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Hybrid Resolution Method for Efficient Depletion Analyses using Explicit Geometry Multigroup Monte Carlo

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Abstract. The hybrid resolution (HR) method is a recently developed calculational algorithm tailored for efficient nuclear reactor analysis by leveraging multigroup (MG) Monte Carlo (MC) coupled with continuous energy MC calculations. While the HR method has demonstrated promising results in various scenarios, an anticipated challenge arises from inconsistencies of MG MC results caused by spatial homogenization when relatively coarse mesh is adopted, particularly in heterogeneous problems characterized by a strong flux gradient. To address this issue, the HR method incorporates MG MC calculations on the same explicit geometry used in continuous energy MC calculations. In other words, this approach preserves accuracy in geometry handling while solely simplifying energy treatment. In our investigation, a 3-dimensional BWR-type fuel assembly was focused on for a comparative study regarding the different geometry treatments in MG MC calculations. Various reactor parameters such as k-effective, power, flux, and atomic densities were estimated, and numerical performance was also compared in terms of the computing time and figure-of-merits. Our evaluation revealed that the explicit geometry-based HR method yielded more consistent and reliable parameters compared to the simplified coarse mesh-based scheme, reducing errors in power and flux distributions by about 10%.

1 Introduction

The hybrid resolution method aims to realize efficient time-dependent nuclear reactor analyses based on the Monte Carlo (MC) simulation [1-2]. This method integrates advantageous features from both high-resolution calculations with continuous-energy MC on explicit geometry and low-resolution calculations with multigroup (MG) MC on a simplified geometry. The high-resolution calculation provides accurate solutions at macro time steps and generates group constants for depletion and MG MC calculations, while the more efficient low-resolution calculation fills a temporal gap between the macro time steps with reliable time-dependent parameters.

This method has proven its efficiency in estimating time-varying reactor parameters in a spatially dependent problem compared with the explicit Euler method and predictor-corrector method [2]. In particular, the MG MC method achieved substantial speed up over the continuous energy MC method through the simplification in energy and geometry treatment. In consequence, this method has substantially improved the performance without requiring excessive time overhead, while providing reliable depletion parameters at each substep.

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However, the homogenization of geometry necessarily entails the loss of the angle dependencies and the spatial importance of neutrons within depletable regions [3]. This disrupts the neutron balance both in spatial and energetic contexts, eventually eroding the equivalence between the continuous energy and MG MC methods. Although the current approach employs form functions to approximate the time-dependent neutron spectrum and flux distribution on explicit geometries, this strategy may lead to inconsistencies with longer depletion steps and in further complicated geometries.

This issue can be suitably addressed by aligning the geometry. The MG MC method is simulated on the same explicit geometry used in continuous energy MC calculations only with energy structure simplification. This approach not only streamlines the entire calculation process of the hybrid resolution method but also enhances the consistency of neutron spectrum and flux distribution within detailed geometry. Moreover, given that the numerical burden associated with reaction type search and cross section calculations typically outweighs that of neutron tracking and geometry treatment, this approach is expected to uphold the efficiency of MG MC calculations without substantial compromise.

This paper discusses the conceptual framework and computational workflow of the HR method within the context of employing two different geometric treatments in the MG MC method. Two distinct schemes are assessed in a single fuel assembly problem characterized by a high dominance ratio. Various reactor parameters are estimated across burnup calculations and compared with reference solutions that rely on the continuous energy MC. The evaluation encompasses a comprehensive analysis of efficiency and performance, focusing on error reduction, including the comparison of total computing time, and corresponding figure-of-merits.

2 Method

2.1 Hybrid resolution with homogeneous coarse mesh-based MG MC

The hybrid resolution method employs low-resolution MC calculations with a few-group energy structure on a simplified mesh-based geometry to bridge the gap between high-resolution MC calculations. Despite a simplification in energy and geometry, the transport calculation still can provide more consistent time-dependent solutions than any other neutronic solvers [4-5] or prediction schemes [6-7] by explicitly simulating the actual neutrons' physical behavior. Furthermore, low-resolution MC calculations can achieve a substantial speed up compared to high-resolution MC calculations, achieving 10-20 times faster calculations depending on scenarios [8]. Therefore, the total computing time can be effectively saved by replacing time-demanding high-resolution MC calculations with the more efficient low-resolution MC calculations.

Nonetheless, careful consideration should be given to the approximation involved in transitioning from high-resolution to low-resolution for a reliable HR method. The standard homogenization process typically assumes that the angular dependence of the flux is separable from its energetic and spatial dependence [9-10]. This assumption causes certain homogenized cross sections, particularly the total cross sections, to be treated as isotopic when they should be angular-dependent. Such a simplification can lead to inaccuracies in the diffusion of neutrons and eventually can fail to accurately represent leakage effects at material interfaces.

$$\bar{\Sigma}_{t,g}^{m} = \frac{\int_{V_m}\int_{E_g}^{E_{g-1}}\int_{4\pi}\Sigma_t(\vec{r},E)\psi(\vec{r},E,\hat{\Omega})dEd\vec{r}d\hat{\Omega}}{\int_{V_m}\int_{E_g}^{E_{g-1}}\int_{4\pi}\psi(\vec{r},E,\hat{\Omega})dEd\vec{r}d\hat{\Omega}} \cong \frac{\int_{V_m}\int_{E_g}^{E_{g-1}}\Sigma_t(\vec{r},E)\phi(\vec{r},E)dEd\vec{r}}{\int_{V_m}\int_{E_g}^{E_{g-1}}\phi(\vec{r},E)\,dEd\vec{r}} \quad (1)$$

where the angular flux can be decoupled with the scalar flux and angular momentum according to the flux separability approximation (FSA)

$$\psi(\vec{r}, E, \hat{\Omega}) \cong \phi(\vec{r}, E) \cdot A(\hat{\Omega}) \tag{2}$$

Another important consideration is that the MG MC calculations provide homogeneous neutron flux homogenized over regions including both depleting and non-depleting (e.g., moderator) materials although fuel regions should only be depleted in burnup calculations. Therefore, the neutron spectrum and flux distribution should be reproduced using the group-dependent homogeneous flux profile and form functions for the subsequent burnup calculation.

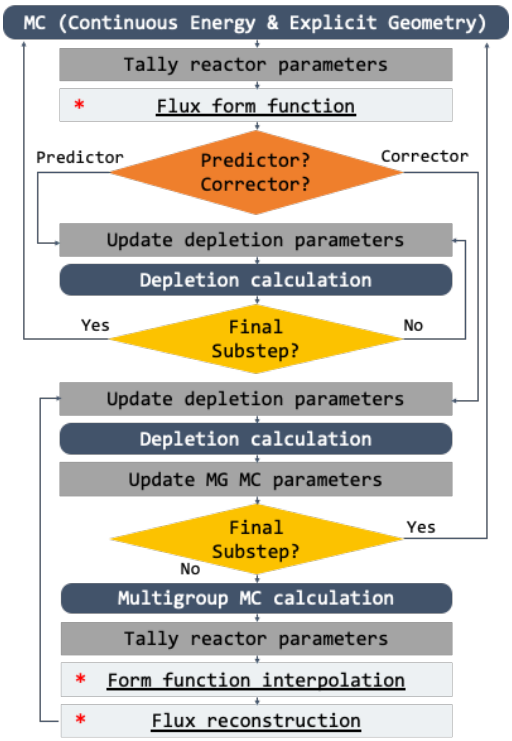

Fig. 1. Flow diagram for hybrid resolution scheme with homogeneous mesh-based MG MC method

Fig. 1 exhibits a flow diagram for the hybrid resolution scheme jointed with simplified mesh grid-based MG MC calculations. This figure focuses on the procedures related to the transition between high-resolution and low-resolution in flux distribution, marked with a red asterisk. From the continuous energy MC calculation, the flux distribution should be calculated based both on explicit geometry (each material m) and mesh grid (each node n) for the depletion and MG MC calculations, respectively:

$$\phi_g^m = \frac{1}{V_m} \int_{V_m} \int_{E_g}^{E_{g-1}} \phi(\vec{r}, E)\, dE d\vec{r} \tag{3}$$

and

$$\phi_g^n = \frac{1}{V_n} \int_{V_n} \int_{E_g}^{E_{g-1}} \phi(\vec{r}, E)\, dE d\vec{r} \tag{4}$$

Then group- and region-wise form functions can be obtained by dividing material-based flux by node-based flux.

$$\text{ff}_{g,m,n} = \sum_{m \in n} V_{m,n} \times \frac{\phi_g^m}{\phi_g^n} \tag{5}$$

where $V_{m,n}$ is the volume fraction of the material m taking over the node n. For example, $V_{m,n}$ equals unity when node n consists solely of material m. These form functions are obtained from every continuous energy MC calculation and later are interpolated for the flux reconstruction at each substep during the depletion period.

The neutron spectrum and flux distribution vary with the change of the isotopic compositions in depleting regions, and the ratio between the material-based flux and node-based flux will be changed with the depletion of the reactor core. Therefore, the form functions at each substep (t_s) should be approximated to reflect the consistent ratios. In our study, the form functions at each substep are estimated at the corrector step to reproduce the high-resolution solutions through quadratic interpolation using the three data points at the previous time step (t_{c-1}), the beginning of the current time step (t_c), and the end of the current time step (t_{c+1}) [7].

$$\begin{aligned}\text{ff}^s = \frac{s}{N_s}\Bigg\{&\left(-\frac{\bar{t}_c^2}{3\bar{t}_{c-1}(\bar{t}_{c-1}+\bar{t}_c)}\right)\text{ff}^{c-1} + \left(1+\frac{\bar{t}_c}{3\bar{t}_{c-1}}\right)\text{ff}^c \\ &+ \left(1-\frac{\bar{t}_c}{3(\bar{t}_{c-1}+\bar{t}_c)}\right)\text{ff}^{c+1}\Bigg\}.\end{aligned} \tag{6}$$

where s signifies the substep index, N_s is the total number of sub-steps, and $\bar{t}$ indicates the time difference between neighboring time steps such as:

$$\bar{t}_c = t_{c+1} - t_c \tag{7}$$

Once the homogeneous flux distribution is obtained from the MG MC calculations, the detailed flux distribution can be regenerated by a reconstruction process:

$$\phi_g^{s,m} = \frac{1}{V_m}\sum_n \text{ff}_{g,m,n}^s \cdot \phi_g^{s,n} \tag{8}$$

Then, the material-based neutron flux is utilized for the depletion calculation.

2.2 Hybrid resolution with explicit geometry-based MG MC

While interpolating form functions offers a straightforward approach to addressing the relationship between high-resolution and low-resolution flux distributions at each substep, it lacks strict consistency due to the nonlinear evolution of neutron spectrum and flux distribution over time. This inconsistency becomes more pronounced with increasing depletion length and geometric complexity.

However, this limitation can be effectively resolved by incorporating explicit geometry into the MG MC simulation. The tedious procedures outlined in equations (2) through (6) can be simply eliminated by using the same explicit geometry as in CE MC calculations. Only procedures related to nuclear data handling and energy condensation require simplification. Therefore, the algorithm of the HR method can be greatly streamlined simply by eliminating the need to calculate the flux distribution at different resolution levels. Instead, flux distributions as well as any other reactor parameters like cross sections can be directly derived on explicit geometry.

One additional benefit is that the accuracy penalty from applying FSA is likely reduced in the explicit scheme. In this approach, the FSA can be relaxed by generating group constants separately for each material, capturing their specific angular dependencies and neutron spectra, rather than collapsing multiple materials into a single homogenized node. This method allows for a more detailed and precise representation of the physical phenomena within each material. Consequently, it enhances the overall fidelity of the simulation, leading to more reliable and accurate predictions.

One expected drawback is the increased computing time required to handle explicit geometry compared to a homogenized mesh grid. Nevertheless, this overhead is expected to be acceptable within the entire burnup calculation. Firstly, MG MC calculations occupy only a fraction of the overall computing time, as the majority is devoted to continuous energy MC transport calculations. Secondly, the computing time spent on determining reaction types, selecting isotopes, and calculating cross sections is typically more dominant than that for searching cells and surfaces and tracking particles. Especially, handling the geometry of lattice-based reactor problems can be highly optimized.

3 Results

3.1 Problem description

A comparative analysis was conducted to evaluate the impact of geometric treatment on multigroup MC calculations in a 3-dimensional BWR-type fuel assembly problem, as illustrated in Fig. 2. This assembly is composed of two types of UO_2 fuel rods with different enrichments arranged in a non-symmetric configuration, alongside two large water holes intended for control rod insertion. In this analysis, the control rods were not considered, and thus the guide tubes were filled with a moderator. The pitch size of the assembly is 12.95 cm, and its height is 381 cm. The moderator represented by boiling water exhibits varying densities with elevation, as depicted in Fig. 2. Note that this analysis does not account for thermal/hydraulic coupling; both material temperature and moderator density remain fixed over time.

The fuel assembly was depleted up to about 5 MWd/kg discharged burnup. In this analysis, various time-dependent reactor parameters were estimated including k-effective, power, neutron flux, and atomic densities. The performance was also evaluated in terms of computing time and figure-of-merits. A reference solution was obtained first using the higher-order predictor-corrector method with tighter depletion steps. On the other hand, the hybrid resolution method was simulated using two different schemes for geometric treatment on the multigroup MC calculation: one with explicit geometry, and another with a homogenized mesh of 10 x 10 x 10. A total of 200,000 histories per cycle and 30 active cycles were simulated in OpenMC with our modules and libraries. Two-group energy structure was used for the multigroup calculation, and each depletion step was divided into 5 sub-steps.

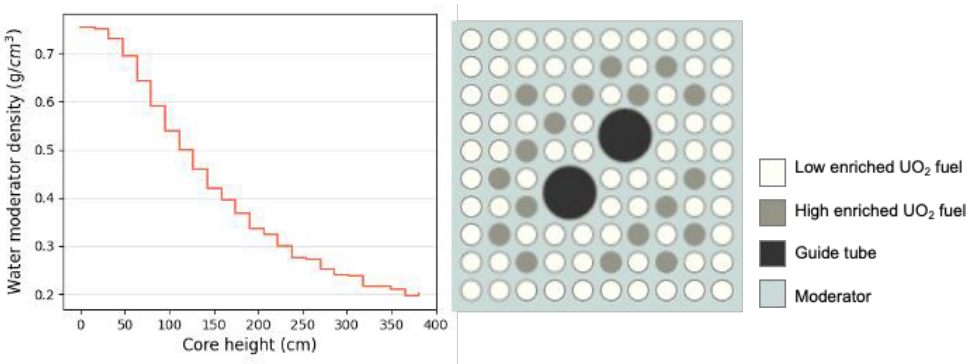

Fig. 2. (a) Moderator density along the axial direction; (b) Radial configuration of the fuel assembly.

3.2 Comparison of various reactor parameters

The pin power distribution was tallied on a 10 x 10 x 10 mesh grid. Notably, this fuel assembly has a strong flux gradient along the axial direction attributed to the varying densities of the moderator. This feature poses challenges in accurately reproducing multigroup MC solutions equivalent to CE MC solutions.

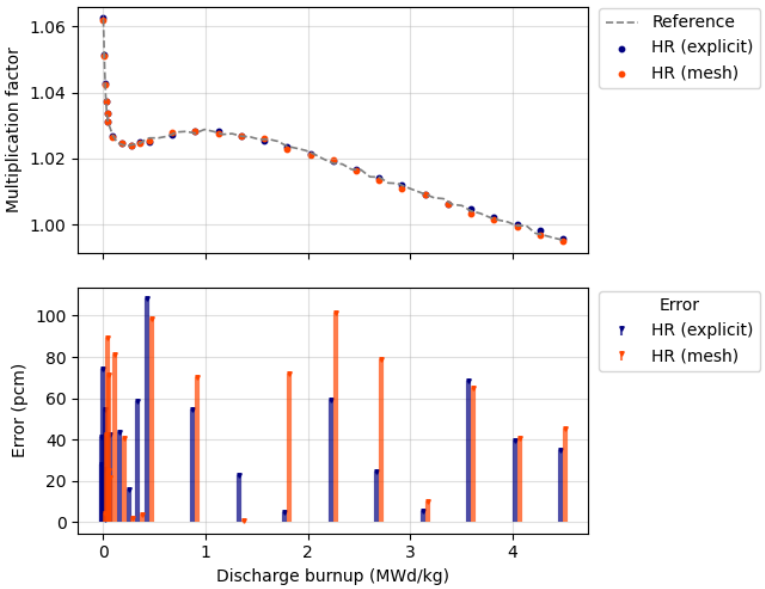

Fig. 3. Time-dependent multiplication factors and corresponding differences with the reference.

Fig. 3 shows the time-dependent k-effective along the depletion and corresponding errors in comparison with the reference solutions. The results of the hybrid resolution methods showed a good agreement with the reference solution. While the errors already fall within a stochastic uncertainty margin ($3\sigma \approx 112.11\ pcm$), the errors will further reduce when tighter steps are used.

Fig. 4 illustrates the relative errors of 3D pin power distribution throughout the depletion simulation. These errors tend to be more significant in the upper core region, likely due to the larger uncertainties stemming from fewer tallies, while the errors appear quite consistent across the depletion timeline. A difference in errors can be observed between the HR schemes

employing the mesh grid and explicit geometry. Specifically, the HR scheme with the mesh grid tends to yield larger errors compared to the scheme with explicit geometry. The mesh grid scheme showed approximately 10% higher errors on average than those of the explicit geometry scheme.

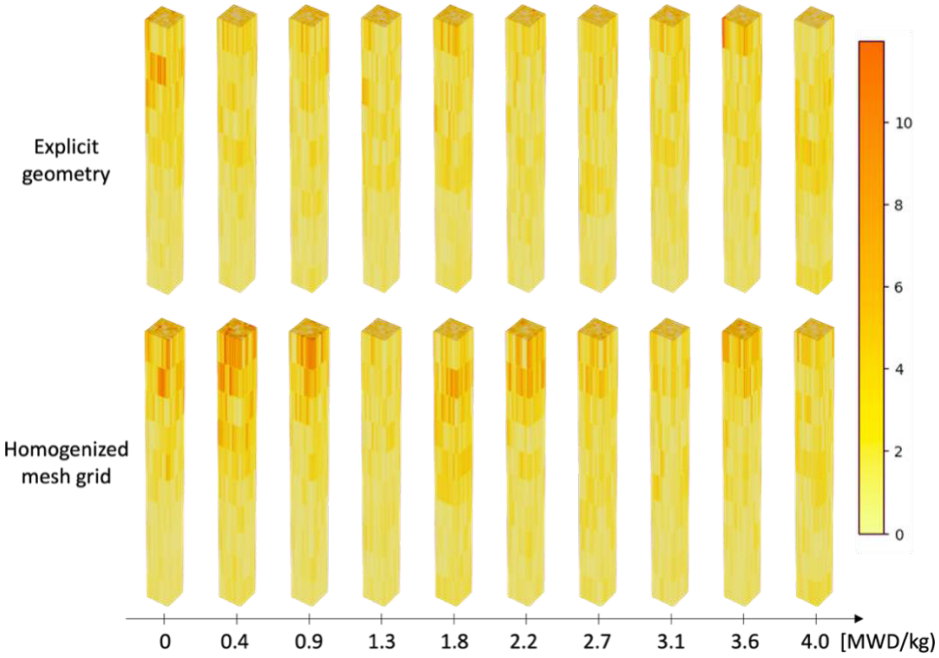

Fig. 4. Relative errors of 3D pin power distribution along the depletion (%).

Fig. 5 compares the average neutron flux values along the depletion simulation. The pin-wise flux distribution was normalized based on the reactor power and averaged across the core. The flux values obtained through the HR methods fluctuate with time and periodically match well with the reference. This result explains that the HR method can give accurate results at every macro depletion step by performing the continuous energy MC simulation, featured by bullet points and vertical grid lines. However, the MG MC calculation tends to underestimate neutron flux values at sub-steps in this problem. This discrepancy is more pronounced in the mesh grid scheme than in the explicit geometry scheme. The explicit geometry scheme constantly demonstrated lower errors over the simulation.

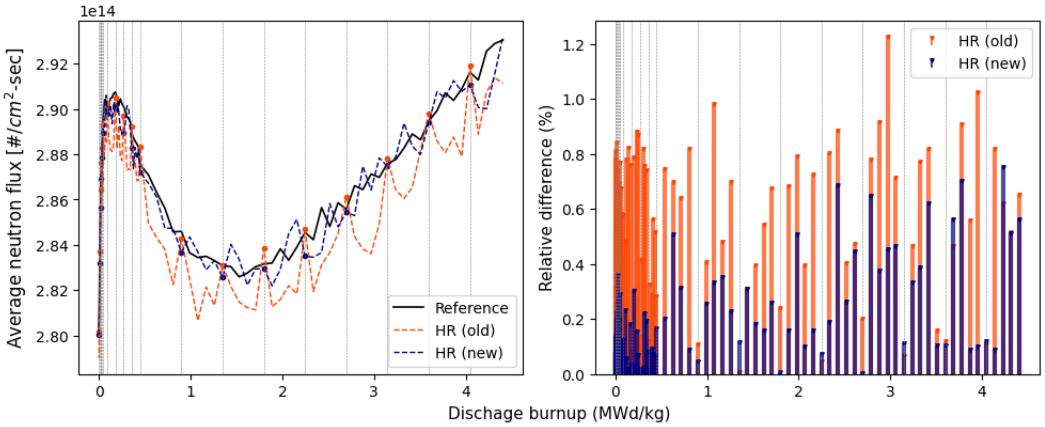

Fig. 5. Time-dependent average neutron flux and corresponding error compared with the reference.

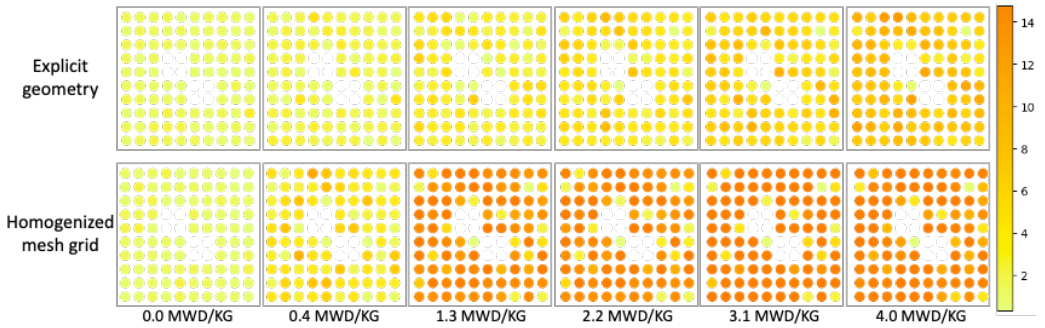

Fig. 6. Error distribution of pin-wise radial flux distribution through the depletion.

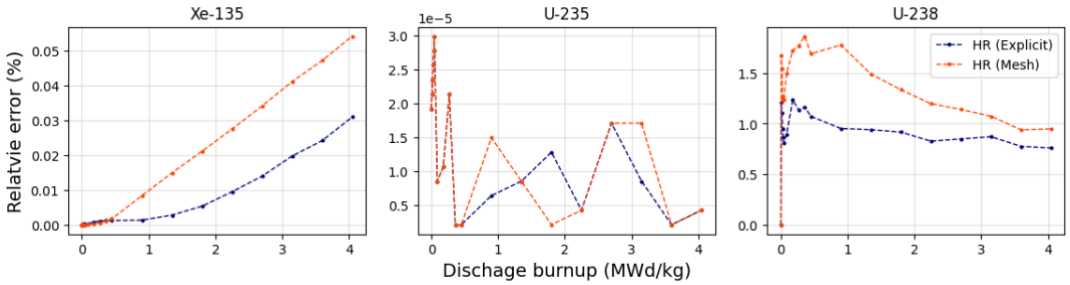

Fig. 7. Relative error of atomic number density for specific isotopes at macro time steps.

Fig. 6 describes the relative errors of the pin-wise radial flux profile with the depletion time. The errors are initially marginal, typically less than 3%. However, the errors get larger after passing the peak point, i.e., the k-effective peak at 1.0 MWd/kg (refer to Fig. 3). During this phase, the reactor state, including k-effective, power, and flux rapidly changes, making it challenging to capture the time-varying trends accurately. Nevertheless, the explicit geometry-based HR method demonstrated closer agreement with the reference than the mesh grid-based HR method. The maximum errors are larger in the mesh grid-based scheme. The errors are estimated to be 10% higher in the mesh grid-based scheme than in the explicit geometry-based scheme.

Last, the atomic densities are compared for several specific isotopes. Fig. 7 shows the relative errors of atomic number densities for Xe-135, U-235, and U-238. While U-235 shows

a good agreement with each other with exceptionally small errors, the errors are larger in the mesh-based scheme for Xe-135 and U-238 isotopes.

3.3 Performance evaluation

The computing load for particle tracking in a complicated geometry will necessarily rise. In other words, the explicit geometry scheme will demand more computational resources than the mesh grid scheme. Fig. 8 illustrates the total computing time allocated to each component. Firstly, the computing time for continuous energy MC calculation remains similar to each other but shows slight variations attributed to uncertainties. Although the numerical cost for the MG MC calculation fairly increased in the explicit geometry scheme compared to the mesh grid scheme, the time overhead accounted for only 9% of the total computing time as the MG MC calculation takes only a small portion of the entire simulation.

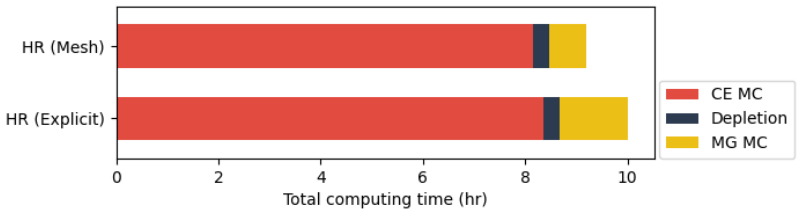

Fig. 8. Comparison of total computing time.

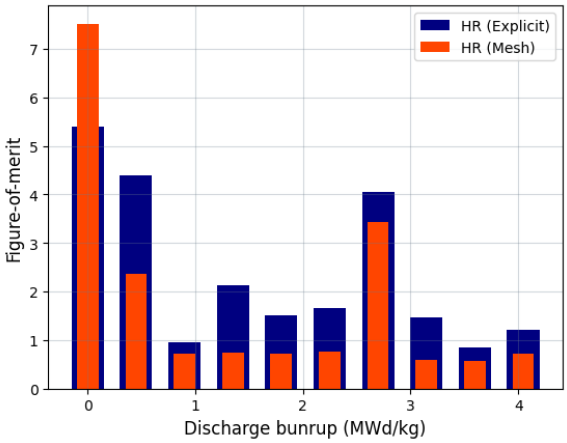

Fig. 9. Figure-of-merit for time-dependent neutron flux.

Overall, the explicit geometry-based HR method demonstrated better performance in evaluating the time-dependent reactor parameters. Fig. 9 presents the figure-of-merits (FOM) for the neutron flux distribution. The FOM was estimated by a reciprocal of the RMS error of the neutron flux multiplied by the computing time in hours at each depletion step. Despite the additional computing time in the MG MC calculation, the explicit geometry-based HR method achieved higher FOMs with improved accuracy throughout the simulation.

Conclusions

The hybrid resolution (HR) method employing explicit geometry-based Monte Carlo calculations has been assessed against the scheme with a simplified mesh-based geometry. A comprehensive analysis was conducted, focusing on various reactor parameters essential for

burnup calculations within a BWR-type fuel assembly problem. The explicit geometry-based approach consistently outperformed the mesh-based scheme for generating more reliable time-dependent parameters. In particular, the explicit geometry-based approach attained a reduction in difference errors for power and flux distributions by more than 10% compared to the mesh-based scheme. Furthermore, the efficiency and performance were evaluated by comparing the computing time and figure-of-merits. Despite the increased computing overhead associated with particle tracking in the more complicated geometry, the total computing time saw only a 9% increment, as the MG MC calculation constituted a small portion of the overall calculation. In consequence, the explicit geometry-based approach maintained higher figure-of-merits throughout the simulation. Further efforts will be dedicated to refining the MG MC solutions by enhancing time-dependent cross sections through burnup.

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