## Institut des Transformations Numériques (ITN) – Manifestation d'intérêt

### "Multi-physics model-free problems in elastoplasticity using heterogeneous local fields"

proposé par
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# 1 Context and scientific objectives:

Engineering materials are increasingly used in industrial applications under different strain rates, temperatures and loading conditions. To ensure in-service robustness and to predict the durability of components, identifying *reliable* and *consistent* models is of prime importance. Besides, macroscopic mechanical behaviour is commonly characterised by the stress-strain curve obtained from uniaxial tests. This identification method – empirical modelling and identification linked with data from uniaxial tests – induces some limitations.

The prevailing simulation paradigm has been to calibrate empirical material models using observational data and then use the calibrated *constitutive model* in calculations. This process of modelling *a fortiori* adds error and uncertainty to the solutions, especially in systems with high-dimensional phase spaces and complex behaviour. This modelling error and uncertainty arise from imperfect knowledge of the form of the material laws, the phase space in which they are defined, and from scatter and noise in the experimental data [1]. Besides, often the models used to fit the data are ad hoc, without a clear basis in physics criterion for their selection, and thus the process of modelling is based in empiricism and arbitrariness. Indeed, the entire process of empirical material modelling, and model validation thereof, is open-ended and no rigorous mathematical theory exists to date that makes it precise and quantitative, *i.e.* the model parameters are user-dependent.

During uniaxial loading, necking originates in smooth samples in a non-controlled location. As a consequence of this geometrical irregularity, a multiaxial stress state within the net cross section of the sample is induced. In notched samples, the multiaxial stress state is theoretically characterized and re-necking could be expected. The multiaxial stress state consists of high levels of hydrostatic stress, for which polymers are known to be sensitive. The stress field should be regarded as an additive decomposition of shear and hydrostatic pressure.

Due to the dissipative effects, the instantaneous temperature of the specimens during mechanical testing is not the same than the room temperature. Depending on the strain rate – among other variables, the heat build-up could be significantly high modifying the mechanical response of the material. Moreover, the heat build-up depending on the geometry and the deformation local field, the temperature rise would be heterogeneous on the surface of the geometry.

In this work, we propose a different paradigm, known as data-driven simulation [2], consisting of formulating calculations directly from experimental material data and pertinent essential constraints and conservation laws, bypassing the empirical material modelling step of conventional computing altogether. Essential constraints and conservation laws such as compatibility and equilibrium remain unchanged, as do all the numerical schemes used in their discretization, such as finite elements, time-integrators, etc. Such conservation laws confer mathematical structure to the calculations, and this mathematical structure carries over to the present data-driven paradigm. However, in data-driven simulation the experimental material-data points are used directly in calculations rather than an empirical material model. In this manner, material modelling empiricism, error and uncertainty are eliminated entirely and no loss of experimental information is incurred.

Whereas the data-driven paradigm has been formulated in the context of computational mechanics and, specifically elastic quasi-static problems [2, 3], we believe that its range and scope is much larger. By contrast, inelastic materials raise the fundamental problem of sampling history-dependent material behaviour [4]. Such sampling should provide appropriate coverage of possible processes and evolutions of the system and is thus likely to result in exceedingly large and complex data sets. The use of tools from Data Science and Big Data management may be expected to be particularly beneficial in dealing with such data sets. Using the local fields – strain and surface temperature – the calculations will consider, for the first time, the global and local response of the material. Furthermore, the *true* temperature of the material will be taken into account.

The scientific objectives envisaged are:

- to propose a new and different simulation framework in which the experimental material-data points are used directly in calculations rather than an empirical material model;
- to avoid material modelling empiricism, error and uncertainty as no loss of experimental information is incurred;
- to implement an efficient data-driven computing and demonstrate the practicality of the approach in the case of thermoplastic polymers;

## 2 Expected results

- Experimental data at two scales:
  - Macroscopic: experimental data from instrumented – DIC and IR – tensile tests will be performed on notched specimens at room and high temperature
  - Microscopic: SEM observations of the microstructure: i) initial; ii) deformed; iii) broken; and possibly by 3D imaging (tomography/laminography) ex or in-situ;
- Model-free simulation taking into account the local fields of deformation and temperature rise;
- Implementation of the model-free paradigm in the in-house simulation interface

## 3 Scientific approach

The scientific approach envisaged for the study is planned as follows:

- for **the first year** (CEMEF), get familiar with all the tools (in the broadest sense):
  - bibliographical study, familiarisation with computer and numerical calculation tools;
  - training on mechanical testing machines and instrumentation – DIC and IR;
  - getting familiar with the experimental database built up and available at the CDM and CEMEF, in order to extract what could be used experimentally in the context of this study;
  - instrumented tests to observe and quantify the heterogeneous deformation and temperature fields;
  - simulation of the tests within an elastic-domain framework (model-free paradigm).
- for **the second year** (MAT), work on the model-free paradigm:
  - Simulation of the tests within a elastic-plastic domain framework using the global response.
  - Minimise the local deformation and temperature rise – local response
  - Simulation of the tests and verification of the agreement with experiments – global and local
  - Implementation of the computational framework in the in-house simulation code;
- For **the third year** (MAT), work on the implementation in the in-house simulation code:
  - Implementation of a general framework in the in-house simulation code.
  - Running of *testing models* and comparing the results issued from the model-free paradigm with the classical elasto-plastic modelling.
  - Considering future prospects, in particular through the use of composite materials (e.g. fibre-reinforced) to at least show whether this is a viable option or not.

The various points are listed in the chronological order in which they are to be completed. Of course, this process is never as linear as that, and some points may be carried out in parallel and/or simultaneously.

# 4 Relevance of the project concerning the objectives & subjects of the ITN

By considering the following issues

- Data-driven computing
- Experimental data with no loss of information
- Coding of new algorithms for insight of a physical phenomena

the project is in line with the objectives and, more especially, with one of the subjects of the ITN: Digital engineering. Indeed, the corresponding research lines are considered: Data Science, Image Processing, High-Performance Computing, Physically-Informed Learning, Mechanical and Multiphysical Systems, Scientific Software.

# 5 Publications by subject

- Local field: [5] [6] [7] [8] [9]
- Digital Image Correlation (DIC): [8] [9] [10] [11]
- Heat build-up: [6] [12] [13] [14]
- Empirical material modeling: [15] [16] [17]

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Applicants should supply the following :

- a detailed resume
- a covering letter explaining the applicant's motivation for the position
- detailed marks
- two references : the name and contact details of at least two people who could be contacted to provide an appreciation of the candidate

to be sent to Centre des Matériaux de l'Ecole des Mines de Paris, B.P. 87 – 91003 EVRY CEDEX, to the attention of recruitment department, and/or by e-mail : recrutement_these@mat.mines-paristech.fr
Skills in experimental characterisation and, especially, **programming language** would be appreciated.

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