Presentation of the OperaHPC project

Marjorie Bertolus, Bruno Michel
marjorie.bertolus@cea.fr, bruno.michel@cea.fr

R2CA School, Bologna, July 4-6, 2023

https://operahpc.eu

Funded by the European Union

OperaHPC: OPEn HPC theRmomechanical tools for the development of eAtf fuels

- Needs
- Objectives and concept
- Partners
- Highlights of project activities
  - ✓ Development of open source HPC codes
  - ✓ Basic research activities
  - ✓ E&T activities

Needs for development and qualification of Generation II-III fuel elements

Needs for GEN II-III fuel elements

- Maintain/increase the safety and production capacity of Gen 2&3 nuclear reactors in an evolving electricity mix brings many new challenges for fuel development
- Gen 2&3 reactor fuels have a large experimental feedback
  - ✓ Continuous evolution of fuel element design and materials
  - ✓ Accelerate this evolution to adapt as quick as possible to the expected changes in the energy sector

Role of fuel performances codes and challenges

- Fuel performance codes: key stones for the fuel licensing, in complement / parallel to irradiation experimental programs
  - ✓ Irradiation capabilities decrease
  - ✓ To meet usage requirements, industrial FPCs need simplifications (empirical modelling)
  - ✓ It takes time to qualify FPCs for new operating conditions or innovative designs

⇨ **Existing 3D simulation tools can start to give some answers**

- Common use of 3D simulation tools and results in industrial context: still challenging
  - ✓ Improvements are needed to reduce the number of empirical parameters
  - ✓ Computation time and access to HPC tools are often limiting issues

Objectives and Approach

Holistic Approach on Fuel Performance codes

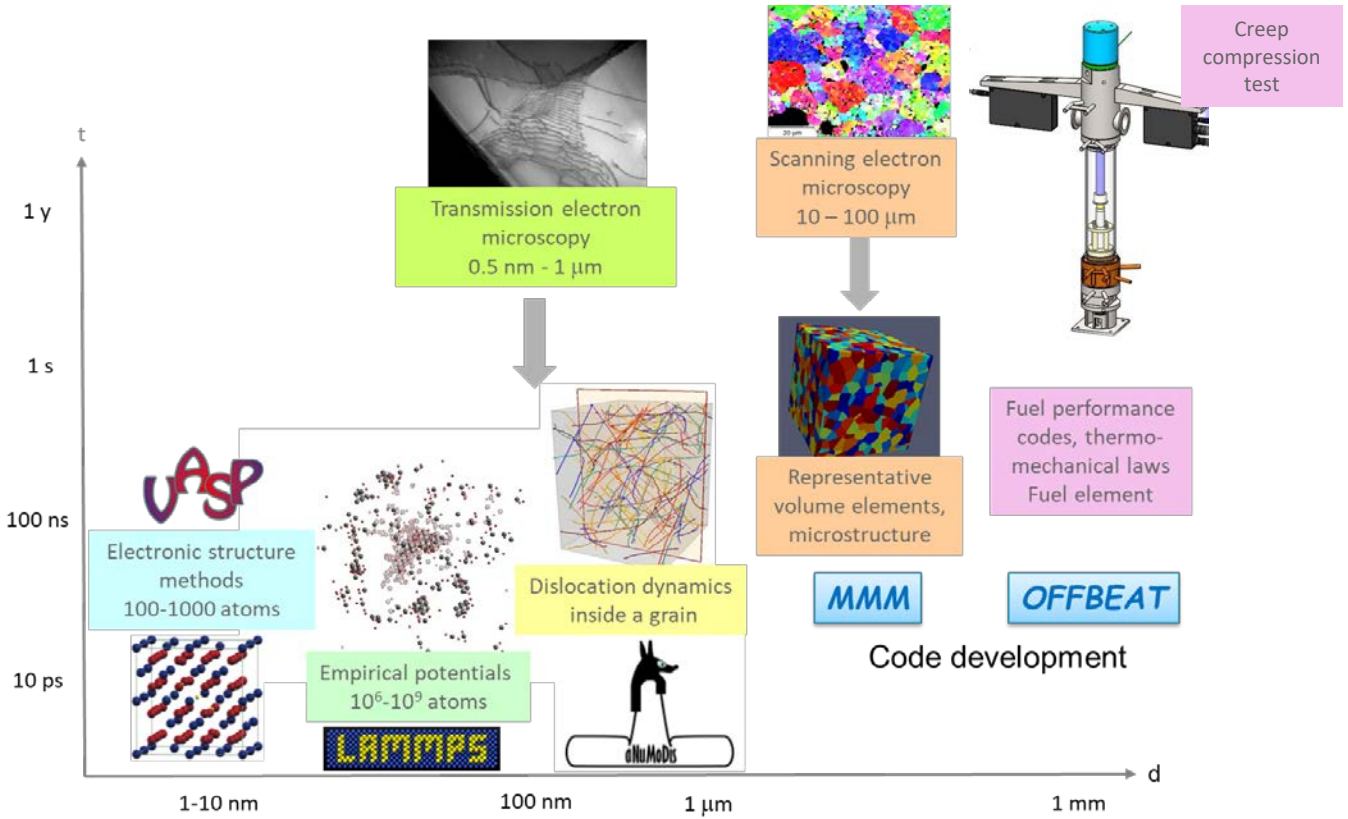
- Whole chain of activities needed to develop and distribute advanced physics-based simulation tools: identification of basic phenomena, determination of missing data, modelling of processes, implementation of models in computational tools, numerical optimization of codes, validation and wide distribution
- Development of tools at the two main relevant scales for the behaviour of the fuel element: the microstructural scale and the fuel rod scale
- Simulation of the thermomechanical behaviour of enhanced Accident Tolerant Fuel elements

OperaHPC Objectives and Concept

Basic Research	Code Development	Industrial application	E&T, dissemination
Study of non-linear mechanical behaviour of fuel under irradiation • Multiscale modelling • Separate effect exp. ↓ Missing data Elementary mechanisms Physics-based models	Numerical methods Multiphysics coupling Parallelization, Uncertainty quantification, QA ↓ Open source 3D HPC simulation tools at microstructure and engineering scale	Time reduction methods Application of codes developed ↓ Improved industrial models, thermo-mechanical behaviour of eATF in normal and DBA conditions	Open data, open source, mobility scheme, MOOC, schools, workshops, end-user group ↓ Transfer of approach, tools and results, training of new gene-ration of researchers and engineers

Approach and tools used by the nuclear community and industry

Coupling of simulation and experimental activities



ABAQUS
ALCYONE
BISON
CYRANO3/MFront
FALCON
FAST
FINIX
LAMMPS
MFEM
MFront
MMM
NUMODIS
OpenFOAM
SCIANTIX
SERPENT
SUBCHANFLOW
TRANSURANUS
VASP
Z-set

Partners

Partners

18 partners representing 7 EU countries + United Kingdom and Switzerland

Complementary organizations

- 9 public nuclear research organisations
- 5 universities
- 2 large industrial partners
- 2 SME

Highlights of Project Activities

Development of Open Source HPC codes

3D high fidelity simulation tools at two scales

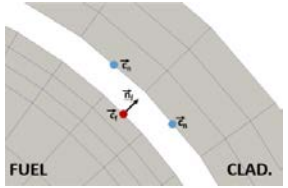
- New 3D mesoscale simulation tool MMM based on representative volume elements: description of complex microstructures, related issues and risk of over-fragmentation in accidental conditions
- 3D fuel rod thermomechanical simulation tool OFFBEAT based on the finite-volume open source HPC library OpenFOAM, coupled with SCIANTIX: Focus on improving computational cost, accuracy and robustness of the non-linear coupling algorithms

+

- a one-way coupling interface between MMM and OFFBEAT
- HPC capabilities for both tools
- Advanced physical models to improve description of fuel behaviour under irradiation: impact of gaseous fission products, cladding oxidation, non-linear mechanical behaviour with as few simplifying assumptions as possible…

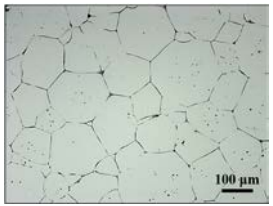
Engineering scale

Rod and pellet-cladding area



Microstructure scale

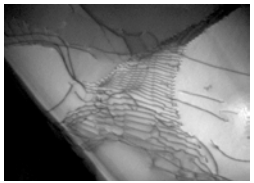
Microcell UO_2 fuel (Kim, NET 50, 253)

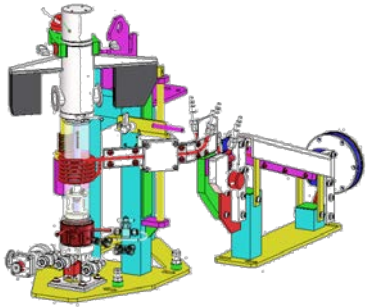


Basic Research Activities

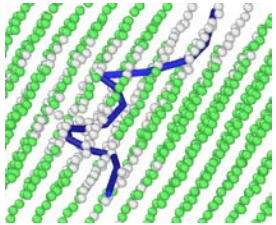
- Extension of the work done in the H2020 INSPYRE project
- Get further insight into non-linear behaviour of irradiated UO_2 fuel (creep, rupture) using an approach combining experimental and modelling investigations

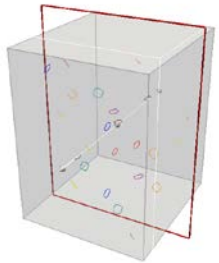
Compression tests on in-pile irradiated UO_2 and characterization of samples before and after tests: SEM-EBSD, TEM





Multiscale modelling of dislocation mobility, hardening, grain boundaries and rupture





Education & Training activities

- Mobility scheme (in collaboration with ENEN2+ Project)
- Two Summer Schools, in collaboration with other European initiatives. First one was ESNMS2022 focused on nuclear materials organized in November 2022 in Cargèse (Corsica) jointly with EERA-JPNM. Second one will take place in 2024 and will focus on FPC
- A MOOC on fuel performance codes: 2 introductory lessons, 1 one on fuel behaviour, 2 on OFFBEAT code (principle and hands on), 1 on SCIANTIX + short videos on specific features, e.g., code coupling

Participants and lecturers of ESNMS 2022

Thank you for your attention

https://operahpc.eu

OperaHPC is funded by the European Union. Views and opinions expressed, however, are those of the author(s) only and do not necessarily reflect those of the European Union or European Commission. Neither the European Union nor the granting authority can be held responsible for them.

User Group

- OperaHPC will interact with the industrial actors in charge of development and licensing of innovative fuels for current European reactors, but also with manufacturers and utilities
- Regular information exchanges will be organised
- The user group will be invited to the final Workshop

Current members

Organisation	Country	Representative	Position
EDF	France	Antoine Ambard	Research engineer
EK-CER	Hungary	Zoltan Hozer	Head of Fuel and Reactor Materials Department,chair of OECD/NEA WGFS
Framatome GmbH	Germany	Wolfgang Schmid	Material designer
TVO	Finland	Arttu Knuutila	Team leader, fuel procurement
Vattenfall	Sweden	Pal Efsing	Senior Specialist in Fracture and Materials Mechanics, professor at KTH
Westinghouse	Sweden	Paul Blair	Principal engineer for fuel rod design methods and methodology

Three main Objectives of OperaHPC

1) Advance the predictive capabilities of state-of-the-art fuel performance codes by
   - Improving significantly the understanding and description of the thermomechanical behaviour under irradiation of UO_2-based fuel elements
   - Transferring the knowledge acquired from basic and applied research into operational tools
2) Advance the numerical capabilities of open source 3D fuel performance codes
   - Add microstructure description to the simulation at the engineering scale
   - Add high Performance Computing (HPC) capabilities
   - Verification, validation, uncertainty quantification
   - Put the improved codes at disposal of the whole research community and industry
3) Transfer the approach and results to users
   - Use results to improve industrial model
   - Prove effectiveness of advanced simulation tools for the licencing of new fuel concepts (eATF)
   - Enhance the link between basic research, open source development and industrial applications
   - Develop training for the next generation of engineers and researchers