M&C 2023 - The International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering · Niagara Falls, Ontario, Canada · August 13 – 17, 2023

Tool developments based on OpenMC toward neutron kinetics and uncertainty propagation with the TFM approach using OpenFOAM mesh and Correlated Sampling

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ABSTRACT

Developments have been performed using the OpenMC neutron transport code for thermohydraulics coupling and nuclear data uncertainty propagation. The main development related to the two applications is the Correlated Samping, this technique allow to propagate the impact of thermal feedback or cross section sampling on the tallies thanks to neutron weigh modifications. The Correlated Sampling is associated to Computer Aided Design (CAD) based mesh and to the Transient Fission Matrix (TFM) approach. Those three elements are presented and allow a global handling of the neutronics-thermohydraulics coupling: the TFM deals with the neutron kinetics using a pre-calculation of the neutron transport stored in matrices, the Correlated Sampling provides the impact of the thermal feedbacks on the matrices, and the CAD mesh is used to define de volumes associated to each bin of the matrices in order to get the results on the same format as the Computational Fluid Dynamics (CFD) code OpenFOAM. Both the implementations and verifications are detailed together with a discussion on the current limitations.

KEYWORDS: OpenMC, Nuclear Data uncertainty, Thermohydraulics, Correlated Sampling, TFM

1. INTRODUCTION

Developments have been performed in the neutron transport code OpenMC [1] for neutron kinetics application and coupling to thermohydraulics. This work relies on previous development on the Transient Fission Matrix (TFM) [2,3] aiming to reduce the neutronics calculation time with the generation of Green functions presenting the neutron transport during a generation. These developments were performed in the neutron transport Serpent2 code [4] and now in OpenMC. This proceeding presents this new implementation, additional features, and an application on a test case study. This development being related to reactor design associated to Molten Salt Reactors (MSR), the main illustration case is the fast version (MSFR) [5].

Different elements detailed below has been added to OpenMC: thermohydraulics mesh reading, correlated sampling and TFM matrices estimation. This paper presents the principle of the implementation together with a discussion on the current limitations.

One of the starting points of Monte Carlo codes is the geometry definition and the thermohydraulics coupling requires specific mesh inputs based on Computer Aided Design (CAD) tools. A coupling to the OpenFOAM [7] Computational Fluid Dynamics (CFD) mesh is presented in section 2. The next step concerns the estimation of the fission matrices for the TFM model and their variation according to density and Doppler effect. A Correlated Sampling (CS) technique has beed implemented in OpenMC during this work for the feedback estimation, including local feedbacks (specific mesh perturbation). It's implementation is presented in section 3 together with a validation on thermal feedback calculation. This implementation is generic and not limited to feedback, thus an application to nuclear data uncertainty is also detailed to validate the implementation. Finally, the estimation of the matrices required for the Transient Fission Matrix approach is detailed in section 4. This implementation is associated the OpenFOAM mesh for the matrices indexing and to the correlated sampling for the local feedback estimation on the matrices elements.

2. OpenFOAM MESH READING

2.1. Implementation

The OpenFOAM thermohydraulics code is a C++ open source project. Multiple solvers exist depending on the case to solve, *e.g.* incompressible, sonic, multiphase... Some of the solvers are based on "multiple regions" and are very convenient for reactor application, the different regions corresponding to the different materials (fuel, reflector, fertile, coolant...). The mesh is defined using different files describing the points positions, the faces (based on three or more points), the cells (based on the faces), and the boundary names (wall, symmetry, inlet, outlet...).

An automatic reading of the OpenFOAM files has been developed using the OpenMC native geometry, allowing to have a direct correspondance between the thermohydraulics and the neutronics cell number. Two types of faces are managed: the triangles, directly converted as an OpenMC plan, and faces defined with four points. The latter comes with a specific management, the four points are not necessarily aligned in a plan for the thermohydraulics code and then neutron loss in the geometry can occur if the face is converted in a single plan. Thus if the difference is larger than the numerical error the corresponding plan is split in two triangular faces. The boundary is adjusted between symmetry and neutron loss according to the name given in OpenFOAM patch. Figure 1 presents an illustration of a Molten Salt Fast Reactor (MSFR) geometry interpretation in OpenMC. Note that even if the mesh reading is based on OpenFOAM format, the mesh itself is generated using ANSYS [8] for better mesh generation capabilities. The fuel region is meshed using a hexahedron dominant mesh and the reflector using tetrahedrons.

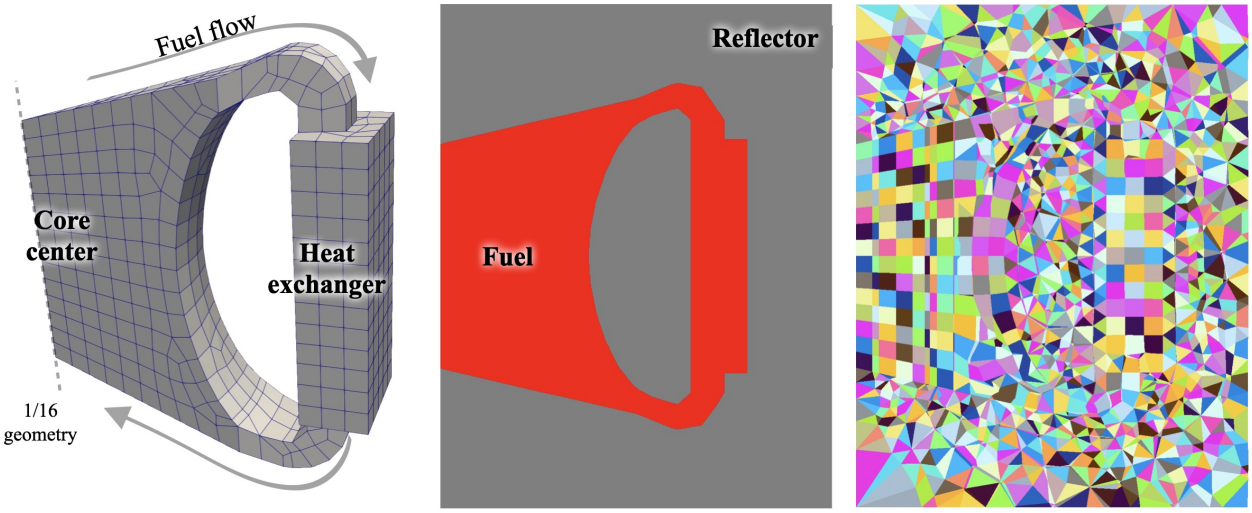

Figure 1: MSFR 1/16 fuel circuit geometry using paraview [9] (left), the OpenMC material (middle), and the corresponding OpenMC cells (right)

The mesh conversion do not requires direct modification in the C++ code of OpenMC, the python interface provides all the required tools for this functionality. Figure 2 presents the influence of the mesh precision on the calculation time. An important increase of computational cost during the first batches has been observed for a large number of meshes. This slowdown is associated to the cell research algorithm when a neutron cross a surface during the tracking procedure. The cells are progressively learning the list of neighbor cells but this process is very slow when the total number of cells is large. For this reason a minor modification had to be implemented in OpenMC on the C++ side. The mesh being conform, each surface is associated during the object creation procedure to its two neighbor cells. In this way the correspondance map is converged before the beginning of the first neutron batch and when a neutron cross a surface, it directly access to the arriving cell. Better results are obtained (curves with the light color on the left and middle plots) with a smaller calculation time for the first batches.

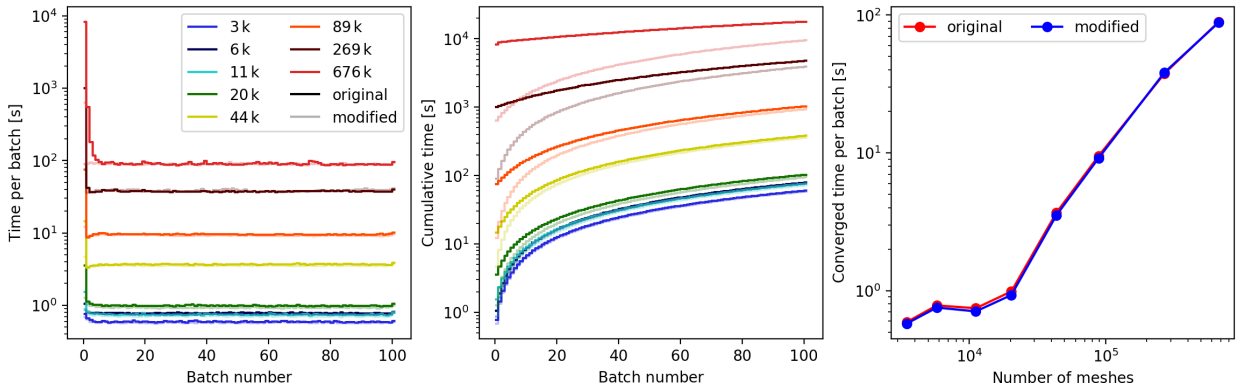

Figure 2: Calculation time for different mesh precision from 3 thousands up to 676 thousands meshes. Time per batch (left) and cumulative time (middle) as a function of the batch number, and converged calculation speed as a function of the number of meshes (right).

2.2. Current limitations

This implementation comes with two main limitations. The first one is due to the requirement to generate a mesh for the whole geometry, including the reflector up to the neutron loss or symmetry plan. The second limitation is the required mesh conformity between the regions: the points and faces need to correspond between the regions (materials) in order to avoid neutron loss.

A third limitation is linked to the OpenMC input file format. The whole geometry being converted in a *xml* ASCII format, the latter increase the file size by a factor 10 compared to the initial *msh* format. This could be tacked in futur by an on the fly conversion from the *msh* file directly in the openMC calculation.

3. CORRELATED SAMPLING IMPLEMENTATION

3.1. Implementation

The Correlated Sampling (CS) allows to estimate in a single calculation the impact of neutron cross section modifications. The main objective of the implementation is the estimation of thermal feedbacks (density and Doppler effect), including local effect such as a perturbation in a single cell. A second application case is the uncertainty propagation of nuclear data uncertainty, the utilisation being identical using random cross section files instead of different temperature for the Doppler broadening.

The correlated sampling consists in modifying the neutron weight according to the ratio of probability to choose or reject an event. For example, considering an interaction after a sampled distance d in a material with a total cross section Σ_{tot} in the analog system and $\Sigma_{\text{tot}}^{\text{pert}}$ in the perturbed system, the weight is modified by the following factor in equation 1. Additional information in the CS process can be found in reference [6] regarding the feedbacks and TFM or reference [10] concerning nuclear data uncertainty propagation.

$$\text{Weight modification factor} = \frac{\Sigma_{\text{tot}}^{\text{pert}} \exp(-\text{d} \cdot \Sigma_{\text{tot}}^{\text{pert}})}{\Sigma_{\text{tot}} \exp(-\text{d} \cdot \Sigma_{\text{tot}})} \tag{1}$$

For a perturbation according to a parameter (e.g. Doppler effect) a weight is associated to each neutron and changes after each interaction. This weight is propagated along the different generation of neutrons in order to take into account the modification on the neutron source due to the perturbation. For this reason a parameter perturbation corresponds to an array of weights. If the user asks to a local perturbation (e.g distribution of the Doppler effect on the mesh), an other dimension is added to the weights and a matrix (array of array) is associated to each neutron. Finally, in the input file the user can ask for different perturbation (such as density and Doppler feedback or material composition), adding an other dimension.

3.2. Application on local feedbacks estimation

In order to check the correlated sampling implementation a simple 1D test has been studied using lithium fluoride molten salt associated to the Th-^{233}U fuel cycle. The system is split in 16 cells (see Figure 3 - left) corresponding to the bins used to tally the fission distribution and to perturb locally the fuel temperature (density or Doppler effect). The plot on the right presents the reactivity variation according to a modification of 1 K in each bin separately. The correlated sampling results is calculated in a single calculation providing an actual temperature modification of 1 K. The reference results (ΔMC - dashed lines) corresponds to 33 different calculations (reference plus 16 calculation for each feedback effect). In order to limit the uncertainty when comparing two independent Monte Carlo calculations, 2 billions of neutrons are propagated per calculation, and the perturbation of each bin is done using +100 K and reduced to +1 K assuming a linear dependence on the density feedback and logarithmic according to the Doppler feedback effect. Concerning the correlated sampling calculation, the number of propagated neutron is also set to 2 billions, and the number of generation used to propagate the perturbed neutron source is set to 30 generations according to the convergence of the Shannon entropy on this geometry.

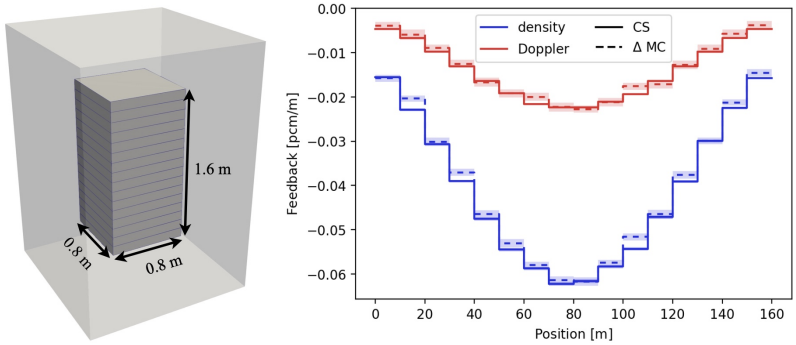

Figure 3: Simplified 1D geometry with 16 bins surrounded with a reflector generated with blockMesh[7] and visualized with paraview on the left, and density (blue) and Doppler (red) reactivity feedback calculated with the correlated sampling (plain line) and reference Monte Carlo (dashed line) on the right.

A second verification test is done in figure 4 on the same calculation, comparing the fission source redistribution according to the perturbation position. Previous study shown that if the perturbation amplitude is not too large and that they are not cross-interacting together the neutron flux shape during a coupled transient can be estimated by summing individual effects [11] for an advance point kinetics approach.

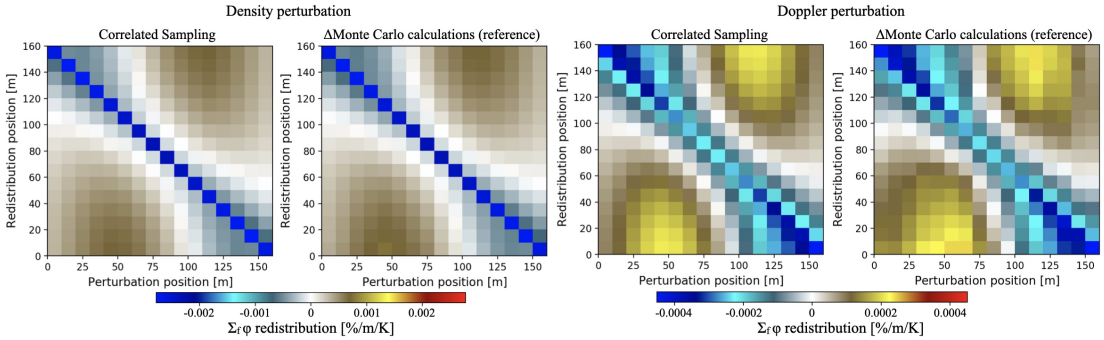

Figure 4: Fission rate redistribution according density (left) and Doppler (right) perturbation, each results is provided for the correlated sampling and direct Monte Carlo calculation.

A very good agreement on obtained on both reactivity feedback and redistribution according to density and Doppler effect.

3.3. Application on nuclear data uncertainty propagation

The correlated sampling implementation is not limited to feedback estimation, the user can provide many different version of a material for a cell. An other application is the nuclear data uncertainty propagation as illustrated in figure 5 with neutron cross section sampling (left plot) according to evaluated cross section covariances. On the middle plot, the y-axis corresponds to the result of the correlated sampling, and the x-axis is a validation with a reference direct Monte Carlo calculation. Note that the amount of neutron is divided by 40 for the CS calculation, providing 7 pcm uncertainty on the multiplication factor compared to 11 pcm for the reference calculation. This result is expected since the neutron follows the same tracks with the CS calculation and then the statistical uncertainty due to the neutron paths is removed.

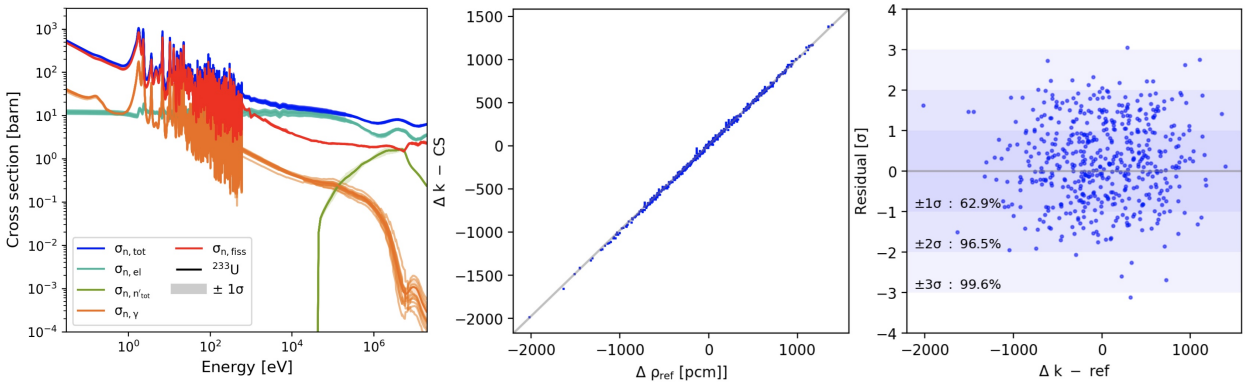

Figure 5: Random cross section sampling on elastic scattering, fission and capture of U^{233} based on ENDF/B-VIII.0 (left), propagation on the k_{eff} of the MSFR reactor (Th-^{233}U cycle): CS as a function of reference calculations (middle) and corresponding residual (right)

For this specific case a very good agreement is observed. This is not necessarily true for any application, especially if the cross section modification is large or if an energy threshold changes in a random cross section. A typical application case can be Bayesian Monte Carlo assimilation. After a preliminary check that the correlated sampling response is correct on a reduced sample, this approach can be very helpful to estimate the quantity of interest (reactivity, reaction rate...) and associate a weight to the random cross section on a very large quantity of samples.

This implementation comes with two main limitations. The CS does not take into account neutron multiplicity and neutron spectrum variation. The corresponding laws being available this should be implemented in futur for nuclear data uncertainty propagation. The second limitation is the probability table management. A temperature modification is not limited to a modification of the probability associated to the tables but also to the cross section factor. The table sampling being independent between the different versions of the materials, the variance on the perturbed neutron weight in then increased.

A third limitation concerns the way random files are provided to OpenMC. The *cross_sections.xml* file link each nucleus to a specific *h5* file, avoiding to the user to manage all the ACE files. Adding perturbed version of the isotopes has been unsuccessful and a temporary solution consists to assign to the next temperature (800, 801, 802...) the random files. Then a classic *h5* file is used for the temperature management, and for specific isotopes a secondary *h5* file is generated for random cross section sampling. A possible solution might be to allow the utilisation of small temperature variation (800.001...) and assign them to the random cross section ACE files to avoid user errors mixing the *h5* files.

4. TRANSIENT FISSION MATRIX (TFM) IMPLEMENTATION

4.1. Implementation

In order to perform kinetic calculations close to the Monte Carlo response with a reduced calculation time, a Green function based approach called Transient Fission Matrix has been developed in previous studies and various application cases [6,13–15]. It consists of different versions of fission matrices containing, for a neutron born in cell j (column of the matrix), the amount of neutron produced by fission in cell i (line of the matrix). The different versions are the cross exchanges between prompt and delayed neutrons (χ_p spectrum to ν_p multiplicity, χ_p to ν_d, χ_d to ν_p, χ_d to ν_d), plus the transport time from j to i, and finally the absorption matrices for interpolation models. In the following the 'prompt to promp' fission matrix is written $\underline{\underline{K}}_{\chi_p \to \nu_p} = \underline{\underline{K}}_{pp}$ and the corresponding time transport matrix is $\underline{\underline{T}}_{pp}$. Once the matrices are estimated, the coupling to the thermohydraulics does not require additional Monte Carlo calculation since the neutron kinetics models consist in using the Green function and adapting the neutron transport to the CFD code output (delayed neutron position and amplitude, temperature and density map).

This TFM approach has been implemented in OpenMC using an arbitrary cartesian or spherical mesh, or using directly the OpenFOAM mesh presented in section 2. All the matrices estimation are performed during a single criticality calculation. Each fission neutron created in the simulation being tagged according to its type (prompt or delayed), an additional tag is added according to the birth cell j. Then the different tallies ($\nu_p \Sigma_f \phi$, $\nu_d \Sigma_f \phi$, $t\nu_p \Sigma_f \phi$, $\Sigma_a \phi$, $leakage$...) are discretized according to the current neutron position i in order to compute the matrices. Note that the estimation occurring during a criticality calculation the source term in j is not flat but corresponds to the actual shape and then allows a better representativity of the Green function according to the system (reactor) response.

The implementation is also coupled to the CS, allowing the estimation in a single calculation of the fission matrices variation according to a global or local variation of density or Doppler broadening (*i.e.* the amount of neutrons created in i for a neutron born in j and assuming a perturbation in cell k). Together with this implementation, additional outputs such as the local feedbacks on the reactivity and flux shapes are also estimated with OpenMC.

For the simple 1D system in section 3.2 the corresponding $\underline{\underline{K}}_{pp}$, $\underline{\underline{K}}_{dp}$ and $\underline{\underline{T}}_{pp}$ are presented in figure 6. The fission matrices have a diagonale dominant shape: considering a neutron created in the position j (column) the probability the create new fission neutron in position i (line) is maximal if $j = i$. Considering the time matrix (right), the larger is the distance between j and i, the larger is the transport time.

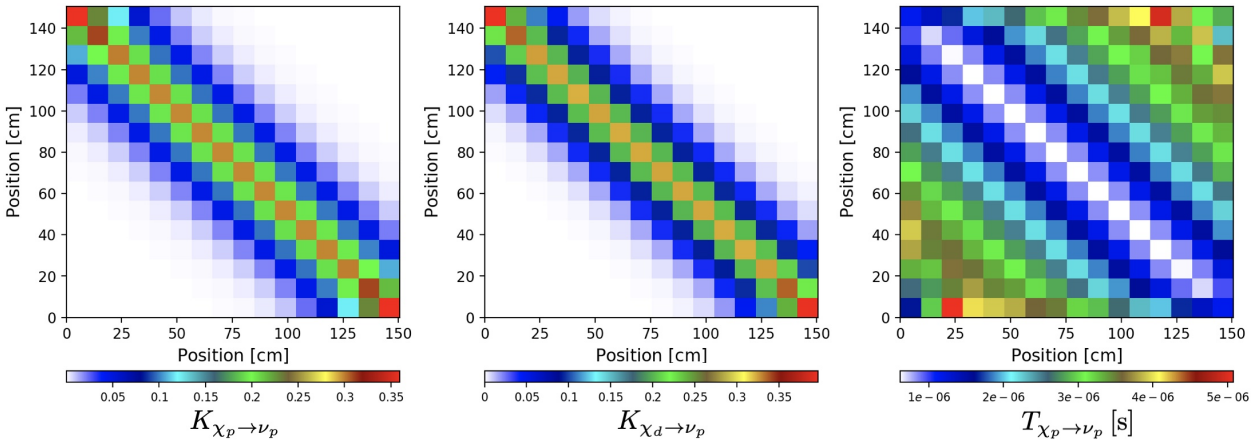

Figure 6: Prompt to prompt (left) and delayed to prompt (middle) fission matrices and prompt to prompt time matrix.

Considering a more complex geometry such as the MSFR shape from the EVOL program [12], the corre-

sponding fission matrix is presented in figure 7. Note that OpenFOAM renumbering the meshes in order to limit the bandwidth, the fission matrix has a global diagonal shape even if this aspect could be improved in futur in order to use sparse matrices.

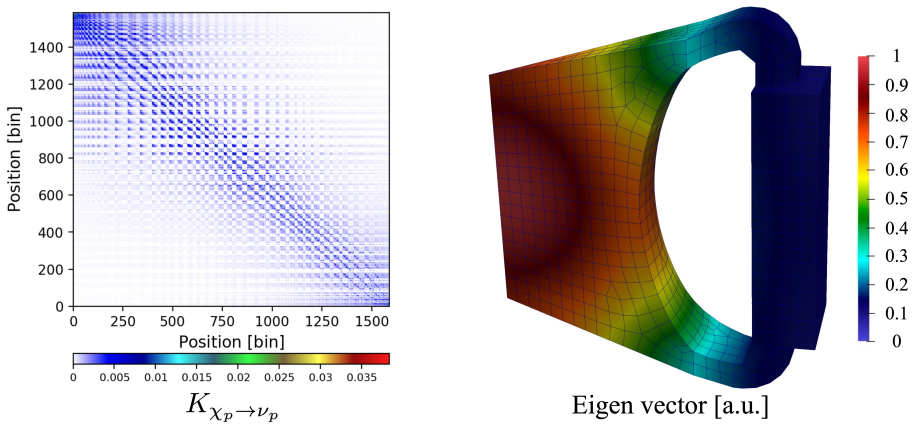

Figure 7: Prompt to prompt fission matrices (left) and eigen vector (right) in the MSFR-EVOL shape geometry.

4.2. Verification

4.2.1. Principle

The TFM approach can be used for different kind of systems from Molten Salt Reactors to PWR reactors using different neutron kinetics models from quasi-static up to direct spatial kinetics. A first verification step of the produced matrices can be performed using global parameters such as the effective fraction of delayed neutron and the effective neutron life time that can be calculated using the fission and time matrices. Those two quantities can be compared to a reference IFP estimation using Serpent2. For this reason we compare the effective kinetic parameters for two MSR configurations with a volume of 4 cubic meter (representative of an AMR version of the MSFR) using an NaCl-$MgCl_2$-$PuCl_3$ eutectic composition:

- the first configuration "Pu" uses an exMOx [REF vidal] plutonium fuel (critical for 58.10% NaCl + 32.46% $MgCl_2$ + 9.44% $PuCl_3$),
- the second configuration "Pu-Am" contains 50% exMOx plutonium, 40%^{241}Am and 10%^{243}Am (critical for 62.99% NaCl + 17.54% $MgCl_2$ + 19.47% (Pu+Am)Cl_3).

This second configuration contains a lot of isotopes with a threshold fission reaction. For this reason a strong difference is expected on the delayed neutron weighting due to the emission at a lower energy.

In order to estimated neutron kinetics parameters we need to build a block matrix $\underline{\underline{K}}_{tot}$ containing the prompt and delayed neutron fission matrices, and its corresponding Eigen vector $\underline{V}_{tot} = (\underline{V}_p \; \underline{V}_d)$:

$$\underline{\underline{K}}_{tot} = \begin{pmatrix} \underline{\underline{K}}_{pp} & \underline{\underline{K}}_{dp} \\ \underline{\underline{K}}_{pd} & \underline{\underline{K}}_{dd} \end{pmatrix} \quad , \quad \underline{\underline{K}}_{tot}\underline{V}_{tot} = k_{eff}\underline{V}_{tot} \tag{2}$$

This matrix contains $(2.n)^2$ elements with n the number of meshes. The transposed matrix $\underline{\underline{K}}^T_{tot}$ corresponds to the backward neutron source propagation and the corresponding Eigen vector $\underline{V}^*_{tot} = (\underline{V}^*_p \; \underline{V}^*_d)$ is the importance map of the prompt and delayed neutron source. Note that the underlying assumption is that the distribution of the adjoint source in the mesh is close to the forward source. This is not necessarily the case

and the mesh size must therefore be sufficiently fine. Then, writing '$\cdot$' the dot product, '$\circ$' the element-wise product and '$\sum \underline{V}$' the sum on all the element of a vector (*i.e.* the meshes), the kinetics parameters are given by:

$$\beta_0 = \frac{\sum \underline{V}_d}{\sum \underline{V}_{tot}} \ , \ \beta_{eff} = \frac{\underline{V}^*_d \cdot \underline{V}_d}{\underline{V}^*_{tot} \cdot \underline{V}_{tot}} \ , \ l = \frac{\sum \left(\underline{\underline{K}}_{pp} \circ \underline{\underline{T}}_{pp} \right) \underline{V}_p}{\sum \underline{\underline{K}}_{pp} \underline{V}_p} \ , \ l_{eff} = \frac{\underline{V}^*_p \left(\underline{\underline{K}}_{pp} \circ \underline{\underline{T}}_{pp} \right) \underline{V}_p}{\underline{V}^*_p \underline{\underline{K}}_{pp} \underline{V}_p} \tag{3}$$

4.2.2. Statistical uncertainty propagation

In order to propagate the statistical uncertainty of the fission matrices up to the kinetic parameters the uncertainty on each term of the matrices can't be used directly. Indeed even if for each term k_{ji} of a matrix has statistical uncertainty $\sigma_{k_{ji}}$ that can be estimated using a standard approach, the correlation with the other terms of the matrix are not zero.

For this reason, all the outputs added to OpenMC in this work (fission matrices, correlated sampling, tally on OpenFOAM mesh...) are provided for each MPI thread separately. Then the standard deviation on each 'quantity of interest' (e.g. β_{eff}) can be obtained as the standard deviation on each 'MPI version' of the raw data (e.g. fission matrices). An optimized approach used below is based on a Jackknife resampling technique in order to avoid threshold effect when the statistics is too low.

4.2.3. Results

The effective kinetic parameters are given in table 1 for the two systems using OpenMC and Serpent2. Note that Serpent2 uses a slightly different geometry based on the *stl* geometry. A very good agreement is obtained, including on the Pu-Am case with a large effect of the adjoint weighing.

Table 1: Effective kinetic parameters calculation using Serpent2 IFP (1.25 billion neutrons) and OpenMC TFM (0.2 billion neutrons)

Case / Method	β_0	β_eff	$l_{fissto fiss}$	l_{eff}
Pu / TFM - OpenMC	317.234 ± 0.003	289.2 ± 0.3	1312.9 ± 0.4	1060.1 ± 0.3
Pu / IFP - Serpent2	317.3 ± 0.2	286.6 ± 0.8	-	1067.0 ± 0.5
Pu-Am / TFM - OpenMC	260.507 ± 0.004	166.1 ± 0.3	378.3 ± 0.1	267.18 ± 0.07
Pu-Am / IFP - Serpent2	261.6 ± 0.2	164.9 ± 0.8	-	265.6 ± 0.2

5. CONCLUSIONS

This work consists in the implementation of additional numerical functionalities in OpenMC for thermo-hydraulics coupling and nuclear data uncertainty propagation. The mesh conversion from the OpenFOAM CFD code allows to define the geometry in Computer Aided Design (CAD) tools as a 3D mesh and the get a direct correspondance between thermohydraulics and neutronics meshes.

The second element is the implementation of a correlated sampling technique. This technique allow to get the tally results associated to n different versions of a material. A very good agreement is obtained on local reactivity feedback and neutron flux redistribution for thermohydraulics coupling problems, and although for nuclear data uncertainty propagation on a MSFR core.

Finally, the estimation of the matrices required for the TFM approach has been implemented in OpenMC. This implementation has been performed in association with the CAD mesh for the matrices index and with

the correlated sampling to estimate global or local density and Doppler feedback effect on the matrices. This implementation has been verified using effective kinetic parameters calculated with the matrices and compared with IFP calculations.

Futur development will focus on the current limitations of this work: the geometry input format that requires large files ; neutron multiplicity, emission spectra and probability tables management for the Correlated Sampling ; and perturbes cross section management for nuclear data uncertainty propagation. Another perspective is the coupling between OpenFOAM and OpenMC for transient calculations and comparison with other tools.

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