Annals of Nuclear Energy 87 (2016) 162–166

Contents lists available at ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

CAD-based Monte Carlo automatic modeling method based on primitive solid

Dong Wang [a,b], Jing Song [a], Shengpeng Yu [a], Pengcheng Long [a], Yongliang Wang [a,*]

[a] Key Laboratory of Neutronics and Radiation Safety, Institute of Nuclear Energy Safety Technology, Chinese Academy of Sciences, Hefei, Anhui 230031, China
[b] University of Science and Technology of China, Hefei, Anhui 230026, China

ARTICLE INFO

Article history:
Received 12 March 2015
Received in revised form 23 July 2015
Accepted 24 July 2015
Available online 10 September 2015

Keywords:
Primitive solid
CAD
Monte Carlo
SuperMC
Automatic modeling

ABSTRACT

Monte Carlo method has been widely used in nuclear design and analysis, where geometries are described with primitive solids. However, it is time consuming and error prone to describe a primitive solid geometry, especially for a complicated model. To reuse the abundant existed CAD models and conveniently model with CAD modeling tools, an automatic modeling method for accurate prompt modeling between CAD model and primitive solid is needed. An automatic modeling method for Monte Carlo geometry described by primitive solid was developed which could bi-convert between CAD model and Monte Carlo geometry represented by primitive solids. While converting from CAD model to primitive solid model, the CAD model was decomposed into several convex solid sets, and then corresponding primitive solids were generated and exported. While converting from primitive solid model to the CAD model, the basic primitive solids were created and related operation was done. This method was integrated in the SuperMC and was benchmarked with ITER benchmark model. The correctness and efficiency of this method were demonstrated.

1. Introduction

In nuclear particle transport simulation, Monte Carlo method has been widely used. The geometry model which should be prepared before simulation can be described in several methods: half space (Briesmeister, 2000; Martz, 2013; Both et al., 2003; Fasso, 2005), primitive solid (Agostinelli et al., 2003; Yican et al., 2015; Song et al., 2014), mesh (Martz, 2013; Agostinelli et al., 2003), CAD model for directly transporting (Tautges et al., 2009), etc. With accurately modeling and intuitively understanding the model, the method mainly used in the Monte Carlo geometry definition is Constructive Solid Geometry method (CSG) (Requicha and Voelcker, 1982) which includes the half space method and the primitive solid method. The half space method constructs solid with half-space surfaces defined in mathematical equations and directions. The primitive solid method constructs solid with Boolean operation, position and rotation. Contract to the half space method, there are some benefits for using the primitive solid method, such as easy to handwrite and understand.

While describing, it is easy to establish a simple model which has less cells and less faces in each cell. But the situation was completely changed while establishing a complex model with many cells and many surfaces in each cell. It is hard to modeling manually which is time consuming and error prone. For reusing the abundant existed CAD model and convenient modeling with CAD modeling tools, an automatic modeling tool for accurate prompt modeling from CAD model is needed. Some previous researches (Grosse and Tsige-Tamirat, 2009; Nasif et al., 2012) of automatic modeling for Monte Carlo simulation had been studied, but most of them focused on half space model. In this paper a newly automatic modeling method for primitive solids was researched for the need of rapid development and various applications of Monte Carlo simulation.

The key conversion of the CAD model and a primitive solid model is the conversion between the boundary representation method (Braid, 1975) and the primitive solid method. The previous research into conversion from CAD model to a half space model is decomposing the CAD model to a convex solid set, and translate to half space geometry according to the boundary surfaces of the convex solids. While converting the CAD model to primitive solid model, the primitive solid can be created according to the boundary surface of the convex solid. While converting primitive solid model to CAD model, it is similar that creating of basic solid to the method of half space but different with movement and rotation.

* Corresponding author at: Key Laboratory of Neutronics and Radiation Safety, Institute of Nuclear Energy Safety Technology, Chinese Academy of Sciences, Hefei, Anhui 230031, China.
E-mail address: yongliang.wang@fds.org.cn (Y. Wang).

http://dx.doi.org/10.1016/j.anucene.2015.07.041
0306-4549/

This method had been studied and integrated in the Super Monte Carlo Simulation Program for Nuclear and Radiation Process, named SuperMC. SuperMC was developed by FDS Team which is an interdisciplinary research team devoting to the research and development of advanced nuclear energy systems, mainly including nuclear reactor physics (Wu et al., 2009), nuclear reactor material (Wu et al., 2002; Wu, 2007; Wu and FDS Team, 2008), nuclear reactor engineering (Wu and FDS Team, 2008; Wu et al., 2011; Wu, 2007), numerical simulation and visualization (Wu et al., 1999; Wu and FDS Team, 2009), medical physics and environmental protection (Yican et al., 2008), etc. It is a CAD-based MC program for integrated simulation of nuclear system by making use of hybrid MC-deterministic method and advanced computer technologies. SuperMC 2.2, the latest version, can perform neutron, photon and coupled neutron and photon transport calculation and integrates automatic modeling and visualization (Wu and FDS Team, 2009; Wu et al., 2006; Hu et al., 2007; Long et al., 2010; Luo et al., 2010; Long et al., 2011; He et al., 2012; Tang et al., 2010). SuperMC/MCAM is the geometry and physics modeling part of SuperMC. Previous version SuperMC/MCAM 4.8 which modeling for MCNP was a mature and efficient modeling program which has been used widely (Li et al., 2007; Zheng et al., 2007; Huang et al., 2006; Lu et al., 2009).

In this paper, the conversion method was described in Section 2. Section 3 introduced the testing method and showed the results. At last, a brief summary was given in Section 4.

2. Conversion algorithm

2.1. CAD to primitive solid conversion

In SuperMC/MCAM, an automatic conversion method which converts CAD model to half space model was implemented. In this method which was based on the CAD model decomposing, a CAD model was imported and decomposed to several disjoint convex solid sets; and then the corresponding surface with direction was generated and transformed to a half space according to each surface of every convex solids. While creating surface based convex solid's surface, the equation of the surface and the direction would be record. Fig. 1 shows an example of a cube with a half cylinder. With this method, this solid would be decomposed into two convex models: a cube and a half cylinder. Then, these convex solids would be processed separately and each surface with its direction would be recorded, and saved in a half space format.

While converting to primitive solids, the improvement of the developing algorithm, which focused on the transform of surfaces of each convex solid, was done based on the above method. While processing a plane half space, a central point on the surface and the equation used to specify the half space would be given. And then the plane half space would be transform to XOY plane and the transform matrix would be recorded. At last a cube would be created and transformed by the inverse of transform matrix to make sure after the movement and rotation, the cube's top surface has the same equation and direction with the plane half space. While processing an inner cylindrical half space, some key parameters including the radius, cylindrical center point and axis would be given. And then a cylinder would be created based on some key parameters. While processing an outer cylindrical half space, some key parameters including the radius, cylindrical center point and axis would be given. And then a cylinder would be created based on some key parameters and a cube would be created with maximum length. Fig. 1 shows the processing of each surface. The processing of converting cone, sphere and torus was similar.

After these primitive solids were created, the Boolean relationships and the movement need to be recorded. The solid was posed at the center of the world after its creation from the half space, and

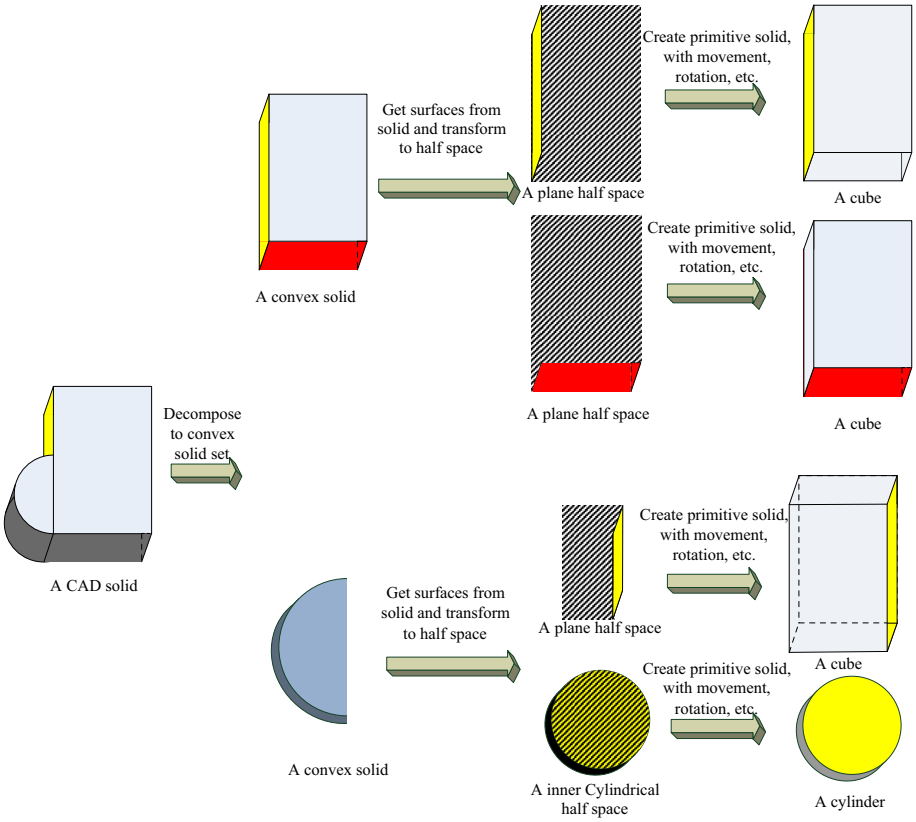

Fig. 1. The processing of each surface in convex solids.

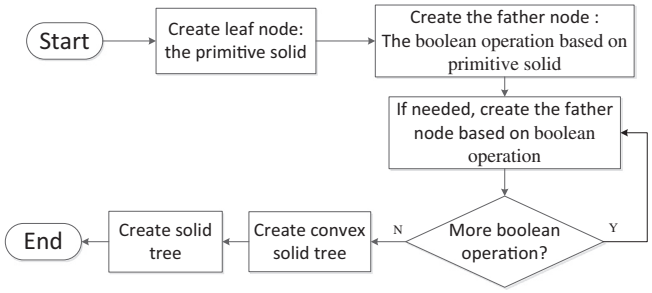

Fig. 2. Flowchart of establishing the geometry tree.

then needed to be moved and rotated according to the half space. Also, the relationships between these solid were recorded which would latter establish a geometry tree. This geometrical tree was established from bottom to top, from primitive solid to the whole model. The flowchart was shown in Fig. 2.

2.2. Primitive solid to CAD conversion

In SuperMC/MCAM, an automatic conversion method which converts half space model to CAD model was implemented. In this method, corresponding solids were created based the half space definition; and then each solid was generated by using the Boolean operation according to the definition of each solid; at last, these solids were output in CAD format.

The key difference between the conversion from half space and primitive solid was mainly in different description. A solid described in half space method was defined as the Boolean operation of several half spaces which were surface with direction, while the same solid described in primitive solid method was defined as the Boolean operation of several primitive solids with movement and rotation. So the key difference was surfaces with direction and solid with movement and rotation.

While processing the primitive solid method, the rotation especially the rotation of the Boolean operating solid must be concerned. To process rotation, procedure follows a sequence as: recording, transferring and operating. For it was hard to record every rotation after several Boolean operations, the rotation matrix was implemented in this research. In this study, the rotation in solid was defined as three rotation angles defined as α, β and γ while rotation axis was $X/Y/Z$ axis by sequence. The matrix was defined as following:

$$\mathrm{Matrix}_X = \begin{matrix} 1 & 0 & 0 \\ 0 & \cos\alpha & \sin\alpha \\ 0 & \sin\alpha & \cos\alpha \end{matrix} \quad (1)$$

$$\mathrm{Matrix}_Y = \begin{matrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ \sin\beta & 0 & \cos\beta \end{matrix} \quad (2)$$

$$\mathrm{Matrix}_Z = \begin{matrix} \cos\gamma & \sin\gamma & 0 \\ \sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{matrix} \quad (3)$$

And the rotation matrix of a primitive solid could be calculated:

$$\mathrm{Matrix}_{\mathrm{primitive}} = \mathrm{Matrix}_X * \mathrm{Matrix}_Y * \mathrm{Matrix}_Z \quad (4)$$

While Boolean operating, the rotation matrix of child solid which participating the Boolean operation should be transferred from the rotation matrix of the Boolean solid named father solid. The equation was as following:

$$\mathrm{Matrix}_{\mathrm{childsolid}} = \mathrm{Matrix}_{\mathrm{FatherSolid}} * \mathrm{Matrix}_{\mathrm{solid}} \quad (5)$$

$\mathrm{Matrix}_{\mathrm{FatherSolid}}$ was the rotation matrix of father solid, and $\mathrm{Matrix}_{\mathrm{child}}$ was the child solid's three axis rotation matrixes; $\mathrm{Matrix}_{\mathrm{childsolid}}$ was the rotation matrix of son solid.

While processing a solid's rotation based the rotation matrix, a rotation axis and the rotation angle was needed. To calculate the rotation axis and the rotation angle, a method which was described by pseudocode as following was implemented.

Pseudocode of get a rotation axis and the rotation angle from rotation matrix

```
// eigenvector of Matrix_Origin which has 3 × 3 elements.
Matrix = Matrix_Origin − | 1 0 0 |
                         | 0 1 0 |
                         | 0 0 1 |
// Simplified the Matrix
For element of each row in Matrix

  For element of each column in Matrix less than main diagonal
   element
    If element unequal to 0.0
      Every element in this row multiplies by first unequal to 0.0
      data in upper row;
      And then subtracts every element which multiplies this
      element in the upper row
    Else continue
    End if
  End For

End For

For element of each row in Matrix
  For element of each column in Matrix element more than main
diagonal element

    If element unequal to 0.0
      Every element in this row multiplies by first unequal to
      0.0 data in lower row;
      Subtract every element which multiplies this element in
      the lower row;
    Else continue
    End if

  End For

End For
// after the matrix had been simplified, calculated eigenvector
// Get the relationship of the three values in eigenvector from the
   simplified matrix
   EV = EigenVectorfromMatrix (Matrix)
   EV = Normalization (EV)
// end of eigenvector
// Get a vector which is perpendicular to eigenvector
   a = CalculateVerticalVector (EV)
   b = a * Matrix_Origin
   θ = arcos(a • b)    // |a| = 1, |b| = 1
// rotate solid with θ and Eigenvector
```

3. Testing

The method of conversion between CAD models and geometry of SuperMC models had been developed, and integrated in SuperMC as SuperMC conversion and inversion modules based on the module architecture of SuperMC. The SuperMC conversion module could convert CAD model to SuperMC input file, and the SuperMC inversion module could invert SuperMC input file to CAD model.

Abundant of models were chosen to validate this method. In this paper, the ITER (International Thermonuclear Experimental Reactor) benchmark model (Li et al., 2007) was chosen for verification. The CAD model was created by CATIA/V5 which was 40° of the whole model and has about 900 cells. As several surfaces were too difficult to directly converted, so some surfaces were cut to several slices and the number of cells were more than 3000 at last.

The visualization comparison of the ITER benchmark model in SuperMC/MCAM between original CAD model and the model inverted from SuperMC input file was taken to check correction generally. After visualization comparison, the volume of each cell in models was compared in order to obtain more persuasive evidence for the correctness of conversion method. Besides visualization and volume comparisons based on geometry, the physical simulation was also done to make sure the simulation used converted input file on SuperMC was as same as MCNP. So simulations with designed material were performed and the results were compared.

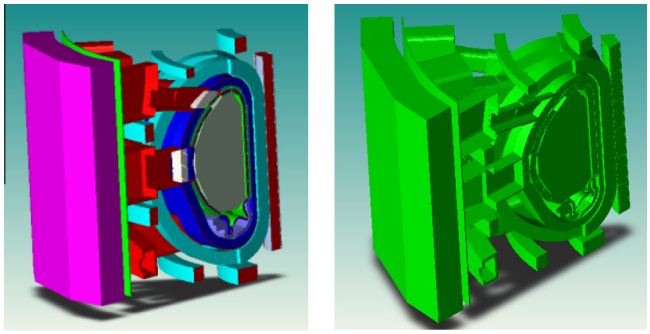

Fig. 3. Visualizations of ITER benchmark model. (a) Original CAD model in SuperMC/MCAM. (b) Model inverted from SuperMC input file in SuperMC/MCAM.

3.1. Visualization and volumes

When comparing the visualizations of the model, the CAD model of ITER benchmark model was imported to SuperMC/MCAM; and then, this model was convert into primitive solid model and then inverted to CAD model. The comparison of visualizations was shown in Fig. 3.

When comparing the volume of the model, the volumes of each cell in the CAD model and the model inverted from SuperMC model were calculated by SuperMC/MCAM. To make the results repeatable, the conversion and inversion were done repeatedly and three volume results were recorded. Fig. 4 shows the comparison of these results. The average relative error of each cell between CAD model and SuperMC model were less than 0.0000513%. The maximum relative error was about 0.0753%.

From Fig. 2, it shown that the shape of original CAD model and the model inverted from SuperMC input file agreed well. From Fig. 3, the average relative error of volume of original CAD model and the model inverted from SuperMC input file was less than 0.00005% although the maximum error was much big than the average. The average error was mainly because of computer's truncation error. And the maximum errors were mainly because some models were wrong converted because of computer's truncation error, for example cone which has very small angle would be converted to cylinder and gets the wrong volumes.

3.2. Neutron flux

After the comparison of visualizations and volumes of the model, preliminary simulation of ITER benchmark model was conducted and the neutron flux was calculated to make sure that the converted SuperMC input file was correct in the simulation. The comparison was between the SuperMC/MCAM converted MCNP input file with designed material and the SuperMC input file with designed material converted from CAD model. The source was a complicated plasma source, and about 67 parts of blanket which was cut to several cells were counted. Fig. 5 shows the comparison of MCNP and SuperMC results. The statics error was about 0.00091 while high than 0.0006 and low than 0.0017, which shows that the results agree to convergence. The average relative deviation of each cell between SuperMC and MCNP was about 6.71384E−06. The maximum relative deviation was less than 2.01104E−05.

From Fig. 5, the neutron flux of blanket in ITER benchmark model between MCNP and SuperMC was listed. The average

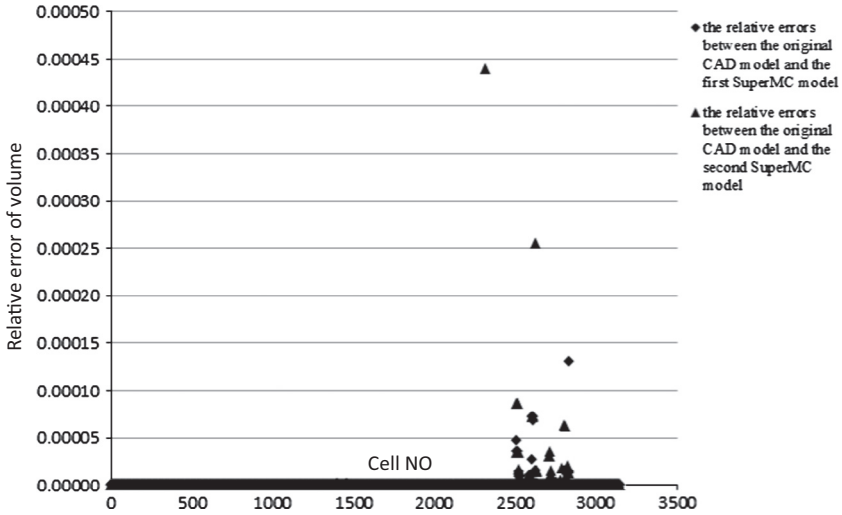

Fig. 4. Relative error of volume of each cell in ITER benchmark model between original CAD model and model inverted from SuperMC input file.

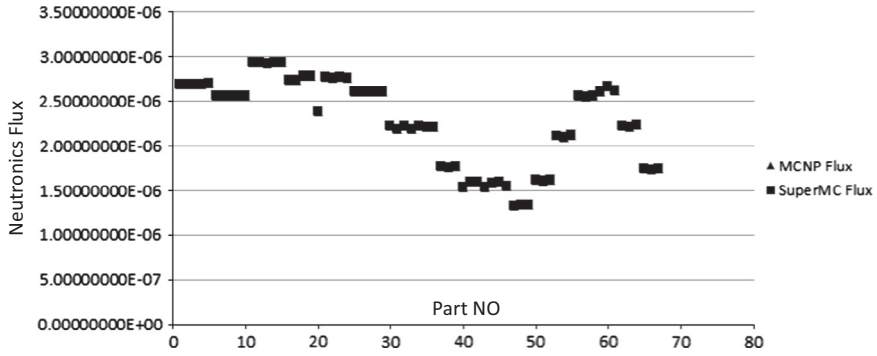

Fig. 5. Neutron flux of cell of blanket in ITER benchmark model between MCNP and SuperMC.

relative deviations were mainly because of the difference between Monte Carlo codes and proved that the converted SuperMC input file could be used in the simulation and agrees well with MCNP. All the test results showed that the conversion method was correct and efficient in the SuperMC simulation.

4. Summary

The method of bi-conversion between CAD models and the Monte Carlo geometry represented by primitive solids has been proposed and integrated in SuperMC/MCAM. The ITER benchmark model was chosen to test the validation, and the correctness and efficiency were demonstrated. Nuclear analysts can effectively and correctly model the Monte Carlo geometry represented by primitive solids to enhance the effectiveness of nuclear analysis for nuclear facilities by using this method.

Acknowledgements

This work was supported by the Strategic Priority Research Program of Chinese Academy of Sciences (No. XDA03040000), the National Natural Science Foundation of China (Nos. 11305205, 11305203 and 11405204), the National Special Program for ITER (No. 2014GB112001).

We would like to express our appreciation for the support of other members of the FDS Team in this work.

References

Agostinelli, S. et al., 2003. GEANT4—a simulation toolkit. Nucl. Instrum. Methods Phys. Res., Sect. A 506 (3), 250–303.

Both, J.P., Mazzolo, A., Peneliau, Y., Petit, O., Roesslinger, B., 2003. User manual for Version 4.3 of the TRIPOLI-4 Monte-Carlo method particle transport computer code.

Braid, I., 1975. The synthesis of solids bounded by many faces. Commun. ACM 18 (4), 209–216.

Briesmeister, J.F., 2000. MCNP – a general Monte Carlo N-particle transport code, Version 4C, LA-13709-M.

Ferrari, A., Sala, P.R., Fasso, A., Ranft, J., 2005. FLUKA: A Multi-particle Transport Code. Stanford Linear Accelerator Center, United States.

Grosse, D., Tsige-Tamirat, H., 2009. Current status of the CAD interface program McCad for MC particle transport calculations. In: Proceedings of International Conference on Mathematics, Computational Methods & Reactor Physics (M&C 2009). American Nuclear Society.

He, Tao, Long, Pengcheng, Zhou, Shaoheng, Zeng, Qin, Hu, Liqin, Wu, Yican, 2012. A method for 3D structured data sets regulation based on image. Recent Adv. Comput. Sci. Inf. Eng. Lect. Notes Electr. Eng. 126, 643–648.

Hu, H., Wu, Y., Chen, M., Zeng, Q., Ding, A., Zheng, S., Li, Y., Lu, L., Li, J., Long, P., FDS Team, 2007. Benchmarking of SNAM with the ITER 3D Model. Fusion Eng. Des. 82, 2867–2871.

Huang, Q., Zheng, S., Lu, L., Hiwatari, R., Asaoka, Y., Okano, K., Ogawa, Y., 2006. Neutronics analysis for a compact reversed shear tokamak CREST. Fusion Eng. Des. 81 (8–14), 1239–1244.

Li, Y., Lu, L., Ding, A., Hu, H., Zeng, Q., Zheng, S., Wu, Y., 2007. Benchmarking of MCAM 4.0 with the ITER 3D model. Fusion Eng. Des. 82 (15–24), 2861–2866.

Long, Pengcheng, Zeng, Qin, He, Tao, Zhang, Junjun, Ying, Dongchuan, Zhou, Shaoheng, Wu, Yican, 2011. Development of a geometry-coupled visual analysis system for MCNP. Prog. Nucl. Sci. Technol. 2, 280–283.

Long, Pengcheng, Zou, Jun, Huang, Shanqing, Qiu, Yuefeng, 2010. Development and application of SN auto-modeling Tool SNAM 2.1. Fusion Eng. Des. 85 (7–9), 1113–1116.

Lu, L., Lee, Y.K., Zhang, J.J., Li, Y., Zeng, Q., Wu, Y.C., 2009. Development of Monte Carlo automatic modeling functions of MCAM for TRIPOLI-ITER application. Nucl. Instrum. Methods Phys. Res., Sect. A 605 (3), 384–387.

Luo, Yuetong, Long, Pengcheng, Wu, Guoyong, Qin, Zeng, Hu, Liqin, Zou, Jun, 2010. SVIP-N 1.0: an integrated visualization platform for neutronics analysis. Fusion Eng. Des. 85 (7–9), 1527–1530.

Martz, Roger L., 2013. The MCNP6 Unstructured Mesh Development Team. The MCNP6 Book on Unstructured Mesh Geometry: User's Guide.

Nasif, H.R., Nasif, Hesham R., Masuda, Fukuzo, Morota, Hidetsugu, Iida, Hitomasa, Sato, Satoshi, Konno, Chikara, 2012. Development of CAD-MCNP interface program GEOMIT and its applicability for ITER neutronics design calculations. Nucl. Technol. 180 (1), 89–102.

Requicha, A.A.G., Voelcker, H.B., 1982. Solid modeling: a historical summary and contemporary. IEEE Comput. Graphic Appl. 2 (2), 9–24.

Song, Jing, Sun, Guangyao, Chen, Zhenping, Zheng, Huaqing, Hu, Liqin, 2014. Benchmarking of CAD-based SuperMC with ITER benchmark model. Fusion Eng. Des. 89 (11), 2499–2503.

Tang, Zhengdao, Long, Pengcheng, Huang, Shanqing, Zou, Jun, Qiu, Yuefeng, 2010. Real-time dose assessment and visualization of radiation field for EAST tokamak. Fusion Eng. Des. 85 (7–9), 1591–1594.

Tautges, Timothy J., Wilson, Paul P.H., Kraftcheck, Jason A., et al., 2009. Acceleration techniques for direct use of CAD-based geometries in Monte Carlo radiation transport. In: International Conference on Mathematics, Computational Methods & Reactor Physics (M&C 2009).

Wu, Y., 2007. Conceptual design and testing strategy of a dual functional lithium-lead test blanket module in ITER and EAST. Nucl. Fusion 47 (11), 1533–1539.

Wu, Y., FDS Team, 2008. Conceptual design of the China fusion power plant FDS-II. Fusion Eng. Des. 83 (10), 1683–1689.

Wu, Y., FDS Team, 2009. CAD-based interface programs for fusion neutron transport simulation. Fusion Eng. Des. 84 (7–11), 1987–1992.

Wu, Y.C., Xie, Z.S., Fischer, U., 1999. A discrete ordinates nodal method for one-dimensional neutron transport numerical calculation in curvilinear geometries. Nucl. Sci. Eng. 133, 350–357.

Wu, Y.C., Qian, J.P., Yu, J.N., 2002. The fusion-driven hybrid system and its material selection. J. Nucl. Mater. 307, 1629–1636.

Wu, Yi-can, Li, Ying, Lu, Lei, Ding, Ai-Ping, Hu, Hai-min, Zeng, Qin, Luo, Yue-tong, Zheng, Shan-liang, Huang, Qun-ying, Chen, Yi-xue, 2006. Research and development of the automatic modeling system for Monte Carlo particle transport simulation. Chin. J. Nucl. Sci. Eng. 26 (1), 20–27.

Wu, Y., Jiang, J., Wang, M., FDS Team, 2011. A fusion-driven subcritical system concept based on viable technologies. Nucl. Fusion 51 (10).

Yican, W., Gang, S., Ruifen, C., et al., 2008. Development of accurate/advanced radiotherapy treatment planning and quality assurance system (ARTS). In: Chinese Phys. C(HEP & NP) 32 (Suppl II), 177–182.

Yican, W., Song, Jing, Zheng, Huaqing, Hao, Lijuan, Long, Pengcheng, Hu, Liqin, FDS Team, 2015. CAD-based Monte Carlo program for integrated simulation of nuclear system SuperMC. Ann. Fusion Energy 82, 161–168.

Zheng, S., Chen, M., Li, J., Zeng, Q., Lu, L., Li, Y., Ding, A., Hu, H., 2007. Neutronics analysis for the test blanket modules proposed for EAST and ITER. Nucl. Fusion 47, 1053–1056.