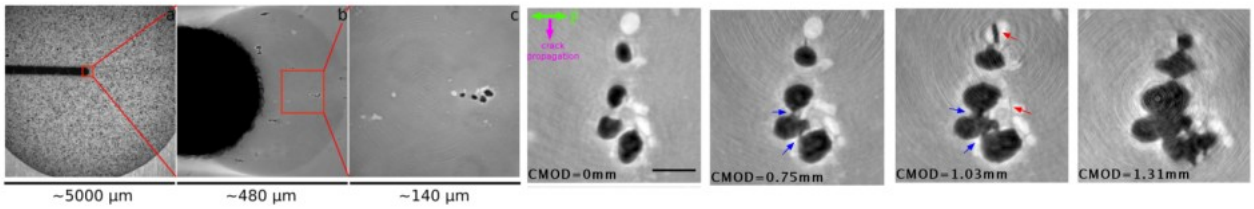
Exploration of damage nucleation models using graph-based deep-learning methods

Master Research Internship at Mines Paris

Context

Strong, formable, damage-tolerant and recyclable materials are crucially needed to reduce CO2 emissions in the transport industry, particularly concerning vehicles with combustion engines but also electric cars. Damage nucleation has gained particular interest in industry as recycling of alloys often leads to higher impurity content and associated amount of brittle intermetallic particles in the alloys. In forming and associated ductile fracture, the damage nucleation on micrometre-sized brittle particles remains poorly understood and hard to predict. Computerized predictions, as well as simulation data, obtained on realistic virtual microstructures, are needed in materials-by-design frameworks that seek to control and enhance the mechanical response of microstructures. Damage evolution is driven by the local stress state, which is itself a complex result of the load distribution within the microstructure of the material. Experimental (4D, i.e. space and time) data, image analysis, meshing tools and full-field computational methods (e.g. finite element) have been developed in an effort to obtain a unified and reliable damage model at the macroscopic scale that works under a wide variety of loading conditions. Nevertheless, the role of stress or strain as well as of particle nature, size and shape remains unclear and hard to predict, yet crucial for formability and fracture. The underlying physics responsible for damage nucleation and evolution is still nowadays an open question. The complexity of such mechanisms suggest that the problems should be tacked at lower scales, i.e. at micrometre scale, which put such study far away from industrial applications. On the other hand, results from literature show that the use of macroscopic phenomenological models do not allow to obtain a generic and unified damage nucleation model, which lead to ad-hoc ingredients that allow to fit some experimental observations. The nucleation of damage and its evolution is currently driven by phenomenological macroscopic laws that are far too simple and cannot accurately reproduce the complexity observed in real systems.

Machine learning techniques could offer alternative strategies to such phenomenological damage laws. Large experimental 4D datasets, of prime importance in this context, are available and can be used in order to develop machine learning pipelines. To train these models and perform inverse identification, experimental observations could be adequately supplemented by simulation data. Yet, this approach suffers from two main drawbacks. First, state-of-the-art micromechanical computations are most often based on meshing of the structures whereas deep-learning pipelines are often based on images. Second, the computational time involved in carrying out 4D simulations on representative volume can be extreme. To address these problems, we propose to use specific graph-based machine-learning methods to leverage existing experimental and computational methods at the microscopic scale, at which the microstructure of the material can be resolved. In particular, Graph Convolutional Networks (GCNs) are deep-learning pipelines that are useful to deal with data generated on fairly-general discrete domains where interdependency between objects is explicitly represented and have lately been adapted to treat mesh-based physical simulation or to deal with crack coalescence and phenomena occurring at the crack tips. The methods yield much more rigorous identification procedures by taking into account mesh-dependency explicitly in PDE solvers, and therefore can be validated unambiguously.



Aluminium sample with a notch, in visible light microscopy image and high/ very high resolution Laminography (left) and development of several voids (black) nucleated at secondary phase particles (white) during loading (right). The scale bar corresponds to 10 µm.

Internship objectives and supervision

This internship will be devoted to developing deep-learning methods that predict material and mechanical parameters based on simulated data obtained using finite element. Model problems and microstructures of increasing complexities will be first considered. Graph-based machine-learning methods, that allow for an exact match between the network and finite element meshes, will be considered. Transfer learning approaches between graphs representing coarse and fine meshes will be implemented and investigated as well as active learning methodologies, where finite element simulations are performed on the fly to train the networks.

The internship work will be jointly supervised by Santiago Velasco-Forero, François Willot (Center for Mathematical Morphology), Daniel Pino Munoz (Centre de mise en forme) and Thilo Morgeneyer (Centre des matériaux)

A student with excellent background in either mechanics, numerical methods or machine-learning techniques is sought for. A publication may be written and submitted to a journal, depending on the internship results. The internship work may be pursued by a PhD thesis.

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