

Overview of the new capabilities in the Monte-Carlo particle-transport code NECP-MCX V2.0

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Abstract. NECP-MCX is a Monte-Carlo particle-transport code developed by the Nuclear Engineering Computational Physics (NECP) Lab. of Xi'an Jiaotong University in 2018. The first version of NECP-MCX is focused on addressing the challenge of deep-penetration radiation-shielding problems. In recent years, new capabilities of unstructured-mesh geometries, dose engine for Boron Neutron Capture Therapy (BNCT), neutron noise analysis, sensitivity analysis, depletion and activation calculation, simulation of randomly dispersed media, homogenization and gamma dose calculation based on point-kernel integral method are implemented in NECP-MCX V2.0. A user interface of NECP-MCX V2.0 is also under active development. This paper will introduce these new capabilities.

1 Introduction

To address the challenges of deep-penetration problems, the first version of NECP-MCX (NECP-MCX V1.0) [1] was developed based on a hybrid Monte-Carlo-Deterministic method, where the deterministic solver is an inhouse three-dimensional parallel discrete ordinate (SN) particle-transport code NECP-Hydra [2]. The language of the input file is eXtensible Markup Language (XML) and the output is Python. The neutron-photon coupling transport calculation functionality was developed based on the continuous-energy ACE-format nuclear library. Both the fixed-source and the critical problems can be solved by NECP-MCX.

NECP-MCX V1.0 was used in more than 20 organizations for research and design. In this process, new demands were proposed by the users. To fulfill the demands of the users, new capabilities were developed and NECP-MCX V2.0 was released. This paper presents a general overview of the new capabilities, including the background and the methodologies.

2 Unstructured mesh geometry

In NECP-MCX V1.0, the Constructive Solid Geometry (CSG) is used, which can handle complex geometries theoretically. However, plenty of human effect is needed to build large complex geometries in engineering applications. Besides, as numerous geometric parameters, like

equation coefficients of surfaces, Boolean operators, etc. should be given by the users, the geometries defined by the users are error-prone.

Considering the powerful modelling capabilities of Computer-Aided Design (CAD) platforms, researchers and engineers widely adopt these platforms to build complex models. In order to utilize the modelling capability of the CAD platforms, researchers have been making efforts to combine CAD platforms and Monte Carlo codes. There are mainly 4 technical routes: performing particle tracking based on the CAD model [3,4], performing particle tracking based on the facet model generated from the CAD model [5,6], converting the CAD model to the CSG model [7–10] and converting CAD model to Unstructured Mesh (UM) geometry [11]. Considering the CSG is still used in NECP-MCX and the simulation of particle transport is the fastest among the four technical routes, the third technical route is adopted in NECP-MCX V2.0. To couple NECP-MCX with Computer-Aided Engineering (CAE) platforms for multi-physics analysis the fourth technical route is also adopted in NECP-MCX V2.0. The third technical route will be introduced in Section 9 and this section focuses on the fourth technical route.

The advantages of UM can be summarized in several aspects. Firstly, plenty of commercial/opensource CAE platforms with a large community can be utilized to generate UM. Secondly, as the UM is widely adopted in Finite Element Method (FEM) analysis, it is easy to accomplish multi-physics simulation based on UM. The disadvantages of the UM are low particle-tracking efficiency and large memory consumption.

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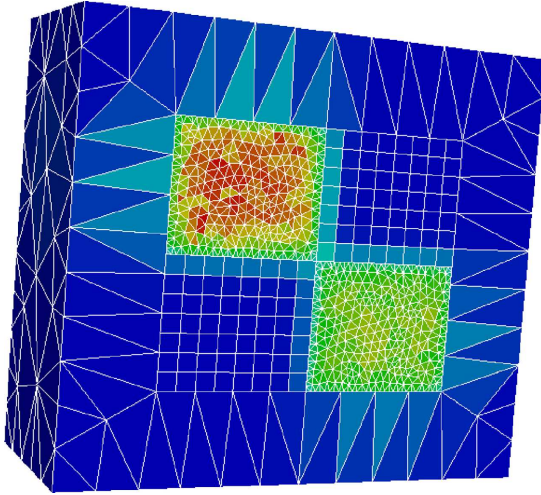


Fig. 1. Flux distribution of the LWR pool benchmark.

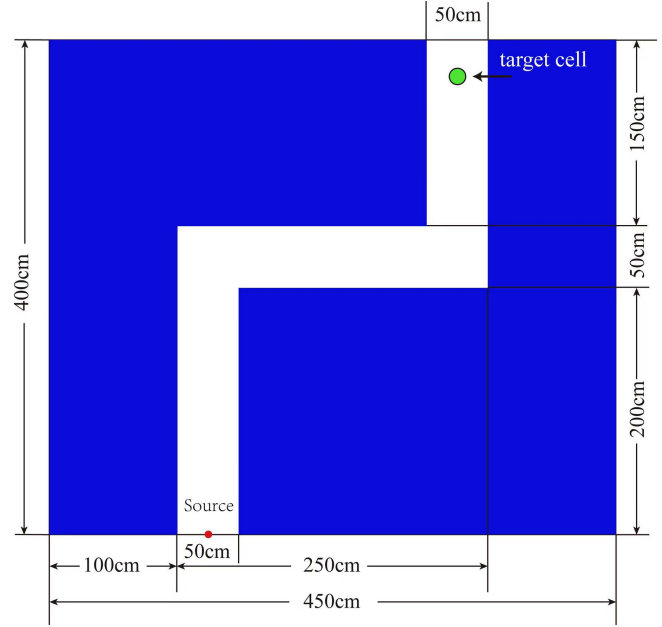
To overcome the disadvantages of the UM, several methods and algorithms were implemented in NECP-MCX V2.0 [12].

To promote the efficiency of UM-based particle tracking, a Mesh-Guided Particle Tracking (MGPT) routine was studied and implemented. The MGPT routine relies on two essential functions: Particle-Mesh Assignment (PMA) and Ray-Mesh Intersection (RMI). To enhance the computational efficiency, these functions are optimized using acceleration techniques, especially employing the block-based spatial kd-tree and neighbour element map.

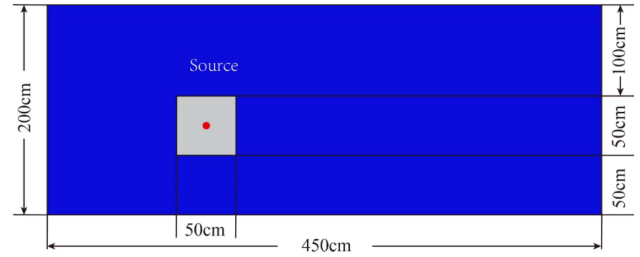
To save memory consumption, the functionality of building a hybrid CSG-UM model was developed in NECP-MCX V2.0. The CSG model and the UM model are built separately by the user and then the UM model is inserted into the CSG model. In particle tracking, the UM is predominant over the CSG, which means that the users do not need to treat the boundary between the CSG and the UM carefully. In this way, the complex components are defined by the UM and the relatively simple components are defined by the CSG, which is much more memory-saving than defining the whole problem by the UM. The flux distribution of the light water reactor (LWR) pool benchmark [13] is given in Figure 1.

3 Hybrid Monte-Carlo-Deterministic method

The Consistent Adjoint Driven Importance Sampling (CADIS) method [14,15] and the Forward-Weighted CADIS (FW-CADIS) [16] were implemented in NECP-MCX V1.0 for automatic variance reduction in simulating deep-penetration radiation shielding problems. For large radiation shielding problems, the number of weight window meshes and the memory consumption will be large. Therefore, a mesh coarsening method based on contribution theory in order to merge the mesh bins with low contributions was implemented [17]. This method can automatically reduce the mesh number and the group number of the weight window.



(a)



(b)

Fig. 2. Geometry of the labyrinthine problem [18]. (a) XZ plane at $Y = 75$ cm. (b) XY plane at $Z = 0.01$ cm.

In NECP-MCX V2.0, to promote the Figure of Merit (FOM) of the CADIS method, the CADIS method was combined with the Next Event Estimator (NEE) and the deterministic transport (DXTRAN) [18]. The CADIS-NEE method performs well in long-distance neutron/photon-transport problems. For the labyrinthine problem as shown in Figure 2 the FOM of CADIS-DXTRAN is about 312.3 times of DXTRAN and 3.3 times of CADIS. The FOM of CADIS-NEE is about 304.8 times of NEE and 3.5 times of CADIS [18].

The CADIS and FW-CADIS were also implemented based on the newly developed UM geometry capability [12]. The deterministic code used is NECP-SUN, which is an in-house SN-discontinuous finite element method (DFEM) code developed by NECP Lab. of Xi'an Jiaotong University. In the UM-based CADIS/FW-CADIS method, the SN-DFEM code, the Monte-Carlo geometry, the Monte-Carlo weight window and the Monte-Carlo source description share the same set of UM. The preliminary results show that the FOM of the UM-based CADIS/FW-CADIS is higher than that of CSG-based CADIS/FW-CADIS [12].

4 Dose engine for BNCT

NECP-MCX V2.0 introduces the function of dose calculation in BNCT. This is the first attempt to apply the code to radiotherapy. Boron Neutron Capture Therapy (BNCT) is a new type of radiotherapy method [19]. This treatment modality utilizes neutrons to eradicate tumour cells enriched with boron-10 which leverages the property of the large reaction cross-section of boron-10 and neutrons. In the treatment planning process, an accurate and efficient dose calculation is necessary [20]. Due to the intricate reaction mechanisms between neutrons and target nuclei, the Monte Carlo particle transport method is commonly employed for neutron transport calculations [21].

When applied to the BNCT treatment planning, the Monte-Carlo neutron transport method needs to overcome several challenges: 1) it requires the capability to handle medical image models which are different from CSG models. The medical image models consist of numerous small units, significantly impacting computation speed and memory; 2) sufficiently fast computation speed is needed to ensure completion of treatment planning within an hour; 3) it should be able to perform calculations under single-node parallel conditions, avoiding the use of excessively large-scale supercomputing resources. To address the aforementioned challenges, NECP-MCX has introduced several new features, resulting in a version specifically designed for BNCT treatment planning systems.

Firstly, a new modelling method which differs from CSG (constructive solid geometry) was developed in NECP-MCX. This method automatically calculates the composition and proportions of materials and elements based on the CT images. The binary-weighted interpolation method was employed to establish material libraries at different levels of detail. Based on this method, a pixel-level acceleration model was generated, aiming to preserve the authenticity of the model's geometry and materials to get an accurate dose result in the later calculation.

Secondly, a new track tracing algorithm was proposed to improve the computational efficiency. In the traditional Monte Carlo methods, surface crossing calculations consume a significant amount of time. It is approximately 80% of the total transport time [22]. The model in the BNCT process is a structured voxel geometry with a lot of voxel bins. This type of model requires a large number of surface crossing calculations in the traditional CSG model process approaches, which leads to low computational efficiency. The new track tracing algorithm takes advantage of the regularity of voxel grids, eliminating the need for per-grid calculations and significantly reducing computational time for geometric calculations. Meanwhile, a new tally strategy was applied in the code, which can get the track length in the corresponding voxel bins during surface crossing calculations. Therefore, tallies can be performed directly without additional judging processes, thereby saving time during the tally.

Third, a batch-based parallel method was applied [23]. In the parallel calculation of the traditional Monte-Carlo transport algorithm, the statistical quantities need to be communicated and summed across the CPU cores for each calculation batch. For the BNCT model with millions of

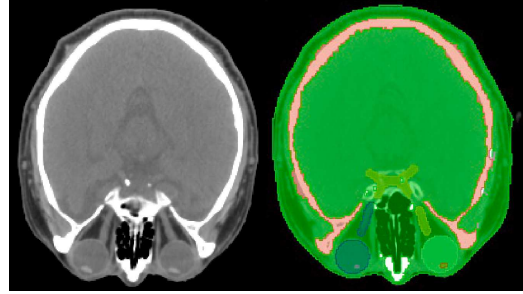


Fig. 3. The CT image and the model slice of the head.

voxel bins, the summation process takes a long time of CPU communication, while a sufficient number of batches is necessary to obtain accurate statistical deviations. To address this issue, a batch-based MPI parallel strategy was applied. In this strategy, each core maintains a set of statistical quantities, which means a whole batch is performed in one core without communication with other cores. After all the batch computations are completed, inter-core communication is performed to sum up the statistical quantities across cores, yielding the total statistical quantities for calculating the results and the corresponding statistical deviations.

To verify the function of dose calculation in BNCT treatment planning, a head phantom is chosen to be the target model. The CT image of the phantom is shown in Figure 3.

The voxel grid consists of $512 \times 512 \times 110$ units, with each unit measuring $0.9766\text{mm} \times 0.9766\text{mm} \times 2.5\text{mm}$ in size. The ROI is contoured by the doctor and shown in the right part.

The neutron beam is set from the upside of the head, the parameter of the neutron is from the Snyder benchmark [24]. It is a generic epithermal neutron beam with 1% fast neutron flux contamination (10 keV to 2 MeV) and 10% thermal flux contamination (1 MeV to 0.5 eV).

The calculation was performed both with NECP-MCX and PHITS. PHITS is a Monte Carlo Particle and Heavy Ion Transport code System developed in Japan [25]. The PHITS has been widely recognized and accepted in the industry for its significant applications in the field of BNCT.

The dose-depth length curve from top to bottom is shown in Figure 4. It shows that the results of NECP-MCX agree well with PHITS.

The total dose difference between MCX and PHITS of one slice is shown in Figure 5, the largest difference between the two codes is 2.49%.

5 Neutron noise analysis

Neutron noise signals from the reactor core contain valuable information about the operation and the maintenance of reactor core. Neutron noise analysis is a very promising technique for the next generation's non-invasive reactor core online monitoring system.

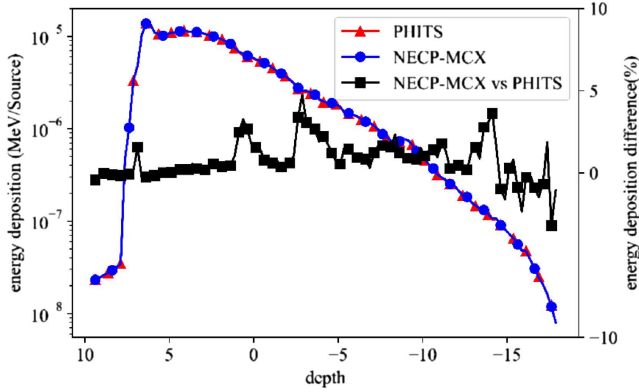


Fig. 4. The dose-depth length curve.

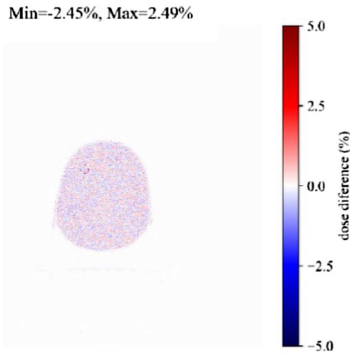


Fig. 5. The total dose difference between NECP-MCX and PHITS of one slice.

Neutron noise calculation has been realized in the NECP-MCX code, including both the traditional direct approach with Rouchon's pseudocross-section method [26] and the novel K-S iteration Monte-Carlo method. The noise source can be defined manually by the user or tallied on mesh during the static calculation for the oscillation-type noise source. The functionality of supporting various noise sources and other functions is under active development.

Traditional neutron noise calculation methods consider the neutron noise problem as a fixed-source problem with fissionable materials, which makes it necessary to simulate all particle histories including tremendous fission particles until no more fission particle is created. The K-S iteration method was originally issued by Raslach and Korobeinikov in 1998 [27] on the deterministic approach, and then integrated into the Monte-Carlo algorithm by Zheng's research on the ADS (Accelerator-Driven Subcritical) system. The K-S iteration method was introduced in the Monte-Carlo method.

Previous works indicated that the K-S iteration has better performance for problems in the subcritical system with external sources [27,28]. The K-S iteration in the Monte Carlo method avoids direct simulation of all particle histories and instead uses an iterative scheme to converge to the final result.

The new Monte-Carlo K-S iteration method was introduced in neutron noise calculation in NECP-MCX. It pro-

vides an iterative scheme for neutron noise calculation, which has shown a better balance of the relative standard deviation between the real part and the imaginary part, and great potential for the acceleration of its convergence.

6 Sensitivity analysis

NECP-MCX V2.0 is capable of calculating sensitivity coefficients of k -eigenvalue [29] and reaction rate ratios [30] to the continuous-energy nuclear data. Currently, cross sections, average neutron yield per fission ν , fission spectrum χ , and Legendre moments of scattering angular distributions [31] are supported for sensitivity analysis. Iterated Fission Probability (IFP) and Contribution-Linked eigenvalue sensitivity/Uncertainty estimation via Track-length importance Characterization (CLUTCH) methods were implemented for the k -eigenvalue sensitivity calculation. Generalized Adjoint Responses in Monte Carlo (GEAR-MC) method including CLUTCH-IFP and CLUTCH-only methods were implemented for generalized sensitivity analysis of reaction rate ratios.

The IFP method is usually encountered with the problem of huge memory usage. To address this problem, the sparse matrix technique and the data decomposition method were implemented in NECP-MCX V2.0 [32]. The sparse matrix technique was used in storing the array of reaction rate scores, which contains a large number of zero values. It turns out that the non-zero values in the reaction rate array only account for $\sim 15\%$ of 44-group energy structure tallies for the Vera 1b problem. Therefore, the sparse matrix technique can reduce nearly 70% usage of memory because the indices of non-zero values need to be stored in addition to the non-zero values themselves. The data decomposition method was used to reduce the memory usage of the IFP method further by distributing data storage of an array of reaction rate scores to different nodes in parallel computing.

Another drawback of the IFP and CLUTCH methods lies in their large variance of sensitivity coefficients of scattering reactions with relatively small cross sections. This is caused by the fact that the scattering term in sensitivity coefficient is tallied based on an analogue estimator and scattering reactions with small cross sections are less likely to happen during one collision, causing large variance of sensitivity coefficients of these reactions. Therefore, the CLUTCH method coupled with forced collisions (CLUTCH-FC) [31] was proposed to increase the occurrence of specific reactions and reduce the variance of sensitivity coefficients of these reactions further. For more practical applications, forced collisions are conducted with multiple scattering reactions simultaneously during one collision. The flow diagram of the forced collision method is shown in Figure 6. The numerical results show that the FOM value of the ^{56}Fe - σ_{inel} reaction calculated by the CLUTCH-FC method can even increase by a factor of 596.29 than that of the CLUTCH method for TMI-1 fuel pin problem in k -eigenvalue sensitivity analysis and a factor of 481.42 in generalized sensitivity analysis. Thus, the newly proposed CLUTCH-FC method is efficient in improving the tally efficiency of sensitivity coefficients of

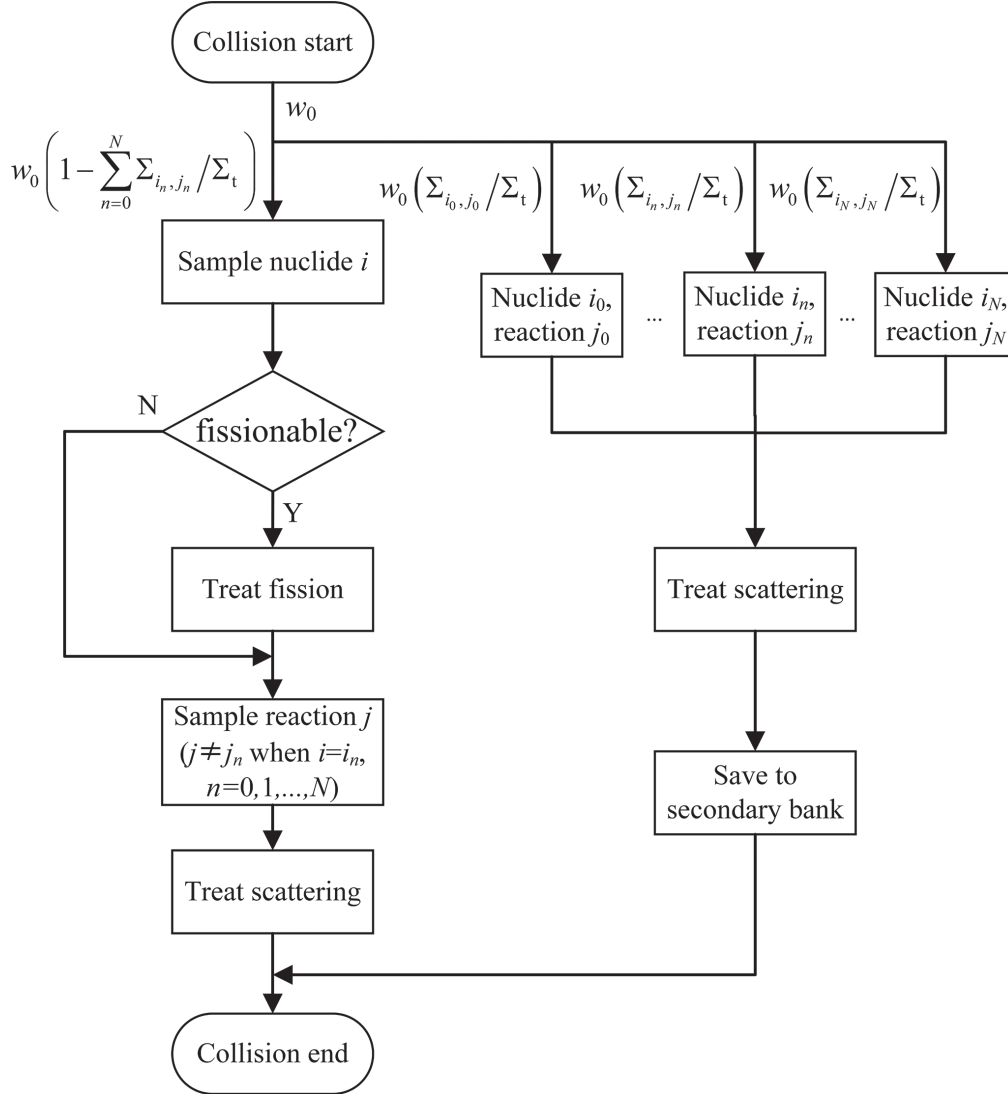


Fig. 6. The flow diagram of the forced collision method from reference [29].

scattering reactions with relatively small cross sections for both k-eigenvalue sensitivity analysis and generalized sensitivity analysis.

7 Depletion and activation calculation

An inhouse depletion/activation solver NECP-Erica [33] developed by NECP Lab. of Xi'an Jiaotong University was coupled internally with NECP-MCX V2.0 for particle-transport-depletion/activation coupling calculation [34]. The “in-memory” data-transfer pattern rather than the pattern of writing and reading external files is adopted to promote the data-transfer efficiency. In the particle-transport-depletion/activation coupling calculation, the predictor-corrector method is used.

The functionality of source-term analysis, including activity calculation, decay-heat calculation and decay-photon source calculation was also developed. Based on

the distribution of the decay-photon source obtained by the source-term analysis, the shut-down dose rate (SDDR) can be obtained with photon-transport calculation.

The capability of depletion/activation calculation was verified based on the natural-Fe activation benchmark [35] and the FNG-dose benchmark [36]. The results of these two benchmarks are given in reference [34]. For the natural-Fe activation benchmark, the atom densities of different isotopes agree well with those obtained by FISPACT-2007. For the FNG-dose benchmark, the errors of the SDDR calculated by NECP-MCX are within 10% compared with the experimental SDDR. The SDDR of the Chinese Fusion Engineering Test Reactor (CFETR) was analyzed by NECP-MCX with the depletion/activation calculation capability. The spatial distribution of the SDDR of CFETR at the shut-down duration of 1 month obtained by NECP-MCX is shown in Figure 7.

The capability of depletion and activation calculation was implemented based on the CSG.

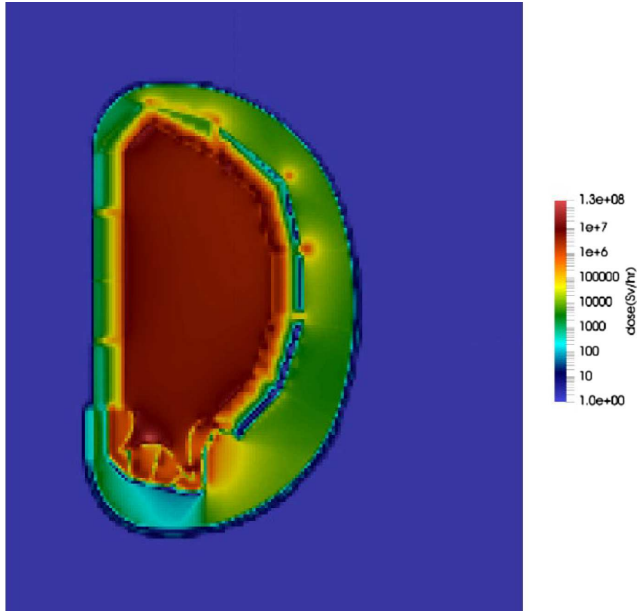


Fig. 7. Spatial distribution of the SDDR of CFETR at the shut-down duration of 1 month [34].

8 Simulation of randomly-dispersed media

The Pebble-Bed type High-Temperature Gas-Cooled Reactor (PB-HTGR) [37] is one of the most promising types of next-generation reactors. The TRI-structural ISOTropic (TRISO) fuel particles are adopted in the PB-HTGR. In the PB-HTGR, the core region is filled with many randomly distributed fuel pebbles and each fuel pebble consists of the graphite matrix where tens of thousands of TRISO fuel particles are filled randomly. In recent research, PWR can be loaded with Fully Ceramic Micro-encapsulated (FCM) fuel to promote safety. In the FCM, the TRISO particles are also randomly distributed.

To simulate the randomly dispersed media, including the fuel pebble and TRISO particles, Several methods, including the regular lattice method, the perturbed lattice method, the chord length sampling method and the explicit modelling method, were developed for the randomly dispersed media simulation in NECP-MCX V2.0 [38]. There are assumptions made in the regular lattice method, the perturbed lattice method and the chord length sampling method. Therefore, the explicit modelling method, which models each randomly distributed TRISO particle explicitly, is usually adopted for the simulation of randomly dispersed media. Two algorithms named the random sequential addition (RSA) algorithm [39] and the Jodrey-Tory (JT) algorithm [40], are implemented in NECP-MCX V2.0 to generate such distribution. Therefore, the users of NECP-MCX V2.0 do not need to generate random distribution themselves.

This capability was verified based on the FCM pin-cell problem, fuel pebble filled with different numbers of TRISO particles and High-Temperature gas-cooled Reactor Pebble-bed Module (HTR-PM).

9 Homogenization

In reactor physics calculation, a two-step analysis is widely adopted. The first step is lattice physics calculation generally based on neutron-transport theory to generate homogenized cross sections. The second step is whole-core neutronics calculation generally based on diffusion theory.

Usually, the neutron-transport solver of lattice physics calculation is based on the deterministic method. However, multi-group approximation is usually made in the deterministic method, which will introduce errors in neutron-transport calculation. In NECP-MCX, the continuous-energy ACE-format nuclear data is used in NECP-MCX, which means that the resonance treatment, one of the main error sources of the deterministic method, is not needed. Therefore, the capability of generating homogenized crosssections was developed in NECP-MCX V2.0 [38].

The homogenized cross-section of different reaction types, the scattering matrix, the fission spectrum and the diffusion coefficients can be obtained by NECP-MCX V2.0. These cross-sections are verified based on HTR-PM and Hualong One reactor.

10 Gamma dose calculation based on point-kernel integral method

The calculation of the gamma radiation dose field is the basis of radiation protection and shielding design. The research on rapid gamma radiation field calculation method can provide effective technical support for radiation protection and radiation shielding design, which is critical to practical application such as decommissioning of nuclear facilities, nuclear waste disposal and equipment maintenance.

In the large-scale radiation shielding problem, the scene is often very complex, and the space is often very large. In some application scenarios, researchers and designers need to evaluate the gamma dose rapidly and neither Monte-Carlo method nor SN method could meet the demand.

Therefore, the capability of gamma dose calculation based on the point-kernel method was developed. The point-kernel integral method is a semi-empirical Green's function convolution method with high computational efficiency. This method is suitable for deep-penetration problems and problems with complex geometry and source. The disadvantage of the point-kernel integral method is that the scattering of particles cannot be accurately considered and the buildup factor needs to be used to correct the scattering. The accuracy of the method is lower than that of the Monte-Carlo method and the SN method.

The development of the point-kernel integral calculation is based on the existing key modules such as geometry, particle, transport, tally and user interface, which are well realized and fully functional. The code of point-kernel integral calculation belongs to the transport module.

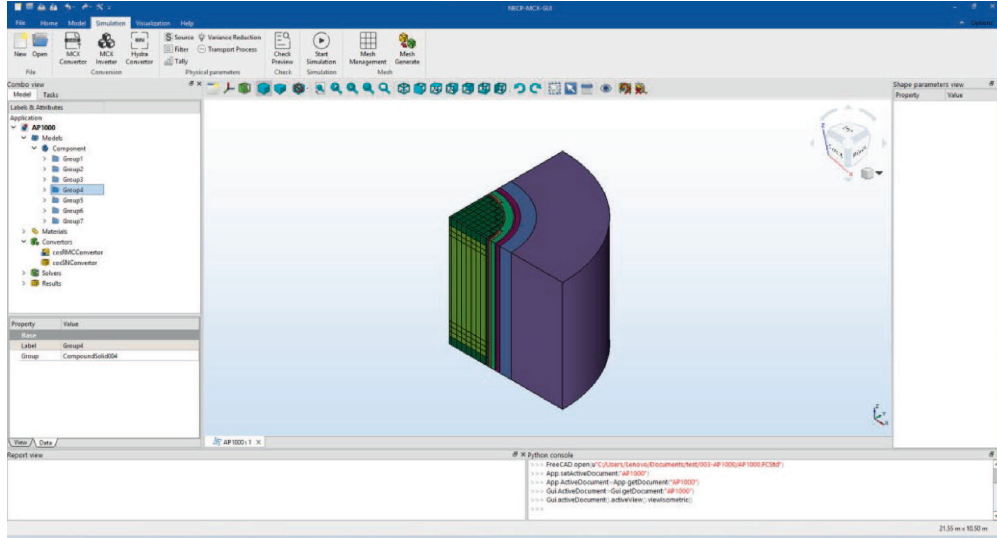


Fig. 8. User interface of NECP-MCX.

The source sampling method for point-kernel calculation is similar to that of Monte-Carlo fixed-source calculation. In point-kernel calculation, the space position (x, y, z) and energy E of the source particle will be sampled based on the source-sampling module of NECP-MCX.

The CSG module is used to calculate the position of particles, calculate the distance to the boundary and deal with the boundary conditions. The ray tracing function required by the point-kernel integral method is realized based on the CSG module.

There are two different parallel simulation flows of the point-kernel integral calculation.

The first is particle parallelism. In this case, the number of sampling particles is more than the number of parallel cores, which is generally the case for problems with volume radiation sources. In this case, the particles will be distributed equally to each core.

The second is mesh parallelism. In this case, the number of sampling particles is less than the number of parallel cores, which generally occurs when there is only a point source in the problem. As the point source only needs to be sampled once, the number of sampling particles is less than the number of parallel cores. In this case it is necessary to distribute meshes equally to each core.

11 User interface

To enhance the capability of NECP-MCX for complex 3D geometries and improve user-friendliness, we developed a graphical user interface (GUI) for NECP-MCX. The GUI is based on the CAD kernel Open CASCADE [41], with FreeCAD [42] serving as the graphical interface framework. The main interface is illustrated in Figure 6 and implemented using C++ and Qt5 coding. Currently, it is compatible with the Windows operating system and is planned for future expansion to multiple platforms.

Presently, the geometric modelling module supports basic body construction, material editing, and auxiliary modelling. The auxiliary modelling feature facilitates the essential CAD-CSG conversion. The physical modelling module enables the interactive setting of physical parameters required for NECP-MCX calculations, including Source, Filter, Tally, Options, etc. The numerical computation module supports the invocation of the NECP-MCX solver installed on the user's local machine to perform calculations. The user interface of NECP-MCX is shown in Figure 8.

12 Conclusion

The development of NECP-MCX started in 2018 from scratch with three developers. The first version of NECP-MCX is aimed at addressing the deep-penetration radiation shielding problem. In recent years, the development of NECP-MCX was driven by the demand of the users and the second version was released in 2024. Therefore, the unstructured-mesh geometry was developed for users familiar with CAD platforms to build complex models. The hybrid Monte-Carlo-Deterministic method was improved in the applications of NECP-MCX to different engineering problems. The geometry, the track tracing algorithm and the parallel algorithm were improved when applied to the BNCT treatment planning. The capabilities of neutron noise analysis and sensitivity analysis are developed for possible application in the future. The capability of the depletion and activation calculation was developed mainly for SDDR analysis of CFETR. The capabilities of randomly-dispersed media and homogenization were developed for the two-step reactor physics analysis of HTR-PM. The point-kernel integral method was developed for rapid gamma dose evaluation of nuclear power plant building. The user interface is still under active development to improve user-friendliness.

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Conflicts of interest

The authors declare that they have no competing interests to report.

Data availability statement

This article has no associated data generated and/or analyzed/Data associated with this article cannot be disclosed due to legal/ethical/other reasons.

Author contribution statement

Conceptualization, Qingming HE; methodology, Qi ZHENG, Jie LI, Zhanpeng HUANG, Jinlong HUANG, Shuai QIN, Hanlin SHU, Heyu PENG, Xuran YANG, Jingwen SHEN; software, Qingming HE, Qi ZHENG; formal analysis, Qingming HE; investigation, Qingming HE; resources, Hongchun WU, Liangzhi CAO; data curation, Qingming HE; writing—original draft preparation, Zhanpeng HUANG, Jinlong HUANG, Shuai QIN, Hanlin SHU, Heyu PENG, Xuran YANG, Jingwen SHEN, Jiandi GUO; writing—review and editing, Qingming HE; visualization, Qi ZHENG, Hanlin SHU, Jinwen SHEN; supervision, Liangzhi CAO, Hongchun WU; project administration, Qingming HE; funding acquisition, Hongchun WU, Liangzhi CAO. All authors have read and agreed to the published version of the manuscript.

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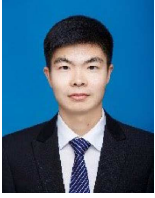
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