Call for 1 PhD candidate

Summary of the position and institute

- A 3-year PhD position
- Thesis director: Prof. Manas V. Upadhyay
- Affiliation: Solid Mechanics Laboratory (LMS), CNRS, Ecole Polytechnique, Institut Polytechnique de Paris
- Tentative start date: September 1, 2024
- Application deadline: February 15, 2024

Ecole Polytechnique is a French public institution of higher education and research. It was established in 1794, during the French revolution, by the mathematician Gaspard Monge. Among its alumni are 3 Nobel prize winners, 1 Fields Medalist, 3 Presidents of France and many CEOs of French and international companies. It was ranked 61st worldwide by the QS World University Rankings 2021 and 2nd by the Times Higher Education Small University Rankings.

LMS is a joint research unit between the Ecole Polytechnique and the French national research center (CNRS). Research at LMS integrates experimental studies as well as the mathematical and numerical modeling of the mechanical and multi-physics behavior of materials and structures over a wide range of spatial and temporal scales.

General context of your project

Dislocations are line-type crystalline defects [1]. They are primary carriers of plastic deformation in all metals and alloys and they have a first order effect in determining the mechanical response of these materials. They are also a primary source of residual stresses in materials. Understanding dislocation dynamics and interactions with other defects is therefore crucial for predicting the material's subsequent mechanical response during processing or under service conditions. This understanding has been primarily gained via continuum-based dislocation dynamics models such as discrete dislocation dynamics and continuum dislocation dynamics.

However, these models require imposing a large set of kinematic and kinetic rules for dislocation presence, motion and interactions with other defects. Any prediction made by them is subject to these imposed rules and removing/adding a rule can drastically change the result. Furthermore, adding a large number of rules for each simulated defect makes large-scale simulations intractable.

For a dislocation dynamics model to be truly predictive, dislocation motion and interactions must be emergent phenomena of the (i) underlying crystal structure instead of imposed rules, (ii) conservation laws (mass, momenta, energy, and topological charge i.e., Burgers' vector), (iii) constitutive laws from non-negative dissipation, and (iv) imposed boundary conditions.

The continuum-based field dislocation mechanics approach [2,3] is currently the state-of-the-art isothermal dislocation initial boundary value problem that models (ii) – (iv) mentioned above and provides (exact) solution for prescribed polar dislocation density fields. However, it lacks topological information from the underlying crystal lattice and cannot keep dislocation cores compact. In other words, it cannot correctly model (i).

Your project and tasks

Title: Modeling dislocation mechanics without imposed kinetic or kinematic rules

Acharya and Viñals [4] recently proposed to remedy this problem by coupling FDM and the phase-field crystal (PFC) approach. PFC is a kind of phase-field approach where the continuous order parameter (say ψ) is related to the atomic number density. PFC employs a free-energy functional of ψ that reproduces a lattice and it is minimized by a periodic ψ of the corresponding lattice symmetry using (L^2/H^{-1}) gradient flow. When modeling dislocations, ψ acts as an indicator function for location of dislocations and importantly, conservation of Burgers vector is an emergent phenomenon of the model. PFC keeps dislocation cores compact and coupled PFC-FDM opens the path to modeling dislocation dynamics without imposed kinetic/kinematic rules under large deformations and at diffusive time scales i.e., under quasi-static loadings.

Your tasks are as follows:

- Thoroughly understand the coupled PFC-FDM theory and perform theoretical developments if necessary.
- Numerically implement the model in a finite element framework inside "FEniCS" FE solver.

- Perform simulations using the model, analyze the results and verify/validate them whenever possible.
- Collaborate with Prof. Jorge Viñals (University of Minnesota, USA), possibly a secondment in the USA
- Write and publish scientific articles in relevant journals
- Present your research at national and international conferences
- Write and successfully defend your PhD thesis at the end of the project

References:
[1] D. Hull and D. J. Bacon, Introduction to Dislocations, *Elsevier Ltd.* (2005) 5th Edition.
[2] A. Acharya, Constitutive analysis of finite deformation field dislocation mechanics *J. Mech. Phys. Solids*. **52**, 301–316 (2004).
[3] R. Arora, X. Zhang, A. Acharya, Finite element approximation of finite deformation dislocation mechanics. *Comput. Methods Appl. Mech. Eng.* **367**, 113076 (2020).
[4] A. Acharya, J. Viñals, Field dislocation mechanics and phase field crystal models. *Physical Review B* 102 (2020) 064109.

Your profile

Necessary
- A Master's degree (Bac+5, for French applicants) in Physics, Mechanical Engineering, Mechanics, Materials Engineering or equivalent obtained after January 2023. Interested candidates graduating before June 1, 2024 can also apply.
- Background in mathematics, specifically solving partial differential equations and functional analysis.
- Programming skills in at least one of the following computer languages: Fortran, Python or C++.
- Good communication (oral and written) skills in English.
- You should be able to work independently as well as in a team. You enjoy working on challenging problems. You should be able to think critically, work diligently and rigorously, and present your ideas in a logical manner.
- You enjoy working in a multi-disciplinary team having an international background.

Not necessary, but a plus
- Experience in using FEniCS
- Research experience and ability to write scientific manuscripts (e.g. master's thesis)
- Experience in the field of dislocations

Interested candidates that **fulfill all the necessary criteria**, please contact send an email to the address below with
- 1-page motivational letter
- Up-to-date and detailed CV
- Contact information of at least 2 referees willing to provide recommendation letters on your behalf

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