Sujet de thèse PR[AI]RIE-PSAI 2025-2028

Acronym	ADDAM		
Project Title	Scientific deep learning for Anomaly Detection in ductile DAmage Modeling applied to metal forming		
Duration	36 months		**Application deadline May 30, 9 a.m.** Selection results between May 30 and June 15.
Keywords	Scientific Machine Learning, XAI, Model Order Reduction, HPC, Point Cloud, Anomaly Detection, Ductile Damage		

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Summary of the project: Damage is a particular form of anomaly in material forming. These anomalies come from materials microstructure heterogeneity that drives ductile damage mechanisms. We propose to combine deep learning for anomaly detection and mechanical modeling of damage. This work is limited to the use of synthetic data produced with mechanical models calibrated in the context of previous work in materials mechanics. However, these models remain imperfect, in particular for dealing with recycled materials or, in general, materials with a high variability of their physical properties. In this case, an anomaly may be caused by unusual properties or an unsuitable mechanical model. The anomalies will be identified as cases out-of-distribution of so-called normal data. The objective of this project is to develop: (i) self-supervised learning of a latent space of normal data, (ii) an anomaly detection task using this latent space, (iii) a final stage of scientific explanation of the causes of anomalies based on explainable AI. All this in the context of large deformations of point cloud.

1. Context of point cloud deformations and main objectives

Scientific machine learning (SciML) is an interdisciplinary field that combines physics-based modeling and scientific computing. In this proposal, we address the following limitations of continuum damage models for metal forming applications [Tekkaya et al., 2020] that are based on partial differential equations and scientific computing: (i) Such physics-based models, with observational data as inputs, are not designed to detect anomalies or modeling errors in real time, even using high performance computing facilities. (ii) Predicting large shape changes of the domain in which PDEs are set up requires complex shape descriptors such as mesh adaptation in finite element models. Such adaptive descriptors hinder the definition of a common ambient space for an extensive statistical analysis of model's predictions.

In this project, we focus our attention on out-of-distribution (OOD) anomaly detection in a statistical framework [Yang et al, 2024]. Our target application is to incorporate more recycled material with stochastic properties into forming processes of aluminum. When considering recycled material, understanding damage is a crucial issue to produce high quality components. Generally speaking, recycling materials makes physics properties of materials more stochastic. For aluminum alloys this conducts to higher contents of intermetallic particles or presence of particles cluster who influence significantly ductile damage mechanisms [Hannard et al., 2016]. To facilitate the definition of a common ambient space, this project considers a point cloud representation [Guo et al, 2020], [Saranti et al., 2024] of shapes and internal states, for both observational data and synthetic data computed by physics-based models. The success of this project will be evaluated in terms of its ability to integrate recent advances in deep learning for point clouds; its ability to detect simulated damage with stress states or geometric defects that do not form part of the training domain.

In this project, the high dimensional data that are the solution of a PDE are a priori down-sampled to a reasonable dimension, about 1000, to facilitate machine learning on 3D point clouds. Data clustering could be a solution for this down-sampling. This down-sampling step is also an answer to another major challenge: the management of huge amounts of data and the environmental impact, which raises questions of sustainability.

Let us refine the details of this project. Our objective is to develop a scientific deep learning approach to anomaly detection in the context of large deformations of point clouds [Beetz et al., 2023], while maintaining a high level of scientific explainability. It is a contribution to Human-Centered Artificial Intelligence [Riedl, 2019], where an AI system helps scientists understand AI predictions in a reasonable time. In this proposal, mechanical submodeling and explainable AI are coupled to understand AI predictions [Tan et al., 2022]. It is a contribution to the development of new, reliable and robust AI methods through hybridization with knowledge specific to mechanics of materials. It is a revolutionary objective. Anomaly detection will be a downstream task using the latent space of a pre-trained model for point cloud deformations. The physics-based model used for the generation of the train dataset is referred to as high-fidelity model (HF-model). This HF-model will be based on Forge finite element simulations which includes enhanced coupled/uncoupled damage models [Bouchard et al. 2011]. Such macroscopic damage models often fail at including microstructure anomalies such as the presence of oriented particles cluster in critical areas that can lead to premature failure [Bouchard et al. 2008].

We consider the following multi-modal data: Input data of the HF-model including shape description, denoted by X_{in}; the down-sampled prediction of the HF-model, denoted by X_{out}. X_{in} includes observational data such as, but not limited to, a point cloud on the surface after deformation of object. The multimodal data (X_{in}, X_{out}) are conventional data in surrogate modeling of physics based model. Being related to the solution of a PDE, this data contains sufficient information to design a submodel around a given zone of interest [Launay et al. 2022].

The train dataset will contain normal data related to normal point cloud deformations understood using a normal HF-model, with low damaged materials. In this dataset, we will consider various constitutive models of different aluminum alloys, that are available in scientific publications and datasets. Normality will be precisely defined according to the application domain. We assume that all anomalies, or their effect, can be observed on 3D point cloud of object surface. A statistical distance to the latent space will serve as an OOD anomaly detection. No anomaly will be a priori defined in that context. The scientific explanation of anomaly detection will be a complementary downstream task. Explaining how data is processed in inference time through the layers of a neural network is beyond the scope of this project.

The explanation aims to answer the following questions: Why was a data instance detected as abnormal/normal? Is it the HF-model or the input data that is causing the anomaly? Can we identify where the anomaly lies in the input data or in the HF-model used to generate the training set? Is the anomaly related to damage of the material? The submodel, equipped with boundary condition from machine learning, will guide the human explanation of anomaly detection. The subdomain of the submodel, will be generated by using Masked autoencoders [Zhang et al, 2022] and eXplainable AI (XAI) [Mulawade et al., 2024]. The proposed scientific explanation process is similar to a digital twining of deep neural network prediction by using mechanical submodels. Here the submodel aims to be a more explainable twin, not a faster digital twin. A good understanding of the data is achieved when the submodel outputs match the anomalous data as a result of submodel calibration.

2. **Reference**

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3 **How to apply**

Send the following documents to david.ryckelynck@minesparis.psl.eu

· a CV;

· a one-page cover letter describing ypur ambitions for the above PhD subject and the relevance of the application in relation to the description of the subject;

· a copy of your latest qualifications