

# Agenda of the ninth **MFront** User Meeting

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## 1 Back to basics: an introduction to **MFront** through isotropic Domain Specific Languages (DSL)

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**Keywords:** **MFront** tutorial, isotropic Behaviours

This introductory talk to **MFront** aims to provide an overview of the basics of **MFront**, as well as a set of best practices through a simple, concrete modeling example.

This presentation, addressed to both novices and experienced users, focuses on the description of isotropic (visco-)plastic behavior laws and their implementation in the **MFront** software, using dedicated parsers for this particular type of material behavior modeling.

In this presentation, detailed information will be given on how **MFront** simplifies the creation of material models using DSLs dedicated to isotropic models, focusing on the following points:

- A detailed analysis of **MFront**'s syntax and functionality for defining isotropic material behavior.

- A practical example of the implementation of material models using MFront, illustrating how the software can be used to specify isotropic behaviour laws.
- The use of the generated libraries and their use with numerical simulation tools.

## 2 Overview of TFEL-4.2 and MGIS-2.2.

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Version 4.2 of TFEL is meant to stabilize the 4.x branches before a new development cycle that will start next year with the 5.x branch (based on C++-20). So does Version 2.2 of MGIS.

Evolutions are focused on new features required by projects support TFEL developments, porting to GPUs of the TFEL/Math and TFEL/Material library, bugs fixing, and documentation.

See this page for a full description: <https://thelfer.github.io/tfel/web/release-notes-4.2.html>

The first chapters of the upcoming MFront book will be presented.

This talk will focus on some of these developments to illustrate their impact on end users and on solvers, notably those based on MGIS.

## 3 First experiences with MFront and MGIS on GPUs

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Graphical Processing Units have attractive raw numerical performances, but can perform poorly in case of complex kernels, such as standard mechanical behaviours.

A key point is the fact that the behavior integration must be performed on a batch of integration points. This requires a deeper integration of MFront and MGIS. As a consequence, the first targets are FFT solvers, such as AMITEX\_FFTP, as:

- The structure of codes based on Fast Fourier Transform allows a clear and a natural separation behaviour integration step from the rest of the code, which is not the case in most FEM based solver.
- The effectiveness of FFT-based methods to solve equilibrium equations, is such that, for non-linear behaviors, a significant part of the simulation time is spent in the behaviour step.

This talk describes our experiences in porting mechanical behaviours implemented using the TFEL/Math and TFEL/Material libraries to GPU devices. The implementations used are slightly modified versions of implementations generated by MFront to avoid some CPUs specific features, such as exception handling. We show that the TFEL/Math and TFEL/Material libraries can be readily used in various GPU parallel programming model such as cuda, kokkos and sycl.

The talk exhibits some early and interesting results for small-strain isotropic (visco-)plastic behaviours, the integration of which can be reduced to a scalar Newton resolution. More complex cases are then described. Solutions to handle behaviours requiring pre- and pos-processing steps (such as orthotropic and/or finite strain behaviours) will be discussed.

The talk concludes on some early thoughts and proposals about integration in FEM based solvers.

## 4 Multiphysics modelling of bonding/debonding phenomena at the pellet-cladding interface in nuclear fuels

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**Keywords:** multiphysics coupling, thermo-chemo-mechanical behaviour, bonding interface, elastic damage, standard materials, nuclear fuel.

In the framework of bonded bodies' multiphysics simulation, we proposed a fully coupled thermo-chemo-mechanical cohesive zone model (CZM). The fully coupled CZM is used for simulating bonding formation, progressive damage up to fracture and friction at the interface of bonded solids under mechanical and thermal cyclic loadings. The mechanical loadings combine tension or compression and shear loadings. The main purpose of this work is to study the influence of the CZM building and the couplings between each physics on the model ability to reproduce the above-mentioned phenomena. The constitutive modelling is performed in full compliance with the thermodynamic principles and with the aim to apply later this modelling on several studies of bonded bodies.

The bonding formation is modelled with an increase of interface stiffness and critical fracture energy in tension and shear. The interface stiffness evolution is enabled by the introduction of a new internal variable that describes the evolution of chemical reactions at the interface under thermomechanical loadings. On top of that, the proposed model describes the thermal flux at the interface as a function of damage and bonding. This thermal flux is formed of the three modes of heat transfer: conduction, convection and radiation. In finite element modelling, the initial gap between solids and non-solid penetration are taken into account with a unilateral contact algorithm. The formulation is very general and hence admits arbitrary geometries and materials.

This work is part of a multiphysics modelling of fuel cladding (mixed oxide - stainless steel) interface in sodium fast nuclear reactors. In this work, various monotonic and cycling loadings are studied in order to show the main features of the model and the differences with other existing models.

## 5 Usage of MGIS in Manta: a case of study

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**Manta** is developed at CEA to be a new generation software for the numerical simulation in mechanics geared toward HPC [1]. **Manta** is meant to be the successor of **Europlexus** and **Cast3M**.

**MGIS** is one of the basis of the so-called end-user API of **Manta**.

Strongly inspired by the **licos** solver of the **Pleiades** platform [2, 3], **MGIS** provides the relevant information to build a dependency graph between models (mechanics, heat transfer, etc.).

This dependency graph is used to check the consistency of the computation. Missing dependencies can be resolved using information provided by the user about the materials or the loadings to which the physical system of interest is subjected.

This talk highlights the role of **MGIS**, associated with this dependencies management algorithm, in providing a streamlined user experience, in particular for complex nonlinear multiphysics simulations.

## 6 Towards an MFfront-based framework for the constitutive modelling of concrete at high strain rates

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**Keywords:** Concrete, Fast transient dynamics, Sympy, Mtest

For more than ten years, the *Laboratoire d’études de DYNAmique* lab at CEA has gathered an in-house knowledge about mesoscale constitutive modelling of concrete at high strain rates through Europlexus [4], which is a finite element software dedicated to fast-transient dynamics.

Across the years, the continuous developments [6] have tried to make it compatible with both experimental and literature results. This was done by adding/modifying the activated mechanisms models (plasticity, damage, strain-rate sensitivity ...). However, there have been no specific efforts done in order to guarantee quality, or to improve code versatility for other uses than simulations, such as constitutive parameters sensitivity analysis with a thirdparty software or constitutive parameters identification.

This talk depicts the first step of a reimplementaion of the constitutive laws through MFfront which embeds a more flexible framework to improve constitutive equations integration accuracy, robustness, computational efficiency and portability. As the equations involved are strongly nonlinear, we propose an innovative way to derivate the numerical scheme, based on symbolic calculations with the SymPy [7] library. After introducing the strategy, verification tests are performed to assess the implementation.

## 7 Microstructure-based modelling of snow viscoplasticity using FFT simulations and MFfront to model crystal plasticity

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**Keywords:** Porous material, Crystal plasticity, Microstructure, X-ray tomography, FFT simulations

The porous structure of snow densifies with time under gravity. Knowledge of snow settlement is essential for many applications such as paleoclimatology and avalanche forecasting [8]. Snow densification is mainly driven by the creep of the ice matrix undergoing viscoplastic deformation. Although the macroscopic behaviour has

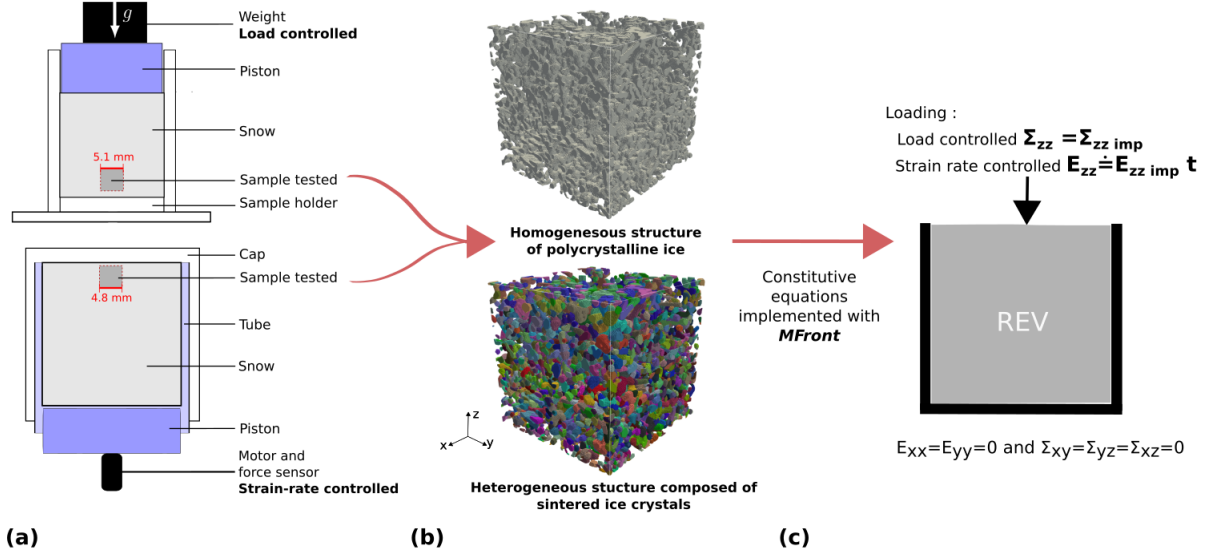


Figure 1: Main workflow. (a) Schematic diagram of the setup associated to the load controlled test (top) and strain-rate controlled test (bottom). (b) Sub-volume on which the simulation was performed: ice-air segmentation for the homogeneous model (top), grain segmentation for the sintered crystals model (bottom). (c) Numerical set-up and boundary conditions.

been previously explored through experiments, little is known about the driving mechanism at the microscale and the influence of the microstructure and crystalline texture on snow viscosity.

In this study, we modelled the elasto-viscoplastic behaviour of snow based on 3D images of its microstructure and the mechanical properties of ice (Fig. 1). We conducted the simulations with a Fast Fourier Transform-based numerical solver (AMITEX\_FFTP, available at <https://amitexfft.github.io/AMITEX/index.html>) to avoid the complex meshing procedure and benefit from high-performance computing facilities. We used two different viscoplastic models for ice at the microscale. The ice matrix in the snow is either considered (i) a homogeneous structure of polycrystalline ice modelled with a 3D Norton-Hoff law [9] or (ii) a heterogeneous structure composed of sintered crystals on which each dislocation plane can be modelled. The behaviour law was implemented in the *MFront* code generation tool for the second model by adapting the Méric-Cailletaud single crystal behaviour brick to the crystal plasticity model for ice [10]. For the first time, this work simulates the behaviour of snow on a crystalline scale, enabling us to identify the possible dominant deformation mechanisms.

We compared our numerical experiments to oedometric compression tests captured by tomography [11]. The model reproduced the increase of viscosity driven by the measured structural changes induced by the progressive settlement. The simulations are closer to the experiments when ice is considered a heterogeneous set of ice crystals rather than homogeneous polycrystalline ice. The numerical experiments on the crystal plasticity model also revealed that the strain is highly localized in the ice matrix, 5 % of the microstructure reaches a vertical stress value higher than 58 times the macroscopic loading. In addition, the strain is driven only by the basal slip system, which represents 99% of the plastic deformation. Overall, this study contributes to developing improved formulations of snow settlement in detailed snowpack simulation tools. It provides a tool to perform mechanical numerical experiments on various snow microstructural patterns.

## 8 Anisotropic damage and gradient-enhanced Eikonal regularization for quasi-brittle materials

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**Keywords:** anisotropic damage, gradient-enhanced, Eikonal non-local, quasi-brittle materials.

Isotropic damage models (e.g., [12]) have proved to be successful in modeling one-dimensional problems or giving an approximation of three-dimensional damage in the case of proportional loading [13]. However, damage in concrete is essentially anisotropic due to some well-known behaviors: strong dissymmetry between tension and compression, unilateral effect, induced anisotropy, etc. Damage is considered to have preferential directions to occur, and this should be described conveniently by tensors instead of a single scalar variable [14].

Many authors have proposed to work with second-order tensors ([15–19]), restricting damage to orthotropic behaviors. Concerning quasi-brittle materials, this assumption is consistent with the phenomenological observations of cracks perpendicular or parallel to the load direction [20].

From a numerical point of view regarding finite element analysis, all the constitutive relations mentioned above hold for a Gauss quadrature point. However, as already well known, simulations at the structure scale with such models will inevitably give mesh-dependent results if no regularization technique is applied. Non-local damage models of integral [21] and gradient-enhanced [22] type have been used for recovering objectivity. Nevertheless, these methods are not capable of reproducing realistic cracking behavior, which is mainly attributed to damage diffusion, initiation and attraction to boundaries [23–28]. These drawbacks are related to the fact that the interactions are considered constant and isotropic in the classic approaches.

To solve this issue, a new class of non-local evolving interactions (or transient internal length) models was developed. [23] proposed one of the first evolving interactions models, where the gradient parameter was supposed to vary in function of the strain but remained isotropic. [29] proposed an internal time integral formulation, introducing some internal length depending on the damage field, which could eventually be anisotropic. Isotropic damage-dependent evolving interactions were considered in [30], where the micromorphic framework is used to derive a similar gradient-enhanced model. [31] developed a stress-based evolving interactions integral model, which could better deal with free boundaries. A gradient-enhanced version of such an anisotropic interactions approach was developed in [32]. [33] proposed an anisotropic transient-gradient approach based on [30], coupling the effect of damage and stress fields in the interactions. Other evolving interactions models exist (e.g., [25, 34]), and the common point of all these approaches is that damage is still considered as an isotropic variable at the behavior level (i.e., a scalar quantity).

Classic non-local models (i.e., with constant internal length) have already been applied to anisotropic damage models. For instance, [35] used the conventional non-local integral approach coupled to a second-order damage tensor constitutive relation. [36] used a classic gradient-enhanced model (based on the strain tensor) to regularize the anisotropic microplane formulation for quasi-brittle materials. A simplified gradient-enhanced regularization of microplane models was proposed in [37], where a scalar quantity is considered in the regularization instead of the strain tensor.

In this work, we propose to couple an evolving anisotropic interactions gradient-enhanced (ENLG) regularization [38] to an anisotropic damage constitutive behavior [19]. The main idea is that the anisotropic behavior in quasi-brittle materials, such as concrete, is induced by damage, while the medium is considered initially isotropic. The induced anisotropy is therefore considered through the ENLG model, where non-local interactions naturally evolve from isotropic to anisotropic in function of a damage-dependent Riemannian metric. The numerical implementation is developed in an in-house finite element code at CEA Saclay based on the FreeFem finite element solver. An implicit algorithm scheme implemented within the MFRONT tool ensures behavior integration at quadrature points, while the communication with the global finite element solver is handled through MGIS. Theoretical and practical aspects are discussed through analyzing numerical simulations (Figure 2) in two and three-dimensional contexts.

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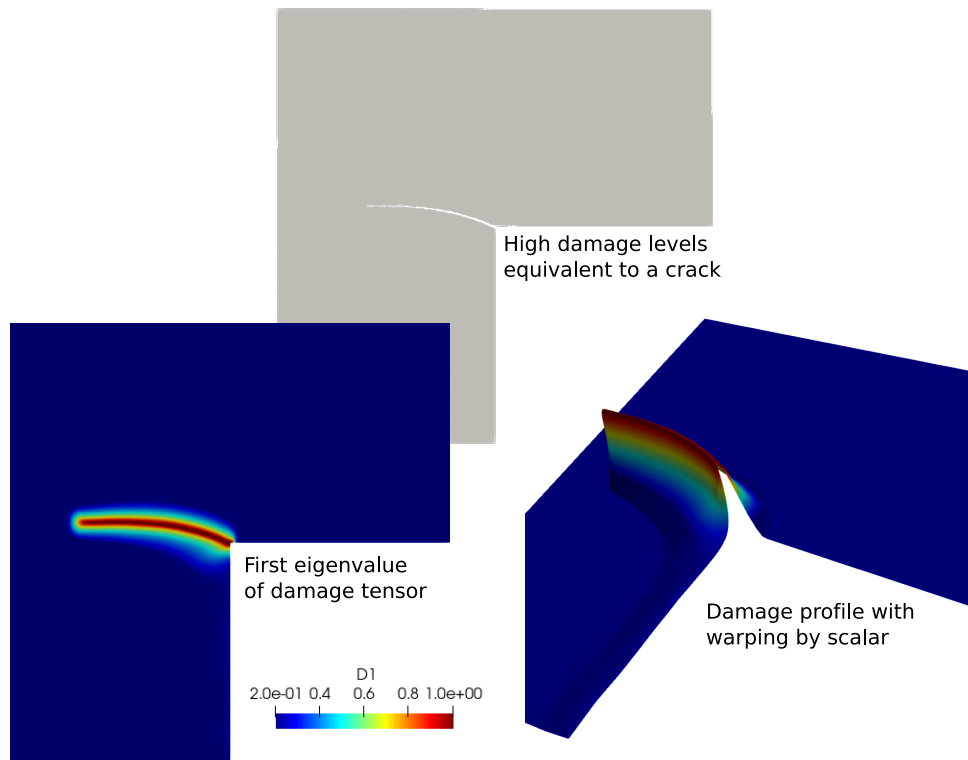


Figure 2: Example of the first damage eigenvalue  $D_1$  color map for the L-shape test and equivalent crack obtained by post-processing techniques.

## 9 Analyse sismique d'un canal par une approche dynamique transitoire simplifiée

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La sûreté des digues et barrages est périodiquement réanalysée dans le cadre d'études de dangers réglementaires. Celles-ci s'appuient sur des études de stabilité dont les situations de chargement sont définies par arrêté ministériel. La situation sismique doit ainsi être justifiée par le calcul pour les ouvrages de grande importance (classes A & B) situés en zone de sismicité 3 et plus.

Conformément aux recommandations de la profession, EDF applique le principe d'approche graduée pour la justification de ces ouvrages allant d'une approche pseudo-statique à une approche dynamique transitoire simplifiée découplant la réponse dynamique de l'ouvrage de l'estimation des déplacements induits. Des développements ont été réalisés ces dernières années par la R&D d'EDF afin d'implémenter ce dernier type d'approche dans `code_aster`: loi d'Iwan développée dans l'environnement `MFront` (présentation au Club-U Mfront en 2016) permettant de décrire la réponse dynamique des sols, et macro-commande `POST_NEWMARK` permettant d'estimer les déplacements irréversibles induits. La première utilisation industrielle de ce développement sur un canal a montré tout son intérêt avec la justification des derniers profils critiques.

## 10 Intégration de MGIS/MFront dans MEF++: interface et cas d'utilisations

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Dans le cadre d’une approche *tout durable*, Michelin tire profit de son expertise et de sa capacité d’innovation dans le domaine des matériaux composites flexibles afin d’étendre son activité au delà du pneumatique. Ainsi, la conception de nouveaux matériaux et la modélisation de leur comportement sont plus que jamais au coeur de l’activité du groupe. Afin d’accompagner cette transformation, des développements sont menés pour favoriser la portabilité et la modularité des outils de modélisation des matériaux.

Dans ce contexte, la suite **MGIS/MFront** a récemment été intégrée au solveur éléments finis **MEF++** [39], co-développé par le laboratoire GIREF de l’Université Laval et par Michelin, avec un double objectif:

- permettre aux concepteurs matériaux d’appeler des lois de comportement externes au solveur, et utilisables dans des environnements variés (prototypage, ajustement de paramètres, etc.)
- favoriser la collaboration autour de la modélisation des matériaux et des structures avec des partenaires industriels et académiques

Cette présentation expose les choix d’implémentation retenus pour appeler des lois de comportement **MFront** dans le solveur **MEF++**. Des cas de validation et d’utilisation sont ensuite présentés, et des perspectives de développement pour étendre la gamme des scénari d’utilisation de **MFront** à Michelin sont finalement proposées.

## 11 A temperature-dependent constitutive model for argillaceous hard soils - weak rocks

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**Keyword:** MFront, OpenGeoSys, temperature dependence, THM analysis.

This talk describes the implementation of a constitutive model through **MFront** to characterise the behaviour of argillaceous hard soils - weak rocks. Particularly, the model is intended to be used in the finite element code **OpenGeoSys**, to perform coupled thermo-hydro-mechanical analyses of underground excavations in the context of deep geological nuclear waste disposal. Special emphasis is placed on the effect that variations of temperature have on the behaviour of these indurated clayey materials.

As identified in previous experimental research, heating saturated clays under drained conditions induces volume changes that depend on the stress history. Normally consolidated clays exhibit thermo-plastic contraction, while overconsolidated and indurated clayey materials show an initial thermo-elastic expansion, followed, at some threshold temperature, by irreversible contractive strains. On the other hand, the strength generally decreases as temperature increases. The implemented constitutive model accounts for the variation of mechanical properties to reproduce the observed behaviour, including the expansion-contraction transition identified in stiff clays. The latter is achieved in the context of multi-surface plasticity, where deviatoric and volumetric yield surfaces are assumed to depend on temperature. Some validation examples are presented, where laboratory tests with temperature variations are simulated both from a constitutive standpoint, with the **MTest** tool, and as a coupled THM boundary value problem in **OpenGeoSys**.

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