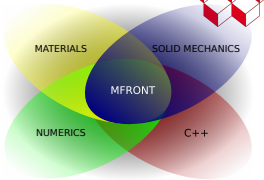

Overview of TFEL 4.2 and MGIS 2.2 and perspectives for TFEL 5.0

MFront User Meeting

06/11/2023

T. Helfer M. Wangermez

CEA, DES, IRESNE, DEC, SESC, LMCP, CADARACHE, FRANCE

Outline

Some highlights of 2023

Overview of `TFEL 4.2` and `MGIS 2.2`

Porting `TFEL` and `MGIS` on GPUs

What's going on for TFEL 5.0 and MGIS 3.0 ?

Conclusions

Addendum

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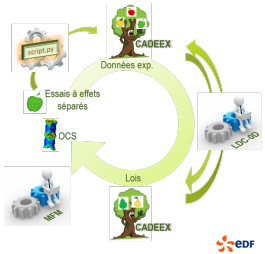

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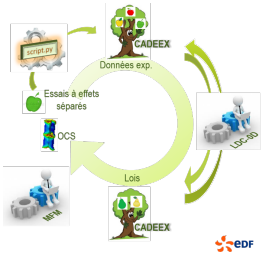

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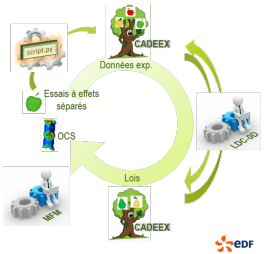

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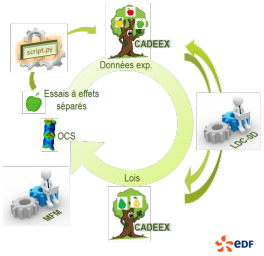

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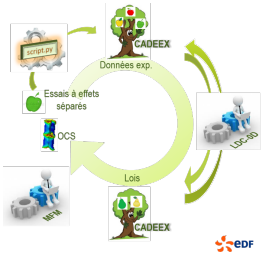

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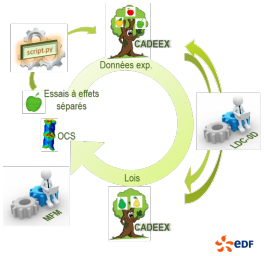

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  - Several training sessions to improve `TFEL` with the `C++` and HPC expert Joel Falcou.

Training sessions

- 3 training sessions are actually planned:
  - 2 training sessions associated in the context of the `MECANUM` project at EDF Lab Saclay:
    - November 2023 and early 2024 (Februar or March).
    - Mostly for engineers at EDF, CEA and Naval Group
  - 1 training session at Cadarache in the context of the `Opera HPC` European project:
    - Mostly targest nuclear engineers from EPFL, VTT, CEA, etc.
- Training sessions are organized **on demand**: typically spanned over two days by groups of around 12 people. The requester must provide rooms, computers, and ~~**beer**~~ meals, etc...

Overview of TFEL 4.2 and MGIS 2.2

Current state of the TFEL 4.x branch

- The TFEL 4.x branch is maturing and starts being used in production.
- TFEL 4.1.x is delivered with:
  - unstable version of code_aster.
  - the upcoming Version 2024 of Cast3M (maybe TFEL 4.2.x).
- Currently, 17 publications based on MFront in 2023 [14, 5, 4, 10, 7, 16, 1, 12, 11, 2, 8, 20, 18, 12, 19, 15, 17].

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  - `3.4.5`: 4 issues fixed.
  - `3.2.9`: 2 issues fixed.
  - `3.1.11`: 6 issues fixed.
  - `3.0.12`: 6 issues fixed.

Issues fixed

- A new release comes with new features and bug fixes.
- Bugs are fixed in the branch corresponding to the release where the bug was introduced and the fix is then spread to newer branches.
  - For instance, if a bug has been introduced in `TFEL 3.2`, the bug is fixed in the `rliv-3.2` branches and spread in the `rliv-3.3`, `rliv-3.4`, `rliv-4.0`, `rliv-4.1` and `master` branches.
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- See the release notes for a description of each issues fixed.
- Creating a release from any of the `rliv` branches is a matter of minutes.

Generalized Gurson-Tvergaard-Needleman yield surface

- The Gurson-Tvergaard-Needleman yield surface can be generalized by replacing the von Mises equivalent stress by another equivalent stress (Hill, Hosford, etc..):

$$S = \left(\frac{\sigma_{eq}}{\sigma_\star}\right)^2 + 2q_1 f_\star \cosh\left(\frac{3}{2} q_2 \frac{\sigma_m}{\sigma_\star}\right) - 1 - q_3 f_\star^2 = 0$$

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- The envisaged syntax is:

```
@Brick "StandardElastoViscoPlasticity" {
    stress_potential : "Hooke" {
        young_modulus : 200e9, poisson_ratio : 0.3
    },
    inelastic_flow : "Plastic" {
        criterion : "GursonTvergaardNeedleman" {
            q1 : 1.5, q2 : 1.0, q3 : 2.2, fc : 0.01, fr : 0.1
        },
        isotropic_hardening : "Linear" {
            R0 : 150e6
        },
        matrix_equivalent_stress: "Hosford"{
            a: 8
        }
    },
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        growth_model : "StandardPlasticModel"
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- The elastic energy release variable, defined as the partial derivative of the free energy with respect to damage, is computed as an auxiliary state variable.

External workspaces for nonlinear solvers

```
template<unsigned short N, typename NumericType>
struct ExternallyAllocatedWorkspace{
  ExternallyAllocatedWorkspace(NumericType* const v)
      : fzeros(v), zeros(v + N), delta_zeros(v + 2 * N), jacobian(v + 3 * N){};
  //! \brief residual vector
  tfel::math::View<tfel::math::tvector<N, NumericType>> fzeros;
  //! \brief current estimate of the unknowns
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- This feature has been introduced to reduce the number of registers used on GPUs.

What's left to end the TFEL 4.x development cycle ?

- Finish support for initialize function (mostly on the MGIS side).
- Finish support for post-processing function (mostly on the MGIS side).
- Support for JIT in MGIS.
- New interfaces:
  - Plaxis: https://github.com/thelfer/tfel/issues/272
  - Flac3D: https://github.com/thelfer/tfel/issues/271

Porting TFEL and MGIS on GPUs

Motivation and challenges

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  - This is the reaons why we focus on a specific use case (FFT solvers) in our early experiments.

Early experiments on GPUs

- Salem Khellal's talk.

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- The most reliable eigen solver in TFEL is based on Jacobi's iterative algorithm. Its usage is strongly adviced when second derivatives of the eigen values are required. This is notably the case for the logarithmic strain framework. A closed formed alternative by Scherzinger et al. is worth investigating [13].

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- JIT compilation to fine-tune the implementation and reduce memory/transfer usage.
- Finite strain strategies consists in pre- and post-processing steps. In particular, the logarithmic strain framework requires the storage of temporary objects between those steps. An external workspace-like strategy is probably required.

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- See also Manta's talk for another point of view.

What's going on for TFEL 5.0 and MGIS 3.0 ?

Port to GPUs

- See the previous challenges !
- Extension of the JIT abilities introduced in TFEL 4.1.

Port to C++ -23

- Time for a great overhaul of `TFEL/Math` and `TFEL/Material` !
  - As always, backward compatibility must be preserved.
- Concepts to replace SFINAE pattern.
  - `trace` implementation in TFEL 4.2:

```
template <typename StensorType>
constexpr std::enable_if_t<implementsStensorConcept<StensorType>(),
                           numeric_type<StensorType>>
trace(const StensorType& s) {
  return s(0) + s(1) + s(2);
}
```

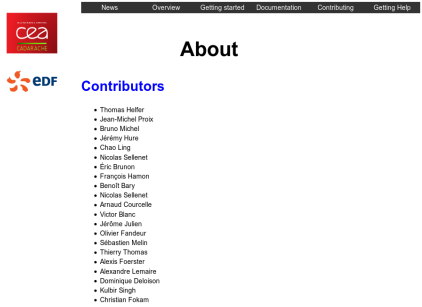
  - `trace` implementation in TFEL 5.0:

```
constexpr auto trace(const StensorConcept auto& s) {
  return s(0) + s(1) + s(2);
}
```

- Multidimensional `operator[]`

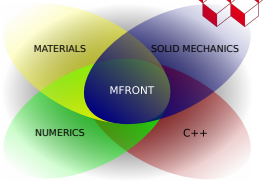
Conclusions

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)

cea iresne



Thanks for you attention ! Any questions?

Initialize functions for behaviours (experimental)

```
@InitializeFunction ElasticStrainFromInitialStress {
  const auto K = 2 / (3 * (1 - 2 * nu));
  const auto pr = trace(sig) / 3;
  const auto s = deviator(sig);
  eel = eval((pr / K) * Stensor::Id() + s / mu);
}
```

- The `@InitializeFunction` keyword introduces a code block that can be used to initialize internal state variables at the very beginning of the computation.
  - A behaviour can define many initialize functions that can be called individually by the calling solver.

Initialize functions for behaviours (experimental)

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@InitializeFunction ElasticStrainFromInitialStress {
  const auto K = 2 / (3 * (1 - 2 * nu));
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  - An initialize function variable can be common to several initialize functions.
- Initialize functions are only supported by the `generic` interface.

Post-processings of behaviours (experimental)

```
// ! principal strains
@PostProcessingVariable tvector<3u,strain> ep;
ep.setEntryName("PrincipalStrain");
// ! compute the principal strain
@PostProcessing PrincipalStrain {
  ep = eto.computeEigenValues();
}
```

- The `@PostProcessing` keyword introduces a code block that can be used to perform computations in a separate step of the behaviour integration.

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- The `@PostProcessing` keyword introduces a code block that can be used to perform computations in a separate step of the behaviour integration.
- The outputs of post-processings are stored in so-called post-processing variables declared by the `@PostProcessingVariable`.

Options to domain specific languages

```
@DSL Default{parameters_as_static_variables : true};
```

- Options to domain specific languages modify their default behaviour:
  - The goal is inhibit some features (for instance, the modification of the parameters from a text file).

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  - Customize the compilation for performances (for instance, treating parameters as static variables).
  - Paves the way toward computations on GPUs and on the fly compilation of behaviours.
- The list of available options for a DSL can be retrieved as follows:

```
$ mfront --list-dsl-options=RungeKutta
```

Options to domain specific languages - II

```
$ mfront --obuild --interface=generic                                \
         --behaviour-dsl-option=parameters_as_static_variables:true \
         --behaviour-dsl-option='overriding_parameters:{T:293.15}'  \
         Plasticity.mfront
```

- DSL options can be specified in a block after the definition of the DSL or on the command line (see `MFrontGallery` project):
  - `--dsl-option`
  - `--material-property-dsl-option`
  - `--behaviour-dsl-option`
  - `--model-dsl-option`

Options to domain specific languages - II

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         --behaviour-dsl-option=parameters_as_static_variables:true \
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  - `--material-property-dsl-option`
  - `--behaviour-dsl-option`
  - `--model-dsl-option`
- DSL Options can also gathered in an JSON-like file:

```
$ mfront --obuild --interface=generic                \
         --behaviour-dsl-options-file=options.json \
         Plasticity.mfront
```

where the file `options.json` file may look like:

```
overriding_parameters : {T : 293.15, dT : 0},
parameters_as_static_variables : true
```

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