TFEL-5.1 and MGIS 3.1

MFront Users Meeting

(1) CEA, DES, IRESNE, DEC, SESC, LMPC, Cadarache, France

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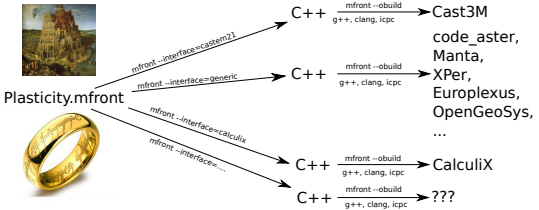
Outline

1. Overview

MFront goals



- `MFront` is a code generation tool dedicated to material knowledge (material properties, mechanical behaviours, point-wise models):
  - Support for small and finite strain behaviours, cohesive zone models, **generalised behaviours**.
  - Point-wise models can also be used to create **post-processings**.
- Main goals:
  - Numerical efficiency (see various benchmarks on the website).
  - Portability: `Cast3M`/`Cyrano`/`code_aster`, `Europlexus`/`AMITEX_FFTP`/`Abaqus`/`CalculiX`/`FEniCS`, `CPU`/`GPU`, `C`/`fortran`/`python`/`Julia`, etc.
  - **Long term support and stability**: `MFront`'s implementations reflects valuable knowledge accumulated over decades about materials and are used in safety critical studies.
  - **Ease of use**: *Longum iter est per praecepta, breve et efficax per exempla* (It's a long way by the rules, but short and efficient with examples).

An example of the `StandardElasticityVicoPlasticity` brick

```
@DSL Implicit;
@Behaviour MohrCoulomAbboSloan3;

@Epsilon 1.e-14;
@Theta 1;

@Brick StandardElastoViscoPlasticity{
  stress_potential : "Hooke" {
    young_modulus : 150.e3,
    poisson_ratio : 0.3
  },
  inelastic_flow : "Plastic" {
    criterion : "MohrCoulomb" {
      c : 3.e1,          // cohesion
      phi : 0.5235987755982999,   // friction angle or dilatancy angle
      lodeT : 0.506145483078356,  // transition angle as defined by Abbo and Sloan
      a : 1e1          // tension cuff-off parameter
    },
    flow_criterion : "MohrCoulomb" {
      c : 3.e1,          // cohesion
      phi : 0.174532925199433,   // friction angle or dilatancy angle
      lodeT : 0.506145483078356,  // transition angle as defined by Abbo and Sloan
      a : 3e1          // tension cuff-off parameter
    },
    isotropic_hardening : "Linear" {R0 : "0"}
  }
};
```

- The `StandardElasticityVicoPlasticity` brick allows to implement complex visco-plastic behaviours with a declarative syntax using predefined components.

An simple example with the Implicit DSL

```
@DSL Implicit;
@Behaviour Norton;
@Brick StandardElasticity;

@MaterialProperty stress E;
E.setGlossaryName("YoungModulus");
@MaterialProperty real ν, A, nn;
ν.setGlossaryName("PoissonRatio");
A.setEntryName("NortonCoefficient");
nn.setEntryName("NortonExponent");

@StateVariable real    p;
p.setGlossaryName("EquivalentViscoplasticStrain");

@Integrator{
  constexpr const auto Mᵉ = Stensor4::M();
  const auto μ = computeMu(E, ν);
  const auto σᵉ = sigmaeq(σ);
  const auto iσᵉ = 1 / (max(σᵉ, real(1.e-12) · E));
  const auto vᵖ = A · pow(σᵉ, nn);
  const auto ∂vᵖ/∂σᵉ = nn · vᵖ · iσᵉ;
  const auto n = 3 · deviator(σ) · (iσᵉ / 2);
  // Implicit system
  fεᵉˡ += Δp · n;
  fp -= vᵖ · Δt;
  // jacobian
  ∂fεᵉˡ/∂Δεᵉˡ += 2 · μ · θ · dp · iσᵉ · (Mᵉ - (n ⊗ n));
  ∂fεᵉˡ/∂Δp = n;
  ∂fp/∂Δεᵉˡ = -2 · μ · θ · ∂vᵖ/∂σᵉ · Δt · n;
} // end of @Integrator
```

- Implicit integration.
- Implicit system:

$$\begin{cases} f_{\underline{\underline{\varepsilon}}^{el}} = \Delta\,\underline{\underline{\varepsilon}}^{el} - \Delta\,\underline{\underline{\varepsilon}}^{to} + \Delta\,p\,\underline{\underline{\mathbf{n}}} \\ f_p = \Delta\,p - A\,\sigma_{eq}^{n} \end{cases}$$

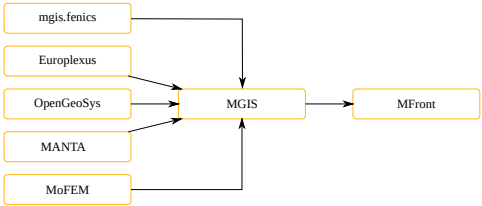
- Jacobian:

$$\begin{cases} \dfrac{\partial f_{\underline{\underline{\varepsilon}}^{el}}}{\partial \Delta\,\underline{\underline{\varepsilon}}^{el}} = \underline{\underline{\mathbf{I}}} + \dfrac{2\,\mu\,\theta\,\Delta\,p}{\sigma_{eq}} \left(\underline{\underline{\underline{\underline{\mathbf{M}}}}} - \underline{\underline{\mathbf{n}}} \otimes \underline{\underline{\mathbf{n}}} \right) \\ \dfrac{\partial f_{\underline{\underline{\varepsilon}}^{el}}}{\partial \Delta\,p} = \underline{\underline{\mathbf{n}}} \\ \dfrac{\partial f_p}{\partial \Delta\,\underline{\underline{\varepsilon}}^{el}} = -2\,\mu\,\theta\,A\,n\,\sigma_{eq}^{n-1}\,\Delta\,t\,\underline{\underline{\mathbf{n}}} \end{cases}$$

- **All programming and numerical details are hidden (by default)**.

- Tensorial operations are provided by the `TFEL/Math` library
- The `TFEL/Material` library provides useful physical functions

Ecosystem



- The `MFrontGenericInterfaceSupport` (`MGIS`) project eases the support of `MFront`'s generated behviours in solvers.
  - Written in `C++`. Interfaces exist for `C`, `Fortran2003`, `python`, `Julia`.
  - Used in `code_aster`, `MFEM/MGIS`, `Europlexus`, `OpenGeoSys`, `XPer`, `Manta`, `dofinx_materials` and many more...
- `MFrontGallery`: a project to compile, test and deploy `MFront` implementations based on the `CMake` build system.
- `TFELMathEnzyme`: a library leveraging `Enzyme` to provide automatic differentiation (experimental).
- `MFrontJIT`: just in time compilation for `MFront`, to be integrated in `MGIS`

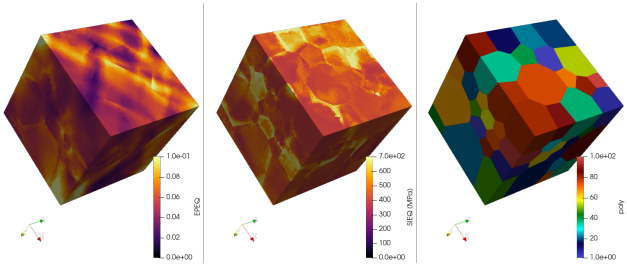
Outline

2. Highlights

Trainings

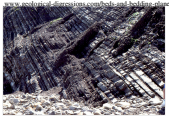
- 2025
  - Centrales Nantes
  - EDF Enery UK, Manchester
  - CEA Saclay (SEMT)
- 2026 (planned)
  - CEA Cadarache (February)

Calculations of aggregates in crystal plasticity with code_aster



- Finite strain single crystal laws
- Phenomenological and physics-based laws successfully implemented in MFront
- Robust and efficient
- "Slowness" inherent in crystalline plasticity formalismwith classical Newton scheme
  - $\approx$ 30 iterations per increment
- Difficulty managing periodic boundary conditions in code_aster
- Plastic incompressibility poorly respected in large transformations?

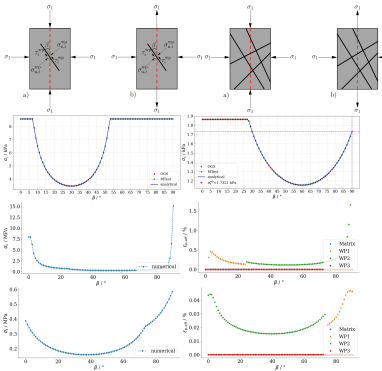
Ubiquitous Joint Model with Three Oblique Joint Sets



$$F^{\mathrm{wp}} = \sigma_{\mathrm{n,i}}^{\mathrm{wp}} \sin\varphi + \left(\tau^m \cos^m\varphi + a^m \sin^m\varphi\right)^{1/m}$$

$$G^{\mathrm{wp}} = \sigma_{\mathrm{n,i}}^{\mathrm{wp}} \sin\psi + \left(\tau^m \cos^m\psi + a_{\mathrm{G}}^m \sin^m\psi\right)^{1/m}$$

$$\sigma_{\mathrm{n,i}}^{\mathrm{wp}} = \boldsymbol{\sigma} : \boldsymbol{n}_{\mathrm{i}}^{\mathrm{wp}} \otimes \boldsymbol{n}_{\mathrm{i}}^{\mathrm{wp}}, \quad \text{and} \quad \tau_{\mathrm{i}} = \sqrt{\boldsymbol{t}_{\mathrm{i}} \cdot \boldsymbol{t}_{\mathrm{i}} - (\boldsymbol{\sigma} : \boldsymbol{n}_{\mathrm{i}}^{\mathrm{wp}} \otimes \boldsymbol{n}_{\mathrm{i}}^{\mathrm{wp}})^2}$$



- Introduces ubiquitous joint Model incorporating three distinct oblique joint sets.
- Captures anisotropic mechanical behaviour arising from multiple non-orthogonal discontinuities.
- Suitable for simulating geomaterials with complex joint networks under various loading conditions.
- Implements tension cutoff criterion to limit unrealistic tensile stresses.
- Coupling with OGS processes.

Ghasabeh and Nagel (2025)
TU Bergakademie Freiberg, Germany

- Implementation available in OGS:
  - https://gitlab.opengeosys.org/MehranGhasabeh/ogs-mg/-/blob/ogs-Oblique/MaterialLib/SolidModels/MFront/UBI3ObliqueTC.mfront?ref_type=heads

Transversely Isotropic Elastoplastic Damage Model

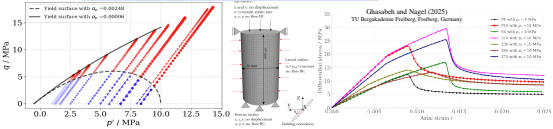
The plastic strain rate is calculated through a flow rule equation

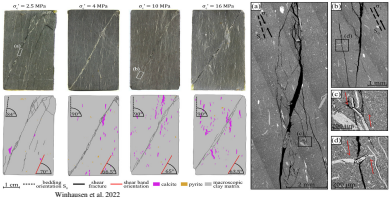
$$\dot{\varepsilon}^{\mathrm{pl}} = \dot{\lambda}\frac{\partial G}{\partial \sigma}$$

The yield and the plastic potential functions are

$$F := \hat{F}(I_1, J_2, \theta, \alpha_p) = J_2 - \frac{(-\alpha_p I_1^n + \gamma I_1^2)}{\sqrt{\exp(\beta_1 I_1) - \beta\cos(3\theta)}}$$

$$G := \hat{G}(I_1, J_2, \theta, \alpha_q) = J_2 - \frac{(-\alpha_q I_1^n + \gamma I_1^2)}{\sqrt{\exp(\beta_1 I_1) - \beta\cos(3\theta)}}$$





Winhausen et al. 2022

- Develops a single plastic surface with capping response.
- Ansisotropic stiffness and strength due to bedding orientation.
- Pre-peak strain hardening.
- Post peak damage evolution for softening.
- Suitable for model developed for clay rock.
- Coupling with OGS processes.

Ghasabeh and Nagel (2025)
TU Bergakademie Freiberg, Germany

- Implementation available in OGS:
  - https://gitlab.opengeosys.org/MehranGhasabeh/ogs-mg/-/blob/ogs-Oblique/MaterialLib/SolidModels/MFront/DesaiTransverselyIsotropicHardeningDamage.mfront?ref_type=heads

MFrontGallery

```
cmake ../MFrontGallery/ -DCMAKE_BUILD_TYPE=Release -Denable-c=ON -Denable-c++=ON -Denable-excel=ON -Denable-fortran=ON  \
-Denable-python=ON -Denable-java=ON -Denable-octave=ON -Denable-generic=ON -Denable-castem=ON -Denable-aster=ON -Denable-cyrano=ON  \
-Denable-ansys=ON -Denable-europlexus=ON -Denable-calculix=ON -Denable-abaqus=ON -Denable-abaqus-explicit=ON -Denable-diana-fea=ON  \
-Denable-zmat=OFF -Denable-fortran-behaviours-wrappers=ON -Denable-mfront-documentation-generation=ON  \
-DCMAKE_INSTALL_PREFIX=/home/th202608/codes/MFrontGallery/master/install
```

- The `MFrontGallery` project provides a `cmake` infrastructure to build, deploy and tests MFront implementations.
  - https://thelfer.github.io/MFrontGallery/web/index.html
  - https://github.com/thelfer/MFrontGallery
- An overview of the project is given in the recently published paper in the Journal Of Opensource Software [2]
- Used in the FailureCriteria project (see J. Hure's talk)

MFEM/MGIS

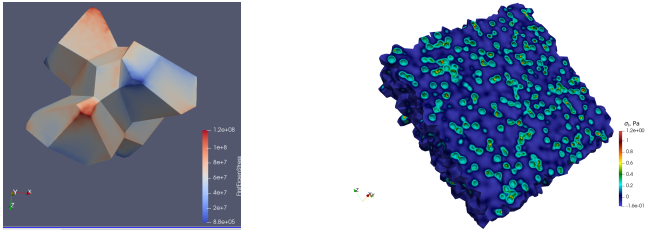


Figure 1: Von Mises equivalent stress of the Cauchy stress in a polycristal (left). Calculation of the first principal stress σ_I induced by a unitary internal pressure in spherical porosities (right).

- The `MFEM/MGIS` project provides an HPC thermomechanical solver for mesocale simulations.
  - `https://thelfer.github.io/mfem-mgis/index.html`
  - `https://github.com/thelfer/mfem-mgis`
  - This solver is developed in the framework of the European Opera HPC project.
- An overview of the project is given in the recently published paper in the Journal Of Opensource Software [1]

Outline

3. Evolutions and new features in TFEL libraries

Some evolutions of the TFEL/Math library

- A static method named `zero` is now available to create fixed-size tensorial objects.

```
constexpr auto s = stensor<2u, double>::zero();
```

- The `View` class allows to interpret a contiguous memory area as a tensorial object. Such views are not efficient on GPUs where coalescent memory access are preferable. The newly introduced `CoalescedView` class offers a solution to this issue. A coalesced view is initialized by an array of pointers to the components of the mapped object, as illustrated in the following snippet:

```
int values[8] = {1, 10, 2, 20, 3, 30, 4, 40};
std::array ptrs{&values[0], &values[2], &values[4], &values[6]};
auto s1 = map<stensor<2u, int>>(ptrs);
```

New library TFELMFrontDatabase

- The TFELMFrontDatabase library provides the MFrontDatabase class which allows to analyse libraries generated by MFront.

```
import mfront.database
db = mfront.database.MFrontDatabase()
r = db.analyseDirectory('/tmp/test-lib/')
epts = db.getEntryPoints(type = 'behaviour',
                         interface = 'generic',
                         material = 'concrete'):
for e in epts:
    print(f"{e.library}: {e.name}")
```

- Entry points can be filtered by name, material, interface and type (behaviour, material property or point-wise model).
- The database can be built from a list of directories or using an environment variable.
- See usage in MGIS later in this talk.

TFEL/Material

- `TFEL/Material`'s evolutions were mainly driven by the developments of the `TFEL/Material/Homogenization` library
  - See A. Martin's talk

Outline

4. Evolutions and new features in MFront

Warnings

- Many warnings have been added to detect potential misuses of `MFront` or known bad practices. A typical example of this feature is the following:

```
$ mfront --interface=generic Plasticity.mfront
[warning]: using the default value for the convergence threshold.
This value is generally considered too loose.
You may want to consider a more stringent value (1e-14 is a good choice).
See the `@Epsilon` keyword for details.
```

- The user has many ways of controlling how warnings are treated, or how to activate/deactivate them.
  - Reporting warnings is activated by default and can be disabled by passing the command line argument `--report-warnings=false` to `MFront`.
  - Warnings are associated with keywords and code blocks. Warnings can be disabled by appending the `safe` option to them:

```
@Epsilon<safe> 1;
```

  - This `safe` option can be ignored by passing the `--ignore-safe` command line argument to `MFront`. This argument is useful when analysing an existing file (written by another person) to question implementation choices.
- **Proposals for new warnings are welcomed !**

Behaviour variables

```
@BehaviourVariable b1 {
  file: "Plasticity.mfront",
  variables_suffix: "1",
  external_names_prefix: "FirstPhase",
  store_gradients: true,
  store_thermodynamic_forces: true,
  shared_external_state_variables: {".+"}
};
```

- Behaviour variables are variables associated with another behaviour.
  - https://thelfer.github.io/tfel/web/behaviour-variable.html
  - `mfront --help-keyword=Default:@BehaviourVariable`
- Behaviour variable is useful in many contexts:
  - It allows switching from a numerical implementation to another, for instance from a fast implementation to a robust one if the fast one diverges.
  - It allows easy implementation of various non-linear homogenization schemes. Tutorials are available on the TFEL website for:
    - Implementing the Sachs/Reuss homogenization scheme.
    - **Implementing the Taylor/Voigt homogenization scheme**.
    - Implementing the β-rule homogenization scheme.
  - Thanks to behaviour variables, the `@Model` keyword now supports point-wise models based on the following DSL: `DefaultModel`, `RungeKuttaModel`, `ImplicitModel`.

Example of usage (Taylor/Voigt homogenization scheme)

```
@Integrator{
  b1.deto=deto;

  constexpr auto b1_smflag = TangentOperatorTraits<MechanicalBehaviourBase::STANDARDSTRAINBASEDBEHAVIOUR>::STANDARDTANGENTOPERATOR;
  const auto r1 = b1.integrate(b1_smflag,CONSISTENTTANGENTOPERATOR);
  StiffnessTensor Dt1 = b1.getTangentOperator();

  b2.deto=deto;

  constexpr auto b2_smflag = TangentOperatorTraits<MechanicalBehaviourBase::STANDARDSTRAINBASEDBEHAVIOUR>::STANDARDTANGENTOPERATOR;
  const auto r2 = b2.integrate(b2_smflag,CONSISTENTTANGENTOPERATOR);
  StiffnessTensor Dt2 = b2.getTangentOperator();

  updateAuxiliaryStateVariables(b1);
  updateAuxiliaryStateVariables(b2);

  sig = f * sig1 + (1 - f) * sig2;
  if (computeTangentOperator_) {
    Dt = f * Dt1 + (1 - f) * Dt2;
  }
}
```

- The simpliest nonlinear homogeneization scheme.
- For the sake of simplicity, error handling has been removed.
- For large number of phases, so-called behaviour variables factories can become handy.
- https://thelfer.github.io/tfel/web/behaviour-variable.html

Stress update algorithm in isotropic DSLs

```
@DSL IsotropicStrainHardeningMisesCreep{
  use_stress_update_algorithm : true
};
```

- Isotropic DSLs all introduced the elastic strain as a state variable. When the elastic material properties are now to be constant in time, then the Hooke law can be written in an incremental form

$$\underline{\sigma}|_{t+\Delta t} = \underline{\sigma}|_t + \lambda \operatorname{tr} \Delta \underline{\epsilon}^{to} + 2\mu \left(\Delta \underline{\epsilon}^{to} - \Delta p \ \ n|_{t+\theta \Delta t} \right)$$

  where λ and μ are the first Lamé's coefficient and the shear modulus, Δp is the increment of the equivalent plastic strain and $n|_{t+\theta \Delta t}$ the flow direction at the middle of the time step.

- The `use_stress_update_algorithm` DSL option prevents the declaration of the elastic strain and switches to this incremental form to compute the stress.

Isotropic harderning rules

```
@DSL IsotropicPlasticMisesFlow{
 use_stress_update_algorithm: true
};
@Behaviour PlasticityWithVoceHardeningRule;
@Epsilon 1e-15;
@ElasticMaterialProperties {
  young_modulus: 150e9,
  poisson_ratio: 0.3
};
@IsotropicHardeningRule "Voce" {R0 : 125e6, Rinf : 500e6, b : 20};
```

- The `@IsotropicHardeningRule` and `@IsotropicHardeningRules` allow to use the isotropic hardening rules available in the `StandardElastoViscoPlasticity` brick.
- If an isotropic hardening rule is defined in the `IsotropicPlasticMisesFlow` DSL, and if no flow rule is defined, the following flow rule is automatically defined:

```
@FlowRule {
  f = seq - R;
  df_dseq = 1;
  df_dp = -dR_dp;
}
```

Removal of the Europlexus interface

- The native Europlexus interface has been removed, as Europlexus now uses the generic interface through MGIS
  - see https://github.com/thelfer/tfel/issues/739 for details.

Outline

5. Evolutions and new features in MGIS library

Overview of MGIS/Function

```
const auto evaluator = pk1_function | as_tensor<3>                    |
                       from_pk1_to_cauchy (F_function | as_tensor<3>) |
                       rotate_backwards (R_function | as_matrix<3,3>);
const auto ok = assign(ctx, sig | as_stensor<3>, evaluator);
```

- This computes the Cauchy stress in the global frame from the first Piola-Kirchhoff stress known in the material frame.
  - This is a typical post-processing for simulation on a polycrystal
- This expression is only valid in `3D`:
  - generated kernels are optimized for specified tensor size
- **Tensorial operations requires to build `MGIS` against the `TFEL`'s libraries**.
- The syntax is strongly inspired by the `std::ranges` library

Overview of MGIS/Function

- MGIS/Function provides a C++-20 interface inspired by std::ranges to create computational kernels which are:
  - composable and easily extensible,
  - constexpr-friendly, multi-thread safe, exception safe, GPU-friendly,
  - adaptable for most data structures, as provided by the targeted solver, language or platform,
  - compatible with various programming models (OpemMP, Kokkos, SYCL, CUDA, parallel STL, hpx, etc.)
  - integrated with the TFEL/Math and TFEL/Material library (Eigen support is feasible),
- MGIS/Function aims at memory safety.
- Two algorithms are provided currently available assign and scalar_reduce.
  - In general, two algorithms are required to build **all** the point-wise operations: std::for_each and std::transform_reduce.
  - Most parallel programming models provides efficient implementations of those algorithms.
  - The efficiency depends on the underlying data structures. In general, the simplier the access to the values, the more efficient will be the implementations.
  - Simple access to values is highly recommended for GPU programming.

Prospects for `MGIS/Function`

- We aim at developing a lot of ready to use modifiers based on `TFEL/Math` and `TFEL/Material`:
  - Hencky strain, Hosford equivalent stress, Hill stress, stress invariants, localization indicators, etc.
  - simple constitutive equations (linear small strain elasticity, Saint Venant-Kirchhoff elasticity, Fourier's law, Euler beam, etc.)
  - homogeneization (see A. Martin's work on `TFEL/Material/Homogeneization`)
- Since most solvers and languages provide simple data structure that are easily mappable with `std::span`, we can provides pre-compiled ready to used post-processings to `MGIS`'s users.
  - Those pre-compiled implementation can be exposed to `python`, `fortran`, `C`, `Julia` (for which bindings already exist).
- The work presented here will be the basis for a first generic interface for GPU's in `MFront`.
  - The behaviour integration will be distinct from the assembly.
  - Such implementation would be directly usage in FFT solvers.
- A nice perspective would be to make `JIT` compilation of kernels.
- Functions and views with coalescent access to data are useful for performances on GPU.

The `integrate_debug` function

- The `integrate_debug` function can be used to generate debug files to analyse integration failures.
  - This remove the need to compile `MFront` behaviours with the `--@GenerateMTestFileOnFailure=true` option.
- This snippet shows that the `integrate_debug` functions can be used as drop-in replacement for the `integrate` function:

```
const auto r = integrate_debug(v, b);
```

- In case of integration failure, a markdown file is generated by default, holding all the information required to reproduce the error.
  - Generating an `MTest` file will require extensions on the `MTest` side to support arbitrary behaviours.
- Even if this shall be superfluous, data on input can be copied to prevent memory corruption.
- If data on input are **not** copied, the cost of using `integrate_debug` shall be negligible compared to `integrate`
- This function is documented and very customizable:
  - https://thelfer.github.io/mgis/web/behaviour-integration-failure-analysis.html

Database of material knowledge

- If `MGIS` is compiled against the `TFEL` libraries, it leverages the `TFELMFrontDatabase` library to provide a function named `loadFromDatabase`:

```
import mgis
import mgis.behaviour as mgis_bv
db = mgis.getDatabase()
db.analyseDirectoriesListedInEnvironmentVariable('MFRONT_GALLERY_LIBRARIES',
                                                 ignore_errors = True)
b = mgis_bv.loadFromDatabase(name='\\w+Elasticity\\w+', material='Wood',
                             hypothesis = mgis.behaviour.Hypothesis.Tridimensional)
```

- Secret dream: see this feature used in `AsterStudy`

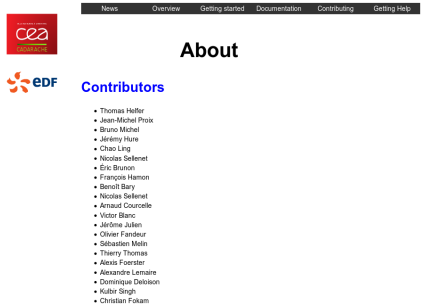
Outline

6. Conclusions and perspectives

Conclusions

- Rewrite code generation in `MFront`
  - Ease extensions of the `StandardElastoViscoPlasticity` brick
- Continue the `MFront` book and improve the documentation.
- Improvement of behaviour variables and behaviour variables factories.
- GPU support:
  - PHD of Tristan Chenaille.
  - Generation of `qfunctions` for `libCEED` and tests in `MFEM` and/or `Ratel`
- Internship dedicated to automatic differentiation and the development of `TFELMathEnzyme`
- Better integration of `MFront`/`MGIS` in `code_aster`:
  - Internship by SIMVIA
- Bindings of `MGIS/Function` in `python`.
- Introduction of `MFrontJIT` in `MGIS`:
  - Integration in `python` for JIT compilations of behaviours described by the `StandardElastoViscoPlasticity` brick

How to contribute



- Citations and illustrations
- Feed-backs, feed-backs, and feed-backs !
  - Please use the forum.
  - Enhancement suggestions (code, documentation, algorithm, etc...)
- Submit new behaviours implementation and tests.
- Submit pages to the gallery.
- Code (for the braves)

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