Agenda of the seventh `MFront` User Meeting

Thomas Helfer

21/10/2021

Contents

1 Overview of `TFEL-4.0` and `MGIS-2.0`.

- Thomas Helfer
  - CEA Cadarache, IRESNE/DES/DEC/SESC/LSC, 13 108 St Paul lez Durance, France.

This talk will:

- Present arious applications of `MFront` during the past year which are not described in the other talks.
- Discuss some new features of Version 4.0 of the `TFEL` project and Version 2.0 of `MGIS`.

Both projects are now based on the `C++-17` standard.

As a consequence, the `TFEL/Math` library have been deeply overhauled. From the end user point of view, the library:

- better handles quantities, i.e. values with units, allowing the compiler to perform dimensional analysis.
- supports higher order objects.

Quantities are now supported by the implicit domain specific languages (DSLs) of `MFront` and the DSL dedicated to material properties.

2 Development of a Novel Damage Model for Concrete Subjected to Creep

- Alexandre Gangnant
  - Sixense necs, Sceaux, France
- Michel Sagno
  - Sixense necs, Sceaux, France
- Jefri Draup
  - EDF Energy R&D UK Centre, Manchester, UK
- Thomas Helfer
  - CEA Cadarache, IRESNE/DES/DEC/SESC/LSC, 13 108 St Paul lez Durance, France.

Concrete exhibits visco-plastic behaviour when subjected to high temperature whilst supporting an external load; this component of plasticity is referred to as load induced thermal strain (LITS), which is also known as transient thermal creep (TTC). LITS phenomena can be important in pre-stressed concrete structures. Indeed, this can potentially lead to a loss in pre-stress, and also residual tensile stress development under transient thermal conditions. Hence, structures which have been subjected to a high temperature thermal loading cycle may experience cracking and subsequent loss of rigidity; this could ultimately lead to a loss of functionality or even structural failure. In addition to that, under pre-stressed structures, basic creep effects might be observed in concrete and could contribute to the failure .

Thus, in a process of catching physical & mechanical phenomena that could occur during the lifetime of a concrete structure (e.g. Pre-stressed concrete vessel of an AGR), a novel model has been developed in order to take into account the damage, creep and LITS phenomena.

Firstly, a damage model (named FLB based on Mazars) coupled with LITS model has been developed using Mfront and tested. Secondly, basic creep has been added to this initial constitutive law. This latter coupled model is based on simple viscoelastic creep model (Burger) in a framework a quasi-brittle material such as concrete. The constitutive behaviour is coupled to the damage law via the total stress tensor. By decomposing the elastic, creep and thermal strains, the damage evolution is driven from the elastic strains and in a proportion of creep strains. Finally, the effective stress is computed and used to obtain the total stress at each iteration with unilateral effect (rigidity recovery due to crack closure) included.

This type of model is most suitable for fully implicit integration schemes and will allow more accurate assessment of structural damage from transient thermal events, such as fire. This work is only based on the coupling damage and creep where thermal effect has been disabled on purpose.

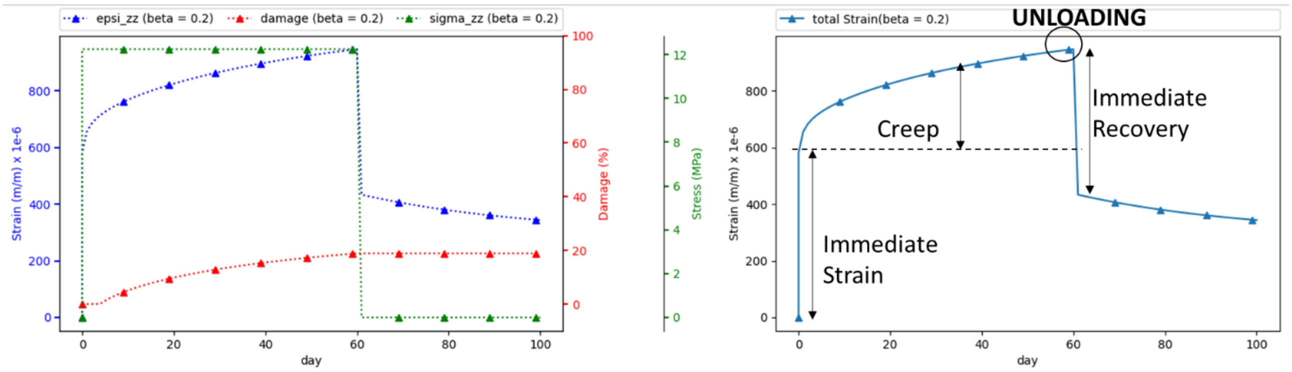

Figure 1: Evolution of creep stains & damage under constant load followed by an unloading by applying the new developed damage creep model

3 A novel approach of using existing implementations of constitutive material models in any numerical code interfacing with `MFront`

- Eric Simo

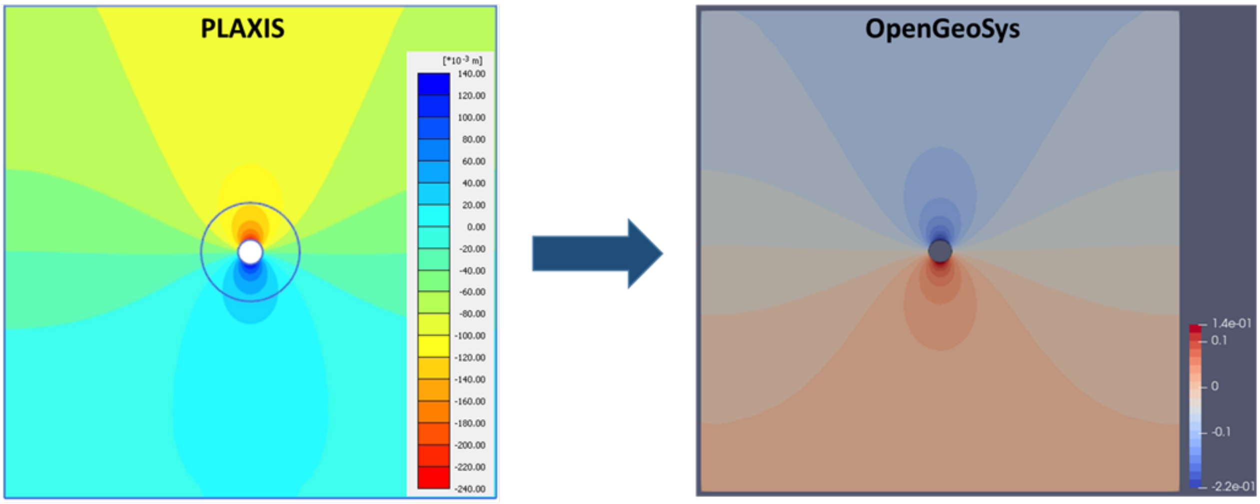

Figure 2: Vertical displacement after the excavation of a gallery in a clay formation using an advanced hypoplastic model

    - BGE Technology, Germany
- Thomas Helfer (CEA)
    - CEA Cadarache, IRESNE/DES/DEC/SESC/LSC, 13 108 St Paul lez Durance, France.
- David Mašín
    - Charles University in Prague Faculty of Science Albertov 6, 128 43 Prague 2, Czech Republic
- Thomas Nagel
    - TU Bergakademie Freiberg, Freiberg, Germany.

A novel approach of using existing implementations of constitutive material models in any numerical code interfacing with `MFront`.

In this work, we developed a novel approach, which consists of using existing constitutive models already available in different finite element codes in any numerical codes interacting with `MFront`. We used for that the versatility of the `C++` language, which allows us to define new kind of interfaces incorporating the legacy implementation code of constitutive equations independently from the programing language used. These interfaces then define the necessary connections between the constitutive models and the solver connected to `MFront`.

At this stage, the approach has been used to make available all kind of constitutive models written in the `UMAT` format in `Fortran` into the code `OpenGeoSys`. The results of a simulation using a `UMAT`-model and the corresponding test procedure to validate this approach will be discussed in this presentation.

4 Implementation of a coupled thermo-elasto-viscoplastic polycrystalline finite element model using `FEniCS` (`mgis.fenics`) and `MFront`

- Nikhil Mohanan
    - Laboratoire de Mécanique des Solides (LMS), CNRS UMR 7649, Ecole Polytechnique, Institut Polytechnique de Paris, 91128 Palaiseau Cedex, France
- Jérémy Bleyer
    - Laboratoire Navier, CNRS UMR 8205, ENPC, Univ Gustave Eiffel, F-77447 Marne-la-Vallée, France
- Thomas Helfer
    - CEA Cadarache, IRESNE/DES/DEC/SESC/LSC, 13 108 St Paul lez Durance, France.
- Manas Upadhyay
    - Laboratoire de Mécanique des Solides (LMS), CNRS UMR 7649, Ecole Polytechnique, Institut Polytechnique de Paris, 91128 Palaiseau Cedex, France

During metal Additive Manufacturing (AM), just after deposition and rapid solidification, the material is subjected to thermal cycling in solid-state with different temperature amplitudes and rates until the end of the AM process. The thermo-mechanical driving forces arising from this Solid-State Thermal Cycling (SSTC) could trigger different micro-mechanisms (e.g., dislocation dynamics, recrystallization, phase transformation, etc.) that can significantly alter the as-solidified microstructure and its subsequent mechanical response.

Our aim is to design and develop a polycrystalline Thermo-Elasto-Viscoplastic Finite Element (T-EVP-FE) model to predict and understand the microstructure evolution and the T-EVP response due to SSTC during AM. This model is intended to act as a base for future developments such as coupling with models for phase transformation, recrystallization, etc.

The T-EVP-FE model has been implemented with the help of `MFront` and `FEniCS` linked together with `MFront Generic Interface Support` (`MGIS`). The `MFront ImplicitGenericBehaviour` DSL is used to model the constitutive behavior while `FEniCS` is used to solve the coupled temperature evolution and equilibrium equations. In this talk, we discuss the T-EVP initial boundary value problem, the `FEniCS-MFront` solution algorithm, key features of the implemented code, and validation with other numerical solutions.

5 Implementation of a polycristalline model to simulate the radiation induced deformation of Zircaloy cladding tubes using the MFront code generation tool

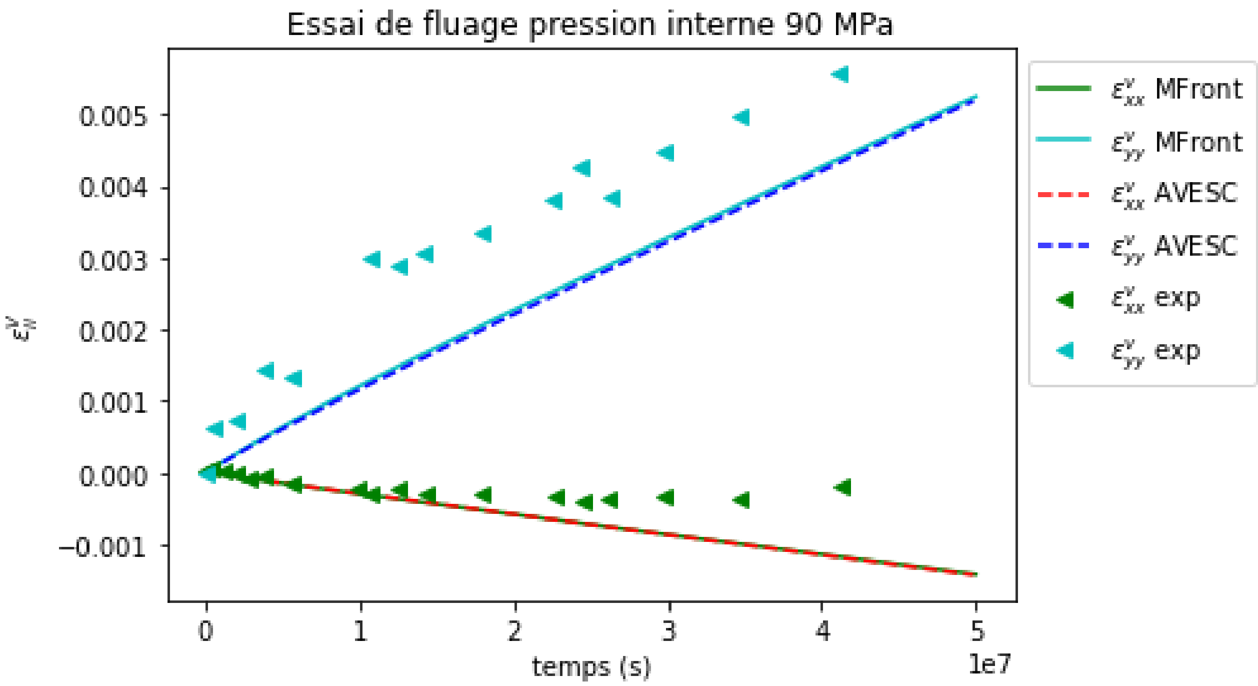

Figure 3: ""

- Cécilia Gicquel
  - CEA Saclay ISAS/DES/DMN/SRMA/LA2M, 91191 Gif-sur-Yvette cedex.
- Renald Brenner
  - CNRS, d'Alembert
- Renaud Masson
  - CEA Cadarache, IRESNE/DES/DEC/SESC/LSC, 13 108 St Paul lez Durance, France.
- Fabien Onimus
  - CEA Saclay ISAS/DES/DMN/SRMA/LA2M, 91191 Gif-sur-Yvette cedex.

The aim of this work is to implement a polycrystalline model in the MFront code generation tool to simulate the radiation induced deformation of cladding tubes made of Zircaloy. Thanks to Mandel's correspondence principle [1] and thanks to an internal variables formulation derived by Ricaud and Masson [2], equivalent to Schapery's collocation method [3], the self-consistent scheme [4] is applied to determine the behaviour of a non-ageing, linear viscoelastic polycrystal. The coefficients of the model are calibrated using the experimental data from Soniak et al. [5]. The numerical simulation is then compared, at the macroscopic and at the local scale, with the quasi-elastic approach developed by Brenner et al. [6] and adapted to in-reactor deformation by Onimus et al. [7].

6 Implementing geomechanical models in `MFront`/`OpenGeoSys` for hydrogeological and geotechnical applications

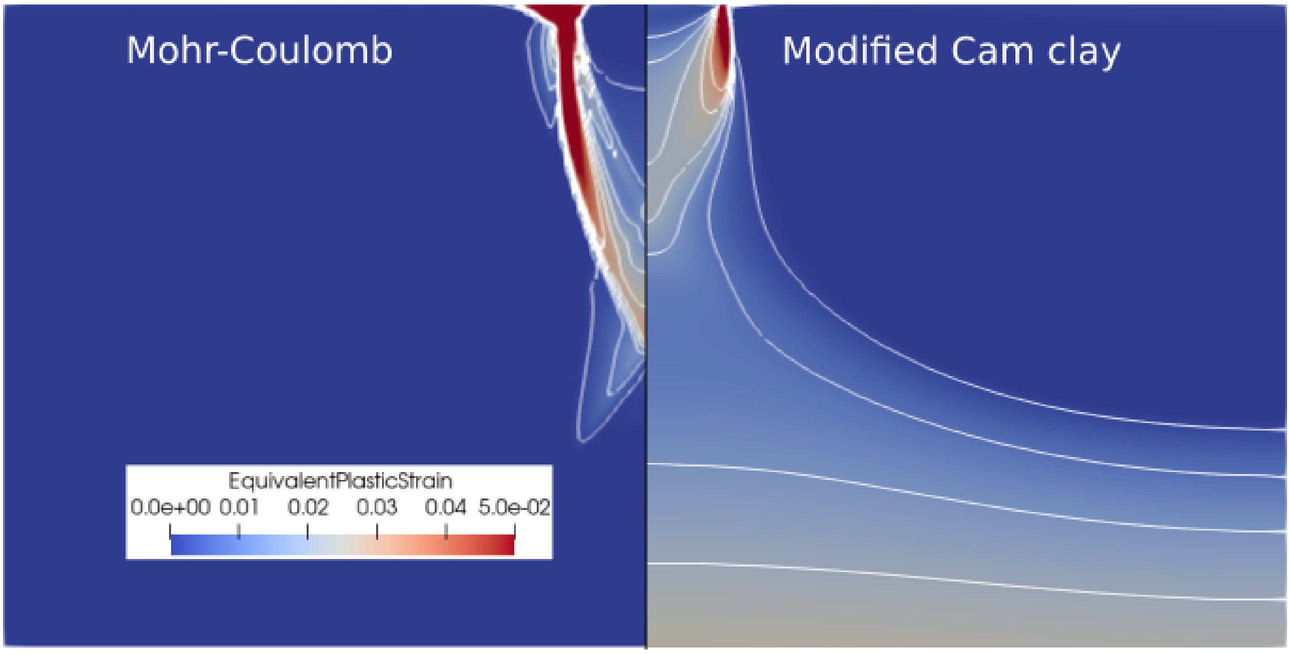

Figure 4: Foundation problem under gravity: Comparison of the Mohr-Coulumb model and the modified Cam clay model at the onset of plastic localization.

- Christian B. Silbermann
  - TU Bergakademie Freiberg, Freiberg, Germany.
- Dominik Kern
  - TU Bergakademie Freiberg, Freiberg, Germany.
- Francesco Parisio
  - TU Bergakademie Freiberg, Freiberg, Germany.
- Thomas Nagel
  - TU Bergakademie Freiberg, Freiberg, Germany.

In order to properly simulate complex hydrogeological or geotechnical processes it is crucial to reasonably capture the mechanical behavior of the geomaterials (soils or rocks, specifically). Mechanically speaking, a constitutive relation is needed for the calculation of the effective stress tensor as part of the constitutive closing of the thermo-hydro-mechanical models used. Therefore, a variety of inelastic (geo)mechanical material models is available in literature, such as the basic and more generally applicable Mohr-Coulomb and Cambridge (Cam) clay models along with more advanced models for specific materials and applications such as models for rock failure in the brittle-ductile transition or for creep in rock salt formations.

Many formulations have in comman that they need to capture effects like elasto-plastic deformation, irreversible (plastic) pore compaction / consolidation, hardening and softening, different loading and unloading stiffness, and temperature dependence. The goal of this work is to highlight recent implementations of geomechanical models in `MFront`/`OpenGeoSys`, such as

- a consistent and clear presentation of the basic modified Cam clay model for cohesive soils
- models for primary, secondary and tertiary creep of rock salt
- rock mechanical models at temperatures and pressures spanning the brittle-ductile transition

This talk describes the implementation of several material models for small strains in the open-source multi-field finite element software `OpenGeoSys` based on `MFront`. For this, the set of constitutive equations and their implementation are outlined. Then, exemplary numerical studies are presented for typical hydrogeological and geotechnical applications demonstrating significant differences with respect to the chosen material model.

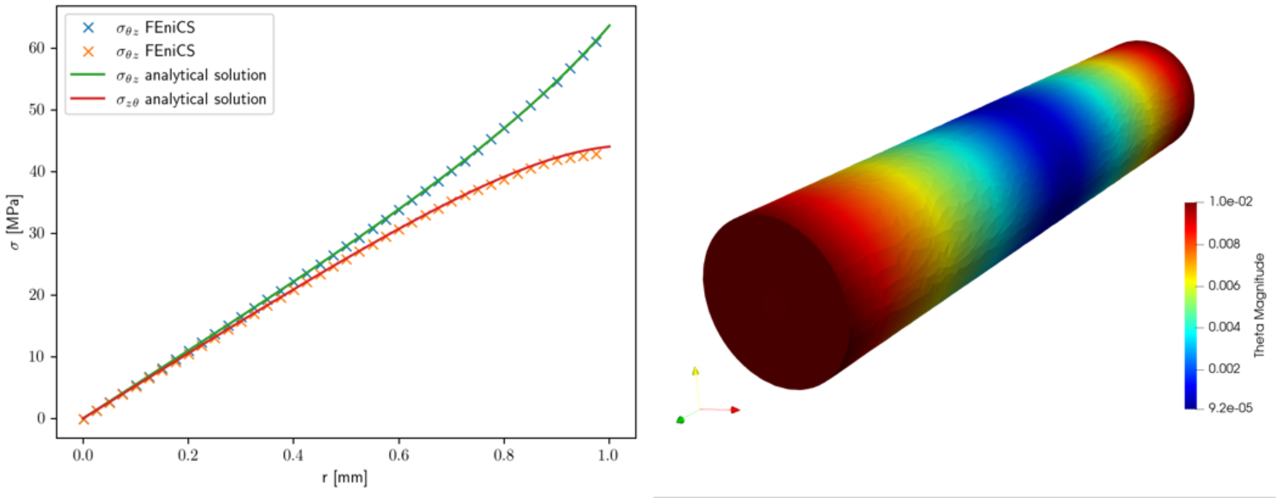

Figure 5: Results obtained for a torsion Test a) Comparison with the analytical solution in elasticity . b) Magnitude of the rotation of the microstructure

7 Validation and performance of Cosserat media in small deformation

- Tamara Dancheva
  - Basque Center for Applied Mathematics
- Raffaele Russo
  - University of the Basque Country
- Flavien Ghiglione
  - MINES ParisTech
- Unai Alonso
  - University of the Basque Country
- Michael Barton
  - Basque Center for Applied Mathematics

In this talk, we will dive into the implementation and performance of a Generalized Continua-based model, more specifically within the framework of Cosserat media [8]. We aim to use this model for simulating the realistic behaviour of metal alloys during the process of machining (a material removal process during which the material undergoes severe plastic deformation). We developed this model using the open-source FEM framework `FEniCS` and `TFEL/MFront` using the `mgis.fenics` module [10]).

We present our work on the validation and performance of the elastic and elastoplastic model ([11], [12]) in small deformation for a representative test case i.e. torsion test of a cylindrical specimen, by comparing the results from FEniCS and TFEL/MFront with the analytical/semi-analytical solution and a solution obtained with the `ZSet` framework, using the `Zebulon` finite element solver.

8 `MFront`, `code_aster` and wood: mechanical behaviors for structural applications and cultural heritage conservation.

- Lorenzo Riparbelli
  - University of Florence, Dagri Dept., Florence, Italy.
- Ioannis Christovasilis
  - Aether Engineering, Florence, Italy.
- Marco Fioravanti
  - University of Florence, Dagri Dept., Florence, Italy.

By its nature, wood has a marked orthotropic behaviour with respect to a cylindrical reference coordinate system, which coincides with the development of its growth rings. Not only its elastic characteristics vary significantly in the three anatomical directions (namely longitudinal, radial and tangential), but it also demonstrates an associated orthotropic viscoelastic behaviour, as well as a strong correlation of its deformation characteristics of shrinkage and swelling with variation of the moisture content.

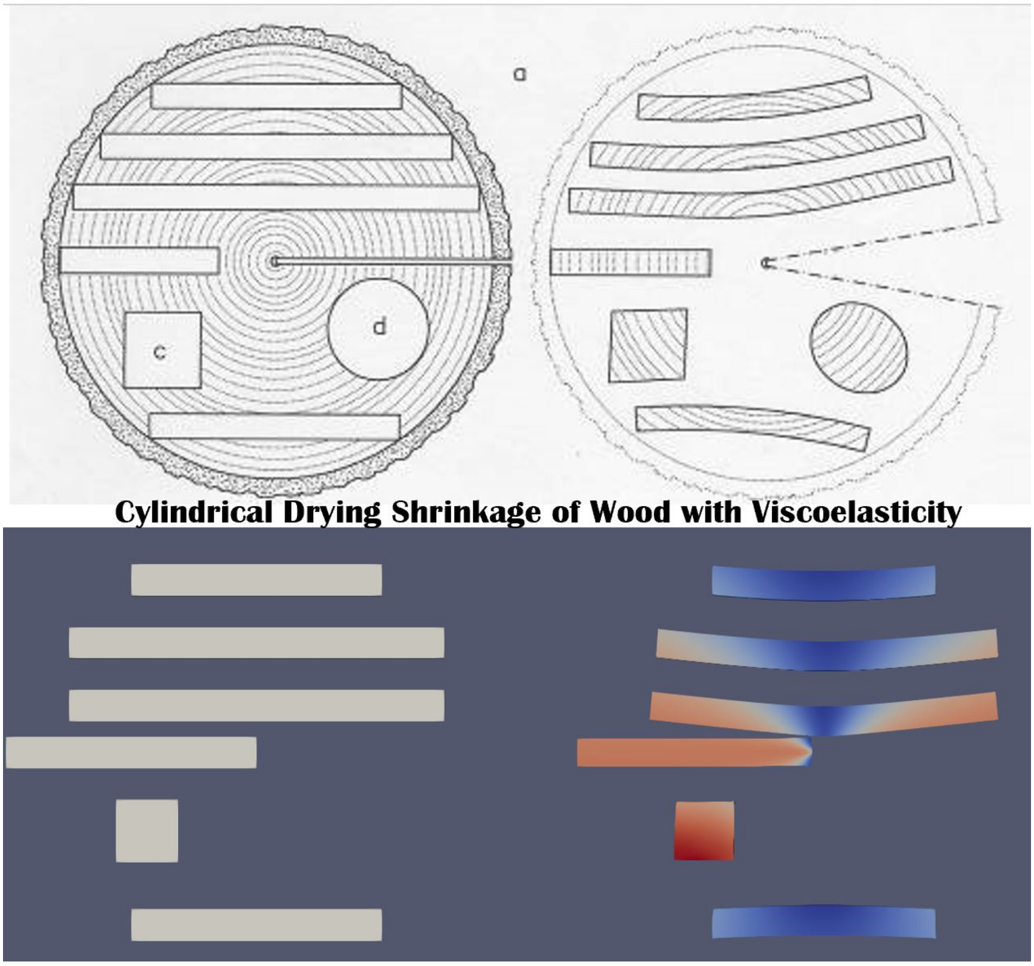

Figure 6: Modelling of Drying schrinkage of wood with `code_aster` and `MFront`

This study shows how, through the use of MFront and the development of dedicated material laws, it is possible to address these issues and simulate these characteristics both for steady-state and transient hygroscopic analyses, allowing to obtain the stress and deformation state and history of the material. Two areas of application are discussed; in the conservation of cultural heritage, specifically renaissance panel paintings, and in structural engineering of timber buildings.

9 Theoretical framework of the friction and wear phenomena through of thermodynamics approaches: application to aeronautical braking

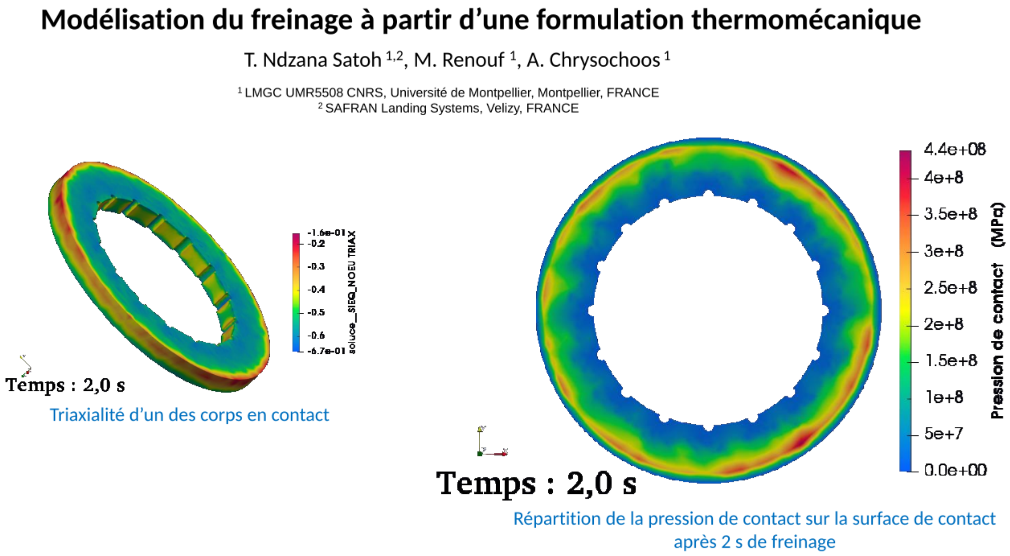

Figure 7: Modelling of braking with `code_aster` and `MFront`

- Thierry Ndzana Satoh
  - LMGC UMR5508 CNRS, Université de Montpellier, Montpellier, France.
  - SAFRAN Landing Systems, Velizy, France
- Mathieu Renouf
  - LMGC UMR5508 CNRS, Université de Montpellier, Montpellier, France.
- André Chrysochoos
  - LMGC UMR5508 CNRS, Université de Montpellier, Montpellier, France.

The limits of Archard's law, stated in [13] to more precisely describe the wear in braking problems is no longer to be demonstrated. The relation of proportionality between the volume of material lost and the associated work as formulated empirically through this law, does not always stick with the physical phenomena observed on the interfaces in contact, in particular in the case of carbon braking systems where the third body trapped in the interface in contact defaults this Archard model. Indeed, wear in these systems, the result of physicochemical processes and complex mechanical and dependent on many parameters which act on time scales and different space. Some studies in the literature come to highlight the close links between energy that is dissipated in the system and the phenomenon of wear [14–16]. By decoupling in this energy the contribution which comes from friction, Zmitrowicz [17–19] or even Dragon-Louiset and Stolz [20] in have shown that it is possible to have an even more description "Real" of the phenomenon of wear.

We propose a theoretical approach to modeling the wear of carbon brake systems from a thermodynamic description of the problem. Quantification of wear debris is estimated from the energy contributions related to the damage of the contact body and the mechanism from a third body potential trapped in the contact. The equations of states and evolutions which govern the model, are written within the framework of generalized standard materials.

10 Implementation of neural network based constitutive models

- Marius Duvillard

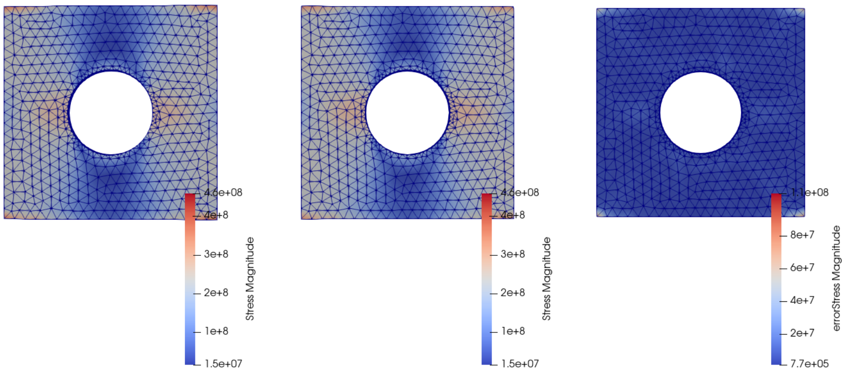

Figure 8: Comparison of results obtained by the Ramberg-Osgood behaviour and an neural network trained on unit tests on a structural test case.

  - CEA Cadarache, IRESNE/DES/DEC/SESC/LSC, 13 108 St Paul lez Durance, France.
- Loïc Giraldi
  - CEA Cadarache, IRESNE/DES/DEC/SESC/LSC, 13 108 St Paul lez Durance, France.
- Thomas Helfer
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The characterization of the material behavior is crucial in the resolution of mechanical problems. For decades, constitutive laws were built thanks to parametric models depending on theoretical formalism [21]. Identifying those parameters and fitting the data is one of the major difficulties. Therefore, modelling error and uncertainty arise from an imperfect knowledge of the functional form of the material laws.

More recently, different kind of data-driven models were introduced with the use of AI, more specifically neural networks [22], or by a minimization problem in the phase space [23]. In the first case, neural networks allow to easily fit the material behavior without strong mathematical *a priori*. Moreover, it has been proved that feedforward neural networks are universal approximators [24], thus they could characterize complex material behaviors.

This talk presents different neural network based constitutive models instead of traditional constitutive law formulations. Neural networks enable to fit the material behavior with an expressive class of functions. The neural network models are directly trained on a synthetic dataset of random load tests in order to find a suitable representation of the material behavior.

We introduce different neural network architectures for constitutive modelling. First, we consider a feedforward network in order to approximate a parametric nonlinear elastic model Ramberg Osgood. Then, in order to cope with history-dependent materials, we consider a recurrent neural network (GRU cells) to model a von Mises elasto-plastic behavior with isotropic linear hardening Isotropic Hardening.

Finally, we demonstrate how to fit a model with `PyTorch`, integrate it in `MFront`, and perform finite elements simulations thanks to the `mgis.fenics` python library. We benckmark machine learning models with classical formulations based on the results of such simulations.

11 The Hybrid High Order method in nonlinear solid mechanics with `MFront` and `MGIS`

- David Siedel
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  - CEA Saclay, ISAS/DES/DM2S/SEMT/LM2S, 91191 Gif-sur-Yvette cedex.
  - Mines ParisTech, PSL University, Centre des matériaux, CNRS UMR 7633, 91003 Évry, France.
- Thomas HELFER
  - CEA Cadarache, IRESNE/DES/DEC/SESC/LSC, 13 108 St Paul lez Durance, France.
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- Nicolas Pignet
  - EDF R&D,
- Jacques BESSON

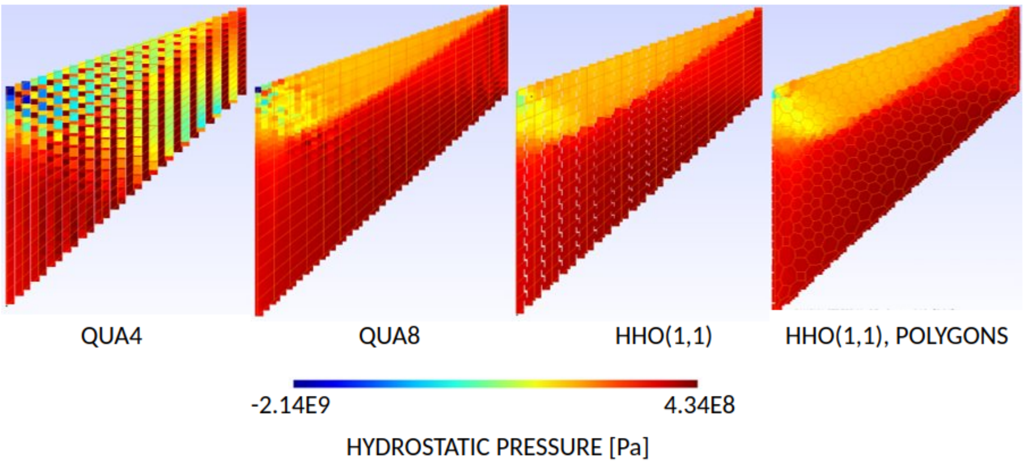

Figure 9: Comparison of the hydrostatic pressure computed using the Hybrid High Order (HHO) method and standard finite elements

– Mines ParisTech, PSL University, Centre des matériaux, CNRS UMR 7633, 91003 Évry, France.

The standard finite element method suffers from volumetric locking when nearly- incompressible materials are considered, leading to spurious oscillations of the hydrostatic pressure. In order to circumvent this phenomenon, the recent HHO (Hybrid High Order) [25, 26] method is considered. This method has several advantages over standard finite elements:

- It is robust to volumetric locking phenomena in primal formulation.
- Polyhedral elements are natively supported.
- The displacements and the strains have the same approximation order.

The HHO method is hybrid as it introduces cell displacement unknowns and faces displacement unknowns which live on the cell boundaries. In the spirit of discontinouous Galerkin methods, displacement can be discontinuous at the cell boundary. Cell unknowns are local and can be condensated during the Newton iterations at the structural scale, hence providing an attractive numerical cost.

Generic implementations of the HHO method have been developped in `C++` (`Disk++` project project, `CERMICS`) and in `Python` (`H2O` project, CEA/MinesParisTech) to solve non- linear mechanics problems. Both implementations can use `MFront` generated behaviour through `MGIS`. The method has also been introduced in industrial solvers `code_aster` and `Cast3M`.

In this presentation, we show the robustness of the HHO method to volumetric locking, using non-linear behaviour laws in finite transformations. Moreover, we show that using the HHO method polyhedral support feature, crystalline plasticity laws can be expressed at the at the element level, with a direct correspondence between a Voronoï cell and an HHO polyhedral element in the mesh.

12 The `MFEM-MGIS` project: coupling of `MFEM` and MGIS for High Performance non linear simulations

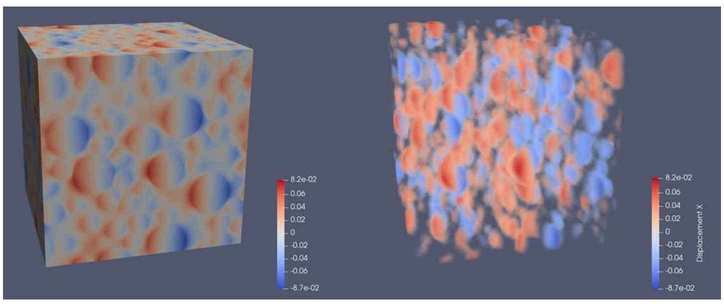

Figure 10: Modelling of 2 000 elastic inclusions in a periodic representative elementary volume with `MFEM-MGIS`

- Guillaume Latu

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The `MFEM-MGIS` library aims at efficiently use supercomputers in the field of implicit nonlinear thermomechanics. Our primary focus is to develop advanced nuclear fuel element simulations where the evolution of materials under irradiation are influenced by multiple phenomena, such as viscoplasticity, damage, phase transitions, swelling due to solid and gaseous fission products.

`MFEM` constitutes the pilar for providing: finite elements abstractions, AMR handling and parallel API.

The `MFEM-MGIS` project is combining `MFEM` with the `MFront Generic Interface Support` library (`MGIS`), an open-source `C++` library that provides convenient data structures to support arbitrarily complex nonlinear constitutive equations generated by the `MFront` code generator.

This talks will discuss the goal of the project, the design of the library (including additions made to `MFEM`) and show early results and benchmarks.

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