Karlsruhe Institute of Technology

KIT advanced approaches for MC modeling and multi-physics coupling

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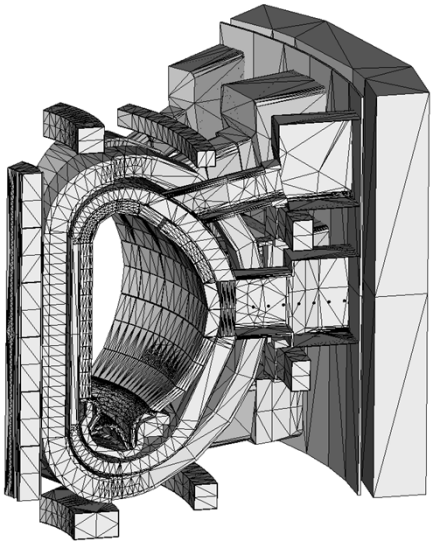
Institute for Neutron Physics and Reactor Technology, KIT



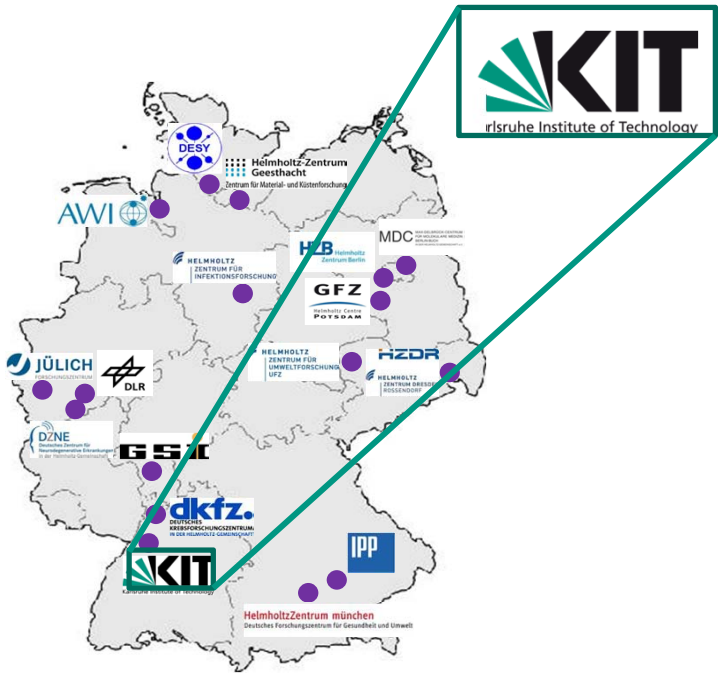
Outline

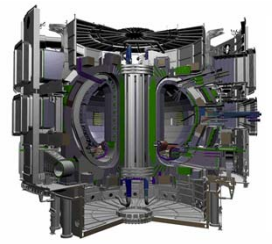
- Introduction
- The integrated system
- Geant4 developements
- Test verifications
- Summary and outlook

Introduction

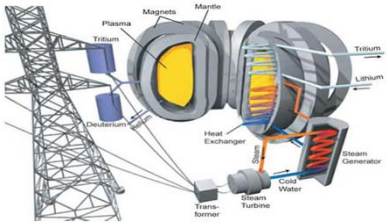
- KIT - Karlsruhe Institute of Technology
  - Created in 2009: University of Karlsruhe + Karlsruhe Research Centre (FZK)
  - One of the 17 largest Helmholtz center

- INR - Institute for Neutron Physics and Reactor Technology
  - Fission: Design optimizations and safety evaluations on LWR and GEN IV reactor
  - Fusion: Nuclear component design, neutronics analysis, fabrication and experiment.

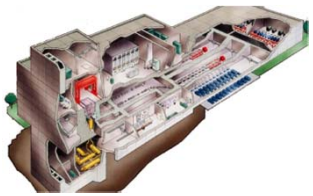




ITER



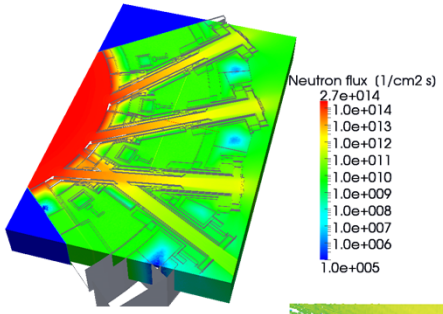
EU DEMO



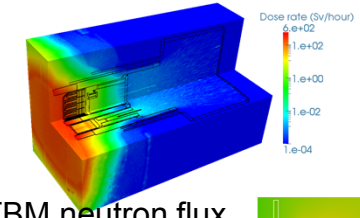
IFMIF

Introduction

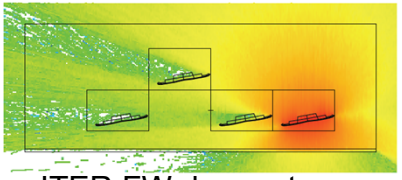
- NK Group – Neutronics and nuclear data
  - Focus on fusion neutronics
- Computational methods and tools
  - McCad: Advance MC modelling program
  - McMeshTran: Multi-physics coupling tool
  - R2S-mesh: Coupled system for shut-down dose rate calculation
- Neutronics analysis
  - ITER, DEMO, IFMIF



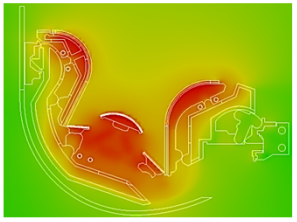
ITER NBI neutron flux



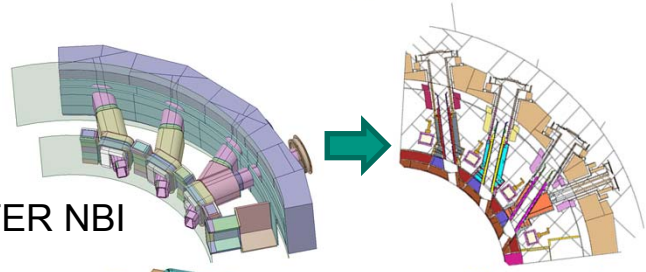
TBM neutron flux



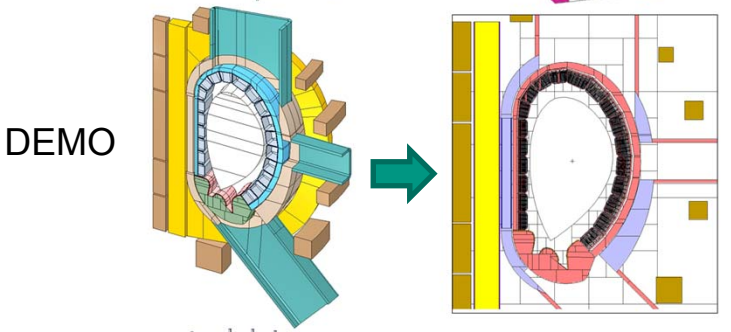
ITER FW dose rate



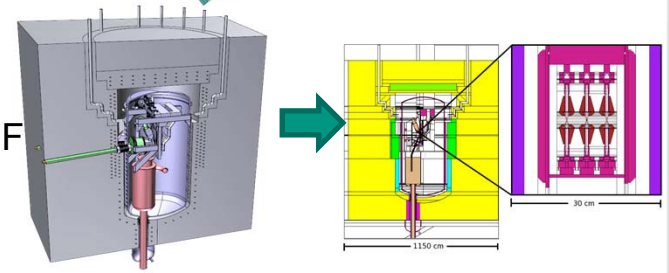
ITER Diverter dose rate



ITER NBI



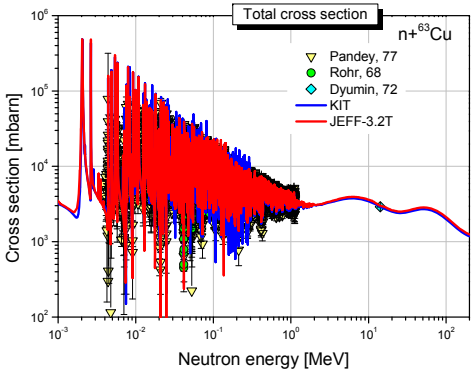
DEMO



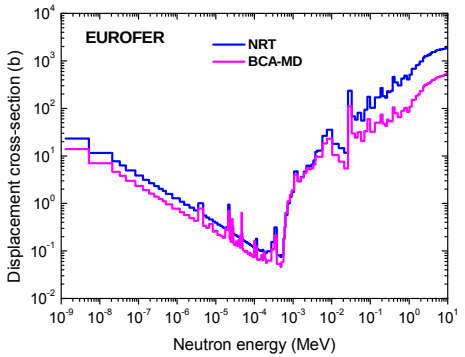
IFMIF

Introduction

- Nuclear data
  - Contributing to JEFF-3.2 library
- Experiment facility
  - Neutron laboratory of the Technical University of Dresden (TUD)
  - Accelerator: 300 kV, 10 mA, up to 10^{12} n/s

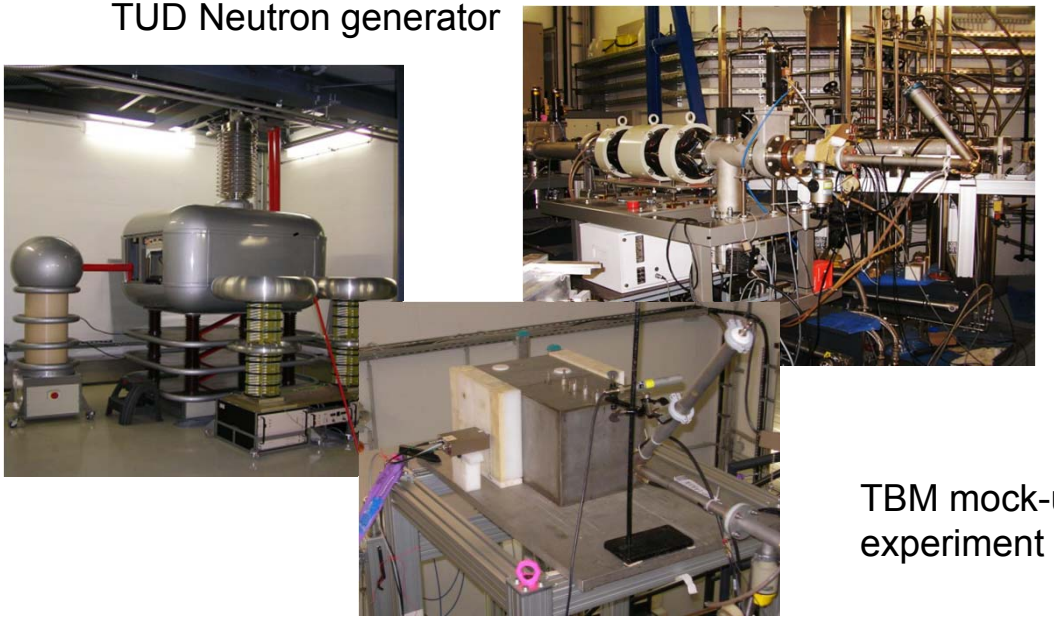


n + ^{63,65}Cu up to 200 MeV

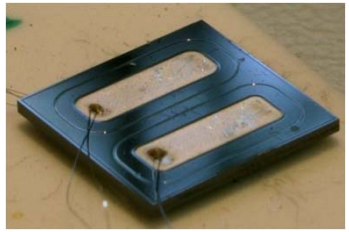


Eurofer steel DPA cross-section data

TUD Neutron generator



TBM mock-up experiment



SiC detector

ISMART

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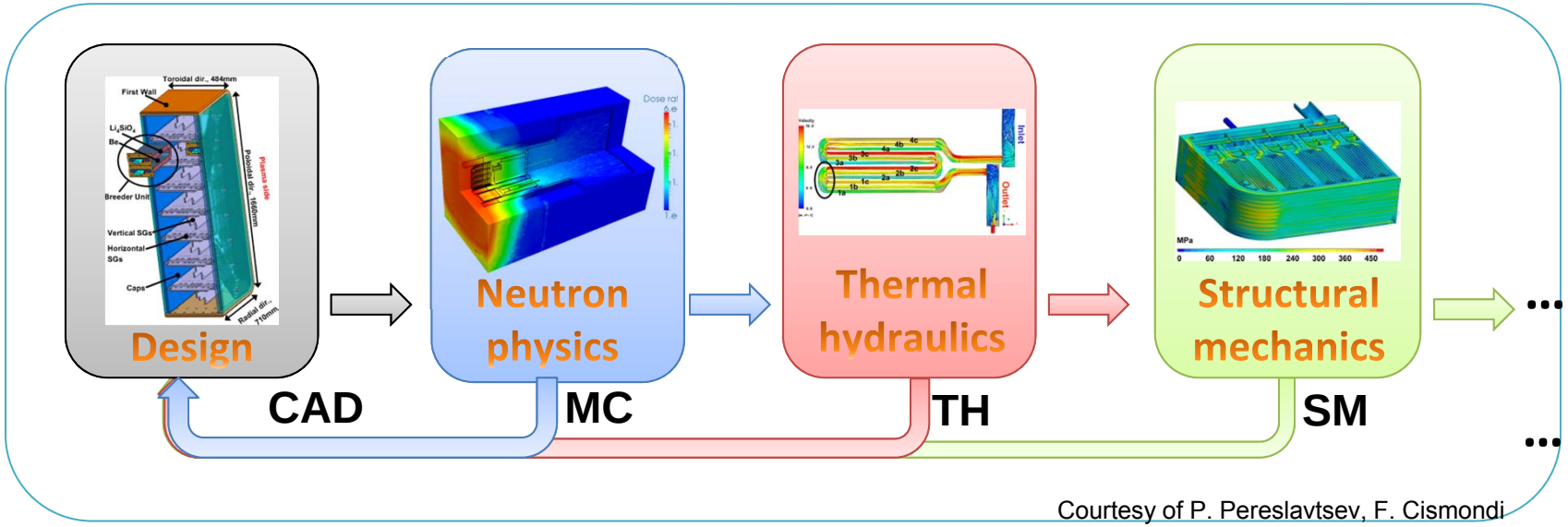
Integrated system

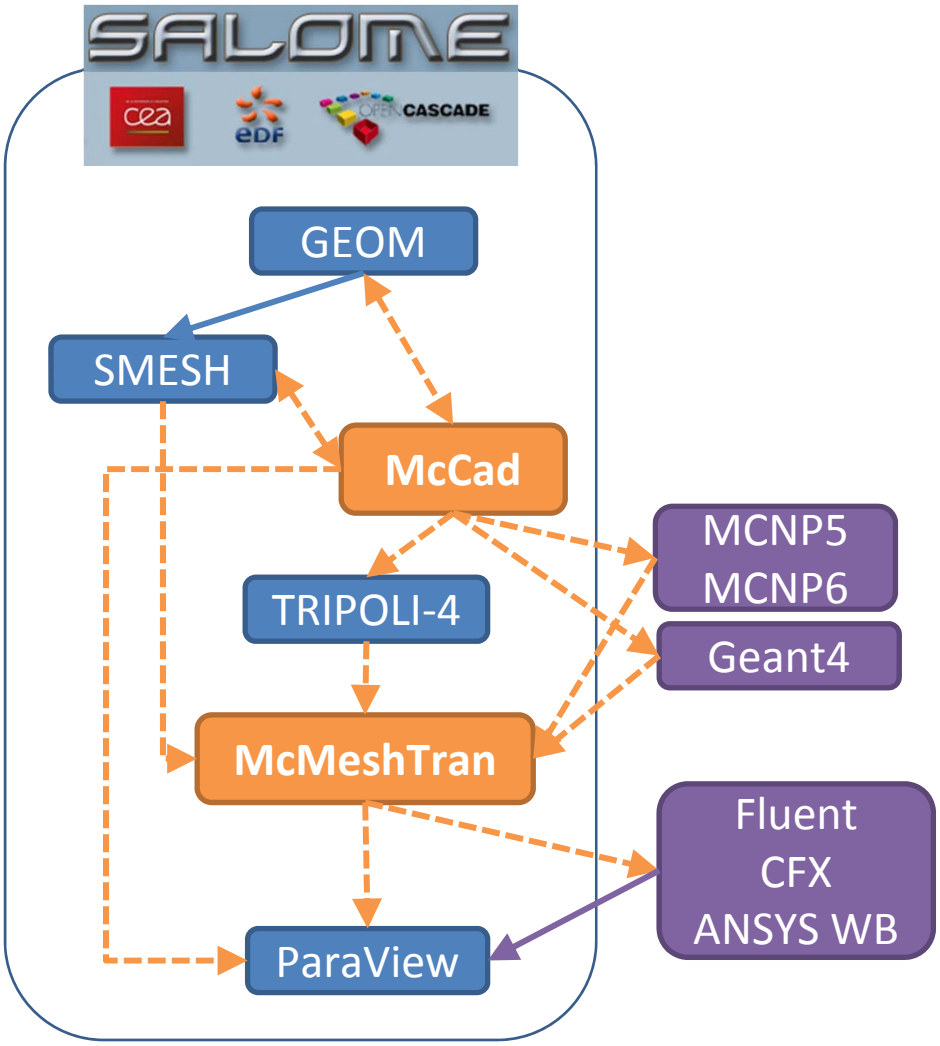


Courtesy of P. Pereslavtsev, F. Cismondi

- CAD conversion tool for Monte Carlo (MC) neutronics codes;
- Data transfer tool for translating MC results for TH/SM codes;
- Implementation and integration of tools into a suitable platform.

Integrated system

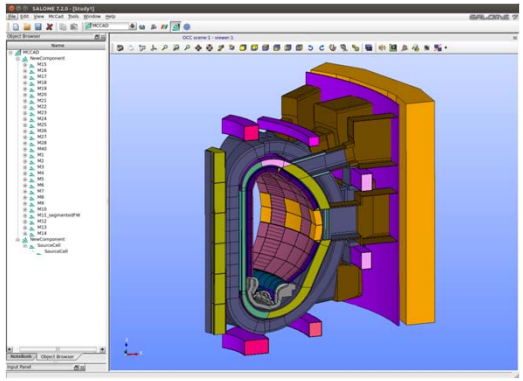
- SALOME
  - Open-source integration platform;
  - GEOM: CAD modelling;
  - SMESH: Mesh generation;
  - ParaView: Data visualization.
- MC codes
  - MCNP5: CSG
  - MCNP6: hybrid CSG and mesh
  - TRIPOLI-4: CSG
  - Geant4: CSG and Tessellated solid
- TH/SM codes
  - Fluent
  - CFX
  - ANSYS Workbench
- Integrated system
  - MC geometry conversion tool
  - MC data transfer tool
  - All the missing links

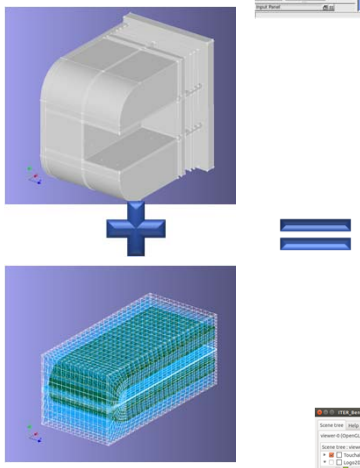


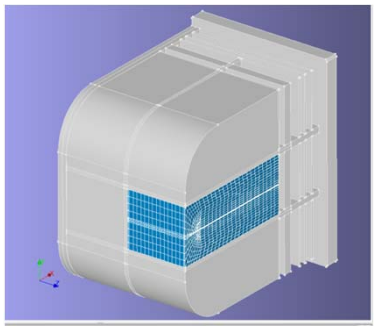
My PhD work!

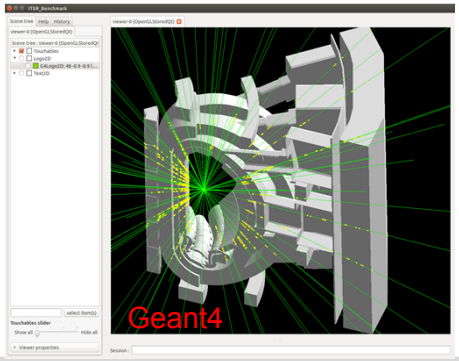
Integrated system-- McCad

- SALOME intergrating version of McCad
  - Integrated GUI;
  - Model persistency using a project file;
  - Internal data sharing with CAD and mesh modules.
- Model processing functions
  - Decomposition
  - Void generation
  - Tessellation
  - Mesh generation
- Hybrid MC geometry support
  - Hybrid CSG& mesh for MCNP6
  - Hybrid CSG& faceted solid for Geant4



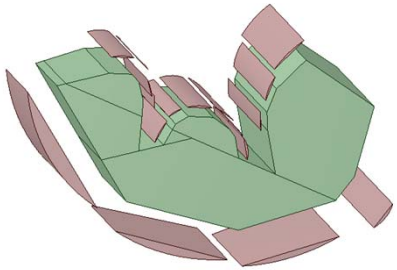




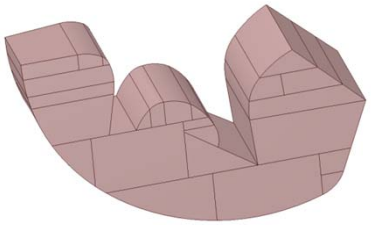


Integrated system-- McCad

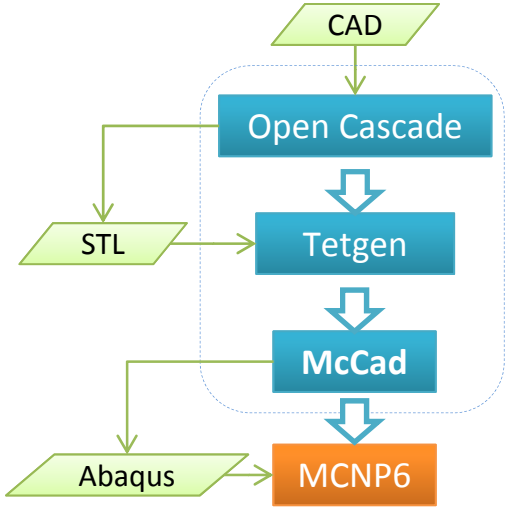
- CSG decomposition algorithm
  - assisting splitting surfaces
  - Optimizing splitting surfaces sorting algorithm
- Mesh generation approach
  - Tessellation-Tetrahedralization (TT)



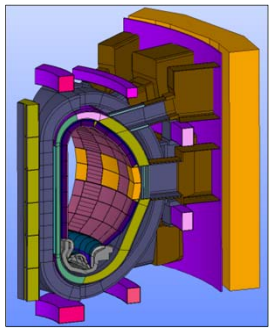
Current algorithm



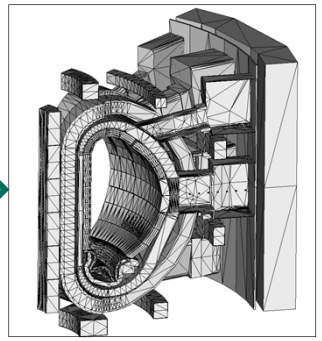
Improved algorithm



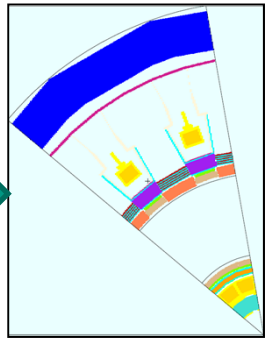
Mesh elements	Meshing time (s) *	Volume dev.
1.5×10^5	4.6	0.11%



ITER Benchmark model (936 solid)



TT unstructured mesh

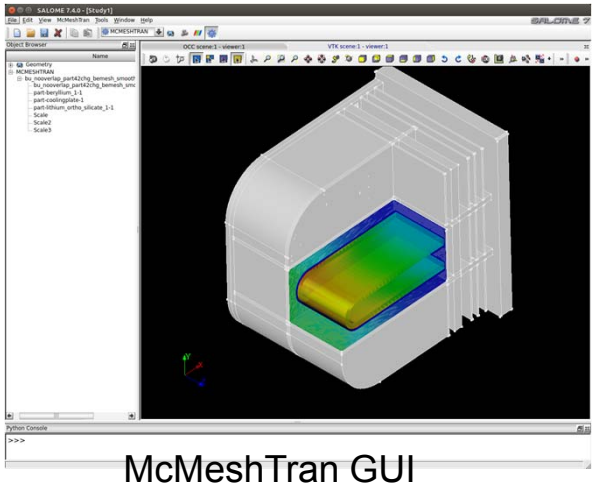


MCNP6 model

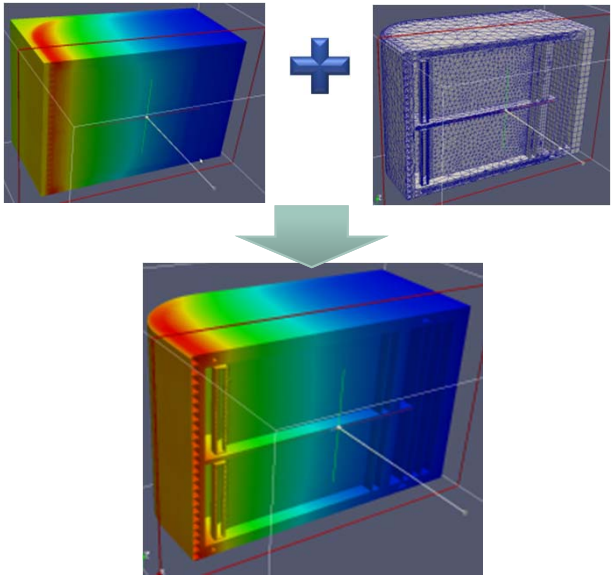
Integrated system-- McMeshTran

- McMeshTran
  - A MC Mesh and data Transformation/ Translation/ Transfer tool;
  - A module in SALOME, sharing meshes with SMESH and data with ParaView
  - Store mesh and data using universal library MED
  - Mathematic calculations, spatial transformation
- Generic interpolation
  - Nearly any mesh to any mesh
  - MED data mapping functions
  - Volume weighted scheme: physical conservative mapping data on cell
  - Point to point scheme: fast mapping data on node

MC result pro-proc. → Data mapping → Interfacing to CFD/FE



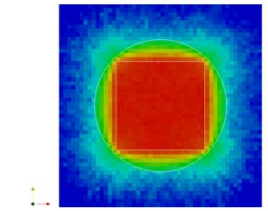
McMeshTran GUI



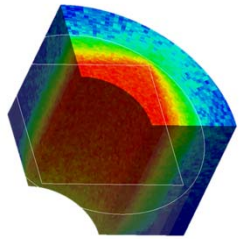
data interpolation

Integrated system-- McMeshTran

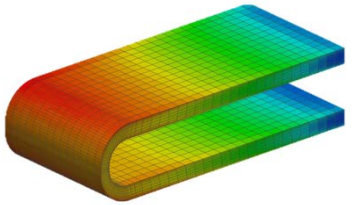
- MC interfaces
  - MCNP5 mesh tally interface
  - MCNP6 unstructured mesh output
  - TRIPOLI-4 interface
  - Geant4 Interface
- TH/SM interfaces
  - Fluent: User Defined Function (C source)
  - CFX: User Fortran (Fortran source)
  - ANSYS Workbench: Comma-separated Value (CSV) format
- Voxel searching algorithm
  - Points are grouped into regular voxels
  - The voxel is firstly located, next find the point inside the voxel
  - The time complexity for locating the voxel is O(1)



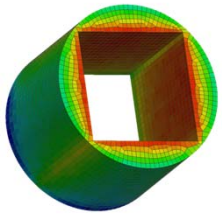
Cartesian mesh



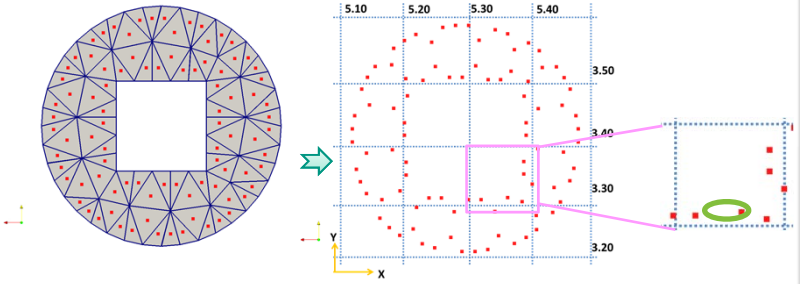
Cylindrical mesh



Structured mesh

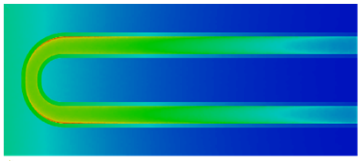


unstructured mesh

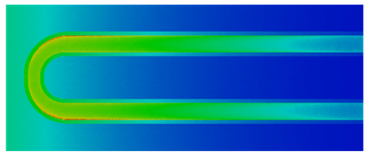


Integrated system– McMeshTran verifications

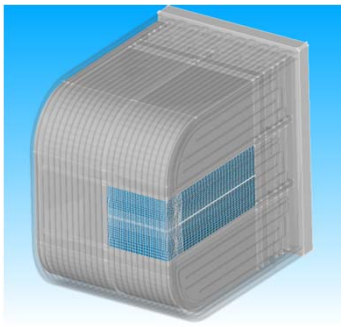
- MCNP5 mesh tally interface
  - Inverted interpolation check
  - Interpolated results agree with MCNP direct-tallied result
- MCNP6 unstructured interface
  - Hybrid CSG and mesh model
  - Unstructured mesh generated by ANSYS-ICEM
- CFD interfaces
  - 1/6 FW model;
  - Nuclear heating is transfered using McMeshTran
  - CFX results are agree with Fluent



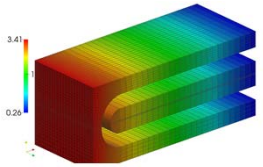
Inverted result



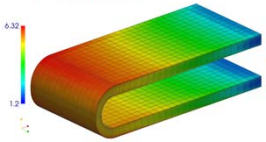
MCNP mix-material tally



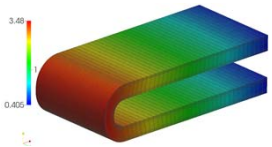
Hybrid CSG and mesh



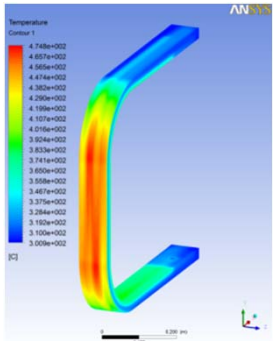
Beryllium



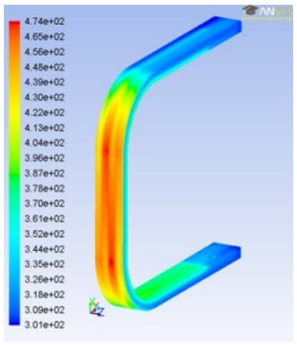
Lithium



Cooling plate



CFX-solid



Fluent-solid

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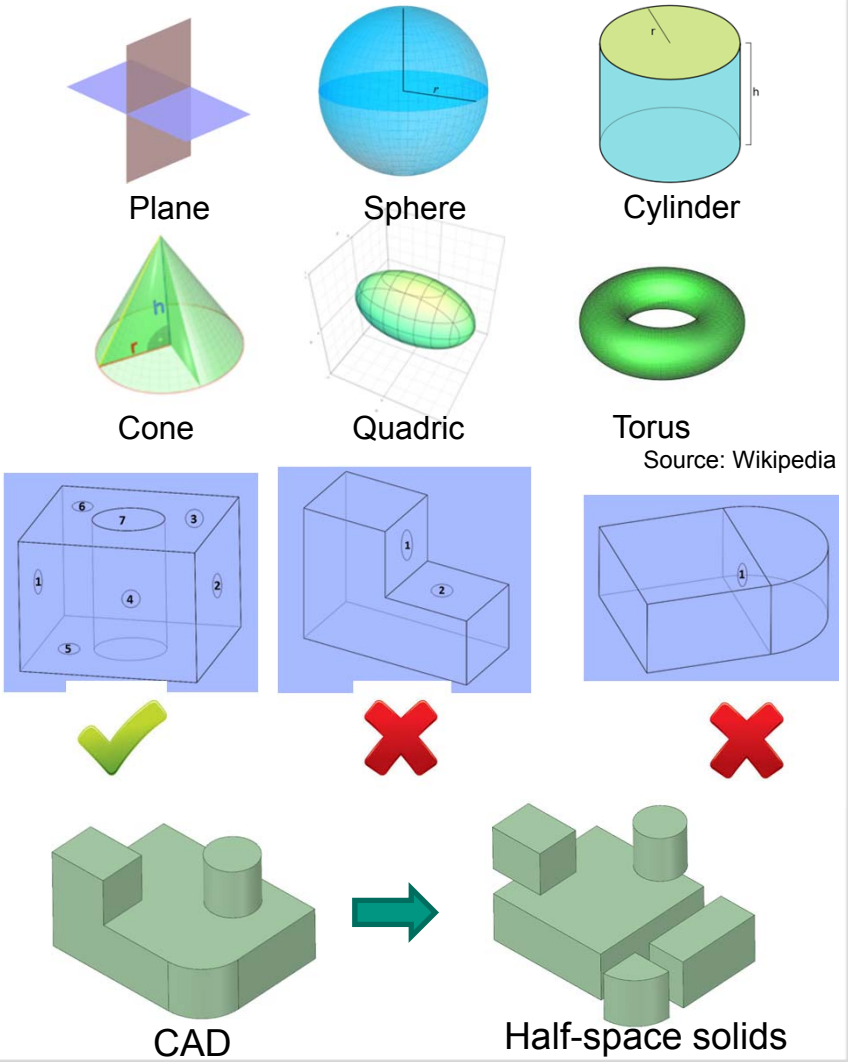
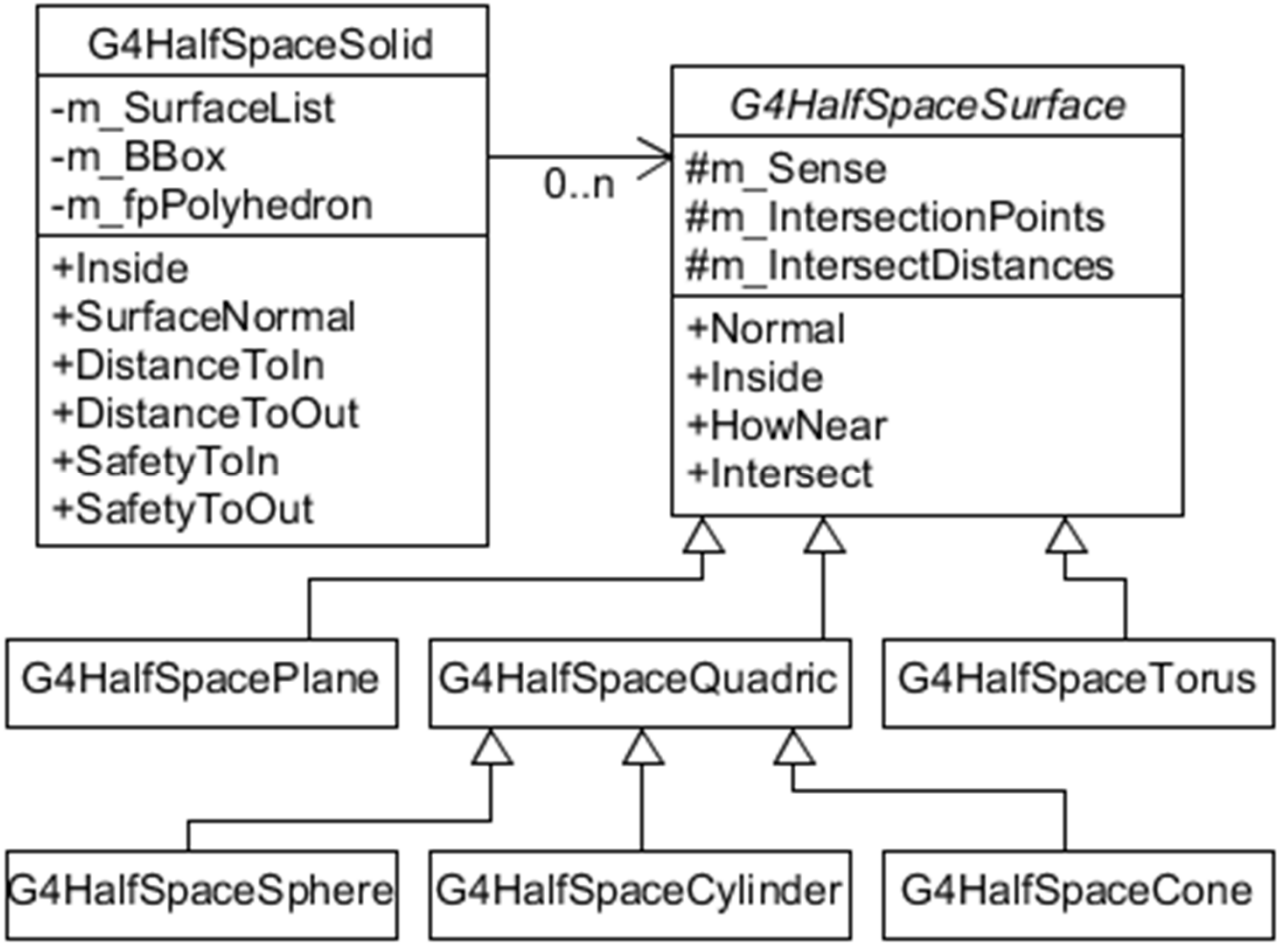
Geant4 developements – Half-space solid

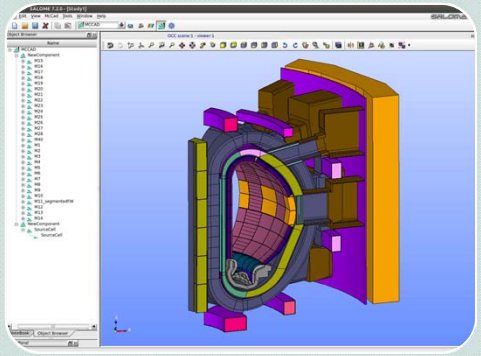
- Half-space surface
  - Common analytic surface
  - Sense: half-space index
    - 1: f(x, y, z) ≥0, positive half-space
    - -1: f(x, y, z) ≤0, negative half-space
- Half-space solid
  - Boolean intersect by half-space surface
  - Complex geometry can be decomposed into half-space solids
  - It is consisted of :
    - A list of half-space surfaces
    - A pre-calculated boundary box
    - Volume and surface area (optional)
    - A polyhedron for visualization.



Geant4 developements -- Half-space solid



Geant4 developements -- Advanced modelling

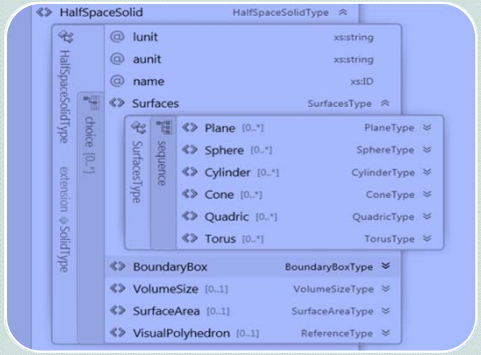


→Interface to export a complete GDML file

→Polyhedron is generated by Open Cascade library

→Material is managed in McCad

→Also able to export Tessellated Solid

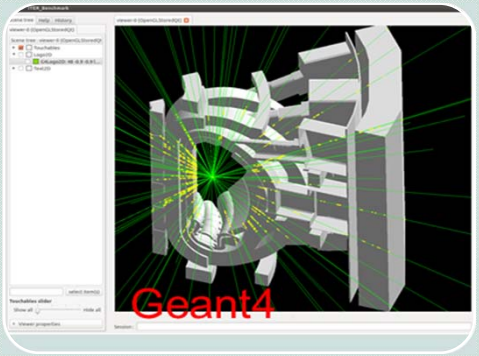


→ Modifying GDML schema to accept new solid type

→Add a Polyhedron type in the Define block

→Add a HalfSpaceSolid type in the solid block

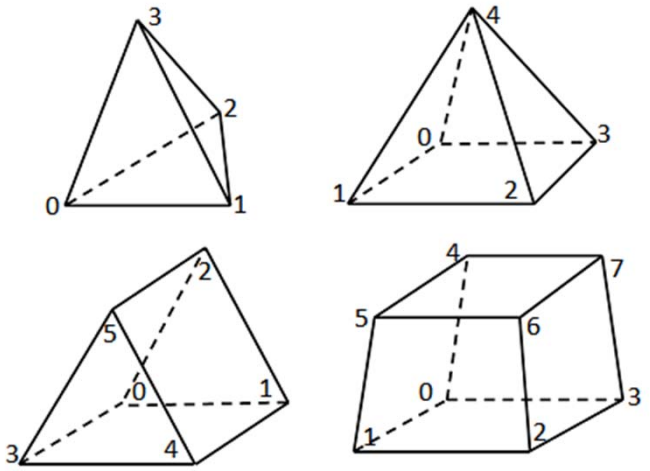
→Union the HalfSpaceSolid using the G4BooleanSolid (not efficient)

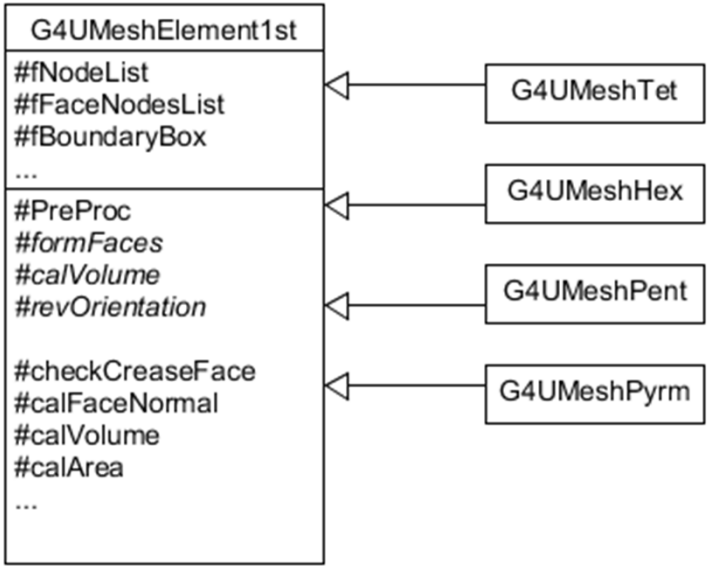


→Modifying Geant4 GDML parser to process new solids

Geant4 developements – Unst. scoring mesh

- First-order elements
  - General type for all convex first-order element
  - Currently implemented four element type
- Preprocess
  - Input: a list of point with indicate order
  - Common preprocess
    - Calculate boundary box
    - Pre-calculate face normal and other params
    - Calculate Area
    - Calculate Center
  - Difference preprocess
    - Form faces
    - Calculate volume
    - Reverse node ordering
- Particle tracking
  - All the required methods
  - General for all convex element type

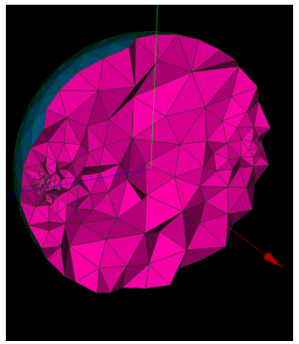




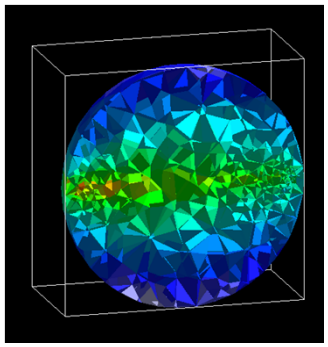
Geant4 developements -- Multi-physics

- Unstructured scoring mesh
  - Based on G4VScoringMesh
    - Use command script
    - Assign Multifunctional detector
  - Able to use all implement elements
  - Visualized the mesh and result
    - In linear or log color map
    - Geant4 have limitation on visualization
- Import mesh / Export results
  - Mesh parser for VTK format
  - Export the results in VTK format

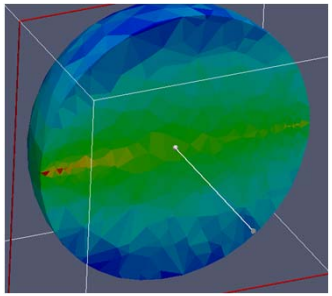
Unstructured mesh



Visualization in Geant4



Export for ParaView



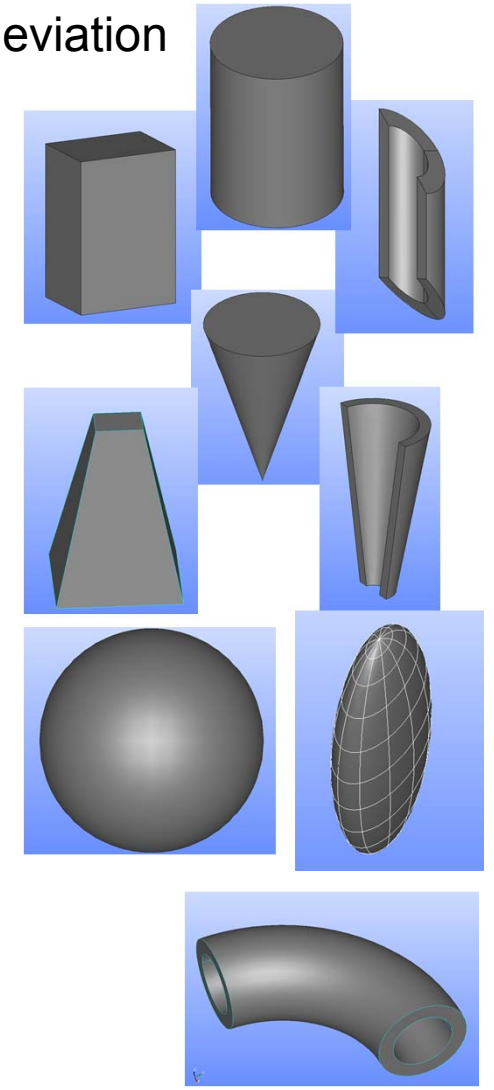
Outline

- Introduction
- The integrated system
- Geant4 developements
- Test verifications
- Summary and outlook

Test verifications

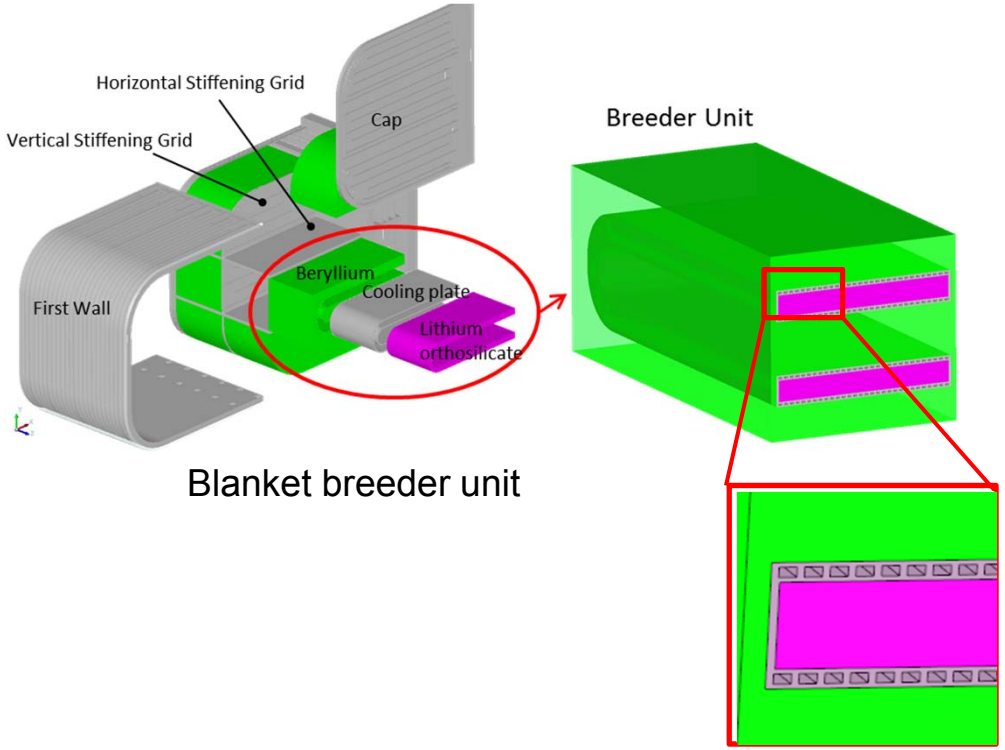
- Compared with Geant4 primitives with Average Absolute Deviation

	Volume (%)	Relative position	Surface normal	Distance to enter	Safety outside	Distance to exit	Safety inside
Box	0.001	Pass	0	6.08×10^{-15}	1×10-9	2.67×10^{-15}	0
Sphere	0.023	Pass	2.56×10^{-33}	8.61×10^{-14}	N/A	7.02×10^{-15}	0
Cylinder	0.012	Pass	3.98×10^{-33}	8.68×10^{-15}	N/A	1.77×10^{-15}	0
Cone	0.156	Pass	7.81×10^{-18}	4.38×10^{-14}	N/A	3.71×10^{-15}	9.03×10^{-11}
Torus	0.163	Pass	4.65×10^{-31}	2.06×10^{-11}	N/A	1.21×10^{-11}	N/A
Trapezoid	0.014	Pass	5.28×10^{-21}	4.96×10^{-10}	N/A	4.54×10^{-10}	2.49×10^{-10}
Tube	0.133	Pass	4.57×10^{-33}	5.54×10^{-15}	N/A	1.12×10^{-15}	4.62×10^{-17}
Cut Tube	0.099	Pass	5.72×10^{-33}	2.28×10^{-14}	N/A	2.25×10^{-15}	2.12×10^{-10}
Cone section	0.123	Pass	1.11×10^{-32}	3.40×10^{-14}	N/A	3.35×10^{-15}	1.16×10^{-15}
Ellipsoid	0.002	Pass	3.86×10^{-33}	2.54×10^{-15}	N/A	1.25×10^{-15}	N/A
Torus section	0.175	Pass	9.20×10^{-31}	1.38×10^{-12}	N/A	1.07×10^{-12}	N/A
UMeshHex Box	0	Pass	0	9.15×10^{-15}	N/A	6.14×10^{-15}	0
UMeshHex Trapozoid	0	Pass	2.59×10^{-32}	2.22×10^{-15}	N/A	3.46×10^{-15}	N/A
UMeshPent Wedge	0.012	Pass	1.22×10^{-32}	4.44×10^{-15}	N/A	1.71×10^{-15}	
UMeshPyrm Pyramid	N/A	Pass	1.16×10^{-23}	-2.65×10^{-10}	N/A	2.22×10^{-10}	1.20×10^{-10}
UMeshTet Tetrahedron	0	Pass	0	0	0	0	0

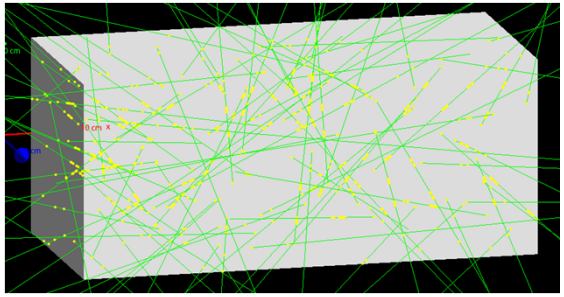


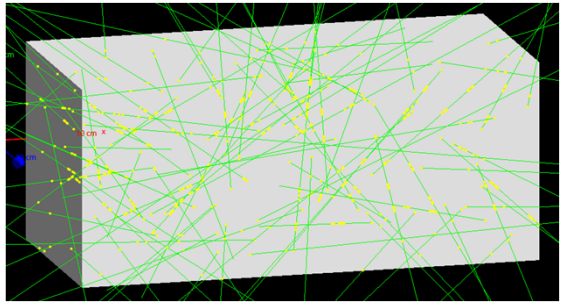
Test verifications

- HalfSpaceSolid vs. Tessellated solid
  - Breeder unit of fusion blanket
  - Complex model with cooling channels
- Calculation
  - Geantino
  - Particles: 1e6
- Time comparison
  - Half-space solid: 86.3 sec (need optimization)
  - Tessellated solid: 78.2 sec



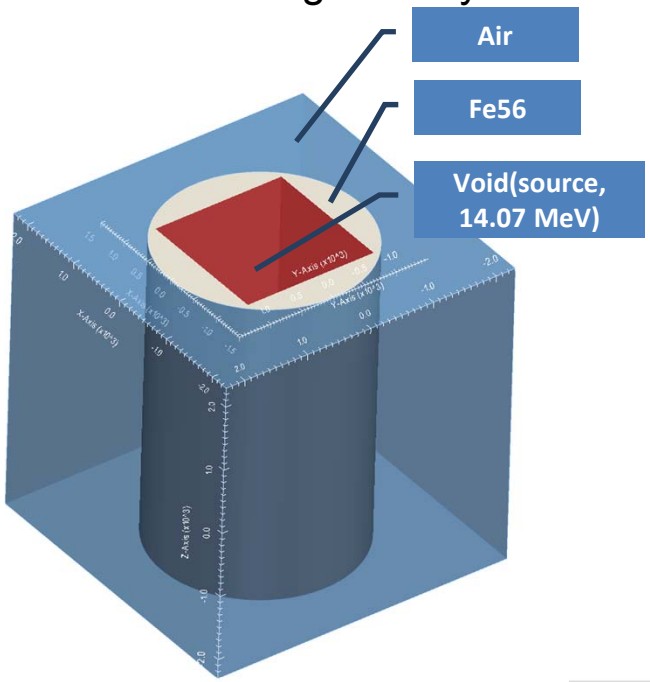
Blanket breeder unit

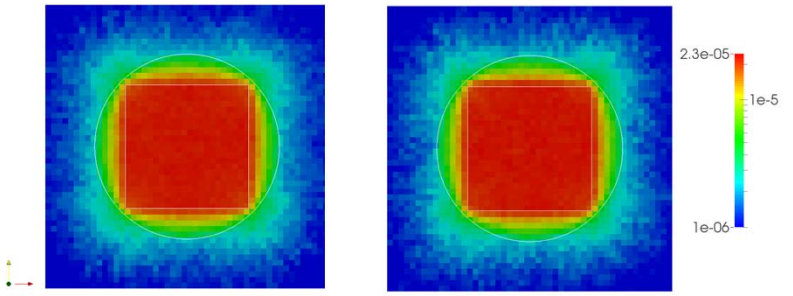




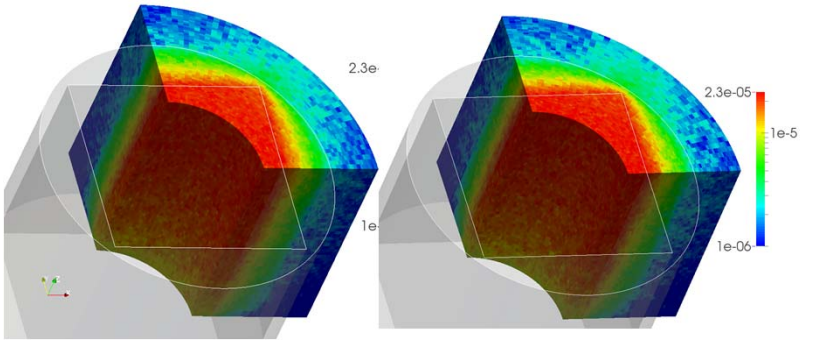
Test verifications

- Test of unstructured scoring mesh using a steel pipe case
  - Orthogonal mesh compared with MCNP5
  - superimposed unstructured mesh tally compared with MCNP6
  - Results agree very well.

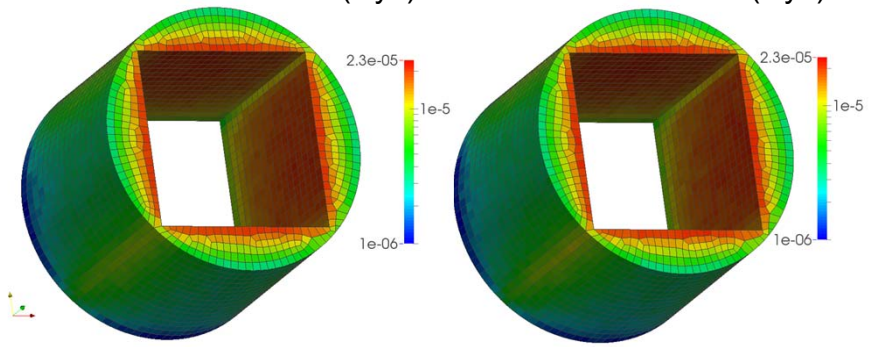




MCNP neutron flux (Cart.) Geant4 neutron flux (Cart.)



MCNP neutron flux (Cyl.) Geant4 neutron flux (Cyl.)



MCNP5 neutron flux (UM) Geant4 neutron flux (UM)

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- Introduction
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Summary

- Summary
  - An CAD based modelling approach has been developed for Geant4 simulation
  - The unstructured mesh scoring function has been developed for multi-physics coupling analysis
  - These functions have been implemented in an integrated system based on SALOME platform.
- Outlook
  - Conduct more tests on the Half-space solid;
  - Make code available;
  - Extend Geant4 for fusion neutronics, e.g implement reflecting boundary, fusion reactor neutron source;
  - Validations of Geant4 for fusion neutronics, e.g. benchmarking, experiment validation, etc.