EMERGENT: dEvelopment of MassivEly paRallel numerical methods for the efficient desiGn of novEl mechaNical meTamaterials

Name of the graduate program (Master 2) : Master mécanique, parcours Modélisation et applications en mécanique (Master's degree, specialization in Modelling and Calculations for theoritical mechanics)
Laboratory for the internship : Laboratoire des Matériaux Composites pour la Construction (LMC2) (Civil Engineering Laboratory)

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Summary :

This project aims to recruit a final-year master's student specialized in theorical mechanics, offering a scholarship and support, with the prospect of completing their internship in the partner laboratory upon achieving strong academic performance. The student will follow courses during the fall semester, and will complete its training by working in the lab for their final internship, during 6 months.

Project EMERGENT aims to revolutionize the design of novel mechanical metamaterials by developing an innovant parallel numerical methodology. To do so, EMERGENT proposes an innovative framework leveraging spectral methods based on Fast Fourier Transform (FFT) and level-set (LS) approaches. FFT-based methods avoid physical-space meshing and inherently satisfy boundary conditions through Fourier series. The LS method captures complex topologies with continuous boundary definitions, ensuring manufacturability. Computational efficiency will be achieved through massively parallel processing using General Purpose Graphics Processing Units (GPGPUs).
The internship involves developing a numerical proof of concept by integrating FFT/LS formulations and parallelizing computations with GPGPU, with applications in 3D-printable materials, cloaking technologies, and advanced metamaterial design.

Project :

The advancement of new metamaterials across various scientific disciplines - such as civil engineering [1, 2], theoretical physics [3, 4], mechanical engineering [5], and acoustics [6] - requires the application of sophisticated numerical methods.
The first essential step is to define and numerically model a Representative Volume Element (RVE) of the material in order to derive the homogenized behavior of the entire material from the computation of the RVE's behavior. Traditionally, the Finite Element Method (FEM) is used to model the RVE [7], which demands specific treatments to ensure compatible boundary conditions (periodic). Secondly, to develop new materials exhibiting unconventional mechanical or physical properties, it is then necessary to optimize the material distribution within the RVE to ensure that the homogenized behavior aligns with the desired properties [7]. Topology optimization algorithms, such as ESO [9] and SIMP [10], are conventionally applied to FEM-discretized RVEs. However, these approaches often result in designs that are difficult - sometimes impossible - to manufacture, display visible elements, and promote stress concentrations. Overcoming this scientific lock is

crucial to allow the manufacture of such materials in accordance with the new 3D printing capabilities for metal, concrete or plastic.

To address these challenges, the team members propose a new methodology in stark contrast to conventional methods mentioned above. First, the numerical model of the RVE will be based on a spectral decomposition instead of FEM formulation. These methods, usually employed in Computational Fluid Dynamics (CFD), are particularly suitable here, as they: i) enable the discretization of Partial Differential Equations (PDEs) without requiring a mesh of the physical space, and ii) are inherently compatible with boundary conditions by a careful choice of spectral base (Fourier series here). Thereafter, level-set-based methods will be employed to capture the RVE’s complex topology. Their mathematical definition of boundaries between different material zones within the RVE allow a continuous – and then manufacturable – description of RVE’s shape, in agreement with the desired homogenized behavior. Finally, given that the numerical calculations can be computationally intensive, massively parallel methodologies are required. The use of emerging general purpose graphical processing unit (GPGPU) computing technologies is being considered in this project, for their computing and energy consuming efficiency.

The objective of this internship is to develop a numerical proof of concept of this new methodology by integrating a coupled Fast Fourier Transform (FFT)/Level-set (LS) formulation for the numerical resolution of the RVE. The whole procedure will be parallelized under the GPGPU paradigm.

The applications of such a theoretical project are numerous. Once the theoretical framework is established, the methodology can be easily adapted to various fields of physics and mechanics: the development of new hyper-viscoelastic materials – even if they are made of classical linear elastic isotropic materials - suitable for 3D printing, the creation of acoustic or visual invisibility cloaks, and more.

Welcoming the student and organizing their stay in France :

The student selected for this program will be awarded a scholarship of €1,000 per month for 10 months. They will study within the Mechanics department, following the "Modeling and Applications in Mechanics" program, during the fall semester.

As part of this program, the student will receive guidance in selecting courses that will provide them with the knowledge needed to successfully complete the internship project. In particular, 2 courses will be followed by the selected student: i) Advanced modelling and calculation techniques for theoritical mechanics (including Finite Elements, Finite Differences, Spectral Decompositions, linear problem solving methods), and (ii) Parallel computations.
Finally, the student will work for six months on the EMERGENT project under the guidance of their supervisors.

<u>Expected skills for candidates</u>:

- Completion of an M1-level program in numerical modeling of mechanical problems,
- Solid knowledge of numerical methods used in mechanics,
- Proficiency in programming with various languages (Python, C, C++, Fortran, laTex).
- Strong written and verbal communication skills in English,
- Adaptability to new environments,
- Ability to work in a team and communicate effectively with supervisors.