SSM
Scuola Superiore Meridionale

MERC PhD Project Proposal 2022/2023

Title of the research project:

Physics-informed machine learning for the multiscale modelling and numerical bifurcation analysis of complex fluids and materials

Keywords (up to five)

Physics-Informed Machine Learning, Manifold Learning, Complex Fluids and Materials, Bridging Micro- Macro Scales, Coarse-Grained Bifurcation Analysis

Supervisors (at least two from two different areas):

Supervisor 1 (Constantinos Siettos, MERC board member, Complex Systems, Physics-Informed Machine Learning, Numerical Analysis)

Supervisor 2 (Pier Luca Maffettone, MPSAMT board member, Dipartimento di Ingegneria chimica, dei Materiali e della Produzione industriale, Rheology, Microfluidics, Soft Matter, CFD simulations)

Supervisor 3 (Yannis Kevrekidis, Dept. of Chemical and Biological Engineering, Dept. of Mathematics and Statistics, Johns Hopkins, Algorithms, Equation-Free computations, Dynamical Systems, Data Mining, Complex Systems Modelling)

Supervisor 4 (Lucia Russo, STEMS, CNR, Agent-based modelling, Bifurcation theory, Spatio-Temporal Dynamics)

Project description (max 5000 characters)

A persistent feature of complex systems in materials science is the emergence of macroscopic, coherent behavior from the interactions of microscopic atoms/molecules- between themselves and with their environment. The implication is that macroscopic rules (description of behavior at a high level) can somehow be deduced from microscopic ones (description of behavior at a much finer level). For some problems (like Newtonian fluid mechanics) the successful macroscopic description (the Navier Stokes equations) predated its microscopic derivation from kinetic theory. In most current fluid-dynamics problems involving complex fluids however, the physics are analyzed at the microscopic level, and the closures required to translate them to a macroscopic scale description are often not available. The construction of effective multiscale dynamical models in the form of ODEs and time-dependent PDEs for the macroscopic/emergent dynamics deriving from the atomistic interactions, which take place in a finer spatio-temporal scale, is at the forefront of current research. In its essence this constitutes the solution of the inverse problem in complex systems modelling leading to physical laws and their closures from data. Such data may come from experiments, or from high dimensional microscopic/multiscale computations such Monte-Carlo, Agent Based, Brownian Dynamics and Molecular Dynamics simulations. An interesting paradigm of such "micro-macro" bridging is the case of liquid crystalline polymers. These are large, anisotropic molecules that generally contain long rigid or semirigid segments that can show phase transitions. In the liquid crystalline state such systems are known to exhibit complex and nonlinear rheological behavior when subjected to shear flows [1-3]. Theoretical and experimental works have shown that, depending on shear rate, several stationary and oscillatory regimes (periodic and even chaotic) can been observed. Rheological predictions of the behavior of such complex fluids often start with the derivation of macroscopic, approximate equations for quantities of interest (order parameters) using various (frequently ad hoc) closure approximations; these closed equations (Ordinary or

Partial Differential Equations) are then analyzed with mathematical techniques for stability and parametric analysis.

State of the art

A key component toward the construction of macroscopic dynamical models in the form of ODEs and PDEs and their analysis from detailed spatio-temporal data is the extraction of the right coarse–grained observables. This is where there have been breakthroughs in the last few years, in terms of numerical analysis, optimization techniques, machine learning and big data. These methods include Diffusion Maps [4] for the identification of the slow manifolds that allow us to identify low-dimensional nonlinear manifolds and their dimensionality Furthermore, theoretical and technological advances over the last few years on physics-informed machine learning have facilitated our ability to discover hidden physical laws in the form of ODEs and PDEs from multiscale/multiphysics high-fidelity observations [5-10]. For complex fluids and materials such as the liquid crystals the state of the art in the modelling are "detailed simulators" such as Brownian and Molecular Dynamics models [11, 12]. These can be used in combination with computational fluid dynamics methods to simulate the behavior of complex fluids in spatially inhomogeneous flows. In particular, for liquid crystals such detailed simulators describe the motion and/or the evolution of the orientation of each molecule under flow in the presence of different potential fields.

Objectives

Our goal in this Thesis is to develop multiscale computational methods to go beyond the state-of-the-art in the modelling and analysis of multiscale/complex fluids and materials with a focus on Liquid Crystals. Based on detailed simulations and possibly available experimental data, we aspire to solve both the inverse and forward problem in the field, thus developing and using physics-informed machine learning algorithms: (a) to discover from microscopic spatio-temporal simulations the closures required to build macroscopic models in the form of ODEs and mesoscopic models in the form of Fokker-Planck (Smoluchowski) PDEs in a closed form, (b) to exploit the arsenal of numerical bifurcation analysis toolkit and Equation-Free approach to systematically investigate the dynamics by computing bifurcation diagrams (see e.g. [13, 14]) with the aim of identifying critical points and manifolds that mark the onset of phase/regime transitions and explaining the emergence of global bifurcations that give rise to spatio-temporal chaos .

This will be accomplished in the following ways:

(a) in black box manner by advancing the existing computational technology with feature extraction algorithms and Manifold learning for identifying the intrinsic dimension of the embedded low-dimensional manifold on which the emergent dynamics evolve and based on a set of appropriate coarse-variables that parametrize the manifold, identify dynamical models of ODEs and PDEs;

(b) gray box, in a multifidelity context, learning better closures of existing approximate dynamical equations obtained analytically under strong and simplified assumptions.

(c) by investigating the dynamics of the constructed continuum models with bifurcation analysis, to detect critical points and manifolds that give rise to phase-transitions, and to unveil more complex phenomena that may arise also due to global bifurcations.

Relevance to the MERC PhD Program (max 2000 characters)

Briefly describe how this project fits within the scope of the MERC PhD program describing its interdisciplinary aspects, relevance in application and beneficiaries.

The proposed research is highly interdisciplinary at the junction between contemporary multiscale complex systems modelling and analysis and mathematical modelling in materials science. Thus, the scientific keystones of the proposed PhD, cut across traditional boundaries between applied mathematics, complex systems, fluid mechanics and soft matter, numerical analysis, microscopic simulations, statistical mechanics and Artificial Intelligence. Through their combination, the proposed approach holds the promise for making a step change to our ability of understanding and analyzing complex systems from data.

The research will also have a far-reaching educational significance through the fundamentally new results that aims to introduce. In the short term, the research will have immediate educational impact on the graduate students and post-doctoral scholars who will be involved in the research.

Key references

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[12] Y. Tao, W. den Otter, KJG Dhont, WJ Briels, 2006, sotropic-nematic spinodals of rigid long thin rodlike colloids by event-driven Brownian dynamics simulations, Journal of chemical physics, 124, 134906.
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[14] F. Gianluca, F. Calabrò, L. Russo, C. Siettos, 2021, A Numerical Solution and Bifurcation Analysis ofNonlinear Partial Differential Equations with Extreme Learning Machines, Journal of Scientific Computing, 89, 44.

Joint supervision arrangements

Describe joint supervision arrangements, e.g. weekly/monthly meetings with one or both supervisors, how will the joint supervision be split etc.

The supervisors are world-wide experts in the various fields of the project, they are collaborating along the research lines of the project since many years, they share common vision and enthusiasm to transfer knowledge and motivation and educate students. They will work closely with the PhD student for the successful completion of the Thesis. The student will meet and discuss on a daily basis with the principal supervisor (C. Siettos), while there will be other regular meetings on a bi-weekly basis with all supervisors, including the period abroad when such meetings will be held remotely.

Location and length of the study period abroad (min 12 months)

The PhD student will spend a period of 12 months at the Laboratory of Prof. Yannis Kevrekidis at Johns Hopkins, USA

Any other useful information

The PhD research project anticipates also the collaboration with world-expert research groups and in particular with the group of Prof. Geroge Karniadakis, Dept. of Mathematics, Brown University and Prof. Athanasios Yannakopoulos, Dept. of Statistics, Athens University of Ecomomics and Business. The student will also benefit with the interactions with these groups through short visits during the period of the PhD Thesis.