



Integrated approach for fusion multi-physics coupled analyses based on hybrid CAD and mesh geometries



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HIGHLIGHTS

- Integrated approach for neutronics, thermal and structural analyses was developed.
- MCNP5/6, TRIPOLI-4 were coupled with CFX, Fluent and ANSYS Workbench.
- A novel meshing approach has been proposed for describing MC geometry.

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ABSTRACT

Coupled multi-physics analyses on fusion reactor devices require high-fidelity neutronic models, and flexible, accurate data exchanging between various calculation codes. An integrated coupling approach has been developed to enable the conversion of CAD, mesh, or hybrid geometries for Monte Carlo (MC) codes MCNP5/6, TRIPOLI-4, and translation of nuclear heating data for CFD codes Fluent, CFX and structural mechanical software ANSYS Workbench. The coupling approach has been implemented based on SALOME platform with CAD modeling, mesh generation and data visualization capabilities. A novel meshing approach has been developed for generating suitable meshes for MC geometry descriptions. The coupling approach has been concluded to be reliable and efficient after verification calculations of several application cases.

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1. Introduction

Neutronic analyses on fusion reactor devices such as International Thermonuclear Experimental Reactor (ITER) and DEMOstration Power Plants (DEMO) require large and complicate neutronic models to be created. The traditional method of creating neutronic models for Monte-Carlo (MC) codes employs conversion tools, e.g. McCad [1] developed in KIT, for converting CAD geometries into Constructive solid geometries (CSG). CSG has advantages in fast particle tracking. However, it is intractable for processing large, complex geometries or spline surfaces. Unstructured mesh (UM) geometry is attractive in solving complex geometry problem, as well as in obtaining nuclear heating distribution which is important for coupled neutronic, thermal hydraulic (TH), and structural mechanical (SM) analyses, i.e. coupled multi-physics analyses. The UM feature has been implemented in MC codes, e.g. MCNP6 [2].

However, the computation time will be huge if the mesh has large amount of mesh elements. How to generate suitable mesh for describing the MC geometry, and create a balance neutronic model with hybrid CSG and mesh geometries, are now becoming important issues.

The coupled multi-physics analyses play an important role in fusion engineering and design. It requires iterative processing of consistent CAD and mesh geometries, transferring and visualization of simulation results. SALOME [3] provides a good solution to realize an integrated platform for processing these data and exchanging them internally, which facilitate the whole multi-physics analyses cycle.

This paper introduces an integrated approach of using hybrid CAD and mesh geometries in coupled multi-physics analyses. The coupling approach and the implementation details are discussed, and at the end several verification calculations were performed.

2. Coupling approach

The complete coupled fusion multi-physics analyses follow several steps: starting from (1) CAD modeling, then (2) mesh

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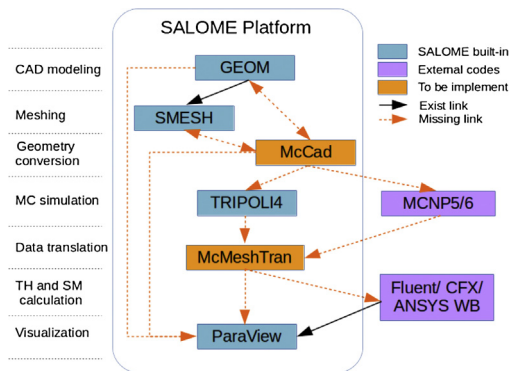


Fig. 1. Workflow of the coupling approach. The enclosed modules are integrated modules in SALOME platform.

generation, (3) MC neutronic model conversion, (4) MC simulation, (5) nuclear heating data translation, (6) thermal hydraulic and structural mechanics calculation, and finally, (7) visualization of the results. Fig. 1 shows the proposed workflow of the entire coupling approach. CAD and mesh are imported or created in SALOME built-in modules GEOM and SMESH, and then provided to the geometry conversion tool McCad for neutronic model conversion. Neutronic calculations are carried out using the MC codes MCNP5, MCNP6 or TRIPOLI-4 [4], simulation results, e.g. nuclear heating distributions, on orthogonal or unstructured meshes are processed by the generic data translation tool McMeshTran [5], which maps the data on MC meshes into target meshes, and then generates interface files for computational fluid dynamics (CFD) codes Fluent or CFX, and finite element method (FEM) SM software ANSYS® Workbench. At last, the visualizations of simulation results are performed with SALOME built-in ParaView module.

Efforts have been made to achieve the seamless coupling of the whole analysis cycle. Based on previous work [1,5], two key modules, McCad and McMeshTran, and all the missing links (dotted arrows in Fig. 1) have been implemented and integrated. McCad has been integrated into SALOME platform by wrapping with a new graphical user interface (GUI), and it has been upgraded to convert hybrid CAD and mesh geometries for MCNP6. McMeshTran has been extended to enable data inflow from MCNP6 and TRIPOLI-4 codes. As important auxiliary for data analysis, a plugin for ParaView has been developed to visualize CAD geometries directly. Furthermore, CAD, mesh, and result data inside SALOME (except for TRIPOLI-4) are exchanged internally using Common Object Request Broker Architecture (CORBA) [6] technology. For those external codes which cannot be integrated, interface files are provided.

3. Implementation details

3.1. Integration of McCad into SALOME

McCad is developed based on Open Cascade (OCC) [7] and Qt4 technology, which are also adopted by SALOME platform. The previous McCad GUI has been replaced with a new SALOME GUI. McCad core classes are inherited and wrapped with new classes using C++ Object-orientated technology, and libraries are dynamically linked with the new GUI (we named it as McCad-SALOME), so that codes can be updated independently. Fig. 2 is the graphic interface of McCad-SALOME. The new features are introduced as follows:

- Geometry solids are organized into a new tree structure of *Components*, *Groups* and *Parts*. A part represents a geometry unit that has a homogenized material and to be converted into a cell or a mesh in MC model; A group consisted of parts with the same

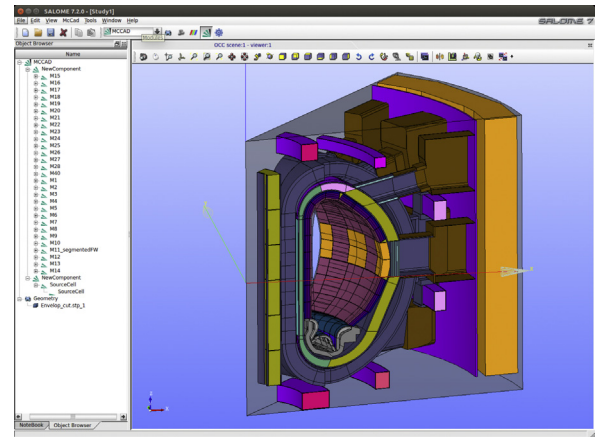


Fig. 2. McCad-SALOME graphic interface.

material; A component consisted of groups for organizing the model in assembly wise.

- Model persistency using a project file. The entire tree structure and its CAD data, meshes and all the attributes are persisted in a project file in HDF [8] format, which is helpful for resuming the process or exchanging data between computers.
- Interactive decomposition. Decomposed CAD solids can be recovered and sent to GEOM for auxiliary cutting.
- Internal data sharing with GEOM and SMESH modules. CAD geometries can be sent to GEOM module for clean-up, simplification and modification; Meshes can be imported/export to SMESH.
- Able to generate and convert unstructured meshes for MCNP6. Components can be chosen to be modeled with mesh while others remained with CSG. Meshes can either be imported, or created by a novel MC mesh generation approach, which will be discussed in next section.

3.2. A novel meshing approach for MC geometry

Unstructured mesh geometry is a state-of-the-art capability in MC codes, therefore it is important to understand which type of mesh is suitable for MC simulation. Unstructured meshes are used either for geometry descriptions, or for result scorings, or both. As for result scorings, meshes generated by common approaches, e.g. finite element (FE) meshes, which have low element aspect ratio and adaptive element size, are considered as high-quality mesh, and able to reveal physical field and its gradient (see, e.g. [9]). However, since MC method does not rely on spatial discretization, aspect ratio and field adaptive element size are not essential for meshes in MC geometry description (or, geometry meshes). Take the first-order tetrahedral meshes in Fig. 3 for illustration, the mesh with high aspect ratio elements in Fig. 3b has less elements and higher

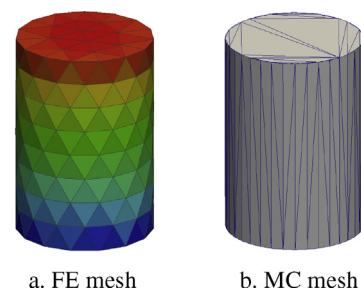


Fig. 3. Comparison of meshes for a cylinder with radius of 1 cm and height of 3 cm. (a) 901 elements, 9.214 cm³; (b) 102 elements, 9.337 cm³.

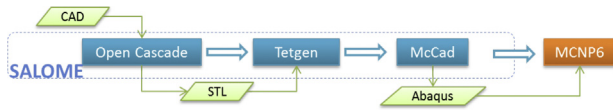


Fig. 4. Workflow of the mesh generation approach.

volume accuracy than the FE mesh in Fig. 3a, thus more preferable for geometry description in MC simulation, regarding the calculation efficiency.

Geometry differences and calculation time are two key aspects for MC geometry meshes. Considering a solid with volume V is meshed using first-order tetrahedral elements, the volumetric difference δ between the mesh geometry and the actual solid is calculated in:

$$\delta = \frac{1}{V} \sum_i^n |V_i - V_i'| \quad (1)$$

where $i = 1, 2, 3, \dots, n$ is the index for mesh elements, n is the total element amount, V_i is the volume of element i , and V_i' is the actual volume the element represents. Theoretically, mesh elements inside the geometry and elements on the planar boundaries have $V_i = V_i'$. When using n_1 to denote these amount of elements, and n_2 to denote amount of elements on non-planar boundaries, n in Eq. (1) can be replaced with n_2 . Assuming that calculation time is increasing monotonically with n , δ can be reduced by increasing n_2 appropriately, whereas n_1 should be kept as small as possible so that the calculation time is reduced. In other word, for creating an *economic* geometry mesh that has small amount of elements and high volume accuracy, mesh elements inside the solid or on planar boundary surfaces should be controlled as less as possible, and elements on non-planar surfaces should be generated in an appropriate way so that the deviation of surface mesh with original surface is reasonably small, meanwhile amount of elements (or, mesh size) is minimized.

To generate such economic mesh for MC geometry description, a so-called *Tessellation-Tetrahedralization* (TT) approach is proposed. The idea is to generate a surface mesh by tessellating (or faceting) a CAD solid, and to use this surface mesh for generating tetrahedral volume mesh conforming to it. Fig. 4 shows the workflow of the approach. The OCC libraries are employed for tessellating CAD solids, and then the surface meshes are exported to STL format files. The accuracy of the surface mesh is controlled with the *Deflection*, which is the maximum allowable deviation for a mesh edge to the surface. Fig. 5 gives an exaggerated illustration. Using the deflection control, the mesh edges are shorter when go along the direction with higher surface curvature, and edges can be longer if the deflection is preserved. At the end, the surface mesh is adaptive to geometry surface. Because an absolute deflection value is not suitable for geometries in different dimensions, the relative deflection (RD) is used which is the deflection value adjusted to the size of the solid.

Then tetrahedral meshes are generated using the open-source meshing tool Tetgen [9]. It is linked by McCad-SALOME with shared libraries. Volume meshes are generated on given surface meshes without mesh refinement, which is called Constrained Delaunay

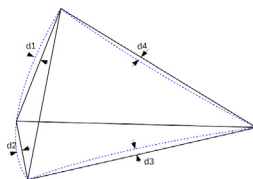


Fig. 5. Using deflection to control the deviation of mesh edge to the original surface.

Tetrahedralization. In this way the geometry accuracy is preserved, and the mesh elements are reduced as well as the meshing time.

Meshes with second-order elements, which have mid-points on the element edges, keep better the surface curvature. However, it requires iterative computation in finding intersection point with quartic element faces in particle tracing, lead to the significant increase of computation time. This approach is intended to create only first-order tetrahedral meshes.

3.3. MCNP6 and TRIPOLI-4 interfaces

Interfaces have been developed for supporting the MCNP6 hybrid geometry feature, including exporting Abaqus meshes and MCNP6 input files. To keep the internal consistency of the model, a geometry part in McCad-SALOME is associated with a MCNP6 pseudo cell, an Abaqus element set, and a mesh instance. Abaqus mesh import interface is provided additionally for checking the mesh, or reusing mesh from other MCNP6 calculation.

Also, McMeshTran interface has been developed for post-processing MCNP6 unstructured mesh results. The interface has been tested to parse the mesh output file with different particle types, element types, energy and time bins, multiplier settings, etc. Besides providing the results on the entire mesh, results for individual instances are also extracted. The meshes and results are stored in McMeshTran using the MED library [10]. As McMeshTran is a generic data translation tool, the nuclear heating results on unstructured mesh can also be exported for TH/SM calculation.

Since TRIPOLI-4 has been integrated into SALOME [11] and has been supported by McCad [12], integrating it in the coupling approach is a further step to fulfill the whole coupled analysis cycle. In this work, an interface for post-processing TRIPOLI-4 mesh tally output has been developed. It is able to process tally mesh on both Cartesian and cylindrical coordinates. The regular mesh used TRIPOLI-4 is converted by McMeshTran into unstructured mesh and stored in the MED library as well.

3.4. Data and CAD interfaces for ParaView

Meshes and data stored in McMeshTran can be internally transferred to SALOME built-in ParaView module via CORBA. MED data is received by a plugin called ParaMEDCorba in the build-in ParaView module, and is translated into VTK multi-block data set for visualization. A similar technique was adopted for visualizing CAD model in ParaView. A ParaView plugin called OCCReader has been developed which tessellates the CAD solids using the similar way as discussed in Section 3.2, and describes the faceted shapes in VTK vtkPolyData for ParaView visualization. CAD geometries can be obtained directly from SALOME GEOM and McCad-SALOME module using internal links, and options are provided for changing the display mode and adjusting tessellation accuracy.

4. Test verifications

4.1. Verifications of the TT meshing approach

Several challenging models have been chosen for testing the efficiency and accuracy of the TT meshing approach in generating geometry meshes. ITER Benchmark model [13] is a 40° sector which is simplified by removing unnecessary details. ITERA-lite 80° model was created as a collaborative effort between the FDS team, ENEA, UKAEA, JAEA, and the ITER Organization. TBM test case is a blanket test case model derived from the conceptual engineering design of the Helium Cooled Pebble Bed Test Blanket Module (HCPB TBM) [14]. Two RD values, 0.01 and 0.001, are adopted, and the meshing time, mesh sizes, volume differences, and lost particles are evaluated. For comparison, ANSYS® Workbench meshing

Table 1
Evaluations on the performances of TT meshing approach.

		CAD Solids	CAD volume (m ³)	Mesh volume (m ³)	Volume difference (%)	Mesh elements	Meshing time (s)	Lost particles ^a
ITER Benchmark	RD = 0.01	932	6.2282 × 10 ³	6.2211 × 10 ³	0.114	1.511 × 10 ⁵	4.6	33/10 ⁸
	RD = 0.001			6.2275 × 10 ³	0.011	5.534 × 10 ⁵	17.1	156/4 × 10 ⁸
ITER A-lite 80°	RD = 0.01	4296	1.7804 × 10 ⁴	1.7836 × 10 ⁴	0.177	4.485 × 10 ⁵	19.9	2/10 ⁸
	RD = 0.001			1.7801 × 10 ⁴	0.015	2.157 × 10 ⁶	45.2	11/3 × 10 ⁷
TBM Test case	RD = 0.01	77	1.6519 × 10 ⁻¹	1.6494 × 10 ⁻¹	0.152	1.410 × 10 ⁵	4.8	0/10 ⁶
	RD = 0.001			1.6517 × 10 ⁻¹	0.010	3.238 × 10 ⁵	8.6	0/10 ⁶
	ANSYS			1.6277 × 10 ⁻¹	1.462	7.624 × 10 ⁵	630.0	0/10 ⁶

^a Lost particles are calculated using MCNP6. Isotropic volumetric source and void materials are applied for ITER benchmark and A-lite 80° models, and surface source is applied for TBM test case. Total simulated neutron histories are given behind the value.

Table 2
Comparisons of meshes and CSG in TBM test case.

	CSG	TT mesh		ANSYS mesh
		RD = 0.01	RD = 0.001	
Processing time (min)	0.94	0.37	0.88	136.45
Simulation time (min)	93.09	483.38	684.14	4646.17
FW heating (W)	3.458 × 10 ⁴ ± 0.05%	3.434 × 10 ⁴ ± 0.17%	3.439 × 10 ⁴ ± 0.17%	3.181 × 10 ⁴ ± 0.13%
Difference ^a	–	0.69%	0.53%	8.01%

^a Using CSG results as reference

software is employed, and the coarsest sizing parameters were set up for generating a tetrahedral mesh for TBM test case. The results are shown in Table 1, which are obtained using a computer with Intel Core i7-4770 (3.40 GHz) cores and 32 GB memory.

Meshing processes using the TT approach were completed within one minute for all the cases. The processes were completed smoothly, just few solids failed due to problems of CAD solids such as very thin slabs, self-penetration, etc. The generated meshes have in general small amount of elements but high geometry accuracy. The increases of RD values improve geometry accuracies while at the meantime induce more elements. Longer time was used in ANSYS® Workbench for generating the mesh, and the volume difference is high than that of TT meshes.

The performances of mesh models for the TBM test case were evaluated by comparing with that of the CSG geometry converted by McCad [5]. In a computing node with 16 cores in the HELIOS supercomputer system at International Fusion Energy Research Centre, Japan, 10⁶ neutrons histories were simulated using MCNP6 parallel computation, and results are listed in Table 2. The simulation time used for TT meshes are around 5–7 times as that of CSG. Time used for processing and simulating ANSYS mesh are much longer than that of CSG, probably due to the larger mesh size. Furthermore, the integral heating results on the first wall (FW) were compared in Table 2. The results of the TT meshes agree well with that of CSG, whereas the result of ANSYS mesh has large discrepancy, thus it seems to be less suitable for MC geometry description. To sum up, the TT approach generates accurate and economic MC geometry meshes with short meshing time.

4.2. Verification of the hybrid geometry approach

The approach of applying hybrid geometries was verified using the TBM test case by replacing one breeder unit (BU) in the CSG neutronic model with unstructured meshes. Well-configured hexahedral meshes for the three subcomponents—beryllium, cooling plates (CP), and lithium-ortho-silicate (OSI) were generated by ANSYS® ICEM for result scoring. The hybrid CAD and mesh model was converted by McCad-SALOME. MCNP6.1 code and FENDL-3.0 [15] cross-section data was employed for neutron transport calculations with identical source and boundaries conditions, materials and data libraries as previous calculations [5]. The heating

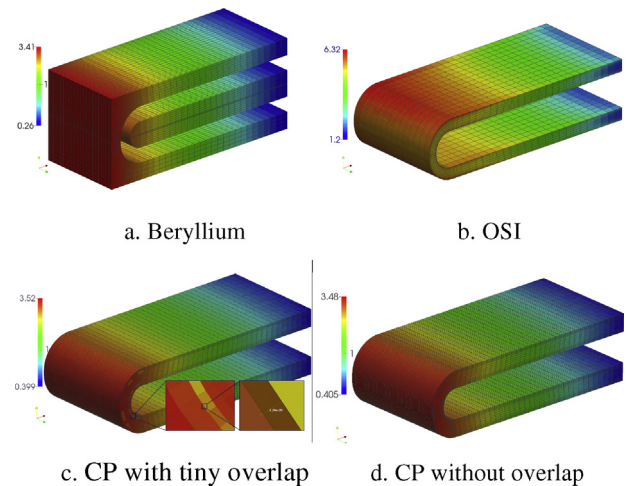


Fig. 6. Heating (W/cm³) of three subcomponents. Relative errors for all the elements are below 3%.

distribution results processed by McMeshTran are shown in Fig. 6, and integrated heating are compared with MCNP5 cell-based integral heating tallies in Table 3.

Table 3 shows that the integrated heating results of MCNP6 unstructured meshes are agree with the MCNP5 cell based tallies. The heating distributions in Fig. 6a and b give correct and smooth heating distributions. However, it is found that heating in Fig. 6c is not distributed smoothly at the lateral plate. By carefully check on the mesh of the lateral plate, a tiny mesh overlap was discovered. Although MCNP6.1 has been implemented with overlap detection and treatment, it might be failed for such small overlapping ($\sim 3 \times 10^{-5}$ mm), which causes particles from the red cell in

Table 3
Integral heating comparison.

Subcomponent	MCNP tally result (W)	MCNP UM result (W)	Diff. (%)
Beryllium	1.5555 × 10 ⁴	1.5787 × 10 ⁴	1.49
CP	1.8036 × 10 ³	1.7596 × 10 ³	2.44
OSI	1.0862 × 10 ⁴	1.0821 × 10 ⁴	0.38

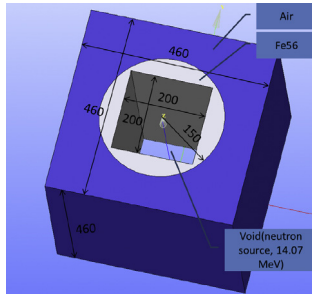


Fig. 7. Test model geometry (dimension unit: cm).

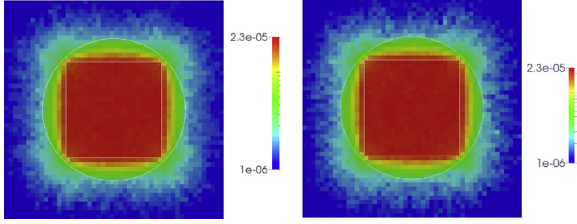


Fig. 8. Normalized neutron flux ($\text{cm}^{-2} \text{s}^{-1}$) results of TRIPOLI-4 (left) and MCNP5 (right).

Fig. 6c goes blindly through the yellow cell. By removing such overlaps, the result for the CP in Fig. 6d becomes smoothly. Therefore, caution should be paid to the mesh overlapping, and improvements on the overlap checking are suggested for MCNP6.1.

4.3. Verification of the TRIPOLI-4 interface

TRIPOLI-4 interface has been verified using a tube model which dimensions, materials and source are illustrated in the Fig. 7. A neutron flux mesh tally has been assigned for the whole geometry with intervals of $50 \times 50 \times 50$ in X, Y, Z direction respectively, and MCNP5-1.6 has been used as well as TRIPOLI-4.8. The results of TRIPOLI-4 in the Fig. 8, which is processed using McMeshTran, show agreement with MCNP5 mesh tally.

4.4. Verification with CFD calculations of the FW

In order to verify the McMeshTran on its coupling capabilities, and also to conduce to a cross-check on the interfaces for CFD codes, CFD calculations for the FW were carried out using both the CFX and Fluent codes. As suggested in [14], the 1/6 FW model was used for the analysis, which is shown in Fig. 9.

Unstructured meshes were generated using the ANSYS Workbench, with around 7.85×10^5 elements in the fluid domain and 7.88×10^5 elements in the solid domain. The volumetric heat source (VHS) was calculated with $5 \times 5 \times 5$ mm mesh tally cells,

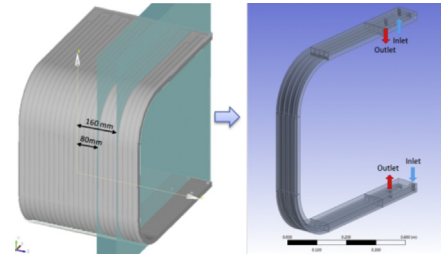


Fig. 9. The FW model for CFD calculations.

and was interpolated into the solid mesh using McMeshTran. The plasma-side surface of the FW was subjected to a 500 kW/m^2 heat flux in radial direction, and decrease to 0 kW/m^2 along the bending portion. The BU-side was assigned with a uniform heat flux of 83 kW/m^2 . Based on the geometry feature, periodic boundary conditions were applied for the lateral surfaces of the model. The other outer surfaces were considered adiabatic thus no heat transfer was assumed toward the outside of the domain. The boundary conditions for one cooling channel are as follows: Inlet temperature 300°C , pressure 80 bar, and mass flow rate 0.1 kg/s . The fluid helium was considered to be incompressible because of the low velocity of $\sim 80 \text{ m/s}$. More detail conditions and material properties can be found in [14].

The conjugate approach was used for solving the heat transfer simultaneously in two domains. The two-equation $k-\omega$ shear stress transport (SST) turbulence model was chosen for closing the CFD equations. The meshes and all the conditions were set identically in both the CFX and Fluent codes. Furthermore, the pressure-based coupled solver was intently chosen in Fluent to keep consistence with CFX. The calculations with the two codes were converged in heat transfer residuals, maximum solid and fluid temperatures, and also the outlet temperatures. The wall distance factor Y^+ has been kept in the region of 30–300 for almost the whole fluid domain.

As the temperature is of most concern in this comparison, the fluid and solid temperature using the two codes were evaluated. From Fig. 10 it can be observed that the CFX and Fluent calculations agree well in the temperature ranges, pattern, and the locations of hotspots both for the fluid and the solid domains. The maximum temperature in the solid and fluid domains and the average outlet temperature results are listed in Table 4. The differences of $1\text{--}2^\circ\text{C}$ are considered to be negligibly small in CFD analyses.

In order to evaluate the contributions of the VHS, the temperature without loading the VHS are also calculated and given in Table 4. Very close temperature raises were obtained using both codes. These results show good evidence for the reliability of the two CFD interfaces.

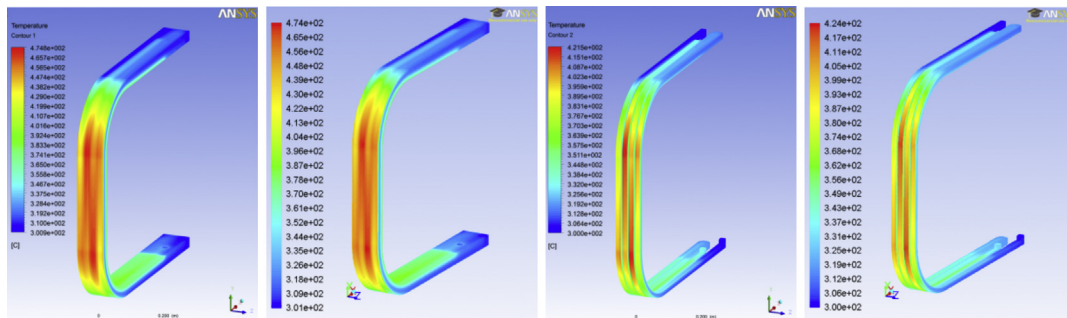


Fig. 10. Temperature distributions (from left to right: CFX-solid, Fluent-solid, CFX-fluid, and Fluent-fluid. Unit: $^\circ\text{C}$).

Table 4
Maximum and outlet temperatures.

	CFX		Fluent		Diff	
	+	–	+	–	+	–
Solid max.	474.81	468.37	473.55	467.12	1.26	1.25
Fluid max.	421.47	415.52	423.59	417.75	2.12	2.23
Outlet avg.	335.45	330.52	334.94	330.41	0.51	0.11

+: with VHS; –: without VHS.

5. Conclusions

An approach that using hybrid CAD and mesh geometries has been developed for fusion multi-physics coupled analysis. Two key modules, the MC geometry conversion tool McCad and the generic data translation tool McMeshTran, have been integrated into the SALOME platform, and interfaces for MC codes MCNP5/6, TRIPOLI-4, CFD codes Fluent and CFX, and structural mechanical software ANSYS Workbench have been developed. A novel TT meshing approach has been proposed for generating economic and accurate MC geometry meshes for MCNP6.

The ITER Benchmark model, the ITER A-lite 80° and the TBM test case model have been employed for verifying the TT meshing approach, and the approach is concluded to be fast and accurate in generate suitable mesh for MC geometry description. The application of hybrid CSG and mesh geometries in MCNP6 has been verified with nuclear heating analysis of the TBM test case. It is found that the tiny overlap in the cooling plate has significant influence on the simulation, which might be failed in MCNP6 overlap treatment. CFD calculations for the FW have been carried out in order to verify the CFD interfaces, and very good agreements on temperature results have been obtained between the CFX and Fluent codes. All these verifications provide good evidences for reliability and efficiency of the system.

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