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CAD-based hierarchical geometry conversion method for modeling of fission reactor cores

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ABSTRACT

The fission reactor core models are usually constructed with abundant nested repeated-structure in several levels. Accordingly, hierarchical descriptions have been adopted in many Monte Carlo (MC) codes to describe fission reactor core efficiently. As the geometry of fission reactor core is more and more complex, modeling for them with some mature Computer-Aided Design (CAD) system becomes more popular. However, the conventional CAD-based MC automatic modeling methods concentrate on decomposing the complex geometries, whereas the hierarchical geometries are neglected. Furthermore, it is time consuming to decompose huge number of geometries in sequence. This paper presents a new method which can generate the hierarchical geometries for MC codes and CAD system in batches. The method can create or gather the hierarchical information as well as other parameters of the models into a dedicated data structure, which can be saved in Geometric Hierarchy Tree (GH-tree). Based on GH-tree, the MC calculation models and CAD models can be generated effectively and accurately. In this paper, the new algorithms were implemented based on the framework of the Super Monte Carlo Simulation Program for Nuclear and Radiation Process (SuperMC), developed by FDS team, and were validated using the models of China Lead-based Research Reactor (CLEAR-I) and IAEA-BN600. The efficiency and accuracy of the new method were demonstrated by the numerical calculation results.

1. Introduction

Over the last two decades, the need of Monte Carlo (MC) methods and its techniques for modeling complex systems are growing (Wu et al., 2014; Vaz, 2010; Cochet et al., 2014). Analytical modeling of complex system is tedious and error-prone (Wu and FDS Team, 2009a; Song et al., 2014). Consequently, many mature CAD-based MC modeling tools are developed to generate MC calculation models, which is actually a Boundary Representation (BREP) to Constructive Solid Geometry (CSG) conversion (Li et al., 2007), because many Monte Carlo codes (Forrest, 2005) uses CSG as their geometry representation system.

The fission reactor core consists of a few types of assemblies, i.e. fuel assembly, control assembly, shield assembly, etc., and each type of assembly is consist of a lattice of fuel rods, control rods and instruments with surrounded coolant (Jain and Tautges, 2014). The geometry of these basic parts has three common features: (1) the basic units of the geometry are easy to be represented by primitive solids; (2) the relationships of different units are rigorous; (3) the large scale geometries are repeated and nested in multiple levels. According to these features, the hierarchical geometries have been adopted in many MC codes to make the calculation model more concise and to accelerate the geometry navigation (Donovan and Tyburski, 2006; Geant4 Collaboration, 2009). For full-core MC transport simulation, modeling of whole reactor cores with millions reaction rate regions is a big challenge, such as the PWR core models proposed by Hoogenboom and William (2009) and BEAVRS benchmark released from MIT (Horelik and Herman, 2013). Furthermore, the optimization of core design and the criticality search need to modify the models frequently, however the MC calculation models always are text-based and not intuitive.

As known, few modeling programs have been developed focus on fission reactor core, among which stand out the Reactor Geometry and Mesh Generator (RGG) toolkit developed by Argonne National Laboratory (Jain and Tautges, 2014) and text-based templates of Serpent (Leppänen et al., 2014). The RGG can generate the whole core three-dimension (3D) model and meshes very quickly by employing an efficient parallel algorithm. However, the MC calculation model cannot be generated by it. The Serpent, which supports text-based templates for modeling the fission

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reactor core, can generate the calculation models conveniently. But the existing models such as CAD models and other MC calculation models cannot be reused and the geometrical complexity is limited by the template. Instead, modeling of the complex geometric structures such as the fission reactor core with mature CAD system will be more conveniently, if the CAD model can be converted into MC calculation model automatically. However, the conventional method (Wu and FDS Team, 2009a) should analysis each solid of the model one by one and decompose them into half-spaces. It usually focuses on the robust decomposition algorithm to the complex surfaces. However, it is not optimal for modeling fission reactor core with the reasons that the hierarchical information of the model cannot be reserved and the huge scale of repeated geometries is a big obstacle to program efficiency.

Consequently, a new CAD-based approach for generating BREP and CSG models of fission reactor core was studied and presented in this paper. The new method reaped huge fruits of the conventional conversion method, which can reuse the exiting CAD model and MC calculation model directly. However, the different is that the new method focuses on concluding the relationships of models and dividing them into corresponding groups in order for converting models in batches. Moreover, the hierarchical geometries were reserved by a dedicated data structure termed as Geometric Hierarchy Tree (GH-tree). The presented method was implemented and tested based on SuperMC which is a general purposed intelligent and multi-functional program for the design and analysis of nuclear system (Song et al., 2014; Sun and FDS Team, 2013). The modeling functional module of SuperMC, which was used widely in nuclear analysis (Qiu et al., 2000; Wu et al., 2011; Wu and FDS Team, 2007a–c, 2009b; Chen and Wu, 2000; Wu, 2002; Wu et al., 2000, 2002), can significantly reduce the manpower and enhance reliability for constructing calculation models of complex geometry (Wu and FDS Team, 2009a; Wu et al., 2013, 2014).

The main procedure and detailed algorithm of this method are presented in Section 2 describes. So for the applications of this method and the test results were demonstrated in Section 3. Finally, the discussion and conclusions were elaborated in Section 4.

2. CAD-based hierarchical geometry conversion method

2.1. Method procedure

The main procedure of CAD-based conversion of fission cores is shown in Fig. 1. The new CAD-based method is embedded into conversion core module which supports two types of conversions: (1) BREP model into CSG and (2) CSG into BREP model. The conversion of BREP model into CSG model generates MC calculation model automatically. In contrast, the conversion of CSG into BREP model can visualize the MC input file and support iterative modification with the two functional modules in GUI where the new BREP model can be created also.

Given the new CAD-based conversion method stands for the purpose of managing geometries in the ideal situation that unique geometric structure is only defined and stored once in memory (Lax et al., 2014), the "meta-geometry" concept is introduced and it is the unique geometry that should be described once, and other geometries can be represented by them with corresponding relationships.

The detailed process of the method is shown in Fig. 2. At the beginning, the fission reactor models with either BREP model or CSG model can be imported through GUI or created as a new model. Considering the BREP models are very intuitive, the meta-geometries can be assigned and the relationships can be built by user control easily. In contrast, the imported MC calculation models of fission reactors are invariably text-based and arduous to image their structures. However, the CSG geometries, physics parameters, hierarchical information and repeated structures of the MC calculation models can be identified and saved automatically based on the shared semantics adapter of SuperMC. In a word, after the fission models are imported or created by GUI, the method collects the parameters to construct a GH-tree for managing all parameters of the whole reactor models.

As shown in Fig. 2, the initial GH-tree should be judged whether it is simplest. According to the three features of fission reactor models, the geometries of them are convenient to be represented by primitive solids, such as cylinder, cube, sphere, hexagonal prisms etc. Because the simplest GH-tree should have the minimum number of meta-geometries and the most concise relationships, the half-space surfaces from decomposing the CAD models and MC calculation models are combined into primitive solids and some redundant nodes are deleted in the GH-tree data structure. In the simplest GH-tree, the creation of geometries can be started at the leaf cell nodes, and by means of the relationships such as Boolean operation, the filling hierarchy, "like-but" relation which describe one cell inherit the geometry of another one (X-5 Monte Carlo Team, 2003), the others geometries can be generated in batches. The generated models are regularly divided into many segments which are affiliated to different levels. The segments improve the flexibility of visualization and calculation, and the user can choose different parts in various precision of models conveniently. The user can observe the models in real time and judge the design if it has met the design requirement. Otherwise many auto modification functions are supported based on the visual models in 3D view and the new MC calculation models can be generated in anytime with the conversion of GH-tree to CSG models. Realistically, the user can't make the decision until they got the tallied results, such as the effective multiplication and the power distributions or the group constant etc.

2.2. Method of creating GH-tree

As shown in Fig. 1, GH-tree is the kernel data structure in the new conversion algorithm where all parameters of fission reactor core, including geometries, material, particle importance and other physics information, are grouped and saved.

First of all, an example is illustrated in Fig. 3 to describe the structure of GH-tree, which is divided into three levels. Universe X (UX) is the top root node of the tree, representing the fission reactor models with three regions, i.e. Cell 1 (C1), Cell 2 (C2) and Cell 3 (C3). The C1 is corresponding with the core region which is filled by the array of two types of assemblies (UY and UZ).

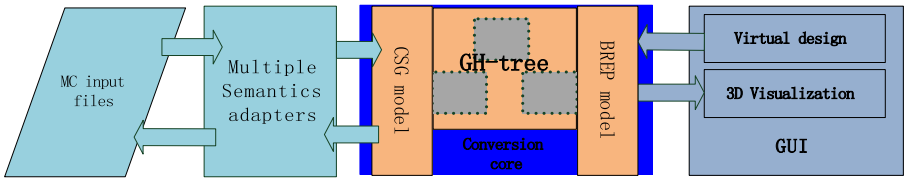


Fig. 1. Main procedure of CAD-based conversion of fission cores.

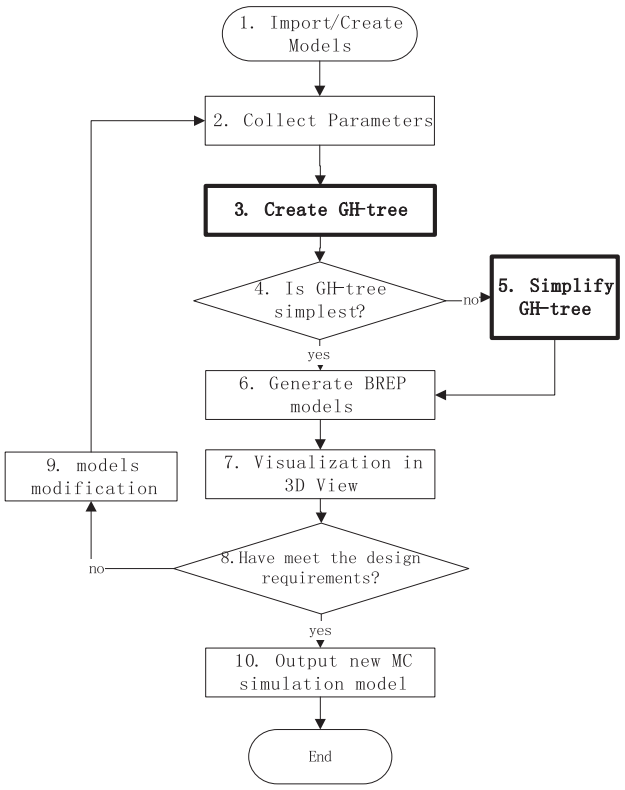


Fig. 2. Flow-chart of the new cad-based conversion.

C2 and C3 are filled by some other support components which can be ignored. Universe Y (UY) stands for fuel assembly, and Cell 4 (C4) is filled by the array of the fuel rod. Cell 5 (C5) is the fuel cladding region. The third level illustrates that the fuel rod is composed by Cell 7 (C7), and Cell 10 (C10) is another type of fuel rod region which inherits the geometry of C7. Cell 6 (C6) is a lattice cell also, which is filled by the array of UZX and UZY. And the Cell 8 (C8) and Cell 9(C9) are two material regions of UZX.

According to the Fig. 3, there are five kinds of nodes in GH-tree. The level node consists of the vector container of universes and the database of meta-geometries. One universe node corresponds to a whole component and regularly has more than one cell nodes. Obviously, one cell node represents a sub-component and always be a unique reaction rate region of the core whose boundary is limited by the meta-geometry quoted from the database. The relations are reserved by fill node or lattice node. In this example, the lattice of UY and UZ is described by the LAT0 node with a two-dimensional array. The FILL0 node which employ a transform vector and a rotation vector to control the position of filling UYX into C4. In the third level, C10 is similar as C7 and they use the same meta-geometry but the transform vector and rotation vector are different. Furthermore, the physics parameters can be related with a cell node, which are reserved by a map container that the index is the number of cell and the value is a class object of physics parameters. In general, one meta-geometry is constructed by a list of primitive solids or half-space surfaces with corresponding Boolean operators.

As shown in Fig. 2, there are two ways to create the GH-tree in different applications. First, for the case of importing the BREP models, after contributing the relationships through the GUI, the meta-geometries and relationships of the fission reactor are confirmed, then the sub-routine only needs to collect the parameters and generate the GH-Tree data structure.

The second method stands for an existing MC calculation model, such as MCNP (X-5 Monte Carlo Team, 2003). The method decomposes it into many basic cells which are described by several half-space surfaces or macro definition solids. The cells belonged to the same universe are set in one group to create a child GH-tree. The universe is the root node and cells are child node which is shown by Fig. 4. In addition, the universes which should be filled in a child cell become the leaf nodes. After subdividing all cells into different child trees, all of them are concatenated by the same universe node and distributed in corresponding levels with the filling relationships.

2.3. Simplification of GH-tree

After getting the initial GH-tree of the fission reactor model, the geometry of a cell is possibly still fragmental. As shown in Fig. 5, C1 node has cited four half-space surfaces from database. In order to reduce the number of meta-geometries and simplify the relationships, the sub-routine employs a two-step method that is depicted as follow.

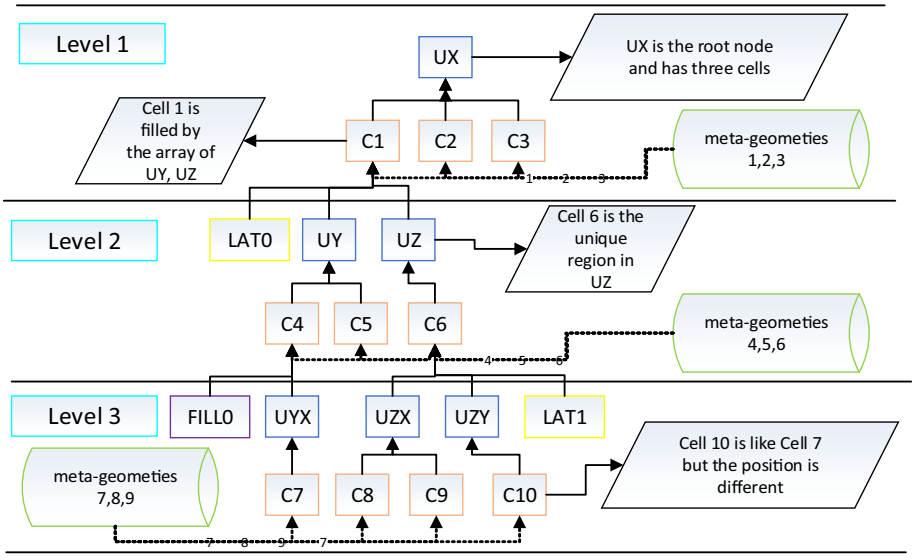


Fig. 3. The structure of GH-tree.

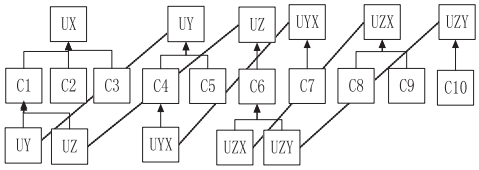


Fig. 4. The child data trees.

In the first step, in order to merge the GH-tree (illustrated in Fig. 5), the paths of GH-tree nodes are changed into several coverage paths, which are traversed by the routine to combine half-space surfaces. The paths are the routes from leaf cell nodes to the top cell nodes, where the universe nodes are all ignored. The detailed combination approach is conceptualized in Fig. 6 and there are three branched paths going to be traversed. In term of considering Cell 3 (C3) and Cell 6 (C6) inherit geometries from C2 and C4 respectively, the routine recognizes that the path 1 is the same as path 3 which shares a same result. Obviously, there are partially overlapping between the path 2 and path 1, the actual executive route and the final results are shown in Fig. 6. In conclusion, the whole processes can be assumed as a finite-state machine, because the types of primitive solid are severely limited and the all situations are predefined such as a plane just combine with another parallel plane, and two couples of parallel planes are combined together which are perpendicular to each other. In spite of the process of combination depending on specific application, the logic of combining operations is finite and the final result is unique.

Afterward the GH-tree has been changed by geometric combinations and the minimum meta-geometries have been confirmed, the relations should be reconstructed in the second step. For high-fidelity simulation, the model is extremely meticulous, where the large-scale of cells is hard to be managed in one group. However, excessive invalid subdivision is inevitable. For my own perspective, it is reasonable for dividing the models into different levels by the relationship of lattice filling, because the fission core is always divided as "Pin → Assembly → Core" three levels, among which the upper level is constructed by the array of components in the lower level.

So the simplification method of the relationship is elaborated as follow:

Giving a relationship which is a part of GH-tree as follow, C0 and C1 both are cell nodes, U1 and U2 are universe nodes, the three "→" are the filling relations:

$$C0 \rightarrow U1 \rightarrow C1 \rightarrow U2 \tag{1}$$

If C1 is not filled by an array of U1, then delete U1, the relationship changes to the follow:

$$C0 \rightarrow C1 \rightarrow U2 \tag{2}$$

In relations (2), C1 is filled by C0, the filling operation can be divided in two Boolean operations. The sign "−" represents Boolean subtraction and the "∪" represents Boolean union and be described by the equation as:

$$C0 \rightarrow C1 = (C1 - C0) \cup C0 \tag{3}$$

In GH-tree, C0 and C1 are two cell nodes which have been related with two meta-geometries and two class objects of physics parameters. The collection $\mathbf{S_0}$ and $\mathbf{S_1}$ are the lists of primitive solids in the meta-geometries. The physics parameters of C0 and C1 can be represented by $\mathbf{P_0}$ and $\mathbf{P_1}$ accordingly. As mentioned in Section 2.2, a cell node is related to physics information by a map container, Then:

$$C0 = \mathrm{map}\langle S_0, P_0\rangle \tag{4}$$

$$C1 = \mathrm{map}\langle S_1, P_1\rangle \tag{5}$$

If $\mathbf{P_1 = 0}$, C1 is a void space, then:

$$C0 \rightarrow C1 = C0 \tag{6}$$

the relationships 1 can be replaced by:

$$C0 \rightarrow U2 \tag{7}$$

Otherwise $\mathbf{P_1 != 0}$, supposing $\mathbf{S_0}$ is a $1 \times m$ matrix that represents m solids, and $\mathbf{S_1}$ is a $1 \times n$ matrix, then:

$$S_0 = (a_1, a_2, a_3 \ldots a_m) \tag{8}$$

$$S_1 = (b_1, b_2, b_3 \ldots b_n) \tag{9}$$

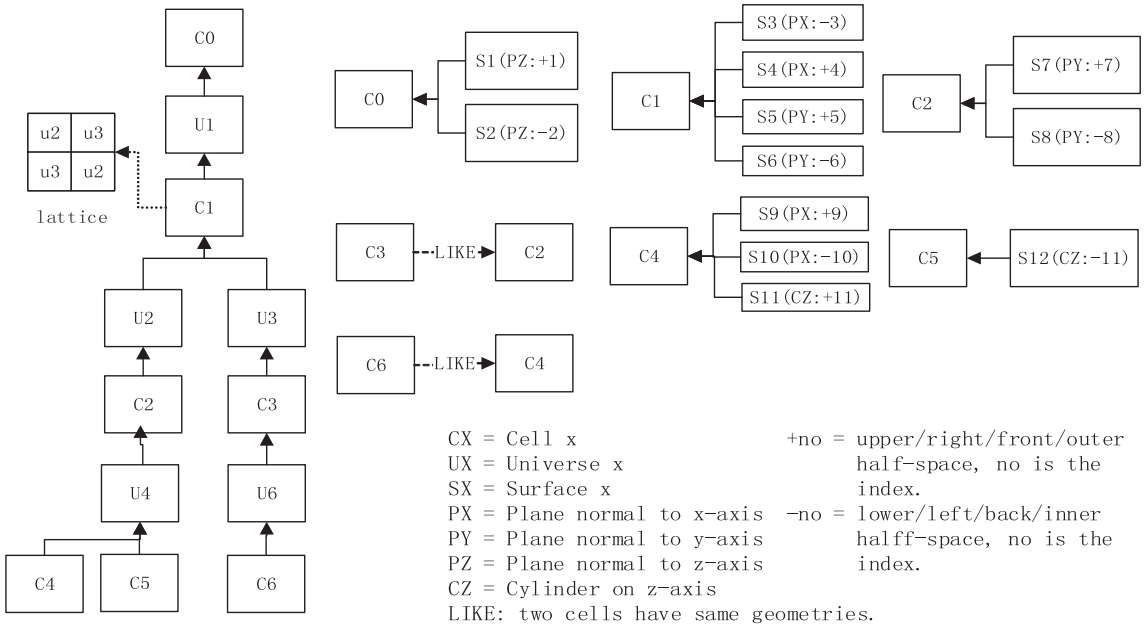


Fig. 5. An initial GH-tree and the fragmental surfaces distributions.

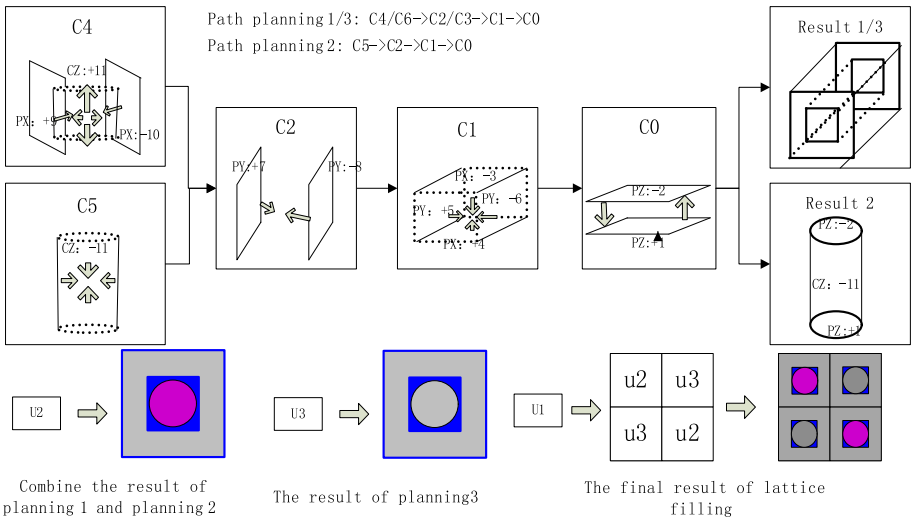


Fig. 6. The processes of combination.

Obviously, Boolean subtraction operations between two solids collections should make each elements from first collection subtract the all solids in the second one. Furthermore, it is clearly that the left region after subtraction belong to C1, so the new region should be related with the physics parameters from C1 to build a new cell which is represented by the character $\mathbf{C1_{new}}$. Then:

$$C1 - C0 = \mathrm{map}\left\langle \left(S_1^T \ldots S_1^T\right)_{n\times m} - (S_0 \ldots S_0)_{n\times m}^T, P1 \right\rangle = C1_{new} \quad (10)$$

According to Eq. (3), the relation can be described as:

$$C0 \rightarrow C1 = C1_{new} \cup C0 \quad (11)$$

As the consequence of Eq. (11), the relationships 1 can be replaced by

$$C0 \rightarrow C1 \rightarrow U2 = C1_{new} \cup C0 \rightarrow U2 \quad (12)$$

The final path in the GH-tree will be replaced as follow:

$$\begin{matrix} C1_{new} \\ C0 \end{matrix} \rightarrow U2 \quad (13)$$

3. Applications and tests

3.1. Modeling of CLEAR-IA

CLEAR-IA was one of the conceptual designs of China Lead-based Research Reactor (Wu and FDS Team, 2014). The three-dimensional CAD model of CLEAR-IA was built with SuperMC as shown in Fig. 7. The different colors represented different materials and components. Taking advantage of the GUI, a user could modify any assembly in the models such as changing the position of a control rod and the configuration of fuel assemblies, or modifying the thickness of shield etc. Based on the new CAD-based method, the CAD model could be transformed very quickly into MC calculation models in repeated-structure format. The comparison of two calculation results for different simulation models including K_{eff} value and the neutron flux of three fuel assemblies (remarked in Fig. 7) was listed in Table 1. One model was generated by the new method and the other was generated by conventional method, both simulated with SuperMC code. According to the reference results with MCNP code, the new method got the closer results than the conventional method. The calculation models which generated by the new method was closer to the MCNP calculation models, because they both employed the repeated-structures and the basic solids which were equal to the macro define in MCNP to describe the geometry. As shown in Table 1, the deviations are compared with MCNP respectively and the statistical errors were unanimous among the three calculations.

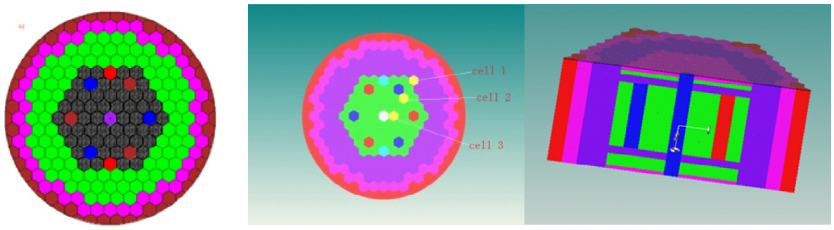
3.2. Modeling of BN600 model

BN600 model (IAEA-TECDOC-1623,2010) was developed by IAEA Coordinated Research Project (CRP), in order to reduce the calculation uncertainties of the LMFR reactivity effects.

In this case, an existing MCNP calculation model of BN600 was transformed into SuperMC calculation model with the two methods with personal computer (Intel(R) core Q9500 2.83 GHz) by two conversions which converted MCNP input file (CSG) into 3D CAD models (BREP) and then generated SuperMC calculation models (CSG). It took only 3 s with the new method, while the conventional method needed 900 s. The neutron fluxes in different cells were shown in Fig. 8. It was clear that the new method saved a lot of modeling time while ensuring the accuracy compared with conventional method and the reference results simulated by MCNP code. The SuperMC code had developed many methods to improve geometry navigation performance (Chen et al., 2015). Realistically, from the simplest GH-tree data structure, the calculation module of SuperMC could get the hierarchical relations and the lists of neighbors. Therefore, the new CAD-based method could generate the optimized models for SuperMC code and accelerate the geometry navigation. In this case, the runtime number of calculation models generated by the new method reduced 2 times compared with that for the model generated by the conventional method.

3.3. Analysis of results

Analyses of the conversion and calculation results were listed in Table 2, while the largest deviation statistics for neutron flux was lower than 0.43% compared with MCNP reference results. With the criticality computation, the particle trajectories were outputted. It was discovered that the deviations which always occurred in the hundreds cycle. By tracing the code, the deviations were triggered by some little truncation errors of geometries. The significance figures of CAD system were always 5 or 6, while these in the MC simulation were more than 13 or 14. However, the new CAD-based method significantly improved the conversion efficiency. Compared with the old method, the conversion time of CLEAR-IA was reduced by 95%, while the BN600 models was



Reference models The visualization of CLEAR-1A in SuperMC/MCAM

Fig. 7. The CLEAR-IA reference model visualized with MCNP plot and the CAD model which is built by SuperMC/MCAM.

Table 1
The calculation results by the models generated by the conventional method and new CAD-based method.

Models	Reference results by MCNP	The conventional modeling method		The new CAD-based modeling method		Statistical error (%)
		Result	Deviation (%)	Result	Deviation (%)	MCNP/SuperMC
K_{eff}	1.0001	0.9999	−0.02	1.0002	+0.01	0.025
Assembly	Neutron flux (1/(cm^2 s))					
Cell-1	1.0377	1.0374	−0.02	1.0377	0	0.02
Cell-2	6.9231	6.9344	+0.16	6.9303	+0.1	0.14
Cell-3	9.6670	9.6494	−0.18	9.6682	+0.01	0.23

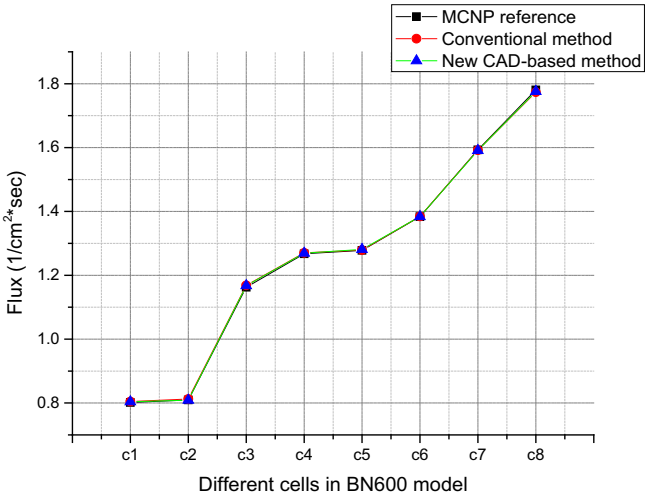


Fig. 8. Neutron fluxes of fuel assemblies in BN600 models.

Table 2
Comparison of the new method with the conventional method.

	Applications	Conversion runtime (s)	Calculation runtime (min)	Conversion memory consumption (MB)
Conventional method	CLEAR-1A	201	234.62	300
	BN600	900	804.79	800
New CAD-based method	CLEAR-1A	10	123.97	58
	BN600	3	443.86	60

reduced by 99.7% because of the fewer number of its meta-geometries than CLEAR-IA had, and the reduction of memory consume were extremely promising. Furthermore, with the case of 10,000 particles, 500 cycles criticality computation, the runtime of the models generated by new method got a remarkable fall with the reason of the calculation model generated by the new method was much simpler and could be directly applied in many algorithms for accelerating geometry navigation.

4. Discussion and conclusions

In this paper, a CAD-based hierarchical geometry conversion method for fission reactor core modeling was presented. This new method could create 3D CAD models and MC calculation models along with the hierarchical information during the conversion between BREP models and CSG models. Furthermore, a special kernel data-structure named GH-tree and a new concept termed meta-geometry were introduced. Based on them, the models could be generated in batches, and be managed in different segments. The new method was verified by CLEAR-IA and BN600 model. The calculation results shown that the new method improved the conversion efficiency up to 300 times and still met the accuracy requirement compared with these of conventional method. Moreover, the calculation model generated by the new method could be used by the calculation module directly even reached much higher performance. However, the method could not recognize the meta-geometries and the relations from CAD models automatically (if the relations were not exited in these CAD models), then the users should establish them manually. And the semantics of some MC codes were extremely complex, which made the semantics adaptor trigger insidious bugs more or less. In the future, a rapid similarity judgment and relation recognition algorithm will be applied in converting the CAD models, and the semantics adaptor will be more intelligent by keeping tests. Then the method will be applied in more complicated reactor core design such as ADS-CLEAR series reactors (Wu et al., 2016) or FDS series reactors (Wu and FDS Team, 2006, 2008; Wu et al., 2006), and more virtual design functions will be studied.

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