Post-doctoral position

Deep learning in materials science : predicting macroscopic properties of a material by analyzing its microscopic structure

Brieuc Conan-Guez, Frédéric Pennerath, Lydia Boudjeloud-Assala
LORIA (Orpailleur)
{brieuc.conan-guez,lydia.boudjeloud-assala}@univ-lorraine.fr,
frederic.pennerath@centralesupelec.fr

Context

Artificial Intelligence, with the advent of *Deep Learning* [1], has recently enabled spectacular advances in various fields of scientific research. It is now currently used in fields such as chemistry and molecular biology, astrophysics, particle physics, health science, etc. The aim of this post-doctoral position is to explore some possible applications of Deep Learning to *materials science* [2].

Structure and properties of polycrystalline materials

Developing new materials, such as high-performance metals and alloys, presents many challenges [3]. One of these is to determine the macroscopic mechanical properties of a material (for instance its ductility) by studying its microscopic structure (atomic composition and structural organization).

In this work, we focus on a specific class of materials, called polycrystalline materials. These materials are made up of millions of invisible grains (ranging in size from a few nanometers to several hundred). Each grain is a regular atomic lattice that can exhibit different symmetries. Neighboring grains differ in shape and spatial orientation (Euler angles). Grain organization determines the material's macroscopic mechanical properties.

When a load (tensile stress) is applied to a material sample, each grain undergoes a stress which results of the interaction stresses produced by its neighbors in order to maintain the cohesion of the sample. To release this mechanical stress, grains have to deform through atomic slippage in the atomic lattice. These slides are likely to leave defects within each grain, known as dislocations.

To study these deformations, materials researchers have different tools at their disposal : they can for instance produce highly detailed images of grains (Euler maps) using electron microscopes (Scanning Electron Microscopes (SEM)). These maps reflect the position, shape and spatial orientation of each grains on the surface of a material [4].

Materials scientists can also rely on numerical simulations using 3D physical models to predict the material's response to stress. These models depend on a number of parameters that need to be specified by the scientists prior to simulation.

These tools are not without their drawbacks. Experimental studies using electron microscopes are very time-consuming. This limits the amount of data that can be acquired. Similarly, physical models require complex partial differential equations to be solved, resulting in very long computation times (many hours).

A research problem in deep learning

The aim of this thesis is to develop new tools based on deep learning techniques to help materials scientists in their research.

A first research direction would be to use classical neural networks as a complement to existing physical models to predict material deformation at the microscopic level. More precisely, an Euler map of the unloaded sample is provided to the predictive model along with the magnitude and direction of the applied load. As a result, the neural network estimates the Euler map of the same sample after deformation. Convolutional neural networks (CNN), the U-Net architecture [5] and spatial transformer networks [6] seem well suited to this task, since Euler maps are numerical tensors.

However, this classical approach does have a drawback. The predictive model is built without any a priori knowledge of physical laws governing the constitution of materials. These fundamental laws must therefore be rediscovered by the model during its learning phase. This requires a very large volume of data, the availability of which is not necessarily compatible with experimental reality.

One possible way of overcoming this obstacle is to use a new class of neural networks, called Physics-Informed Neural Networks (PINN) [7]. For a PINN-type network, the architecture of the model is no different from that of a classical network. However, the error function used during the training phase, is adapted to inject a priori knowledge of physical laws into the model. More precisely, the error function is the sum of two terms : one term that measures how well the model fits experimental data (as in a classical neural network), and a second term that measures how well the model conforms to physical reality. One of the advantage of PINN networks, is that they require a smaller volume of data than classical approaches.

Required work

1. state of the art on deep learning applied to materials science
2. development of neural predictive models
3. the design of these models will be guided by knowledge acquired in materials science

Required Skills

— thesis in computer science, with skills in machine learning and data science
— Proficiency in Python and Pytorch/Tensorflow
— skills in materials science would be a plus

Additional information

- the postdoctoral researcher will be part of the team for the MAMIE NOVA project (Machine LeArning for MIcromEchanics : A NOVel Approach), which is funded by the ANR (National Agency for Research)
- two research laboratories are involved :
  - LORIA laboraty (Laboratoire Lorrain de Recherche en Informatique et ses Applications) - team Orpailleur
  - LEM3 laboratory (Laboratoire d'Etude des Microstructures et de Mécanique des Matériaux)
- a team of supervisors from computer science and materials science
  - Brieuc Conan-Guez (MCF - LORIA), Frédéric Pennerath (MCF - LORIA), Lydia Boudjeloud-Assala (PR - LORIA)
  - Antoine Guitton (PR - LEM3) - Vincent TAUPIN (CNRS - LEM3) - Benoît BEAUSIR (MCF - LEM3)
- location : LORIA - Metz, CentraleSupelec
- remuneration : project MAMIENOVA
- duration : 2 years

To apply

Please send your detailed CV and a cover letter to the addresses :

- Brieuc Conan-Guez : brieuc.conan-guez@univ-lorraine.fr
- Frédéric Pennerath : frederic.pennerath@centralesupelec.fr
- Lydia Boudjeloud-Assala : lydia.boudjeloud-assala@univ-lorraine.fr
- Antoine Guitton : antoine.guitton@univ-lorraine.fr

Recommendation letters are not required, but please include the contact information of your references. You can also provide a published article on machine learning.

Références

[1] Ian J. Goodfellow, Yoshua Bengio, and Aaron Courville. *Deep Learning*. MIT Press, 2016.

[2] S. Sandfeld. *Materials Data Science*. Springer Charm, 2024.

[3] Hull D. and Bacon D.J. *Introduction to Dislocations (Fifth Edition)*. Butterworth-Heinemann, 2011.

[4] Dipendra Jha, Saransh Singh, Reda Al-Bahrani, Wei-keng Liao, Alok Choudhary, M. Graef, and Ankit Agrawal. Extracting grain orientations from ebsd patterns of polycrystalline materials using convolutional neural networks. *Microscopy and Microanalysis*, 24 :497–502, 10 2018.

[5] Olaf Ronneberger, Philipp Fischer, and Thomas Brox. U-net : Convolutional networks for biomedical image segmentation. In Nassir Navab, Joachim Hornegger, William M. Wells III, and Alejandro F. Frangi, editors, *Medical Image Computing and Computer-Assisted Intervention - MICCAI 2015 - 18th International Conference Munich, Germany, October 5 - 9, 2015, Proceedings, Part III*, volume 9351 of *Lecture Notes in Computer Science*, pages 234–241. Springer, 2015.

[6] Max Jaderberg, Karen Simonyan, Andrew Zisserman, and Koray Kavukcuoglu. Spatial transformer networks, 2016.

[7] M. Raissi, P. Perdikaris, and G.E. Karniadakis. Physics-informed neural networks : A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational Physics*, 378 :686–707, 2019.