

Towards Uncertainty Quantification : Efficient Surrogate Models In Coupled Fluid-Structure Interaction For Fuel Assembly Bow

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ABSTRACT

In the core of nuclear reactors, fluid-structure interaction and intense irradiation lead to the progressive deformation of fuel assemblies. When this deformation becomes significant, it can result in additional costs and extended fuel unloading and reloading operations. Therefore, it is essential to develop effective fuel management strategies that minimize excessive deformation and interactions between fuel assemblies. However, accurately predicting deformation and the interactions that arise between fuel assemblies remains challenging due to the complex interdependencies of various phenomena, including neutronics, thermal-hydraulics, and thermomechanics, each subject to inherent uncertainties. This work presents a comprehensive approach to address these challenges by focusing on the coupling between hydraulic and thermomechanical phenomena within a pressurized water reactor. An initial sensitivity analysis was conducted to determine the most influential parameters, first in hydraulic models [A. Abboud et al., BEPU 2024, 272], and then in mechanical models [A. Abboud et al., M&C 2025, 46282]. To effectively manage uncertainties over several reactor power cycles, it is useful to have accurate surrogate models. Using this information, the coupled simulation aims to synergistically integrate hydraulic and mechanical effects, along with their interactions, to achieve a more accurate modeling of fuel assembly deformation while capturing the dependencies of each model to its uncertain parameters. Furthermore, this study goes beyond standard parameter uncertainties by addressing epistemic factors, such as the convergence algorithms and criteria used in the coupled simulations. By analyzing these coupled effects and the associated uncertainties, this work is intended to provide a deeper understanding of the interaction between hydraulic and mechanical behaviors, enhancing the reliability and accuracy of predictive simulations. Ultimately, this integrated modeling approach will help to improve reactor management by informing more robust fuel management strategies and reducing risks related to fuel assembly deformation.

Keywords: Uncertainty Quantification, Fluid-Structure Interaction, Thermomechanics, Thermal Hydraulics, Assembly bow

1. INTRODUCTION

1.1. Modeling the fluid-structure interaction of fuel assembly bow

Fuel assembly bowing, a significant issue in nuclear reactor cores first identified in the 1990s, stems from incomplete rod cluster insertion (Anderson et al., 2005 [1]), prompting revisions in core management

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(Kerkar and Paulin, 2008 [2]; Grard, 2015 [3]). The deformation arises from complex physical phenomena, including neutronics, mechanics, and hydraulics (Karlsson and Manngard, 1999 [4]; de Lambert et al., 2019 [5]; Wanninger et al., 2018 [6]), complicating accurate modeling. Irradiation creep affects rod-to-grid and guide thimble-to-grid links (Fidleris, 1988 [7]; Scholz and Matera, 2000 [8]), influencing rod curvature. Residual forces from friction between rods and grid dimples and springs create nonlinear interactions, while factors like thermal expansion and rod elongation increase compression forces, exacerbating bowing. Hydraulic forces, driven by coolant flow, also play a primary role in deformation (Wanninger, 2018 [6]), leading to research on fluid-structure interaction (FSI) modeling. FSI can be studied dynamically (Ricciardi et al., 2009 [9]) or quasi-statically, which is relevant for long timescales such as fuel assembly bowing. The quasi-static approach computes static equilibria over time, often using partitioned two-way coupling between mechanics and hydraulics solvers (Benra et al., 2011 [10]). Simulating a full PWR core with 241 assemblies requires substantial computational resources, making simplified models necessary. High-fidelity simulations using CSM and CFD remain impractical for uncertainty quantification for full-core simulations. To address this, beam and shell theories provide simpler structural models, and porous media formulations enable efficient fluid modeling (Wanninger et al., 2018 [6]), allowing industrial simulations within feasible timeframes. Recent focus has been on 1D models of hydraulic networks for fuel assembly bowing. These simpler models, producing nonlinear systems with minimal computational dimensions, were first applied by Stabel and Dressel (2011) [11] using a pipe-based model. De Lambert et al. ([12], [13]) further advanced this approach with a hydraulic network formulation incorporating local flow redistributions near spacer grids, using optimized hydraulic resistances to represent flow dynamics accurately.

1.2. Summary of the objectives of this article

This article develops a methodology for coupling hydraulic and mechanical surrogate models using Gaussian process-based metamodels to simulate an entire irradiation cycle. The objective is to enhance the efficiency of simulations by leveraging surrogate models to reduce computational time while maintaining predictive accuracy. The study addresses key challenges in the coupling process, including managing the temporal aspects of mechanical metamodels over an 18-month cycle, transitioning from a single to multiple assemblies, and ensuring accurate fluid-structure interactions. A dual-loop coupling strategy is introduced, incorporating an internal mechanical loop for handling inter-assembly contact and a global fluid-structure interaction loop to stabilize the coupling between hydraulic and mechanical models. This work aims to provide a robust framework for efficiently simulating fuel assembly behavior over irradiation cycles, which will be further validated through comparisons with reference codes. The focus is on improving the computational efficiency of simulations, particularly for use in sensitivity analyses and uncertainty quantification.

2. DESCRIPTION OF REFERENCE MODELS

The deformation of fuel assemblies is simulated using two computational codes: the hydraulic code Phorcys and the thermomechanical code DAAC. Phorcys uses a hydraulic network model that calculates lateral and vertical pressure losses as a function of the reactor core geometry at a given time [14]. This means that Phorcys operates with hydraulic boundary conditions and depends on the current deformations of the assemblies, which are predicted by the mechanical code. For the mechanical simulations, the CEA developed the computational code DAAC. This code employs a simplified thermomechanical model of a fuel assembly (FA), validated against a more detailed model. The behavior of the 264 rods in the assembly is effectively represented by a single equivalent rod with aggregated stiffness properties. While a second set of beams represents the skeleton, a skeleton-rod connection is implemented at each grid level to account for the nonlinear and coupled forces and moments resulting from contact and friction. The figure 2 illustrates the rod-to-grid connection using six red connection elements linking the grid mid-plane (shown in grey) to the rod surface, on the middle, the mesh of the upper part of the simplified fuel assembly model is depicted,

while on the right, the cyclic axial load curve reflects the plasticity and friction of the hold-down system, supported by a pink connection element. The model accounts for thermal expansion, irradiation-induced growth, creep, and variations in grid clamping forces over the course of irradiation [15]. The coupling of hydraulic and mechanical models using partitioned codes involves an iterative convergence loop. This approach requires significant computational time, and its stability calls for control.

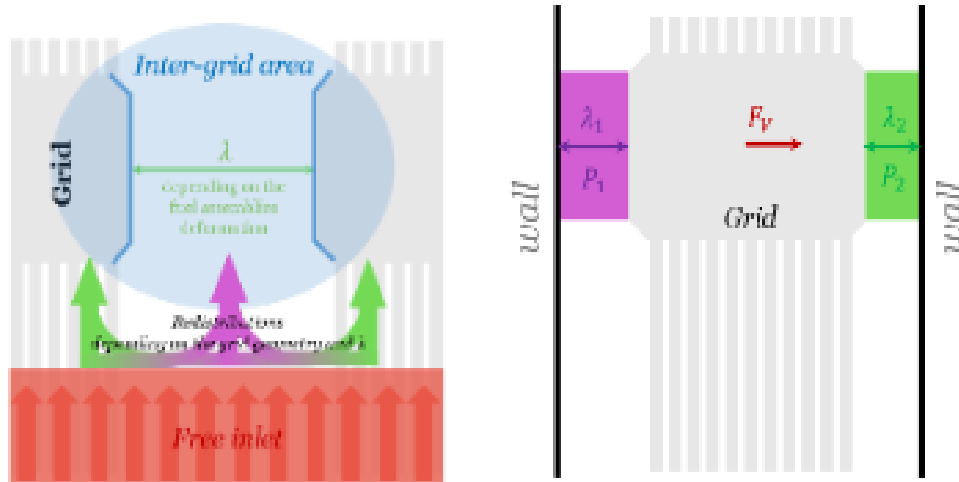


Figure 1. Flow redistribution in the core (left), lateral hydraulic force (right) (From [14])

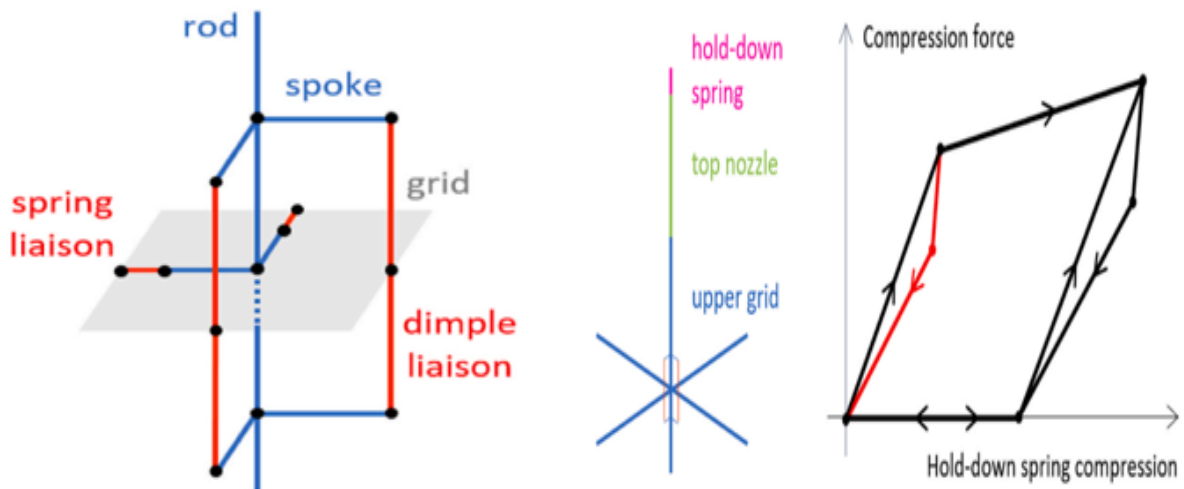


Figure 2. Rod-to-Grid Link with Connection Elements (left) and Cyclic Axial Load Curve (right) (From [16])

3. PREDICTION ACCURACY OF FUEL ASSEMBLY BOW USING THE THERMOMECHANICAL SURROGATE MODELS

The ability to represent spacer grid displacement variations using three Gaussian processes (GP) was demonstrated in a study conducted on a **single isolated assembly**. These processes predict variations in the modal amplitudes of the three main deformation modes, namely C , S , and W , for the periods before and after irradiation. More specifically, the second process is expressed in terms of modal velocity during the irradiation phase, where the hydraulic force F_h is not constant. In this section, a validation of the surrogate model prediction results will be performed by comparing the predictions of the three combined surrogate models with the actual mechanical calculations obtained from the code. In other words, this involves calculating the difference between the reel spacer grid displacement $U_G(z)$ and the predicted $\hat{U}_G(z) = \sum_{i=1}^3 C_i U_i(z)$, where $z = 1, \dots, 10$ represents the spacer grid number, and the C_i are the predicted modal coefficients for C, S, W modes respectively. To assess the predictive performance of the surrogate models, comparative calculations were performed by plotting the predicted displacements along with their 95% credible intervals ($\pm 2\sigma(z)$, where $\sigma^2(z)$ is the predictive variance of the GP model $\hat{U}_G(z)$) and calculating the root mean square error (RMSE) between observed and predicted values. Out of the 2000 predictions analyzed, only 14 fell outside the credible interval, indicating that approximately 99% of the predictions were consistent with expectations. Residuals, representing the discrepancies between observed and predicted values, were analyzed using the infinity norm to identify the cases with the highest prediction errors. Figures, 3,4 and 5 illustrates three representative examples: a prediction with minimal error, a case corresponding to the RMSE, and an extreme case falling outside the 95% credible interval. These findings demonstrate the robustness of the surrogate models and their ability to provide reliable predictions with a very low proportion of significant errors, thereby enabling their potential use in simulating a complete cycle by chaining the three successive surrogate models.

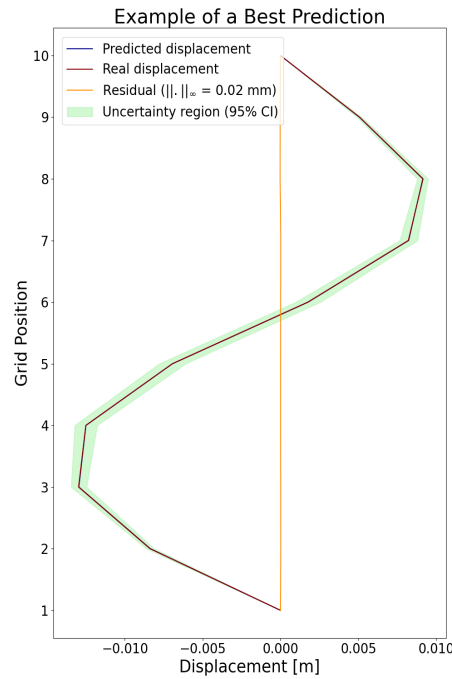


Figure 3. Best prediction

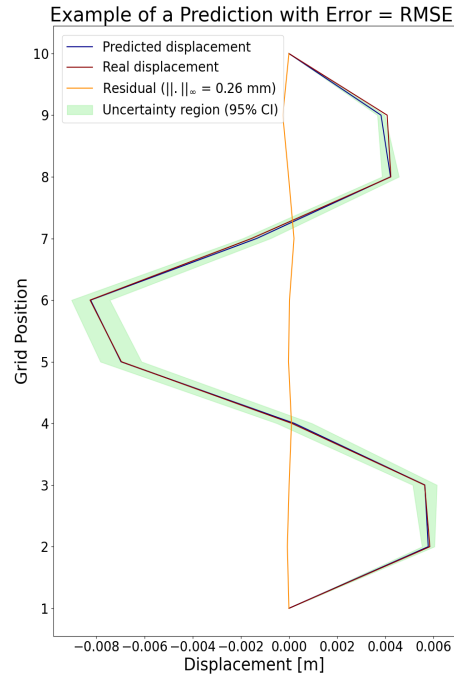


Figure 4. Prediction error equal to RMSE

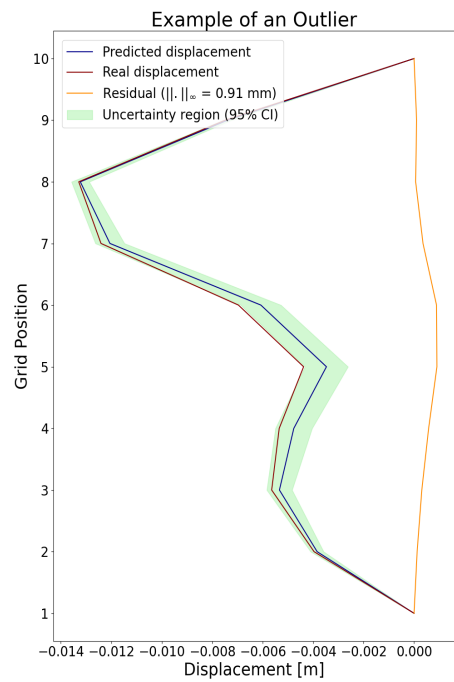


Figure 5. Worst outlier among 2000 simulations

4. SURROGATE MODELS COUPLING FOR FUEL ASSEMBLY BOW SIMULATION

In a previous study on hydraulic contributions, GP-based surrogate models [17] were developed and tested to predict hydraulic forces at each spacer grid level in fuel assemblies. These processes take as input the assembly deformation parameters, which influence the calculation of hydraulic forces, along with temperature, boundary conditions, grid resistance, and an epistemic parameter, all considered uncertain. These elements are preserved for metamodel construction within the framework of uncertainty propagation to improve simulation accuracy. A second study on mechanical behavior [15], also utilizing Gaussian processes, developed three mechanical surrogate models to predict assembly deformation, with results extended in this paper. These processes take as input hydraulic forces, which influence fuel assembly bow calculations, as well as initial assembly deformations, temperature, fast neutron flux, creep and growth constants, grid clamping, and forces from the hold-down system, all considered uncertain. These elements are similarly retained for metamodel construction to refine uncertainty propagation and enhance predictive precision. This section aims to establish a methodology for coupling these two surrogate models, significantly reducing computation times for uncertainty quantification.

4.1. Surrogate models coupling strategy

The primary objective is to leverage the speed of metamodels to increase the number of calculations in sensitivity analysis. Achieving this goal requires overcoming several key challenges. First, managing the temporal aspects of the mechanical metamodels is critical, particularly in developing an approach that allows simulating a complete cycle from metamodels constructed over a one-month period. Another challenge involves transitioning from a single connected assembly to multiple assemblies, which requires addressing penetration and contact between the assemblies. The strategy for coupling the metamodels within a fluid-structure interaction must also be robustly defined. Finally, ensuring the prediction accuracy of these coupled metamodels is essential to guarantee the reliability of the results in complex simulations.

4.2. Temporal management of mechanical surrogate models

The objective is to simulate a complete irradiation cycle over 18 months, using three distinct metamodels: one for the pre-irradiation phase, one for the irradiation phase, and one for the post-irradiation phase. To achieve this, metamodel 1 is used for the pre-irradiation phase, followed by the use of metamodel 2 at each time step, which corresponds to a month of irradiation. Finally, metamodel 3 predicts the behavior during the post-irradiation phase. As shown in Figure 6, by chaining these three metamodels, a full irradiation cycle simulation can be performed.

4.3. Switching from one fuel assembly to several

To simulate a row of n fuel assemblies based on a metamodel constructed from a single isolated assembly, it is crucial to implement a methodology to manage the contact between the assemblies and to prevent interpenetration [18]. A penalization approach was chosen to avoid penetration at the spacer grid levels of assemblies, until stabilization is achieved. This approach is detailed below and it relies on the penalty function $f(x) = 500(1 - \exp^{-\lambda x})$, where x represents the penetration depth (see Figure 7). The exponential function was selected to avoid sudden changes in forces, ensuring a smooth progression. The 500 factor was chosen to limit the force to 500 N, thereby preventing instabilities in the row simulation. Additionally, λ is chosen so that the slope at zero is equal to 10^7 N/m to ensure contact precision. The method requires successive iterations of the contact loop, as shown in Figure 8.

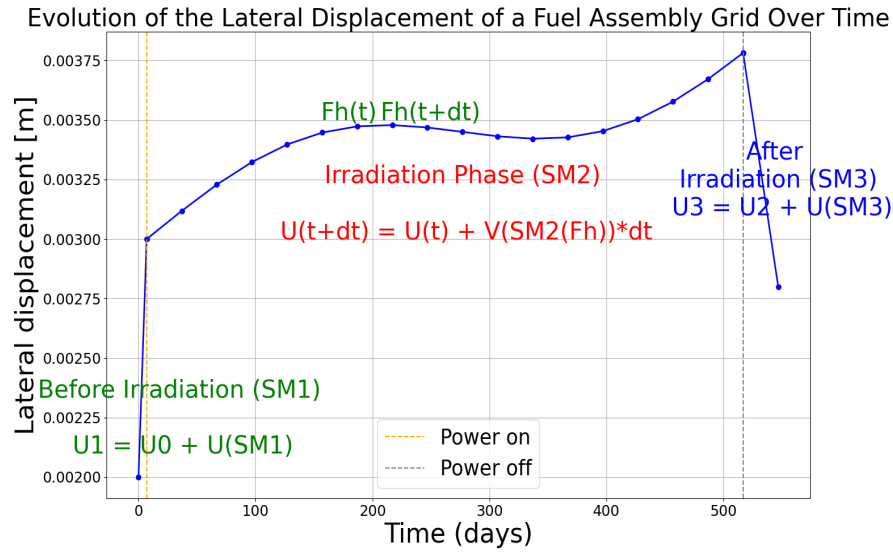


Figure 6. Cumulative temporal management of mechanical surrogate models

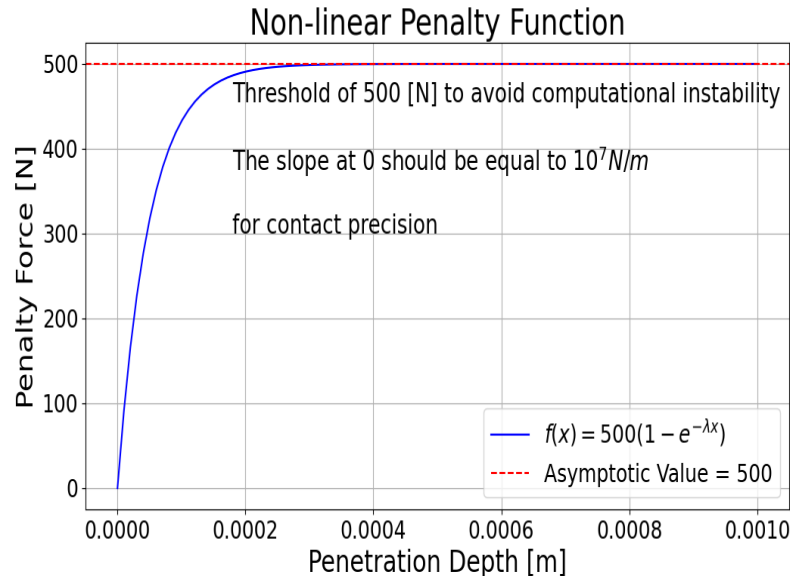


Figure 7. Nonlinear penalty function

4.4. FSI coupling strategy for surrogate models

The implemented coupling strategy relies on a dual-loop system, combining an internal mechanical loop and a global fluid-structure interaction (FSI) loop (see Figure 8). **Internal Mechanical Loop:** This loop employs the nonlinear penalty method to prevent inter-assembly penetration. The process begins with the generation of an initial deformation for a row of n assemblies, followed by the detection of potential penetrations. In the event of contact, the penalty method generates nonlinear contact forces. These corrected forces are then

combined with hydraulic forces and introduced into the mechanical metamodells, which generate updated modal coefficients. These coefficients are projected onto a finite element basis to compute new assembly deformations. When the displacement solution is stable the algorithm is considered converged. Otherwise, the mechanical and penalty iterations continue. **FSI Coupling Loop:** A relaxation method is employed on hydraulic forces to stabilize the coupling between the mechanical and hydraulic models. This approach helps to ensure smooth convergence by gradually updating the solution, preventing oscillations in the iterative process. Once a stable mechanical solution (U_j) is achieved in the internal mechanical loop, it is transferred to the hydraulic metamodells, which compute updated hydraulic forces. These forces are subsequently fed into the mechanical metamodells, initiating a new mechanical loop. The FSI coupling is evaluated: if the difference between two consecutive iterations ($\|U_{j+1} - U_j\|$) is below a predefined tolerance ϵ , the FSI coupling is considered converged, and a solution at $t + \Delta t$ is obtained. This process is repeated at each time step t , particularly during the irradiation phases where $t = \text{month of irradiation}$. The grid clamping value is updated after irradiation step using an interpolation method that relates grid clamping to cumulative fluence following the trend given in Figure 9.

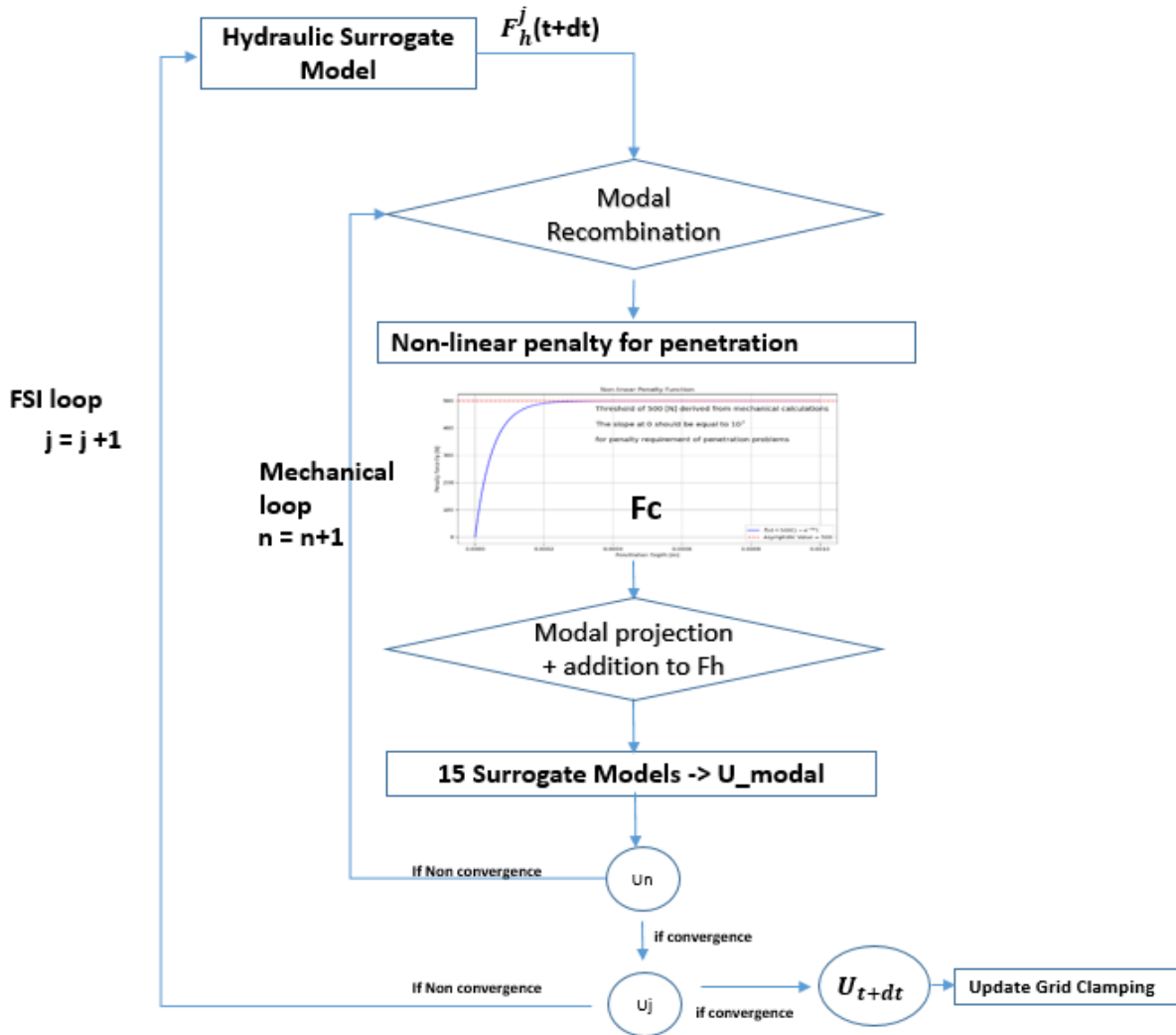


Figure 8. FSI coupling, and mechanical intern loop illustration

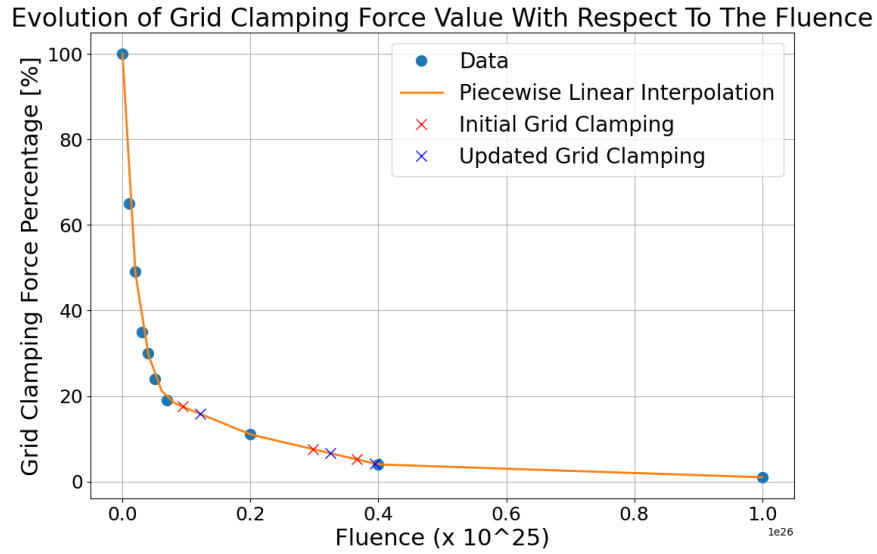


Figure 9. Grid clamping curve interpolation with respect to the fluence

4.5. Verification of the mechanical loop

The primary objective is to perform calculations on a row of 15 fuel assemblies (FA) to compare the results obtained using the metamodels with those from reference codes over a complete irradiation cycle. This study aims to compare the final deformations of the assemblies and evaluate the predictive accuracy of the coupled metamodels. To achieve this, the input parameters for the mechanical metamodels are selected based on a realistic cycle configuration. This configuration assumes approximately 33% beginning cycle, 33% at Cycle 2, and 33% at Cycles 3 and 4, ensuring a homogenized power profile for improved fuel management. Additionally, the input parameters are adjusted according to the age of the assemblies (see Table I). Modal coefficients are utilized to generate the initial deformations specific to each assembly's age, while the grid clamping value of the grids is determined individually for each assembly. These choices ensure representative conditions and behavior in the calculations throughout the entire cycle.

Assembly Type	Standard Deviation of Modal Coefficients	Grid Clamping Force Mean (N)	Standard Deviation of Grid Clamping Force (N)
New	$\sigma_C = 0.0002, \sigma_S = 0.0001, \sigma_W = 0.00005$	100% of initial value	1 % of initial value
One Cycle	$\sigma_C = 0.002, \sigma_S = 0.001, \sigma_W = 0.0005$	27% of initial value	5 % of initial value
Two or Three Cycles	$\sigma_C = 0.005, \sigma_S = 0.003, \sigma_W = 0.001$	14% of initial value	10 % of initial value

Table I. Input parameter laws based on the age of the assemblies

4.6. Verification of the nonlinear penalization method

To validate the nonlinear penalty method applied on a complete row of fuel assemblies (FA), a specific test was conducted on the mechanical loop. The objective of this test was to assess the method's ability to effectively manage the mechanical interactions between fuel assemblies. The procedure involves generating an initial deformation of the 15 assemblies, simulating their mechanical state prior to insertion into the reactor core, in order to replicate the initial deformations at the beginning of the cycle. This initial deformation leads, from a numerical perspective, to penetration zones between the assemblies. The goal is to verify whether the mechanical loop is capable of detecting these penetration zones, calculating the necessary

contact forces, and adjusting the positions of the assemblies to eliminate the interpenetrations. These forces must not only prevent any inter-assembly penetration but also ensure the overall mechanical stability of the system. This test is a crucial step in validating the reliability and accuracy of the nonlinear penalty method in a realistic simulated context. The test conducted demonstrates the ability and efficiency of the nonlinear penalty method in terms of mechanical stability and convergence rate, requiring only 8 iterations in less than a few seconds. An example of these results is provided in Figures 10 and 11.

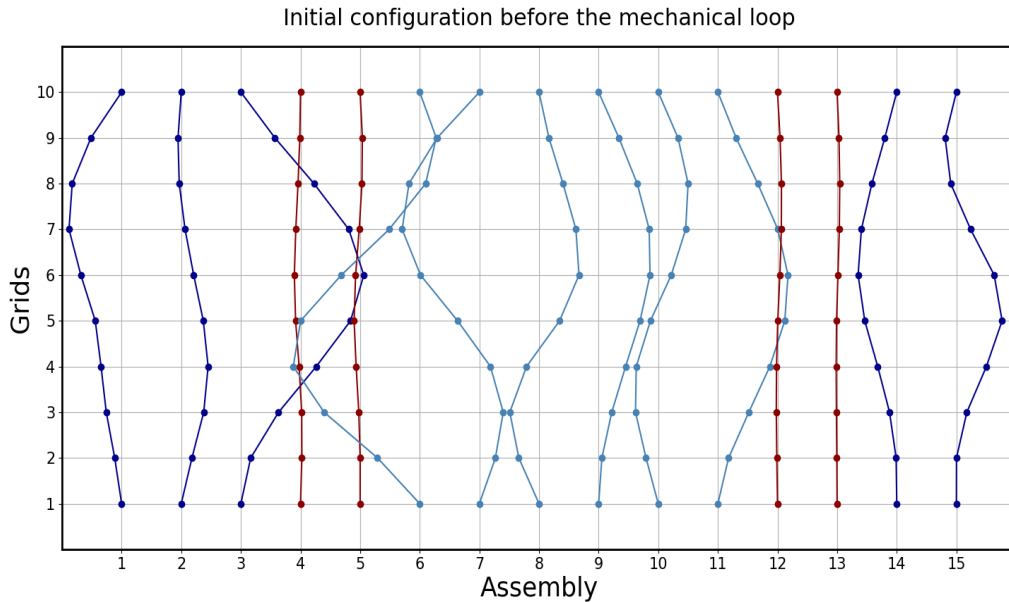


Figure 10. Example of a penetrated deformation before the mechanical loop

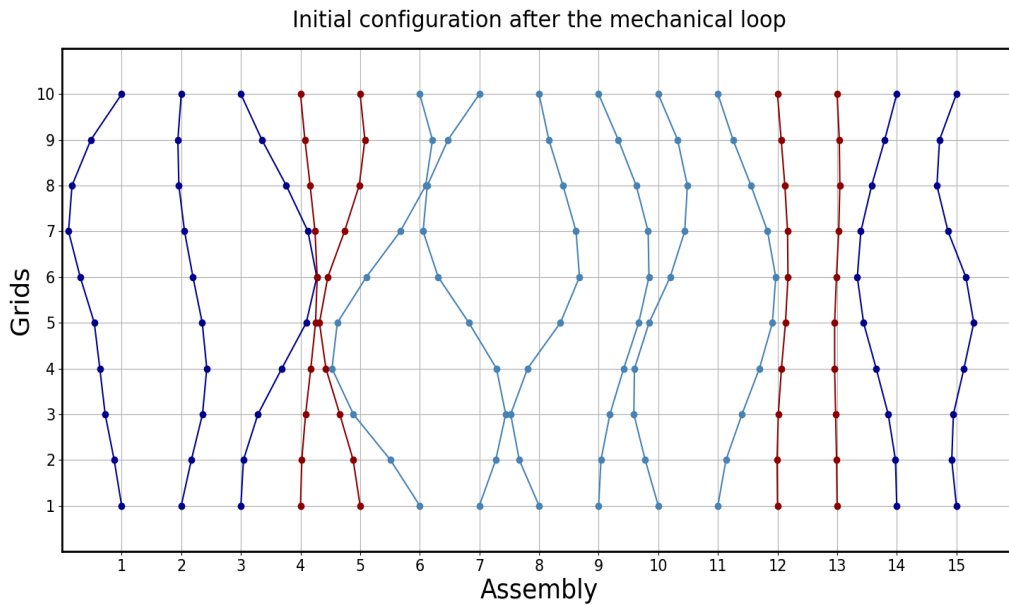


Figure 11. Non-penetrated deformation after mechanical loop convergence

4.7. Comparison of coupled surrogate models prediction with coupled reference codes

The objective of this study is to evaluate the predictive capability of coupled metamodels by comparing them with coupled reference codes. The simulations were conducted starting from an initially undeformed fuel assembly configuration. Both models—the coupled metamodels and the reference codes—were subjected to identical hydraulic boundary conditions. The same input parameter values were used for the mechanical metamodels, including temperature, creep and growth constants, holddown system forces, fast neutron flux, and grid clamping force. The initial grid clamping force was set to its maximum standard value at the start, as the assemblies were considered new and undeformed, having not yet undergone irradiation. Two tests were performed: the first with symmetric hydraulic boundary conditions (see Figure 12) and the second with asymmetric conditions (see Figure 13) to introduce additional complexity and assess the robustness of the coupled metamodels. The simulations were carried out over a complete 18-month cycle, with the clamping force value updated at each time step. The results presented correspond to the end of the cycle, after the system has cooled down and the upper plate has been opened.

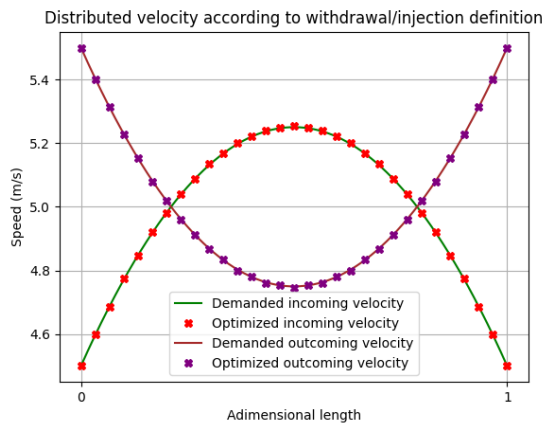


Figure 12. Symetric hydraulic boundary conditions profiles

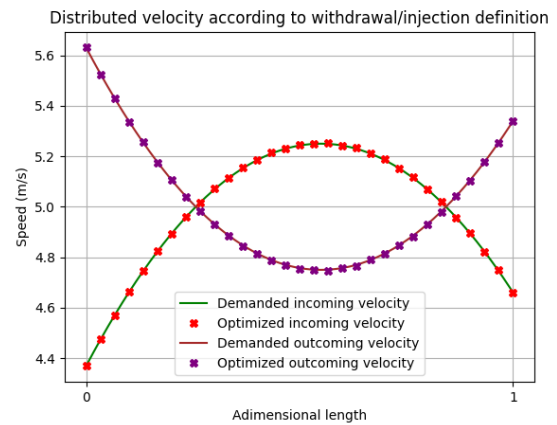


Figure 13. Assymetric hydraulic boundary conditions profiles

4.8. Results and discussions

First, the computation time required to simulate the deformation of assemblies over an 18-month cycle using coupled reference codes exceeds one hour, whereas the simulation using coupled metamodels takes only one minute. This represents a 60-fold time reduction, confirming the efficiency of metamodels and justifying their use for sensitivity analyses in future studies. Since statistical methods require a large number of simulations, the computational efficiency of metamodels makes them particularly advantageous. The results presented in Figures 14 and 15, in the case of a symetric hydraulic boundary conditions, demonstrate good agreement between simulations performed with coupled reference codes and those using coupled metamodels. As expected, the shape and symetry of the row pattern are very similar in both simulations. Furthermore, in the more complex case, with an asymmetric hydraulic boundary conditions profile (see Figures 16 and 17), a consistent correlation between the predictions of coupled metamodels and reference codes was found, with a similar 60-fold computational speedup. A slight discrepancy between metamodel predictions and reference simulations is observed. However, this difference is expected and can be attributed to several factors. Two main sources of uncertainty accumulate over a full cycle simulation. The first arises from the metamodels themselves: uncertainty in the hydraulic metamodels affects the accuracy of hydraulic force calculations,

which are subsequently transmitted to the mechanical metamodells. Additionally, uncertainties in the three mechanical metamodells, particularly the second mechanical metamodell, which simulates the irradiation phase and is repeatedly called throughout the cycle, contribute to error accumulation. The second source of uncertainty is epistemic in nature, stemming from modeling choices and numerical coupling algorithms, especially convergence criteria values.

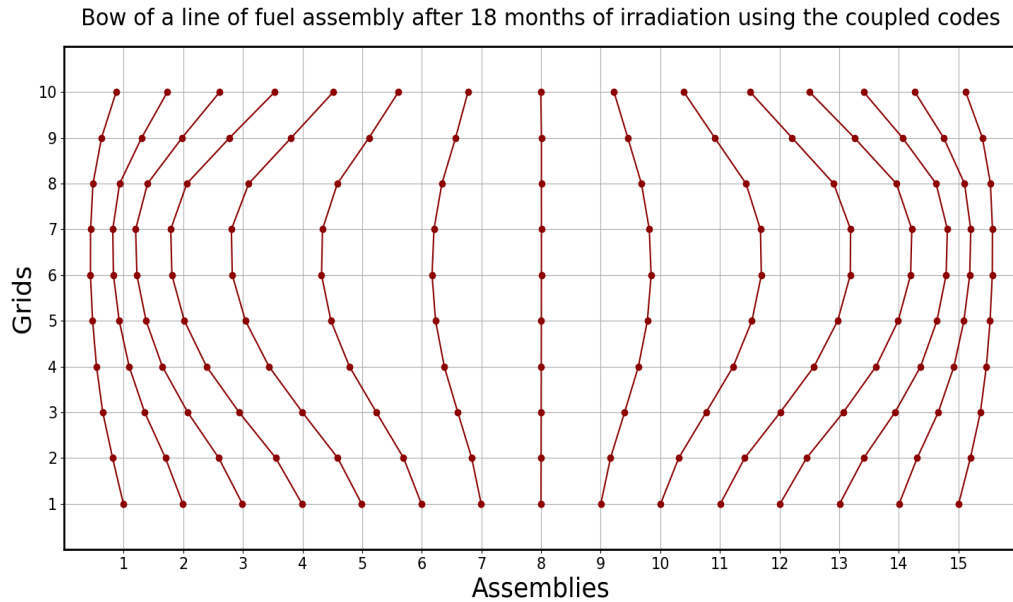


Figure 14. Results of the cycle simulation using coupled reference codes with symmetric hydraulic boundary conditions

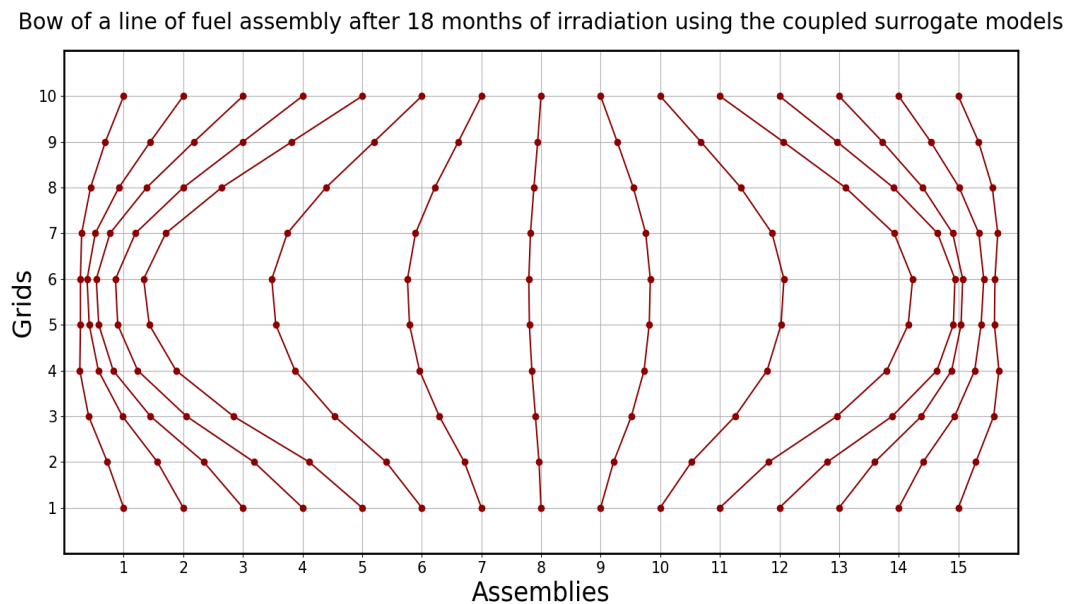


Figure 15. Results of the cycle simulation using coupled surrogate models with symmetric hydraulic boundary conditions

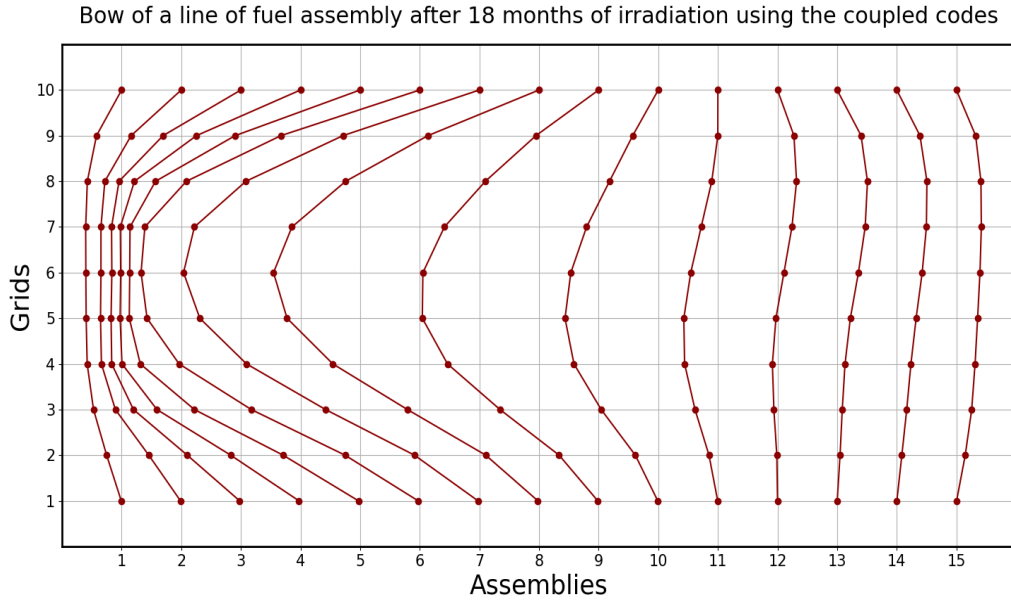


Figure 16. Results of the cycle simulation using coupled reference codes with asymmetric hydraulic boundary conditions

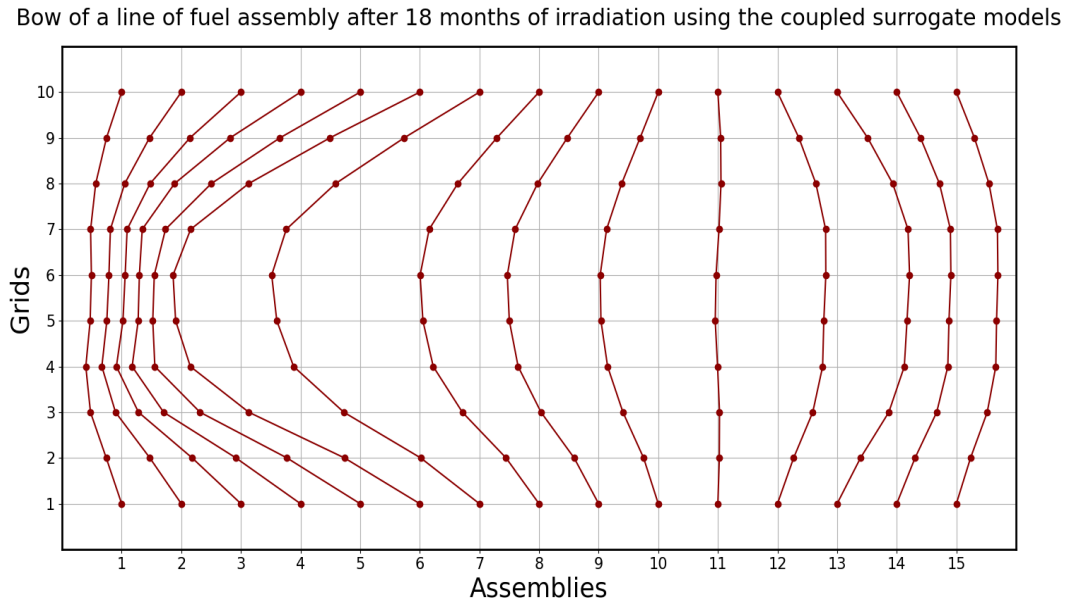


Figure 17. Results of the cycle simulation using coupled surrogate models with asymmetric hydraulic conditions

4.9. Conclusions

The results obtained demonstrate the ability of coupled metamodels to accurately reproduce simulations from reference codes, while providing a significant computational time reduction. This computational efficiency paves the way for their use in more complex analyses, particularly in the context of uncertainty

quantification.

5. CONCLUSION

This study developed a methodology for coupling two surrogate models, hydraulic and thermomechanical, using Gaussian process-based metamodels to simulate an entire irradiation cycle. The mechanical surrogate models were first validated by comparing their predictions with those from mechanical reference code DACC. This validation confirmed the models' ability to simulate fuel assembly bow, making them reliable for coupling with hydraulic models. The coupling strategy was designed to address several key challenges, such as managing the temporal aspects of the mechanical models over an 18-month irradiation cycle. This was achieved by using three distinct metamodels, representing the pre-irradiation, irradiation, and post-irradiation phases, which were chained together for a full cycle simulation. Additionally, a nonlinear penalization method was implemented to avoid inter-assembly penetration, at the spacer grid levels. A robust fluid-structure interaction (FSI) strategy was also developed, utilizing a dual-loop algorithm consisting of an internal mechanical loop and a global FSI loop. This algorithm ensured proper inter-assembly contact and stability during the iterative process, with mechanical and hydraulic forces exchanged iteratively to ensure convergence. Finally, a comparison of the coupled surrogate models with reference codes demonstrated that the surrogate models reproduced the results with sufficient accuracy, with a 60-fold reduction in computational time. The models performed well under various hydraulic boundary conditions, and while some discrepancies were observed, these were attributed to uncertainties in the surrogate models and those attributed to coupling criteria. Overall, the coupled surrogate models were shown to be an effective and efficient complement to traditional methods, offering significant time savings and predictive accuracy, enabling broader sensitivity analyses and uncertainty quantification in future studies.

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