Abstracts of the eleventh MFront User Meeting

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1 Overview of TFEL-5.1

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Version 5.0 is a port to the TFEL library to C++-20 which a major overhaul of the TFEL/Math and TFEL/Material libraries

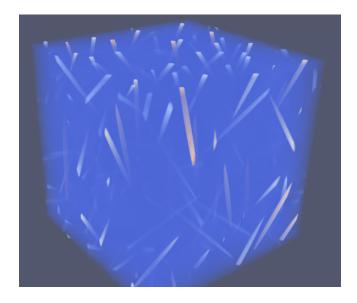
See this page for a full description: https://thelfer.github.io/tfel/web/release-notes-5.0.html

2 The new TFEL/Material/Homogenization library, application to 'mean-field' homogenization schemes on particulate and polycrystalline composites

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The ANOHONA project gathers some of the best french experts in the mean-field homogenization. One of the main goals of the project is to democratize, simplify the implementation of the resulting constitutive equations, and bridge the gap between academic research and industrial studies.

In this talk, we will present the functionalities of the new TFEL/Material/Homogenization library. This module provides widely used tools of mean-field homogenization for linear materials:



- Effective properties given by classical schemes (Mori-Tanaka, dilute scheme, self-consistent scheme, ...)
- Eshelby and Hill tensors for various ellipsoidal inclusions, including isotropic and anisotropic matrix
- Computation of mean strains and localisation tensors

This module is available in C++ and Python:

```
polarizations=[]
crystal=Polycrystal()
for grain in grains:
    crystal.addGrain(grain)
    P=np.array([1.,1.,1.,0.,0.,0.])
    polarizations.append(P)
E=np.array([1.,0.,0.,0.,0.])

hSC=computeSelfConsistent(crystal,polarizations,E)
print(hSC.stiffness)
print(hSC.mean_strains)
```

This module is directly usable in MFront to implement nonlinear constitutive equations based on mean-field homogenization schemes (linear comparison composite). Particularly, three examples will be treated:

- Implementation of an incremental variational scheme for a fiber-reinforced microstructure with linear/non-linear visco-elasticity.
- Implementation of an additive interaction law for an elasto-viscoplastic polycrystal.
- Implementation of Berveiller-Zaoui type homogenized behaviour on a polycrystal with arbitrary local behaviours.

As a perspective, a new brick, dedicated to mean-field homogenization, is under-development, allowing to implement such constitutive equations with a minimum of code.

3 Elasto-Visco-Plastic behavior law for irradiated low alloy steels

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In this talk, we present a new mechanical behavior law designed for irradiated polycrystalline low alloys steels. The law concatenates multiscale modeling results over several time and space scales, coupled with the Taylor homogenization rule. It accounts for temperature, strain rate, initial and irradiated microstructure. Starting from a complete set of constitutive equations describing crystal plasticity of irradiated ferritic steels, simple assumptions and approximations are made to integrate these equations over the homogenized Taylor polycrystal. The final flow equation incorporates lattice friction, Hall-Petch effect, static and dynamic aging, forest strengthening and irradiation hardening controlled by the size and density of solute clusters.

For the MFront implementation, we selected the ImplicitII Domain Specific Language. We present this specific implicit scheme and the special precautions to be taken to avoid divergence and numerical inefficiency. Finally, we illustrate the interface of the MFront behaviour with code_aster computations.

4 Constitutive equations for porous ductile materials in MFront

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The nucleation, growth, and coalescence of voids are major physical mechanisms involved in the ductile fracture of metal alloys. Modeling this failure mode and predicting ductile tearing requires constitutive equations that involve porosity as an additional state variable. Many constitutive equations have been proposed in the literature, but only a few are available in finite element solvers. To capitalize on these laws and provide a state-of-the-art, easy-to-use numerical implementation of constitutive equations for porous materials, the MFront StandardElastoViscoPlasticity brick was extended to porous materials a few years ago. First, this extension's capabilities will be reviewed in terms of ductile tearing predictions using different FEM solvers (Cast3M, MANTA, and code_aster) and FFT solvers (AMITEX_FFTP). Second, advanced constitutive equations to be included in the StandardElastoViscoPlasticity brick in the near future will be described.

5 Identification of material parameters using a heterogeneous test and the FEMU method: application to a viscoplastic behavior law

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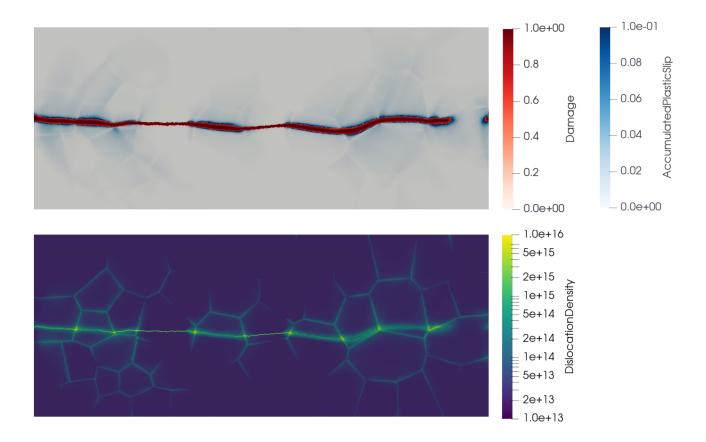
Numerical simulation, and in particular the finite element method, has become a central tool in the sheet metal forming industry.

Accurately simulating these processes requires a precise description of the mechanical behavior of metallic sheets. Identifying the parameters of advanced constitutive models—including anisotropy, hardening, and viscoplasticity—traditionally relies on quasi-homogeneous mechanical tests, from which only limited information can be extracted. A promising alternative to these time-consuming experimental campaigns is the Material Testing 2.0 approach. It combines heterogeneous mechanical tests with full-field measurement techniques, enabling inverse identification of material parameters from the observed kinematic fields.

This work follows that approach by identifying the parameters of a viscoplastic constitutive model for a Dual Phase DP600 steel, using a heterogeneous test performed under quick loading conditions and processed via the Finite Element Model Updating method.

6 Crystal plasticity coupled to brittle fracture

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Recent advances in experimental methods now enable detailed characterization of bulk microstructures and internal crack networks in millimeter-scale samples. Concurrently, mathematical and computational tools have progressed to effectively model the nucleation and propagation of cracks in brittle materials. Among these, the phase-field method has undergone significant extensions to better reflect physical phenomena. These developments include the incorporation of anisotropic fracture energy landscapes, coupling with plastic deformation mechanisms [1], and interactions with diffusing chemical species.

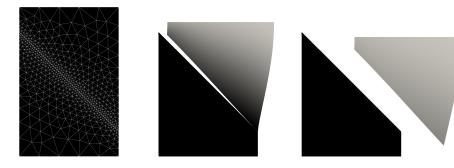
In this seminar, we narrow our focus to the microstructural scale, particularly in materials where brittle fracture is driven by localized plastic activity such as silicon-iron alloys, tungsten, and steels at cryogenic temperatures. Foundational studies by Hall [2] and Petch [3] demonstrated the influence of grain size on yield and fracture strength, highlighting prominent size effects. However, the impact of grain boundaries and grain size on fracture toughness remains less well understood, especially given the observed non-monotonic relationship between grain size and fracture toughness in the micrometer range [4].

We present recent progress in modeling the interplay between crystal plasticity and brittle fracture. Specifically, we examine how stress heterogeneities and singularities, originating from dislocation interactions and their interactions with grain boundaries, can act as precursors to fracture. To this end, we introduce a modeling framework that captures plasticity-induced brittle failure while incorporating an intrinsic material length scale. This length scale is shown to be critical for reproducing characteristic grain-size-dependent behavior observed during crack initiation and propagation in polycrystalline materials. Our approach employs a crystal plasticity constitutive behaviour implemented in MFront, which is seamlessly integrated with the finite element library FEniCS via the mgis.fenics interface.

- [1] Brach, S., Tanné, E., Bourdin, B., and Bhattacharya, K. Computer Methods in Applied Mechanics and Engineering 353 (2019): 44-65.
- [2] Hall, E. O. Proceedings of the Physical Society. Section B 64.9 (1951): 747.
- [3] Petch, N. J. Progress in Metal Physics 5 (1954): 1-52.
- [4] Reiser, J., and Hartmaier, A. Scientific reports 10.1 (2020): 2739.

7 MFront Cohesive Zone Models for code_aster

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We present the implementation of a nonlinear Cohesive Zone Model (CZM) in MFront, designed to study the mechanical behavior of soil and rock joints.

The constitutive equations are solved using a dual Lagrangian approach. This allows us to consider properly rigid – plastic behaviours, in constrast to purely penalized approaches. 2D finite element simulations powered by code_aster demonstrate the robustness of the proposed model.

Furthermore, we extend the CZM framework to poromechanics, allowing for a fully coupled hydro-mechanical analysis.

8 Resolution strategies for brittle and fatigue phase field damage model

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The phase-field damage model is a coupled problem involving two unknowns: damage and displacement. It can be solved using a monolithic approach - where both unknowns are treated simultaneously, at the risk of potential convergence issues due to the lack of convexity of the model's functional -or using a staggered approach, in which each sub-problem is solved sequentially while keeping the other unknown fixed (at the cost of a potentially very slow convergence).

Various strategies have been explored in recent years, aiming either to preserve the robustness of a monolithic algorithm, even in unstable phases, or to accelerate the convergence of staggered schemes.

In this work, we use the flexibility of the MFront code and its coupling with the Manta solver to test these different strategies, with the goal of improving the computational efficiency of phase-field approaches for brittle fracture and for high cycle fatigue crack propagation.

9 References