HPC modelling for nuclear safety assessment

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HPC modelling for nuclear safety assessment

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Abstract. High Performance Computing (HPC) has taken on an increasingly important role in recent years since it enables to model efficiently the complex behaviour of Systems, Components, and Structures (SSCs) and their interactions, and to perform simulations of the operational scenarios faster. Particularly in the nuclear field, HPC is currently used and expected to be utilized in nearly all areas, such as design optimization, safe and long-term safe operation, integrity evaluation, etc. The latter, as an example, requires an exhaustive SSCs assessment, which in turn requires higherfidelity models, both in terms of resolution and physics, increased knowledge of the physics of the phenomena or mechanisms affecting them, parametric studies, and better estimation of margins by reducing uncertainties and optimising operations.

In this paper some case studies are presented and described.

The first case consists in the modelling of creep behaviour of a fuel element. Finite Element Modelling (FEM) on hardware designed for parallel computation allows to simulate increasingly complex physical systems and reduce the computation time of the performed transient non-linear analyses. Results point out on the reliable prediction of creep behaviour obtained with a surrogate model. Understanding the thermo-mechanical properties of structural and nuclear materials and their changes provided essential for the plant safe operation as well as the Uncertainty Quantification (UQ).

The second case deals with a thermal-hydraulics application in support of Generation IV (GEN IV) Liquid Metal Fast Reactors (LMFRs). Results from RANS calculations will be compared with experimental data for a selected steady-state condition occurring in a rod-bundle geometry. UQ analyses are especially performed using deterministic sampling techniques to assess how much the results are affected by uncertainties in the input parameters.

1. Introduction

High-Performance Computing (HPC) is used practically in all areas of nuclear energy, as e.g. supporting the design and design improvement/retrofitting, enhancing material behaviour prediction, and understanding, safe operation, and life plant management of nuclear power plants whether fission or fusion. HPC is assuming an ever-increasingly important role in modelling as it enables us to perform simulations efficiently and faster of the behaviour of systems, structures, and components (SSCs), under operational scenarios, coupling various and different physics and scales [1]. Furthermore, the development of these new techniques combined with the availability of large computational resources has also allowed a significant development of new methods of machine learning and predictive analysis.

Figure 1 shows the three main areas of HPC (and scalable data science) [2] that can be applied in many scientific fields: algorithms, systems, and applications. The integration of all of them is essential to ensure HPC system operates more efficiently.

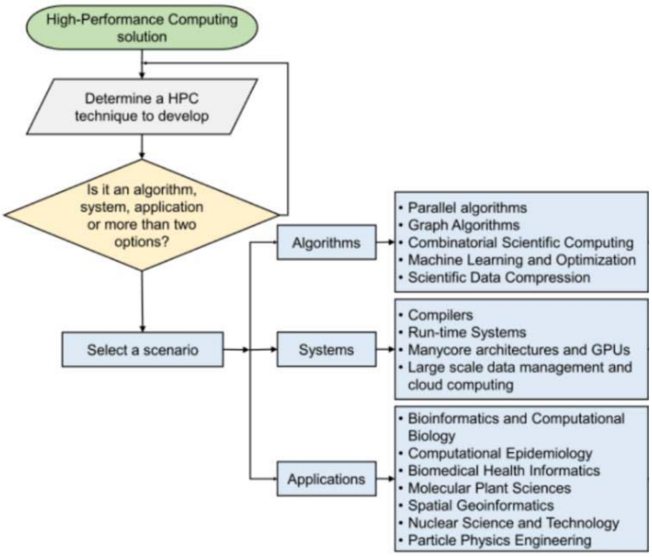


Figure 1. HPC data science organization (courtesy from [2]), which can be applied in many scientific fields

The adoption of HPC comes with its own set of challenges and limitations, such as e.g., the complex infrastructure and platform requirements, the scalability issues, the integration of multiple processors and accelerators, and the adoption of conventional/unconventional processor architectures required for non-intensive or heavy computations. Moreover, to perform multiphysics and multiscale simulations (heavy workloads), which can be characterized by the difficulty of precise prediction, with parallel programming, a robust and even more complex platform and cluster design is needed.

Another important aspect to consider is also the complexity of porting the existing codes, models and tools or rewriting them from scratch for the new architecture or fuel performance code (e.g., improving the reduced order models machine learning-based or surrogate models as did in the OPERA HPC project [3]) to cope with limitations and issues with programming and debugging tools for the accelerators.

By analysing the state of the art, it appears that HPC applications in the nuclear sector focus on the accuracy of simulation and reliability of data, used for validation purposes. Particularly, numerical modelling used for nuclear safety design and operation requires high-fidelity simulations. Advance the predictive capabilities of the numerical codes will improve significantly the understanding of component behaviour in a large variety of conditions. The knowledge acquired will be transferred into operational tools obtained an optimization of the plant operation.

The study of Shams et al. [5] focuses on the description of HPC facility at the Świerk Computing Centre (P) detailing the hardware configuration and software used for nuclear reactor design and safety and the computational requirements/capabilities.

Varè et al. [6] discusses the digitalization and virtual reality as key technologies to improve safety and performance of nuclear power. The study of Bakosi [7] describes the FE modelling by HPC of complex-geometry 3D flows and provides an overall fast numerical scheme based on an equivalent 1D finite volume scheme. This allows an effective use the computing resources even in the presence of hardware heterogeneities and dynamic parallel computational load. The study of Iannone [8] describes the infrastructure, providing technical details, and the performances of MARCONI, the new European HPC facility for Fusion, allowing modelling to exploit the latest available CPU technologies.

In this paper instead HPC is used to identify some key points for better estimation of safety margins by reducing simulation uncertainties and optimizing the plant operation. The paper consists of two main parts. The first one presents the improved HPC FE modelling of the creep mechanism of a fuel element, accounting for the thermo-mechanical loading during steady-state operation and transients, complex physical systems, and non-linear analyses material behaviour. The second part describes a thermal-hydraulics application (RANS calculations) in support of Generation IV (GEN IV) Liquid Metal Fast Reactors (LMFRs). This activity was carried out in the frame of the PNNR Flagship Project 4.2 "HPC tools for the simulation of nuclear systems".

2. FE creep modelling

Severe thermo-mechanical environments, such as relatively high temperatures, differential pressures, and corresponding hoop stress, influence largely the material behaviour of reactor components as microstructure is naturally dependent on the temperature and stress level it is facing during its lifetime.

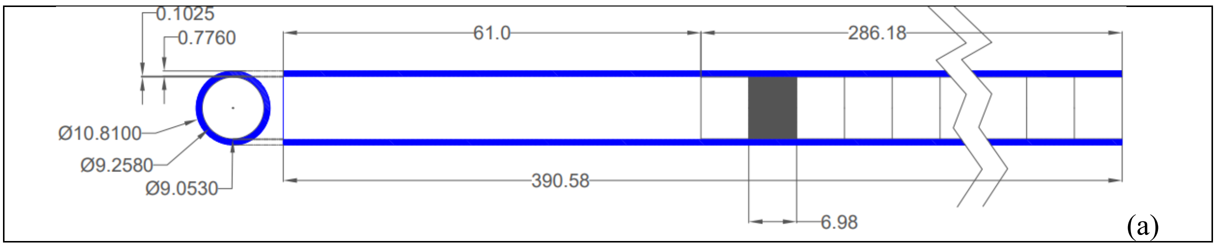
As a results, important deformation mechanisms such as swelling, creep, pellet-clad interaction, fuel-overfragmentation and cracking can occur. Of all these, creep of fuel cladding is certainly the dominant mechanism of slow irreversible deformation process under the influence of stresses below the yield stress [9] [10].

From continuum point of view, a reliable prediction of creep requires the definition of the mechanical equilibrium equations, appropriate constitutive equations, not only based on Norton-Bailey model (e.g. for primary creep stage), and suitable initial and boundary conditions. Therefore, it is necessary to employ a new and flexible HPC modelling integrating possibly experimental, and in-line operational data in ways not possible with traditional experimentally based paradigm.

Figure 2 shows the overall dimensions of a PWR fuel rod and the FE model (only a section) that was developed starting from this geometry: the cladding and fuel gap is 0.1025 mm; the plenum's nominal height (61.0 mm) is filled with Helium at 2.31 MPa.

As first step, a mesh sensitivity study has been performed by varying the element types (i.e., shell, solid) and the mesh sizes (e.g., 960, 1920, 3840, and 4320 elements), and the core counts to determine the appropriate mesh density for accurate results. Given the axisymmetric geometry and considering the purpose of determining the performance of a reduced order model, it is believed that the model implemented with 4320 3D solid elements is the most appropriate for representing the thermo-mechanical behaviour of the fuel rod.

Analyses were executed on Workstation 1 (W1) - Intel(R) Core (TM) i9-10920X CPU @ 3.50GHz, 3504 MHz with 24 cores, and Workstation 2 (W2) - Intel(R) Core (TM) i9-9820, 3.30GHz-Turbo-Boost 4.20GHz.



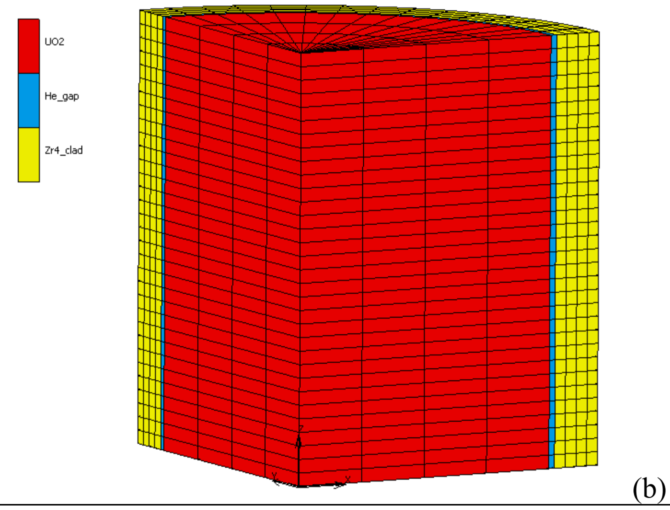


Figure 2. Fuel rod (UO2 pellet plus Zr-4 cladding) dimensions [mm] (a) and FE model (b). In the figure the red volume is the UO2 pellet, the light blue part represents the He gap, while the yellow annular volume represents the Zr-4 cladding.

Non-linear thermo-mechanical analyses were performed to simulate plasticity and creep mechanisms which are the most important responsible for accumulation of irreversible damage in the fuel rod. The secondary creep, which is characterized by a constant strain rate, is generally more important for temperatures in the range of 40 % and 70% of the melting temperature; at higher temperatures the creep mechanism is diffusion of atoms or Cobble or Nabarro-Herring creep, with a formula similar to the Norton law but with m=1 [12] [4]. To simulate creep and ensure unconditional stability regardless the time step, the fully implicit viscoplastic Maxwell model with creep strain rate ($\dot{\varepsilon}$) was implemented [12], [14]. The coefficients of the equation of the implicit power law model combined with regular plasticity are $A = 3.41\times10^{-33}$; $n = 3.3$; $m = 0.2$; $k = 0.8$. The UO2 behaviour was assumed isotropic with thermo-mechanical properties that automatically updated throughout the entire transient. This is supported by the recent studies on the fuel mechanical behaviour [15]. The boundary conditions reflect the typical normal operation conditions of the fuel rod [16], as e.g. coolant temperature and pressure equal to 287.7 °C and 15.52 MPa respectively, specific linear mean power of 42 kW/m, and the rod/pellets restraints [17]. The axial symmetry was also imposed. Staggered solution and the multifrontal direct solver were used for FE creep solution (0.01-time step, 200 increments) [18].

Using parallel processing, HPC-based FE model can distribute computational tasks across multiple processors, significantly reducing the analysis time.

Because of high thermal gradients within the pellet, internal thermal stresses are developing in the fuel. If one assumes that the average strength of a typical oxide fuel is about 150 MPa [19], one will find that the fuel pellet starts to fragment when the differential temperature across the surface of the pellet is higher than 120° C, i.e. under nominal conditions.

Results showed that the outward radial displacement of about $4 \cdot 10^{-5}$ m obstructing half gas gap. Moreover, the Von Mises stress overcome the allowable stress intensity [20] of 6 % and 30 % in the pellet and cladding respectively. The maximum value equivalent creep strain rate (of about $1.3\cdot10^{-4}$ s^{-1}) appeared in the innermost part of the pellet (see Figure 3), as expected, and aligns with reference [21]. In addition, from HPC standpoint, findings showed that increasing the number of cores high performance in terms of calculation time is obtained. However, no significant computational enhancement was observed beyond 8 cores.

Figure 4 shows the performance plots for the three discretized FE model; the vertical axis, termed “wall time”, is the actual time taken from the start to the end of the simulation.

W1 resulted 15% to 20% faster than W2 to run complex nonlinear creep analyses. This difference in terms of performance is even more marked for models with a high number of elements.

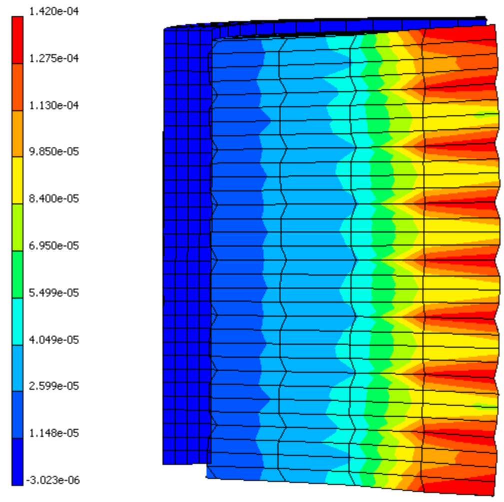


Figure 3. Equivalent creep strain (contour plot). The system unit is [hr^{-1}]. The external annular sector in blue represents the cladding deformation. The internal volume having a color ranging from red to blue represents the deformation of the pellet

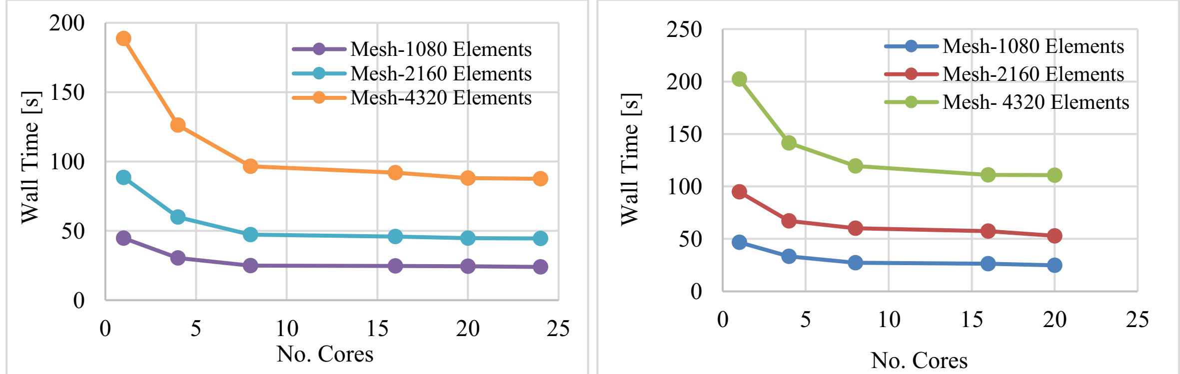


Figure 4. W1(left) and W2 (right) performance for the three discretized FE model

3. Thermal-hydraulics modelling and application

Concerning the thermal-hydraulics applications, the present paper focuses on CFD uncertainty quantification analyses in support of the development of GEN IV NPPs. In particular, a selected operating condition from the NACIE-UP Fuel Pin Simulator (FPS) [22], whose Fuel Pin Simulator (FPS) sketch design is reported in Figure 5 is considered. The FPS is a 19 rods wire wrapped electrically heated bundle in which LBE flows as the primary coolant. A simulation of this component allowing for a fine representation of each detail would require a very large computational cost, in the range of 50-100 million cells.

A nodalization for such a detailed model was developed, but its computational effort was later considered too large to be adopted for the copious number of calculations required for uncertainty quantification analysis. Therefore, a new model (see [23] for more reference), opting for a coarser representation of the wrapped wire geometry but allowing for the creation of a structured mesh, was developed to reduce the computational effort. The total cell count for the reduced cost model is in the range of 5 million.

Figure 6 shows a sample temperature distribution predicted by the code, the coarse shape of the wires, clearly not round, can be easily spotted in the referred figure.

As reported in [23], despite its reduced level of detail of the considered geometry, the model provides suitable capabilities in reproducing the thermal-hydraulic behaviour of the component at a definitively smaller computational cost. A validation of the approach was thus achieved.

Reducing the computational cost per run is very important for uncertainty quantification analyses owing to the large number of operating conditions to be considered in the excitation matrix. Indeed, excitation matrices, to prove their consistency with the addressed data, should fulfil several moments of the selected parameter distributions (average, variance, skewness…). This goal is typically achieved performing hundreds of calculations adopting a Montecarlo sampling, something that may lead to an incredibly large computational effort when dealing with CFD analyses. To prevent this, deterministic sampling methods were recently proposed in literature [24] providing tools to obtain uncertainty quantification analyses with a limited amount of selected operating conditions.

One of the key points of the deterministic sampling is the selection of a set of operating conditions fulfilling, by construction, the relevant moments of the addressed parameters distributions.

Figure 7 reports the excitation matrix considered for the present application obtained adopting the modified 4th order Hadamard approach, together with the considered variance for each investigated parameter.

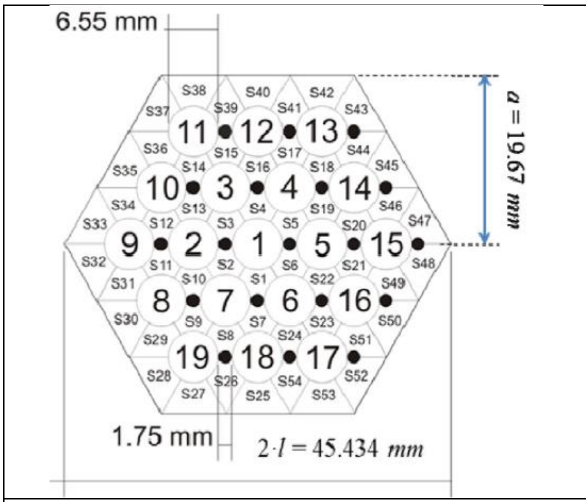


Figure 5. NACIE-UP facility sketch, taken from [23]

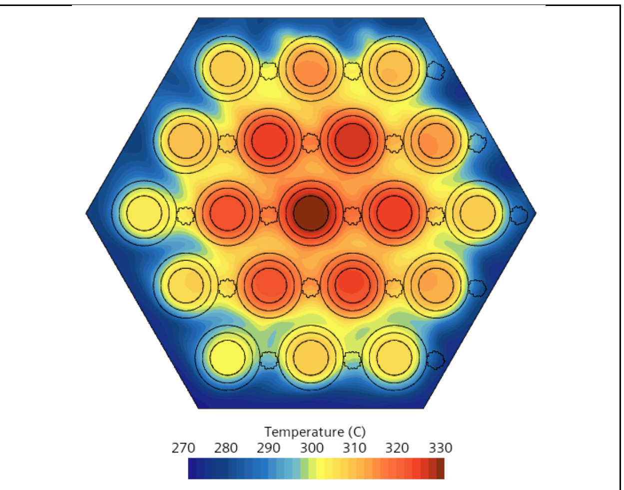


Figure 6. Temperature distribution for the FPS mid-section predicted by the reduced cost model.

$$\boldsymbol{\Sigma}_{\mathrm{HAD}}^{T} = \begin{pmatrix} \mathit{Sample} & \dot{\mathbf{m}}_{\mathrm{LBE}} & \mathbf{T}_{\mathrm{IN,FPS}} & \mathbf{Q}_{\mathrm{eff}} & \mathbf{Q}_{\mathrm{pre}} \\ HAD01 & \sigma_1 & \sigma_2 & \sigma_3 & \sigma_4 \\ HAD02 & -\sigma_1 & \sigma_2 & -\sigma_3 & \sigma_4 \\ HAD03 & \sigma_1 & -\sigma_2 & -\sigma_3 & \sigma_4 \\ HAD04 & -\sigma_1 & -\sigma_2 & \sigma_3 & \sigma_4 \\ HAD05 & \sigma_1 & \sigma_2 & \sigma_3 & -\sigma_4 \\ HAD06 & -\sigma_1 & \sigma_2 & -\sigma_3 & -\sigma_4 \\ HAD07 & \sigma_1 & -\sigma_2 & -\sigma_3 & -\sigma_4 \\ HAD08 & -\sigma_1 & -\sigma_2 & \sigma_3 & -\sigma_4 \end{pmatrix}$$

$\sigma_1 = \sigma_{mflow} = \pm 5\%$ *of the reference flow*
$\sigma_2 = \sigma_{Tin} = \pm 1.5°C$ *Inlet temperature uncertainty*
$\sigma_3 = \sigma_{power\_Active} = \pm 10\%$ *of the reference Active region supplied power*
$\sigma_4 = \sigma_{power\_Upstream} = \pm 4\%$ *of the reference Upstream region supplied power*

Figure 7. The 4th order modified Hadamard excitation matrix considered in the present work.

For each row, representing a distinct run, a perturbation of ±σ from the reference value is considered for each investigated parameter; e.g. for HAD01 the mass flow is $m_{flow1} = m_{flow,ref} + \sigma_{mflow}$ and for HAD02 the mass flow is $m_{flow2} = m_{flow,ref} - \sigma_{mflow}$.

The input parameters were selected after a sensitivity analysis process reporting that they are the most affecting the calculation outputs. Sigma values were instead provided by the experimentalists.

As it can be observed, this matrix allows investigating the effect of four input parameters while intrinsically assuring the fulfilment of mean and variance. This is confirmed by performing the average on each column, which turns to be zero, meaning that, on average, the reference mass flow rate is applied, i.e. thus fulfilling the considered distribution requirement on the zeroth moment (the average).

Figure 8 reports a sample of the results obtained for the calculations performed considering the first 4 rows of the excitation matrix. Here a comparison between the experimental measurements and the predicted values for temperature values inside the FPS is performed. On the x-axis the thermocouple number is reported, a label reporting its location inside the FPS is also included in the figure.

Results show that both overestimating and underestimating trends are predicted, thus reassuring about the approach capability in fulfilling the zeroth moment requirement (average). Figure 9 reports instead the result of the performed UQ approach obtained assembling all the predicted trends (HAD01 to HAD08) and calculating their average and root mean square. These values can be compared with experimental data showing that sufficiently reliable results were obtained, and the predicted uncertainty ranges size seems reasonable. A general increase of uncertainty is observed moving from left to right (i.e. from the inlet to the outlet) suggesting that a build-up of the uncertainty occurs along the axial direction. Almost all the experimental data lay in a ±σ range from the calculated average, thus suggesting that the adopted CFD model and approach are suitable for the addressed application. Further analyses are expected to be performed on other selected operating conditions and adopting different deterministic sampling approaches to further investigate and validate the considered UQ approach.

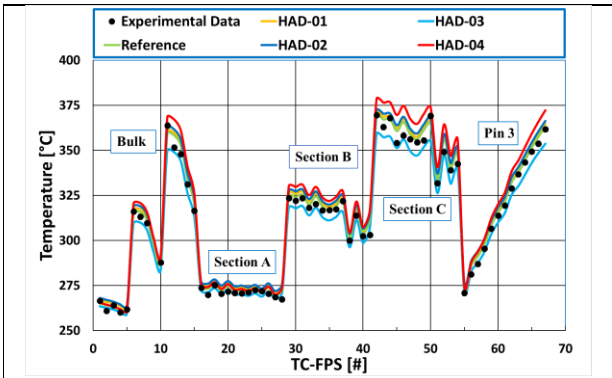


Figure 8. Experimental data vs. CFD predictions for the first 4 rows of the excitation matrix.

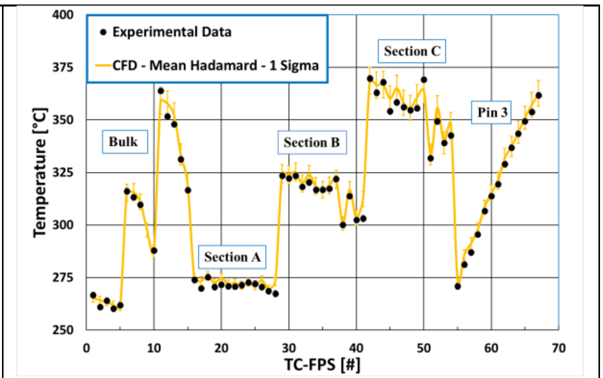


Figure 9. Results of the performed uncertainty quantification analysis.

4. Summary

Advantages and disadvantages of HPC have been explored with reference to two different application cases: thermo-mechanical analysis of creep for clad-pellet interaction and CFD uncertainty quantification analyses in support of the development of GEN IV NPPs. On the positive side, it emerged that HPC offers unparalleled computational power enabling to tackle complex problems and process massive amounts of data and complex operations with speed and efficiency. However, the adoption of HPC also comes with its own set of challenges and limitations, such as the complex infrastructure and platform requirements, energy consumption, scalability issues, integration of multiple processors and accelerators, and the adoption of conventional and/or unconventional processor architectures which are required for non-intensive and heavy computations, respectively.

The findings showed that increasing the number of cores results in significant improvements in calculation time is obtained: W1 resulted 15% to 20% faster; performances increase with the model complexity. However, no significant computational enhancement was observed beyond 8 cores.

Results obtained from CFD uncertainty quantification analyses performed by considering the modified Hadamard excitation matrix show that both overestimating and underestimating trends are predicted (Figure 8), thus reassuring about its capability in fulfilling the first momentum requirement. As for UQ approach, sufficiently reliable results were obtained, and the predicted uncertainty ranges size seems reasonable. The main aim of the performed work is promoting the use of CFD in safety assessment analyses for nuclear power plants.

Further analyses are expected to be performed to investigate e.g. challenges posed by the development and integration of machine learning, AI, and deep learning techniques, and to quantify the uncertainty of predictions obtained by multi-scale and multi-physics approaches.

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