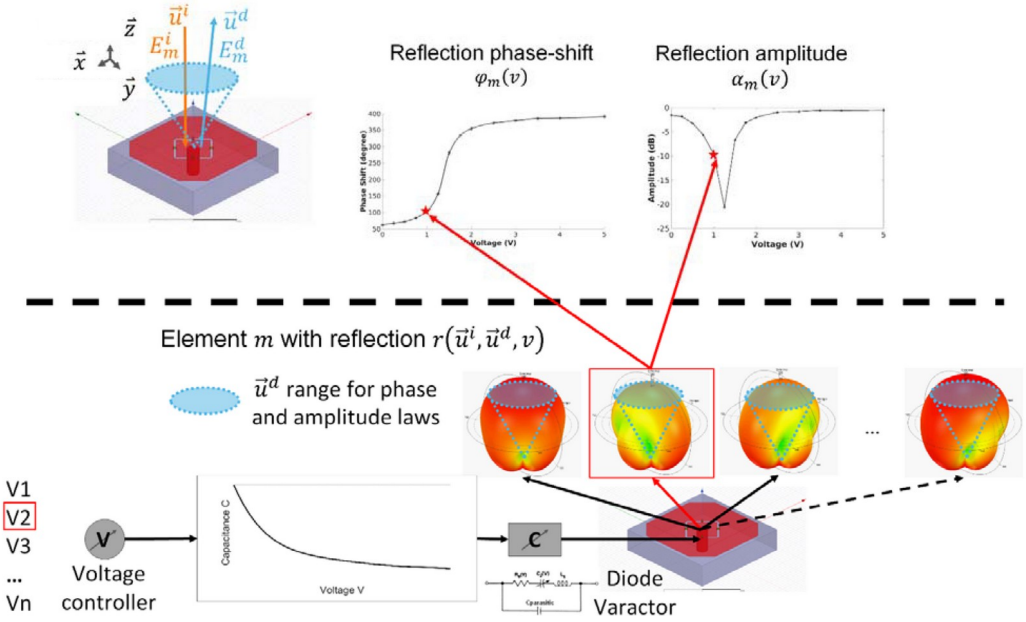
Required background of the student: Electromagnetism, telecommunication

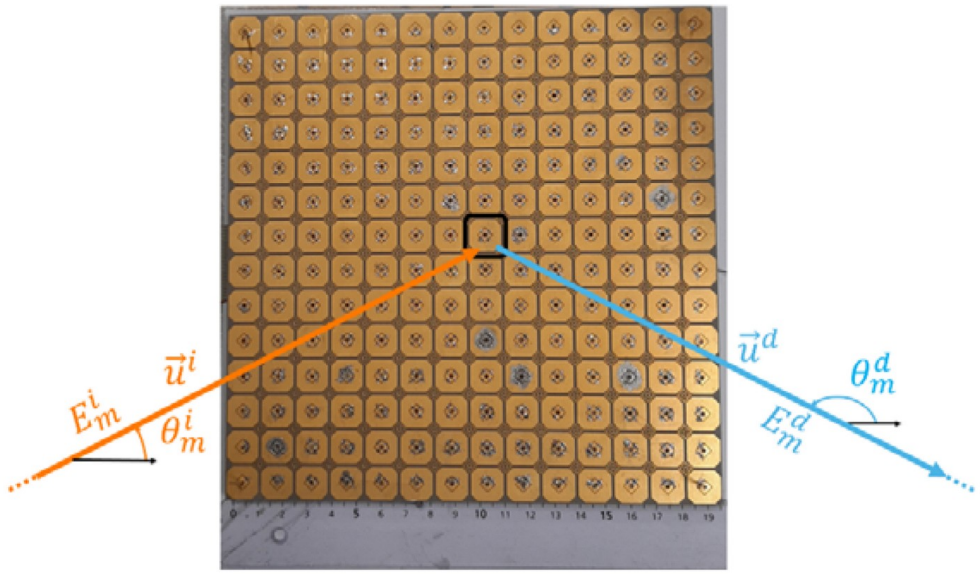
A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. R Fara, DT Phan-Huy, P Ratajczak, A Ourir, M Di Renzo, J De Rosny, “Reconfigurable intelligent surface-assisted ambient backscatter communications–experimental assessment”, IEEE international conference on communications workshops (ICC), 2021.
2. R Fara, P Ratajczak, DT Phan-Huy, A Ourir, M Di Renzo, J De Rosny, ‘A prototype of reconfigurable intelligent surface with continuous control of the reflection phase’ IEEE Wireless Communications 29 (1), 70-77, 2022.
3. AV Nikulin, A Vignaud, NI Avdievich, D Berrahou, J de Rosny, A Ourir, ‘Open birdcage coil for head imaging at 7T‘, Magnetic Resonance in Medicine 86 (4), 2290-2300, 2021.
4. K Rachedi, A Ourir, DT Phan-Huy, J de Rosny, ‘Reconfigurable compact antenna for spatial modulation mimo communications‘, International Journal on Communications Antenna and Propagation 9 (3), 218, 2020.
5. Kwon Hoyeong, et al, Nonlocal Metasurfaces for Optical Signal Processing, Phys. Rev. Lett., 121(17), pp 173004, 2018.

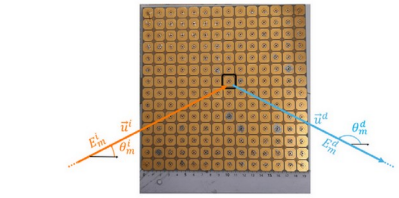
Illustrations :

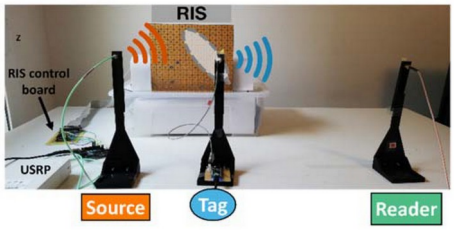
Reflection phase-shift and amplitude of the element m for fixed $\vec{u}^i$ and for $\vec{u}^d$ for in the range of the phase-shift and amplitude laws

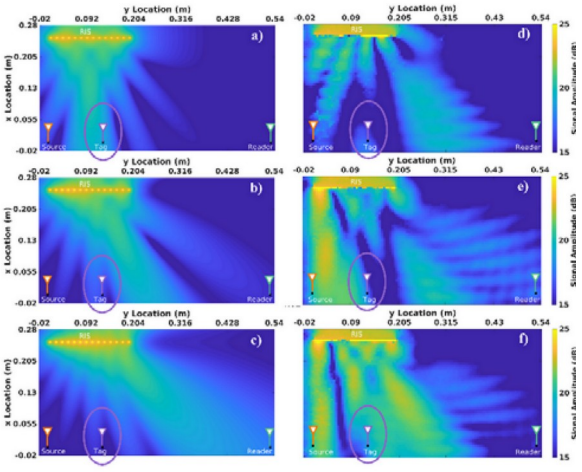




RIS with M elements


$\vec{u}^i$
E_m^i
θ_m^i
$\vec{u}^d$
θ_m^d
E_m^d


RIS
z
RIS control board
USRP
Source
Tag
Reader


y Location (m)
x Location (m)
a)
b)
c)
d)
e)
f)
RIS
Source
Tag
Reader
Signal Amplitude (dB)

A Prototype of Reconfigurable Intelligent Surface with Continuous Control of the Reflection Phase

Modeling, Full-Wave Electromagnetic Characterization, Experimental Validation, and Application to Ambient Backscatter Communications

R. Fara[1,2], P. Ratajczak[2], D.-T. Phan-Huy[2], A.Ourir[3], M. Di Renzo[1] and J. De Rosny[3]
[1]*Université Paris-Saclay, CNRS, CentraleSupélec, Laboratoire des Signaux et Systèmes,*
3 rue Joliot-Curie, 91192, Gif-sur-Yvette, France
[2]*Orange Labs Networks,* Châtillon & Sophia-Antipolis, France
[3]*ESPCI Paris, PSL University, CNRS, Institut Langevin*, Paris, France
romain.fara@orange.com

***Abstract*—With the development of the next generation of mobile networks, new research challenges have emerged, and new technologies have been proposed to face them. On the one hand, the reconfigurable intelligent surface (RIS) technology is being investigated for partially controlling the wireless channels. The RIS is a promising technology for improving the signal quality by controlling the scattering of the electromagnetic waves in a nearly passive manner. On the other hand, ambient backscatter communications (AmBC) is another promising technology that is tailored for addressing the energy efficiency requirements for the Internet of Things (IoT). This technique enables low-power communications by backscattering ambient signals and, thus, reusing existing electromagnetic waves for communications. RIS technology can be utilized in the context of AmBC for improving the system performance. In this paper, we report a prototype of an RIS that offers the capability of controlling the phase shift of the reflected waves in a continuous manner, and we characterize its characteristics by using full-wave simulations and through experimental measurements. Specifically, we introduce a phase shift model for predicting the signal reflected by the RIS prototype. We apply the proposed model for optimizing an RIS-assisted AmBC system and we demonstrate that the use of an RIS can significantly improve the system performance.**

Keywords—Ambient backscatter communications; 6G, Internet of Things, Reconfigurable intelligent surface, metasurface.

INTRODUCTION

The development of each generation of mobile networks has improved the efficiency of wireless communications. From the second generation (2G) to the fifth generation (5G) of mobile networks, the performance of wireless communication systems has improved, thanks to research and development efforts on the design and optimization of the transmitters and receivers. However, the propagation channel separating the transmitters and receivers has inherently been perceived as not controllable and sometimes unfavorable to the propagation of the electromagnetic (EM) waves. This is one of the challenges that have been identified for next generation mobile networks [1].

Recently, the reconfigurable intelligent surface (RIS) technology has been proposed and investigated for application to wireless communications [2]. An RIS is a planar structure that comprises a large number of unit cells that are capable of scattering (e.g., reflecting) the EM signals in a controlled manner [3]. An RIS can modify the phase-shift, the amplitude or even the polarization of the incident signal thanks to a smart controller that tunes the response of each unit cell. Notably, the RIS technology is nearly passive, as it is completely based on the scattering of the EM waves and does not require power amplifiers for signal transmission. Indeed, some energy is only required for the smart controller and for enabling the reconfigurability of the RIS. Therefore, an RIS can mitigate the interference or improve the signal quality at some specific and localized network locations. The RIS technology shows promising potential for application in future networks, as it can partially control and shape the propagation channels as one desires. The deployment of RISs can, therefore, improve the signal reliability in a nearly passive manner, without additional densification of the network elements and without the use of active antennas at the transmitters and receivers. RISs can be combined with existing technologies like multiple-input multiple-output (MIMO) systems, millimeter-wave (mmWave) communications, terahertz (THz) communications, machine learning (ML) and artificial intelligence (AI) for enhancing the performance of sixth generation (6G) networks [3].

In particular, the RIS technology can be employed for enhancing the performance of another promising technology, especially in the context of the Internet of Things (IoT): ambient backscatter communications (AmBC) [4]. In AmBC, a device, named tag, transmits data to another device, named reader, without generating additional EM waves. In simple terms, the tag is illuminated by an ambient signal source, such as a TV tower, a WiFi hotspot, or even a base station, and such received signal is then backscattered by the tag. The tag is able to modulate the backscattered signal by implicitly transmitting its own message. The modulated signal is detected by the reader, which can decode the tag's message. A simple tag modulates the backscattered signal according to two possible states: (i) a backscattering state, when the tag antenna is short-circuited, and (ii) a transparent state, when the tag antenna is open-circuited

[5]. Since AmBC systems inherently reuse the ambient signals and do not transmit additional EM waves for communications, they are considered a suitable technology for very low power applications [6]. However, the tag-to-reader link may be inherently interfered by the ambient signal. Also, the tag may not backscatter a strong enough signal to the reader, if, e.g., it is located in a deep fade of the ambient signal [7]. AmBC is, therefore, a promising technology, yet it has some limitations.

To overcome the just mentioned limitations, AmBC can be assisted by an RIS. For example, the authors of [8] show that the phase shifts of an RIS can be optimized to compensate for the multipath effect of the propagation channel, in order to reduce the interference and to increase the signal quality at the reader. In [9], an RIS plays the role of the tag and is used to backscatter the message to the reader. Since many unit cells are available at the RIS, the backscattered signal is enhanced and can be more easily detected. This principle is demonstrated experimentally in [10], and it is shown to significantly improve the system performance. Also, the authors of [11] report that, in cognitive networks, an RIS can improve the performance of the tag-to-reader link by maximizing the signal at the tag's location [12].

Therefore, recent research works have demonstrated that the RIS technology is a suitable candidate for improving the performance of AmBC. In [12], in particular, we have experimentally demonstrated that the tag-to-reader link can be enhanced by creating a passive reflected beam that improves the signal quality at the tag's and reader's locations. Similar to MIMO systems [13] but in a nearly passive manner, an RIS beamforms the reflected signal to assist the transmission of the tag. The experiments conducted in [12] utilize an RIS prototype that comprises 196 reconfigurable unit cells, each capable of phase-shifting the reflecting signal in a controlled manner. This is realized by using varactor diodes that control the phase response of the unit cells, which enables a continuous tuning of the phase shifts of the reflected signal. Even though the principle has been experimentally validated in [12], the RIS has not been completely characterized and, in particular, no equivalent model for the phase shift and amplitude response of the reflection coefficient was given. This is, however, essential for utilizing the RIS prototype in wireless communications.

In this paper, we focus on this specific and important aspect, and introduce a simplified model for the phase and amplitude response of the reflection coefficient of a voltage controlled RIS prototype. Based on the proposed model, we evaluate its suitability and accuracy in the context of RIS-assisted AmBC. In particular, the validation of the model is performed through full-wave simulations in Ansys HFSS and through experimental measurements. We demonstrate that the complex EM behavior of each unit cell can be modeled with simple equations that depend on the control voltage applied to the unit cells. Based on the proposed model for the unit cell, we propose a method to create a large codebook to realize passive beamforming. For given locations of the source, tag, and reader, the unit cells of the RIS are appropriately tuned to reflect and maximize the signal towards desired spots. We demonstrate that the signal scattered by the RIS can be well approximated by the linear combination of the contribution of each unit cell (based on the proposed model). Also, we prove that an RIS with a continuous phase-shift tuning capability can improve the performance of AmBC. We discuss the accuracy of the proposed (simple) model for the phase shift and compare it, with the aid of full-wave simulations, against more complex models that account for a finer-grained modeling of the response of the unit cells. We show that the proposed simplified model is sufficiently accurate for first-order analysis of RIS-assisted communications within a given range for the angles of incidence and reflection.

The paper is organized as follows. First, we introduce the RIS prototype with continuous phase-shifting capability and discuss its characteristics. Then, we describe a method to define a large codebook for realizing passive beamforming through controllable phase-shifting. Subsequently, we illustrate the RIS-assisted AmBC principle and compare the predictions from the proposed phase shift model against accurate full-wave simulations with Ansys HFSS. Finally, we conclude the paper.

RIS Prototype with Continuous Phase-Shifting

As illustrated in Fig. 1, the RIS prototype comprises 14×14 unit cells. Each unit cell is a reflecting conductive patch that can be reconfigured independently of the others. In particular, the unit cell is a three-dimensional patch on a dielectric substrate. The patch is made of two conductive areas separated by an annular slot. The inner and outer areas are connected to each other with four MA46H120 varactor diodes. The specific arrangement of the varactor diodes ensures the adjustment of the capacitance of the unit cell, which provides the desired tunability of the reflection coefficient of the unit cell. In detail, in the reverse configuration, the capacitance of a varactor diode is inversely proportional to the junction voltage. Thus, the capacitance of the unit cell can be tuned by controlling the voltage applied to the four varactors. As illustrated in Fig. 1, the unit cell can be reconfigured by applying different voltages to the four varactor diodes, which, in turn, enables the configuration of the reflection coefficient.

In the realized unit cell structure, four varactors are used for each unit cell for ensuring a good symmetry of the radiation pattern. All unit cells have identical design and size, i.e., 14×14 mm. They are engineered to operate in the frequency range 5.15-5.75 GHz [13, 14], which yields a cell size of approximately a quarter of the signal wavelength. The unit cell structure is characterized through full-wave simulations in Ansys HFSS under periodic boundary conditions. In detail, the results are obtained by considering an infinitely large surface that is a periodic repetition of a unit cell configured to realize a given reflection coefficient. Thus, a homogeneous infinite surface is simulated with the desired unit cell configuration, which ensures the correct definition of reflection coefficient.

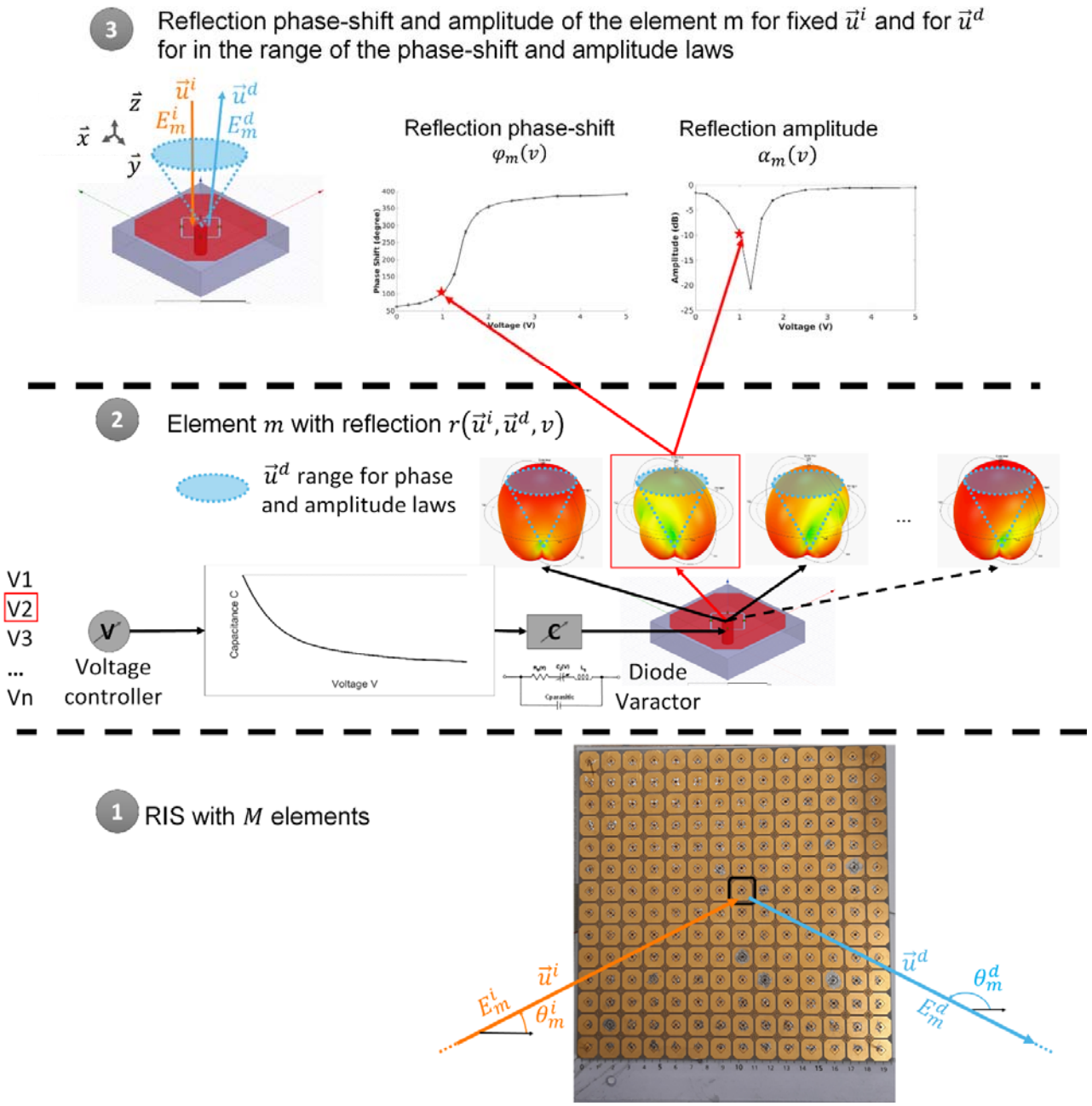


Fig. 1. Unit cell with a voltage-controlled tunable reflection coefficient $r(\vec{u}^i, \vec{u}^d, v)$. Full-wave simulation results under periodic boundary conditions [14, 15]

As illustrated in Fig. 1, the desired reflection coefficient of each unit cell can be obtained through the voltage-controlled capacitance that characterizes each unit cell. More precisely, if the m^{th} unit cell is illuminated by an electric field E^i whose direction of incidence is $\vec{u}^i$, the reflected electric field towards the direction of departure $\vec{u}^d$ can be written as $E^d = E^i \cdot r(\vec{u}^i, \vec{u}^d, v)$, where v is the voltage applied to the unit cell, $\vec{u}^i$ and $\vec{u}^d$ are unit-norm vectors defined by the azimuth and elevation angles of incidence (θ^i, φ^i) and departure (θ^d, φ^d), respectively, in spherical coordinates, and $r(\cdot)$ is the reflection coefficient.

To characterize the unit cell and to introduce an EM-consistent model for $r(\vec{u}^i, \vec{u}^d, v)$ that can be utilized in wireless communications, we study the scattering properties of the unit cell, as a function of $\vec{u}^i, \vec{u}^d,$ and v, by using the Ansys HFSS EM software under periodic boundary conditions and through

measurements conducted with the RIS prototype. As far as the full-wave simulations are concerned, the reflection coefficient of each unit cell is indirectly characterized as a function of the capacitance c of the varactor diodes. As far as the experimental characterization through measurements is concerned, the reflection coefficient of each unit cell is directly characterized as a function of the voltage v applied to the varactor diodes. Since the capacity of each varactor diode is voltage-controlled, as illustrated in Fig. 1, c and v are directly related to each other, i.e., $v = v(c)$ or $c = c(v)$. This relation is not necessary in this paper, but it can be derived through measurements.

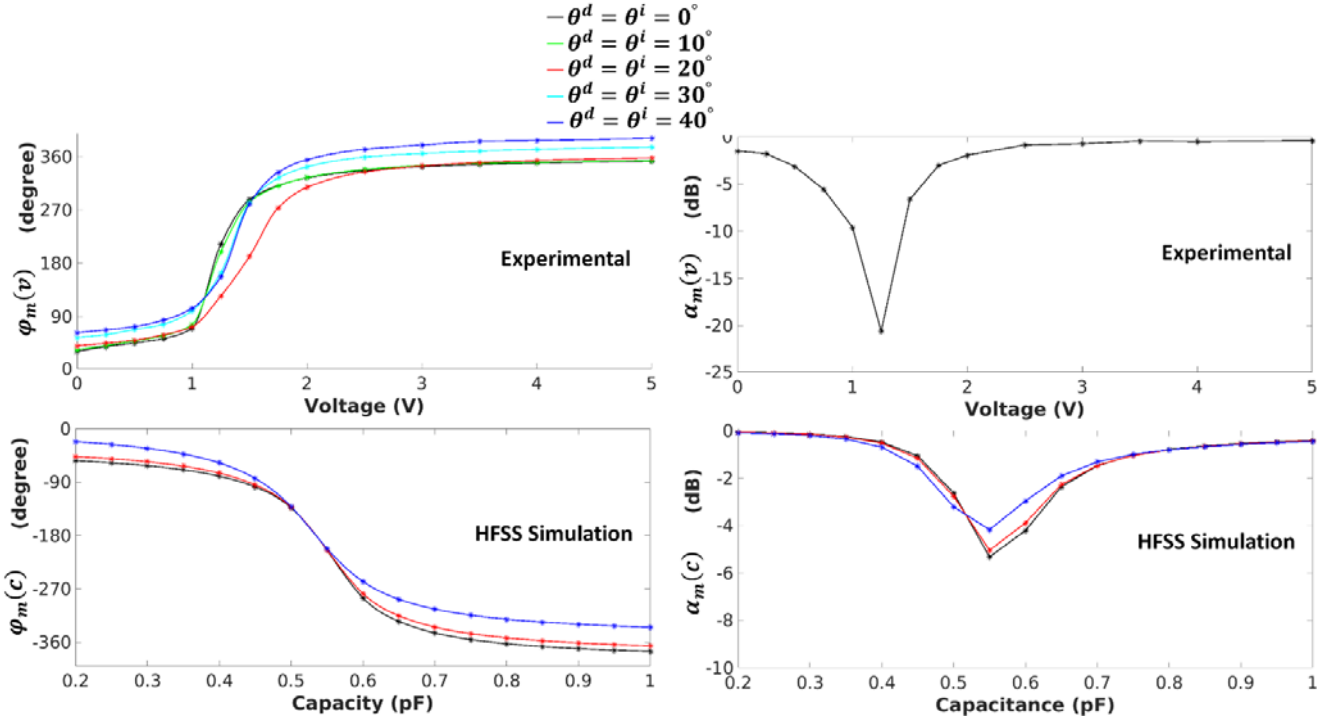


Fig. 2. Phase and amplitude of $r(\vec{u}^i, \vec{u}^d, v)$ as a function of v and for fixed $\vec{u}^i$ and $\vec{u}^d$ ($\varphi^i = 0, \varphi^d = 180$ degrees). HFSS simulations vs. experimetal measurements.

The characterization of the reflection characteristics of the unit cell is illustrated in Fig. 2 for various elevation angles of the incident and reflected electric field. The figure reports, in particular, the phase $\varphi_m(\cdot)$ and the amplitude $\alpha_m(\cdot)$ of the reflection coefficient as a function of the capacitance of the varactor diodes (HFSS simulations) and the junction voltage (prototype experiments). From the results illustrated in Fig. 2, we evince that both the phase and the amplitude of the reflection coefficient of each unit cell are almost independent of the angle of incidence and reflection, if the deflection angle is less than 40 degrees. Within this range of angles, notably, the radiation pattern of the unit cell can be assumed to be almost omnidirectional. For wider angles of deflection, on the other hand, Fig. 1 shows that the radiation pattern of the unit cell is not omnidirectional, but it depends on the angle of incidence and reflection. As expected, Fig. 2 shows that the reflection coefficient can be adjusted by appropriately controlling the junction voltage in the range 0-5 V, which corresponds to a capacity in the range 0.2-1 pF.

By considering, therefore, angles of incidence and reflection no larger than 40 degrees with respect to the normal to the unit cell, a simple model for the reflection coefficient of the unit cells can formulated as follows:

$$r(\vec{u}^i, \vec{u}^d, v) \approx r(v) \approx g_0 \alpha_m(v) e^{j\varphi_m(v)} \qquad (1)$$

where g_0 denotes the unit cell (constant) gain, and $\alpha(v)$ and $\varphi(v)$ denote the amplitude and the phase of the unit cell reflection coefficient, respectively, which can be configured in a continuous manner as a function of the voltage v that is applied to the varactor diodes.

The relation in (1) has been experimentally characterized with the aid of the RIS prototype and some experimental measurements. The obtained functions, $\alpha(v)$ and $\varphi(v)$, are reported in Table I as a function of the voltage v. Table I is valid only for angles less than 40 degrees for which the RIS was designed, optimized, and engineered.

TABLE I. EXPERIMENTAL CHARACTERIZATION OF THE REFLECTION COEFFICIENT IN (1): $\alpha(v)$ AND $\varphi(v)$ AS A FUNCTION OF v.

Voltage [V]	$\alpha(v)$ [dB]	$\varphi(v)$ [degrees]
0	-1.517	32.798
0.25	-1.807	40.854
0.5	-3.156	46.807
0.75	-5.59	53.543
1	-9.576	70.32
1.25	-20.563	-167.158
1.5	-6.615	-73.171
1.75	-3.029	-49.627
2	-1.959	-35.908
2.5	-0.874	-23.263
3	-0.749	-16.087
3.5	-0.469	-12.663
4	-0.528	-9.925
5	-0.439	-6.906

By analyzing Table I, we observe that the amplitude and the phase of the reflection coefficient are not independent of each other, since they both depend on the control voltage. In particular, the amplitude of the reflection coefficient has the smallest value in correspondence of the range of major variation of the phase of the reflection coefficient (see Fig. 2).

In this section, we have characterized the phase and amplitude response of the RIS prototype, and have introduced a simple model for the reflection coefficient of each unit cell, based on full-wave simulations, under the modeling assumption of periodic boundary conditions, and experiments. We have demonstrated the main capabilities of the designed RIS prototype: The phase-shift induced by each unit cell can be continuously controlled as a function of the control voltage applied to the unit cell. This feature can be exploited in order to control the angle of reflection of the incidence signal and to beamform the reflected signal towards the desired direction. This is analyzed and experimentally validated next.

RIS CODEBOOK DESIGN FOR ACCURATE BEAMSTEERING

From the EM characterization of the unit cell in Fig. 1 and Fig. 2, we evince that it is possible to treat an RIS as a black-box that comprises several identical and voltage-controlled unit cells, each capable of independently changing the amplitude and phase of the incident signal. By appropriately optimizing all the unit cells of the RIS, the incident signal can be partially controlled and steered towards desired locations, in order to enhance or null the received signal in a nearly passive manner, without power amplification, without decoding and reencoding the incident signal, and without requiring radio frequency chains. If the operation of the RIS prototype is restricted to angles of incidence and reflection smaller than 40 degrees (for which our prototype was designed), Table I constitutes the proxy between the EM world and the wireless communications world.

An appropriately optimized RIS can, therefore, steers the reflected signal towards desired directions or specified locations. Assuming, for example, that the locations of the transmitter and RIS are known, we can pre-design a codebook of beamforming vectors that provide the exact configuration of the phase shifts of every unit cell of the RIS in order to steer the reflected signal towards a receiver that is located in a given position. This is obtained by ensuring that the signals scattered by each unit cells add up coherently in correspondence of the desired receiver location. Then, given an area of interest, a location-dependent codebook for nearly passive beamforming can be engineered.

A simple approach to realize an RIS that focuses the reflected signal towards a specified location, in line-of-sight of both the RIS and the transmitter, is to ensure that (i) the phase shift applied by each unit cell is optimized to guarantee that the signals reflected by all the unit cells add up coherently at the location of the receiver and (ii) each unit cell adds an additional phase shift that ensures that signal reflected form the RIS adds up coherently with the signal emitted by the transmitter at the location of the receiver. Our proposed RIS prototype enables these two functionalities simultaneously. Based on Table I, this can be realized by controlling the junction voltage of each unit cell, so as to apply a cell specific phase shift and an addition constant RIS phase shift.

More precisely, let E^S be the transmitted electric field at the transmitter (source) location S and let E^P be the RIS-reflected electric field at the predefined location P. Based on (1), under the assumption of free-space propagation, we have:

$$E^P = E^S \sum_{m=1}^{M} \frac{\lambda e^{j\left(2\pi \frac{d_m^{S-RIS}}{\lambda}\right)}}{4\pi d_m^{S-RIS}} [g_0 \alpha_m(v) e^{j\varphi_m(v)}] \frac{\lambda e^{j\left(2\pi \frac{d_m^{Ris-P}}{\lambda}\right)}}{4\pi d_m^{Ris-P}} \qquad (2)$$

where M is the total number of unit cells of the RIS, d_m^{S-RIS} and d_m^{RIS-P} are the transmission distances between the source and the m^{th} cell of the RIS, and between the m^{th} cell of the RIS and the predetermined target location P, respectively, and λ is the signal wavelength. Finally, j denotes the imaginary unit.

From (2), we evince that the phase shift that corresponds to the optical path-length associated with the m^{th} unit cell at the target location P is as follows:

$$b_m^{(P)} = e^{-j2\pi \frac{d_m^{S-Ris} + d_m^{Ris-P}}{\lambda}} \qquad (3)$$

From (3), in order to ensure that the signals scattered by all the unit cells are phase-aligned with the transmitted signal at the target location P, the phase shift that each unit cell of the RIS needs to apply to the incidence signal is $\varphi_m = b_m^{(P)} - \psi^{(P)}$,

where $\psi^{(P)}$ is the uniform phase of the transmitted signal observed at the target location P.

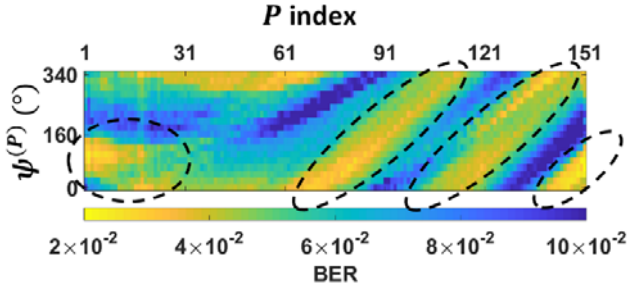


Fig. 3. Experimental measurements of the BER for all possble values of the predefined locations (p=1,2,…,151) and phase shifts $\psi^{(P)}$ (in the range 0-360 degrees). The experimetnal setup is illustrated in Fig. 4.

An illustration of the bit error rate (BER) performance of an RIS-assisted communication system, deployed by using our RIS prototype, is illustrated in Fig. 3 as a function of several target locations (P index) and RIS phase shifts $\psi^{(P)}$. A photo of the considered system setup for application to AmBC is given in Fig. 4. The experimental results in Fig. 3 are obtained by pre-designing the beamforming codebook in (3) in correspondence of 151 possible locations of a target receiver, and by then measuring the BER, at a specified location, by testing the 151 pairs of phase shifts $\left(b_m^{(P)}, \psi^{(P)}\right)$ of the RIS codebook. From Fig. 3, we observe that there are multiple pairs $\left(b_m^{(P)}, \psi^{(P)}\right)$ that provide good BER performance. In particular, the pairs depicted in yellow correspond to possible configurations of the RIS that enchance the link performance, as compared to the same system setup in the absence of RIS.

It is worth mentioning that the performance enhancement offered by RIS-assisted communications can be further improved (with respect to the results illustrated in Fig. 3), since the beamforming design in (3) is sub-optimal and the simplest one that can be applied, since it accounts only for the different optical path-lengths of the signal scattered by the unit cells.

RIS-ASSISTED AMBC: UNIT CELL MODELING ACCURACY

In AmBC, the system performance highly depends on the power level of the signal received at the tag. Since a tag is a passive device, the amount of power that is backscattered is ultimately determined by the amount of power that the tag receives from the transmitter (the source in Fig. 4). In this context, an RIS can be utilized to passively beamform the signal emitted by the source towards the tag, so as to enhance the amount of power received and, therefore, the amount of power that is backscattered towards the receiver (the reader in Fig. 4). To this end, the RIS needs to be appropriately optimized in terms of beamforming vector and uniform phase shift, i.e., the optimal pair $\left(b_m^{(P)}, \psi^{(P)}\right)$ needs to be identified, where P denotes the location of the tag in the considered example.

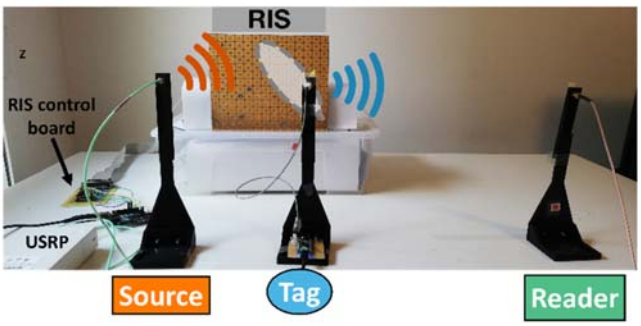


Fig. 4. Illustration of the considered testbed for RIS-assisted AmBC.

Therefore, it is important to use an accurate model for the RIS in order to enable a simple but accurate design of the configuration of the unit cells. In Table I, we have introduced a simple model for the amplitude and phase of the reflection coefficient of each individual unit cell of the RIS, as a function of the control voltage. The objective of this section is to evaluate the accuracy of the model introduced in Table I, as compared with full-wave simulations performed with Ansys HFSS. The results of this analysis are illustrated in Fig. 5.

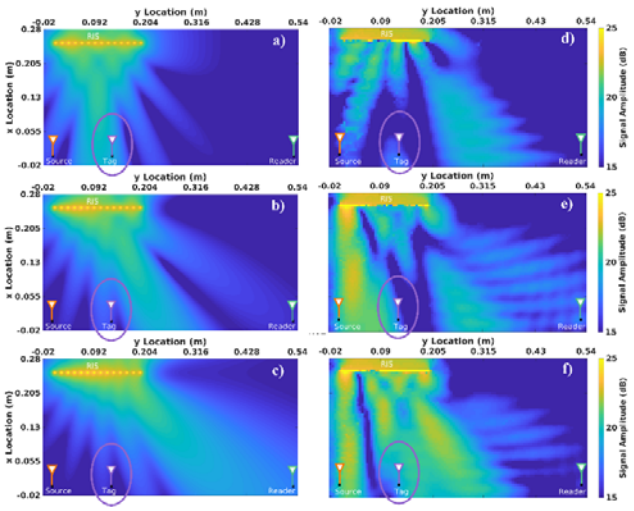


Fig. 5. Illustration of the field scattered by the RIS for three different beamforming pairs $\left(b_m^{(P)}, \psi^{(P)}\right)$ that mininize the BER in Fig. 3: (a)-(c) shows the results obtained with the simple model in Table I and (d)-(f) show the results obtained through full-wave simulations in Ansys HFSS.

The results reported in Fig. 5 are obtained as follows.

- ***Simplified model in Table I***. Given the locations of the source, tag, RIS, and reader in Fig. 4, three pairs $\left(b_m^{(tag)}, \psi^{(tag)}\right)$ that minimize the BER in Fig. 3 are considered. The optimal beamforming vector and uniform phase shift are identified by using the simplified model for the RIS in Table I, and the simple analytical model for the scattered field in (2). In particular, we assume $g_0 = 1$ but we account for the fact that the amplitude of the reflection

coefficient of each unit cell is not independent of the applied phase shift (and the unit cell control voltage).

- ***Full-wave simulations in Ansys HFSS.*** We simulate the entire RIS structure in Ansys HFSS by considering the actual scattering from each unit cell as illustrated in Fig. 1. The same three pairs $\left(b_m^{(tag)}, \psi^{(tag)}\right)$ as for the simplified model are considered, but no assumption on the modeling of the unit cells is made. In particular, the analytical models in Table I and (2) are not assumed, and the mutual coupling among the unit cells of the RIS is considered. In addition, the finite size of the RIS is taken into account in the full-wave simulations and no periodic boundary conditions at the unit cell level are applied in this case.

The results illustrated in Fig. 5 show, as expected, that some differences exist between the predictions obtained by using Table I and (3), as compared with those obtained with accurate full-wave simulations. We note, however, that the simplified model for the RIS in Table I well predicts the direction of the reflected beam of interest. More precisely, we observe that a hot spot can be clearly observed in correspondence of the location of the tag (circled in purpled color in Fig. 5), which confirms the signal enhancement provided by the RIS at the target location. Also, this is in agreement with the experimental results reported in Fig. 3. The mismatch between the simple model in Table I and the full-wave simulations in Ansys HFSS can be reduced by enriching the model for the RIS proposed in Table I at the expenses of a higher modeling and optimization complexity. Also, it needs to be mentioned that the tag in Fig. 5 is located near the boundary of Fraunhofer's far-field, which in part justifies the mismatch in Fig. 5.

CONCLUSION

In this paper, we have described a prototype of an RIS whose unit cells that can be digitally and individually tuned through a control voltage. By appropriately configuring the voltage, the phase of the scattered field of each unit cell can be optimized. We have characterized the electromagnetic behavior of the individual unit cells of the RIS under the assumption of periodic boundary conditions, and have proposed a simple voltage-dependent model for the reflection coefficient of the unit cells. If the angles of incidence and reflection are confined in the range ±40 degrees, we have shown that the unit cells can be assumed to have an almost omnidirectional and unit-gain radiation pattern, while the amplitude of the reflection coefficient depends on the applied phase shift through the control voltage. We have compared the proposed simple model against full-wave simulations and have shown that, despite simple, the proposed model can be successfully employed for first-order optimization of the RIS. Finally, by capitalizing on the proposed model for the RIS and method for optimizing its nearly passive beamforming codebook, we have substantiated through experimental measurements that an RIS can enhance the performance and reliability of AmBC systems.

ACKNOWLEDGMENT

This work has been supported in part by the European Commission through the H2020 RISE-6G project under grant agreement number 101017011.

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Non-local Intelligent Metasurfaces of Low Energy Telecommunication Applications

The growth of interest in metasurfaces has led to novel and interesting possibilities for imaging and telecommunication applications. Metasurfaces have unique abilities for blocking, absorbing, concentrating, dispersing, or guiding waves, from microwave through visible frequencies. Our team has realized theoretical and experimental research in this domain that spreads from fundamental explorations of physics to actual device design [1-4]. Recently, optical analog signal processing using non-local metasurfaces has been gaining significant attention as a way to overcome the speed and energy limitations of digital techniques [5]. Most fabricated metasurfaces are passive, meaning that they cannot be tuned post fabrication. In contrast, reconfigurable intelligent surfaces (RIS) allow the dynamic control of its properties under external incidence [2] (See figure 1). They could be useful in applications ranging from free space optical communications to holographic displays, and depth sensing.

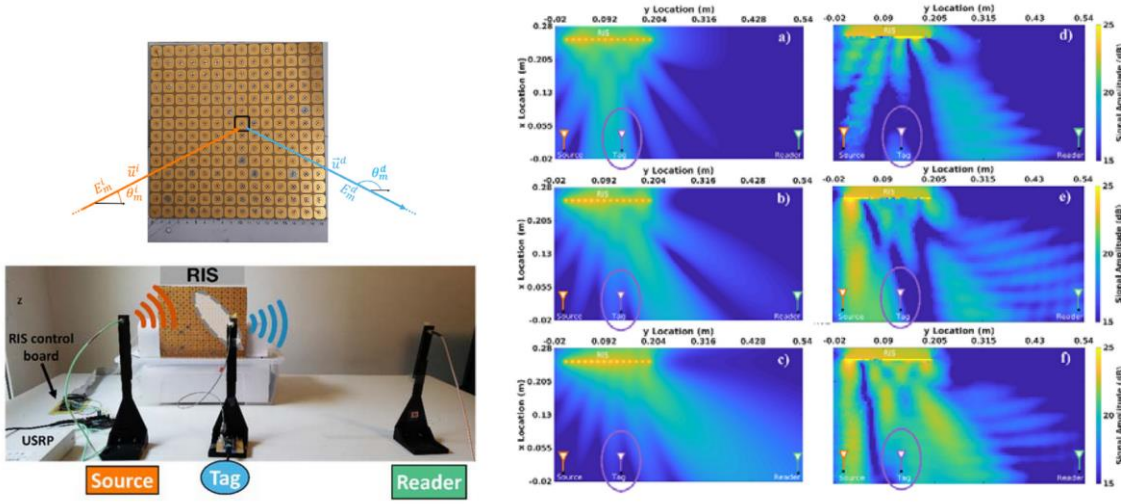


Figure 1: The fabricated RIS (Top left). The backscattering communication setup (bottom left). The electromagnetic field Map for different configurations of the RIS (Right).

Here, we propose to study the behavior of non-local RISs in the microwave regime. The investigation will include the design, the modeling and the characterization of such structures. The aim is to propose original non-local RISs concepts for novel application systems.

The candidate will be involved in the analytical and numerical modelling and the development of non-local RISs that can be used either as antennas, backscatterers or as intelligent reflectors. Then, the candidate will build setups to characterize the RISs and to investigate potential applications. Numerical simulations and experimental validations will be performed for the different studies.

[1] R Fara, DT Phan-Huy, P Ratajczak, A Ourir, M Di Renzo, J De Rosny, “Reconfigurable intelligent surface-assisted ambient backscatter communications–experimental assessment”, IEEE international conference on communications workshops (ICC), 2021.

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Advisor(s): Abdelwaheb Ourir (a.ourir@espci.fr), Julien de Rosny (Julien.derosny@espci.fr)

Keywords: microwaves, metasurfaces, reconfigurable intelligent surfaces, telecommunicaion.

Expected profile:
The candidates need to be familiar with signal processing and electromagnetism. Knowledge of photonics and metamaterials is a plus.

ParisTech

ESPCI PARIS PSL

TITLE: IRREVERSIBLE ALGORITHMS FOR PHYSICAL MODELING

Topic number : ***2023_026***

Field : Physics, Optics, Mathematics and their applications,

Subfield:

ParisTech School: ESPCI Paris - PSL
Research team: PCT https://turner.pct.espci.fr/~amaggs/index2.html
Research lab: GULLIVER - Voyages expérimentaux et théoriques en matière molle
Lab location: Paris
Lab website:https://www.gulliver.espci.fr/?-home-

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Maggs Anthony anthony.maggs@espci.fr
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Molecular modeling (research rooted in particle-based computation) is central to our understanding of the material world. Its methods allow one to investigate complex phenomena in biophysics and materials research, and to describe the fundamental phase behavior of the universe that surrounds us. Molecular modeling has provided methods for many other fields, from astrophysics to hydrodynamics, statistical mechanics and field theory. Molecular modeling is an interdisciplinary research field, in which the development of algorithms plays an important role. Improved sampling methods, constrained ensembles, and novel approaches beyond molecular dynamics stand out in their promise for the future. Although the principal methods have been developed for over half a century, disruptive development continues to take place. An example is the irreversible Markov-chain Monte Carlo methods which violate the fundamental detailed-balance condition yet converge towards equilibrium. They illustrate that past algorithms were overly restrictive. Radically new Markov-chain Monte Carlo algorithms have already led to the resolution of long-standing controversies (as for example in two-dimensional melting studied through the use of irreversible Markov chains). We wish to extend these methods to standard interaction potentials in soft-matter physics, in the belief that this can lead to highly

efficient codes that explore equilibrium configurations under irreversibility conditions.

Required background of the student: physics with mathematical applications

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Hard-disk pressure computations—a historic perspective,

https://doi.org/10.1063/5.0126437

Journal of Chemical Physics, Botao Li Yoshihiko Nishikawa, Philipp Höllmer, Louis Carillo, A. C. Maggs ,Werner Krauth

2. Multithreaded event-chain Monte Carlo with local times

https://doi.org/10.1016/j.cpc.2020.107702

Computer physics communications, Botao Li, Synge Todo, A.C. Maggs, Werner Krauth.

3. Large-scale dynamics of event-chain Monte Carlo

https://doi.org/10.1103/PhysRevE.105.015309

Physical Review, A. C. Maggs and Werner Krauth

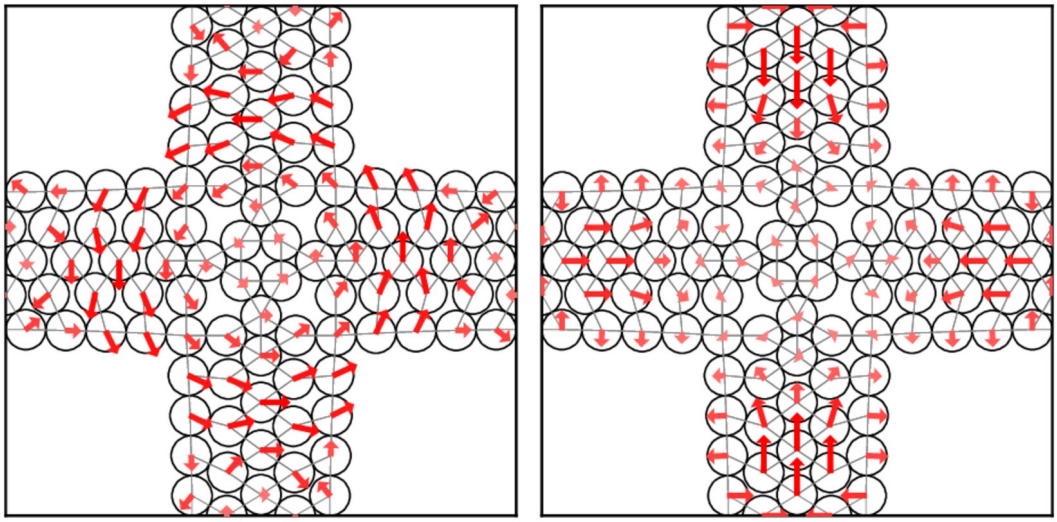
4. Sparse Hard-Disk Packings and Local Markov Chains,

https://doi.org/10.1007/s10955-022-02908-4

Journal of Statistical Physics, Philipp Höllmer, Nicolas Noirault, Botao Li, A. C. Maggs & Werner Krauth.

5.

Illustrations :



ParisTech

Arts et Métiers

TITLE: DYNAMICS, STABILITY AND TRANSITION TO TURBULENCE OF SEPARATION BUBBLES IN FLOWS OF VARYING DENSITY

Topic number : ***2023_027***

Field : Material science, Mechanics and Fluids, ,

Subfield:

ParisTech School: Arts et Métiers
Research team:
Research lab: DynFluid
Lab location: Paris
Lab website:https://dynfluid.ensam.eu/

Contact point for this topic: Arts et Métiers

Advisor 1: BEN HASSAN SAÏDI Ismaïl ismail.benhassansaidi@ensam.eu
Advisor 2: ROBINET Jean-Christophe jean-christophe.robinet@ensam.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: When a boundary layer is subjected to a sufficiently strong adverse pressure gradient, it leads to the creation of an unsteady separation bubble. These separation bubbles are the seat of several complex and interrelated dynamical phenomena of both linear and non linear nature (linear instabilities, triadic interactions, etc.). As a result, the dynamics of these separation bubbles is known to be broadband with, in particular, phenomena of low characteristic frequencies leading to oscillating loads on adjacent structures detrimental for engineering systems performances and safety. Moreover, when the incoming boundary layer is laminar, the unsteady dynamics of the separation bubble can lead to the transition to turbulence of the boundary layer. In both these respects, the physical understanding of the dynamics of these flows is an important issue for various practical applications.

In this context, several past works were devoted to the understanding of the physical mechanisms underlying the onset of the low frequency unsteady regime of separation bubbles for constant density flows. In particular, the seminal works of Rodriguez et al. 2021 have shown that the low frequency unsteadiness of these flows could be due to a secondary global instability of a first stationary 3D unstable mode.

The aim of this thesis is to carry out a similar study for flows with variable density. More precisely, we will aim at constructing the bifurcation scenario of non forced transitional separation bubbles. In the context of flows with variable density, previous studies already highlighted a global instability with respect to three dimensional disturbances leading to a bifurcation from a 2D steady state to a 3D steady state of the separation bubble when the adverse pressure gradient is bigger than a threshold value. In this project, we will perform global stability analyses of the 3D steady state in order to determine if a bifurcation towards a 3D unsteady state with a frequency consistent with the low frequency breathing of the bubble exists.

The understanding of the physical mechanisms at the origin of the low frequency unsteadiness of separated bubbles in flows of variable density, which is the objective of this thesis, has for ultimate goal the possibility of controlling this phenomenon in order to improve the performances and to make more reliable the concerned industrial systems.

Required background of the student: The desired candidate has a research master's degree with a specialization in fluid mechanics or applied mathematics. The candidate must be interested in the physical analysis and understanding of flow dynamics. A good experience and a taste for analysis and numerical simulation tools are essential.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Rodríguez, D., Gennaro, E., & Souza, L. (2021). Self-excited primary and secondary instability of laminar separation bubbles. Journal of Fluid Mechanics, 906, A13. doi:10.1017/jfm.2020.767

2. S. Cherubini, J.-Ch. Robinet, P. De Palma, F. Alizard; The onset of three-dimensional centrifugal global modes and their nonlinear development in a recirculating flow over a flat surface. Physics of Fluids 1 November 2010; 22 (11): 114102. https://doi.org/10.1063/1.3500677

3. V. Theofilis; Global linear instability. Annual Review of Fluid Mechanics January 2011; 43:319-352. https://doi.org/10.1146/annurev-fluid-122109-160705

4.

5.

Illustrations :

PhD. Thesis proposal

Dynamics, stability and transition to turbulence of separation bubbles in flows of varying density

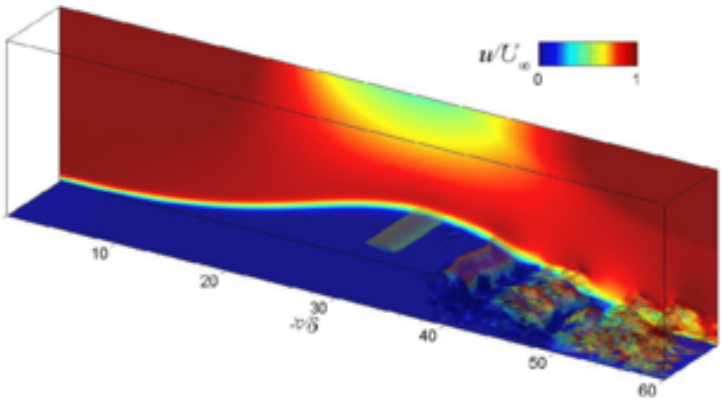


Figure 1: 3D structures in separated flow from Seo et al. 2018

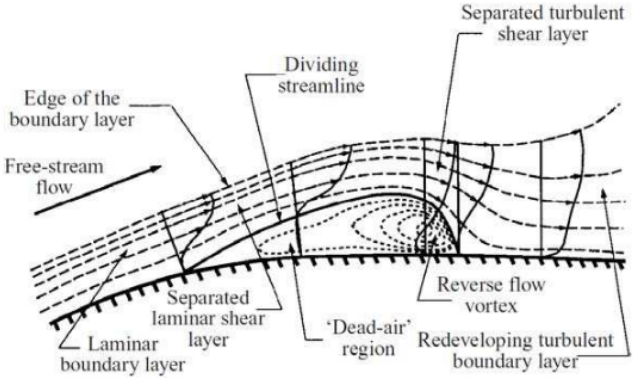


Figure 2: Scheme of a separated flow from Horton (1968)

Subject:

When a boundary layer is subjected to a sufficiently strong adverse pressure gradient, it leads to the creation of an unsteady separation bubble. These separation bubbles are the seat of several complex and interrelated dynamical phenomena of both linear and non linear nature (linear instabilities, triadic interactions, etc.). As a result, the dynamics of these separation bubbles is known to be broadband with, in particular, phenomena of low characteristic frequencies leading to oscillating loads on adjacent structures detrimental for engineering systems performances and safety. Moreover, when the incoming boundary layer is laminar, the unsteady dynamics of the separation bubble can lead to the transition to turbulence of the boundary layer. In both these respects, the physical understanding of the dynamics of these flows is an important issue for various practical applications.

In this context, several past works were devoted to the understanding of the physical mechanisms underlying the onset of the low frequency unsteady regime of separation bubbles for constant density flows. In particular, the seminal works of *Rodriguez et al. 2021* have shown that the low frequency unsteadiness of these flows could be due to a secondary global instability of a first stationary 3D unstable mode.

The aim of this thesis is to carry out a similar study for flows with variable density. More precisely, we will aim at constructing the bifurcation scenario of non forced transitional separation bubbles. In the context of flows with variable density, previous studies already highlighted a global instability with respect to three dimensional disturbances leading to a bifurcation from a 2D steady state to a 3D steady state of the separation bubble when the adverse pressure gradient is bigger than a threshold value. In this project, we will perform global stability analyses of the 3D steady state in order to determine if a bifurcation towards a 3D unsteady state with a frequency consistent with the low frequency breathing of the bubble exists.

The understanding of the physical mechanisms at the origin of the low frequency unsteadiness of separated bubbles in flows of variable density, which is the objective of this thesis, has for ultimate goal the possibility of controlling this phenomenon in order to improve the performances and to make more reliable the concerned industrial systems.

Location of the thesis: The candidate will be enrolled at the Ecole Nationale Supérieure de Arts et Métiers and will carry out his/her research at the DynFluid laboratory (http://dynfluid.ensam.eu/).

Candidate profile: The desired candidate has a research master's degree with a specialization in fluid mechanics or applied mathematics. The candidate must be interested in the physical analysis and understanding of flow dynamics. A good experience and a taste for analysis and numerical simulation tools are essential.

Contact: For more information and to apply (CV and cover letter), please contact :

- Jean-Christophe ROBINET: jean-christophe.robinet@ensam.eu
- Ismaïl BEN HASSAN SAÏDI: Ismail.benhassansaidi@ensam.eu

Bibliography:

1 Rodríguez, D., Gennaro, E., & Souza, L. (2021). Self-excited primary and secondary instability of laminar separation bubbles. *Journal of Fluid Mechanics*, *906*, A13. doi:10.1017/jfm.2020.767

2 S. Cherubini, J.-Ch. Robinet, P. De Palma, F. Alizard; The onset of three-dimensional centrifugal global modes and their nonlinear development in a recirculating flow over a flat surface. *Physics of Fluids* 1 November 2010; 22 (11): 114102. https://doi.org/10.1063/1.3500677

3 V. Theofilis; Global linear instability. *Annual Review of Fluid Mechanics* January 2011; 43:319-352. https://doi.org/10.1146/annurev-fluid-122109-160705

TITLE: HIGHER-ORDER CONTINUUM MECHANICS THEORIES TO PREDICT SMALL SCALE EFFECT ON THE VIBRATION PROPERTIES OF NANOSTRUCTURES

Topic number : ***2023_028***

Field : Material science, Mechanics and Fluids, ,

Subfield:

ParisTech School: Arts et Métiers
Research team: Écoulements complexes
Research lab: LAMPA - Laboratoire angevin de mécanique, procédés et innovation
Lab location: Angers
Lab website:https://lampa.ensam.eu/accueil-lampa-100748.kjsp

Contact point for this topic: Arts et Métiers

Advisor 1: El Baroudi Adil adil.elbaroudi@ensam.eu
Advisor 2: Le Pommellec Jean Yves jeanyves.lepommellec@ensam.eu
Advisor 3: Ammar Amine amine.ammar@ensam.eu
Advisor 4:

Short description of possible research topics for a PhD: Vibration modes in nanostructures present a major interest in characterization of the materials properties. In particular, virus is known to resonate in the confined-acoustic dipolar mode with microwave of the same frequency. Indeed, investigating the vibrational modes of viruses has been motivated by the possibility of using ultrasonic waves to destroy or to inactivate a virus present in a living organism. The vibration of a free homogeneous and isotropic sphere was studied by Lamb using the theory of elastic media. However the free sphere model used to interpret the experimental results is a rough approximation of the actual environmental conditions of nanoparticles. A more general theory based on higher-order continuum mechanics for accurately predicting the vibration modes of nanosphere embedded in a viscoelastic media is the subject of this thesis. Several constitutive laws of the viscoelastic medium must be considered in order to obtain a more realistic model.

Required background of the student: Physics, Mechanics, Applied Mathematics

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Analytical approach for predicting vibration characteristics of an embedded elastic sphere in complex fluid
2. A note on the spheroidal modes vibration of an elastic sphere in linear viscoelastic fluid
3. Vibration properties of an elastic gold nanosphere submerged in viscoelastic fluid
4. Small-scale effects on the radial vibration of an elastic nanosphere based on nonlocal strain gradient theory
5. Love waves characteristics in viscoelastic fluid loaded surface layer : comparison between Jeffrey and Maxwell-Jeffrey models

Illustrations :

ParisTech

TITLE: IMPROVING THE DATA EFFICIENCY OF MACHINE LEARNING MODELS WITH DESCRIPTORS DERIVED FROM QUANTUM CHEMISTRY

Topic number : ***2023_029***

Field : Chemistry, Physical chemistry and Chemical Engineering, Information and Communication Science and Technology,

Subfield:

ParisTech School: Chimie ParisTech - PSL
Research team: Chemical Theory and Modeling https://www.quanthic.fr
Research lab: I-CLEHS - Institute of chemistry for life and health
Lab location: Paris
Lab website:https://www.chimieparistech.psl.eu/recherche/les-laboratoires/i-clehs/

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Stuyver Thijs thijs.stuyver@chimieparistech.psl.eu
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Traditional machine learning (ML) algorithms tend to require lots of training data. However, by introducing domain knowledge, one can dramatically improve the data efficiency -- as well as generalizability -- of these models. As such, in one of the main research lines within our research group, we aim to augment ML models with descriptors stemming from quantum chemical calculations to facilitate their application to domains for which only limited data is available.
A potential PhD project within the group consists of investigating the connection between the roughness of molecular property landscapes and the inclusion of domain knowledge inspired descriptors. The roughness/smoothness of molecular property landscapes, i.e., the evolution of the target property as one traverses a selected feature space, has often been connected to the inherent “modellability” of the target property. Featurizations that give rise to smooth activity landscapes ought to result in machine learning models requiring relatively few data points, whereas rough landscapes ought to result in models requiring many data points to reach an acceptable accuracy. In this project, we would first investigate how the inclusion of physics inspired descriptors

affects the roughness of activity landscapes, and subsequently we would determine whether changes in roughness can be used as an unbiased metric to select informative descriptors for a ML model.

Required background of the student: (computational) chemistry, with at least some programming experience and an interest in machine learning/artificial intelligence

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. T. Stuyver, C. W. Coley, Quantum chemistry-augmented neural networks for reactivity prediction: Performance, generalizability, and explainability, J. Chem. Phys. 2022, 156, 084104.
2. M. Aldeghi, D. E. Graff, N. Frey, J. A. Morrone, E. O. Pyzer-Knapp, K. E. Jordan, C. W. Coley, Roughness of molecular property landscapes and its impact on modellability. J. Chem. Inf. Model. 2022, 62, 4660-4671.
3. Z. Tu, T. Stuyver, C. W. Coley, Predictive chemistry: machine learning for reaction deployment, reaction development, and reaction discovery. Chem. Sci. 14, 226-244.
4.
5.

Illustrations :

ParisTech

TITLE: ENHANCED PASSIVITY AND CORROSION RESISTANCE OF MULTI PRINCIPAL ELEMENT ALLOYS

Topic number : ***2023_030***

Field : Chemistry, Physical chemistry and Chemical Engineering, ,

Subfield:

ParisTech School: Chimie ParisTech - PSL
Research team: PCS
Research lab: IRCP - Institut de Recherche de Chimie de Paris
Lab location:
Lab website:https://www.ircp.cnrs.fr/

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: mercier Dimitri
DIMITRI.MERCIER@CHIMIEPARISTECH.PSL.EU
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Multi principal element alloys (MPEA), also called high entropy alloys (HEA), is a new class of metallic alloys (first elaborated in 2004) having a great interest as engineering alloys. Their mechanical properties have been widely studied and currently a detailed approach of the design of these alloys (microstructure, composition) allows elaborating specific alloys with excellent mechanical properties, that may outperform those of conventional alloys. In contrast to the mechanical properties, the surface reactivity of these materials, and particularly their corrosion resistance, has only been slightly studied. Different studies have shown that the original “Cantor” alloy does not provide good corrosion resistance, due to its high (equimolar) Mn content. Combining what we know of the origin of the corrosion resistance of Ni and Fe-based stainless alloys, and applying a thermodynamic approach for the composition optimization, our research group was able to design and synthesize two new single-phase HEA/MPEA alloys containing molybdenum, which show excellent corrosion resistance. The purpose of this research program is to understand the detailed relationship between alloy composition, surface reactivity and corrosion behavior (passivity, passivity breakdown, localized corrosion resistance) of MPEA/HEA alloys with high Cr and Mo

contents, and explore a range of compositions that can be maintained as single fcc phase after rapid cooling or contain Mo-rich secondary phases. The surface oxides (native and passive films), which are key factors for the corrosion resistance, will be characterized for the different alloy compositions by advanced surface analysis techniques, including X-ray Photoelectron Spectroscopy (XPS) and Time-of-Flight Secondary Ion Spectrometry (ToF-SIMS), combined with electrochemical measurements. A focus will be placed on the stability and the growth mechanisms of these layers using an original approach developed by our research group, using in situ isotopic labelling ($^{18}O_2$).

Required background of the student: Corrosion Science, Surface Science, Materials Science, Electrochemistry

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. X. Wang et al., Origin of enhanced passivity of Cr-Fe-Co-Ni-Mo multi-principal element alloy surfaces, npj mat deg, 13, 2023, 10.1038/s41529-023-00330-z
2. X. Wang et al., Enhanced passivity of Cr-Fe-Co-Ni-Mo multi-component single-phase face-centred cubic alloys: design, production and corrosion behaviour, Cor Sci, 200, 2022, 10.1016/j.corsci.2022.110233
3. L. Wang, Study of the surface oxides and corrosion behaviour of an equiatomic CoCrFeMnNi high entropy alloy by XPS and ToF-SIMS, Cor Sci, 167, 2020, 10.1016/j.corsci.2020.108507
4.
5.

Illustrations :

TITLE: GENERATIVE A.I. (CHATGPT AND GPT-4) FOR GOOD, BAD AND BUSINESS

Topic number : ***2023_031***

Field : Information and Communication Science and Technology, Design, Industrialization,

Subfield:

ParisTech School: Arts et Métiers
Research team: Présence et innovation https://lampa.ensam.eu/equipe-p-i-132195.kjsp?RH=1415871394252&RF=1478611858411
Research lab: LAMPA - Laboratoire angevin de mécanique, procédés et innovation
Lab location: Angers
Lab website:https://lampa.ensam.eu/accueil-lampa-100748.kjsp

Contact point for this topic: Arts et Métiers

Advisor 1: Richir Simon Simon.Richir@ensam.eu
Advisor 2: SCHMIDT Colin colin.schmidt@univ-lemans.fr
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: The Ph.D. candidate's research will explore the ethical dilemmas posed by contemporary Artificial Intelligences (A.I.) and their impact on society. This will involve a thorough analysis of questions related to privacy, bias, and employment disruption, illustrated through concrete case studies and real-world scenarios.

Additionally, the study will investigate how A.I., specifically Generative A.I., can spur economic growth in underserved regions. The candidate will provide practical examples of how A.I. technologies can be harnessed to promote economic development in these areas, highlighting the transformative potential of A.I.

In essence, this research will shed light on the ethical challenges associated with A.I. while showcasing the tangible benefits and innovative possibilities it offers, supported by a compelling technological example.

Required background of the student: Cognitive Science, Artificial Intelligence, Human-Computer Interaction, Psychological and Philosophical Analysis of Society, Generative Grammar

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Extensions of mind: relating to data and others, AH '20: Proceedings of the 11th Augmented Human International Conference May 2020 https://doi.org/10.1145/3396339.3396402
2. JAYESH S. PILLAI, COLIN SCHMIDT, SIMON RICHIR (2013), Achieving Presence through Evoked Reality, Frontiers in Psychology, 02/2013; 4:86.
DOI:10.3389/fpsyg.2013.00086
3. SCHMIDT C.T.A. (2013), “L’homme entendu. Explorations terminologiques”, in KLEINPETER E. (Ed.) L’humain augmenté, Paris: CNRS
Editions, collection «Les Essentiels d’Hermès».
4. SCHMIDT C.T.A. (Ed.) (2009), "Computation in the Natural World", Special Issue of Minds and Machines, vol. 19 n° 4, Springer ; this issue

features the work of Margaret A. BODEN, Lorenzo MAGNANI and Mark BISHOP amongst other scholars, 117 pages
5. SCHMIDT C.T.A. (2008), "Redesigning Man?", Pieter E. VERMAAS, Peter KROES, Andrew LIGHT, Steven A. MOORE, (eds.)Philosophy and Design:
From Engineering to Architecture, pp. 209-216: Philosophy of Science section, Springer Science, Dordrecht. ISBN 978-1-4020-6590-3 (Print) 978-1-4020-6591-0

Illustrations :

TITLE: USE OF EMULSIFIED ZEROVALENT IRON FOR SOIL REMEDIATION : EXPERIMENTAL INVESTIGATION AT THE DARCY SCALE

Topic number : ***2023_032***

Field : Environment Science and Technology, Sustainable Development, Geosciences, Material science, Mechanics and Fluids, Energy, Processes

Subfield:

ParisTech School: Arts et Métiers
Research team: Porous media
https://www.i2m.u-bordeaux.fr/Recherche/TREFLE-Transferts-Fluides-Energetique/Groupe-Milieux-Poreux
Research lab: I2M - Institut de Mécanique et d'ingénierie
Lab location: Bordeaux
Lab website:https://www.i2m.u-bordeaux.fr/

Contact point for this topic: Arts et Métiers

Advisor 1: AHMADI-SENICHAULT Azita azita.ahmadi@ensam.eu
Advisor 2: RODRIGUEZ DE CASTRO Antonio antonio.rodriguezdecastro@ensam.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Urban and agricultural environments are more and more contaminated by chlorinated organic solvents, pesticides, nitrates, heavy metals, etc. Such pollutants, which initially impact surface soils, eventually seep into groundwater. Soil pollution also reduces the amount of land available for agriculture as food and feed crops uptake soil contaminants. It is therefore essential to restore degraded soils to ensure water and food sovereignty. Unlike site remediation processes by excavation, in situ treatments do not require the movement of soil and are cost-effective. Suspensions of granular zerovalent iron (ZVI) can be injected in the soil to reduce halogenated organic pollutants and react with pesticides, herbicides, aromatic hydrocarbons, azo dyes and heavy metals. Nevertheless, ZVI is very susceptible to corrosion in an aqueous medium. This PhD thesis will assess the efficiency of vectorizing ZVI using an emulsified nonpolar phase (e.g., vegetal oil), which is expected to mitigate corrosion during delivery. Also, emulsified oil droplets and organic pollutants are miscible, which promotes contact between the

reagent and the pollutant to trigger the chemical reaction. Furthermore, the biodegradation of pollutants can be stimulated by using vegetable oils in the carrier emulsions. A series of 1D experiments will be performed using sand columns and the effective properties at the Darcy scale, i.e., residual saturation of the pollutant, apparent viscosity of the emulsion and relative permeabilities will be quantified through gamma-ray attenuation and pressure drop measurements, for different process conditions. The rate of degradation of the pollutants will be quantified by chromatography of the effluents. Then, the effects of gravity force, porosity gradients and stratification will be evaluated during flow through metric-scale 2D and 3D tanks filled with layers of different permeabilities. These experiments will provide criteria to select the controllable parameters, preventing the uneven spread of ZVI in heterogeneous soils and stability loss.

Required background of the student: A solid theoretical and experimental understanding of the fundamentals of fluid mechanics is required. The principles of mathematical programming and numerical methods must be known. Performing experiments requires dexterity, autonomy and meticulousness.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Gallo A., Bianco C., Tosco T., Tiraferri A., Sethi R. (2019). Synthesis of eco-compatible bimetallic silver/iron nanoparticles for water remediation and reactivity assessment on bromophenol blue. Journal of Cleaner Production, 211.

2. Mohammadian S., Krok B., Fritzsche A., Bianco C., Tosco T., Cagigal E., Mata B., Gonzalez V., Diez-Ortiz M., Ramos V., Montalvo D., Smolders E., Sethi R., Meckenstock R.U. (2021). Field-scale demonstration of in situ immobilization of heavy metals by injecting iron oxide nanoparticle adsorption barriers in groundwater. Journal of Contaminant Hydrology, 237, 103741

3. Mondino F., Piscitello A., Bianco C., Gallo A., de Folly D'Auris A., Tosco T., Tagliabue M., Sethi R. (2020). Injection of Zerovalent Iron Gels for Aquifer Nanoremediation: Lab Experiments and Modeling. Water 12, 826.

4. Rodríguez de Castro, A., Ben Abdelwahed, A., Bertin, H. (2023): Enhancing pollutant removal from contaminated soils using yield stress fluids as selective blocking agents. Journal of Contaminant Hydrology 255, 104142.

5. Rodríguez de Castro, A., Goyeau, B. (2022). Numerical analysis of the pore-scale mechanisms controlling the efficiency of immiscible displacement of a pollutant phase by a shear-thinning fluid. Chemical Engineering Science 251 117462.

Illustrations :

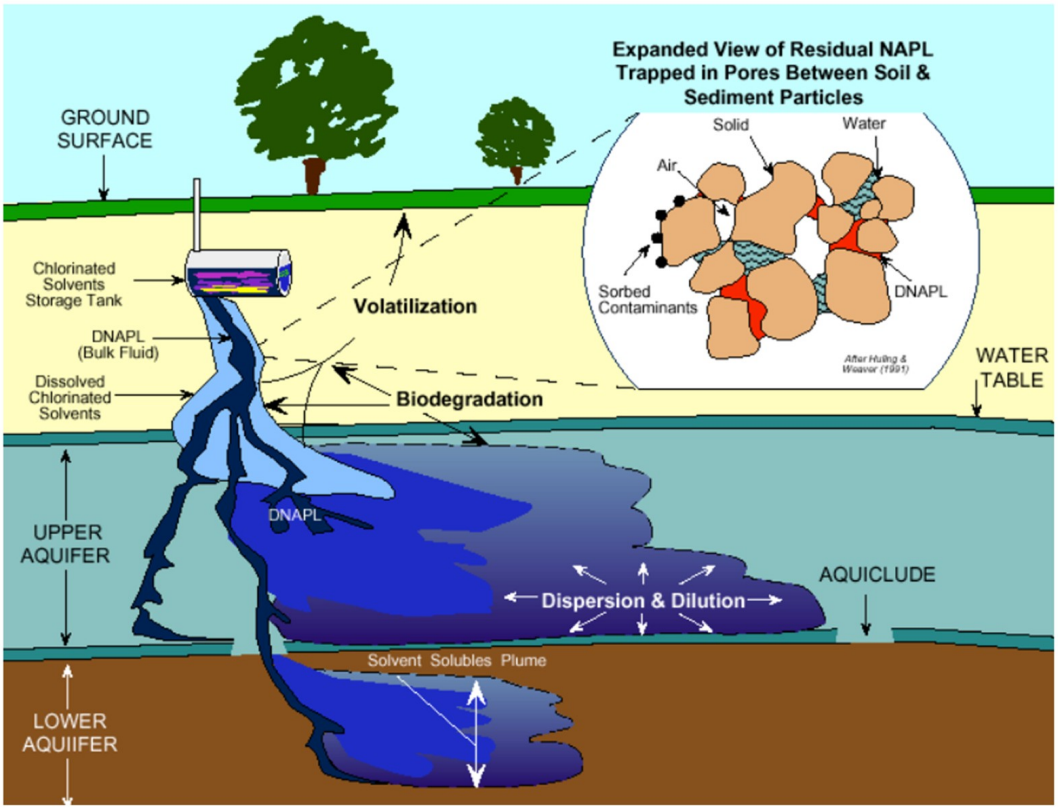


Figure 1 *Spread of a Dense Non-aqueous Phase Liquid pollutant (DNAPL) in a soil. From "EPA. Monitored natural attenuation of petroleum hydrocarbons. U.S. EPA Remedial Technology Fact Sheet, EPA/600/F-98/021, May 1999."*

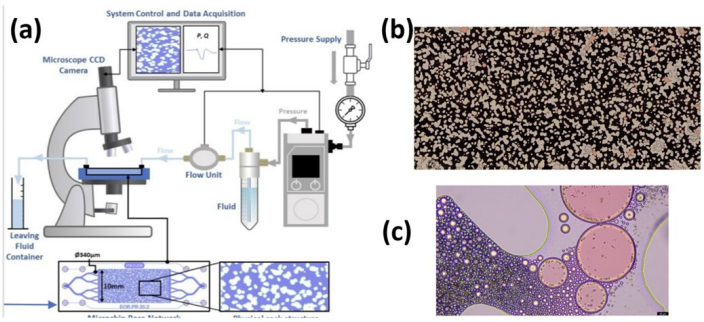


Figure 3 *(a) Microfluidic setup used at I2M to study the displacement of a pollutant oil by an emulsion. (b) Image showing the positions of solid (yellow), resident pollutant oil (red) and emulsion (black) after emulsion flooding. All the micromodel is dispalayed (2 x 1 cm). (c) Zoom on a smaller region (0.5 x 0.25 mm) showing the interfaces between oil, solid and emulsion phases.*

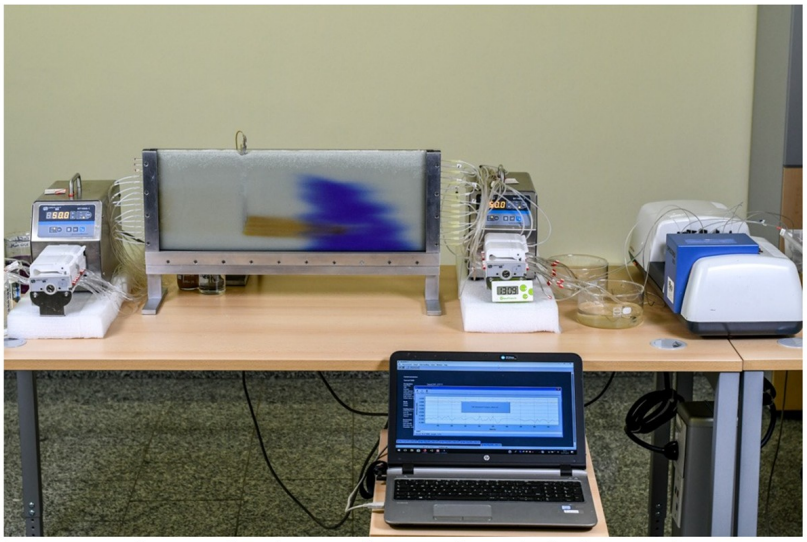


Figure 4 *Experimental setup for the simulation of emulsified zerovalent iron injection and propagation in 2D vertical geometry (Groundwater Engineering Group – Politecnico di Torino)*

Use of emulsified zerovalent iron for soil remediation : experimental investigation at the Darcy scale

Urban and agricultural environments are more and more contaminated by chlorinated organic solvents, pesticides, nitrates, heavy metals, etc. Such pollutants, which initially impact surface soils, eventually seep into groundwater. Soil pollution also reduces the amount of land available for agriculture as food and feed crops uptake soil contaminants. It is therefore essential to restore degraded soils to ensure water and food sovereignty. Unlike site remediation processes by excavation, in situ treatments do not require the movement of soil and are cost-effective. Suspensions of granular zerovalent iron (ZVI) can be injected in the soil to reduce halogenated organic pollutants and react with pesticides, herbicides, aromatic hydrocarbons, azo dyes and heavy metals. Nevertheless, ZVI is very susceptible to corrosion in an aqueous medium. This PhD thesis will assess the efficiency of vectorizing ZVI using an emulsified nonpolar phase (e.g., vegetal oil), which is expected to mitigate corrosion during delivery. Also, emulsified oil droplets and organic pollutants are miscible, which promotes contact between the reagent and the pollutant to trigger the chemical reaction. Furthermore, the biodegradation of pollutants can be stimulated by using vegetable oils in the carrier emulsions. A series of 1D experiments will be performed using sand columns and the effective properties at the Darcy scale, i.e., residual saturation of the pollutant, apparent viscosity of the emulsion and relative permeabilities will be quantified through gamma-ray attenuation and pressure drop measurements, for different process conditions. The rate of degradation of the pollutants will be quantified by chromatography of the effluents. Then, the effects of gravity force, porosity gradients and stratification will be evaluated during flow through metric-scale 2D and 3D tanks filled with layers of different permeabilities. These experiments will provide criteria to select the controllable parameters, preventing the uneven spread of ZVI in heterogeneous soils and stability loss.

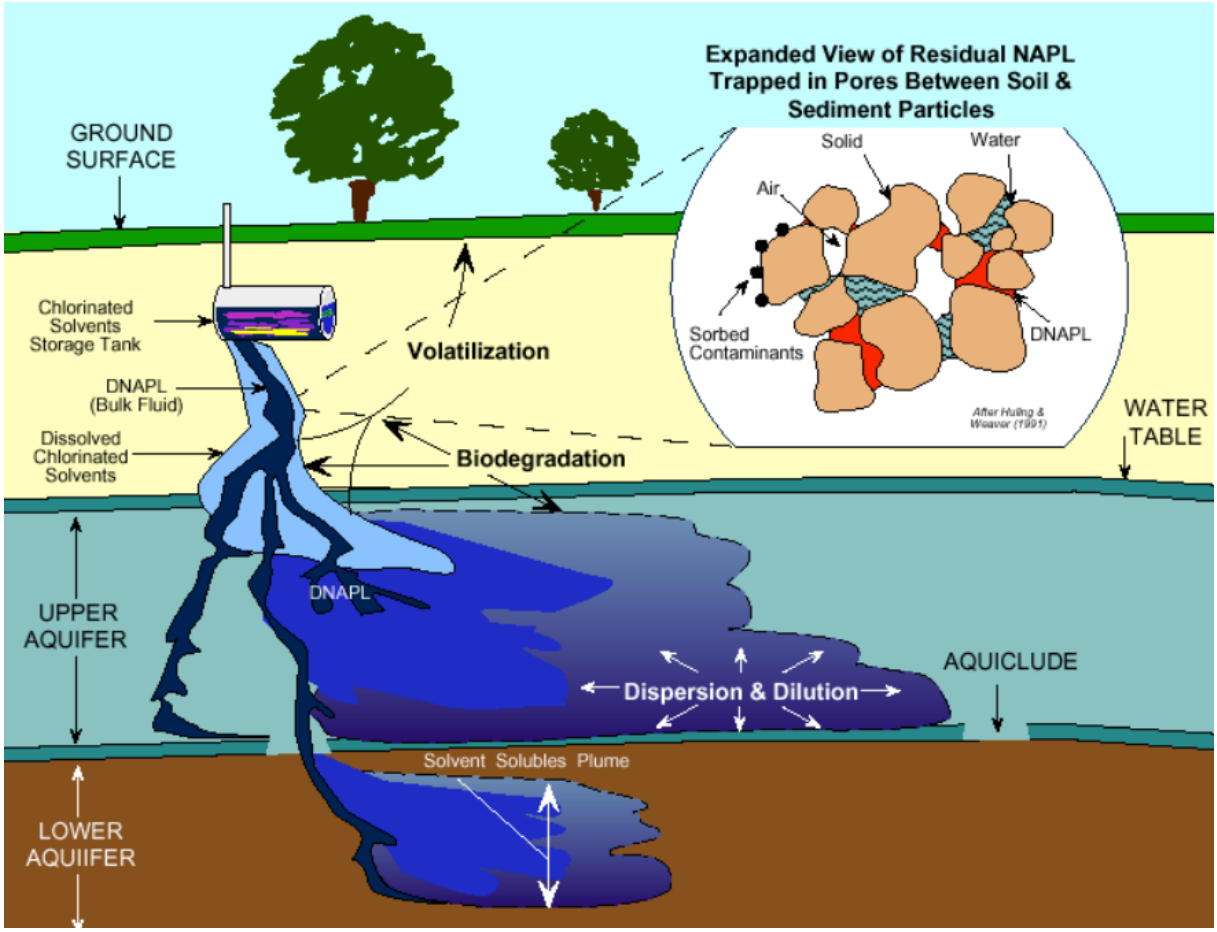


Figure 1 *Spread of a Dense Non-aqueous Phase Liquid pollutant (DNAPL) in a soil. From "EPA. Monitored natural attenuation of petroleum hydrocarbons. U.S. EPA Remedial Technology Fact Sheet, EPA/600/F-98/021, May 1999."*

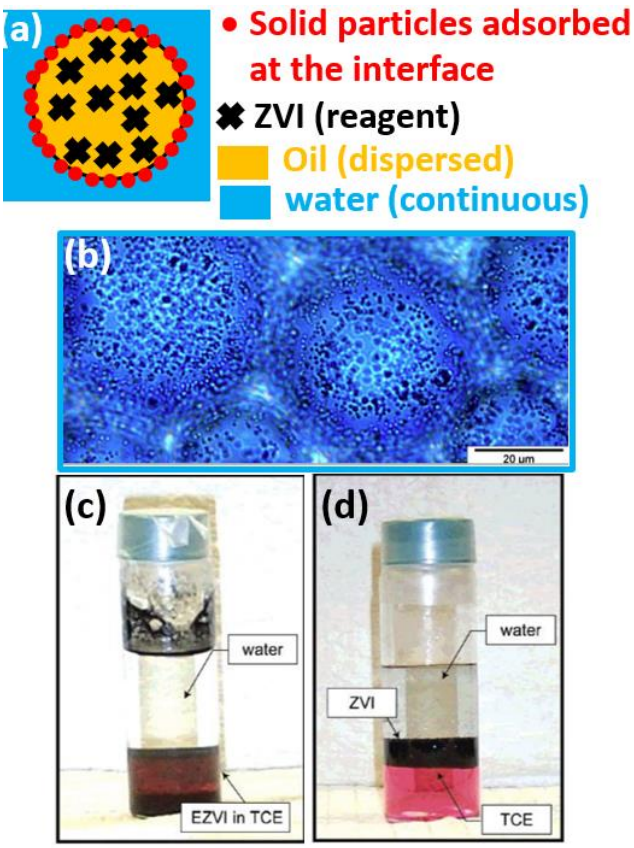


Figure 2 *(a) Schematic view of an oil-in-water Pickering emulsion loaded with ZVI. (b) Optical microscope image of a real Pickering emulsion. (c,d) Batch experiments showing best mixing of emulsified ZVI (EZVI) with TCE pollutant as compared with ZVI in aqueous suspension (from Quinn J, Geiger C, Clausen C, Brooks K, Coon C, O'Hara S, Krug T, Major D, Yoon WS, Gavaskar A, Holdsworth T. Field demonstration of DNAPL dehalogenation using emulsified zero-valent iron. Environ Sci Technol. 2005 Mar 1;39(5):1309-18)*

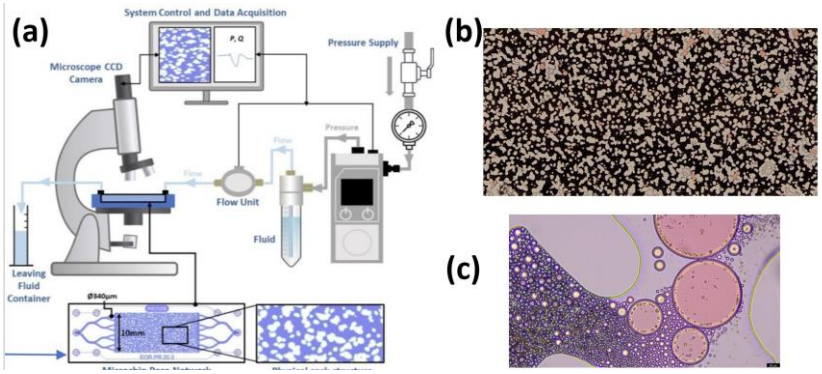


Figure 3 *(a) Microfluidic setup used at I2M to study the displacement of a pollutant oil by an emulsion. (b) Image showing the positions of solid (yellow), resident pollutant oil (red) and emulsion (black) after emulsion flooding. All the micromodel is dispalayed (2 x 1 cm). (c) Zoom on a smaller region (0.5 x 0.25 mm) showing the interfaces between oil, solid and emulsion phases.*

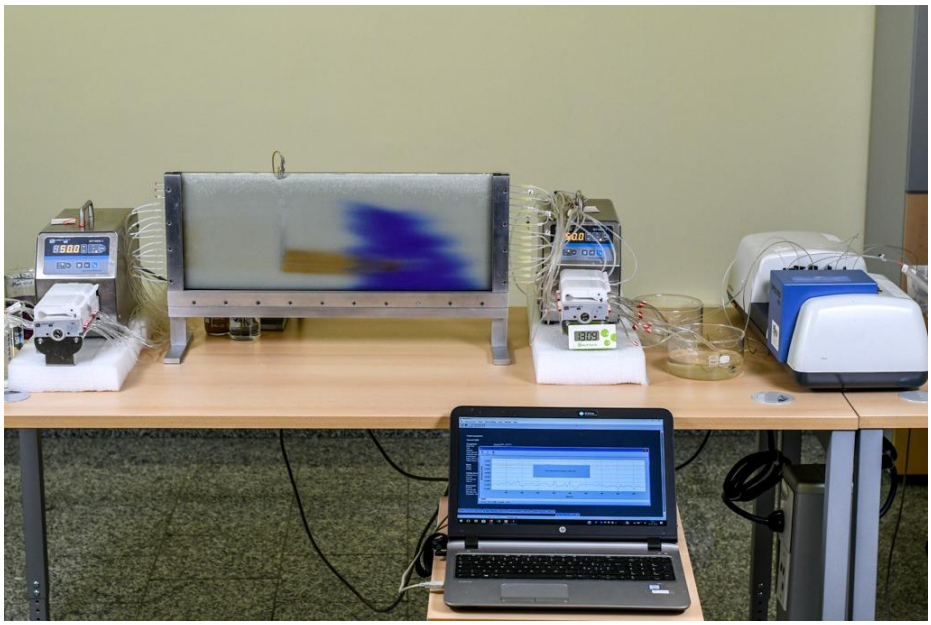


Figure 4 *Experimental setup for the simulation of emulsified zerovalent iron injection and propagation in 2D vertical geometry (Groundwater Engineering Group – Politecnico di Torino)*

References

Gallo A., Bianco C., Tosco T., Tiraferri A., Sethi R. (2019). Synthesis of eco-compatible bimetallic silver/iron nanoparticles for water remediation and reactivity assessment on bromophenol blue. Journal of Cleaner Production, 211.

Mohammadian S., Krok B., Fritzsche A., Bianco C., Tosco T., Cagigal E., Mata B., Gonzalez V., Diez-Ortiz M., Ramos V., Montalvo D., Smolders E., Sethi R., Meckenstock R.U. (2021). Field-scale demonstration of in situ immobilization of heavy metals by injecting iron oxide nanoparticle adsorption barriers in groundwater. Journal of Contaminant Hydrology, 237, 103741.

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Rodríguez de Castro, A., Ben Abdelwahed, A., Bertin, H. (2023): Enhancing pollutant removal from contaminated soils using yield stress fluids as selective blocking agents. Journal of Contaminant Hydrology 255, 104142.

Rodríguez de Castro, A., Goyeau, B. (2022). Numerical analysis of the pore-scale mechanisms controlling the efficiency of immiscible displacement of a pollutant phase by a shear-thinning fluid. Chemical Engineering Science 251 117462.

Tran Ngoc, T.D., Ahmadi, A. Bertin, H. (2020), Non-Fickian dispersivity investigation from numerical simulations of tracer transport in a model double-porosity medium at different saturations, Journal of Contaminant Hydrology 234, 103678.

ParisTech

Arts et Métiers Sciences et Technologies

TITLE: MULTI-SCALE INVESTIGATION OF CAPILLARY-DRIVEN EVAPORATIVE COOLING

Topic number : ***2023_033***

Field : Energy, Processes, Design, Industrialization, Material science, Mechanics and Fluids

Subfield:

ParisTech School: Arts et Métiers
Research team: Porous media
https://www.i2m.u-bordeaux.fr/Recherche/TREFLE-Transferts-Fluides-Energetique/Groupe-Milieux-Poreux
Research lab: I2M - Institut de Mécanique et d'ingénierie
Lab location: Bordeaux
Lab website:https://www.i2m.u-bordeaux.fr/

Contact point for this topic: Arts et Métiers

Advisor 1: RODRIGUEZ DE CASTRO Antonio
antonio.rodriguezdecastro@ensam.eu
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: An effective strategy to control the increase in urban surface temperature and create a comfortable thermal environment consists in passively cooling urban vertical surfaces (building walls and fences) by means of evaporation. The vertical motion of the heat carrier fluid is traditionally generated by a pump, which consumes energy. To reduce power consumption, innovative capillary-driven evaporative cooling systems have drawn much attention. These systems rely on the capillary action of a porous material to transport the heat carrier fluid (often water) against gravity to an upper surface. Once on the upper surface, and/or during its flow through the porous material, the fluid evaporates, absorbing heat from the nearby surface and cooling it. This energy-efficient and environmentally friendly cooling method can be used in many applications, including air-conditioning, passive cooling of urban environments, cooling of solar panels, electronics cooling and crop cooling in agriculture. However, the design of advanced porous materials capable of supplying water at a suitable flow rate while achieving high cooling power requires a deep

understanding of the phenomena occurring at different scales, ranging from the pore scale to the scale of the application. The objective of this PhD is to model these phenomena based on cutting-edge numerical simulations and their experimental validation. To do so, a set of Direct Numerical Simulations and Pore-Network Modelling simulations will be conducted. The proposed models will be validated through microfluidic and real scale experiments.

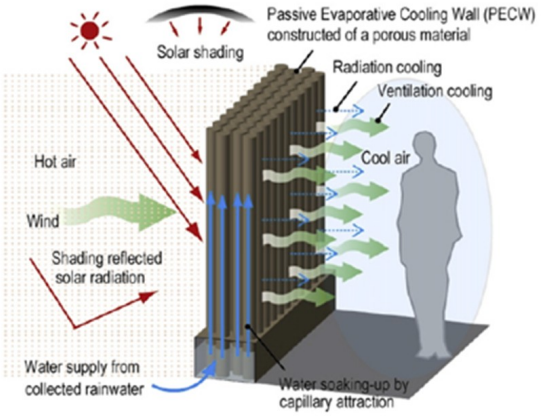
Required background of the student: A solid theoretical and experimental understanding of the fundamentals of fluid mechanics is required. The principles of Computational Fluid Dynamics must be known. Performing experiments requires dexterity, autonomy and meticulousness.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Alberghini, M., Boriskina, S. V., Asinari, P., Fasano, M.,(2022). Characterisation and modelling of water wicking and evaporation in capillary porous media for passive and energy-efficient applications. Applied Thermal Engineering, 208, 118159.
2. He, J., Hoyano, A. (2010) Experimental study of cooling effects of a passive evaporative cooling wall constructed of porous ceramics with high water soaking-up ability. Building and Environment 45, 461-472.
3. Panda, D., Bhaskaran, S., Paliwal, S., Kharaghani, A., Tsotsas, E., Surasan, V. K. (2020): Pore-scale physics of drying porous media revealed by Lattice Boltzmann simulations, Drying Technology.
4. Rodríguez de Castro, A., Agnaou, M. Gostick, J. (2023). Predicting Shear-thinning Fluid Flows in Porous Media using Pore Network Modeling: Simulations and Experimental Validation. Transport in Porous Media 149, 453–478.
5. Velasco-Gómez, E., Tejero-González, A., Jorge-Rico, J., Rey-Martínez, F. R. (2020). Experimental investigation of the potential of a new fabric-based evaporative cooling pad. Sustainability, 12(17), 7070

Illustrations :

(a)



(b)

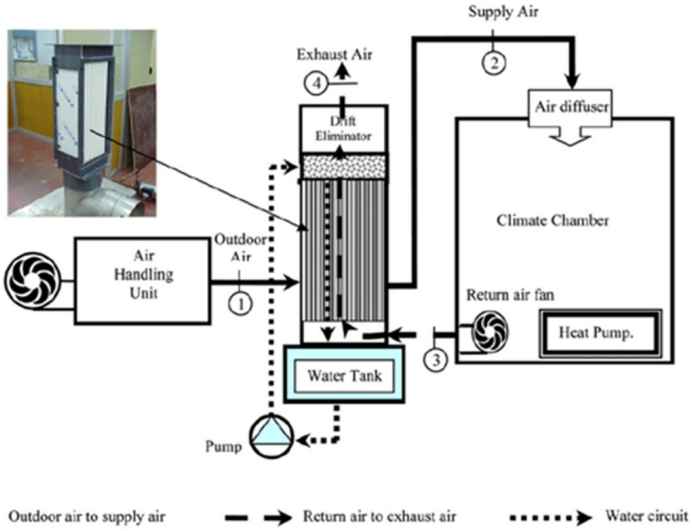


Figure 1 *Schematic description of a passive evaporative cooling system constructed with a porous material with high capillary absorption capacity. From He and Hoyano (2010).* (b) *View of a semi-indirect evaporative recuperator made with ceramic Pipes. From Velasco-Gómez, E, et al. (2020).*

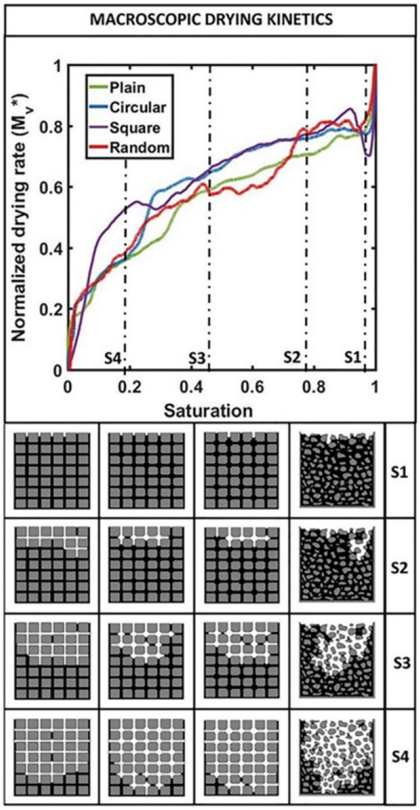


Figure 2 *(Top) Macroscopic drying kinetics during isothermal drying of four different porous media (plain, circular, square, and random arranged from left to right) (bottom) Phase distribution in respective porous media (S1: 0.97; S2:0.78; S3: 0.45; S4:0.21). The normalized drying rate (M v) is the ratio of drying rate at a particular period of time (or saturation) and the initial drying rate at S =1. It is implemented so as to compare the drying curves of four different porous media. From Panda et al. (2020).*

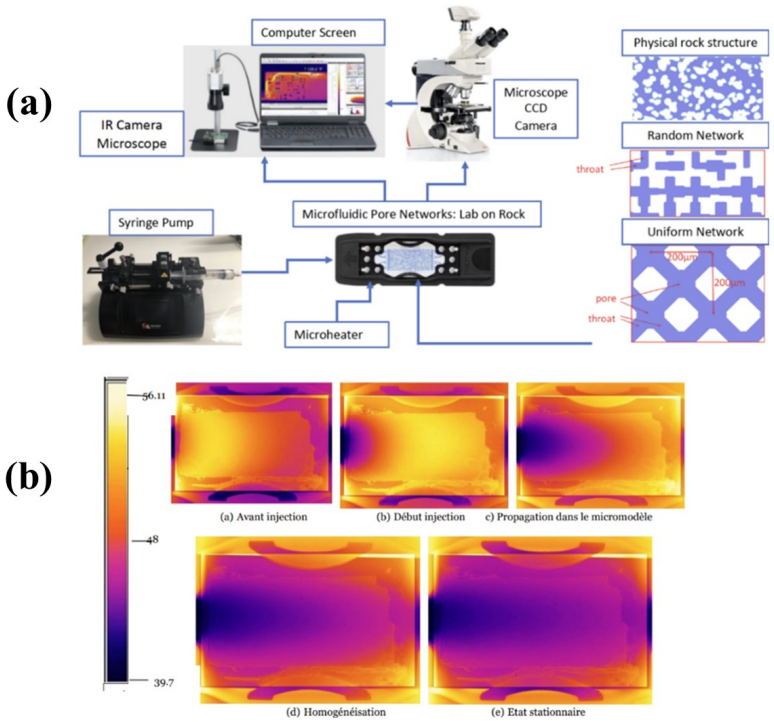


Figure 3. *(a) Schematic view of the microfluidic device designed and implemented at I2M laboratory to perform measurements of the equivalent thermal coefficient. The geometry of the microchannels can be chosen (examples of uniform, random and representative networks of a rock are provided). (b) Surface temperature maps (in °C) measured by infrared termography during the injection of a cold liquid into a micromodel heated by Joule effect, as measured at I2M laboratory.*

Multi-scale investigation of capillary-driven evaporative cooling

An effective strategy to control the increase in urban surface temperature and create a comfortable thermal environment consists in passively cooling urban vertical surfaces (building walls and fences) by means of evaporation. The vertical motion of the heat carrier fluid is traditionally generated by a pump, which consumes energy. To reduce power consumption, innovative capillary-driven evaporative cooling systems have drawn much attention. These systems rely on the capillary action of a porous material to transport the heat carrier fluid (often water) against gravity to an upper surface. Once on the upper surface, and/or during its flow through the porous material, the fluid evaporates, absorbing heat from the nearby surface and cooling it. This energy-efficient and environmentally friendly cooling method can be used in many applications, including air-conditioning, passive cooling of urban environments, cooling of solar panels, electronics cooling and crop cooling in agriculture. However, the design of advanced porous materials capable of supplying water at a suitable flow rate while achieving high cooling power requires a deep understanding of the phenomena occurring at different scales, ranging from the pore scale to the scale of the application. The objective of this PhD is to model these phenomena based on cutting-edge numerical simulations and their experimental validation. To do so, a set of Direct Numerical Simulations and Pore-Network Modelling simulations will be conducted. The proposed models will be validated through microfluidic and real scale experiments.

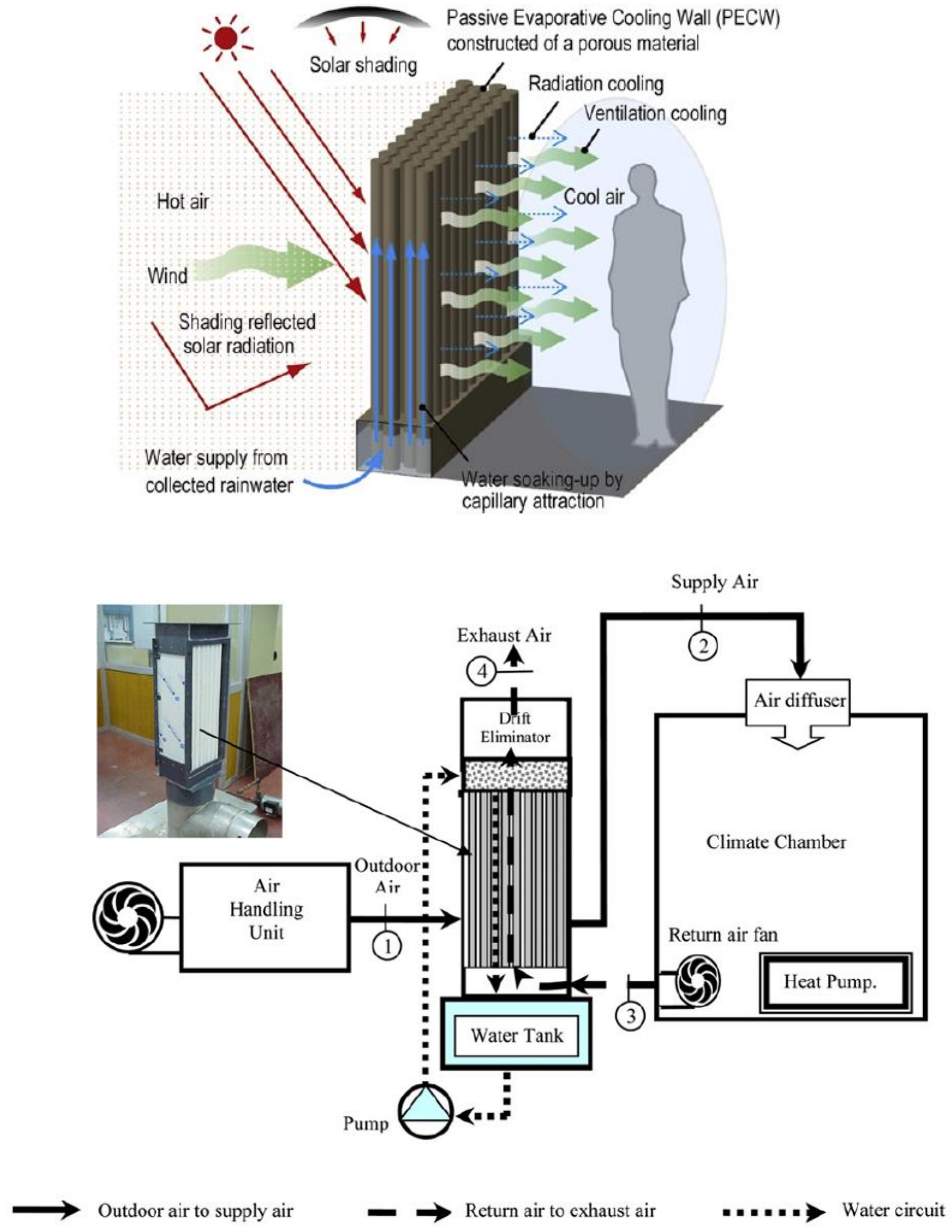


Figure 1 *Schematic description of a passive evaporative cooling system constructed with a porous material with high capillary absorption capacity. From He and Hoyano (2010).* (b) *View of a semi-indirect evaporative recuperator made with ceramic Pipes. From Velasco-Gómez, E, et al. (2020).*

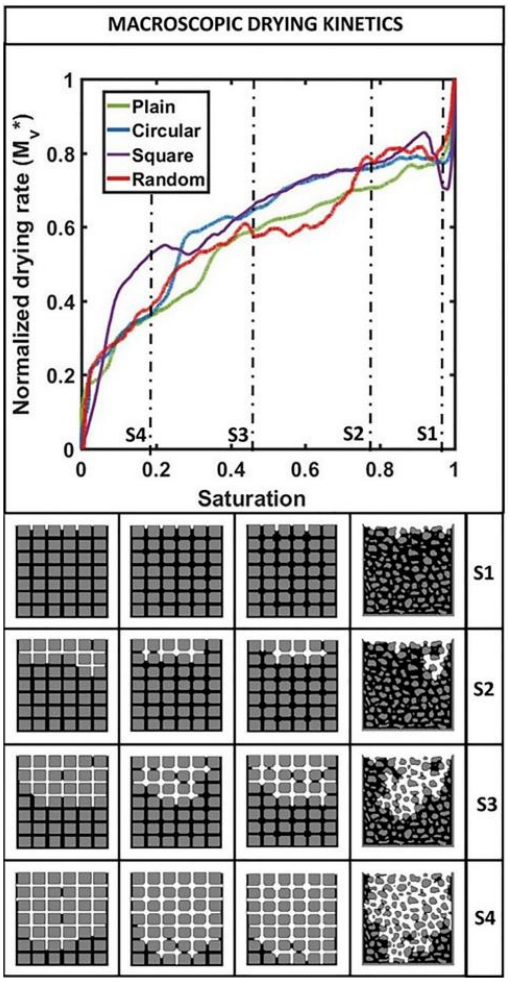


Figure 2 *(Top) Macroscopic drying kinetics during isothermal drying of four different porous media (plain, circular, square, and random arranged from left to right) (bottom) Phase distribution in respective porous media (S1: 0.97; S2:0.78; S3: 0.45; S4:0.21). The normalized drying rate (M_v) is the ratio of drying rate at a particular period of time (or saturation) and the initial drying rate at S =1. It is implemented so as to compare the drying curves of four different porous media. From Panda et al. (2020).*

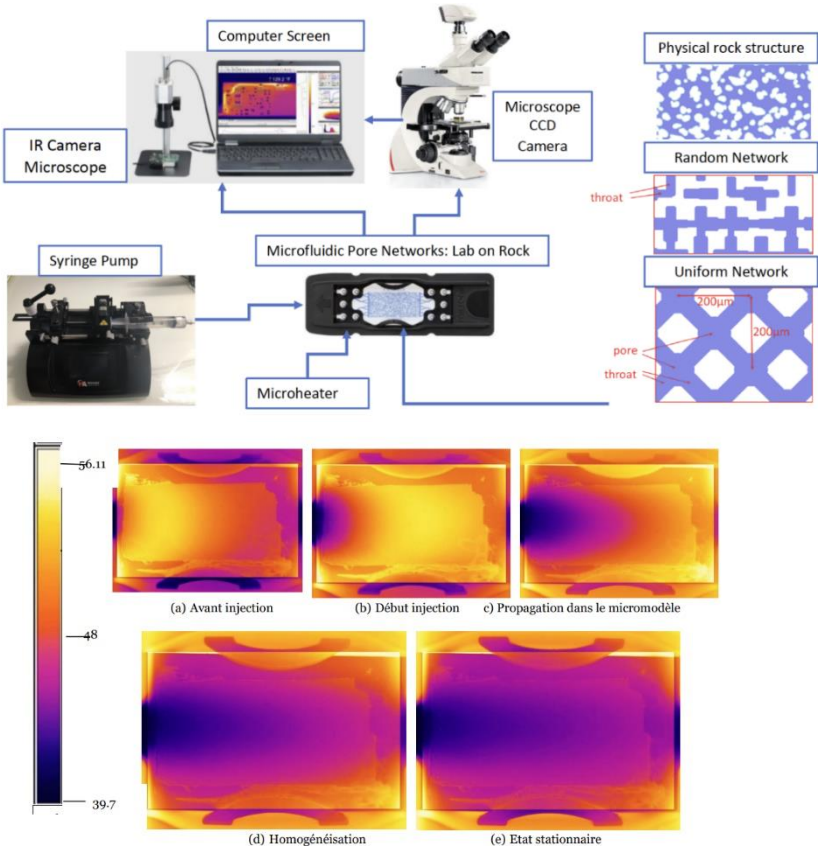


Figure 3. *(a) Schematic view of the microfluidic device designed and implemented at I2M laboratory to perform measurements of the equivalent thermal coefficient. The geometry of the microchannels can be chosen (examples of uniform, random and representative networks of a rock are provided). (b) Surface temperature maps (in °C) measured by infrared termography during the injection of a cold liquid into a micromodel heated by Joule effect, as measured at I2M laboratory.*

Research fields

Energy, Processes; Design, Industrialization; Material Science, Mechanics and Fluids.

References

Alberghini, M., Boriskina, S. V., Asinari, P., Fasano, M.,(2022). *Characterisation and modelling of water wicking and evaporation in capillary porous media for passive and energy-efficient applications*. Applied Thermal Engineering, 208, 118159.

He, J., Hoyano, A. (2010) *Experimental study of cooling effects of a passive evaporative cooling wall constructed of porous ceramics with high water soaking-up ability*. Building and Environment 45, 461-472.

Panda, D., Bhaskaran, S., Paliwal, S., Kharaghani, A., Tsotsas, E., Surasan, V. K. (2020): *Pore-scale physics of drying porous media revealed by Lattice Boltzmann simulations*, Drying Technology.

Rodríguez de Castro, A., Agnaou, M. Gostick, J. (2023). *Predicting Shear-thinning Fluid Flows in Porous Media using Pore Network Modeling: Simulations and Experimental Validation*. Transport in Porous Media 149, 453–478.

Velasco-Gómez, E., Tejero-González, A., Jorge-Rico, J., Rey-Martínez, F. R. (2020). *Experimental investigation of the potential of a new fabric-based evaporative cooling pad*. Sustainability, 12(17), 7070

ParisTech

TITLE: HARNESSING TANDEM CATALYSIS FOR THE SYNTHESIS OF BIOBASED POLYMERS FROM RENEWABLE RESOURCES

Topic number : ***2023_034***

Field : Chemistry, Physical chemistry and Chemical Engineering, ,

Subfield:

ParisTech School: Chimie ParisTech - PSL
Research team: http://www.ircp.cnrs.fr/la-recherche/equipe-cocp/
Research lab: IRCP - Institut de Recherche de Chimie de Paris
Lab location:
Lab website:http://www.ircp.cnrs.fr/

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Thomas Christophe
christophe.thomas@chimieparistech.psl.eu
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Tandem catalysis is one of the strategies used by Nature for building macromolecules. However, these biological processes rely on highly complex biocatalysts thus limiting their industrial applications. In the same biomimetic spirit, we want to initiate a research effort to synthesize biodegradable polymers via tandem catalytic transformations, where “activated” monomers are synthesized from raw materials (in one or more steps) and subsequently (co)polymerized. The objectives for this are clear: not only can a reduction in workload, waste, and energy consumption be achieved, but also the synthesis of complex products that are otherwise difficult to obtain (e.g., because of thermodynamic hurdles) comes within reach. In other words, the combination of chemistries may allow the direct synthesis of macromolecules with high structural complexity. Therefore, we want to direct investigative efforts toward the synthesis of new renewable monomers and the subsequent catalytic conversion of these monomers into their corresponding polymers. The general idea is to use a tandem procedure of combining the synthesis of new biomass-derived monomers with subsequent polymerization by well-defined metal-based catalysts, aiming at novel polymeric materials.

Required background of the student: (macro)molecular chemistry : synthesis and characterization techniques

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Tandem synthesis of alternating polyesters from renewable resources, C. Robert, F. de Montigny, C. M. Thomas, Nature Comm., 2011, 2, 586

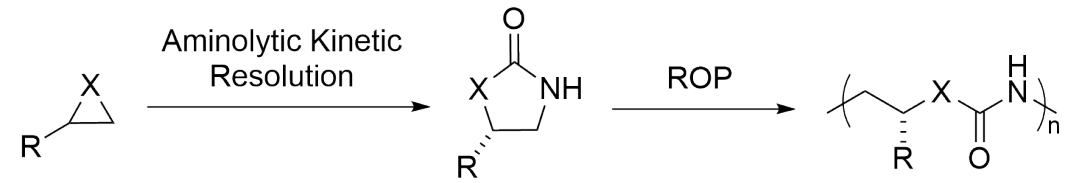
2. Mechanistic Aspects of the Polymerization of Lactide Using a Highly Efficient Aluminum(III) Catalytic System, C. Robert, T. E. Schmid, V. Richard, P. Haquette, S. K. Raman, M.-N. Rager, R. M. Gauvin, Y. Morin, X. Trivelli, V. Guérineau, I. del Rosal, L. Maron, C. M. Thomas, J. Am. Chem. Soc. 2017, 139, 6217-6225

3. Polymerization of rac-Lactide Using Achiral Iron Complexes: Access to Thermally Stable Stereocomplexes
P. Marin, M. J.-L. Tschan, F. Isnard, C. Robert, P. Haquette, X. Trivelli, L.-M. Chamoreau, V. Guérineau, I. del Rosal, L. Maron, V. Venditto, C. M. Thomas , Angew. Chem. Int. Ed. 2019, 58, 12585-12589

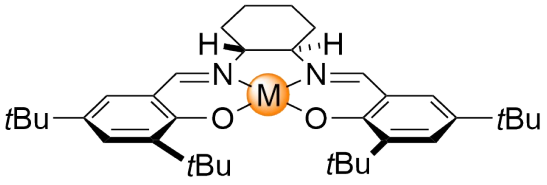
4. Access to Highly Stereodefined 1,4-cis-Polydienes by a Orthogonal Tandem Catalytic Polymerization, D. Fiorito, M. Simon, C. M. Thomas, C. Mazet, J. Am. Chem. Soc. 2021, 143, 13401-13407

5. Multicatalytic Transformation of (Meth)acrylic Acids: a One-Pot Approach to Biobased Poly(meth)acrylates, H. Fouilloux, W. Qiang, C. Robert, V. Placet, C. M. Thomas, Angew. Chem. Int. Ed. 2021, 60,19374-19382

Illustrations :



X = O, NR



M = Al-Cl
M = Co

TITLE: ECO-EFFICIENT PROCESSES FOR THE SYNTHESIS OF SUSTAINABLE POLYMERS

Topic number : ***2023_035***

Field : Chemistry, Physical chemistry and Chemical Engineering, ,

Subfield:

ParisTech School: Chimie ParisTech - PSL
Research team: COCP http://www.ircp.cnrs.fr/la-recherche/equipe-cocp/
Research lab: IRCP - Institut de Recherche de Chimie de Paris
Lab location: Paris
Lab website:http://www.ircp.cnrs.fr/

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Gauvin Regis regis.gauvin@chimieparistech.psl.eu
Advisor 2: Thomas Christophe
christophe.thomas@chimieparistech.psl.eu
Advisor 3:
Advisor 4:

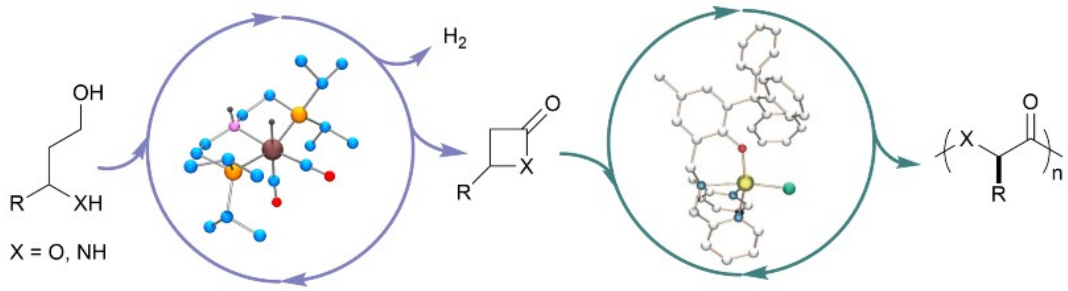
Short description of possible research topics for a PhD: The development of new methods to transform biomass into resources suitable for polymer production remains a crucial obstacle on the way to a more sustainable chemical economy. In this regard, the creation of renewable polymers through one-pot catalysis represents an important tool to support more sustainable plastics production. In this project, hydrogen borrowing, a clean atom-economical technology, will be harnessed in a first step to synthesize lactones or lactames monomers from biosourced raw materials. These will then be polymerized through stereoselective ring opening polymerization, providing novel polyesters or polyamides. An intense emphasis will be placed on the design of new organometallic catalysts based on Earth-abundant metals, as well as on establishing the physicochemical properties of the polymers.

Required background of the student: (macro)molecular chemistry : synthesis and characterization techniques, molecular catalysis

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Fouilloux, H.; Rager, M.-N.; Ríos, P.; Conejero, S.; Thomas, C. M. Angew. Chem., Int. Ed. 2022, 61, e202113443
2. Upitak, K.; Thomas, C. M. Acc. Chem. Res. 2022, 55, 2168
3. a) Robert, C.; De Montigny, F.; Thomas, C. M. Nat. Commun. 2011, 2, 586. b) Fouilloux, H.; Qiang, W.; Robert, C.; Placet V.; Thomas, C. M. Angew. Chem., Int. Ed. 2021, 60, 19374.
4. Nguyen, D. H.; Trivelli, X.; Capet, F.; Paul, J.-F.; Dumeignil, F.; Gauvin R. M. ACS Catal., 2017, 7, 2022.
5. Marin, P.; Tschan, M. J.-L.; Isnard, F.; Robert, C.; Haquette, P.; Trivelli, X.; Chamoreau, L.-M.; Guérineau, V.; del Rosal, I.; Maron, L.; Venditto, V.; Thomas C. M. Angew. Chem. Int. Ed. 2019, 58, 12585.

Illustrations :



ParisTech

TITLE: DESIGN OF BIOCOMPATIBLE AND BIODEGRADABLE POLYMER-COATED NANOPARTICLES AS VECTORIZING AGENTS

Topic number : ***2023_036***

Field : Chemistry, Physical chemistry and Chemical Engineering, ,

Subfield:

ParisTech School: Chimie ParisTech - PSL
Research team: COCP http://www.ircp.cnrs.fr/la-recherche/equipe-cocp/
Research lab: IRCP - Institut de Recherche de Chimie de Paris
Lab location:
Lab website:http://www.ircp.cnrs.fr/

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Gauvin Regis regis.gauvin@chimieparistech.psl.eu
Advisor 2: Thomas Christophe
christophe.thomas@chimieparistech.psl.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: The design of efficient vectorizing agents is at the cornerstone of modern pharmaceutical agents. In this view, the tailoring of specific (molecular) objects by covalent bonding with polymer chains is of major interest, to confer them significant compatibility with physiological environments.

In this view, biocompatible and biodegradable polymers are ideal candidates as components within such advanced formulations. These can be most efficiently prepared using ring opening polymerization (ROP) of lactones or lactides into polyesters or polylactic acid mediated by organometallic initiators. On the top of that, immobilization of organometallics on inorganic surfaces via surface was demonstrated to boost stereoselectivity of these considered polymerization processes. In this project, we propose to combine surface organometallic chemistry and ROP of polar monomers to design specific nanoobjects by “growing from” or “growing on” approaches, where chain growth is mediated by specifically designed supported organometallic entities. The ultimate goal will be the development of biopolymer-coated nanoparticles for future implementation into drug delivery systems.

Required background of the student: materials and (macro)molecular chemistry : synthesis and characterization techniques

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. N. Soliman, L. K. McKenzie, J. Karges, E. Bertrand,M. Tharaud, M. Jakubaszek, V. Guérineau,B. Goud, M. Hollenstein, G. Gasser, C. M. Thomas, Chem. Sci., 2020, 11, 2657-2663.

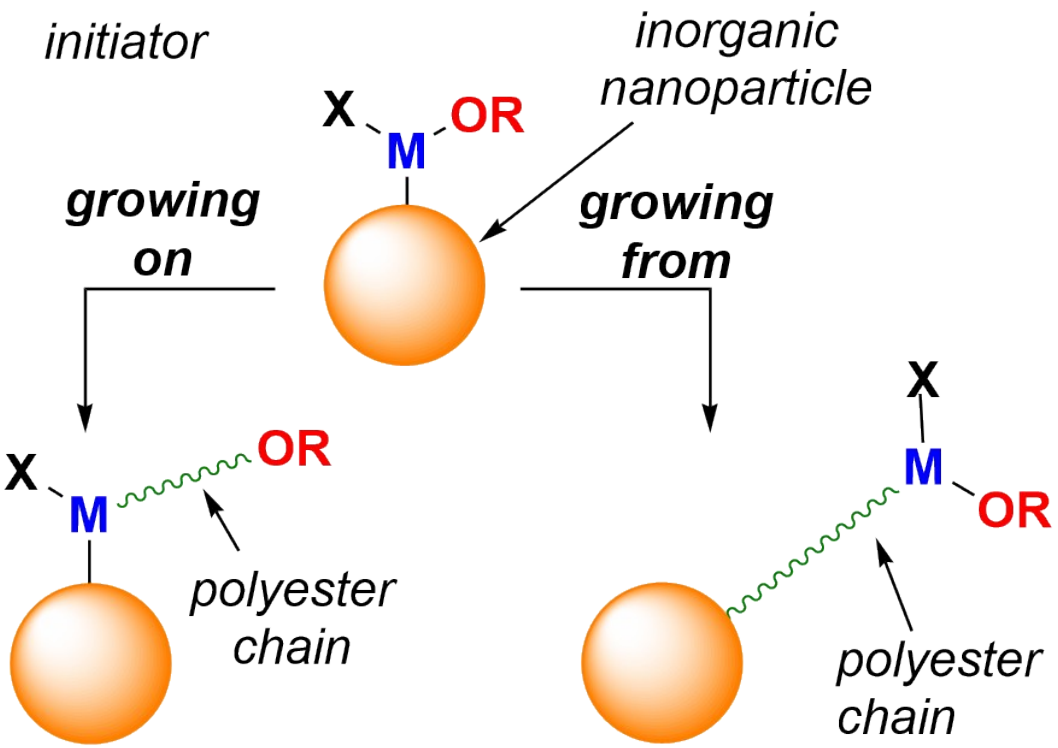
2. P. Marin, M. J.-L. Tschan, F. Isnard, C. Robert, P. Haquette, X. Trivelli, L.-M. Chamoreau, V. Guérineau, I. del Rosal, L. Maron, V. Venditto, C. M. Thomas, Angew. Chem. Int. Ed. 2019, 58, 12585-12589

3. M. J.-L. Tschan, R. M. Gauvin, C. M. Thomas, Chem. Soc. Rev., 2021, 50, 13587-13608.

4. N. Ajellal, G. Durieux, L. Delevoye, G. Tricot, C. Dujardin, C. M. Thomas, R. M. Gauvin, Chem. Commun. 2010, 46, 1032-1034

5.

Illustrations :



ParisTech

Arts et Métiers

TITLE: AI-BASED ADAPTIVE PROCESS MONITORING IN SMART MANUFACTURING

Topic number : ***2023_037***

Field : Design, Industrialization, Energy, Processes, Information and Communication Science and Technology

Subfield: Porcess Control and Optimization, Applied Mathematics

ParisTech School: Arts et Métiers
Research team:
Research lab: LCFC - Laboratoire de conception, fabrication, commande
Lab location: Metz
Lab website:http://lcfc.ensam.eu/

Contact point for this topic: Arts et Métiers

Advisor 1: HOMRI Lazhar lazhar.homri@ensam.eu
Advisor 2: ZOUHRI Wahb
Advisor 3: DANTAN Jean-Yves jean-yves.dantan@ensam.eu
Advisor 4:

Short description of possible research topics for a PhD: With the emergence of industry 4.0 and data-driven approaches usage within smart manufacturing systems, statistical process control (SPC) should be adapted by considering feedbacks and knowledge from users and process, in order to improve the product development, to ensure its quality and reliability and to identify process drifts or anomalies. Dynamic process control constantly drives process improvement by focusing on extracting knowledge from gathered data (signals)for immediate actions, ensuring therefore more efficiency and schedule adherence.
It could automatically analyse the process and send alerts for immediate assessment. By continually leading improvements, systems performance and quality are thus maximized.
In fact, undefined anomalies usually result into a breakdown of the equipment or a fault in the working of the equipment. Therefore, adopting a new anomaly detection approach for process control will lead to test's cost reduction and allow a quick identification of anomalies and unexpected patterns.
Moreover, the derived knowledge can be used to improve the product

design specifications and defining its verification and validation plans to build functional and reliable models.

Required background of the student: Statistics, Computer Science, Mechanical Engineering, Industrial Engineering.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. CIANCIO, Vincent, HOMRI, Lazhar, DANTAN, Jean-Yves, et al. Development of a flexible data management system, to implement predictive maintenance in the Industry 4.0 context. International Journal of Production Research, 2023, p. 1-17.
2. Ciancio V., Homri L., Dantan J.-Y., Siadat A., 2020. Towards prediction of machine failures: overview and first attempt on specific automotive industry application. IFAC-PapersOnLine 53, 289-294. 2020.
3. Zouhri, W., Dantan, J. Y., Häfner, B., Eschner, N., Homri, L., Lanza, G., Theile, O. & Schäfer, M. (2020). Optical process monitoring for Laser-Powder Bed Fusion (L-PBF). CIRP Journal of Manufacturing Science and Technology, 31, 607-617
4. Himeur Y., Ghanem K., Alsalemi A., Bensaali F., Artificial intelligence-based anomaly detection of energy consumption in buildings: A review, current trends and new perspectives, Applied Energy 287, 2021.
5. Bassetto S., Siadat A., Martin P., Adavanced Process Control Application Modelling. CIRP Intelligent Computation Manufacturing Engineering, Jul 2002, ischia, Italy

Illustrations :

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Design, Industrialization

Subfield: Industrial Eng, Mechanical Eng.

Title: AI-based Adaptive Process Monitoring in Smart Manufacturing

ParisTech School: Arts et Métiers Sciences et Technologies

Advisor(s) Name: Lazhar HOMRI, Wahb ZOUHRI, Jean-Yves DANTAN
Advisor(s) Email: *lazhar.homri@ensam.eu*
Research group/Lab: *LCFC*
Lab location: *Arts et Metiers Campus of Metz*
(Lab/Advisor website): *http://lcfc.ensam.eu/*

Short description of possible research topics for a PhD:

With the emergence of industry 4.0 and data-driven approaches usage within smart manufacturing systems, statistical process control (SPC) should be adapted by considering feedbacks and knowledge from users and process, in order to improve the product development, to ensure its quality and reliability and to identify process drifts or anomalies.

Dynamic process control constantly drives process improvement by focusing on extracting knowledge from gathered data (signals)for immediate actions, ensuring therefore more efficiency and schedule adherence. It could automatically analyse the process and send alerts for immediate assessment. By continually leading improvements, systems performance and quality are thus maximized.

In fact, undefined anomalies usually result into a breakdown of the equipment or a fault in the working of the equipment. Therefore, adopting a new anomaly detection approach for process control will lead to test's cost reduction and allow a quick identification of anomalies and unexpected patterns.
Moreover, the derived knowledge can be used to improve the product design specifications and defining its verification and validation plans to build functional and reliable models.

Required background of the student: Statistics, Computer Science, Mechanical Engineering, Industrial Engineering.

Key words: Manufacturing Quality Management, Anomaly Detection, Artificial Intelligence

A list of 5 (max.) representative publications of the group:

1. Ciancio V., Homri L., Dantan J.-Y., et al. Development of a flexible data management system, to implement predictive maintenance in the Industry 4.0 context. International Journal of Production Research, 2023, p. 1-17.

2. Ciancio V., Homri L., Dantan J.-Y., Siadat A., 2020. Towards prediction of machine failures: overview and first attempt on specific automotive industry application. IFAC-PapersOnLine 53, 289-294. 2020.
3. Zouhri, W., Dantan, J. Y., Häfner, B., Eschner, N., Homri, L., Lanza, G., Theile, O. & Schäfer, M. (2020). Optical process monitoring for Laser-Powder Bed Fusion (L-PBF). CIRP Journal of Manufacturing Science and Technology, 31, 607-617
4. Himeur Y., Ghanem K., Alsalemi A., Bensaali F., Artificial intelligence-based anomaly detection of energy consumption in buildings: A review, current trends and new perspectives, Applied Energy 287, 2021.
5. Bassetto S., Siadat A., Martin P., Adavanced Process Control Application Modelling. CIRP Intelligent Computation Manufacturing Engineering, Jul 2002, ischia, Italy

ParisTech

Arts et Métiers

TITLE: TOLERANCE ALLOCATION MULTI-OBJECTIVE OPTIMIZATION MODEL FOR SUSTAINABLE AND INTELLIGENT MANUFACTURING

Topic number : ***2023_038***

Field : Design, Industrialization, Energy, Processes,

Subfield:

ParisTech School: Arts et Métiers
Research team:
Research lab: LCFC - Laboratoire de conception, fabrication, commande
Lab location: Metz
Lab website:http://lcfc.ensam.eu/

Contact point for this topic: Arts et Métiers

Advisor 1: HOMRI Lazhar lazhar.homri@ensam.eu
Advisor 2: DANTAN Jean-Yves
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Sustainable and smart manufacturing has become a strategic focus as industries have begun exploring new ways to use resources efficiently, improve product quality, and reduce energy consumption. Energy is utilized at every stage of a product's life cycle. The efficiency of the resulting products is ultimately influenced by the conditions in which they are designed, manufactured, and assembled. Tolerancing decisions can profoundly impact the product quality, production costs, energy consumption, and the waste amount, generated in mass production. Tolerance allocation considers design requirements, performance indicators, and manufacturing capabilities in a common multi-objective model.
With the introduction of precision manufacturing technology, traditional tolerance optimization models that only consider cost and quality can no longer meet the requirements. The issue of optimizing energy consumption in the manufacturing process should be more considered. Therefore, the tradeoffs between manufacturing cost, quality loss, and energy consumption during processing are considered as objective functions. A multi-objective optimization model for tolerance allocation is defined based on cost, quality, and energy consumption, that aims to serve as a surrogate model when data gathering and analysis.

Required background of the student: Mechanical Engineering, Optimization, Programming

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Khezri, A., Homri, L., Etienne, A., & Dantan, J. Y. (2023). Hybrid cost-tolerance allocation and production strategy selection for complex mechanisms: simulation and surrogate built-in optimization models. Journal of Computing and Information Science in Engineering, 23(5), 051003.
2. Dantan, J.-Y. and Eifler, T., 2021, Tolerance allocation under behavioural simulation uncertainty of a multiphysical system. CIRP Annals, 70, 127-130
3. Wang, Y., Huang, A., Quigley, C. A., Li, L., & Sutherland, J. W. (2021). Tolerance allocation: Balancing quality, cost, and waste through production rate optimization. Journal of Cleaner Production, 285, 124837.
4. Natarajan, J., Sivasankaran, R., & Kanagaraj, G. (2018). Bi-objective optimization for tolerance allocation in an interchangeable assembly under diverse manufacturing environment. The International Journal of Advanced Manufacturing Technology, 95, 1571-1595.
5. Etienne, A., Dantan, J.-Y., Siadat, A. and Martin, P., 2009, Activity-Based Tolerance Allocation (ABTA)–driving tolerance synthesis by evaluating its global cost. International journal of production research, 47, 4971-4989.

Illustrations :

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Design, Industrialization

Subfield: Mechanical Eng., Industrial Eng., Process Eng.

Title: Tolerance Allocation Multi-Objective Optimization model for Sustainable and Intelligent Manufacturing

ParisTech School: Arts et Métiers Sciences et Technologies

Advisor(s) Name: Lazhar HOMRI, Jean-Yves DANTAN
Advisor(s) Email: *lazhar.homri@ensam.eu*
Research group/Lab: *LCFC*
Lab location: *Arts et Metiers Campus of Metz*
(Lab/Advisor website): *http://lcfc.ensam.eu/*

Short description of possible research topics for a PhD:

Sustainable and smart manufacturing has become a strategic focus as industries have begun exploring new ways to use resources efficiently, improve product quality, and reduce energy consumption. Energy is utilized at every stage of a product's life cycle. The efficiency of the resulting products is ultimately influenced by the conditions in which they are designed, manufactured, and assembled. Tolerancing decisions can profoundly impact the product quality, production costs, energy consumption, and the waste amount, generated in mass production. Tolerance allocation considers design requirements, performance indicators, and manufacturing capabilities in a common multi-objective model.

With the introduction of precision manufacturing technology, traditional tolerance optimization models that only consider cost and quality can no longer meet the requirements. The issue of optimizing energy consumption in the manufacturing process should be more considered. Therefore, the tradeoffs between manufacturing cost, quality loss, and energy consumption during processing are considered as objective functions.
A multi-objective optimization model for tolerance allocation is defined based on cost, quality, and energy consumption, that aims to serve as a surrogate model when data gathering and analysis.

Required background of the student: Mechanical Engineering, Tolerancing, Optimization, Computer science

Key words: Tolerancing, Cost, Energy, Optimization, AI.

A list of 5 (max.) representative publications of the group:

1. Khezri, A., Homri, L., Etienne, A., & Dantan, J. Y. (2023). Hybrid cost-tolerance allocation and production strategy selection for complex mechanisms: simulation and surrogate built-in optimization models. Journal of Computing and Information Science in Engineering, 23(5), 051003.
2. Dantan, J.-Y. and Eifler, T., 2021, Tolerance allocation under behavioural simulation uncertainty of a multiphysical system. CIRP Annals, 70, 127-130.
3. Wang, Y., Huang, A., Quigley, C. A., Li, L., & Sutherland, J. W. (2021). Tolerance allocation: Balancing quality, cost, and waste through production rate optimization. Journal of Cleaner Production, 285, 124837.
4. Natarajan, J., Sivasankaran, R., & Kanagaraj, G. (2018). Bi-objective optimization for tolerance allocation in an interchangeable assembly under diverse manufacturing environment. The International Journal of Advanced Manufacturing Technology, 95, 1571-1595.
5. Etienne, A., Dantan, J.-Y., Siadat, A. and Martin, P., 2009, Activity-Based Tolerance Allocation (ABTA)–driving tolerance synthesis by evaluating its global cost. International journal of production research, 47, 4971-4989.

ParisTech

ESPCI PARIS PSL

TITLE: SPIN-LATTICE COUPLING IN THE QUANTUM PARAELECTRIC EUTIO3

Topic number : ***2023_039***

Field : Physics, Optics, Material science, Mechanics and Fluids, Chemistry, Physical chemistry and Chemical Engineering

Subfield:

ParisTech School: ESPCI Paris - PSL
Research team: Quantum Matter https://qm.lpem.espci.fr/
Research lab: LPEM - Laboratoire Physique et d'études des matériaux
Lab location: Paris
Lab website:https://lpem.spip.espci.fr/

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Fauqué Benoît benoit.fauque@espci.fr
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Engineering heat conductivity in solids has been a long-term challenge for physicists. Of particular interest is the design of low thermal conductivity materials for thermoelectric or thermal barrier devices. Last year we have identified EuTiO3 , a quantum paraelectric materials which becomes antiferromagnetic at low temperature, has a novel material with a remarkable low thermal conductivity. In this PhD we propose to conduct the first study by inelastic neutron scattering of its lattice and magnetic spectrum, and their interplay on a dedicated large single crystal. This work will be complemented by thermal transport at low temperature and up to 16T and magnetic suceptibility measurements. DFT calculations will be also performed to guide the interpretation of the experimental resuslts. This PhD project will bring crucial information on the origin of the remarkable low thermal conductivity of EuTiO3 and its multiferroic properties .

Required background of the student: material science , condensed matter physic, good knowledge on quantum and statistcal physic

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. A. Jaoui, Phys. Rev. Materials 7, 094604 (2023)
2. B. Fauqué, Phys. Rev. B 106, L140301 (2022)
3. C. Collignon et al., Phys. Rev. Materials 5, 065002 (2021)
4. Clément Collignon et al., Phys. Rev. X 10, 031025 (2020)
5. X. Li et al.,Phys. Rev. Lett. 124, 105901 (2020)

Illustrations :

TITLE: PHYSICALLY DATA STRUCTURED AND PHYSICALLY INFORMED DATA-DRIVEN MODELING FOR STRUCTURAL HEALTH MONITORING OF THIN STRUCTURES USING ULTRASONIC WAVES

Topic number : ***2023_041***

Field : Information and Communication Science and Technology, Material science, Mechanics and Fluids,

Subfield:

ParisTech School: Arts et Métiers
Research team:
Research lab: PIMM - Laboratoire Procédés et ingénierie en mécanique et matériaux
Lab location:
Lab website:https://pimm.artsetmetiers.fr/

Contact point for this topic: Arts et Métiers

Advisor 1: Fakhreddine Ababsa fakhreddine.ababsa@ensam.eu
Advisor 2: Marc Rebillat
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Structural Health Monitoring (SHM) is dedicated to the continuous and non-invasive monitoring of structures integrity, ensuring safety and optimal performances through on-site real-time measurements. Typically, a SHM approach for thin structures relies on the utilization of transducers, such as piezoelectric (PZT), bonded on the structure under examination and that can either send and received ultrasonic waves within the structure to be inspected. Thus, the data collection process associated with the SHM of thin structures using ultrasonic waves generate large datasets composed of many time series associated with all the PT paths available on the structure that need to be processed using robust and efficient techniques in order to determine the presence of the damage and their properties (nature, position, size, etc.). Machine Learning (ML) methods are well suited to this kind of application and are increasingly used by the SHM community. For example, data-driven models are used to further understand how ultrasonic waves propagating within thin structures react to different conditions and to explain the underlying physics. However, their performance depends greatly on the quality of the input

data and generalization performances are limited by the low amount of data available for learning, especially regarding damaged cases. However, besides available experimental or numerical data, physical knowledge regarding the structure to be inspected and ultrasonic propagation can also be used to structure input data or to tailor more efficient data-driven models. Furthermore, all the time series associated with the available PZT paths are correlated as they monitor the same structure, but this correlation is merely exploited to properly structure input data.
In this PhD proposal, we will thus investigate new ways of structuring data that increase the accuracy of data driven SHM algorithms and that are based on the physical knowledge related with the structure to be inspected. In particular, the generation of key images from physics-based signals corresponding to all the available PZT paths will be investigated. We will also study how to robustly integrate them into an advanced deep learning model dedicated to image processing and thus benefiting from all the readily associated available tools. The developed algorithms will be validated on both numerical and experimental data. It is expected to demonstrate that by using a physical way to structure data, performances of SHM algorithms can be reduced as well as the amount of data required for their training.

Required background of the student:

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Image processing through deep learning after DI extraction for the SHM of aeronautic composite structures using Lamb waves. S Husain, M Rébillat, F Ababsa. Sixteenth International Conference on Quality Control by Artificial Vision. 2023

2. Experimental Damage Localization and Quantification with a Numerically Trained Convolutional Neural Network. H Postorino, E Monteiro, M Rebillat, N Mechbal. European Workshop on Structural Health Monitoring. 2022

3. Unsupervised damage clustering in complex aeronautical composite structures monitored by Lamb waves: An inductive approach. A Rahbari, M Rébillat, N Mechbal, S Canu. Engineering Applications of Artificial Intelligence. 2021

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Illustrations :

ParisTech

ESPCI PARIS PSL

TITLE: DIFFUSIO-OSMOSIS ON HETEROGENEOUS SURFACES FOR BLUE ENERGY

Topic number : ***2023_042***

Field : Material science, Mechanics and Fluids, Chemistry, Physical chemistry and Chemical Engineering, Environment Science and Technology, Sustainable Development, Geosciences

Subfield:

ParisTech School: ESPCI Paris - PSL
Research team: MIE - Innovative materials for energy https://www.mie.espci.fr/spip.php?rubrique2
Research lab: CBI - Chimie, Biologie et Innovation
Lab location: Paris
Lab website:https://www.cbi.espci.fr/home-40/

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Tregouet Corentin corentin.tregouet@espci.fr
Advisor 2: Colin Annie annie.colin@espci.fr
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Osmosis is the phenomenon responsible for spontaneous liquid transfers through porous membranes separating water reservoirs with different salinities. Diffusio-osmosis describes the flow on a charged surface immerged in a gradient of salinity. In specific conditions, these phenomena enable the generation of electrical currents between two reservoirs of brine and fresh water. Based on this principle, the production of electricity where sea water meets fresh water from the river: this is called the Blue Energy. The available blue energy to be harvested worldwide is estimated to be 1 TW, which represents not less than 10 times the total solar-energy consumption. Therefore, Blue Energy has the potential to be a game changer for the energy transition. Before being able to harvest efficiently this energy, it is necessary to finely understand the fluxes occurring in the membrane, but also how it couples with the upstream and downstream fluxes. More specifically, complex effects at the entrance and the exit of nanopores result from couplings between ion concentrations, electric fields, electrostatic forces, pressure and flow, described by the advection-diffusion equation and Navier-Stokes. The aim of this PhD is to

study how the modification of the membrane surface (roughness, conductivity, charge, etc) can enhance the overall fluxes of ions, and therefore, the harvested electrical power.

Required background of the student: The candidate must be an experimentalist, with a background in physics, fluid mechanics or chemical engineering.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Brahmi, Y., & Colin, A. (2022). New membrane and electrode assembly concept to improve salinity energy harvesting. Energy Conversion and Management, 254, 115297.

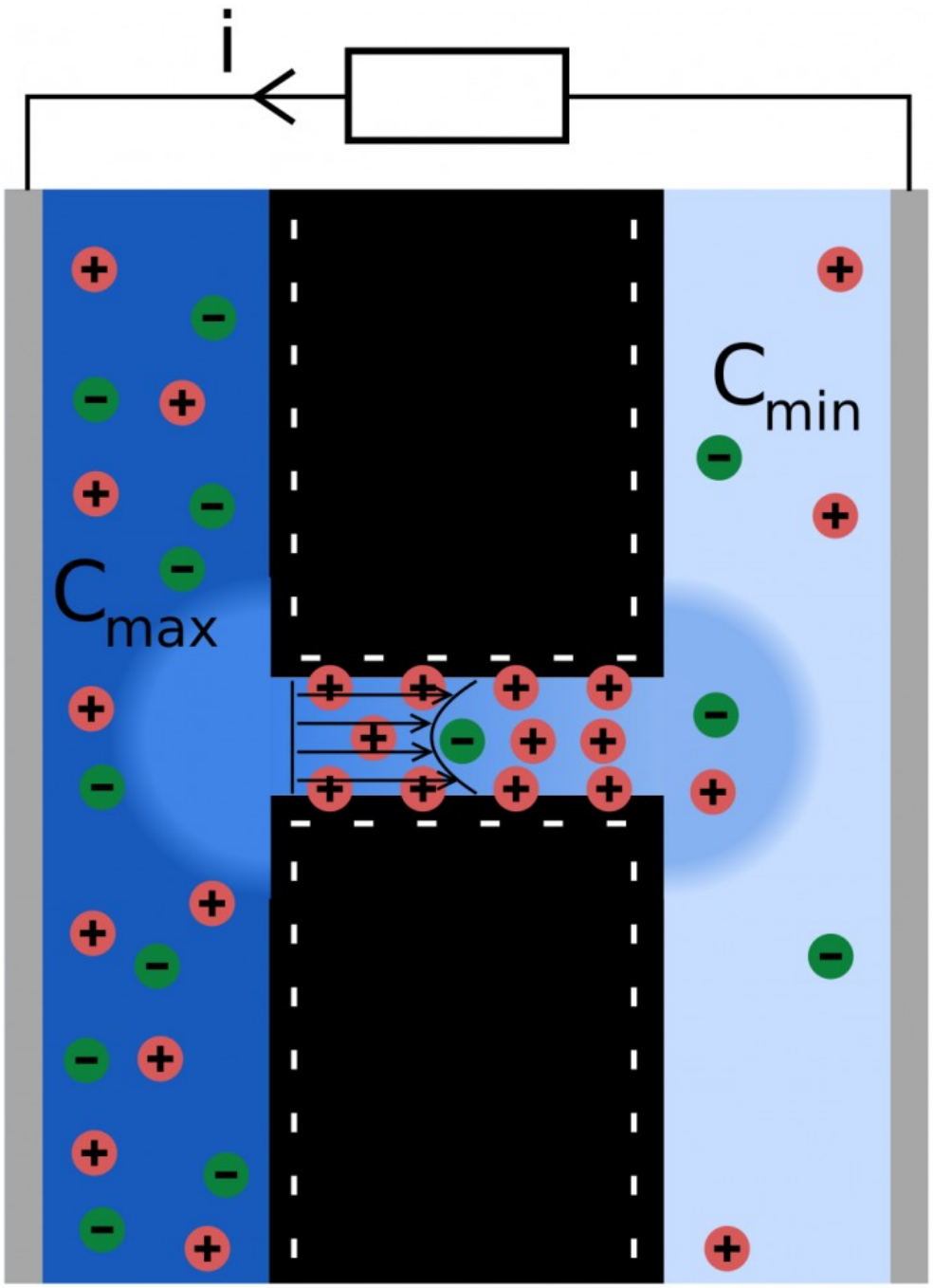
2. Siria, A., Bocquet, M., & Bocquet, L. (2016). New avenues for the large-scale harvesting of blue energy. Nature Reviews Chemistry, 1(0091).

3. Gao, J., Liu, X., Jiang, Y., Ding, L., Jiang, L., & Guo, W. (2019). Understanding the Giant Gap between Single-Pore- and Membrane-Based Nanofluidic Osmotic Power Generators. Small, 15(11), 1–8.

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Illustrations :


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ParisTech

ESPCI PARIS PSL

TITLE: ENHANCING THE MECHANICAL PROPERTIES OF POLYOLEFIN BLENDS BY EXPLOITING SUPRAMOLECULAR COASSEMBLY

Topic number : ***2023_043***

Field : Chemistry, Physical chemistry and Chemical Engineering, Material science, Mechanics and Fluids,

Subfield:

ParisTech School: ESPCI Paris - PSL
Research team: Macromolecular Chemistry and Design (CDM)
Research lab: C3M - Chimie Moléculaire, Macromoléculaire, et Matériaux
Lab location: Paris
Lab website:https://www.mmc.espci.fr

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Van Zee Nathan nathan.van-zee@espci.psl.eu
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: The vast majority of plastics collected through recycling programs is not actually reused. It is generally too expensive to transform most recovered plastic waste into useful materials, a consequence of the limitations of current reprocessing technology. Of particular note, polyethylene (PE) and polypropylene (PP) are the most widely used and unfortunately among the least reused polymers today. The main reasons for this situation is that objects made from polyolefins are difficult to rapidly sort and that untreated blends of PE and PP have poor mechanical properties. PE and PP are incompatible polymers and thus exhibit minimal interfacial adhesion between each other. All reported methods for enhancing the properties of such blends are limited by difficult disadvantages, such as high costs, non-scalable processing requirements, and mediocre mechanical properties. In this proposed thesis project, we aim to overcome these issues by exploring unconventional strategies to generate strong interfacial adhesion between incompatible polyolefins while utilizing processing conditions that are relevant to the plastics industry. The key innovation will be focused on engineering the crystallization at the polymer-polymer interface by exploiting novel supramolecular

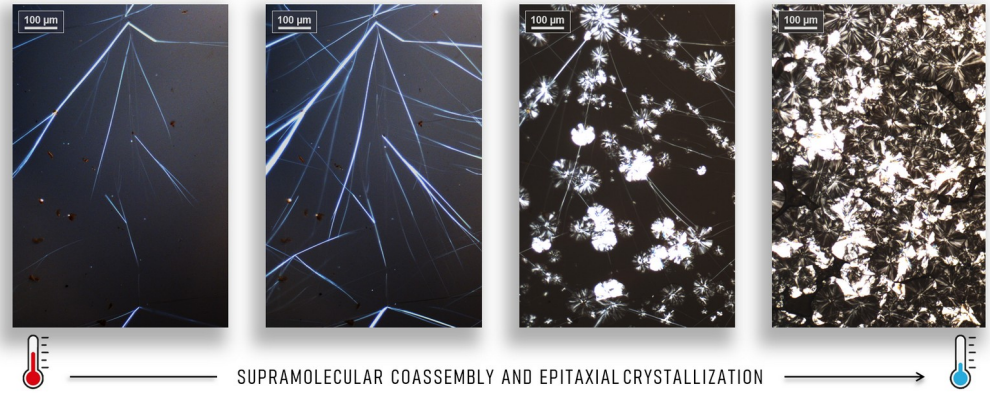
coassemblies. This project will be interdisciplinary, as it will encompass supramolecular chemistry, organic synthesis, physical chemistry, and materials science. We hope to develop new fundamental design principles for enhancing interfacial adhesion on the basis of the creative application of X-ray scattering, microscopic, rheological, calorimetric, and mechanical testing techniques.

Required background of the student: The student should ideally have a background in supramolecular chemistry. Additional experience in organic synthesis, physical chemistry, and/or materials science is highly advantageous.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. G. J. M. Formon, S. Storch, A. Y.-G. Delplanque, B. Bresson, N. J. Van Zee, R. Nicolaÿ. Overcoming the Tradeoff Between Processability and Mechanical Performance of Elastomeric Vitrimers. Adv. Funct. Mater. 2023, 2306065.
2. N. J. Van Zee*, M. F. J. Mabesoone, B. Adelizzi, A. R. A. Palmans, E. W. Meijer. Biasing the screw-sense in supramolecular co-assemblies featuring multiple helical states. J. Am. Chem. Soc. 2020. 142, 20191.
3. M. Maaz, A. Riba-Bremerch, C. Guibert, N. J. Van Zee, R. Nicolaÿ. Synthesis of polyethylene vitrimers in a single step: Consequences of graft structure, reactive extrusion conditions, and processing aids. Macromolecules 2021, 54, 2213.
4. B. Adelizzi, N. J. Van Zee, L. N. J. de Windt, A. R. A. Palmans, E. W. Meijer. The future of supramolecular copolymers unveiled by reflecting on covalent copolymerization. J. Am. Chem. Soc. 2019, 141, 6110–6121.
5. N. J. Van Zee, B. Adelizzi, M. F. J. Mabesoone, X. Meng, A. Aloi, R. H. Zha, M. Lutz, I. A. W. Filot, A. R. A. Palmans, E. W. Meijer. Potential enthalpic energy of water in oils exploited to control supramolecular structure. Nature 2018, 558, 100–103.

Illustrations :



SUPRAMOLECULAR COASSEMBLY AND EPITAXIAL CRYSTALLIZATION

TITLE: VIRTUAL HISTOLOGICAL STAINING AND TRIDIMENSIONAL RECONSTRUCTION FOR AUTOMATED ANALYSIS OF TISSUE BIOPSY FOLLOWING DYNAMIC FULL-FIELD OPTICAL COHERENCE TOMOGRAPHY IMAGING

Topic number : ***2023_044***

Field : Information and Communication Science and Technology, Life and Health Science and Technology,

Subfield: 3D modelling for medical images

ParisTech School: Arts et Métiers
Research team: XR team https://institutchalon.ensam.eu/
Research lab: LISPEN - Laboratoire d'ingénierie des systèmes physiques et numériques
Lab location: Chalon-sur-Saône
Lab website:http://lispen.ensam.eu/

Contact point for this topic: Arts et Métiers

Advisor 1: LOU Ruding ruding.lou@ensam.eu
Advisor 2: MALDINEY Thomas thomas.maldiney@ch-chalon71.fr
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Urgent recourse to biopsy analysis might be of precious help to obtain rapid histopathological diagnosis and guide the management of several medical conditions in critically ill patients. Among them, brain biopsy to explore neurological diseases of unknown etiology (1), lung biopsy for undiagnosed acute respiratory failure (2), skin biopsy for severe dermatological manifestations (3), and kidney biopsy for acute kidney injury of unknown origin (4) are some of the most relevant indications in critical care. Unfortunately, conventional biopsy analysis requires multiple preparation steps, including fixation, sectioning, and staining, all responsible for a significant delay between histopathological diagnosis and initiation of the appropriate treatment (5).
To circumvent such limitation, interferometric tissue examination with dynamic full-field optical coherence tomography (D-FF-OCT) has recently demonstrated its ability to avoid these biopsy processing steps and return high-definition imaging of various tissues in less than an hour, in comparison to conventional biopsy analysis that requires a minimum of

24 hours and often up to several days of analysis (6–8). Yet, D-FF-OCT biopsy analysis necessitate a novel and specific training for pathologists, as well as critical adaptation of both interpretative reading and diagnostic criteria, to achieve proper and high-quality histopathological diagnosis. All these constraints ultimately increase the risk of delaying the delivery of definitive results, thus lead to the consideration of an automated analysis and interpretation of these D-FF-OCT data. If convolutional neural network was already reported to transform wide-field autofluorescence images into images that are equivalent to those obtained with conventional histological stainings (9), there is to our knowledge no previous report of the potential application of such method to the analysis of D-FF-OCT images.

The aim of this PhD thesis is to design a deep-learning-based automated method such as convolutional neural network to transform D-FF-OCT images into biopsy images that match those obtained following conventional histological stainings with the aim to significantly improve both time and diagnosis accuracy of D-FF-OCT-based analysis of tissue biopsy. In addition, the project intends to investigate the potential of tridimensional reconstruction of tissue models from these D-FF-OCT-images, as well as interactive and intuitive virtual reality tissue cartography, to help pathologists visualizing the underlying histopathological lesions (10–12).

The present PhD thesis will exploit a collection of D-FF-OCT images acquired throughout the course of ongoing multicenter and prospective clinical trials dedicated to the evaluation of D-FF-OCT performances for the analysis of both kidney (NCT05728216, https://clinicaltrials.gov/study/NCT05728216) as well as skin biopsies (NCT05608902, https://clinicaltrials.gov/study/NCT05608902).

References:

1. Mathon B, Favreau M, Degos V, Amelot A, Le Joncour A, Weiss N, et al. Brain Biopsy for Neurological Diseases of Unknown Etiology in Critically Ill Patients: Feasibility, Safety, and Diagnostic Yield. Critical Care Medicine. 2022 Jun;50(6):e516–25.

2. Philipponnet C, Cassagnes L, Pereira B, Kemeny JL, Devouassoux-Shisheboran M, Lautrette A, et al. Diagnostic yield and therapeutic impact of open lung biopsy in the critically ill patient. Palaniyar N, editor. PLoS ONE. 2018 May 25;13(5):e0196795.

3. Badia M, Casanova JM, Serviá L, Montserrat N, Codina J, Trujillano J. Dermatological Manifestations in the Intensive Care Unit: A Practical Approach. Critical Care Research and Practice. 2020 Sep 26;2020:1–12.

4. Augusto JF, Lassalle V, Fillatre P, Perrotin D, Meziani F, Schenck-Dhif M, et al. Safety and diagnostic yield of renal biopsy in the intensive care unit. Intensive Care Med. 2012 Nov;38(11):1826–33.

5. Rastogi V. Artefacts: A Diagnostic Dilemma – A Review. JCDR . 2013 ; Available from: http://www.jcdr.net/article_fulltext.asp?issn=0973-709x&year=2013&volume=7&issue=10&page=2408&issn=0973-709x&id=3541

6. Maldiney T, Greigert H, Martin L, Benoit E, Creuzot-Garcher C, Gabrielle PH, et al. Full-field optical coherence tomography for the diagnosis of giant cell arteritis. Meckel S, editor. PLoS ONE. 2020 Aug 31;15(8):e0234165.
7. Quénéhervé L, Olivier R, Gora MJ, Bossard C, Mosnier JF, Benoit a la Guillaume E, et al. Full-field optical coherence tomography: novel imaging technique for extemporaneous high-resolution analysis of mucosal architecture in human gut biopsies. Gut. 2021 Jan;70(1):6–8.
8. Maldiney T, Garcia-Hermoso D, Sitterlé E, Chassot JM, Thouvenin O, Boccara C, et al. Dynamic full-field optical coherence tomography for live-cell imaging and growth-phase monitoring in Aspergillus fumigatus. Front Cell Infect Microbiol. 2023 Jul 12;13:1183340.
9. Rivenson Y, Wang H, Wei Z, De Haan K, Zhang Y, Wu Y, et al. Virtual histological staining of unlabelled tissue-autofluorescence images via deep learning. Nat Biomed Eng. 2019 Mar 4;3(6):466–77.
10. Said SAE, Atta HMA, Hassanien AE. Interactive soft tissue modelling for virtual reality surgery simulation and planning. IJCAET. 2017;9(1):38.

11. Liimatainen K, Latonen L, Valkonen M, Kartasalo K, Ruusuvuori P. Virtual reality for 3D histology: multi-scale visualization of organs with interactive feature exploration. BMC Cancer. 2021 Dec;21(1):1133.
12. Lu L, Wang H, Liu P, Liu R, Zhang J, Xie Y, et al. Applications of Mixed Reality Technology in Orthopedics Surgery: A Pilot Study. Front Bioeng Biotechnol. 2022 Feb 22;10:740507.

Required background of the student: Computer sciences, Image processing, Virtual Reality

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Maldiney T, Garcia-Hermoso D, Sitterlé E, Chassot JM, Thouvenin O, Boccara C, et al. Dynamic full-field optical coherence tomography for live-cell imaging and growth-phase monitoring in Aspergillus fumigatus. Front Cell Infect Microbiol. 2023 Jul 12;13:1183340.
2. Maldiney T, Greigert H, Martin L, Benoit E, Creuzot-Garcher C, Gabrielle PH, et al. Full-field optical coherence tomography for the diagnosis of giant cell arteritis. Meckel S, editor. PLoS ONE. 2020 Aug 31;15(8):e0234165.
3. Liimatainen, K., Latonen, L., Valkonen, M. et al. Virtual reality for 3D histology: multi-scale visualization of organs with interactive feature exploration. BMC Cancer 21, 1133 (2021). https://doi.org/10.1186/s12885-021-08542-9
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Illustrations :

ParisTech

Arts et Métiers Sciences et Technologies

PHD RESEARCH TOPIC FOR APPLYING THE CSC SCHOLARSHIP

Field: ***Information and Communication Sciences and Technologies***

Subfield: Computer sciences, Medical Imaging, Image processing, Virtual Reality.

Title: Virtual histological staining and tridimensional reconstruction for automated analysis of tissue biopsy following dynamic full-field optical coherence tomography imaging

Doctoral college: Arts et Métiers Sciences et Technologies

Advisor(s) Name:	Dr. Ruding Lou	Dr. Thomas Maldiney
Advisor(s) Email:	ruding.lou@ensam.eu	thomas.maldiney@ch-chalon71.fr
Research group/Lab:	LISPEN	LIPNESS
Lab location:	Chalon-sur-Saône	Dijon
(Lab website):	http://lispen.ensam.eu/	http://inserm-u1231.u-bourgogne.fr/

Short description of possible research topics for a PhD:

Urgent recourse to biopsy analysis might be of precious help to obtain rapid histopathological diagnosis and guide the management of several medical conditions in critically ill patients. Among them, brain biopsy to explore neurological diseases of unknown etiology (1), lung biopsy for undiagnosed acute respiratory failure (2), skin biopsy for severe dermatological manifestations (3), and kidney biopsy for acute kidney injury of unknown origin (4) are some of the most relevant indications in critical care. Unfortunately, conventional biopsy analysis requires multiple preparation steps, including fixation, sectioning, and staining, all responsible for a significant delay between histopathological diagnosis and initiation of the appropriate treatment (5).

To circumvent such limitation, interferometric tissue examination with dynamic full-field optical coherence tomography (D-FF-OCT) has recently demonstrated its ability to avoid these biopsy processing steps and return high-definition imaging of various tissues in less than an hour, in comparison to conventional biopsy analysis that requires a minimum of 24 hours and often up to several days of analysis (6–8). Yet, D-FF-OCT biopsy analysis necessitate a novel and specific training for pathologists, as well as critical adaptation of both interpretative reading and diagnostic criteria, to achieve proper and high-quality histopathological diagnosis. All these constraints ultimately increase the risk of delaying the delivery of definitive results, thus lead to the consideration of an automated analysis and interpretation of these D-FF-OCT data. If convolutional neural network was already reported to transform wide-field autofluorescence images into images that are equivalent to those obtained with conventional histological stainings (9), there is to our knowledge no previous report of the potential application of such method to the analysis of D-FF-OCT images.

The aim of this PhD thesis is to design a deep-learning-based automated method such as convolutional neural network to transform D-FF-OCT images into biopsy images that match those obtained following conventional histological stainings with the aim to significantly improve both time and diagnosis accuracy of D-FF-OCT-based analysis of tissue biopsy. In addition, the project intends to investigate the potential of tridimensional reconstruction of tissue models from these D-FF-OCT-images, as well as interactive and intuitive virtual reality tissue cartography, to help pathologists visualizing the underlying histopathological lesions (10–12).

The present PhD thesis will exploit a collection of D-FF-OCT images acquired throughout the course of ongoing multicenter and prospective clinical trials dedicated to the evaluation of D-FF-OCT performances for the analysis of both kidney (NCT05728216, https://clinicaltrials.gov/study/NCT05728216) as well as skin biopsies (NCT05608902, https://clinicaltrials.gov/study/NCT05608902).

References:

1. Mathon B, Favreau M, Degos V, Amelot A, Le Joncour A, Weiss N, et al. Brain Biopsy for Neurological Diseases of Unknown Etiology in Critically Ill Patients: Feasibility, Safety, and Diagnostic Yield. Critical Care Medicine. 2022 Jun;50(6):e516–25.

2. Philipponnet C, Cassagnes L, Pereira B, Kemeny JL, Devouassoux-Shisheboran M, Lautrette A, et al. Diagnostic yield and therapeutic impact of open lung biopsy in the critically ill patient. Palaniyar N, editor. PLoS ONE. 2018 May 25;13(5):e0196795.

3. Badia M, Casanova JM, Serviá L, Montserrat N, Codina J, Trujillano J. Dermatological Manifestations in the Intensive Care Unit: A Practical Approach. Critical Care Research and Practice. 2020 Sep 26;2020:1–12.

4. Augusto JF, Lassalle V, Fillatre P, Perrotin D, Meziani F, Schenck-Dhif M, et al. Safety and diagnostic yield of renal biopsy in the intensive care unit. Intensive Care Med. 2012 Nov;38(11):1826–33.

5. Rastogi V. Artefacts: A Diagnostic Dilemma – A Review. JCDR [Internet]. 2013 [cited 2023 Sep 17]; Available from: http://www.jcdr.net/article_fulltext.asp?issn=0973-709x&year=2013&volume=7&issue=10&page=2408&issn=0973-709x&id=3541

6. Maldiney T, Greigert H, Martin L, Benoit E, Creuzot-Garcher C, Gabrielle PH, et al. Full-field optical coherence tomography for the diagnosis of giant cell arteritis. Meckel S, editor. PLoS ONE. 2020 Aug 31;15(8):e0234165.

7. Quénéhervé L, Olivier R, Gora MJ, Bossard C, Mosnier JF, Benoit a la Guillaume E, et al. Full-field optical coherence tomography: novel imaging technique for extemporaneous high-resolution analysis of mucosal architecture in human gut biopsies. Gut. 2021 Jan;70(1):6–8.

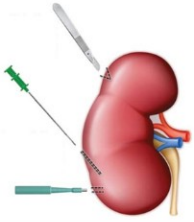
8. Maldiney T, Garcia-Hermoso D, Sitterlé E, Chassot JM, Thouvenin O, Boccara C, et al. Dynamic full-field optical coherence tomography for live-cell imaging and growth-phase monitoring in Aspergillus fumigatus. Front Cell Infect Microbiol. 2023 Jul 12;13:1183340.

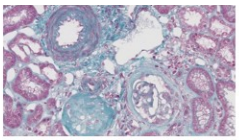
9. Rivenson Y, Wang H, Wei Z, De Haan K, Zhang Y, Wu Y, et al. Virtual histological staining of unlabelled tissue-autofluorescence images via deep learning. Nat Biomed Eng. 2019 Mar 4;3(6):466–77.

10. Said SAE, Atta HMA, Hassanien AE. Interactive soft tissue modelling for virtual reality surgery simulation and planning. IJCAET. 2017;9(1):38.

11. Liimatainen K, Latonen L, Valkonen M, Kartasalo K, Ruusuvuori P. Virtual reality for 3D histology: multi-scale visualization of organs with interactive feature exploration. BMC Cancer. 2021 Dec;21(1):1133.

12. Lu L, Wang H, Liu P, Liu R, Zhang J, Xie Y, et al. Applications of Mixed Reality Technology in Orthopedics Surgery: A Pilot Study. Front Bioeng Biotechnol. 2022 Feb 22;10:740507.

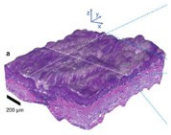




Standard analysis

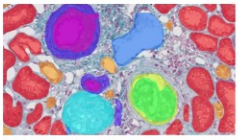


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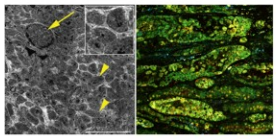


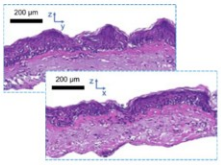
3D virtual model

Artificial Intelligence (AI)



AI





ParisTech

ESPCI PARIS PSL

TITLE: HIGH-THROUGHPUT SELECTION AND COMPUTATIONAL DESIGN OF CATALYTIC ANTIBODIES

Topic number : ***2023_045***

Field : Chemistry, Physical chemistry and Chemical Engineering, Life and Health Science and Technology, Physics, Optics

Subfield:

ParisTech School: ESPCI Paris - PSL
Research team:
Research lab: GULLIVER - Voyages expérimentaux et théoriques en matière molle
Lab location: Paris
Lab website:https://www.gulliver.espci.fr/

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Rivoire Olivier olivier.rivoire@espci.fr
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: A major challenge is to design on-demand catalysts for arbitrary reactions with specificities and efficiencies comparable to natural enzymes. Catalytic antibodies, obtained by selecting antibody repertoires for high affinity to transition state analogues, can potentially meet this challenge. The feasibility and generality of the approach was extensively demonstrated in the 1980s and 1990s, but while catalytic antibodies thus obtained could be as specific as enzymes, they were always inferior in catalytic efficiency. This conclusion, however, rests on indirect selection methods and low-throughput characterization of catalytic efficiencies. Today, more powerful experimental techniques are available to directly select large protein libraries for in vitro catalytic activity. Coupled with high-throughput sequencing, these methods provide large datasets that can be analyzed by machine learning to guide the generation of interesting variants. We propose to apply these recent experimental and computational approaches to reassess the potential of catalytic antibodies.

Required background of the student: A strong quantitative background is required, for example in physics, chemistry or engineering. Previous experience in molecular biology, microfluidics or machine learning would be a plus, but is not necessary if the candidate is willing to learn these techniques.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Hilvert, D. Critical analysis of antibody catalysis. Ann. Rev. Biochem. 69, 751–793 (2000)

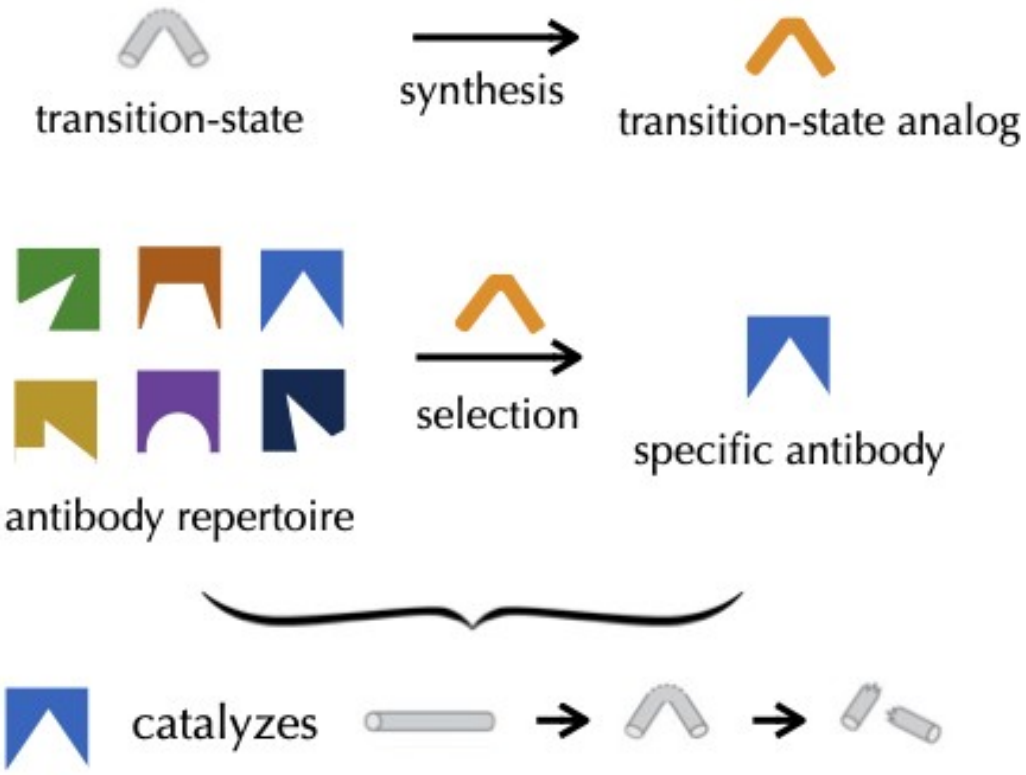
2. Agresti, J. J. et al. Ultrahigh-throughput screening in drop-based microfluidics for directed evolution. Proc. Nat.l Acad. Sc. 107, 4004–4009 (2010)

3. Kinney, J. B. & McCandlish, D. M. Massively parallel assays and quantitative sequence–function
relationships. Ann. Rev. Gen. Human Gen. 20, 99–127 (2019)

4. Schulz, S. et al. Parameters and determinants of responses to selection in antibody libraries. PLoS
Comp. Biol. 17, e1008751 (2021)

5.

Illustrations :


transition-state
synthesis
transition-state analog
selection
specific antibody
antibody repertoire
catalyzes

PhD Proposal – High-throughput Selection and Computational Design of Catalytic Antibodies
Supervisors: Olivier Rivoire & Clément Nizak
Laboratory: Gulliver, ESPCI, PSL Université, Paris, France

High-throughput Selection and Computational Design of Catalytic Antibodies

A major challenge is to design on-demand catalysts for arbitrary reactions with specificities and efficiencies comparable to natural enzymes. Catalytic antibodies, obtained by selecting antibody repertoires for high affinity to transition state analogues, can potentially meet this challenge. The feasibility and generality of the approach was extensively demonstrated in the 1980s and 1990s, but while catalytic antibodies thus obtained could be as specific as enzymes, they were always inferior in catalytic efficiency. This conclusion, however, rests on indirect selection methods and low-throughput characterization of catalytic efficiencies. Today, more powerful experimental techniques are available to directly select large protein libraries for in vitro catalytic activity. Coupled with high-throughput sequencing, these methods provide large datasets that can be analyzed by machine learning to guide the generation of interesting variants. We propose to apply these recent experimental and computational approaches to reassess the potential of catalytic antibodies.

Context

The development of efficient catalysts is central in several industrial sectors, for instance for the synthesis of pharmaceutical compounds and the development of renewable energies. Enzymes produced by living organisms currently surpass in efficiency and selectivity chemical catalysts used in the industry, but are limited to a subset of biological reactions under particular conditions. A major challenge is to design on-demand catalysts that rival natural enzymes. The field of **catalytic antibodies (CA)**[1, 2] is an approach to this challenge based on two elements:

(i) Our theoretical understanding of chemical processes: Theoretically, a chemical reaction amounts to crossing a barrier of free energy separating the desired product(s) from the available reactant(s)/substrate(s). The unstable state on top of the barrier defines the **transition state (TS)** and, according to Pauling's principle, enzymes lower the barrier by stabilizing it relative to the substrate(s) [3]. The TS is a theoretical construct, but chemists can design **transition-state analogs (TSA)** that mimic the geometry and charges of the TS, but are stable [4].

(ii) Our ability to harness the power of immune systems to obtain proteins (**antibodies**) that can bind any desired molecular target [5].

These two elements have led to the proposal that CAs can be obtained by immunization of animals with TSAs [6]. The first experimental demonstration in the mid-eighties [7, 8] led to a flurry of works that have confirmed the generality of the approach by producing CAs for ~ 100 different chemical reactions, including reactions for which no natural enzyme is known, such as the Diels-Alder reaction [9]. As shown in Fig. 1A for a case with some of the best data [10], discrimination for TSAs (measured by the ratio K_m/K_i of the dissociation constant to the substrate K_m over the dissociation constant to the TSA K_i) correlates well, as theoretically predicted, with catalytic activity (measured by the ratio $k_{\rm cat}/k_{\rm uncat}$ of the catalytic rate $k_{\rm cat}$ over uncatalyzed reaction rate $k_{\rm uncat}$). However, while CAs can rival with enzymes in substrate specificity they have much lower catalytic efficiency [11]: rate enhancements $k_{\rm cat}/k_{\rm uncat}$ are of order 10^6-10^{12} and up to 10^{17} for natural enzymes, but typically in the range 10^2-10^5 for CAs [12].

The origins of this limitation have been extensively debated [11, 12, 13]. One issue may be that immunization selects for affinity to the TS rather than discrimination between the TS and substrate. As illustrated in Fig. 1B, affinity for the TSA (K_i) shows no systematic correlation with catalytic activity ($k_{\rm cat}$). Another issue may be the imperfect similarity of TSAs to TSs. In fact, even if the TSA is a good analog to the TS, there are many ways in which an antibody can bind to it, not all expected to be as relevant for catalysis. Other hypotheses include the limited selection cycles to which CAs have been subject compared to natural enzymes, or an intrinsic limitation of antibody molecules, but no definitive conclusion has been

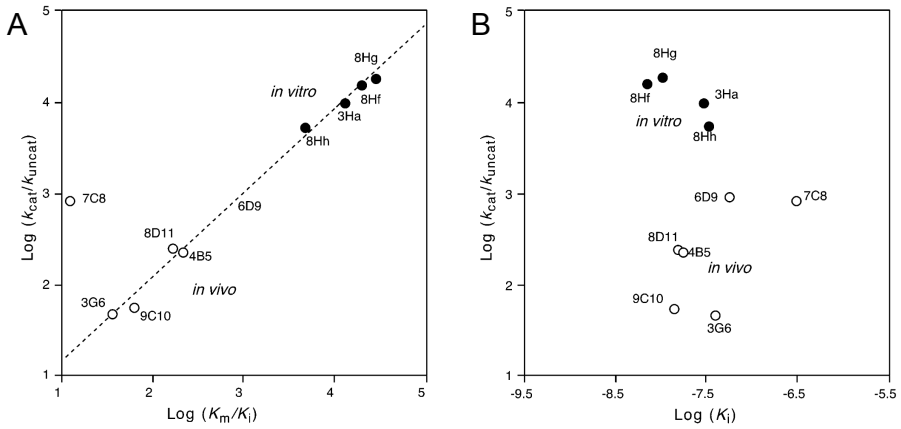


Figure 1: Data illustrating the current state of the art [10] – **A.** CAs obtained by *vivo* immunization against a TSA (in white) and further *in vitro* DE (in black), show the expected correlation between discrimination for the TSA (K_m/K_i) and catalytic efficiency ($k_{\rm cat}/K_m$). One CA (7C8), however, appears subject to different constraints. We propose to redraw such a graph with $\sim 10^5$ points to get a far more comprehensive appreciation of the potential of CAs. **B.** CAs were obtained by selecting for their affinity to the TSA (low K_i) but this graphs shows this selective pressure to be only poorly correlated to catalytic efficiency (large $k_{\rm cat}$). We propose to directly select for discrimination (large K_m/K_i) and for catalytic activity (large $k_{\rm cat}$) using, respectively, new computational and experimental approaches.

reached [12, 13]. In the absence of breakthrough, the field has been nearly abandoned by chemists since the early 2000s, although immunologists have since identified numerous natural antibodies with catalytic activities [14], including proteolytic activities that were thought to be too challenging for antibodies [15].

Since the mid-1990s, a purely empirical approach has come to dominate protein engineering, **directed evolution (DE)**, which mimics Darwinian evolution by experimentally subjecting a population of proteins to cycles of diversification (mutations) and selection [16]. Invented contemporarily to CAs, antibody phage display consists in the *in vitro* selection of antibody libraries for binders against a specified antigen, thus reproducing the evolutionary process by which antibodies are produced by immune systems [17]. Phage display was shown to advantageously replace [18] or complement [19] *in vivo* immunization. Fig. 1A thus illustrates how CAs that have additionally undergone *in vitro* selection by phage display (in black) can improve on those obtained by *in vivo* immunization (in white) [10]. Selecting directly for catalytic activity has also been the object of many efforts, but is experimentally challenging. All methods developed in the context of CAs have been indirect, and therefore subject to confounding factors [12, 13]. General methods for the direct, *in vitro* selection for catalytic activity at a large scale have only more recently been developed [20]. The currently most powerful technology, droplet microfluidics, uses custom microfluidic devices to express enzymes genes individually in pL-droplets, assay expressed enzymes for activity with an optical (absorbance or fluorescence) readout, and sort droplets according to measured activity, typically at kHz-rates, thus allowing the screening of 10^5 enzyme genes/day [21, 22].

DE is very powerful but, as currently implemented, has important limitations: it necessitates a good starting point [23], i.e., a protein that already has detectable activity, and is time and labor intensive, which limits the number of cycles that can be performed. DE is therefore well suited to the engineering of existing enzymes, but not to the generation of radically new enzymes. DE can, however, be coupled to other approaches. For instance, the computational design of proteins based on the principle of free energy minimization can produce novel enzymes with modest but sufficient activity to serve as starting points for DE [24]. Of notice, however, the novel enzymes obtained in this way most often work by mechanisms that differ from the mechanism that the computational method sought to implement [25].

In the past years, **machine learning (ML)** has been revolutionizing protein design [26]. Generative models based on databases of natural sequences have for instance been applied to produce enzymes with new sequences [27]. Yet, as the models are trained on natural enzymes, the activity of the generated enzymes do not depart from existing activities. ML can also be coupled to DE through **high-throughput**

sequencing (HTS), which provides data on the composition of a population of proteins at the scale of 10^5-10^7 sequences [28]. ML can turn this data into quantitative models predicting biophysical properties from sequences [29].

The two supervisors, **Olivier Rivoire (OR) and Clément Nizak (CN)**, have been at the forefront of these recent developments:

(1) OR and CN have demonstrated how the *in vitro* selection of antibody libraries by phage display can be combined with HTS to produce large, quantitative datasets amenable to insightful statistical analyses [30, 31]. Most recently, we have shown how to combine HTS datasets from selections against multiple targets to infer generative ML models of antibody binding and specificity [32]. With these models, we computationally designed and experimentally validated antibodies that strongly bind one target and much less another target. With this approach, antibodies can be selected for discrimination rather than for affinity.

(2) During his time at ESPCI (2013-2021), CN has gained a strong expertise in droplet microfluidics [33, 34, 35]. In the past few years, CN and OR have been working together to combine this technology with HTS to probe the mutational landscape of an enzyme (trypsin), and map substrate-specificity of hundreds of enzymes in the same family (serine proteases) [36].

(3) For the past 15 years, OR has been collaborating with the Ranganathan lab at the University of Chicago to analyze protein sequences with statistical models [37, 38], with a recent focus on generative ML models [39]. OR has also developed theoretical models addressing the principles of catalysis [40, 41].

Objectives

We propose to combine our experimental and computational expertises for a renewed understanding of the potential of CAs. As illustrated in Fig. 1, previous studies were limited to the characterization of very few antibodies, making any general conclusion tentative. We propose to produce graphs analogous to Fig. 1 with significantly improved sampling, both quantitatively and qualitatively, by characterizing $> 10^4$ CAs obtained by direct selection for discrimination and for catalytic activity.

To this end, we will take well-characterized CAs, with known affinities for their substrate and TSA, that catalyze the hydrolysis of esters [42, 43, 44, 10], which is the most common type of reaction catalyzed by reported CAs [11]. Esterase activity of these CAs can be measured optically (see below), allowing direct selection for catalytic activity using droplet microfluidics [45, 46]. We will randomly mutagenize these CAs in their antigen-binding site to generate libraries of size 10^5-10^7, as in our previous work [30]. We will then select these libraries by two methods:

(i) High-throughput *in vitro* selection for affinity to the TSA, as well as to non-hydrolyzable analogs of the substrate, using phage display as in Fig. 1 with additional HTS readout as in our previous works [30, 31]. Using our most recent results [32], we will infer from HTS data from these experiments a ML model that can generate antibodies with specific binding profile, namely strong affinity for the TSA (low K_i) and weak affinities for the substrate (high K_m).

(ii) High-throughput *in vitro* selection for catalysis using a droplet microfluidics set-up that we have already developed for another project [36]. Esterase activity of CAs will be monitored optically either by absorbance reporting product concentration [42, 44], or fluorescence reporting the inhibition of in vitro expression of a fluorescent protein by the product, which is the antibiotic chloramphenicol [10, 47]. Here again, we will analyze the results by HTS to infer kinetic constants, in particular, k_{cat}.

These two approaches will not only produce candidate CAs at a large scale but, as importantly, in new ways that have not been so far implemented, but should be more conducive to the production of efficient CAs, namely (i) direct selection for TSA discrimination (as opposed to previous selection for TSA affinity) and (ii) direct selection for catalysis (as opposed to previous indirect approaches). The catalytic efficiency of antibodies produced by method (i) will be assayed by method (ii) and, reciprocally, the binding profile of antibodies produced by method (ii) will be assayed by method (i). This will reveal at the scale of 10^4-10^5 different antibodies the quantitative relationship between the binding profile and the catalytic efficiency of CAs. Using our computational ML methods to design antibodies with desired binding profile [32], we will then be able to turn this knowledge into a method to generate computationally more efficient CAs.

Laboratory and supervisors

The project will take place in the Gulliver laboratory at ESPCI-Paris and will be co-supervised by two CNRS researchers:

Olivier Rivoire (OR), is a theoretical physicist with a background in statistical physics and > 15 years of experience in analyzing protein sequences [37, 38, 39] and modeling protein biophysics [40, 41], with a particular interest in enzymatic catalysis.

Clément Nizak (CN) has a strong expertise in phage display, droplet microfluidics and high-throughput sequencing, which will be used in the project. His current work involves combining droplet microfluidics and HTS to map mutational landscapes of enzymes.

More information about the laboratory and the team can be found at:
`https://www.gulliver.espci.fr/`
`http://statbio.net/`

Required background of the student

A strong quantitative background is required, for example in physics, chemistry or engineering. Previous experience in molecular biology, microfluidics or machine learning would be a plus, but is not necessary if the candidate is willing to learn these techniques.

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ParisTech

ESPCI PARIS PSL

TITLE: EXPLORING NEW CONCEPTS FOR POLYMER UPCYCLING USING SOLVENT-FREE PROCESSES

Topic number : ***2023_046***

Field : Chemistry, Physical chemistry and Chemical Engineering, ,

Subfield:

ParisTech School: ESPCI Paris - PSL
Research team:
Research lab: C3M - Chimie Moléculaire, Macromoléculaire, et Matériaux
Lab location: Paris
Lab website:https://www.mmc.espci.fr/spip.php?rubrique79

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Nicolaÿ Renaud renaud.nicolay@espci.psl.eu
Advisor 2: Van Zee Nathan nathan.van-zee@espci.psl.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: The world production of plastics reached 391 Mt in 2021. Between 2009 and 2019, an additional 138 Mt was produced, representing an increase of more than 50% in ten years. Thus, the recycling and upcycling of plastic is increasingly critical, from an economic, environmental and societal point of view.
With this project we are aiming to develop new solvent-free approaches to upcycle polymers and polymer blends into materials with improved chemical and mechanical properties. This PhD will build on recent studies from our team to produce vitrimers via reactive processing. The unique properties of vitrimers make them recognized as a new class of polymeric materials from the fundamental point a view, and in practical terms, as a new way of controlling and solving problems of processing, chemical resistance, mechanical strength and recycling of plastic materials.

Required background of the student: The candidate should hold a master degree in organic chemistry or polymer science, and have keen interest in molecular chemistry, polymer functionalization, polymer characterization (chemical, physico-chemical and mechanical).

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. M. Röttger, T. Domenech, R. Van der Weegen, A. Breuillac, R. Nicolaÿ, L. Leibler “High-performance vitrimers from commodity thermoplastics through dioxaborolane metathesis” Science 2017, 356, 62. DOI: 10.1126/science.aah5281
2. G. J. M. Formon, S. Storch, A. Y.-G. Delplanque, B. Bresson, N. J. Van Zee, R. Nicolaÿ “Overcoming the Tradeoff Between Processability and Mechanical Performance of Elastomeric Vitrimers” Adv. Funct. Mater. 2023, 2306065. DOI: 10.1002/adfm.202306065
3. N. J. Van Zee, R. Nicolaÿ “Vitrimers: Permanently crosslinked polymers with dynamic network topology” Prog. Polym. Sci. 2020, 101233. DOI: 10.1016/j.progpolymsci.2020.101233
4. M. Maaz, A. Riba-Bremerch, C. Guibert, N. J. Van Zee, R. Nicolaÿ “Synthesis of Polyethylene Vitrimers in a Single Step: Consequences of Graft Structure, Reactive Extrusion Conditions, and Processing Aids” Macromolecules 2021, 54, 2213. DOI: 10.1021/acs.macromol.0c02649
5. A. Breuillac, A. Kassalias, R. Nicolaÿ “Polybutadiene Vitrimers Based on Dioxaborolane Chemistry and Dual Networks with Static and Dynamic Cross-links” Macromolecules 2019, 52, 7102. DOI: 10.1021/acs.macromol.9b01288

Illustrations :

ParisTech

ESPCI PARIS PSL

TITLE: BIOPHYSICS OF THE CELL CORTEX

Topic number : ***2023_047***

Field : Physics, Optics, Life and Health Science and Technology,

Subfield:

ParisTech School: ESPCI Paris - PSL
Research team:
Research lab: PMMH - Physique et mécanique des Milieux Hétérogènes
Lab location: Paris
Lab website:https://www.pmmh.espci.fr/-Home-

Contact point for this topic: ESPCI Paris - PSL

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Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: The actin cytoskeleton is a key player for mammalian cells mechanics and migration, as well as in the control of their shape. Of particular interest is the actin cortex, a dense thin layer of actin filaments and myosin motors associated to the plasma membrane. Animal cell's mechanics is believed to be largely prescribed by the properties of the cortex, but its precise contribution and the dependence on its rapid renewal and its active contraction is not fully understood. We recently developed a new technique, the "cell pincher", to directly probe the mechanics and dynamics of cell cortex using two mutually attracted magnetic microbeads. Our results revealed for the first time that actin cortex thickness in live cells present myosin II-dependent fluctuations around an average value of a couple of hundred nanometers. These fluctuations are very large with amplitude comparable to the average cortex thickness (Laplaud et al Science Advances 2020). The same technique allows quantifying elastic and viscous properties by imposing transient forces on the cortex through the beads and measuring the resulting deformations. Our setups combine the cell-pincher with control of the adhesion state on micro-patterns, quantitative spinning disk microscopy, and a nano-indenter to measure whole-cell mechanics. Cell biology expertise is assured by a close collaboration with the group of Matthieu Piel in Institut Curie.

This context makes possible to determine the evolution of the thickness, the active fluctuations and the viscoelastic properties of the cortex when the cell undergoes changes in its morphology to enable different functions. These functions includes migration, where the cell's front and back acquire different properties, during adhesion, when the part in contact with the substrate is different from its apex, or during cell cycle, where the cell rounds before mitosis. Additionally, measuring independently the viscoelastic properties of the cortex and of the whole cell will help determine how the first dictates the second.

Required background of the student: We are looking for curious and enthusiastic candidates with a physical or biophysical background to join the team and tackle these ambitious questions. Prior experience with microscopy experiments, data analysis, cell culture and cell mechanics is a plus but is not required.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Valentin Laplaud et al. Pinching the cortex of live cells reveals thickness instabilities caused by myosin II motors.Sci. Adv.7,eabe3640(2021).DOI:10.1126/sciadv.abe3640

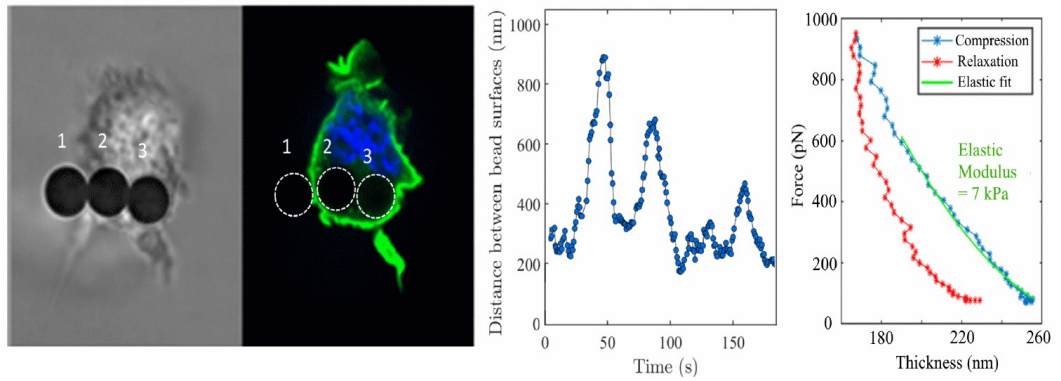
2. The distance between the plasma membrane and the actomyosin cortex acts as a nanogate to control cell surface mechanics
Sergio Lembo, Léanne Strauss, Dorothy Cheng, Joseph Vermeil, Marc Siggel, Mauricio Toro-Nahuelpan, Chii Jou Chan, Jan Kosinski, Matthieu Piel, Olivia Du Roure, Julien Heuvingh, Julia Mahamid, Alba Diz-Muñoz

bioRxiv 2023.01.31.526409; doi:
https://doi.org/10.1101/2023.01.31.526409

3. The membrane-actin linkers ezrin, radixin, and moesin are dispensable for macrophage migration and cortex mechanics
Perrine Verdys, Javier Rey Barroso, Joseph Vermeil, Martin Bergert, Thibaut Sanchez, Arnaud Métais, Thomas Mangeat, Elisabeth Bellard, Claire Bigot, Jean-Philippe Girard, Isabelle Maridonneau-Parini, Christel Vérollet, Frédéric Lagarrigue, Alba Diz-Muñoz, Julien Heuvingh, Matthieu Piel, Olivia Du Roure, Véronique Le Cabec, Sébastien Carréno, Renaud Poincloux
bioRxiv 2023.07.27.550674; doi:
https://doi.org/10.1101/2023.07.27.550674

4. Planade J, Belbahri R, Boiero Sanders M, Guillotin A, du Roure O, Michelot A, et al. (2019) Mechanical stiffness of reconstituted actin patches correlates tightly with endocytosis efficiency. PLoS Biol 17(10): e3000500. https://doi.org/10.1371/journal.pbio.3000500
5.

Illustrations :



ParisTech

TITLE: ASYMMETRIC CATALYSIS TOWARD BIORELEVANT ARCHITECTURALLY NOVEL NATURAL AND UNNATURAL PRODUCTS

Topic number : ***2023_048***

Field : Chemistry, Physical chemistry and Chemical Engineering, ,

Subfield: Chemistry

ParisTech School: Chimie ParisTech - PSL
Research team: CSB2D (Catalysis, Synthesis of Biomolecules and Sustainable Development)
Research lab: I-CLEHS - Institute of chemistry for life and health
Lab location: Paris
Lab website:https://iclehs.fr/

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Vidal Virginie virginie.vidal@chimieparistech.psl.eu
Advisor 2: Phansavath Phannarath phannarath.phansavath@chimieparistech.psl.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Our group develops new catalytic processes for the synthesis of natural products and targets of biological interest. We have been interested in the development of novel methods for synthetic efficiency and atom- and step-economical processes using transition metal-catalyzed reactions as they provide a direct and selective way toward the synthesis of highly valuable products. The research program will be dedicated to the development of asymmetric catalytic methods in a context of sustainable development for carbon-carbon and carbon-hydrogen bond forming reactions using asymmetric hydrogenation (AH) or asymmetric transfer hydrogenation reactions (ATH) through dynamic kinetic resolution (DKR) to target scaffolds of biorelevant molecules of medicinal interest. The PhD research program aims at developing new catalytic asymmetric approaches to address long-standing problems in the synthesis of chiral key intermediates to access natural products and pharmaceutical drugs.

Required background of the student: Experience in organic/organometallic synthesis

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. B. He, P. Phansavath, V. Ratovelomanana-Vidal. Org. Chem. Front. 2021, 8, 2504–2509

2. He, B.; Phansavath, P.; Ratovelomanana-Vidal, V. Org. Chem. Front. 2020, 7, 975

3. He, B.; Phansavath, P.; Ratovelomanana-Vidal, V. Org Lett 2020, 21, 3276

4. Zheng, L.-S.; Férard, C.; Phansavath, P.; Ratovelomanana-Vidal, V. Org Lett 2019, 21, 2998

5. Zheng, L.-S.; Férard, C.; Phansavath, P.; Ratovelomanana-Vidal, V. Chem. Commun. 2018, 54, 283

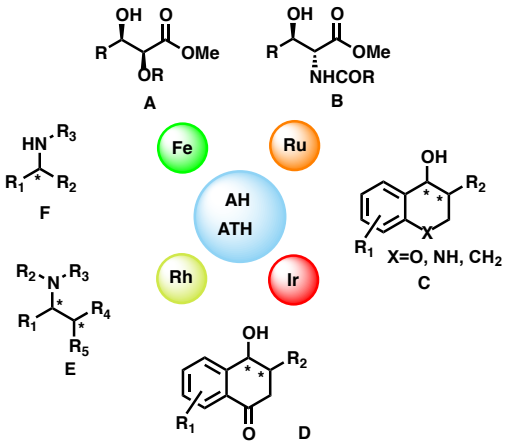
Illustrations :

Research Topic for the ParisTech/CSC PhD Program

Field : *Chemistry, Physical Chemistry and Chemical Engineering*
Subfield: *Organic Chemistry, Catalysis*
Title: *Asymmetric Catalysis toward BioRelevant Architecturally Novel Natural and Unnatural Products*
ParisTech School: *Chimie ParisTech*
Advisor(s) Name: *Virginie VIDAL, Phannarath PHANSAVATH*
Advisor(s) Email: *virginie.vidal@chimieparistech.psl.eu*
Research group/Lab: *i-CLeHS – CSB2D Team, Chimie ParisTech*
(Lab/Advisor website): *Institute of Chemistry for Life and Health Sciences (i-CLeHS), CSB2D Team - https://www.chimieparistech.psl.eu/*

Short description of possible research topics for a PhD:

Our group develops new catalytic processes for the synthesis of natural products and targets of biological interest. We have been interested in the development of novel methods for synthetic efficiency and atom- and step-economical processes using transition metal-catalyzed reactions as they provide a direct and selective way toward the synthesis of highly valuable products. The research program will be dedicated to the development of asymmetric catalytic methods in a context of sustainable development for carbon-carbon and carbon-hydrogen bond forming reactions using asymmetric hydrogenation (AH) or asymmetric transfer hydrogenation reactions (ATH)[1] through dynamic kinetic resolution (DKR)[2] to target scaffolds of biorelevant molecules of medicinal interest.[3] The PhD research program aims at developing new catalytic asymmetric approaches to address long-standing problems in the synthesis of chiral key intermediates such as **A**-**F** to access natural products and pharmaceutical drugs.



Required background of the student: experience in organic/organometallic synthesis.

Related recent publications of the group:

(1) "Asymmetric Hydrogenation and Transfer Hydrogenation", Wiley-VCH Verlag GmbH, Weinheim, Germany, P. Phansavath, V. Ratovelomanana-Vidal, Eds, p 1-384, **2021**. (2) (a) R. Molina-Betancourt, L. Bacheley, A. Karapetyan, G. Guillamot, P. Phansavath, V. Ratovelomanana-Vidal, *ChemCatChem* **2022**, *14*, e202200595. (b) R. Molina-Betancourt, P. Phansavath, V. Ratovelomanana-Vidal, *Molecules* **2022**, *27*, 995-1010. (c) R. Molina-Betancourt, P. Phansavath, V. Ratovelomanana-Vidal, *J. Org. Chem.* **2021**, *86*, 12054–12063. (d) R. Molina-Betancourt, Echeverria, P.-G.; Ayad, T.; Phansavath, P.; Ratovelomanana-Vidal, V. *Synthesis* **2021**, 53, 30-50. (e) R. Molina-Betancourt, P. Phansavath, V. Ratovelomanana-Vidal, *Org. Lett.* **2021**, *23,* 1621–1625. (f) B. He, P. Phansavath, V. Ratovelomanana-Vidal. *Org. Chem. Front*. **2021**, *8*, 2504–2509. (g) He, B.; Phansavath, P.; Ratovelomanana-Vidal, V. *Org. Chem. Front.* **2020**, *7*, 975. (h) He, B.; Phansavath, P.; Ratovelomanana-Vidal, V. *Org Lett* **2020**, *21*, 3276. (i) Zheng, L.-S.; Férard, C.; Phansavath, P.; Ratovelomanana-Vidal, V. *Org Lett* **2019**, *21*, 2998. (j) Zheng, L.-S.; Férard, C.; Phansavath, P.; Ratovelomanana-Vidal, V. *Chem. Commun*. **2018**, *54*, 283. (3) Ayad, T.; Phansavath, P.; Ratovelomanana-Vidal, V. *Chem. Rec*. **2016**, *16*, 2750.

ParisTech

Arts et Métiers Sciences et Technologies

TITLE: DAMAGE TOLERANT ACTIVE CONTROL

Topic number : ***2023_049***

Field : Mathematics and their applications, Material science, Mechanics and Fluids, Information and Communication Science and Technology

Subfield: Predictive maintenance and active control of vibration

ParisTech School: Arts et Métiers
Research team: DYSCO https://pimm.artsetmetiers.fr/equipes/dysco
Research lab: PIMM - Laboratoire Procédés et ingénierie en mécanique et matériaux
Lab location: Paris
Lab website:https://pimm.artsetmetiers.fr/

Contact point for this topic: Arts et Métiers

Advisor 1: Mechbal Nazih nazih.mechbal@ensam.eu
Advisor 2: Rebillat Marc marc.rebillat@ensam.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Predictive monitoring or conditioned based maintenance (CBM) is a real Holy Grail for both reliability experts and financiers. By monitoring the state of degradation of structures through various indicators, it enables maintenance actions to be spaced out on average, while paradoxically reducing the risk of failure. Structural Health Monitoring (SHM) has become a key issue in many sectors of innovative industry. It is based on so-called "intelligent" structures, consisting of a sensor and actuator network and a real-time acquisition and control architecture. In practice, sensors and actuators need to have as little impact as possible on the mass and mechanical properties of the structure to be controlled. These constraints have naturally prompted research into the use of piezoelectric materials. Once instrumented, the structure must be capable of detecting, locating and quantifying damage. But is it capable of limiting its evolution? Was it capable of preventing or delaying its onset? The answer to these questions lies in the use of the same PZT elements for active spatial control, to reduce the vibratory stresses (in and around the damaged area) that could accelerate the propagation of damage or trigger others. This multimodal use of active elements opens the way to a number of theoretical and practical developments. It is helping to

accelerate the industrial deployment of SHM systems, offering new possibilities for improving reliability and optimizing maintenance. Damage Tolerant Active Control (DTAC) is a young field of research . It focuses on the development of integrated approaches to reduce vibration while monitoring structural integrity, identifying possible damage, and reconfiguring the control law. The first function of a DTAC system is to detect and localize damage and to provide the possibility of containing the evolution of the damage by spatially configuring the control law to favor rejection around the damaged zone over the rest of the structure (see illustrations). A DTAC system thus offers the possibility of improving the resilience of the structure. At present, very few works address this multimodality in the use of active elements for structural monitoring. The Indeed, DTAC aims to properly formalize the problem of vibration attenuation with a view to improving the operational lifetime of a structure, by tackling several scientific hurdles:

• Stability. Various disturbance rejection strategies have been proposed, requiring theoretical formalization of the conditions for stability and interaction with the SHM module (active or passive approach). Most SHM approaches are so-called "open-loop" approaches. So how can they be used in a closed-loop context?

• Placement. Another point concerns the study of observability and spatial controllability for the optimal placement of active elements in view of a multimodal approach (SHM and CA) and the extension of robust estimation theory to take account of the "spatial" dimension.

• Active control and fatigue. Repeated exposure to the vibratory stresses generated by the DTAC system can lead to an accelerated ageing of the structure, affecting its durability and thus hindering its use. How can we optimize the impact of vibrations generated by the control system on fatigue and therefore on the structure's operational life?

• Validation. Numerical and experimental validation is required. Experimental validation requires special devices for implementing SHM systems based on acoustic waves and reconfigurable control laws, requiring real-time measurement of vibration wave propagation.

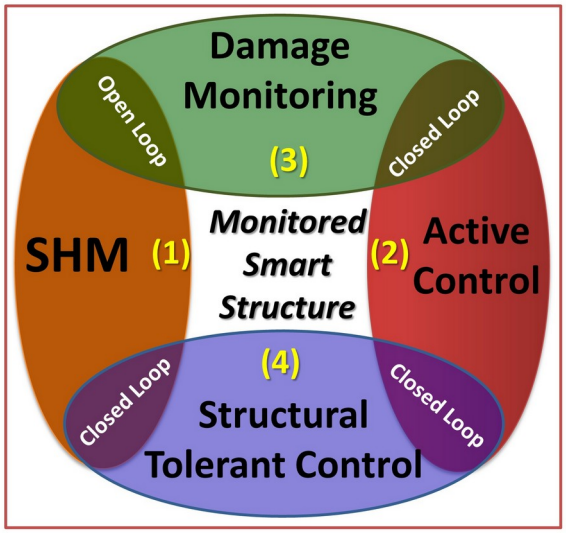
On the basis of the initial work carried out, the aim of this thesis is to propose one or more DTAC systems enabling the above questions to be answered. Starting with a specific case study and use case, the aim is to develop an SHM system whose frequency spectrum lies outside the bandwidth of the control law (Lamb wave-based methods, for example), coupled with active control laws designed to attenuate vibrations spatially (in specific - damaged - zones of the structure) while minimizing the fatigue induced by their actions.

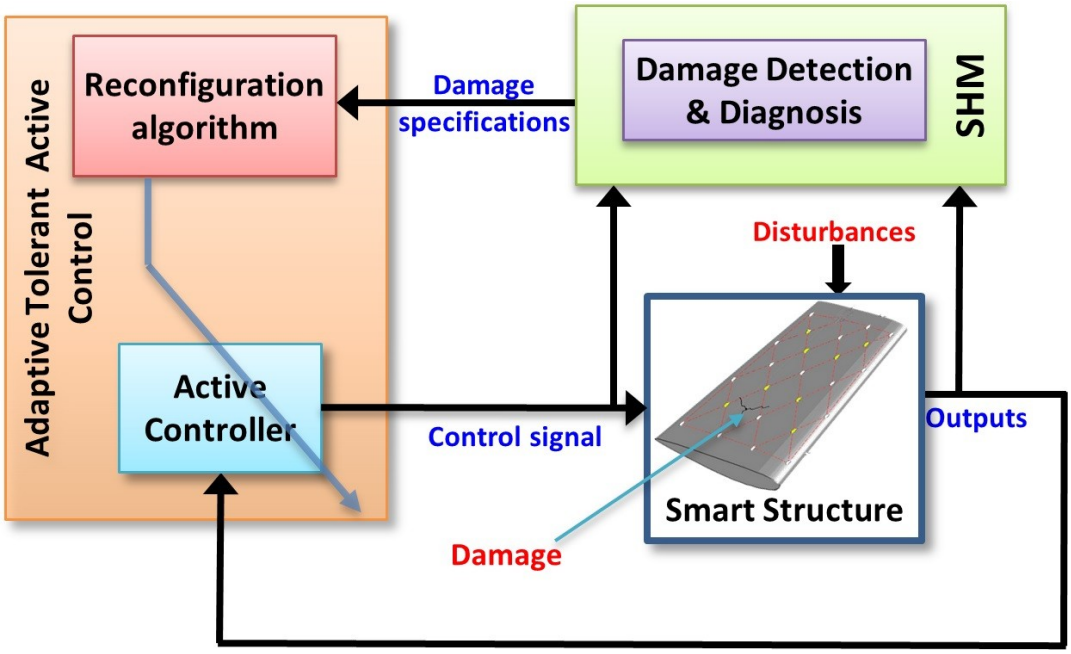
Required background of the student: Structural dynamics, Control Theory

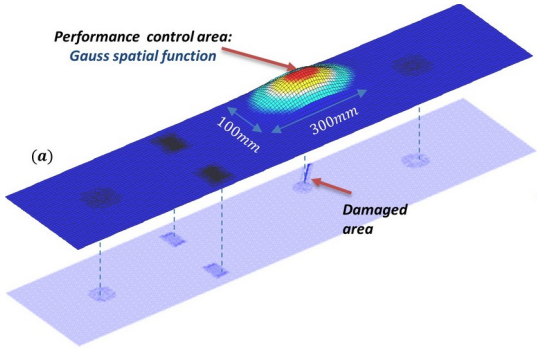
A list of 5 (max.) representative publications of the group: (Related to the research topic)

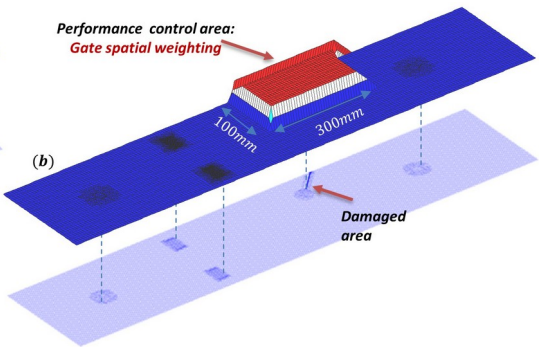
1. N. Mechbal et E. Nobrega, «Spatial H∞ Approach to Damage Tolerant Active Control,» Structural Control and Health Monitoring, vol. 22, n° %19, p. 1148–1172, 2015a.
2. H. Genari, N. Mechbal, G. Coffignal et E. Nóbrega, «A Reconfigurable Damage-Tolerant Controller Based on a Modal Double-Loop Framework,» Mechanical Systems and Signal Processing, n° %1 88, pp. 334-353, 2017.
3. H. Genari, N. Mechbal, G. Coffignal et E. Nóbrega, «Damage-Tolerant Active Control Using a Modal H∞ Norm-Based Methodology,» Journal of Control Engineering Practice, n° %160, pp. 76-86, 2017.
4. N. Mechbal et E. Nobrega, «Damage Tolerant Actice Control: Concept and State of Arts,» chez 8th IFAC Symposium on Fault Detection, Supervision and Safety of Technical Processes (SAFEPROCESS), Mexico, 2012
5. M. Rébillat and N. Mechbal, "Damage localization in geometrically complex aeronautic structures using canonical polyadic decomposition of Lamb wave difference signal tensors" SHM Journal, 2019 10.1177/1475921719843453

Illustrations :


Damage
Monitoring
(3)
Open Loop
Closed Loop
SHM (1)
Monitored
Smart
Structure
(2) Active
Control
(4)
Closed Loop
Closed Loop
Structural
Tolerant Control


Adaptive Tolerant Active Control
Reconfiguration algorithm
Damage specifications
Damage Detection & Diagnosis
SHM
Disturbances
Active Controller
Control signal
Outputs
Smart Structure
Damage


Performance control area:
Gauss spatial function
100mm
300mm
(a)
Damaged area


Performance control area:
Gate spatial weighting
100mm
300mm
(b)
Damaged area

TITLE: EFFICIENCY ENHANCEMENT OF THE COMPRESSED AIR ENERGY STORAGE (CAES) PROCESS

Topic number : ***2023_050***

Field : Energy, Processes, Physics, Optics, Environment Science and Technology, Sustainable Development, Geosciences

Subfield:

ParisTech School: Arts et Métiers
Research team:
Research lab: LIFSE - Laboratoire Ingénierie des Fluides Systèmes Energétiques
Lab location: Paris
Lab website:https://lifse.artsetmetiers.fr

Contact point for this topic: Arts et Métiers

Advisor 1: DELIGANT Michaël michael.deligant@ensam.eu
Advisor 2: PEREIRA Michaël michael.pereira@ensam.eu
Advisor 3: SPECKLIN Mathieu mathieu.specklin@ensam.eu
Advisor 4:

Short description of possible research topics for a PhD: The intermittent nature of renewable energy has pushed in recent years the need for efficient, reliable, low-cost and scalable energy storage technologies. Given its relatively high efficiency and its low environment impact, electro-mechanical storage appears as a good candidate. CAES (Compressed Air Energy Storage), which belongs to this family, is a promising technology but requires high compression ratio to be competitive.
This PhD research aims at analyzing the CAES process and at designing versatile and innovative technologies in order to improve its overall efficiency. CAES systems involve specific mechanical devices (pumping system, compression/expansion chamber, turbines, etc) and a strong coupling between different fields of applied physics, such as thermal management, turbo-machinery, multiphase flow, material science, etc. A global and systemic approach is thus necessary to carry out this research project.
The proposed research requires the combination of 3 different types of approaches. Firstly, as the thesis will be mainly experimental, the student will be prompted to carry out tests. An experimental rig capable of

achieving high-pressure ratio has already been set up in the LIFSE laboratory. Secondly, system modeling based on 0-D / 1-D lumped models will be developed in order to optimize the full system. Data obtained from experimental measurements will be used to validate the model. Finally, computational fluid dynamics is also considered to analyze local heat transfers occurring in CAES.
The thesis will be mainly experimental, but will also involve numerical modeling. An experimental rig capable of achieving high-pressure ratio has already been set up in the LIFSE laboratory. The student will therefore be prompted to carry out tests.

Required background of the student: Physics / Fluid Dynamics / Thermodynamics

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Deligant, M., Huebel, M., Djaname, T.-N., Ravelet, F., Specklin, M., Kebdani, M. Design and off-design system simulation of concentrated solar super-critical CO2 cycle integrating a radial turbine meanline model. Energy Reports (2022), https://doi.org/10.1016/j.egyr.2022.07.141.
2. Specklin, M., Deligant, M., Sapin, P., Solis, M., Wagner, M., Markides, C. N., Bakir, F., Numerical study of a liquid-piston compressor system for hydrogen applications, Applied Thermal Engineering, 216 (2022), pp118946, https://doi.org/10.1016/j.applthermaleng.2022.118946
3. M.A. AitChikh, I.Belaidi, S.Khelladi, J.Paris, M.Deligant}, and F.Bakir. Efficiency of bio- and socio-inspired optimization algorithms for axial turbomachinery design.
4.
5.

Illustrations :

RESEARCH TOPIC FOR THE PARISTECH / CSC PHD PROGRAM

Field: Physics, Energy, Processes
Subfield: Applied Physics

Title:

Efficiency enhancement of the compressed air energy storage (CAES) process

ParisTech School: Arts et Métiers - Institute of Technology

Advisor(s) Name: Dr. Mathieu Specklin
Dr. Michaël Pereira
Dr. Michaël Deligant

Advisor(s) Email:
mathieu.specklin@ensam.eu
michael.pereira@ensam.eu

Research group/Lab: Laboratory of Fluids Engineering and Energy Systems (LIFSE)
Lab location: 151 Boulevard de l'hôpital 75013 PARIS
Lab Website: https://lifse.artsetmetiers.fr

Short description of possible research topics for a PhD :

The intermittent nature of renewable energy has pushed in recent years the need for efficient, reliable, low-cost and scalable energy storage technologies. Given its relatively high efficiency and its low environment impact, electro-mechanical storage appears as a good candidate. CAES (Compressed Air Energy Storage), which belongs to this family, is a promising technology but requires high compression ratio to be competitive.

This PhD research aims at analyzing the CAES process and at designing versatile and innovative technologies in order to improve its overall efficiency. CAES systems involve specific mechanical devices (pumping system, compression/expansion chamber, turbines, etc) and a strong coupling between different fields of applied physics, such as thermal management, turbo-machinery, multiphase flow, material science, etc. A global and systemic approach is thus necessary to carry out this research project.

The proposed research requires the combination of 3 different types of approaches. Firstly, as the thesis will be mainly experimental, the student will be prompted to carry out tests. An experimental rig capable of achieving high-pressure ratio has already been set up in the LIFSE laboratory. Secondly, system modeling based on 0-D / 1-D lumped models will be developed in order to optimize the full system. Data obtained from experimental measurements will be used to validate the model. Finally, computational fluid dynamics is also considered to analyze local heat transfers occurring in CAES.
The thesis will be mainly experimental, but will also involve numerical modeling. An experimental rig capable of achieving high-pressure ratio has already been set up in the LIFSE laboratory. The student will therefore be prompted to carry out tests.

Required background of the student:
Physics / Fluid Dynamics / Thermodynamics

A list of representative publications of the group:

1. Specklin, M., Deligant, M., Porcheron, S., Wagner, M., Bakir, F., (2019) Experimental study and modelling of a high-pressure ratio liquid piston compressor, *14th International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics* Wicklow, Ireland

2. Deligant, M., Huebel, M., Djaname, T.-N., Ravelet, F., **Specklin, M.**, Kebdani, M. Design and off-design system simulation of concentrated solar super-critical CO2 cycle integrating a radial turbine meanline model. Energy Reports (2022), https://doi.org/10.1016/j.egyr.2022.07.141.

3. **Specklin, M.,** Deligant, M., Sapin, P., Solis, M., Wagner, M., Markides, C. N., Bakir, F., Numerical study of a liquid-piston compressor system for hydrogen applications, *Applied Thermal Engineering*, 216 (2022), pp118946, https://doi.org/10.1016/j.applthermaleng.2022.118946

4. M.A. AitChikh, I.Belaidi, S.Khelladi, J.Paris, M.Deligant}, and F.Bakir.
Efficiency of bio- and socio-inspired optimization algorithms for axial turbomachinery design.

5. Smoothed particle hydrodynamics: A consistent model for interfacial multiphase fluid flow simulations. Journal of Computational Physics}, 358:53—87, 2018.

6. Deligant, M., Sauret, E., Danel, Q., & Bakir, F. (2020). Performance assessment of a standard radial turbine as turbo expander for an adapted solar concentration ORC. *Renewable Energy*, *147*, 2833-2841.

7. Deligant, M., Danlos, A., Podevin, P., Clenci, A., & Guilain, S. (2017, October). Surge detection on an automotive turbocharger during transient phases. In *IOP Conf. Ser. Mat. Sci. Eng*. (No. 12082).

ParisTech

TITLE: PHD RESEARCH POSITION ON EFFICIENCY OF PERFORMIC ACID (AN OXIDIZING AGENT) ON ANTIBIOTIC RESISTANCE BACTERIA (ARB) AND GENES (ARGS)

Topic number : ***2023_051***

Field : Environment Science and Technology, Sustainable Development, Geosciences, ,

Subfield:

ParisTech School: Ecole des Ponts ParisTech
Research team:
Research lab: LEESU - Laboratoire Eau environnement et systèmes urbains
Lab location: Champs-sur-Marne
Lab website:https://www.leesu.fr/

Contact point for this topic: Ecole des Ponts ParisTech

Advisor 1: Bressy Adèle adele.bressy@enpc.fr
Advisor 2: Jusselme My Dung jusselme@u-pec.fr
Advisor 3: Moilleron Régis moilleron@u-pec.fr
Advisor 4:

Short description of possible research topics for a PhD: We are pleased to announce a unique opportunity for a highly motivated and dedicated PhD. researcher to join our research team in investigating the efficiency of Performic acid, an oxidizing agent, in combating Antibiotic-Resistant Bacteria (ARB) and Genes (ARG). This research position offers an exciting and challenging environment to make a meaningful contribution to the critical issue of antimicrobial resistance, which poses a significant threat to public health worldwide.
The rise of antimicrobial resistance is a global concern, and finding novel approaches to address it is of paramount importance. Performic acid, known for its strong oxidizing properties, has shown promise in reducing the presence of indicator microbial pathogens. However, its effectiveness against antimicrobial resistance remains unassessed.
This Ph.D. project aims to comprehensively investigate and understand the efficacy of Performic acid as a potential solution to combat antimicrobial resistance.

Required background of the student: microbial ecology, environmental monitoring, environmental chemistry, molecular biology, biotechnology,

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Tadesse BT et al. BMC Infectious Diseases 17, 616 (2017)
2. Gehr, R. et al. Water Sci. Technol. 59, 89–96 (2009)
3. Chhetri, R. K. et al. Sci. Total Environ. 677, 1–8 (2019)
4.
5.

Illustrations :

Object: **Proposition of thesis subject – ParisTech-CSC program**

Créteil, September 20, 2023

Part A/ Thesis subject:

Thesis title: Efficiency of performic acid (an oxidizing agent) on antibiotic resistance bacteria (ARB) and genes (ARGs)

State of the art and background of the research: Accelerated use of **biocides and antibiotics** leads to an increase in the concentration of organic micropolluants in urban wastewater, which promotes the development of **antimicrobial resistance (AMR)** including antibiotic resistant genes (ARGs) and bacteria (ARB). AMR has been recognized as a public health challenge in the 21st century. The 2017 World Health Organization (WHO) report identified the antibiotic resistant infections as the greatest risk to health with more than 700,000 deaths per year worldwide. Antimicrobial resistance will claim approximately to 10 million lives in Europe and about US$100 trillion in the US per year by 2050 (Tadesse et al., 2017). Different treatment methods have been attempted to eliminate ARB and ARGs from wastewater, such as chlorination and UV disinfection, ozonation, advanced oxidation processes and membrane bioreactors. However, AMR treatment efficiencies in real-scale WWTPs were observed at low degrees, only 2–3 logs of ARGs reduction, and in some cases, no reduction was registered. Besides, divergent responses to the treatment were also noticed, implying that only limited types of AMR are being inactivated (Paruch et al., 2021). Moreover, the increased usage of UV light doses, ozone and chlorine in order to maximize the efficiency raises concerns regarding the huge energy cost and excess hazardous chemical residues. Therefore, further optimization of operating conditions is required to obtain adequate AMR removal efficiency.

Recently, **performic acid** (PFA, HCO_3H), a **powerful oxidizing agent containing active oxygen (25.8%)**, has gained growing interest in **wastewater disinfection** thanks to its **high oxidizing property** (Chhetri et al., 2019). PFA disinfection mechanisms are based on the release of highly **reactive oxygen species** (**ROS**) (i.e., **hydroxyl ($HO^{\bullet}$) and peroxide ($O_2^{\bullet-}$)**) (Gehr et al., 2009) that can create the chemical reactions (*i.e.*, breaking of bonds) on biomolecules such as protein, enzyme, lipid and DNA leading to alter microbial metabolisms and damage the structure of microbial cells. PFA is put in use and has become the **most relevant disinfectant agent at the industrial level due to the low costs of implementation and operation** as well as **negligible formation of disinfection by-products (DBPs**) in comparison to chlorine-based disinfectants that drive more than 600 DBPs, among which there are many toxic compounds (Richardson et al., 2007). PFA has recently been studied at laboratory scale as disinfecting agent targeting **indicator microorganisms** and used at full-scale in European countries including Spain, Italy, Finland, Germany and France (Campo et al., 2020). Currently, the Norovirus project led by the Syndicate of Thau (France) is in progress in which Leesu is a partner. In this project, PFA was used to treat norovirus, the main cause of acute gastroenteritis in humans, in wastewater discharge. Apart from this project, very little research has been investigated on the effect of PFA against the inactivation

of antibiotic resistance genes (ARGs), emerging pathogenic such as viruses and bacteria. The project aims to study the mechanisms and effectiveness of the new technology disinfection using performic acid in reducing resistance genes and/or resistant bacteria.

Work goals: Based on the facts stated above, the research work in this thesis is designed with the three principal objectives: mapping the sources of ARB/ARGs and characterising the micropollutants emerging (i.e. biocides and antibiotics) **(*objective#1*),** investigating the disinfectant effectiveness of PFA on ARB/ARGs **(*objective#2*),** monitoring the dissemination of ARB/ARGs into the environment (***objective#3*).**

Methodology:

Objective#1: Mapping the sources of ARB/ARGs and characterising the micropollutants emerging. Wastewater samples from four wastewater treatment plants (WWTPs) belonging (*Seine aval, Seine amont, Seine centre,* and *Seine Grésillons*) in the Ile-de-France region will be collected for the two years (2024 and 2025) at four seasons including spring, summer, autumn and winter. Collected samples will be subjected for the screening of ARB and ARGs. The identification and quantification of ARB and ARGs will be conducting employing qPCR, RT-qPCR and Next-Generation Sequencing (NGS) technology. In parallel, non-target screening will be using to quantify micropollutants from antibiotic and biocide groups in these samples. Through bioinformatic analysis and computational modelling, we will evaluate the relationship between the biological and chemical datasets to predict the link between ARG/ARGs and micropollutants.

Objective#2: Investigating the effectiveness of PFA on ARB/ARGs. To study the disinfection efficiency of the PFA, both laboratory and *in situ* experiments will be conducted. For laboratory experiments, wastewater samples collected from four WWTPs that are detailed in *objective#1* will be used for disinfection experiment. In this approach, various parameters like temperature, pH, contact time, PFA concentration, and levels of ARB/ARGs will be taken into account. On the other hand, the sampling campaign will be designed to evaluate the PFA-disinfection efficiency under real conditions, at an industrial scale. Indeed, we will take advantage of the alternative disinfection method involving PFA-disinfection process that the SIAAP have been implemented in June 2023 at the *Seine amont* WWTP (Fig. 1). **ARB/ARGs** will be estimated at different time intervals before and after PFA injection during dry and wet weather conditions/periods using the same protocols that will be set up in *objective#1*.

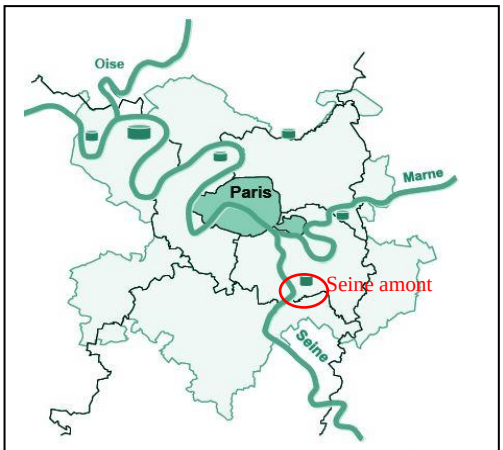


Figure 1: Seine water network and location of SIAAP-WWTPs

Objective#3: Monitoring the dissemination of ARB/ARGs into the environment. Samples from the Seine River watershed including (i) surface waters at different depths, ii) sediments and iii) shellfishes will be collected at the discharge point of treated wastewater

with PFA (*Seine amont* WWTP) which are detailed in *objectif#2* and along the Seine River upstream and downstream. We aim at evaluating the dissemination of ARB/ABGs into the environment through identification and quantification of the ARB and the fate of ARGs in these samples.

Expected outcomes

- This research proposal will provide a clear base line on the population and genomic diversity of ARB/ARGs present in the main WWTPs of Ile-de-France (France), which are the greatest French WWTPs. With this genetic information, we can tackle these biological risks in an efficient way.
- The results obtained in this present project will provide relevant information on an emerging disinfectant technology for wastewater treatment using PFA. The results concerning the evaluation of wastewater treatment performance toward the elimination of pathogenic agents will be of great interest to national and international plant managers.
- If the project confirms the efficacy of performic acid on ARG/ABGs, the technology will be made available in the market to treat urban wastewater, especially hospital wastewater that carries various pathogenic agents.
- Monitoring and post treatment assessment will be helpful in assuring the quality of treated wastewater and interpreting the effectiveness of PFA in the wastewater treatment process.
- It is also important to note that results obtained will be published in international "Open access" journals (e.g., *Nature, Water Research, Environmental Science & Technology*) which will benefit the entire community of researchers to industrial structures.

National/international and academic/industrial collaborations

The research theme of this thesis project is part of the OPUR program concerning the task "Identification and Quantification of Micropollutants" leaded by Adèle Bressy (researcher in Ecole des Ponts ParisTech) and part of the project WOx-Patox (*Wastewater treatment with an Oxidizing agent: efficiency on emerging Pathogens and antibiotic resistance genes (ARGs) and microbial ecoToxicology of the receiving water ecosystem*) leaded by My Dung Jusselme (Associate Professor, Leesu, UPEC) in collaboration with national/international and academy/industrial partners including (i) the chemists and biologists of Leesu, (ii) the Siaap (the greater Paris Sanitation Authority), (iii) the OSU-EFLUVE, an observatory of the sciences of the universe (ENPC ParisTech/UPEC) and Salles lab leading by Prof. Joana Falcao Salles (Faculty of Science and Engineering, University of Groningen). In this context, the PhD student will have an opportunity to broaden his/her horizons and create new relationships/networks.

Teaching and research competences acquired related to this thesis for later contribution in home country

The PhD student to be recruited for CSC program-2024 (return in 2027-2028) for this project will gain knowledge on the presence and quantity of ARGs/ARB in wastewater and their potential release to the environment. She/he will have access to new, powerful, eco-friendly and economical technologies for wastewater treatment. With this exposure, she/he can conduct research efficiently on wastewater treatment in China.

Regarding laboratory techniques, the PhD student will be trained in **numerous techniques in laboratory including molecular biology, bioinformatics and computational biology involved in the biological data analysis particularly DNA, RNA and protein sequences and software to analyze data such as R.** With this background in laboratory techniques, she/he can put at the service of teaching in the form of **practical work and applique in research in order meet the objective of the new projects**.

Time scale of the thesis project

The work schedule for this thesis project has been established in Fig. 2.

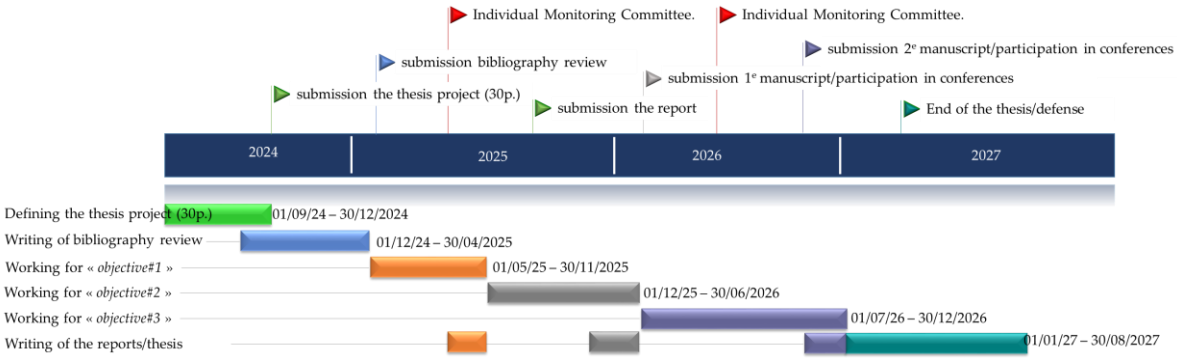


Figure 2: Time scale of the thesis project

Bibliographie

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Karpova, T. et al. Water Sci. Technol. 68, 2090–2096 (2013).
Chhetri, R. K. et al. Sci. Total Environ. 677, 1–8 (2019).
Gehr, R. et al. Water Sci. Technol. 59, 89–96 (2009).
Richardson, S. D. et al. Mutation Research - Reviews in Mutation Research (2007).
Campo, N. et al. Water Res. 169, 115227 (2020).

Part B/ Laboratory:

The PhD student to be recruited will carry out his/her thesis in the Water, Environment, and Urban System Laboratory (Leesu). Leesu is a multidisciplinary research group composed of researchers and teacher-researchers of the Ecole des Ponts ParisTech and the University Paris Est Creteil (UPEC) from different disciplines including microbiology, chemistry, ecotoxicology and hydrology. The research object of Leesu is urban water. In the global

context of increasing consumption of water and global changes such as climate, pollution, and urbanism, Leesu lab develops a multi- and interdisciplinary research, an applied and involved research in water sciences in order to protect groundwater and aquatic ecosystems and to optimize water resources. Numerous projects conducted at Leesu, in the past and currently, contribute to the management of urban water polluted by micropollutants and microbial pathogens. Leesu is the member of the "Comité Experts Priorisation (CEP)", of the Anses (Agence National de Sécurité Sanitaire Alimentaire) expert committee on water, and of the working group of the "Association Scientifique and Technique pour l'Eau and l'Environnement" (ASTEE). Leesu in collaboration with national and international, academy and operational partners leads or is involved in different research programs including OPUR (Observatory of Urban Pollutants in Île-de-France), PIREN-Seine (Interdisciplinary Research Program on water and the environment in the Seine basin), LABEX Urban Futures, MeSeine Innovation and in several research projects including LIFE ADSORB (European project), Phyte'Up (Winner of the Call for Expression of Interest, Grand Paris), MIDI (Microorganisms: actors governing the degradation of Diuron in sewage sludge during biological treatment, EC2CO project from CNRS). Leesu is currently conducting research projects to develop non-targeted screening tools for micropollutants and their degradation products by physical, chemical and biological reactions.

The present thesis project is integrated into the project WOx-PaTox (*Wastewater treatment with an Oxidizing agent: efficiency on emerging Pathogens and antibiotic resistance genes (ARGs) and microbial ecoToxicology of the receiving water ecosystem*). The Wox-PaTox project presents a multidisciplinary scientific endeavor at the crossroad between microbial ecology, microbial toxicology, environmental chemistry and social sciences to respond to the growing demand for water and the threats to water security by emerging contaminants (both biotic and abiotic) through discharges of treated wastewater. This is one of the three major research axes of the Leesu. The research theme of this thesis project is one of the three work packages of the Wox-PaTox project in which the efficiency of performic acid treatment on emerging pathogen and antibiotic resistance genes during wastewater treatment will be treated. Moreover, the research theme of the present thesis application is a continuity of three PhD projects in progress at Leesu lab. The first one was undertaken by Claudia Paijens (co-supervised by A. Bressy and R. Moilleron, in program OPUR); this study focused on characterizing the biocides present in urban water. The second one is carried out by Sadia Bagagnan (co-supervised by M.D. Jusselme and R. Moilleron, in the framework of the program MeSeine Innovation) and the research is concerned with the microbial ecotoxicology of the receiving environment (i.e., the Seine River) receiving the wastewater treated with PFA. The last one is being conducted by Christelle Nabintu-Kajoka (co-supervised by J. Le Roux, in the program OPUR), this work focuses on the generation of by-products during wastewater treatment by PFA (Fig. 3).

The Leesu lab disposes of all the necessary equipment in both analytical biology and chemistry platforms for the realization of this research project. For biological analysis, we have shaking culture incubators for microbial culture, Nanovue for DNA quantification, FastPrep and centrifuge for DNA extraction, thermocycler/real-time thermocycler (qPCR) and digital PCR for DNA amplification. Moreover, the Leesu dispose the equipment for

chemical analysis including liquid chromatography coupled to tandem mass spectrometry (UPLC-MS/MS), Ultra high performance liquid chromatography system coupled to a high resolution hybrid mass spectrometer (UPLC-IMS-Q-TOF), in close collaboration with the Prammics analytical platform (OSU Efluve), etc.

The cost for the realization of this thesis project will be covered by the MeSeine innovation (45k), Mocopée programs led and financed by Siaap (45k) and others such as Biocid@Home, OPUR.

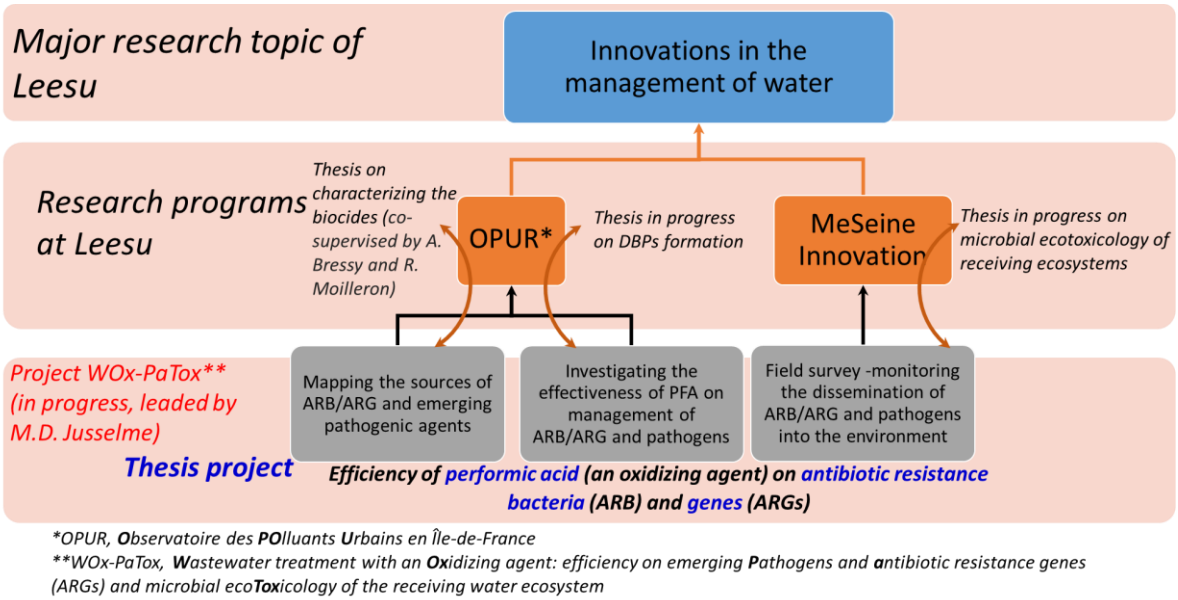


Figure 3: Scientific integration into Leesu

Part C/ Thesis supervisors

The PhD student to be recruited will carry out his/her thesis under the supervision of Adèle BRESSY (Researcher at ENPC), Régis Moilleron (Professor, Director of Leesu) and My Dung Jusselme (Associate Professor at UPEC),

- Dr. Adèle Bressy (https://www.leesu.fr/bressy-adele) is a researcher at ENPC, Leesu. She works on micropollutants, in particular biocides. Her research projects focus on (i) the non-targeted quantification of emerging micropollutants in urban waters, (ii) the investigation of the emission, the transfer and the fate of biocides in urban waters and (iii) the quantification of micropollutants in domestic waters and the search for ways to reduce the emission of these biocides to the environment. She is currently involved in several research programs and projects including ANR-Biocid@Home, BiociDust, BRIQUE, and OPUR program and has supervised 5 PhD thesis so far, and has published 30 scientific papers.
- Prof. Régis Moilleron (https://www.leesu.fr/moilleron-regis) is the director of Leesu since 2014. His researches have been focused on (i) the fate of organic micropollutants in urban environment and (ii) technology in treatment of wastewater. He is currently

involved in several research programs and projects including MeSeine innEAUvation program, OPUR program, Phyte'up project, MIDI project and others. He has supervised more than 20 PhD thesis so far, he has published more than 70 scientific papers.

- Associate Prof. My Dung Jusselme (https://www.leesu.fr/jusselme-my-dung) has joined leesu since 2019. Her research activities focus on (i) microbial ecotoxicology, (ii) interactions between microorganisms and micropollutants and (iii) new technology for disinfection of WWTP effluents using performic acid. She is currently leaded the project MIDI (**MI**croorganisms: actors governing the degradation of **DI**uron in sewage sludge during secondary treatment) funded by EC2CO funding. She participates in the program of MeSeine Innovation led by the SIAAP in which she is the co-supervisor of a Ph.D student working on spatiotemporal dynamics of microbial communities in the Seine River surface water. She has published 15 scientific papers.

Support career advancement. The PhD student, with the support of his/her supervisors, will have the opportunity to participate in teaching (64h equiv. TD per year) of statistical tools, structural biochemistry, microbiology and energy metabolism, intended for 1st and 2nd year undergraduate students. This will strengthen his ability to express himself in public, particularly in front of the students, and improve the quality of his teaching. With this baggage of experience, the PhD student will be able to participate effectively and quickly in teaching and scientific research once he/she returns to China. The PhD student will work under the supervision of 3 research/teacher-researchers from the Leesu lab and with researchers from other national/international laboratories. After returning to China, he/she will be able to continue working with them to develop the new research projects aimed at improving wastewater treatment technology, water quality and thus the health of the Chinese population.

ParisTech

ESPCI PARIS PSL

TITLE: COLLECTIVE ACTUATION OF A COLLOIDAL ELASTIC MATRIX

Topic number : ***2023_052***

Field : Material science, Mechanics and Fluids, Physics, Optics, Chemistry, Physical chemistry and Chemical Engineering

Subfield: Soft Matter, Active Matter

ParisTech School: ESPCI Paris - PSL
Research team: Olivier Dauchot
Research lab: GULLIVER - Voyages expérimentaux et théoriques en matière molle
Lab location: Paris
Lab website:https://www.gulliver.espci.fr

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Dauchot Olivier olivier.dauchot@espci.fr
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Collective actuation has been reported as a new kind of collective dynamics taking place when polar active particles are embedded in an elastic solid. It was first obtained experimentally and described theoretically for a system of centimetric active agents connected by springs. Shortly later, the same dynamics were reported in a biofilm of bacteria suspended in a viscoelastic matrix. This confirms that collective actuation is a generic phenomenon that can be observed in very different active systems, at very different scales. One can therefore envision the design and synthesis of self-actuable materials
The main goal of this project it to transpose the ingredients allowing for collective actuation from the centimetric scale to the micron scale, taking advantage of self-propelled Janus colloids. Here also one expects the strain field induced by the active forces to induce an elasto-active feedback, eventually leading to some form of collective actuation. Unveiling such a process would be a major breakthrough both in our understanding of living bodies and towards the design of new functional materials.

Required background of the student: A good knowledge of colloidal and interface science is mandatory. Being at ease with micro-manipulation, confocal microscopy is necessary too. Finally mentoring data- processing using Matlab or python is important.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Chemical Physics of Active Matter O. Dauchot, H. Löwen J. Chem. Phys. 151, 114901 (2019)

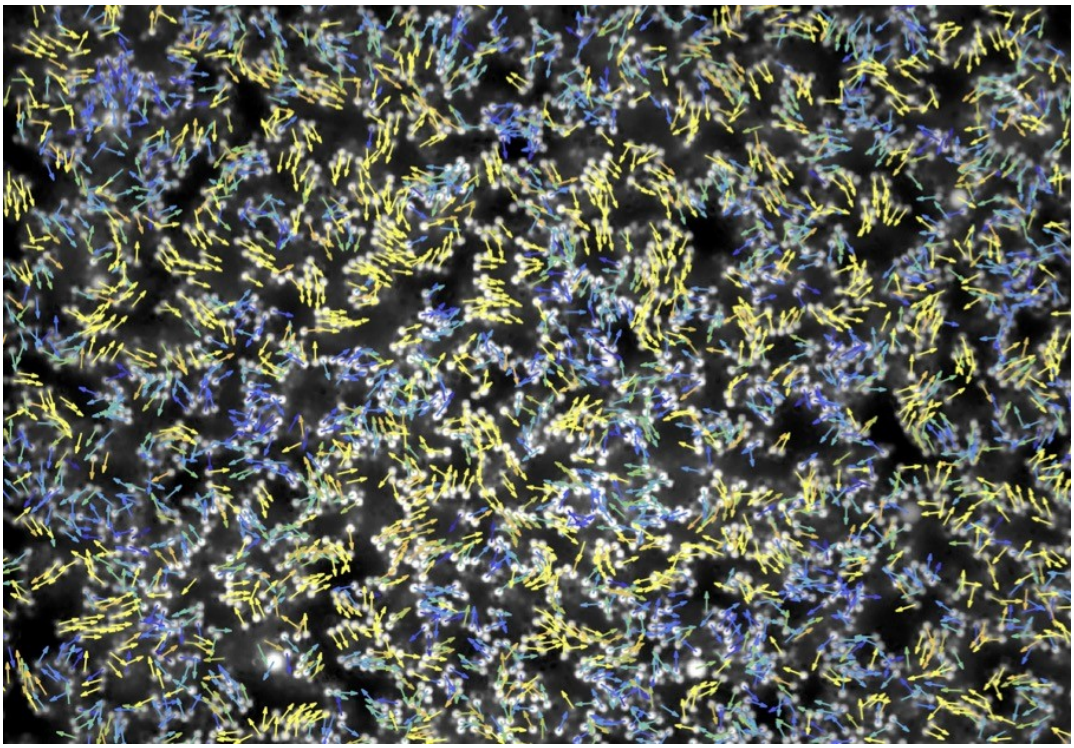
2. Interrupted Motility Induced Phase Separation in Aligning Active Colloids. Marjolein N. van der Linden, Lachlan C. Alexander, Dirk G. A. L. Aarts, Olivier Dauchot
Phys. Rev. Lett. 123, 098001 (2019)

3. Selective and collective actuation in active solids. Baconnier, Paul, Dor Shohat, C. Hernández López, Corentin Coulais, Vincent Démery, Gustavo Düring, and Olivier Dauchot. Nature Physics 18, no. 10 (2022): 1234-1239.

4. Reconfiguration, Interrupted Aging and Enhanced Dynamics of a Colloidal Gel using Photo-Switchable Active Doping. Wei, Mengshi, Matan Ben Zion, and Olivier Dauchot, Phys. Rev. Lett. 131, 018301

5. Active versus passive hard disks against a membrane: Mechanical pressure and instability. Junot, G., G. Briand, R. Ledesma-Alonso, and Olivier Dauchot. Physical review letters 119, no. 2 (2017): 028002.

Illustrations :



RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Physics, Optics
Subfield: (Chemistry, Colloidal Sciences) ***Title***: Collective actuation of a colloidal elastic matrix
ParisTech School: ESPCI Paris | PSL

Advisor(s) Name: Olivier Dauchot
Advisor(s) Email: olivier.dauchot@espci.fr
Research group/Lab: Gulliver Lab
Lab location: Paris
(Lab/Advisor website): https://www.gulliver.espci.fr

Short description of possible research topics for a PhD: (10-15 lines in English + optional figure)

Collective actuation has been reported as a new kind of collective dynamics taking place when polar active particles are embedded in an elastic solid. It was first obtained experimentally and described theoretically for a system of centimetric active agents connected by springs. Shortly later, the same dynamics were reported in a biofilm of bacteria suspended in a viscoelastic matrix. This confirms that collective actuation is a generic phenomenon that can be observed in very different active systems, at very different scales. One can therefore envision the design and synthesis of self-actuable materials

The main goal of this project it to transpose the ingredients allowing for collective actuation from the centimetric scale to the micron scale, taking advantage of self-propelled Janus colloids. Here also one expects the strain field induced by the active forces to induce an elasto-active feedback, eventually leading to some form of collective actuation. Unveiling such a process would be a major breakthrough both in our understanding of living bodies and towards the design of new functional materials.

Required background of the student: (What should be the main field of study of the applicant before applying?)

A good knowledge of colloidal and interface science is mandatory. Being at ease with micro-manipulation, confocal microscopy is necessary too. Finally mentoring data-processing using Matlab or python is important.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. *Chemical Physics of Active Matter* O. Dauchot, H. Löwen J. Chem. Phys. **151**, 114901 (2019)
2. *Interrupted Motility Induced Phase Separation in Aligning Active Colloids*. Marjolein N. van der Linden, Lachlan C. Alexander, Dirk G. A. L. Aarts, Olivier Dauchot Phys. Rev. Lett. 123, 098001 (2019)
3. *Selective and collective actuation in active solids*. Baconnier, Paul, Dor Shohat, C. Hernández López, Corentin Coulais, Vincent Démery, Gustavo Düring, and Olivier Dauchot. *Nature Physics* 18, no. 10 (2022): 1234-1239.

4. *Reconfiguration, Interrupted Aging and Enhanced Dynamics of a Colloidal Gel using Photo-Switchable Active Doping*. Wei, Mengshi, Matan Ben Zion, and Olivier Dauchot, Phys. Rev. Lett. 131, 018301
5. *Active versus passive hard disks against a membrane: Mechanical pressure and instability*. Junot, G., G. Briand, R. Ledesma-Alonso, and Olivier Dauchot. Physical review letters 119, no. 2 (2017): 028002.

ParisTech

TITLE: INVESTIGATING TWIP AND TRIP EFFECTS IN TI AND ZR METASTABLE ALLOYS VIA ADVANCED IN-SITU METHODS

Topic number : ***2023_053***

Field : Material science, Mechanics and Fluids, ,

Subfield:

ParisTech School: Chimie ParisTech - PSL
Research team: Métallurgie Structurale
Research lab: IRCP - Institut de Recherche de Chimie de Paris
Lab location: Paris
Lab website:https://www.ircp.cnrs.fr/la-recherche/equipe-ms/

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: SUN Fan fan.sun@chimieparistech.psl.eu
Advisor 2: Vermaut Philippe philippe.vermaut@chimieparistech.psl.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: The phenomena of Twinning Induced Plasticity (TWIP) and Transformation Induced Plasticity (TRIP) are pivotal in enhancing the mechanical properties of titanium and zirconium alloys. The metastable states of these alloys allow diverse twinning and martensitic transformations under external stress. The metastable phase is modulated by factors such as alloying elements, chemical composition, grain structure, and secondary phase precipitation. Recent studies in our lab have demonstrated the potential for simultaneous or independent activation of TWIP and TRIP effects in alloys, depending on their structural variances and beta phase stability. In this PhD research, a new method developed in our lab, termed Transformation Partition Mapping (TPM), will be employed to quantify mechanical twinning and martensitic transformation distributions, relative to grain orientation across alloys of differing metastabilities. Further insights on the TPM method can be found from our latest publications in the references. Additionally, advanced in-situ characterizations via Transmission Electron Microscopy (TEM) under tensile deformation will be conducted as a complementary method to in-situ Electron Backscatter Diffraction (EBSD) statistics. The objective of this research activities is to elucidate the fundamental mechanisms underlying 332-type twinning, beta-orthorhombic

martensitic transformation, secondary phases, and their interplay with conventional dislocation glide. This thesis, scheduled for a 48-month study of experimental investigation, will predominantly be conducted within the Métallurgie Structurale team at Chimie-Paristech.

Required background of the student: Master's degree in Material Science and Engineering or Metallic Materials
Background in electron microscopy and physical metallurgy
Proficient in English communication and writing
Competent in collaborative teamwork and project management

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. B. Qian, S.A. Mantri, S. Dasari, J. Zhang, L. Lilensten, F. Sun, P. Vermaut, R. Banerjee, F. Prima, Mechanisms underlying enhanced strength-ductility combinations in TRIP/TWIP Ti-12Mo alloy engineered via isothermal omega precipitation, Acta Mater. 245 (2023). https://doi.org/10.1016/j.actamat.2022.118619.
2. Tang, Junhui; Zorgati, Ahmed; Gaillard, Jean-Baptiste; Vermaut, Philippe; Prima, Frédéric; Sun, Twinning-induced plasticity (TWIP) effect in multi-phase metastable beta Zr-Nb alloys, J. Mater. Sci. Technol. 139 (2023) 120–125. https://doi.org/https://doi.org/10.1016/j.jmst.2022.07.062.
3. B. Qian, M. Yang, L. Lilensten, P. Vermaut, F. Sun, F. Prima, In-situ observations of a hierarchical twinning–detwinning process in stress-induced α ″ -martensite of Ti-12Mo alloy, Mater. Res. Lett. 10 (2022) 45–51. https://doi.org/10.1080/21663831.2021.2013967.
4. B. Qian, L. Lilensten, J. Zhang, M. Yang, F. Sun, P. Vermaut, F. Prima, On the transformation pathway in TRIP/TWIP Ti–12Mo alloy, Mater. Sci. Eng. A. 822 (2021) 141672. https://doi.org/10.1016/j.msea.2021.141672.
5. J. Zhang, Y. Fu, Y. Wu, B. Qian, Z. Chen, A. Inoue, Y. Wu, Y. Yang, F. Sun, J. Li, F. Prima, Hierarchical {332}<113> twinning in a metastable β Ti-alloy showing tolerance to strain localization, Mater. Res. Lett. 8 (2020) 247–253. https://doi.org/10.1080/21663831.2020.1745920.

Illustrations :

ParisTech

TITLE: INVESTIGATIONS OF MECHANICAL PROPERTIES AND CORROSION DYNAMICS OF ZN-BASED BIORESORBABLE ALLOYS

Topic number : ***2023_054***

Field : Material science, Mechanics and Fluids, Life and Health Science and Technology, Chemistry, Physical chemistry and Chemical Engineering

Subfield:

ParisTech School: Chimie ParisTech - PSL
Research team: Métallurgie Structurale
Research lab: IRCP - Institut de Recherche de Chimie de Paris
Lab location: Paris
Lab website:https://www.ircp.cnrs.fr/la-recherche/equipe-ms/

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: SUN Fan fan.sun@chimieparistech.psl.eu
Advisor 2: Ogle Kevin kevin.ogle@chimieparistech.psl.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Bioresorbable alloys are emerging materials designed for temporary load-bearing biomedical implants in cardiovascular and orthopedic applications. Zinc (Zn), an essential human nutrient, exhibits biodegradability within tissue environments. In comparison to magnesium (Mg) and iron (Fe), Zn manifests a better balance of dissolution rate and mechanical strength, making it as a viable base metal for alloy innovation. Through alloying with diverse elements, a significant enhancement in alloy strength can be achieved, primarily attributed to the emergence of secondary phases. Consequently, the evolution of phase constitution and alloy composition impacts corrosion behavior. Hence, a comprehensive understanding of the alloying effects on both mechanical attributes and corrosion dynamics is essential to design an alloy with balanced performance. This project will combine fundamental research activities in physical metallurgy and surface electrochemistry to define the correlations among chemical composition, microstructure, mechanical properties, and corrosion dynamics. The investigation will contain a wide range of experimental methodologies including thermomechanical treatments, mechanical testing, thermodynamic

assessments, microstructural analyses (utilizing SEM/TEM/EDX/EBSD), and electrochemical measurements (such as potentiodynamic polarization, impedance measurement, Atomic Emission Spectroelectrochemistry, etc.). Scheduled over a 48-month timeframe, the bulk of the research will develop at IRCP of Chimie-Paristech, in close association with Sorbonne University, Beihang University and Peking University.

Required background of the student:

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Y. Zhang, C. Roux, A. Rouchaud, A. Meddahi-pell, V. Gueguen, C. Mangeney, F. Sun, G. Pavon-djavid, Y. Luo, Recent advances in Fe-based bioresorbable stents : Materials design and biosafety, Bioact. Mater. 31 (2024) 333–354. https://doi.org/10.1016/j.bioactmat.2023.07.024.
2. H. Yang, B. Jia, Z. Zhang, X. Qu, G. Li, W. Lin, D. Zhu, K. Dai, Y. Zheng, Alloying design of biodegradable zinc as promising bone implants for load-bearing applications, Nat. Commun. 11 (2020) 1–16. https://doi.org/10.1038/s41467-019-14153-7.
3. K. Ogle, Atomic emission spectroelectrochemistry: Real-time rate measurements of dissolution, corrosion, and passivation, Corrosion. 75 (2019) 1398–1419. https://doi.org/10.5006/3336.
4.
5.

Illustrations :

ParisTech

Arts et Métiers

TITLE: ZONAL STRUCTURES AND TURBULENCE IN BURNING PLASMAS

Topic number : ***2023_055***

Field : Physics, Optics, ,

Subfield:

ParisTech School: Arts et Métiers
Research team:
Research lab: LIFSE - Laboratoire Ingénierie des Fluides Systèmes Energétiques
Lab location: Paris
Lab website:https://www.devinci.fr/research-center/

Contact point for this topic: Arts et Métiers

Advisor 1: Biancalani Alessandro alessandro.biancalani@devinci.fr
Advisor 2: Gurcan Ozgur ozgur.gurcan@lpp.polytechnique.fr
Advisor 3:
Advisor 4:

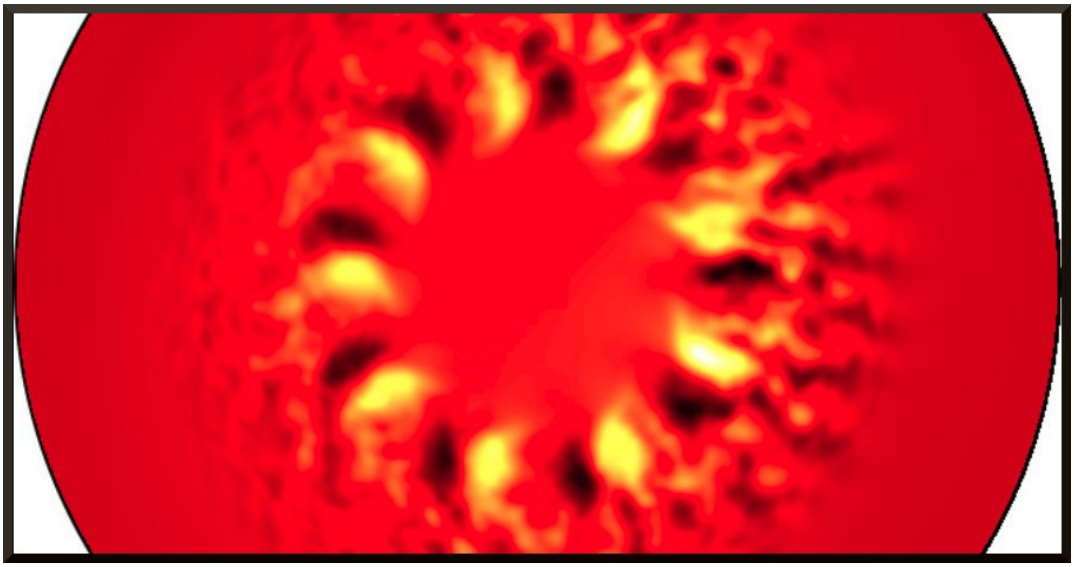
Short description of possible research topics for a PhD: Magnetized plasmas are an example of problems rich of nonlinear physics, similarly to neutral fluids, but more complex, due to the possible coexistence of different kinds of waves and instabilities. Understanding the formation and saturation of turbulence in magnetic confinement plasma experiments is a necessary step towards the achievement of a comprehensive theoretical model. Micro-turbulence in tokamak plasmas generates meso-scale zonal, i.e. axisymmetric, structures (ZSs), analogously to the formation of zonal bands parallel to the equator in planets like Jupiter. In this project, the PhD candidate will study the nonlinear interaction of turbulence and ZSs by means of numerical simulations with different theoretical models. Direct numerical simulations are at the edge of what is feasible with the existing supercomputers . Reduced models, capable of predicting the transport mechanisms
with less numerically demanding calculations, are the proper tool for scans in the parameter space, and for understanding the fundamental physics of the this rich nonlinear dynamics . In particular, the PhD candidate will extend the existing theoretical models to the regimes of burning plasmas, i.e. hot plasmas in the presence of a high concentration of highly energetic ions .

Required background of the student: Degree in physics. Knowledge of plasma physics, and numerical methods.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. A. Biancalani, A. Bottino, A. Di Siena, O. Gurcan, T. Hayward-Schneider, F. Jenko, P. Lauber, A. Mishchenko, P. Morel, I. Novikau, F. Vannini, L. Villard, A. Zocco, "Gyrokinetic investigation of Alfven instabilities in the presence of turbulence", Plasma Physics and Controlled Fusion 63, 065009 (2021)
2. Ö. D. Gürcan and P. H. Diamond, "Zonal flows and pattern formation", J. Phys. A. Math. Theor. 48, 293001 (2015), DOI 10.1088/1751-8113/48/29/293001
3. A Mishchenko, et al. "Numerical tools for burning plasmas", Plasma Phys. Control. Fusion 65, 064001 (2023), DOI 10.1088/1361-6587/acce68
4. L. Chen and F. Zonca, "Theory of Alfvén waves and energetic particle physics in burning plasmas", Nucl. Fusion 47, S727 (2007), DOI 10.1088/0029-5515/47/10/S20
5.

Illustrations :



ParisTech

TITLE: FOAM-MICP: FOAM MEDIATED MICROBIOLOGICALLY INDUCED CALCITE PRECIPITATION

Topic number : ***2023_056***

Field : Environment Science and Technology, Sustainable Development, Geosciences, Material science, Mechanics and Fluids, Life Science and Engineering for Agriculture, Food and the Environment

Subfield:

ParisTech School: Ecole des Ponts ParisTech
Research team: Rheophysics and Porous Media
https://navier-lab.fr/en/research/rheophysique-et-milieux-poreux/
Research lab: Laboratoire NAVIER (mécanique, physique des matériaux et des structures, géotechnique)
Lab location: Champs-sur-Marne
Lab website:https://navier-lab.fr/en/

Contact point for this topic: Ecole des Ponts ParisTech

Advisor 1: PITOIS Olivier olivier.pitois@univ-eiffel.fr
Advisor 2: TANG Anh-Minh anh-minh.tang@enpc.fr
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: The Microbiologically Induced Calcite Precipitation (MICP) method involves injecting bacteria and other compounds into soils, where the bacteria are nucleation sites to precipitate CaCO3 that acts as a cement between the grains. A new step has just been reached at Navier Laboratory with the development of bio-calcifying liquid foams. The use of such liquid foam in high-permeability soils (e.g. sands) has been shown to promote a robust pendular-like regime, which is reminiscent of the pendular regime in unsaturated media: bacteria concentrate in those precursor liquid bridges between the grains where bio-cementation takes place. This new potential method, that we call Foam-MICP, remains to be validated in terms of mechanical strength provided in various soils. This is the purpose of the present project. The experimental approach will consist in optimizing the way the method is applied, e.g. filling the pore space with bacteria-loaded foam or introduction of the bacteria/nutriment after the foam filling step, foam liquid fraction, duration of one treatment, … For each sample, the precipitation will be followed by ultrasound methods

coupled with classical mechanical tests. X-Ray Tomography will be used to assess the distribution of $CaCO_3$ precipitate. In addition, mechanical tests will be performed at the scale of two foam-embedded grains to determine the resulting precipitate-induced adhesion force.

Required background of the student: Background in condensed matter physics, material science (physics/chemistry) or soil mechanics. A taste in experimental work is expected. A background in biotechnologies is not necessary, this aspect will be dealt with by the support team.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. I. Cantat, O. Pitois, et al., “Foam: Structure and Dynamics“, Oxford University Press (2013) ISBN: 978-0-19-966289-0.

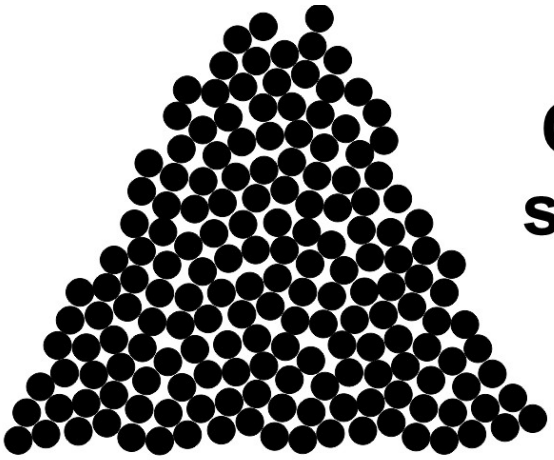
2. Ceccaldi M., Pitois O., et al., Liquid relative permeability through foam-filled porous media: Experiments, Physical Review Fluids (2023) 8, 024302

3. Pitois O., et al. Daisy-shaped liquid bridges in foam-filled granular packings, Journal of Colloid and Interface Science (2023) 638, pp. 552-560

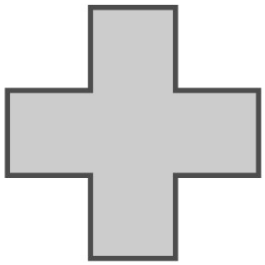
4. Galvani N., Pitois O., et al., Hierarchical bubble size distributions in coarsening wet liquid foams. PNAS (Proceedings of the National Academy of Sciences of the United States of America) (2023) 120, e2306551120

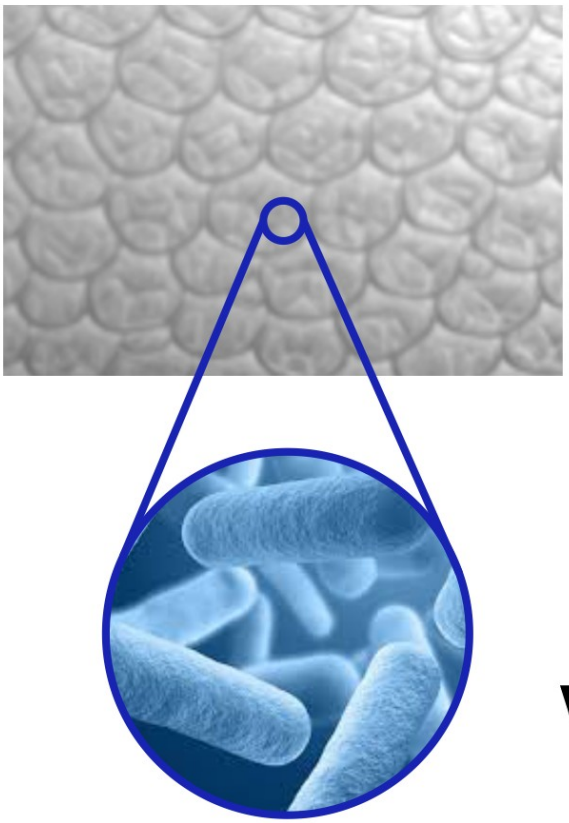
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Illustrations :



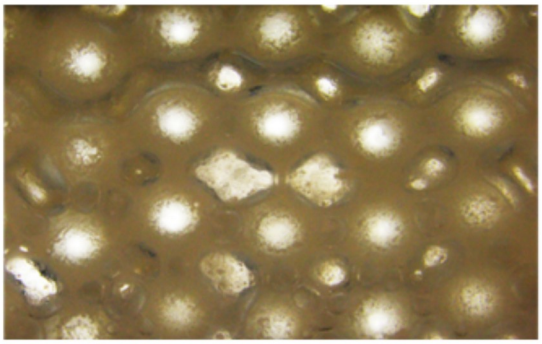
Cohesionless soil (e.g. sand)

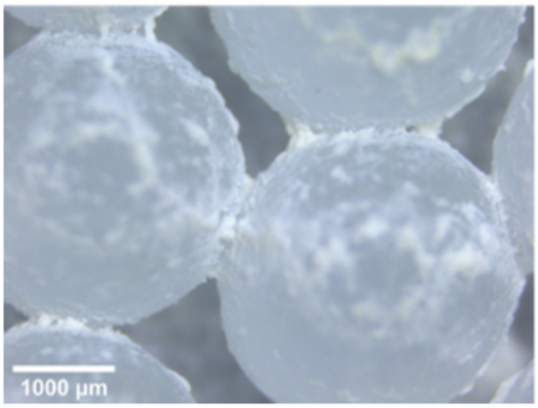


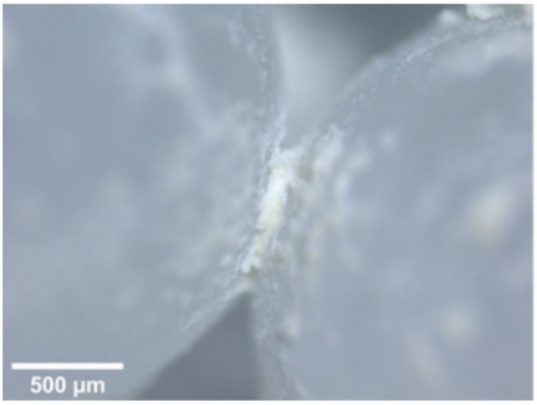


Liquid foam loaded with bacteria









The Foam-MICP method: (Left) View from the wall of foam-filled granular packing. The liquid foam contains bacteria and nutriments. (Center, Right) View of the resulting $CaCO_3$ bridges formed at contact between grains after one treatment.

ParisTech

ESPCI PARIS PSL

TITLE: PHOTON THERMALIZATION IN DISORDERED SCATTERING MEDIA

Topic number : ***2023_057***

Field : Physics, Optics, ,

Subfield:

ParisTech School: ESPCI Paris - PSL
Research team:
https://www.institut-langevin.espci.fr/valentina_krachmalnicoff and
https://www.institut-langevin.espci.fr/romain_pierrat
Research lab: Institut Langevin
Lab location: Paris
Lab website:https://www.institut-langevin.espci.fr/home

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Krachmalnicoff Valentina valentina.krachmalnicoff@espci.fr
Advisor 2: Pierrat Romain romain.pierrat@espci.fr
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: In this project we propose to study photon thermalization towards Bose-Einstein condensation in a solution of dyes in which the cavity is replaced by a strongly scattering medium. The study will be performed theoretically, numerically and experimentally. We will explore different regimes in which the light emitted by the fluorophores/scattering medium ensemble shows either a fluorescent spectrum or a thermalized spectrum or Bose-Einstein condensation. This will be achieved by changing the density of molecules and the properties of the scattering medium.

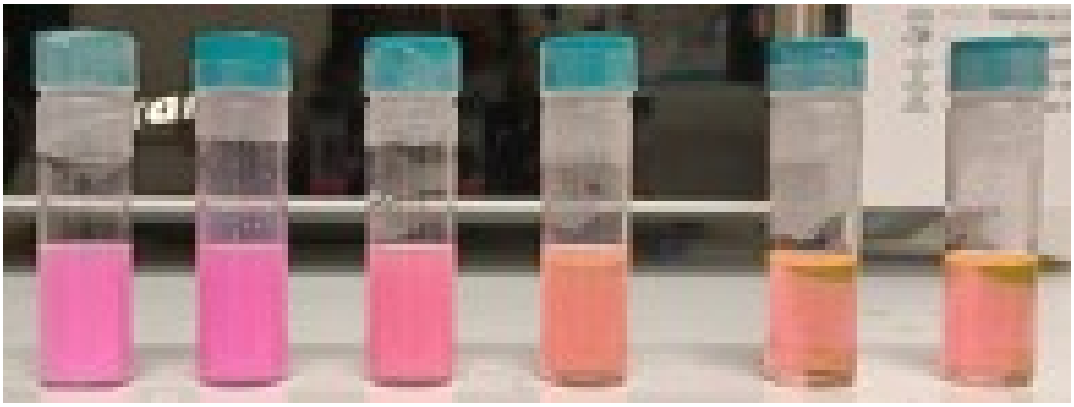
Required background of the student: A solid background in optics and computational physics is needed, background in nanophotonics and quantum optics is a plus. A taste for experimental physics, theoretical physics and simulations is expected. Good level of English.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. H. Cao, Random Lasers: Development, Features and Applications, Opt. Photon. News 16, 24 (2005)

2. D. S. Wiersma, The physics and applications of random lasers, Nat. Phys. 4, 359 (2008)
3. J. Klaers, J. Schmitt, F. Vewinger, and M. Weitz, Bose–Einstein condensation of photons in an optical microcavity, Nature 468, 545 (2010)
4.
5.

Illustrations :



Photon thermalization in disordered scattering media

Supervisors: Valentina Krachmalnicoff, Romain Pierrat
valentina.krachmalnicoff@espci.fr – romain.pierrat@espci.fr
Co-supervisor: Yannick De Wilde, Remi Carminati
Host Institute: Institut Langevin, ESPCI Paris, 1 rue Jussieu, 75005 Paris
https://www.institut-langevin.espci.fr/

Coupling quantum emitters to photonic cavities is a common way to control light-matter interaction and produce light sources operating in different regimes, from spontaneous emission in LEDs to stimulated emission in lasers. Multiple scattering in a disordered medium is another and apparently simple way to enhance the interaction between an ensemble of emitters immersed within the medium and the emitted light. When the size of the medium exceeds the scattering mean free path, photons undergo a diffusive random walk that increases the probability of absorption and emission by the fluorophores, thus mimicking the effect of a cavity. This idea led to the concept of random laser, that has been demonstrated in a large variety of configurations, from colloidal suspensions in a dye solution to infiltrated powders or white paints [1, 2].

Since photons are bosons, they can undergo Bose-Einstein condensation which is a phase transition characterized by a macroscopic population of the ground state of the system. A crucial step towards Bose-Einstein condensation is thermalization. While for massive particles, thermalization is the result of inter-particle collisions, for non-interacting photons the key mechanism is emission-absorption cycles of a reservoir of fluorescent molecules. Bose-Einstein condensation of photons in a cavity filled with dye molecules has been observed relatively recently [3], and came well after the condensation of atomic gases (1995) or polaritons in semiconductor microcavities (2002).

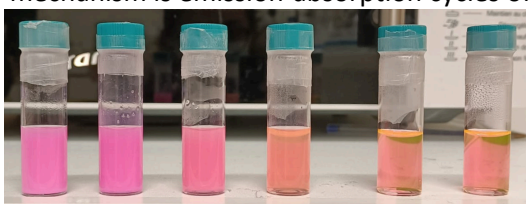


Figure: solution containing fluorescent dyes and scattering particles for different concentrations of scattering particles (higher on the left of the picture).

In this project we propose to study photon thermalization towards Bose-Einstein condensation in a solution of dyes in which the cavity is replaced by a strongly scattering medium. Diffusion ensures that photons undergo an adequate number of absorption and emission cycles to thermalize with the dye solution.

The study will be performed theoretically, numerically and experimentally. We will explore different regimes in which the light emitted by the fluorophores/scattering medium ensemble shows either a fluorescent spectrum or a thermalized spectrum or Bose-Einstein condensation. This will be achieved by changing the density of molecules and the properties of the scattering medium.

We are accepting applications from students with different background and motivation, ranging from quantum optics and nanophotonics to physical-chemistry, and from fundamental research to applied sciences interests. For more information, please contact Valentina Krachmalnicoff at valentina.krachmalnicoff@espci.fr or Romain Pierrat at romain.pierrat@espci.fr

References:

[1] H. Cao, Random Lasers: Development, Features and Applications, Opt. Photon. News **16**, 24 (2005).
[2] D. S. Wiersma, The physics and applications of random lasers, Nat. Phys. **4**, 359 (2008).
[3] J. Klaers, J. Schmitt, F. Vewinger, and M. Weitz, Bose–Einstein condensation of photons in an optical microcavity, Nature **468**, 545 (2010).

ParisTech

ESPCI PARIS PSL

TITLE: STUDYING CAVITATION OF SOFT CONFINED LAYERS WITH FORCE-SENSITIVE MOLECULES (MECHANOPHORES)

Topic number : ***2023_058***

Field : Material science, Mechanics and Fluids, Physics, Optics, Chemistry, Physical chemistry and Chemical Engineering

Subfield: Polymer Science

ParisTech School: ESPCI Paris - PSL
Research team: Soft Polymer Networks https://www.simm.espci.fr/-Soft-Polymer-Networks-.html
Research lab: SIMM - Sciences et ingénierie de la matière molle
Lab location: Paris
Lab website:https://www.simm.espci.fr/-Home-.html

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Creton Costantino costantino.creton@espci.psl.eu
Advisor 2: Barthel Etienne etienne.barthel@espci.psl.eu
Advisor 3:
Advisor 4:

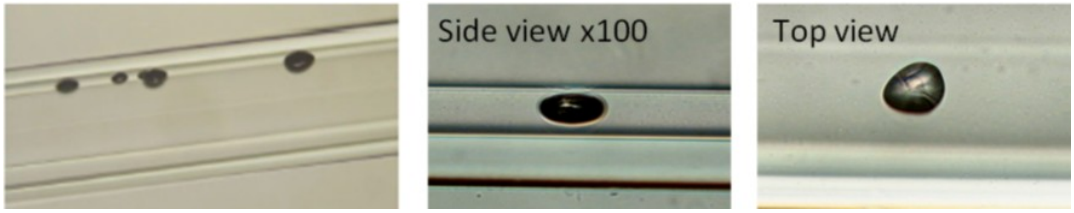
Short description of possible research topics for a PhD: Our group has recently developed a new method to detect and quantify molecular damage in crosslinked elastomers giving an unprecedented vision of fracture in fully transparent soft materials. The objective of this thesis is to apply this method to the problem of cavitation in soft confined layers, a situation occurring in seals and coatings exposed to a hydrostatic stress. We have recently developed a home-made set-up able to apply in controlled conditions a nearly hydrostatic stress on soft (MPa modulus) thin layers (100-500 µm). Combining model elastomers labeled with force-sensitive mechanophores with finite element modeling and cavitation testing, we will tackle the old but unsolved problem of the criterion for nucleation of cavities in confined conditions and of the orientation of subsequent crack growth. While the failure of polymers in uniaxial tension is clearly related to polymer chain extension, the failure in hydrostatic tension occurs at very low strains and relatively low stresses and a proper criterion is currently beyond reach. The thesis will involve material synthesis, mechanical testing in various conditions, finite element modeling and optical observations with confocal microscopy.

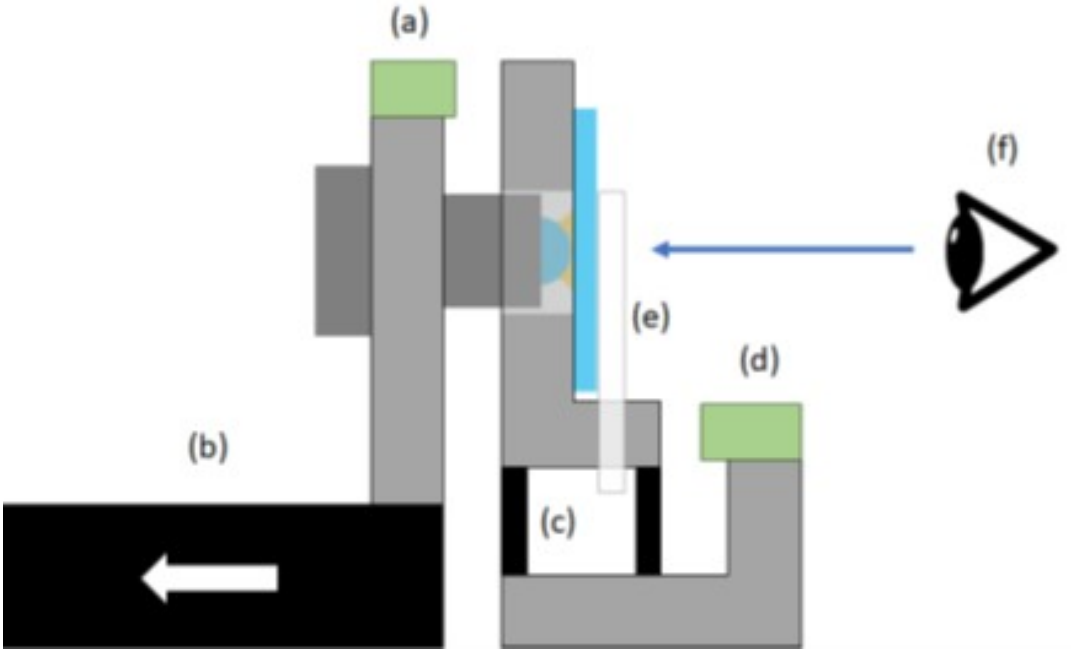
Required background of the student: Pirmary back ground in materials science, mechanics or physics with interest in material sythesis

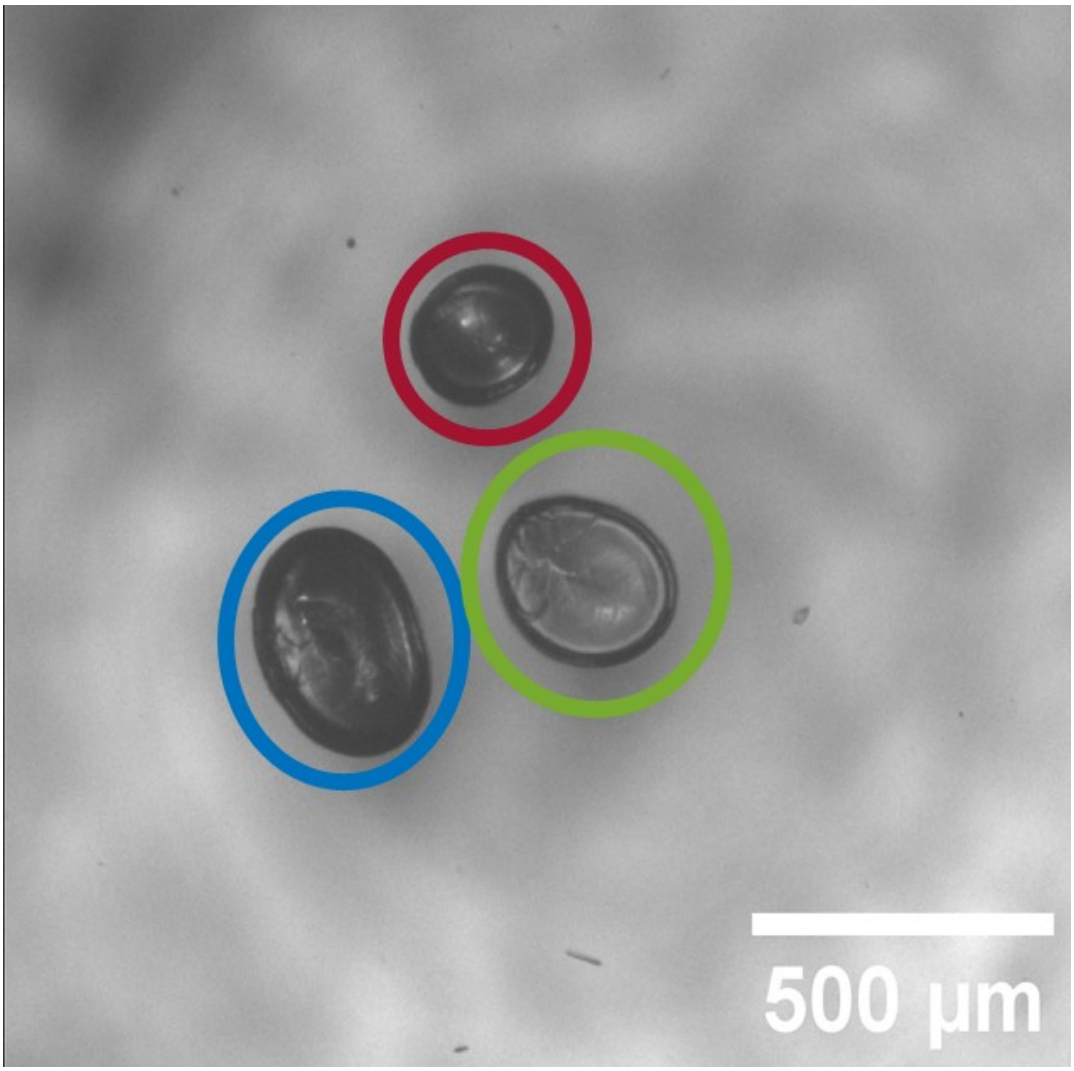
A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Ducrot, E., Chen, Y., Bulters, M., Sijbesma, R. P. & Creton, C. Toughening Elastomers with Sacrificial Bonds and Watching them Break. Science 344, 186-189 (2014).
2. Morelle, X. P., Sanoja, G. E., Castagnet, S. & Creton, C. 3D fluorescent mapping of invisible molecular damage after cavitation in hydrogen exposed elastomers. Soft Matter 17, 4266-4274 (2021).
3. Slootman, J. et al. Quantifying and mapping covalent bond scission during elastomer fracture. Physical Review X 10, 041045 (2020).
4. Elziere, P., Dalle-Ferrier, C., Creton, C., Barthel, E. & Ciccotti, M. Large strain viscoelastic dissipation during interfacial rupture in laminated glass. Soft Matter 13, 1624-1633 (2017). https://doi.org:10.1039/C6SM02785G
5. Sanoja, G. E. et al. Why is mechanical fatigue different from toughness in elastomers? The role of damage by polymer chain scission. Science Advances 7, eabg9410 (2021). https://doi.org:doi:10.1126/sciadv.abg9410

Illustrations :


Side view x100
Top view


(a)
(f)
(e)
(d)
(b)
(c)


500 µm

ParisTech

TITLE: BIOCIDES IN URBAN RUNOFF: MEASUREMENT AND MODELLING FOR EMISSION AND FATE ASSESSMENT AT THE NEIGHBOURHOOD LEVEL

Topic number : ***2023_059***

Field : Environment Science and Technology, Sustainable Development, Geosciences, Chemistry, Physical chemistry and Chemical Engineering,

Subfield:

ParisTech School: Ecole des Ponts ParisTech
Research team:
Research lab: LEESU - Laboratoire Eau environnement et systèmes urbains
Lab location: Champs-sur-Marne
Lab website:https://www.leesu.fr/

Contact point for this topic: Ecole des Ponts ParisTech

Advisor 1: Gromaire Marie-Christine marie-christine.gromaire@enpc.fr
Advisor 2: Bressy Adèle adele.bressy@enpc.fr
Advisor 3:
Advisor 4:

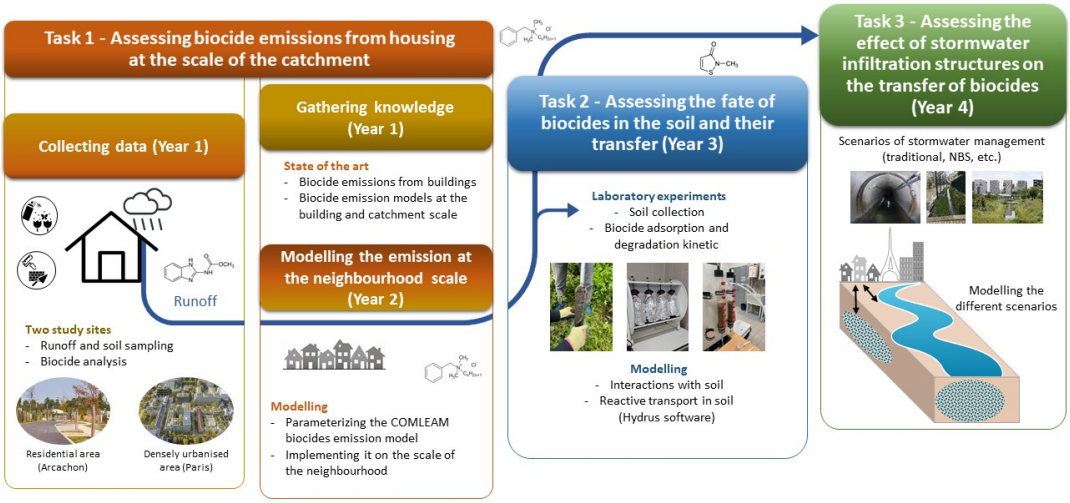
Short description of possible research topics for a PhD: Biocidal substances are widely used in building materials particularly as fungicides, algaecides, demossing agent or insecticides and for pest control. Although biocide emissions from construction materials have been extensively studied in the laboratory or on the scale of test benches, few studies have quantified emissions at the scale of an urban neighbourhood and addressed the link between urban emissions of biocides, their fate in the stormwater management system and their transfer to the surface or underground aquatic environment. The development of measures to control stormwater at source that promote on-site infiltration of urban runoff raises concerns about the fate of biocides in the soil of infiltration systems and their potential transport to the groundwater. The objectives for this thesis proposal are (i) to assess biocide emissions from housing at the scale of a residential neighbourhood; (ii) to assess the fate of biocides in the soil; and (iii) to assess the effect of stormwater infiltration structures on the transfer of biocides into the environment.

Required background of the student: Masters degree in environmental sciences or hydrology. The candidate must show a high interest for lab experiment and modelling.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Paijens C., Tedoldi D., Frère B., Mailler R., Rocher V., Moilleron R., Bressy A. (2022). Biocidal substances in the Seine River: contribution from urban sources in the Paris megacity. Environ. Sci.: Water Res. Technol., 2022,8, 2358-2372, doi:10.1039/d2ew00253a, https://enpc.hal.science/hal-03772400v1
2. Paijens C., Bressy A., Frère B., Tedoldi D., Mailler R., Rocher V., Neveu P., Moilleron R. (2021). Urban pathways of biocides towards surface waters during dry and wet weathers: Assessment at the Paris conurbation scale. Journal of Hazardous Materials, 2021, 402, pp.123765, doi:10.1016/j.jhazmat.2020.123765, https://enpc.hal.science/hal-02934934v1
3. Tedoldi D., Chebbo G., Pierlot D., Kovacs Y., Gromaire M.-C. (2016). Impact of runoff infiltration on contaminant accumulation and transport in the soil/filter media of Sustainable Urban Drainage Systems: A literature review. Science of The Total Environment 569–570, 904–926, doi:10.1016/j.scitotenv.2016.04.215
4. Tunqui Neira J.-M., Gromaire M.-C., Chancibault K., Chebbo C. (2023). Toward a comprehensive functional typology of stormwater control measures for hydrological and water quality modeling purposes. Blue-Green Systems, 5 (1), pp.41-56, doi:10.2166/bgs.2023.026, https://enpc.hal.science/hal-04149255v1
5. Flanagan K., Branchu P., Boudahmane L., Caupos E., Demare D., Deshayes S., Dubois P., Meffray L., Partibane C., Saad M., Gromaire M.-C. (2019). Retention and transport processes of particulate and dissolved micropollutants in stormwater biofilters treating road runoff. Science of the Total Environment, 656, pp.1178-1190, doi:10.1016/j.scitotenv.2018.11.304, https://enpc.hal.science/hal-02065392v1

Illustrations :



PhD thesis proposal for the ParisTech – CSC program

Biocides in urban runoff: measurement and modelling for emission and fate assessment at the neighbourhood level

PhD proposed in the Leesu laboratory in École des Ponts ParisTech (ENPC)

1 Summary of the thesis project

1.1 Background and objectives

While the use of pesticides in urban environments is becoming increasingly controlled, biocidal substances are being used more and more, particularly as fungicides, algaecides, demossing agent or insecticides in building materials and for pest control (ANSES, 2019; Paijens et al., 2020a). These biocides are emitted in runoff from buildings, discharged onto the ground or into the stormwater management system and reach the environment, with a potentially negative impact on aquatic and terrestrial ecosystems (Kresmann et al. 2018; Paijens et al. 2020a). However, these urban emissions of biocides and their impact on receiving environments are poorly documented. Claudia Paijens' (2019) thesis work at Leesu has shown (i) that biocides are ubiquitous in urban waters, posing a risk to the aquatic environment, (ii) that an increase in biocide flows between upstream and downstream of the Paris conurbation has been observed for several molecules, and (iii) that the presence of several biocides is related to stormwater flows, likely via leaching from building materials (Paijens et al, 2020b, 2021). Although biocide emissions from construction materials have been extensively studied in the laboratory or on the scale of test benches (Bollmann et al., 2016; Burkhardt al., 2011; Gromaire et al, 2015), few studies have quantified emissions at the scale of an urban neighbourhood and addressed the link between urban emissions of biocides, their fate in the stormwater management system and their transfer to the surface or underground aquatic environment (Burkhardt et al., 2011; Gallé et al., 2020; Paijens et al., 2020a).

The development of measures to control stormwater at source that promote on site infiltration of urban runoff raises concerns about the fate of biocides in the soil of infiltration systems and their potential transport to the groundwater. As predominantly hydrophilic molecules, biocides should not be strongly retained by the soil, unlike the micropollutants generally studied in runoff, such as metals and polycyclic aromatic hydrocarbons (Tedoldi et al., 2016). In addition, biocides can evolve into transformation products (TPs), which are poorly documented and represent an unknown risk of exposure for receiving environments. Very diffuse runoff management, in nature based solutions (NBS) constructed with adapted/engineered soils, could allow temporary retention and biodegradation of biocides, but the real importance of these processes has not been assessed to date.

In this context, we have identified several objectives for this thesis proposal: (i) **assess biocide emissions from housing at the scale of a residential neighbourhood;** (ii) **assess the fate of biocides in the soil;** (iii) **assess the effect of stormwater infiltration structures on the transfer of biocides into the environment** (See Figure 1).

1.2 Scientific challenges

- Development of laboratory experiments to assess the kinetics of adsorption and degradation of biocides in the soils of infiltration structures and in water.
- Parametrisation and validation of models on different scales: (i) COMLEAN model of biocide emissions from buildings on a neighbourhood scale, (ii) Hydrus model for biocide transfer in infiltration structures and soils adjacent to buildings,
- Determination of scenarios of stormwater management on the scale of an urban district

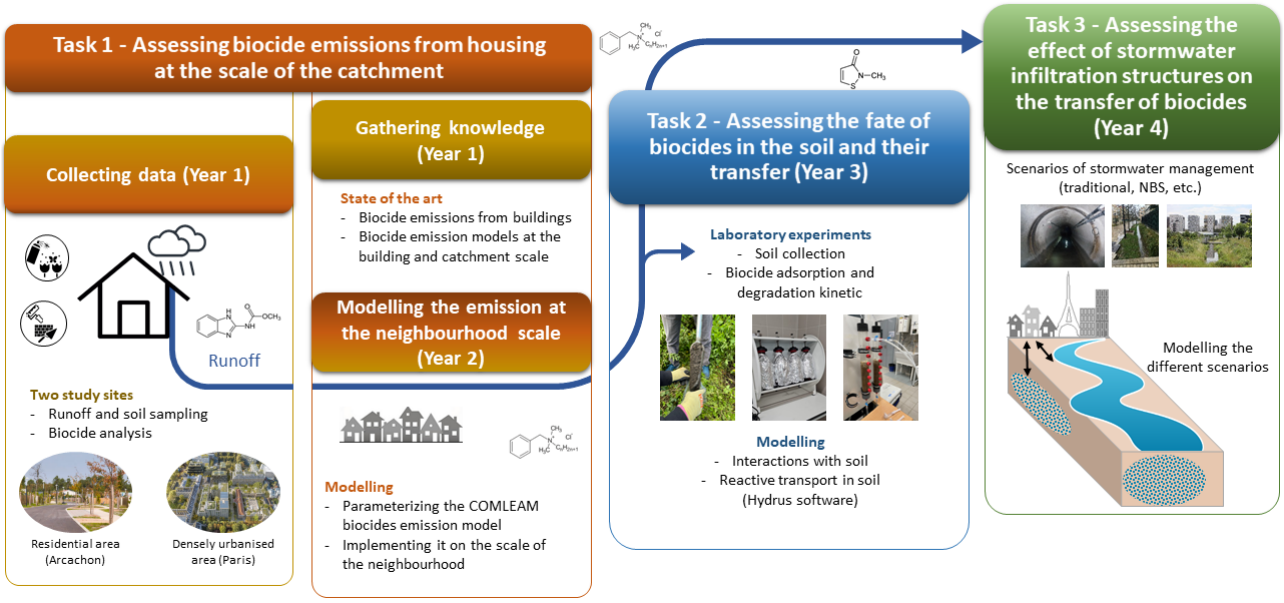


Figure 1 : Different tasks of the PhD proposal

1.3 Methodology

The thesis will be conducted as part of several research projects already funded: ANR Biocid@Home (Biocides at home: emissions, potential exposure and reduction solutions, 2021 – 2025) and the Francilian Observatory in Urban Hydrology (OPUR). It will be based in particular on experimental data acquired on two sites instrumented respectively in a residential area near Arcachon and in a recent dense urban area near Paris. Samples of run-off (at the building level, from stormwater drains and in the infiltration structures) as well as the soils infiltrating it, will be collected at different points of these neighbourhoods and analysed to quantify biocides and their transformation products. Data on the use of biocides is also being collected through field surveys.

The first few months of the thesis will be used (i) to review the state of the art in modelling the emission, transfer and fate of biocides emitted by buildings in runoff; (ii) to consolidate the database required for the modelling by identifying the various useful parameters and their values; and (ii) setting up the monitoring framework. The transfer processes from buildings to receiving environments will then be modelled in two stages. Year 1 will involve parameterising the COMLEAM biocides emission model (www.comleam.ch) and implementing it on the scale of the catchment areas, in collaboration with Prof. Burkhardt. The model will be calibrated and validated using survey data and runoff analysis. The second stage (year 2) involves modelling the fate of biocides in soils

and their transfer to groundwater. Laboratory experiments to estimate the adsorption and degradation of biocides, based on the soil samples collected on site, will be required and modelled. Reactive transport in the unsaturated zone of the soil will be modelled, on the scale of the infiltration structure and more widely on the scale of the neighbourhood, using Hydrus software and validated by comparison with on-situ data of soil contamination. The final stage (year 3) will focus on the scenario of runoff water management on the scale of a residential neighbourhood, by comparing traditional 'all-pipe' management and different variants of at-source stormwater management (the more or less diffuse nature of the management structures, the type of structure, the nature of the soil of the structures, etc.). The results of the models and scenarios will be interpreted in year 3 and translated into operational results. (See Figure 1)

The data required for the modelling is currently being acquired by the different projects and will be completed by the PhD student for the Parisian study site. The COMLEAN model is being made available by its developer, Prof. Burkhardt, a partner in the Biocid@Home project. The Hydrus software is already in use at Leesu.

1.4 Expected results and exploitation

The expected results are (i) an integrated model of the emission, transfer and fate of biocides from buildings to the underground, at a district scale; (ii) an assessment of the effectiveness of at-source stormwater management facilities in limiting the spread of biocides to groundwater.

The results will be published in the form of scientific articles and presentations at international conferences, as well as articles aimed at technical services and public authorities.

1.5 Bibliography

ANSES. (2019). Étude Pesti'home (www.anses.fr/en/system/files/2019Pestihome.pdf)
Bollmann U. E. *et al.* (2016). Environmental Science & Technology 50:4289–4295
Burkhardt M. *et al.* (2011). Water Science and Technology 63:1974–1982.
Kresmann S. *et al.* (2018). Science of The Total Environment 625:900–908.
Paijens C. *et al.* (2020a). Environmental Science and Pollution Research 27:3768–3791.
Paijens C. *et al.* (2020b). Water, Air, & Soil Pollution 231:210.
Paijens C. *et al.* (2021). Journal of Hazardous Materials 402:123765.
Tedoldi D. *et al.* (2016). Science of The Total Environment 569–570:904–926.

2 Organisation and implementation of the project

2.1 Laboratory presentation and resources available

The Water, Environment and Urban Systems lab (Leesu, www.leesu.fr) is a French research laboratory in environmental sciences, specialized in studying water and its management in urban and peri-urban environments. It is a joint laboratory between École des Ponts ParisTech and Université Paris-Est Créteil. Leesu's main focus of research is water in the city. Facing the challenge of making the city sustainable and resilient in the context of global changes, the lab aims to gain a better understanding of water and contaminant flows in the urban environment and to develop

innovative concepts for water and soil management. Through interdisciplinary and multi-scale approaches, Leesu focuses on different aspects of global changes: climate, hydrology, urban planning and architecture, regulations, practices, uses, management methods, pollution. Leesu's research relies on experiments and demonstrators to study the impact of global changes, the dissemination of innovations, the emergence of new sectors, the brakes and levers, the positioning of users and territorial compatibility. Leesu is committed to transferring its knowledge to local authorities, the industry and the general public. LEESU has all the equipment needed to perform this project: analytical instruments, lab-scale pilots and field work equipment, Hydrus licence.

Location: Laboratoire Eau, Environnement et Systèmes Urbains (Leesu) - École des Ponts, 6-8 avenue Blaise Pascal, 77455 Champs-sur-Marne, France

2.2 Thesis supervisors

The PhD student will be supervised by **Pr. Marie Christine GROMAIRE and Dr. Adèle BRESSY**, tenured researchers in École des Ponts ParisTech (marie-christine.gromaire@enpc.fr ; adele.bressy@enpc.fr). Marie-Christine Gromaire (50% supervision) is an expert in urban hydrology and modelling, while Adèle Bressy (50% supervision) is a specialist in environmental chemistry and the fate of micropollutants in the environment. Both areas of expertise are required for the thesis.

- Pr. Marie-Christine Gromaire (https://www.researchgate.net/profile/Marie-Christine-Gromaire) is a top grade researcher at ENPC, Leesu. Her research topic is mainly on water and contaminant fluxes associated with urban runoff, and their source control in sustainable urban drainage system (SUDS). In recent years, she focused on the study of hydrological and physico-chemical processes within nature-based solutions for stormwater management (NBSsw), as well as on the effects of a NBSsw in the city. Within the OPUR observatory of urban hydrology (https://www.leesu.fr/opur/), which she has co-managed since its creation, she is co-piloting the research topic on evaluation and improvement of SUDS performance at the facility scale, as well as the development of a long-term observatory of SUDS at the district scale, and contributing to modelling developments on the evaluation of SUDS deployment at the urban scale. She has supervised 15 PhD thesis so far, and has published 100 scientific papers.
- Dr. Adèle Bressy (https://www.researchgate.net/profile/Adele-Bressy) is a researcher at ENPC, Leesu. She works on micropollutants, in particular biocides. Her research projects focus on (i) the non-targeted quantification of emerging micropollutants in urban waters, (ii) the investigation of the emission, the transfer and the fate of biocides in urban waters and (iii) the quantification of micropollutants in domestic waters and the search for ways to reduce the emission of these biocides to the environment. She is currently involved in several research programs and projects including ANR-Biocid@Home, BiociDust, BRIQUE, and OPUR program and has supervised 5 PhD thesis so far, and has published 30 scientific papers.

2.3 Expected collaborations

- **Prof. Michael Burkhardt** (HSR University of Applied Sciences Switzerland), provision of the COMLEAN emission model (www.comleam.ch) and support for its parameterisation and use.
- **Pr. Noureddine Bousserrhine and Dr. Julien Le Roux,** Université Paris-Est Créteil, laboratory experiments on the adsorption and degradation kinetics of biocides

ParisTech

TITLE: MULTICOMPONENT TRANSFORMATIONS INVOLVING ACETYLENIC COMPOUNDS MEDIATED BY NEW LOW-VALENT IRON CATALYSTS

Topic number : ***2023_060***

Field : Chemistry, Physical chemistry and Chemical Engineering, ,

Subfield:

ParisTech School: Chimie ParisTech - PSL
Research team: Catalysis, Synthesis of Biomolecules and Sustainable Development
Research lab: I-CLEHS - Institute of chemistry for life and health
Lab location: Paris
Lab website:https://iclehs.fr/

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: LEFEVRE Guillaume
guillaume.lefevre@chimieparistech.psl.eu
Advisor 2: VIDAL Virginie virginie.vidal@chimieparistech.psl.eu
Advisor 3: PHANSAVATH Phannarath
phannarath.phansavath@chimieparistech.psl.eu
Advisor 4:

Short description of possible research topics for a PhD:
Multicomponent reactions are pivotal transformations in organic chemistry since they allow the introduction of a large structural diversity in one-pot conditions. In a green chemistry context, the development of sustainable and low-cost catalysts able to promote such transformations is moreover particularly appealing. We recently developed in our groups a novel reduced iron-based platform featuring a formal Fe(0) center associated with a non-innocent bidentate nitrogen-containing bulky ligand (N,N). This (N,N)2Fe(0) complex displays a remarkable affinity for unsaturated compounds such as alkynes and alkenes, and promotes efficiently alkyne cyclotrimerization reactions.

In order to capitalize on those results, we aim at investigating a larger scope of transformations mediated by this new complex. A first task will be to synthesize a family of new functionalized (N,N)' ligands involving a variety of electron-withdrawing and electron-donating substituents on the original (N,N) platform. This will allow access to a variety of (N,N)2'Fe(0) complexes with modulate stereoelectronic properties. Those

paramagnetic complexes will be characterized by paramagnetic 1H NMR, as well as by X-Ray Diffraction analysis and elemental analysis. In a second time, their ability to catalyze several multicomponent transformations involving acetylenic compounds and olefins will be investigated. A particular focus will be put on the synthesis of cyclic enones by Pauson-Khand methodology, as well as the synthesis of heterocyclic compounds by condensation of alkynes, alcohols and amidines. Click-chemistry condensation of organic azides with alkynes will also be investigated.

Required background of the student: Organic and organometallic chemistry

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Robin, M., Bakas, N., Clisson, A., Chamoreau, L.-M., Haddad, M., Ratovelomanana-Vidal, V., Neidig, M. L., Lefèvre, G. ACS Catal. 2023, 13, 4882

2. Parisot, W.; Huvelle, S.; Haddad, M.; Lefèvre, G.; Phansavath, P.; Ratovelomanana-Vidal, V. Org. Chem. Front. 2023, 10, 1309

3. Huvelle, S.; Matton, P.; Tran, C.; Rager, M.-N.; Haddad, M.; Ratovelomanana-Vidal, V. Org. Lett. 2022, 24, 5126

4.

5.

Illustrations :

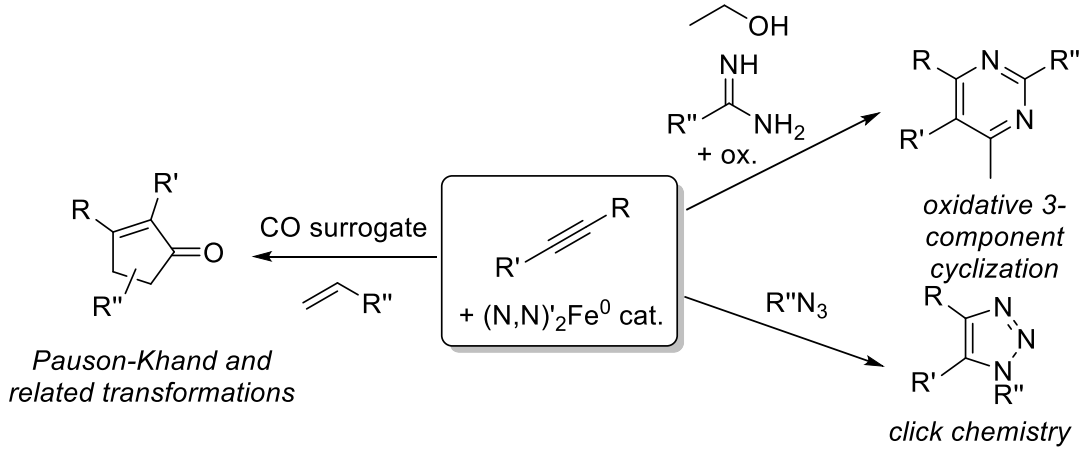
Multicomponent transformations involving Acetylenic Compounds mediated by new Low-Valent Iron Catalysts

Laboratory : *i-CLeHS – UMR 8060 équipe Catalyse, Synthèse de Biomolécules et Développement Durable, CSB2D (Chimie ParisTech, PSL University, 11 rue Pierre et Marie Curie, 75005 Paris).*

PhD Advisors : Guillaume Lefèvre, Virginie Vidal, Phannarath Phansavath

Multicomponent reactions are pivotal transformations in organic chemistry since they allow the introduction of a large structural diversity in one-pot conditions. In a green chemistry context, the development of sustainable and low-cost catalysts able to promote such transformations is moreover particularly appealing. We recently developed in our groups a novel reduced iron-based platform featuring a formal Fe(0) center associated with a non-innocent bidentate nitrogen-containing bulky ligand (N,N). This $(N,N)_2Fe(0)$ complex displays a remarkable affinity for unsaturated compounds such as alkynes and alkenes, and promotes efficiently alkyne cyclotrimerization reactions.[1],[2]

In order to capitalize on those results, we aim at investigating a larger scope of transformations mediated by this new complex. A first task will be to synthesize a family of new functionalized (N,N)' ligands involving a variety of electron-withdrawing and electron-donating substituents on the original (N,N) platform. This will allow access to a variety of $(N,N)_2'Fe(0)$ complexes with modulate stereoelectronic properties. Those paramagnetic complexes will be characterized by paramagnetic ^1H NMR, as well as by X-Ray Diffraction analysis and elemental analysis. In a second time, their ability to catalyze several multicomponent transformations involving acetylenic compounds and olefins will be investigated. A particular focus will be put on the synthesis of cyclic enones by Pauson-Khand methodology, as well as the synthesis of heterocyclic compounds by condensation of alkynes, alcohols and amidines. Click-chemistry condensation of organic azides with alkynes will also be investigated (Scheme 1).



Scheme 1

Related recent selected publications of the group :

[1] a) Robin, M., Bakas, N., Clisson, A., Chamoreau, L.-M., Haddad, M., Ratovelomanana-Vidal, V., Neidig, M. L., Lefèvre, G. *ACS Catal.* **2023***, 13*, 4882 ; b) Rousseau, L., Desaintjean, A.; Knochel, P., Lefèvre, G. *Molecules* **2020**, *25*, 723. c) Rousseau, L., Herrero, C., Clémancey, M., Imberdis, A., Blondin, G., Lefèvre, G. *Chem. Eur. J.* **2020**, *26*, 2417; d) Cahiez, G., Lefèvre, G., Moyeux, A., Guerret, O., Gayon, E., Guillonneau, L., Lefèvre, N., Gu, Q., Zhou, E. *Org. Lett.* **2019**, *21*, 2679; e) Desaintjean, A., Belrhomari, S., Rousseau, L., Lefèvre, G., Knochel, P. *Org. Lett.* **2019**, *21*, 8684; [2] a) Parisot, W.; Huvelle, S.; Haddad, M.; Lefèvre, G.; Phansavath, P.; Ratovelomanana-Vidal, V. *Org. Chem. Front.* **2023**, *10*, 1309; b) Huvelle, S.; Matton, P.; Tran, C.; Rager, M.-N.; Haddad, M.; Ratovelomanana-Vidal, V. *Org. Lett.* **2022**, *24*, 5126; c) Review: Matton, P. Huvelle, S. Haddad, M., Phansavath, P., Ratovelomanana-Vidal, *Synthesis* **2022**, 54, 4 and cited references. See also d) Tran, C., Haddad, M., Ratovelomanana-Vidal, V. *Synthesis* **2019**, *51*, 2532; e) Tran, C., Haddad, M., Ratovelomanana-Vidal, V. *Synlett* **2019**, *30*, 1891; f) Ye, F., Haddad, M., Ratovelomanana-Vidal, V., Michelet, V. *Org. Lett.* **2017**, *19*, 1104; g) Ye, F., Tran, C., Jullien, L., Le Saux, T., Haddad, M., Michelet, V., Ratovelomanana-Vidal, V. *Org. Lett*. **2018**, *20*, 4950.

ParisTech

ESPCI PARIS PSL

TITLE: MICROFLUIDICS FOR ALGAE SELECTION

Topic number : ***2023_061***

Field : Chemistry, Physical chemistry and Chemical Engineering, Life and Health Science and Technology,

Subfield:

ParisTech School: ESPCI Paris - PSL
Research team: MIE https://www.mie.espci.fr/spip.php?rubrique2
Research lab: CBI - Chimie, Biologie et Innovation
Lab location: Paris
Lab website:https://www.cbi.espci.fr/accueil-22/

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: COLIN Annie annie.colin@espci.fr
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: The culture of microalgae allows to transform CO2 into molecules of high added value.
In new generation bioreactors, algae are subjected to high constraints.

In this thesis, we will develop tools to quantify the constraints applied to algae and to quantify the effect of the constraints on the metabolism of the algae, its development, the photosynthesis reactions.
To achieve this objective, we will take advantage of classical rheology tools but also of microfluidic tools.
A planar cell under a microscope will allow us to apply controlled stresses and to measure the viscosity of the suspension as a function of the algae concentration.
When the shear is stopped, the displacement of the algae and their ability to reproduce will be analyzed.
To probe the effect of elongational flows, controlled microfluidic geometries will be used, and the algae will be made to circulate in constrictions. The microfluidic tools will also allow us to analyze swimming and stress resistance on isolated algae. .
We are looking for a candidate with expertise in complex fluid rheology

and/or algae culture. Knowledge of microfabrication/microfluidics would be appreciated but not necessary.

Required background of the student: We are looking for a candidate with expertise in complex fluid rheology and/or algae culture. Knowledge of microfabrication/microfluidics would be appreciated but not necessary.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Goyon, J., Colin, A., Ovarlez, G., Ajdari, A., & Bocquet, L. (2008). Spatial cooperativity in soft glassy flows. Nature, 454(7200), 84-87.

2. Guillot, P., Panizza, P., Salmon, J. B., Joanicot, M., Colin, A., Bruneau, C. H., & Colin, T. (2006). Viscosimeter on a microfluidic chip. Langmuir, 22(14), 6438-6445.

3.

Engl, W., Roche, M., Colin, A., Panizza, P., & Ajdari, A. (2005). Droplet traffic at a simple junction at low capillary numbers. Physical review letters, 95(20), 208304.

4.

5.

Illustrations :

ParisTech

ESPCI PARIS PSL

TITLE: LATTICE DYNAMICS AND ELECTRON-PHONON COUPLING IN HIGH DIELECTRIC CONSTANT QUANTUM MATERIALS

Topic number : ***2023_062***

Field : Physics, Optics, Material science, Mechanics and Fluids,

Subfield:

ParisTech School: ESPCI Paris - PSL
Research team: Optical conductivity https://www.lpem.espci.fr/ocg/
Research lab: LPEM - Laboratoire Physique et d'études des matériaux
Lab location: Paris
Lab website:https://www.lpem.espci.fr/ocg/

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Lobo Ricardo lobo@espci.fr
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Quantum materials are those that require quantum mechanics concepts to describe their macroscopic properties. These include superconductors, magnetic materials, heavy-fermions, and topological insulators, to name a few. The remarkable properties of these materials often come from particular electronic band structures with little influence from the underlying lattice. In some cases, however, the electron coupling to the crystalline lattice plays a major role. High dielectric constant materials are an example of physical properties that need the electron interaction with the lattice to account for its properties. A high dielectric constant affects how the electron senses the electrical crystal field and, hence, the collective electronic phenomena. SrTiO3 is a classic example of such materials, in which superconductivity can appear with extremely low charge densities. KTaO3 is another recent example of a high dielectric function material having a large electron-lattice interaction. The subject of this work is to study the optical (infrared, visible and UV) properties of these materials down to low temperatures. The main goal is to understand the phonon structure, eventually with a polar soft-mode, and its interactions with the electronic transport. As the ircrystal lattice is strongly sensitive to deformation, optical spectra at high pressures will complement this data.

Single crystals can be made at LPEM and the candidate is expected to participate in their synthesis and growth.

Required background of the student: Physics, materials sciences

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. https://scholar.google.com/citations?hl=en&user=H-o5WgUAAAAJ
2. https://scholar.google.com/citations?hl=en&user=4k9_fEMAAAAJ
3. See above list
4.
5.

Illustrations :

ParisTech

ESPCI PARIS PSL

TITLE: NEUROMORPHIC DEVICES USING VANADIUM DIOXIDE

Topic number : ***2023_063***

Field : Physics, Optics, Material science, Mechanics and Fluids,

Subfield:

ParisTech School: ESPCI Paris - PSL
Research team: Micro & Nano Characterization team (MNC)
https://www.espci.psl.eu/recherche/labos/lpem/mnc/index.html
Research lab: LPEM - Laboratoire Physique et d'études des matériaux
Lab location: Paris
Lab website:https://www.lpem.espci.fr/spip.php?rubrique45

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: AIGOUY Lionel lionel.aigouy@espci.fr
Advisor 2: ZIMMERS Alexandre azimmers@espci.fr
Advisor 3: CHEN Zhuoying zhuoying.chen@espci.fr
Advisor 4:

Short description of possible research topics for a PhD:
Neuromorphic electronic circuits are designed to mimic the behavior of biological neural networks, enabling them to process information in a brain-inspired manner (see Fig.1). To save energy, the creation of these circuits will be unavoidable as the use of AI software expands . In recent years, transition metal oxides have emerged as very promising candidates for neuromorphic devices . (i) By manipulating oxygen vacancies in materials such as TiO2 using electrical pulses, they exhibit non-volatile memory properties, mimicking artificial synapses . (ii) Other materials with inherent insulating to metal transition (IMT) have shown spiking behavior, resembling artificial neurons . At the ESPCI Paris, we possess the expertise to produce high-quality epitaxial thin films of vanadium dioxide (VO2), a material known for displaying both memory and spiking characteristics around room temperature . The PhD subject will involve the fabrication of VO2 thin films, the design of electrical spiking transport measurements at the micron scale, and ultimately, controlling these devices using an optical laser beam in a microscope setup (see Fig.2). This laser writing approach will allow, for the first time, the control of these neuromorphic devices (memory and spiking) and integrating them into a network.

Required background of the student: The PhD candidate must have a solid academic background in physics and chemistry and express strong interest in scientific experiments and analysis.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Neuromorphic Computing: From Materials to Systems Architecture / Report of a Roundtable Convened to Consider Neuromorphic Computing Basic Research Needs (2015), https://www.osti.gov/servlets/purl/1283147
2. del Valle, J. et al. Challenges in materials and devices for resistive-switching-based neuromorphic computing. J. Appl. Phys. 7 (2018); 124 (21): 211101
3. Basak, S. et al., Spatially Distributed Ramp Reversal Memory in VO2. Adv. Electron. Mater (2023), 2300085. Adv. Electron. Mater cover, Volume 9, Issue 10, https://onlinelibrary.wiley.com/journal/2199160x
4. Fang, Z. et al. Tuning the Resistance of a VO2 Junction with a Focused Laser Beam and Atomic Force Microscopy, Submitted (2023)
5.

Illustrations :

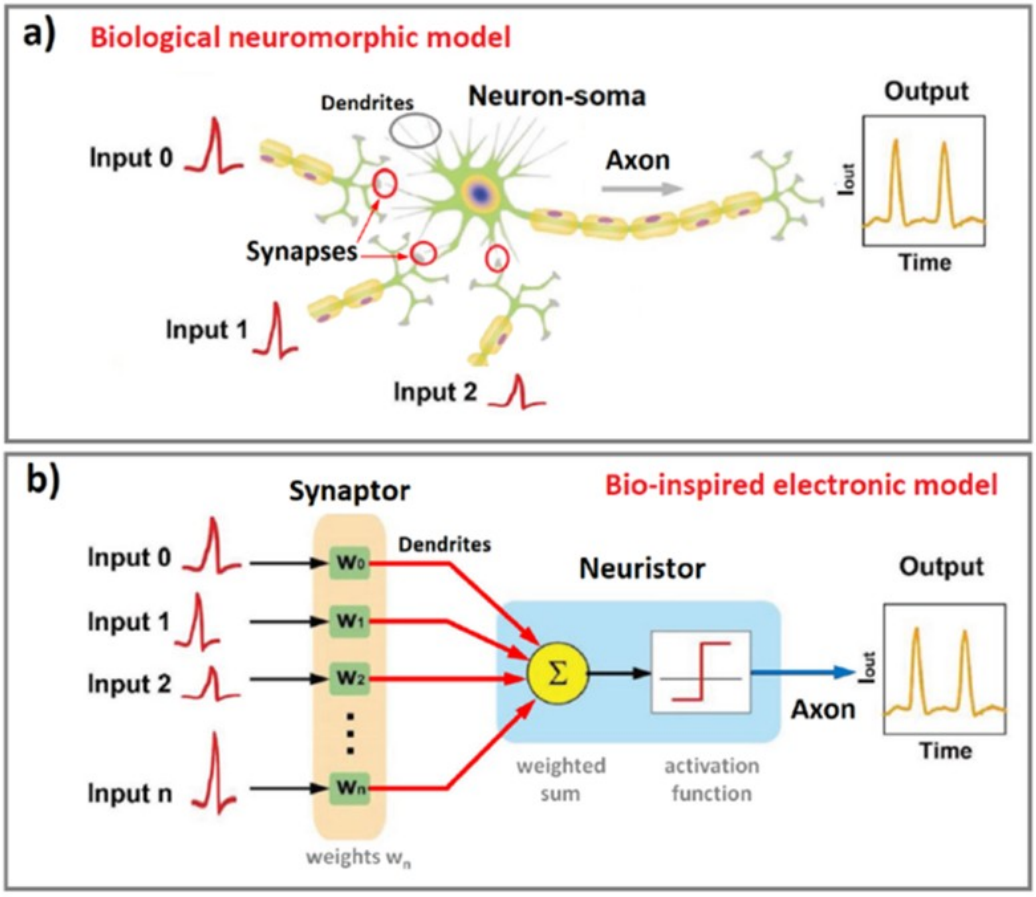


Figure 1: Schematic illustration of a neuromorphic system. a) Biological model: the neuron cell body receives inputs from other neurons via synapses. b) Bio-inspired electronic model: the electronic neuristor accumulates inputs generated by multiple pre-synaptic neuristors, the weights of which are modulated by memristive synaptors.

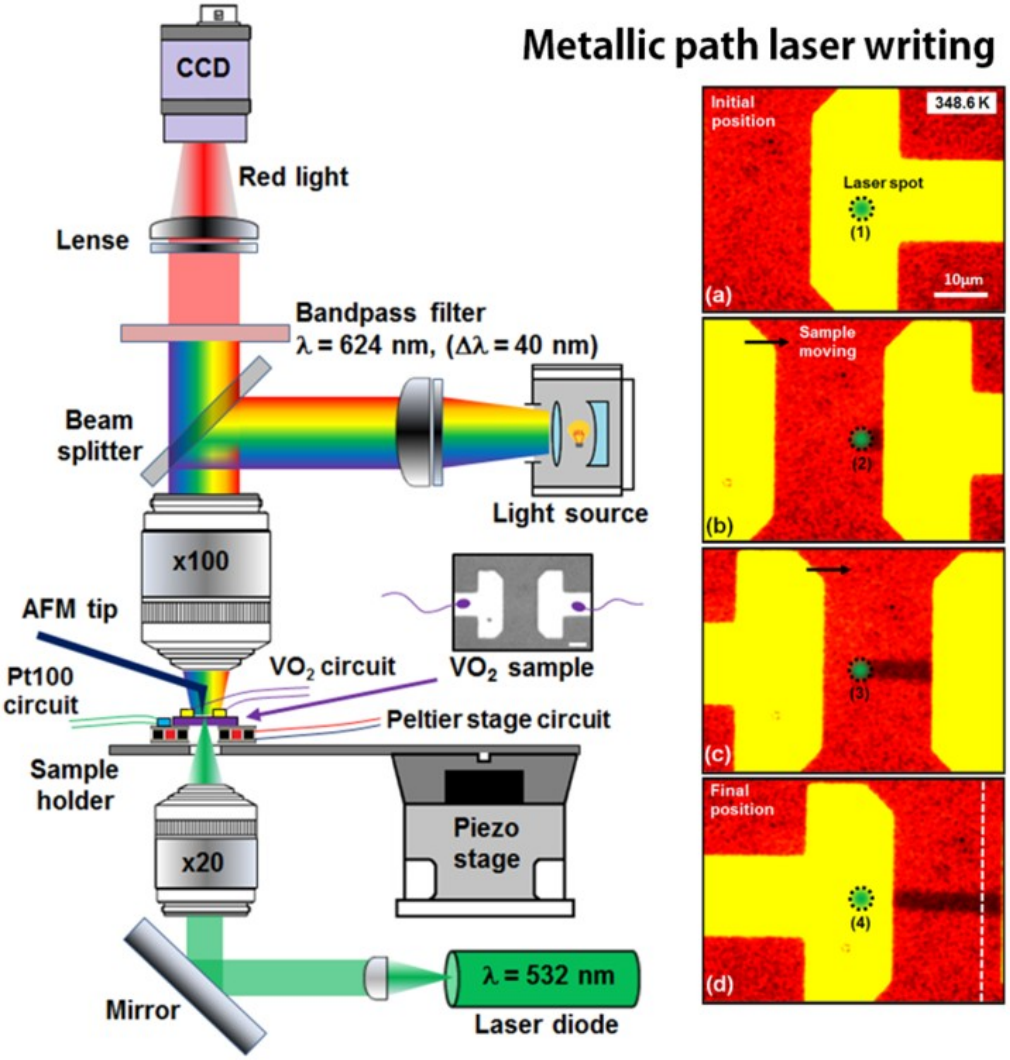


Figure 2: Left: Sketch of the optical setup combining observation of the VO_2 film from the top and laser illumination from the bottom (adapted from Ref [4]). Right: Optical microscopy images (a, b, c, d) captured when scanning the junction with the laser spot (indicated by the dotted green circle). As the laser is scanned through the 20μm junction, a dark metallic path is created inside the red insulating VO_2. This laser writing will allow the control of neuromorphic devices (memory and spiking) on the micron scale.

Neuromorphic devices using vanadium dioxide

L. Aigouy, A. Zimmers, Z. Chen, LPEM, ESPCI Paris, 10 rue Vauquelin 75005 Paris France

contact : azimmers@espci.fr

Neuromorphic electronic circuits are designed to mimic the behavior of biological neural networks, enabling them to process information in a brain-inspired manner (see Fig.1). To save energy, the creation of these circuits will be unavoidable as the use of AI software expands [1]. In recent years, transition metal oxides have emerged as very promising candidates for neuromorphic devices [2]. (i) By manipulating oxygen vacancies in materials such as TiO_2 using electrical pulses, they exhibit non-volatile memory properties, mimicking artificial synapses [2]. (ii) Other materials with inherent insulating to metal transition (IMT) have shown spiking behavior, resembling artificial neurons [2]. At the ESPCI Paris, we possess the expertise to produce high-quality epitaxial thin films of vanadium dioxide (VO_2), a material known for displaying both memory and spiking characteristics around room temperature [3-4]. The PhD subject will involve the fabrication of VO_2 thin films, the design of electrical spiking transport measurements at the micron scale, and ultimately, controlling these devices using an optical laser beam in a microscope setup (see Fig.2). This laser writing approach will allow, for the first time, the control of these neuromorphic devices (memory and spiking) and integrating them into a network.

Required background of the student: The PhD candidate must have a solid academic background in physics and chemistry and express strong interest in scientific experiments and analysis.

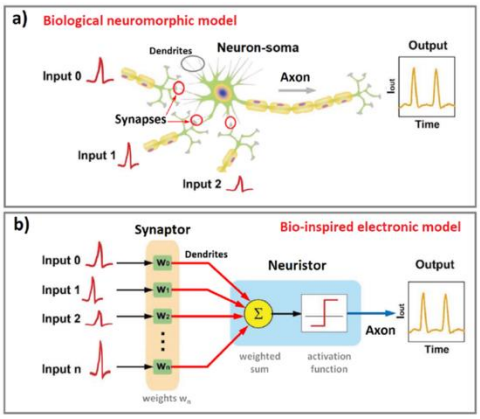


Figure 1: Schematic illustration of a neuromorphic system. a) Biological model: the neuron cell body receives inputs from other neurons via synapses. b) Bio-inspired electronic model: the electronic neuristor accumulates inputs generated by multiple pre-synaptic neuristors, the weights of which are modulated by memristive synaptors.

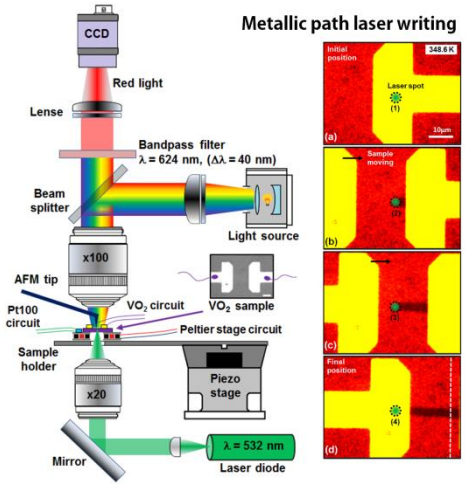


Figure 2: Left: Sketch of the optical setup combining observation of the VO_2 film from the top and laser illumination from the bottom (adapted from Ref [4]). Right: Optical microscopy images (a, b, c, d) captured when scanning the junction with the laser spot (indicated by the dotted green circle). As the laser is scanned through the 20µm junction, a dark metallic path is created inside the red insulating VO_2. This laser writing will allow the control of neuromorphic devices (memory and spiking) on the micron scale.

[1] Neuromorphic Computing: From Materials to Systems Architecture / Report of a Roundtable Convened to Consider Neuromorphic Computing Basic Research Needs (**2015**), https://www.osti.gov/servlets/purl/1283147

[2] del Valle, J. *et al.* Challenges in materials and devices for resistive-switching-based neuromorphic computing. J. Appl. Phys. 7 (**2018**); 124 (21): 211101.

[3] Basak, S. *et al.*, Spatially Distributed Ramp Reversal Memory in VO_2. Adv. Electron. Mater (**2023**), 2300085. Adv. Electron. Mater cover, Volume 9, Issue 10, https://onlinelibrary.wiley.com/journal/2199160x

[4] Fang, Z. *et al.* Tuning the Resistance of a VO_2 Junction with a Focused Laser Beam and Atomic Force Microscopy, Submitted (**2023**).

ParisTech

ESPCI PARIS PSL

TITLE: MICRO-OBJECTS IN INTERACTION WITH VISCOELASTIC FLUIDS

Topic number : ***2023_064***

Field : Material science, Mechanics and Fluids, Physics, Optics, Life Science and Engineering for Agriculture, Food and the Environment

Subfield:

ParisTech School: ESPCI Paris - PSL
Research team: Comlex Suspension
Research lab: PMMH - Physique et mécanique des Milieux Hétérogènes
Lab location: Paris
Lab website:http://www.pmmh.espci.fr

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: DU ROURE OLIVIA olivia.duroure@espci.psl.eu
Advisor 2: LINDNER ANKE anke.lindner@espci.psl.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Fluid-structure interaction is ubiquitous in nature and industrial applications. It describes the non linear coupling between an object and the surrounding fluid: Under flow objects are oriented, rearranged or deformed leading to complex transport properties and non trivial macroscopic properties at the scale of the suspension. In our group, we have performed an extensive experimental study of this problem when a microscopic fiber, flexible or rigid, is transported in a Newtonian fluid in microfluidc channels. We have gained an important knowledge on the morphological dynamics that can emerge , on the long term behavior and on the fiber sorting potential .
In this PhD project ,we propose to extend this approach to study the impact of non Newtonian properties of the fluid. Typically we aim at studying how the object dynamics is changed when the fluid is viscoelastic by using polymer solution. We expect dramatic changes specifically in presence of obstacles (see figure) as the flow will be spatially more complex than in their absence. Such studies will help to better understand the flow of industrial and everyday materials (biological liquids, fiber-reinforced rubbers, food suspensions…) but also open new route for sorting and separation issues.

Required background of the student: physics or hydrodynamics or soft matter or microfluidics

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Liu Yanan et al. PNAS 2018. doi.org/10.1073/pnas.1805399115

2. Chakrabarti et al Nature Physique 2020. doi.org/10.1038/s41567-020-0843-7

3. Bonacci et al. Journal Fluid Mechancis 2022. doi:10.1017/jfm.2022.1040

4. Li, Zhibo PhD thesis

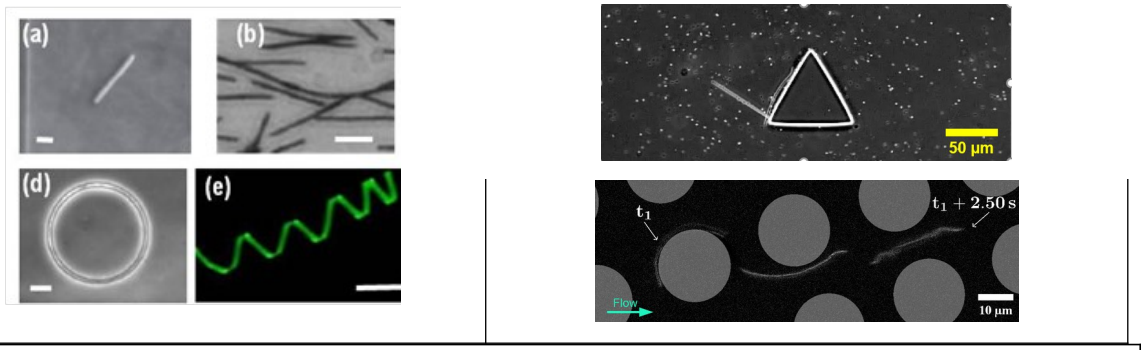
5.

Illustrations :

Laboratory name : PMMH-ESPCI
CNRS identification code : UMR 7636
Supervision : Anke Lindner and Olivia du Roure
e-mail : anke.lindner@espci.psl.eu, olivia.duroure@espci.psl.eu
Web page: https://blog.espci.fr/oliviaduroure/ and https://blog.espci.fr/alindner/
Internship location: PMMH-ESPCI, Jussieu Campus, Central Paris

Micro-objects in interaction with viscoelastic fluids

Fluid-structure interaction is ubiquitous in nature and industrial applications. It describes the non linear coupling between an object and the surrounding fluid: Under flow objects are oriented, rearranged or deformed leading to complex transport properties and non trivial macroscopic properties at the scale of the suspension. In our group, we have performed an extensive experimental study of this problem when a microscopic fiber, flexible or rigid, is transported in a Newtonian fluid in microfluidc channels, in simple flow geometries [1, 2] and recently in more complex configurations [3, 4]. We have gained an important knowledge on the morphological dynamics that can emerge [1, 2], on the long term behavior [5] and the fiber sorting potential [4].



Left : Model particles: fabricated by (a & d) projection lithography, (b) self-assembly of magnetic colloids, (e) nanoparticles spiral (courtesy A. Crosby, UMass). The scale bar represents 10 µm. Right : Interaction of a rigid fiber with one triangular obstacle (top) and of an flexible filament with an array of circular obstacles (bottom).

In this PhD project ,we propose to extend this approach to study the impact of non Newtonian properties of the fluid. Typically we aim at studying how the object dynamics is changed when the fluid is viscoelastic by using polymer solution. We expect dramatic changes specifically in presence of obstacles (see figure) as the flow will be spatially more complex than in their absence. Such studies will help to better understand the flow of industrial and everyday materials (biological liquids, fiber-reinforced rubbers, food suspensions…) but also open new route for sorting and separation issues.

Briefly, we propose to study the individual or collective dynamics of rigid or flexible fibers or disks in selected viscoelastic flows, as a function of the nature of the particles and the geometry of the flow. Precise control of the particle properties will be made possible by the use of novel micro-fabrication techniques (see Fig. 1a) coupled to the use of well controlled microfluidic flow geometries.

[1] Liu et al. PNAS 2018 [2] Chakrabati et al Nature Physics 2020
[3] Bonacci et al JFM 2022, [4] Zhibo Li, PhD thesis, Li et al. in preparation [5] Bonacci et al, in preparation.

ParisTech

ESPCI PARIS PSL

TITLE: PROBING SOLID/ELECTROLYTE INTERFACES WITH SINGLE-CHARGE NANOFLUIDICS

Topic number : ***2023_065***

Field : Chemistry, Physical chemistry and Chemical Engineering, Material science, Mechanics and Fluids, Physics, Optics

Subfield:

ParisTech School: ESPCI Paris - PSL
Research team:
Research lab: SIMM - Sciences et ingénierie de la matière molle
Lab location: Paris
Lab website:simm.espci.fr/

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Comtet Jean jean.comtet@espci.fr
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Ionic charge transport processes at the interface between solid surfaces and liquid electrolytes are at the heart of a number of energy and environment related applications (blue energy, super-capacitors and batteries, nanofiltration…). However, our fundamental understanding of these dynamic interfacial processes remains poor, due to the strong experimental barriers related to the exploration of ionic charge dynamics at the intimate scale of the interface.
In this context, we recently demonstrated that optically active defects hosted at the surface of 2D hexagonal Boron Nitride (hBN) crystals can be used as optical markers to track the motion of single H+ proton charges at the hBN/water interface (see figure). Using Single Molecule and Super-Resolution Microscopy techniques, we could reveal single proton trajectories through the successive activation of fluorescent defects at the surface of the crystal, bringing novel molecular insights on charge dynamics at these interfaces.
The aim of this PhD position is to take advantage of this unique experimental system, to investigate out-of-equilibrium transport processes at the scale of the single interfacial charge. We will combine these single-molecule microscopy techniques with ionic and fluidic

transport measurements in micro and nanofluidic devices. This unique combination will allow us to access to the dynamics of single proton charges on the solid surface under out-of-equilibrium fluidic and electric forcings and correlate it with ensemble transport in the channel. We will then extend these strategies to other materials. These measurements at ultimate scales will allow us to gain unprecedented molecular-scale insights on charge transport processes at flowing, electrically driven and confined solid/liquid interfaces.

Required background of the student: We are looking for a strongly motivated experimentalist, with a background in one of the following domains: Physics, Soft Matter, Optics, Electrochemistry, Chemical Engineering or Material Science.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Science Advances (2021), 7(40), eabg8568.

(https://doi.org/10.1126/sciadv.abg8568)

2. Nature Nanotechnology (2020), 15(7), 598-604.

(https://doi.org/10.1038/s41565-020-0695-4)

3. Nature Materials (2023), 1-7. (https://doi.org/10.1038/s41563-023-

01658-2)

4.

5.

Illustrations :

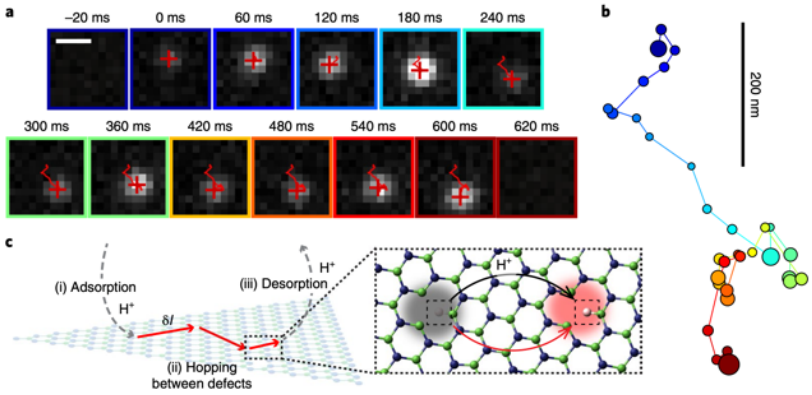
CSC PhD position

Probing solid/electrolyte interfaces with single-charge nanofluidics

Ionic charge transport processes at the interface between solid surfaces and liquid electrolytes are at the heart of a number of energy and environment related applications (blue energy, super-capacitors and batteries, nanofiltration…). However, our fundamental understanding of these dynamic interfacial processes remains poor, due to the strong experimental barriers related to the exploration of ionic charge dynamics at the intimate scale of the interface.

In this context, we recently demonstrated that optically active defects hosted at the surface of 2D hexagonal Boron Nitride (hBN) crystals can be used as optical markers to track the motion of single H^+ proton charges at the hBN/water interface (see figure). Using Single Molecule and Super-Resolution Microscopy techniques, we could reveal single proton trajectories through the successive activation of fluorescent defects at the surface of the crystal, bringing novel molecular insights on charge dynamics at these interfaces.

The aim of this PhD position is to take advantage of this unique experimental system, to investigate out-of-equilibrium transport processes at the scale of the single interfacial charge. We will combine these single-molecule microscopy techniques with ionic and fluidic transport measurements in micro and nanofluidic devices. This unique combination will allow us to access to the dynamics of single proton charges on the solid surface under out-of-equilibrium fluidic and electric forcings and correlate it with ensemble transport in the channel. We will then extend these strategies to other materials. These measurements at ultimate scales will allow us to gain unprecedented molecular-scale insights on charge transport processes at flowing, electrically driven and confined solid/liquid interfaces.



References

Science Advances (2021), **7***(40)*, eabg8568. (https://doi.org/10.1126/sciadv.abg8568)
Nature Nanotechnology (2020), **15***(7)*, 598-604. (https://doi.org/10.1038/s41565-020-0695-4)
Nature Materials (2023), 1-7. (https://doi.org/10.1038/s41563-023-01658-2)

Keywords and Recruitment terms

Single Molecule Fluorescence Microscopy, Super-Resolution, Micro and Nano-Fluidics, Electro-kinetics, 2D-materials, Solid/Liquid Interfaces.

We are looking for a strongly motivated experimentalist, with a background in one of the following domains: Physics, Soft Matter, Optics, Electrochemistry, Chemical Engineering or Material Science.

Contact

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10, Rue Vauquelin, 75005 Paris, France
https://blog.espci.fr/jcomtet/

ParisTech

TITLE: MULTISCALE EXTREMES OF LONG-RANGE DEPENDENT GEOPHYSICAL DATA

Topic number : ***2023_066***

Field : Environment Science and Technology, Sustainable Development, Geosciences, Mathematics and their applications, Information and Communication Science and Technology

Subfield:

ParisTech School: Ecole des Ponts ParisTech
Research team:
Research lab: HM & Co - Hydrologie Météorologie et Complexité
Lab location: Champs-sur-Marne
Lab website:https://hmco.enpc.fr

Contact point for this topic: Ecole des Ponts ParisTech

Advisor 1: TCHIGUIRINSKAIA Ioulia ioulia.tchiguirinskaia@enpc.fr
Advisor 2: SCHERTZER Daniel Daniel.Schertzer@enpc.fr
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Geophysical data of all kinds (in-situ, remote sensing, simulations) are rapidly becoming more available, with increasingly high precision and resolution, thanks to new measurement and computing technologies, as well as open data policies. At the same time there are increasingly pressing issues to address in mitigating and adapting to climate change while ensuring sustainable development, with a logical emphasis on the extremes (e.g., how to reduce the 20% of most extremes).
However, these data often exhibit extreme variability with long-range dependence over a wide range of space-time scales that require methodological advances. Indeed, classical extreme value theory only concerns short-range dependences and classical extreme observables are highly scale dependent.
Based on the expertise of the HM&Co laboratory in stochastic multifractal processes possessing both long-range dependencies and scale invariances, it is proposed to define and validate new extreme observables which will be scale independent and easily implementable in Deep Learning, to improve the predictability and forecasting of long-range dependent geophysical data.

Required background of the student: Stochastic processes, data science, informatics. A first part of the thesis will be devoted to update knowledge in those domains.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. 1. Lovejoy, S. and Schertzer, D. (2013), The Weather and Climate: Emergent Laws and Multifractal Cascades. Cambridge U.K.: Cambridge University Press., 491 p
2. 2. Tchiguirinskaia, I., Schertzer, D. and Lovejoy, S. (2013), Multifractals and Physically Based Estimates of Extreme Floods. Montreal: CEATI International Inc., 120 p
3. 3. Schertzer, D. & Tchiguirinskaia, I. (2020), A century of turbulent cascades and the emergence of multifractal operators. Earth Sp. Sci. 7, e2019EA000608
4. 4. Marsan, D., Schertzer, D. & Lovejoy, S. (1996), Causal space-time multifractal processes: Predictability and forecasting of rain fields. J. Geophys. Res. 101, 26,333-26, 346
5. 5. Zhou, H., Schertzer, D., Tchiguirinskaia, I. (2023). Combining variational mode decomposition and recurrent neural network to predict rainfall time series, evaluating the performance by universal multifractals. Submitted to Hydrology and Earth System Sciences

Illustrations :

ParisTech

Arts et Métiers

TITLE: EXTENDED REALTY FOR REAL-TIME VISUALIZATION OF INTRAVENOUS FLUID FLOW

Topic number : ***2023_067***

Field : Material science, Mechanics and Fluids, Information and Communication Science and Technology, Life and Health Science and Technology

Subfield: Digital Health, Diagnostic and therapy

ParisTech School: Arts et Métiers
Research team:
Research lab: LIFSE - Laboratoire Ingénierie des Fluides Systèmes Energétiques
Lab location: Paris
Lab website:HTTPS://LIFSE.ARTSETMETIERS.FR/

Contact point for this topic: Arts et Métiers

Advisor 1: GARBAYA Samir samir.garbaya@ensam.com
Advisor 2: KHELLADI Sofiane Sofiane.KHELLADI@ensam.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Despite the big interest of the research community on dynamic 3D visualization of fluids such as blood flow in the veins and injected drugs, high-fidelity representation models still not achieved. The fluids' flow in human body is inherent to physico-chemical properties specific to each patient. Hence, the personalization of models is necessary for the accuracy and efficiency of intervention. This PhD project will focus on the development of real-time interactive simulation for intravenous fluid flow using augmented reality. The research work includes geometric data acquisition, 3D modelling of human body limbs/organs and dynamic visualization of fluid flow and its interactions with deformable shapes/surfaces. The objective is to define and identify personalized digital markers of the intravenous flow for specific fluids which could be validated in diagnostic and therapeutic contexts.

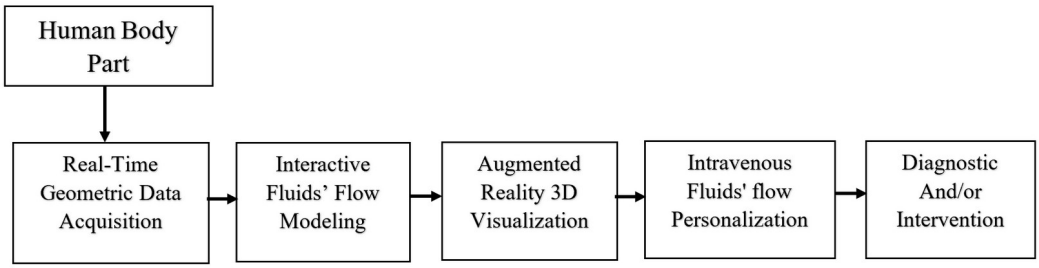
Required background of the student: Applicants must have completed a Master of Engineering in a discipline related to mechanical engineering/computer science. Prospective applicants must have skills in

Computational Fluid Dynamics, 3D geometric modelling, Augmented Reality/Virtual reality and Real-time Dynamic Visualization.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Paul Tamayo-Serrano, Samir Garbaya and Pierre Blazevic, “Gamified In-Home Rehabilitation for Stroke Survivors: Analytical Review”, the International Journal of Serious Games, ISSN: 2384-8766, Volume 5, Issue 1, March 2018. DOI: https://doi.org/10.17083/ijsg.v5i1.224
2. Boumrah, M., Garbaya, S. & Radgui, A. “Real-time visual analytics for in-home medical rehabilitation of stroke patient—systematic review”, Medical & Biological Engineering & Computing (2022). https://doi.org/10.1007/s11517-021-02493-w, ISSN 1741-0444
3. Ulises Zaldívar-Colado, Samir Garbaya, Paúl Tamayo-Serrano, Xiomara ZaldívarColado and Pierre Blazevic., "A Mixed Reality for Virtual Assembly”, 26th IEEE International Symposium on Robot and Human Interactive Communication (ROMAN2017), August 28 - September 1, 2017, Lisbon, Portugal
4. M. Boumrah, S. Garbaya, and A. Radgui, “Real-Time Visual Analytics for Remote Monitoring of Patient’s Health ,” WSCG’203 -. International Conference in Central Europe on Computer Graphics, Visualization and Computer Vision’2023, Prague, Czech Republic
5. Nehla Ghouaiel, Samir Garbaya, Jean-Marc Cieutat, Jean-Pierre Jessel, "Mobile Augmented Reality in Museums: Towards Enhancing Visitor's Learning Experience", Vol. 17 No. 1 (2017) 21-31, https://doi.org/10.20870/IJVR.2017.17.1.2885

Illustrations :



Augmented Reality-Based Interactive Visualization of Intravenous Fluids' Flow

TITLE: THE EXPANSION OF HUMAN EXPERIENCE: SYNTHESIS OF MODERATE TRANSHUMANISM, TECHNOLOGY AND MIND

Topic number : ***2023_068***

Field : Design, Industrialization, Information and Communication Science and Technology,

Subfield: Design, Robotic

ParisTech School: Arts et Métiers
Research team: Présence & inovation https://lampa.ensam.eu/les-equipes-de-recherche-100787.kjsp?RH=1415871394252&RF=1415871394252
Research lab: LAMPA - Laboratoire angevin de mécanique, procédés et innovation
Lab location: Angers
Lab website:https://lampa.ensam.eu/le-laboratoire-100789.kjsp?RH=1415871305167&RF=1415870871805

Contact point for this topic: Arts et Métiers

Advisor 1: Colin Schmidt colin.schmidt@univ-lemans.fr
Advisor 2: RICHIR Simon simon.richir@ensam.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: This thesis aims to explore the extension of human experience through the integration of the mind, information technology, and telecommunications, while addressing the necessary adaptations to meet future challenges. Artificial intelligence, robotics/cobotics and other enticing technological endeavours offer a wide range of scenarios for the citizens of tomorrow, providing new services and fresh perspectives.

Social and Ethical Acceptability: This research places particular emphasis on the social and ethical dimensions of expanding human experience. Social and ethical acceptability is crucial in guiding the development and implementation of these new technologies. Implications for daily life, cultural values, privacy, security, and justice are among the areas that will be explored in depth.

ENSAM LAMPA ParisTECH laboratory is considering a research

framework (PEPR eNSEMBLE project, with a budget of 38 million Euros) that would potentially enhance the available academic resources and open up new opportunities for digital explorations for cooperation.

Ultimately, this research aims to contribute not only to technological advancements but also to foster a better understanding of the social and ethical implications of expanding human experience through technology. The ideal candidate should be prepared to embrace these exciting multidisciplinary challenges.

Required background of the student: Desired Candidate Profile: Minimum equivalent to French M2 by research. The ideal candidate for this thesis should demonstrate a strong interest in Philosophy, Artificial Intelligence, Technology, and minimalist Transhumanism. A solid understanding of the ethical and social issues related to technology is an essential asset. In addition, multidisciplinary skills are required to navigate through fields such as computer science, sociology, cognitive psychology, design, law, and economics. The candidate should also be open to collaboration and innovative research, as this thesis aims to push the boundaries of knowledge in the constantly evolving field of "intelligent objects" serving human everyday mental explorations.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Extensions of mind: relating to data and others, AH '20: Proceedings of

the 11th Augmented Human International Conference May 2020

https://doi.org/10.1145/3396339.3396402

2. JAYESH S. PILLAI, COLIN SCHMIDT, SIMON RICHIR (2013),

Achieving Presence through Evoked Reality, Frontiers in Psychology,

02/2013; 4:86.

DOI:10.3389/fpsyg.2013.00086

3. SCHMIDT C.T.A. (2013), “L’homme entendu. Explorations

terminologiques”, in KLEINPETER E. (Ed.) L’humain augmenté, Paris:

CNRS

Editions, collection «Les Essentiels d’Hermès»

4. SCHMIDT C.T.A. (Ed.) (2009), "Computation in the Natural World",

Special Issue of Minds and Machines, vol. 19 n° 4, Springer ; this issue

features the work of Margaret A. BODEN, Lorenzo MAGNANI and Mark

BISHOP amongst other scholars, 117 pages
5. SCHMIDT C.T.A. (2008), "Redesigning Man?", Pieter E. VERMAAS,

Peter KROES, Andrew LIGHT, Steven A. MOORE, (eds.)Philosophy and

Design:
From Engineering to Architecture, pp. 209-216: Philosophy of Science

section, Springer Science, Dordrecht. ISBN 978-1-
4020-6590-3 (Print) 978-1-4020-6591-0

Illustrations :

ParisTech

TITLE: NEW CLASS OF ELECTROCHEMICAL APTASENSORS FOR EARLY DISEASE DIAGNOSIS

Topic number : ***2023_069***

Field : Chemistry, Physical chemistry and Chemical Engineering, Life and Health Science and Technology,

Subfield:

ParisTech School: Chimie ParisTech - PSL
Research team: SEISAD https://iclehs.fr/research/seisad/
Research lab: I-CLEHS - Institute of chemistry for life and health
Lab location: Paris
Lab website:https://www.chimieparistech.psl.eu/recherche/les-laboratoires/i-clehs/

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: GRIVEAU Sophie sophie.griveau@chimieparistech.psl.eu
Advisor 2: SLIM Cyrine cyrine.slim@chimieparistech.psl.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Early diagnosis of diseases such as cancer, and the urgent need to be able to detect very low levels of tumor biomarkers, will lead to the development of new biosensors dedicated to molecular recognition and detection of biomarkers at very low concentrations in biological fluids.
The objective of the thesis is to design biosensors using a novel class of grafted polymers, surface-attached hydrogel thin films on conductive transducer as a biocompatible matrix for biomolecule immobilization. From biomolecules, aptamers constitute an attractive alternative to antibodies due to their high affinity and excellent specificity for a target or a family of selected targets. It is also possible to functionalize them with specific chemical functions and/or with a tag to label the aptamers, for their further immobilization and/or for their analysis.
The immobilization of the aptamer onto surface-attached hydrogel thin films by covalent attachment provides a biodegradable shelter, providing the aptamer excellent environments to preserve its active and functional structure while allowing the detection of biomarkers. For improved sensitivity and higher stability of the sensor, a high density of immobilized aptamer is enabled.

Within a constant miniaturization effort, we will tend towards the transposition of this work, towards microfluidic electrochemical biosensors on real matrices due to their miniature, portable, and low-cost systems as well as high throughput and automation. The integration of electrochemical sensors into microfluidic formats with the incorporation of unique materials for detection will be explored in this project. The development of these systems would bring significant advantages over current systems in terms of sensitivity, rapidity, and cost for early diagnosis.

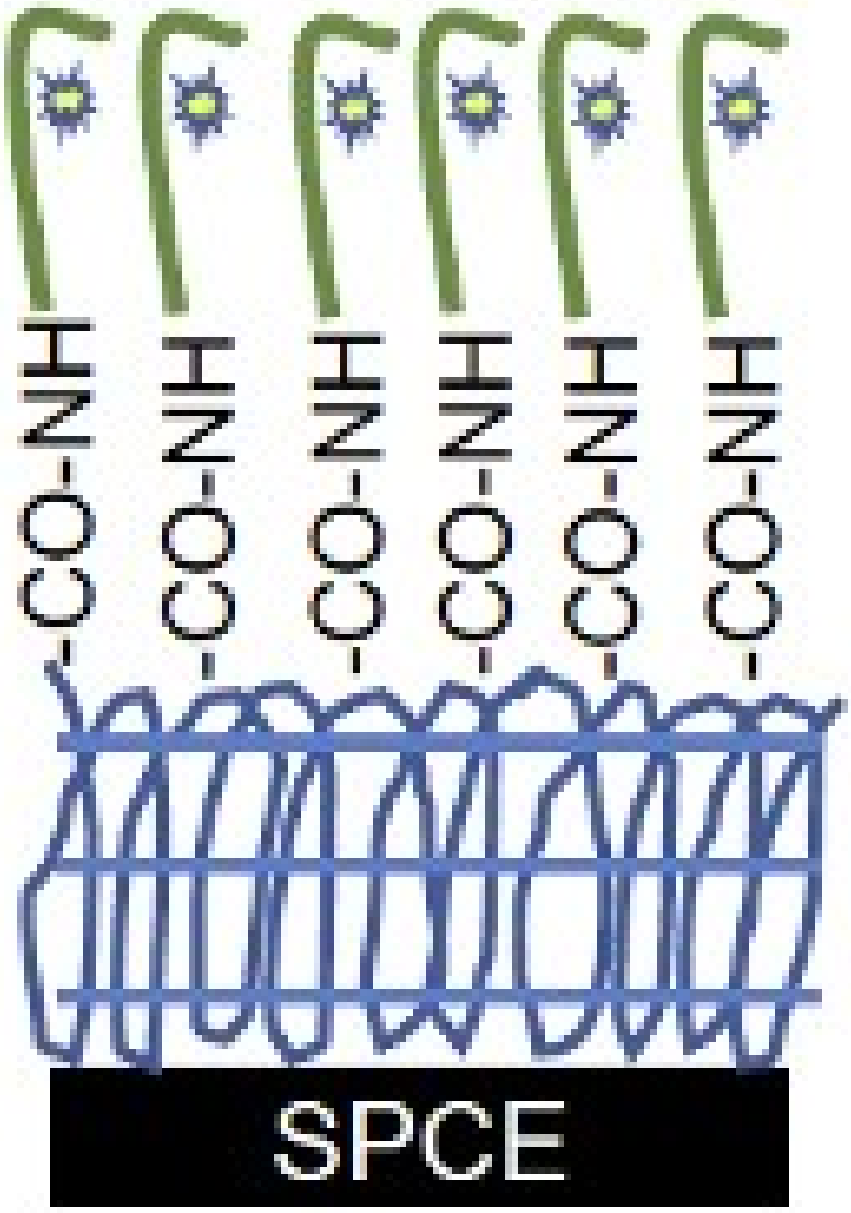
Required background of the student: Physical chemistry, ideally background in basic electrochemistry

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. 1- Kassahun, G.; Griveau, S.; Juillard, S.; Champavert, J.; Ringuedé, A.; Bresson, B.; Tran, Y.; Bedioui, F.; Slim, C. Poly(acrylic acid) hydrogel matrix based impedimetric aptasensor for the detection of diclofenac. Langmuir 36 (2020) 827–836.
2. 2- Quinton, D., Girard, A., Thi Kim, L. T., Raimbault, V., Griscom, L., Razan, F., Bedioui, F. (2011). On-chip multi-electrochemical sensor array platform for simultaneous screening of nitric oxide and peroxynitrite. Lab on a Chip, 11(7), 1342–1350
3. 3- Griveau, S., & Bedioui, F. (2013). Electroanalytical methodologies for the detection of S-nitrosothiols in biological fluids. The Analyst, 138(18), 5173–81
4. 4- Ramirez-Garcia, G., Martinez-Alfaro, M., Gutierrez-Granados, S., Alatorre-Ordaz, A., Griveau, S., & Bedioui, F. (2015). Electrochemical assessment of possible melatonin effect on nitric oxide production from kidneys of sub-acute lead treated rats. Electrochimica Acta, 166, 88–92
5. 5- Slim, C., Ratajovà, E., Griveau, S., Kanoufi, F., Ferraro, D., Perréard, C., Bedioui, F. (2015). Two-step local functionalization of fluoropolymer Dyneon THV microfluidic materials by scanning electrochemical microscopy combined to click reaction. Electrochemistry Communications, 60, 5–8

Illustrations :




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ParisTech

Arts et Métiers Sciences et Technologies

TITLE: MODELING CONTROL PARAMETERS FOR THROMBOSIS FORMATION IN VENTRICULAR ASSIST DEVICES

Topic number : ***2023_070***

Field : Life and Health Science and Technology, ,

Subfield:

ParisTech School: Arts et Métiers
Research team:
Research lab: LIFSE - Laboratoire Ingénierie des Fluides Systèmes Energétiques
Lab location: Paris
Lab website:https://lifse.artsetmetiers.fr

Contact point for this topic: Arts et Métiers

Advisor 1: KOUIDRI SMAINE smaine.kouidri@ensam.eu
Advisor 2: SPECKLIN MATHIEU mathieu.specklin@ensam.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD: Heart failure is a widespread and deadly disease in the modern world. Due to a shortage of donors, various long-term therapies have been implemented for the treatment of end-stage heart failure. Among them, ventricular assistance exhibits survival rates comparable to those achieved with a heart transplant. However, many clinical complications associated with ventricular assistance still disrupt the lives of patients, sometimes endangering their prognosis. One common complication involves the formation of thrombosis within these devices, which must be optimized to extend their implantation duration. The objective of the theoretical and numerical research work to be conducted during this thesis concerns the modeling of thrombosis that develops under the operating conditions of the cardiac assist device, taking into account the specific hemodynamic constraints of this device.

Required background of the student: Fluids Mechanics, Mechanical Engineering

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. L. Marcel, M. Specklin, S. Kouidri, The Evolution of Long-Term Pediatric Ventricular Assistance Devices, Expert Review of Medical Devices, 2021, Vol 18(8), pp. 783-798, doi.org/ 10.1080/17434440.2021.1947245
2. J. Song , S. Kouidri, F. Bakir, Numerical study of hemodynamic and diagnostic parameters affected by stenosis in bifurcated artery, Computer methods in biomechanics and biomedical engineering, June 2020
3. J. Song , S. Kouidri, F. Bakir, Numerical study on flow topology and hemodynamics in tortuous coronary artery with symmetrical and asymmetrical stenosis, Biocybernetics and Biomedical Engineering, January 2021
4.
5.

Illustrations :