OPERA HPC

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Abstract

This document contains the second electronic newsletter

OPERA HPC

NEWSLETTER

Issue 2

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MESSAGE FROM THE COORDINATOR

The annual meeting of the OperaHPC project was held on November 20-21 in Cordoba, co-organized by CEA and CIEMAT. At the end of the second year, activities are under progress according to the plan with very fruitful common work between the members of the consortium. This newsletter is the opportunity to recall our main objectives and to do a first summary of the results obtained at mid-project.

The objectives of the project are to contribute to the fuel performance code qualification using advanced simulation tools with physically based modelling and high performance computing capabilities. The main idea is to address the challenging topic of reducing the licensing period for the qualification of enhanced accident tolerant fuels with an acceleration of the transfer between research, development and end users of the fuel performance codes. To do so, the project's strategic objectives are

- basic research activities with a focus on the fuel pellet mechanical properties,
- the development of open source fuel performance codes enabling advanced 3D simulation using High Performance Computing capabilities,
- the improvement of the current industrial models with Machine Learning type techniques
- representative industrial studies of eATF elements for PWR and VVER using improved codes,
- education and training activities and dissemination of the project's results.

The basic research activities in WP1 and WP2 address the development of an experimental set-up to perform creep tests on irradiated fuel samples, the determination of physical data on fuel mechanical properties by complementary experimental characterizations and multiscale modelling and the improvement of physics-based mechanical laws for fuel and cladding.

The design of the mechanical set-up for creep test experiments was completed. A new mechanical device will be used to perform a compression test on a small irradiated fuel specimens at high temperature in a hot cell of the LECA-STAR lab at the IRESNE institute of the CEA. In parallel, fuel samples irradiated at 13 and 37 GWd/tM were selected and prepared to start the detailed characterization using the Scanning and Transmission Electron Microscopes available in the microanalysis unit of the LECA-STAR hot lab. In particular, the type and quantity of dislocations induced by irradiation were characterized. These results, presented in the public deliverable D1.1 of the project, constitute the input data needed by micro-mechanical models to estimate the irradiation induced hardening.

To contribute to the understanding of the effect of irradiation on the fuel creep behaviour, the dislocation mobility was studied using Classical Molecular Dynamics (CMD) and Dislocation Dynamics simulations. The results of these simulations enabled the development of a cross slip law that describes the complex behaviour of screw dislocations in the three gliding modes of UO_2. The fracture toughness K_{IC} was also computed using CMD simulations of a tensile test with an ellipsoidal notch of few nanometres. These simulations shows that the energy needed for the surface separation can include, in some conditions, a dissipative phase change in the stress concentration zone ahead of the crack tip.

The improvement of physics-based mechanical laws for fuel and cladding has also started in the framework of the WP2. The state-of-the-art analysis was shared between the partners and it was decided to use the crystal plasticity framework and the NTFA homogenization technique for the description of the UO_2 polycrystalline microstructure and to use the open source tool MFront for the numerical implementation of the new mechanical laws developed in the WP2. The focus of the application will be on an eATF coated cladding with a surrogate model describing the heterogeneity due to the thin external chromium coating.

The codes developed in the WP4 of the project, OFFBEAT and MMM, are devoted to the fuel rod engineering scale and to the heterogeneous material microstructure scale, respectively. To complete the OFFBEAT multi-physic modelling for fission gas behaviour and irradiation effects, developments are also performed in the SCIANTIX code. Then, a prototype tool is developed in order to take advantage of the Smooth Particle Method for the simulation of phenomena where the geometry update question is challenging for Finite Volume or Finite Element methods. The WP3 activities will enable the integration of these open source codes in the existing computational framework of legacy fuel performance codes and core or assembly scale simulation tools.

The OFFBEAT code computational scheme refers to a cell-centred finite-volume approach to solve the nonlinear solid mechanics. This is combined with a framework for thermal analysis and with numerical developments concerning the treatment of the gap heat transfer and contact, based on a mapping algorithm that allows the use of independent non-conformal meshes for fuel and cladding. The developments performed during the first two years of the OperaHPC project concern the improvement of the physical models needed for an advanced description of the fuel behaviour under irradiation. More specifically, the cladding integrity assessment under PCMI has been improved thanks to a large strain formulation as well as a semi-implicit approach for thermomechanical contact, hydrogen transport and hydride precipitation in the cladding.

The MMM code is a 3D simulation tool devoted to the solid mechanics analysis of a Representative Volume Element of heterogeneous materials. The modelling approach is based on the MFEM-MGIS Finite Element solver enabling High Performance computing for nonlinear mechanics. The objectives of the MMM application are to describe the fuel mechanical behaviour under irradiation for polycrystalline and porous microstructures. Three representative study cases have been defined to address respectively: the UO_2 viscoplastic behaviour, the fuel fragmentation induced by fission gases over pressurized bubbles and the viscoplastic behaviour of an eATF Ceramic-Metallic fuel microstructure.

At the end of October 2024 the first beta versions of the OFFBEAT and MMM codes were made available on their open source repository. The Verification and Validation process of these two codes is ongoing. A 3D simulation benchmark is performed to compare OFFBEAT to the CEA-EDF-FRAMATOME code ALCYONE and to the American code BISON. Detailed results on the Pellet Cladding Mechanical Interaction are available to contribute to the verification of the new 3D computation scheme of OFFBEAT.

In the WP6, which is devoted to the improvement of current industrial models, a computational time reduction strategy based on machine learning techniques, as well as the industrial models and fuel performance codes targeted, were described in a public deliverable. In this document, the state of the art of machine learning and surrogate models methods is given with preliminary applications dedicated to pellet cladding mechanical interaction and fission gas behaviour. The next step is to build learning databases using the 3D OFFBEAT and MMM simulation codes. At the end of the second year, the OFFBEAT simulations have started in order to provide a detailed description of the pellet cladding gap evolution including a possible recovery of pellet fragment relocation after gap closure. MMM simulations are also under progress for fuel fragmentation induced by over pressurized fission gases bubbles.

Finally, the applicative objective of the project in WP7 is to demonstrate the capacity of 3D simulation and improved modelling to investigate a set of industrial PWR and VVER elements in representative conditions. Six different configurations were defined in order to address questions related to state-of-the-art and enhanced Accident Tolerant Fuel designs. During the two first years, the WP7 activity was focused on the computation of irradiation loading history for the VVER configurations. New assessments at the core scale were performed to describe the nominal irradiation conditions for various fuel assembly configurations, as well Reactivity Insertion Accident conditions with Cr coated cladding and a Loss Of Coolant accident with a large breach in a cold leg.

The education and training activities in the WP8 spans a large program going from the basic research up to industrial applications through the fuel performance codes development and machine learning techniques. A significant number of mobilities between the partners have also been organized. Concerning the dissemination and exploitation of the Project's developments and results, an open science approach was chosen, including publications, open source codes and FAIR data management. One strength of this approach is to capitalize all the developments and results obtained in the project in open source codes available for the partners and beyond for the fuel performance code and material science communities. At the end of the second year, 32 publications were prepared, 13 papers in peer review journals and 19 conference presentations, and beta versions of the OFFBEAT and MMM codes are available on open source repositories. A first meeting has been organized with the End User Group, which is composed of industrial actors in charge of the development and licensing of innovative fuels for current European reactors (manufacturers, utilities and TSOs) in order to define the main topics of interest for them.

After these two first years, the OperaHPC project has already produced many significant results, on schedule, as well a large number of communications at scientific events and towards the industrial community. A significant number of education and training activities have also been organised. The first period project review has confirmed with no ambiguity the success of our collaboration.

I would like to thank all the contributors of the project for their involvement and their excellent scientific contributions.

RESEARCH BEYOND BORDERS: FROM POLITECNICO DI MILANO TO EPFL

Giovanni Zullo, a PhD student at Politecnico di Milano, undertook two research mobilities at EPFL in October 2023 and February-March 2024 as part of the OperaHPC project.

During his first mobility, Giovanni collaborated with Alessandro Scolaro to couple SCIANTIX 2.0, an open-source meso-scale code for fission gas behavior, with OFFBEAT, an open-source integral thermo-mechanical fuel performance code. This integration ensured the code suite was operational and ready to support the project activities. Alongside this achievement, Giovanni deepened his expertise in the OFFBEAT code, laying a robust foundation for his subsequent research efforts.

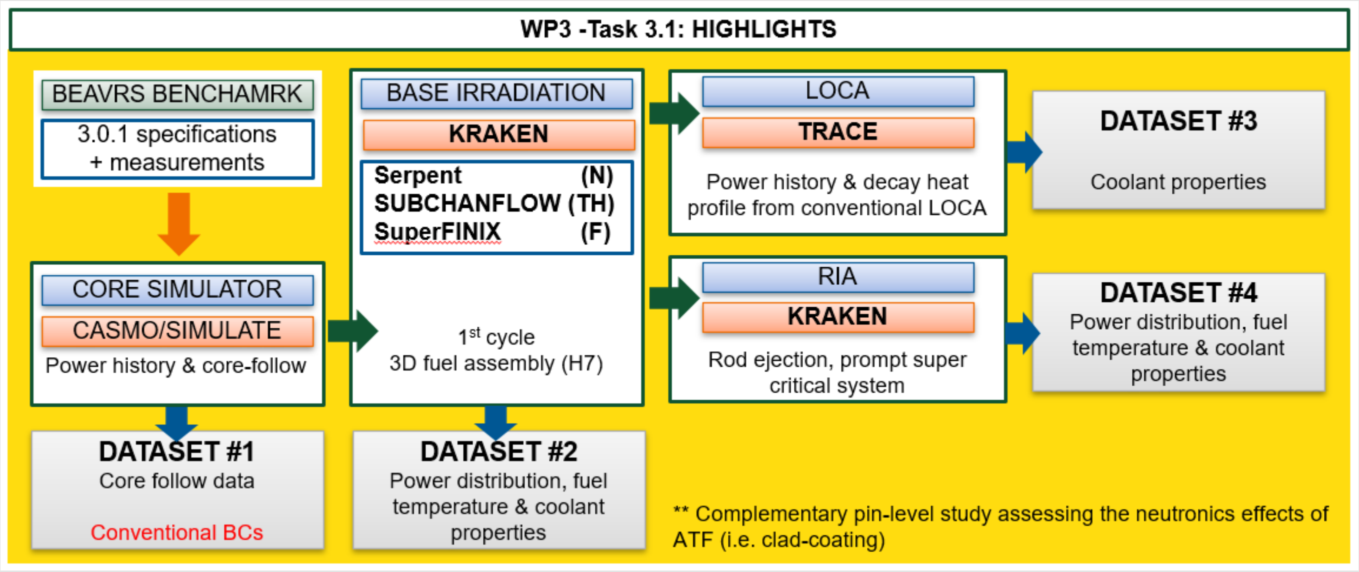
In the following months, Giovanni focused on verification and validation activities, including the assessment of new validation cases of significance to the OperaHPC project. During his second mobility, he finalized the integral-scale validation of SCIANTIX 2.0, showcasing its capabilities in modelling fission gas behaviour in light water reactor fuel rods when coupled with various fuel performance codes such as OFFBEAT, TRANSURANUS, and FRAPCON/FRAPTRAN. This work, conducted in collaboration with CIEMAT and JRC-Karlsruhe, resulted in a disseminated publication in the Journal of Nuclear Materials: Zullo, G., Pizzocri, D., Scolaro, A., Van Uffelen, P., Feria, F., Herranz, L. E., & Luzzi, L. (2024). Integral-scale validation of the SCIANTIX code for Light Water Reactor fuel rods. Journal of Nuclear Materials, 601, 155305.

In addition to this, Giovanni developed a novel modelling methodology to describe intragranular fission gas diffusion in UO_2 fuel matrix during the high-burnup structure (HBS) restructuring. This advancement enables SCIANTIX to seamlessly capture the formation and evolution of the HBS, including the transition from non-restructured to high-burnup structure fuel. The methodology is now primed for testing within the coupled SCIANTIX-OFFBEAT framework, further enhancing the predictive capabilities of the project computational tools. This work has also been disseminated and published in Nuclear Engineering and Design: Zullo, G., Scolaro, A., Barani, T., & Pizzocri, D. (2024). Two-phase modeling for fission gas sweeping in restructuring nuclear oxide fuel. Nuclear Engineering and Design, 429, 113602.

This mobility was partially supported by the ENEN2plus project, which is funded by the European Union (Grant number 101061677) .

High-Fidelity Boundary Conditions for Transient Calculations

We are pleased to announce the successful development of 3D high-fidelity boundary condition datasets tailored for dedicated loss-of-coolant accident (LOCA) and reactivity-initiated accident (RIA) scenarios. This effort builds on the well-established BEAVRS benchmark, using state-of-the-art computational tools to support detailed simulations with the OFFBEAT fuel performance code. These datasets enable comparison of conventional (1.5D) and advanced 3D boundary condition models, shedding light on the impact of varying resolutions.



What's next?

These high-fidelity datasets provide a critical foundation for advancing fuel behaviour modeling, offering a robust verification framework for OFFBEAT and other solvers. The comparison of 1.5D and 3D boundary conditions at various resolutions will further enhance our understanding of transient reactor dynamics.

We look forward to applying these tools to refine predictive capabilities and support innovative fuel designs for safer and more efficient reactor operations.

Interested?

- The generation of the high-fidelity boundary conditions and the results are described in D3.1.
- The boundary conditions datasets are available at https://doi.org/10.5281/zenodo.14525347.
- Riku Tuominen, Ville Valtavirta "Coupling of Serpent, SUBCHANFLOW and SuperFINIX for transient simulations". M&C 2025 conference. Denver, CO, USA. April-30, 2025 (accepted).
- Computational tools:
  - ➢ Serpent multi-purpose three-dimensional continuous energy neutron and photon transport Monte Carlo code, VTT

    Serpent 2.2. available at: OECD / NEA Data Bank (Package-ID NEA-1923) and RSICC (Code package CCC-872)
  - ➢ Kraken multi-physics computational framework, VTT

    Kraken 1.2 available at OECD / NEA Data Bank (Package-ID NEA-1924) and RSICC (Code package CCC-877)

EVENTS

The third edition of the European School on Nuclear Materials (ESNMS 2024) took place from October 27 to November 2, 2024 at the IESC in Cargèse, Corsica, France.

The school covered multiscale modelling from advanced electronic structure theory to continuum modelling as well as sophisticated characterization of materials phenomena in the nuclear materials science context to give the students the best possible toolbox for their future careers as nuclear materials scientists. All types of nuclear materials were treated.

It was co-organized by CEA and KTH as part of the co-funded European partnership on Nuclear Materials CONNECT-NM and it brought together world-leading European scientists, including several participants of OperaHPC.

Upcoming The NuFuel 2025 workshop (Research into nuclear fuel in Europe) will be hosted at the Delft University of Technology (Delft, The Netherlands) on September 16-18, 2025.

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