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The MFEM/MGIS solver: overview and applications to large-scale simulations at mesoscale

Tommaso Barani[(1)], Raphaël Prat[(2)], Thomas Helfer[(3)], Bruno Michel[(4)], Guillaume Latu[(5)]

[(1)] *CEA, DES, IRESNE, DEC, SESC, Cadarache, F-13108 Saint-Paul-Lez Durance, France, tomaso.barani@cea.fr*
[(2)] *CEA, DES, IRESNE, DEC, SESC, Cadarache, F-13108 Saint-Paul-Lez Durance, France, raphael.prat@cea.fr*
[(3)] *CEA, DES, IRESNE, DEC, SESC, Cadarache, F-13108 Saint-Paul-Lez Durance, France, thomas.helfer@cea.fr*
[(4)] *CEA, DES, IRESNE, DEC, SESC, Cadarache, F-13108 Saint-Paul-Lez Durance, France, bruno.michel@cea.fr*
[(5)] *CEA, DES, IRESNE, DEC, SESC, Cadarache, F-13108 Saint-Paul-Lez Durance, France, guillaume.latu@cea.fr*

Abstract — In this work, we present the main characteristics and salient traits of the MFEM/MGIS solver, and some applications focused on micromechanical modeling developed within the framework of the European OperaHPC project.

Keywords: HPC simulations. Mesoscale simulations. Nuclear fuel modelling.

Introduction

The MFEM/MGIS solver aims to efficiently use supercomputers to describe coupled multiphysics phenomena with a particular focus on thermo-mechanics. The authors primarily aim at describing the nuclear fuels at mesoscale (see example below), but MFEM/MGIS is versatile and can address more general cases.

This open-source library relies on several components as prerequisites: the MFEM (Modular Finite Element Methods) library (1, 2), the MGIS (MFront Generic Interface Support) library (3), and the MFront code generator (4).

Thanks to the features embedded within MGIS and MFront and specific developments, MFEM/MGIS adds several mechanical features compared to a pure MFEM approach. The library tackles some peculiarities of nonlinear mechanics, including the support of complex constitutive laws and some boundary conditions, and introduces dedicated post-processings.

About MFEM

MFEM is a finite element library designed for current supercomputers and exascale supercomputers. It provides many useful features for carrying out state-of-the-art simulations: support for curvilinear meshes, high-order approximation spaces and different families of finite elements, interfaces to several types of parallel solvers (including matrix-free ones), preconditioners, and native support for adaptive mesh refinement (AMR).

Originating from the applied mathematics and parallel computing communities, MFEM offers both performance and a large panel of advanced mathematical features. In particular, one can easily switch from one linear solver to another (direct or iterative), which is essential for the targeted applications within the PLEIADES platform (5), dedicated to microstructure and mesoscale modeling of nuclear fuel. MFEM/MGIS provides an alternative to the previously used thermomechanical solver in PLEAIDES for large-scale simulations.

Statement of need

The native solid mechanics examples in `MFEM` are mostly limited to simple constitutive equations such as elasticity and hyperelasticity without internal state variables. This is insufficient to address many engineering studies and, in particular, complex nuclear fuel simulations.

The aim of the `MFEM/MGIS` project is to combine `MFEM` with the `MFrontGenericInterfaceSupport` (`MGIS`) project, an open-source `C++` library that handles all the kinds of behaviours supported by the open-source `MFront` code generator.

In the field of nonlinear mechanics, this encompasses arbitrary complex behaviours that can describe damage, plasticity, and viscoplasticity in both small or finite strain analyses. Generalized behaviours such as variational approaches to fracture are also supported by `MFEM/MGIS`.

The `MGIS` data structures are used to add support for partial quadrature functions to `MFEM`, a feature needed to store internal state variables for each material.

Outline

Section 1 gives a general overview of the project.

The abilities and the versatility of the solver are demonstrated through the description of two complex families of simulations in Section 2:

- Section 2.1 describes two simulations of a polycrystal subjected to a macroscopic uniaxial stress state.
- Section 2.2 introduces a recent model that describes the fragmentation of the uranium matrix due to the pressurized bubbles generated by irradiation. This simulation illustrates the flexibility of how the solver handles boundary conditions.

1 Overview of `MFEM/MGIS` features

This section provides a high-level overview of the project. The interested reader may refer to the project's website for further information, including installation guide, documentation, tutorials, and benchmarks: https://thelfer.github.io/mfem-mgis/index.html

An overview of the project is given in a dedicated paper (6).

`MFEM/MGIS` is written in `C++20` language. As the application targets mechanical engineers, it provides a high level of abstraction, focused on the physical aspects of the simulation and hiding most numerical details by default.

The API is declarative and primarily based on data structures similar to `python` dictionaries, which inherently limits direct use of C++. In particular, such data structures are used to instantiate nonlinear evolution problems, behaviour integrators, post-processings, and boundary conditions.

1.1 Multiphysics simulations: Fuel Pellet Fragmentation

`MFEM/MGIS` enables setting nonlinear multiphysics simulations using a staggered approach. Heat transfer, mechanics, and damage gradient models are currently implemented, but the code is extensible, and other physics can be added.

As an example, Figure 1 highlights the application of `MFEM/MGIS` to the description of fuel pellet fragmentation made of uranium dioxide, which is a brittle material, due to high thermal gradients during the reactor startup using a damage gradient model.

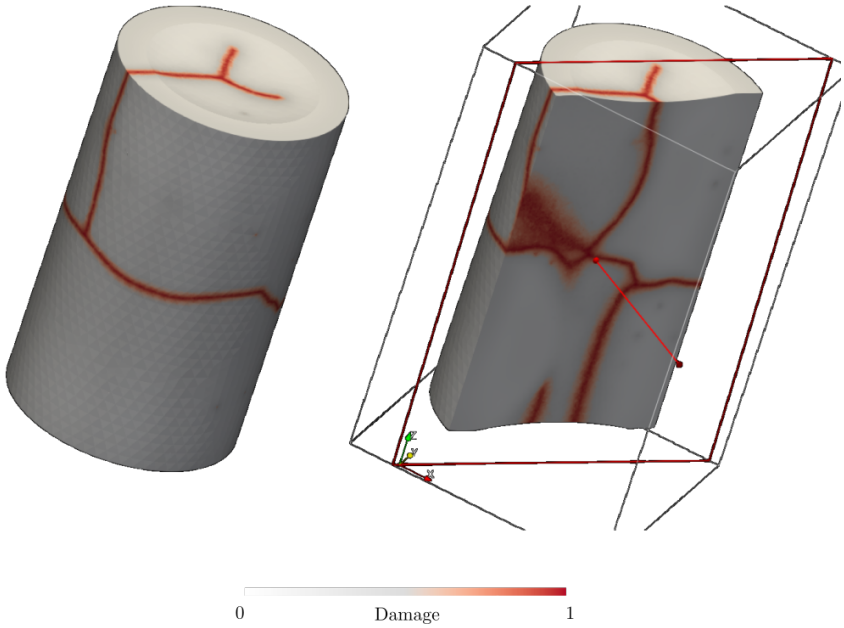

Figure 1: Fuel pellet fragmentation during the reactor startup using a damage gradient model. This simulation couples heat transfer, mechanics, and a micromorphic damage gradient model. The mechanical problem required $2\,10^7$ degrees of freedom, see D. Siedel's PhD thesis for more details (7). The simulation ran at the TGCC supercomputer on 2,048 processes.

1.2 The `NonLinearEvolutionProblem` class

The main class of `MFEM/MGIS` is called `NonLinearEvolutionProblem` and describes the evolution of the materials of the physical system of interest over a single time step for a given phenomenon.

Currently, `MFEM/MGIS` provides built-in support for mechanics, heat transfer, and micromorphic damage.

The following snippet declares a new nonlinear evolution problem:

```
mfem_mgis::NonLinearEvolutionProblem problem(
    {{"MeshFileName", "fuel.msh"},
     {"FiniteElementFamily", "H1"},
     {"FiniteElementOrder", 6},
     {"UnknownsSize", 1},
     {"Hypothesis", "Tridimensional"},
     {"Parallel", true}});
```

As the unknown is scalar (according to the `UnknownsSize` parameter), this problem can be used to describe heat transfer or micromorphic damage.

The `NonLinearEvolutionProblem` class supports both sequential and parallel computations and lets the user exploit a large subset of `MFEM` abilities, including the use of finite elements of arbitrary orders.

A staggered approach for multiphysics simulations can be set up by using several instances of `NonLinearEvolutionProblem`.

1.3 The `PeriodicNonLinearEvolutionProblem` class

`MFEM/MGIS` provides a specialized version for the `NonLinearEvolutionProblem` for periodic computations named `PeriodicNonLinearEvolutionProblem`, which is meant to evaluate the macroscopic behaviour of a Representative Volume Element (RVE), assuming periodic boundary conditions on the boundaries. This class allows managing the evolutions of the macroscopic gradients (strain

in small strain analysis, deformation gradient in finite strain analysis, temperature gradient in heat transfer analysis) and passing them to behaviour integrators.

Note

Anticipating Section 2.1, it is worth noting that directly imposing the macroscopic stress state is not allowed: a dedicated algorithm shall be set up.

1.4 Post-processings

Various post-processings are available. Here are some examples of post-processings that were recently added to `MFEM/MGIS`:

- `ComputeResultantForceOnBoundary`: Compute the resultant of the inner forces on a boundary.
- `ComputeMeanThermodynamicForcesValues`: Compute the macroscopic stress and strain for each material.
- `ParaviewExportIntegrationPointResultsAtNodes`: Paraview post processing files of partial quadrature functions, like the ones associated with the internal state variables.

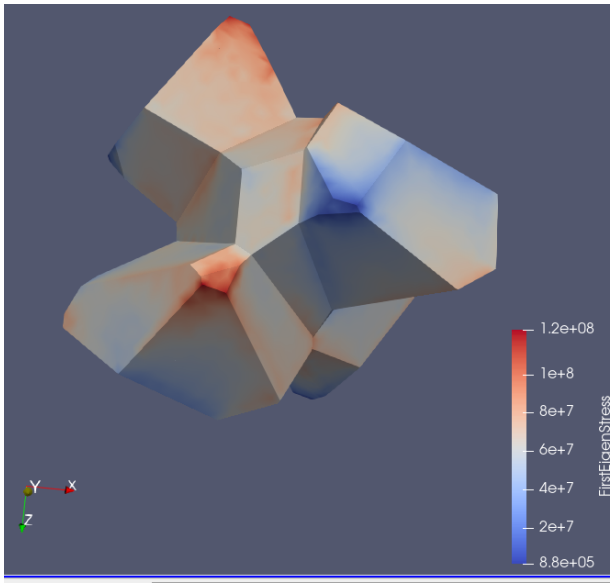

Figure 2: Von Mises equivalent stress of the Cauchy stress in a polycristal.

Many post-processings leverage the `MGIS/Function` library: Figure 2 shows the results of the computation of von Mises equivalent stress of the Cauchy stress based on the following code:

```
const auto ok = pk1 | as_tensor<N> | from_pk1_to_cauchy(F | as_tensor<N>) | vmis | seq;
```

where `N` is the space dimension.

2 Applications to large scale simulations of nuclear fuels at mesoscale

2.1 Polycrystal under macroscopic uniaxial stress state

Most experimental data about the viscoplastic behaviour of uranium dioxide, the main nuclear fuel used in french power reactors, are accessible through the analysis of uniaxial compressive tests (8).

The simulations described in this section are meant to reproduce a macroscopic uniaxial stress state representative of uniaxial compressive tests, allowing comparisons of RVE simulations with a polycrystal to macroscopic results.

2.1.1 Constitutive equations and crystal orientation

The simulations considered assume that each UO_2 grain follows a finite strain crystal plastic behaviour, which is detailed in the reference (8).

The orthotropic material basis for each grain is specified as input to the crystal plasticity constitutive model. This basis is precomputed from the grain Euler angles, defining its crystallographic orientation relative to the sample reference frame.

This test case is available on github.

2.1.2 Loading and algorithm used to impose a macroscopic uniaxial stress state

The macroscopic deformation gradient in the direction of the loading is imposed. The off-diagonal components of the macroscopic deformation gradient are imposed.

At each time step, the fixed-point algorithm is used to determine the two remaining components of the macroscopic deformation gradient, in order to converge toward a uniaxial stress state. If the current prediction of those components does not lead to an uniaxial stress state, a correction of those components is made assuming an elastic behaviour of RVE. The macroscopic elastic properties are derived from the single crystal elastic constant given above with the mean values of the Voigt and Reuss bounds for an isotropic polycrystal. While this correction may seem very crude, good prediction from previous time steps allows convergence in a few iterations.

2.1.3 Post-processings and verifications

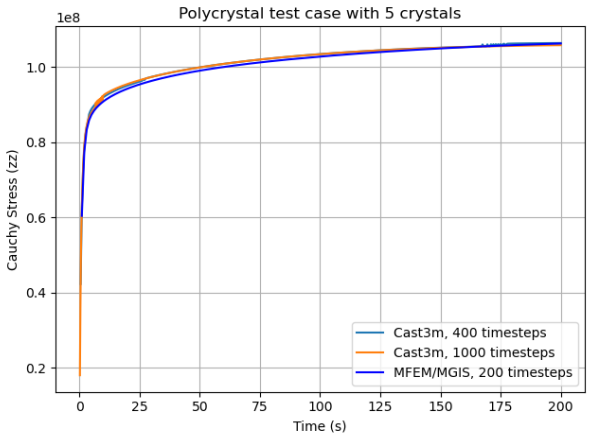

Figure 3: Comparison of macroscopic stress/strain curves between `Cast3M` and `MFEM/MGIS`

Figure 3 compares the results by `MFEM/MGIS` and the `Cast3M` solver (9) (used within the PLEIADES platform) on a small polycrystal containing only 5 grains due to limitations of the `Cast3M` solver regarding large-scale simulations. This comparison demonstrates that the fixed-point algorithm described in the previous section is correctly implemented.

2.2 Simulation of pressurized gas bubbles in uranium dioxide

A representative application of the `MFEM/MGIS` framework, developed within the OperaHPC european project, involves simulating pressurized inclusions in a uranium dioxide matrix, characteristic of UO_2 nuclear fuel microstructures at high burnup. This test case examines a RVE containing spherical porosities subjected to internal pressure within an effectively infinite elastic medium. The simulation imposes periodic boundary conditions with zero macroscopic displacement gradient, which constrains volumetric expansion and induces a macroscopic compressive hydrostatic stress state.

The internal stress field resulting from a pressure p_{in} applied on the porosity boundaries can be determined using the elastic superposition principle, which relates the stress state under

combined internal pressure and hydrostatic compression to the stress-free periodic boundary condition:

$$\overline{\overline{\sigma}}\left(p_{in}-p_{hyd},0\right)=\overline{\overline{\sigma}}\left(p_{in},p_{hyd}\right)+p_{hyd}\,\overline{\overline{I}}$$

with $\overline{\overline{I}}$ being the identity tensor and p_{hyd} the resulting hydrostatic stress.

2.2.1 Application to Fission Gas Release

This framework enables the assessment of transient fission gas release from the porosities through an overfragmentation mechanism. The fracture criterion is evaluated based on purely elastic stress calculations, wherein the principal stresses are computed at each material point. Crack initiation occurs when the maximum principal stress near bubble i, $\sigma_I^{\max}\big|_i$, exceeds the material rupture stress:

$$\sigma_I^{\max}\big|_i(p_{in})>\sigma_R$$

The maximum principal stress is evaluated at distance $R+\delta$ from the bubble center, where R represents the bubble radius and δ corresponds to the distance to the first Gauss integration point in the finite element discretization. The fractional fission gas release (FGR) for bubbles with uniform internal pressure p_{in} is then calculated as:

$$\mathrm{FGR}=\frac{\sum_i\left[V_i\,\middle|\,\left(\sigma_I^{\max}\big|_i(p_{in})\right)>\sigma_R\right]}{\sum_{i=1}^{n}V_i}$$

This formulation assumes that upon crack initiation, unstable propagation occurs, releasing the entire gas content from the affected bubble.

2.2.2 Computational case

The presented testcase consists of 5157 equal spheres of radius 0.85 μm, randomly dispersed in a RVE of 50 μm of size, resulting in a 11% volumetric porosity. The boundary conditions for the problem are periodical, and we consider a null macroscopic displacement gradient. The spherical cavities are not meshed, and we impose a uniform internal pressure on their surface, equal to 1 Pa in this testcase. The resulting finite element problems consists of 898×10^6 degrees of freedom. Figure 4 represents the first principal stress calculated in the microstructure.

This test case is available on github.

3 Conclusion and future works

This paper presents the `MFEM/MGIS` HPC application designed to address large-scale thermo-mechanical simulation and recent supercomputers. Based on an open source software stack, it allows the fine representation of microstructure in full 3D in the field of nuclear fuel modeling.

On the one hand, `MGIS` and `MFront` bring support for complex nonlinear behaviours such as damage, plasticity, and viscoplasticity capabilities. On the other hand, `MFEM` provides advanced finite element schemes and parallel performance (tested on several thousands of cores until now).

In the short term, the pressurized gas bubbles will be used in the `OperaHPC` project for the validation of the fission gas release assessment and for the computation of a learning data base needed for the development of a surrogate model for fuel over-fragmentation. The polycrystal test case will be validated with experimental strain stress curves measured during creep compression test on UO_2 fuel pellets, and will also be used for a representative study of advanced fuel microstructure behaviour during a power transient in a PWR reactor.

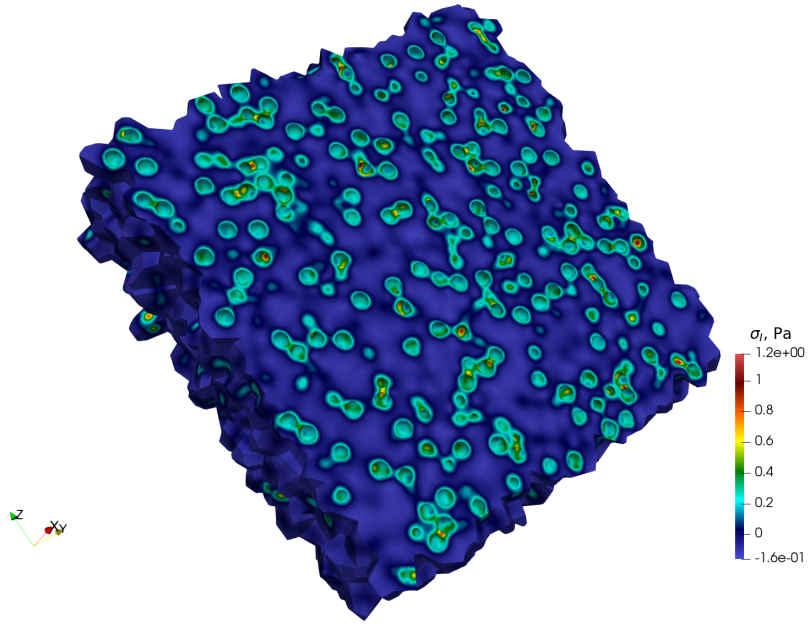

Figure 4: Calculation of the first principal stress σ_I induced by a unitary internal pressure (1 Pa) applied in the spherical porosities.

Acknowledgements

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