Agenda of the sixth MFront User Meeting

Thomas Helfer

25/11/2020

Contents

1 Overview of `TFEL-3.4` and `MGIS-1.2`. T. Helfer, G. Marois. (13h30-14h00)

This talk will present the new features of Version 3.4 of the `TFEL` project.

1.1 Version 3.4 of the `TFEL` project

This talks will present some new features and improvements introduced during the development of Version 3.4 of the `TFEL/MFront` project.

Figure 1 illustrates some noticeable applications of `TFEL/MFront` not presented in any of the subsequent talks.

The major features of this version are:

- A better support of the implicit resolution of generalised behaviours, in particular regarding the computation of the consistent tangent operator [3]. Examples of this features will be presented in Talks 3 and 7 and in references [4–7].
- An extension of the `StandardElastoViscoPlasticity` brick to porous materials. This is discussed in Talk 5.

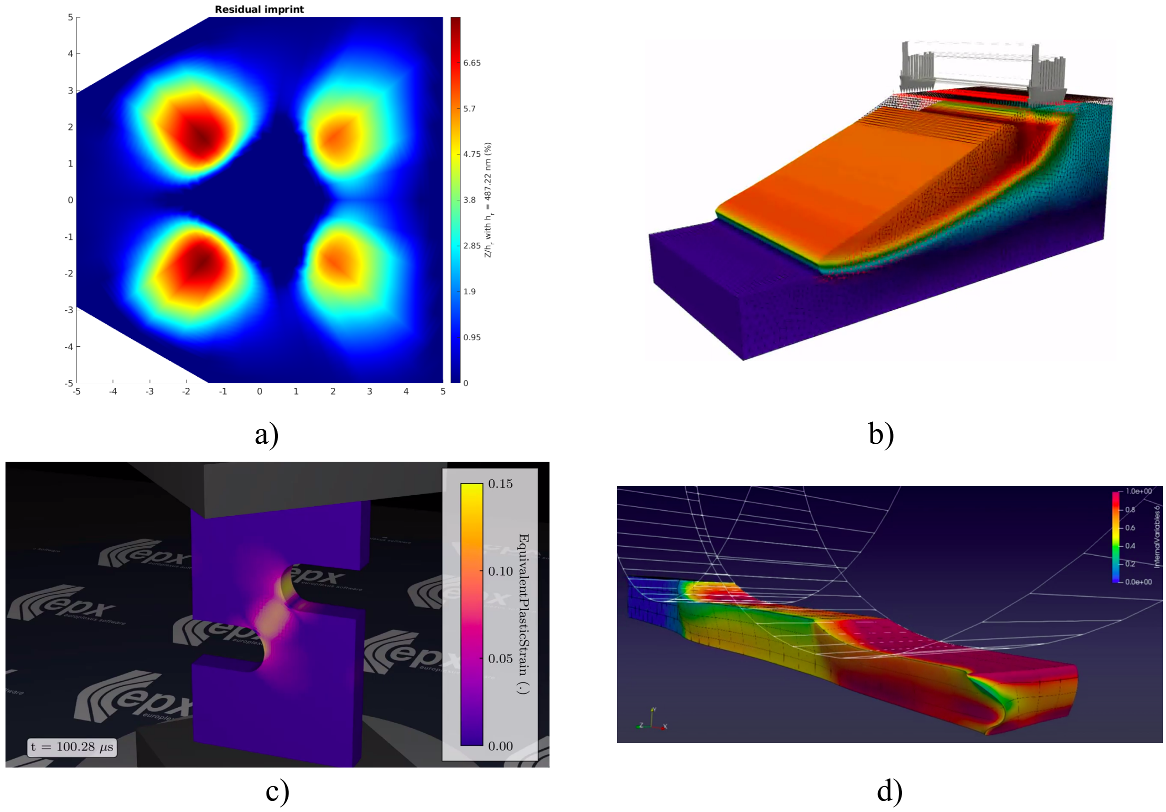


Figure 1: Noticeable applications of `MFront` and `MGIS` in 2020. a) Normalised residual topography after an indentation test on a single crsytal of copper with Méric-Cailletaud' finite stain behaviour [1] using `Ansys` (courtesy of A. Bourceret, FEMTO) b) Slope failure analysis with strength reduction in `OpenGeoSys` (courtesy of T. Deng and T. Nagel, [2]) c) Integration of the `MGIS` integration in `Europlexus` (courtesy of P. Bouda, CEA) d) Simulation of rolling using the innovative CEA' proto-application `MEFISTO` (courtesy of O. Jamond, CEA)

- The ability to store MFront behaviours in a madnex file. madnex is a data model based on HDF5 file format that was originally designed by EDF as part of their in-house projects for capitalising their experimental data and which is now being shared among the main actors of the french nuclear industry with the aim of becoming the de facto standard to exchange experimental data, MFront implementations and unit tests of those implementations. Documentation is available here: http://tfel.sourceforge.net/madnex.html.
- The MFront' generic interface now exports functions to rotate gradients in the material frame before the behaviour integration and rotate the thermodynamics forces and the tangent operator blocks in the global frame after the behaviour integration. Such functions are particularly useful for generalised behaviours.

A special effort has been set on the documentation with many new tutorials [3–11].

In order to increase the community of developers, a first tutorial showing how a new stress criteria can be added to the StandardElastoViscoPlasticity brick has been published [12]. Other similar tutorials are being considered.

1.2 Version 1.2 of the MGIS project

mgis.fenics The mgis.fenics python module, developed by J. Bleyer and discussed in depth in Talk 3, is the major development of this version.

Orthotropoic behaviours This version also provide a better support for orthotropic behaviours, following the developments made in MFront' generic interface. Prior to this version, orthotropy had to be handled by the calling solver, which implied:

- rotating the gradients in the material frame before the behaviour integration.
- rotation the thermodynamics forces and the tangent operator blocks in the global frame after the behaviour integration.

MFront' generic interface now exports appropriate functions which are seamlessly integrated in MGIS.

Integration in new solvers MGIS has been tested in a growing number of solvers and numerical platforms:

- MoFEM, see Talk 6.
- NairnMPM, see Talk 2.
- esys.escript.
- Kratos Multiphysics. A dedicated application has been developed in the mfront/application branch with the help of Vicente Mataix Ferrándiz and Riccardo Rossi.
- DUNE. Small and finite strain examples are available here: https://github.com/thelfer/dune-mgis

An MFEM application is currently under heavy developments here: https://github.com/thelfer/mfem-mgis.

2 Implementing a shear-transformation-zone model in MPM and SPFEM using MFront. Ning Guo, Wenlong Li (14h00-14h30)

In this study, we have implemented a shear-transformation-zone (STZ) model in both the material point method (MPM) and the smoothed particle finite element method (SPFEM) using MFront, a code generator for the efficient implementation of constitutive models, to study the large-deformation problems of geomaterials.

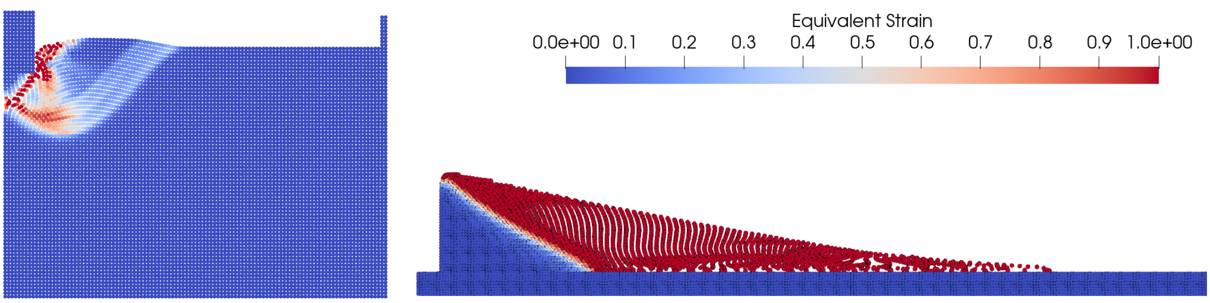


Figure 2: Equivalent strain contour from the MPM simulations: the footing (left) and the column collapse (right)

The applicability of the STZ model in simulating geomaterials and the efficiency of the MFront interface are demonstrated with two examples, namely, the footing and the granular column collapse problems (See Figure 2).

3 Binding MFront with FEniCS for automated formulation and resolution of generalized non-linear behaviours. J. Bleyer, T. Helfer (14h30-15h00)

In this talk, we will present a python package called mgis.fencis [13] which provides a binding between MFront [14] and FEniCS [15, 16], a finite-element library dedicated to the automated formulation and resolution of PDEs.

Using this package, we alleviate the difficulties of implementing complex material constitutive laws in FEniCS by relying on the MGIS project [17]. The development of this package enabled to test MFront recent extension to generalized behaviours.

Typical applications involve for instance fully coupled non-linear thermoelasticity or phase-field models of fracture.

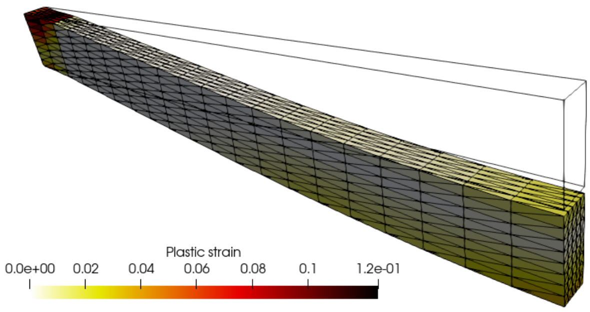


Figure 3: An example of finite strain plastic results with the mgis.fencis module

A set of tutorials provide an overview of the features of the module and its usage:

- Stationnary non-linear heat transfer [9].
- Stationnary non-linear heat transfer: 3D problem and performance comparisons [10].
- Transient heat equation with phase change [6].
- Monolithic transient thermoelasticity [4].
- Small-strain von Mises elastoplasticity [8].
- Finite-strain elastoplasticity within the logarithmic strain framework [18]. See also Figure 3.
- Multiphase model for fiber-reinforced materials [5].
- Phase-field approach to brittle fracture [11].

We will also mention the current limitations which are planned to be resolved when adapting the package to the next-generation FEniCS-x project.

4 One application of the MGIS project to the a variational problem resolution modelling a damaged elasto-plastic material. V. Alves Fernandes, G. Bacquaert, J. Bleyer, D. Kondo, C. Maurini, S. Raude, F. Voldoire (15h00-15h30)

The analysis of soil materials leads to the need to formulate highly nonlinear constitutive laws. In this presentation, the mgis.fenics project is efficiently used to implement a regularized model coupling elasto-plasticity and damage, initially proposed by J.-J. Marigo and K. Kazymyrenko in [19].

The numerical strategy to solve the mechanical problem is based on the interaction between the FEniCS and MFront environments. On the one hand, benefiting from the local integration of MFront, the elasto-plastic problem is treated. In another time, the damage problem is solved in FEniCS with the help of the TAO optimization software library.

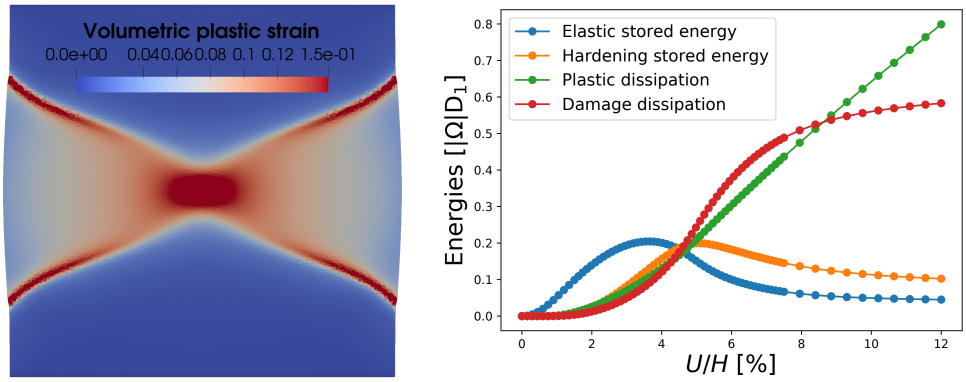


Figure 4: From a simulated compression under axisymmetric conditions, the final volumetric plastic field (at U/H=12%) and the evolution of every stored and dissipated energy part supplied by the external mechanical work.

Solving these two successive sub-problems ensures the resolution of a well-posed variational problem, by providing a physically acceptable solution (respecting equilibrium equations, plasticity and damage criteria). Typical numerical simulations to geomaterials are illustrated and commented on. See Figure 4 for a first example.

The need to complexify the initial model to account for a richer phenomenology (cyclic and hydromechanical behavior mainly) is finally briefly discussed.

5 Extension of the `StandardElastoViscoPlasticity` brick to porous materials. M. Shokeir, J. Hure, T. Helfer (16h00-16h30)

This talk presents an extension of `MFront`' `StandardElastoViscoPlasticity` brick to constitutive equations developed for porous materials.

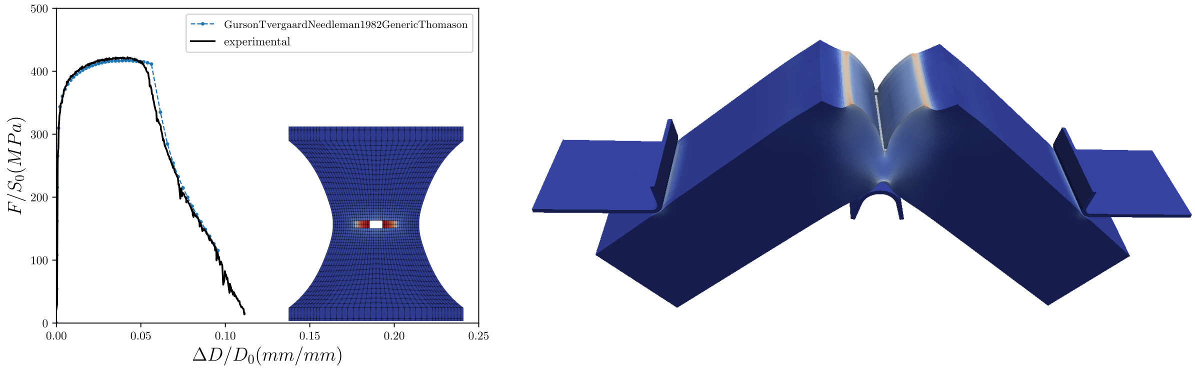
Porous plasticity models describe the nucleation, growth and coalescence of voids, accounting for the porosity as an additional state variable. These models are used to perform numerical simulations of ductile fracture of metals.

From a numerical point of view, the implementation of these constitutive equations based on implicit schemes is known to be challenging for various reasons, such as strong evolutions of state variables, singular yield surfaces when the porosity reaches a critical value, and / or thresholds for evolutions laws. An innovative fully implicit numerical algorithm has been set-up based on an accelerated fixed-point method to handle these challenges.

Gurson-Tvergaard-Needleman and Rousselier yield criteria have been implemented and validated, along with several nucleations laws. Complex constitutive equations of porous visco-plasticity can now be implemented in a few lines in a very intuitive and readable way, as follows:

```
@Brick StandardElastoViscoPlasticity{
  stress_potential : "Hooke" {young_modulus : 200e3, poisson_ratio : 0.3},
  inelastic_flow : "Plastic" {
    criterion : "GursonTvergaardNeedleman1982" {
      f_c : 0.01, f_r : 0.10, q_1 : 2, q_2 : 1, q_3 : 4
    },
    isotropic_hardening : "Linear" {R0 : 200.}
  },
  porosity_evolution : {
    nucleation_model : "Chu-Needleman 1980 (stress)" {
      fn : 0.1, sigm : 20, sn : 10, fmax : 0.1
    }
  }
};
```

Additional constitutive equations for porous materials can also be added by the user, as described in [12]. The Gurson-Tvergaard-Needleman model implemented in the brick has been used to perform the numerical simulations of ductile tearing using the finite-element solver `Cast3M`.



a) b)

Figure 5: a) `Cast3M` simulation of a Notched Tensile sample of an AA6061-T6 found in the core of Jules Horowitz Reactor and comparison of simulation result with experimental data. b) `Cast3M` simulation of a Charpy test on the PWR reactor core vessel' steel

The first example is the modelling of the 6061-T6 aluminum alloy which is the material for the vessel-rack assembly of the Jules Horowitz Reactor (JHR). This alloy, as many others, undergoes damage by void nucleation and extremely rapid coalescence. This makes it difficult for researchers to model such a behaviour. However, the innovative accelerated fixed-point method allows the user to model such harsh behaviours. As depicted in Figure 5 a), simulations are performed on axisymmetric notched samples and compared to experimental results in order to calibrate the parameters of the model.

The second example deals with the low alloy steel used for Reactor Pressure Vessel (RPV) of Pressurized Water Reactor (PWR), where impact tests are simulated, as illustrated in Figure 5 b), and compared to numerical results.

6 MoFEM: An open source, parallel finite element library - MFront integration. Karol Lewandowski, Lukasz Kaczmarczyk (16h30-17h00)

`MoFEM` (Mesh-oriented Finite Element Method) is a C++ library for managing complexities related to the finite element method (FEM) [20].

`MoFEM` is developed to provide a finite element library incorporating modern approximation approaches and data structures for engineers, students and academics.

`MoFEM` is specifically designed to solve complex engineering problems, enabling seamless integration of meshes that comprise multiple element types and element shapes, which are typically encountered in industrial applications.

In the first part of this talk, we will present a brief introduction to `MoFEM` library, focusing attention on the `MoFEM` software design, and examples applications.

In the second part of the presentation, a `MoFEM` user module integrating `MFront` behaviours library will be demonstrated. Using off-the-shelf `MoFEM` operators and bilinear form integrators results in clean and concise implementation, allowing for usage of multiple material models on different parts of the finite element mesh. The performance of the module will be shown with numerical examples. See Figure 6 for a first example.

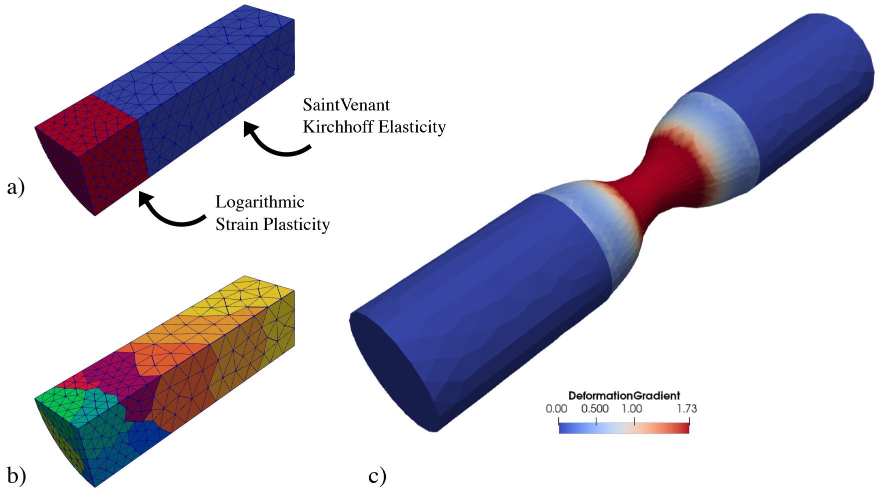


Figure 6: Example necking of a rod with two `Mfront` behaviours. a) Discretised one eighth of the geometry. b) Parallel domain decomposition. c) Deformed specimen and distribution of deformation gradient.

7 Implementation of constitutive models for clay rocks and bentonite-based materials using MFront for safety and performance assessments of HLW-repositories in clayey formations. Eric Simo, P. Herold, M. Mánica, T. Helfer, D. Masin, T. Nagel (17h00-17h30)

Argillaceous formations are currently being considered in several countries as a possible host medium for deep geological disposal of high- and intermediate-level and long-lived nuclear waste [21]. They exhibit desirable features such as low hydraulic conductivity, low molecular diffusion, and significant radionuclide retention capacity [22]. Particularly, in Germany, rock salt, clay rock as well as crystalline rock are being considered for the final disposal of high-level waste in accordance with the site selection act [23]. In step one of the first phase of the site selection procedure, the German Waste Management Organisation, Bundesgesellschaft für Endlagerung mbH (BGE), identified and proposed nine clay formations (so-called sub-areas) as potential repository sites based on a defined set of of geoscientific criteria and requirements [24].

In clay formations, bentonite materials are considered as the main sealing component of the engineered barrier system. This is particularly due to their swelling capacity upon hydration, which helps to close remaining gaps and voids at the sealing location, and thus ensure confinement of the disposed radioactive waste.

In repository conditions, clay rocks and bentonite materials will be subjected to coupled thermo-hydro-mechanical loads, which can potentially compromise their sealing capacity if certain tolerances are exceeded. The understanding of the complex thermo-hydro-mechanical behaviour of clay materials is therefore necessary for the safety assessment of repository systems. Constitutive models able to reproduce such material behaviour are needed for the numerical based safety and performance assessments of repository systems.

The development of material models for clay rocks and bentonite-based materials has been addressed in the past two decades by several researchers; see for instance [25–27] for clay rocks and [28–33] for bentonite constitutive models. For this purpose, BGE funded the research project PIONIER which takes advantage of multiple experimental investigations on clays and bentonite materials in the work packages GAS and HITEC of the European Joint Programme on Radioactive Waste Management – EURAD, to deal with such constitutive models. The approaches proposed by [25] for clay rocks and [28, 29] for bentonite have been selected by the authors for further development and implementation in the numerical code `OpenGeoSys` [34, 35]. The implementation will be carried out in MFront, a code generation tool for constitutive modelling [14, 17]. The complexity of the considered material behaviour requires addressing several numerical challenges. For instance, a new concept has been developed to use `MFront` as a wrapper to integrate an existing implementation of a constitutive equation in a solver supported by `MFront`[7]. The concept has been successfully validated for the hypoplastic model for bentonite by [28, 29]. For clay rocks, theoretical works are being carried out to incorporate a nonlocal plasticity approach within the `MFront-OpenGeoSys` framework. The latter is necessary for the implementation of the nonlocal plasticity model proposed by [25].

The present contribution intends to give an overview to the implementation strategies for the two selected models within the MFront framework and their application in the scope of the project PIONIER.

8 About the speakers

Thomas Helfer is an engineer at CEA in the Fuel Simulation Laboratory at Cadarache, France and the main developer of `TFEL/MFront` and `MGIS`. https://www.researchgate.net/profile/Thomas_Helfer.

Goustan Bacquaert is a PhD student working at EDF Lab Paris-Saclay, supervised by the École des Ponts PariTech and the Sorbonne Université. His work focuses on the modelling of soil behaviours, both theoretically and numerically, for structural engineering studies.

Jérémy Hure is a researcher at CEA in the Department of Materials for Nuclear Applications, working on fracture mechanics of irradiated materials. http://jeremy.hure.free.fr

Mohamed Shokeir is a PhD student at CEA & École des Mines Paristech on the influence of radiation damage on the fracture toughness of aluminum alloys - computational methods on the AA6061-T6. https://www.linkedin.com/in/mohamed-shokeir-897b2614a

Ning Guo is an Assistant Professor at Zhejiang University in the Department of Civil Engineering. He is working on computational geomechanics and multiscale modeling of geomaterials.

Wenlong Li is a PhD student in civil engineering department at Zhejiang University.His research focus is modeling granular materials,especially sand.

Karol Lewandowski is a research associate at University of Glasgow, a key contributor to the finite element library `MoFEM`. His current research interest lies in plasticity and contact mechanics for incremental cold flow forming simulations.

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