Nuclear Data Needs for Fusion Neutronics Applications

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October 11th, 2022

IAEA Technical Meeting on the Compilation

of Nuclear Data Experiments for Radiation Characterization

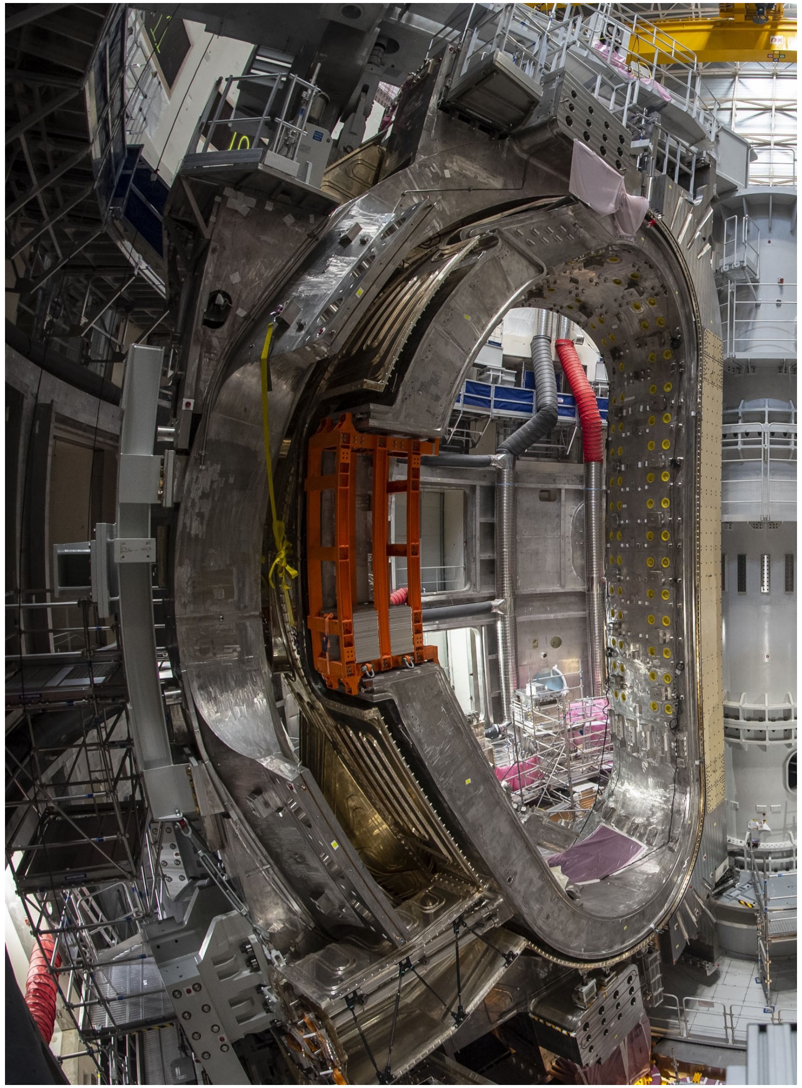
Vienna, Austria

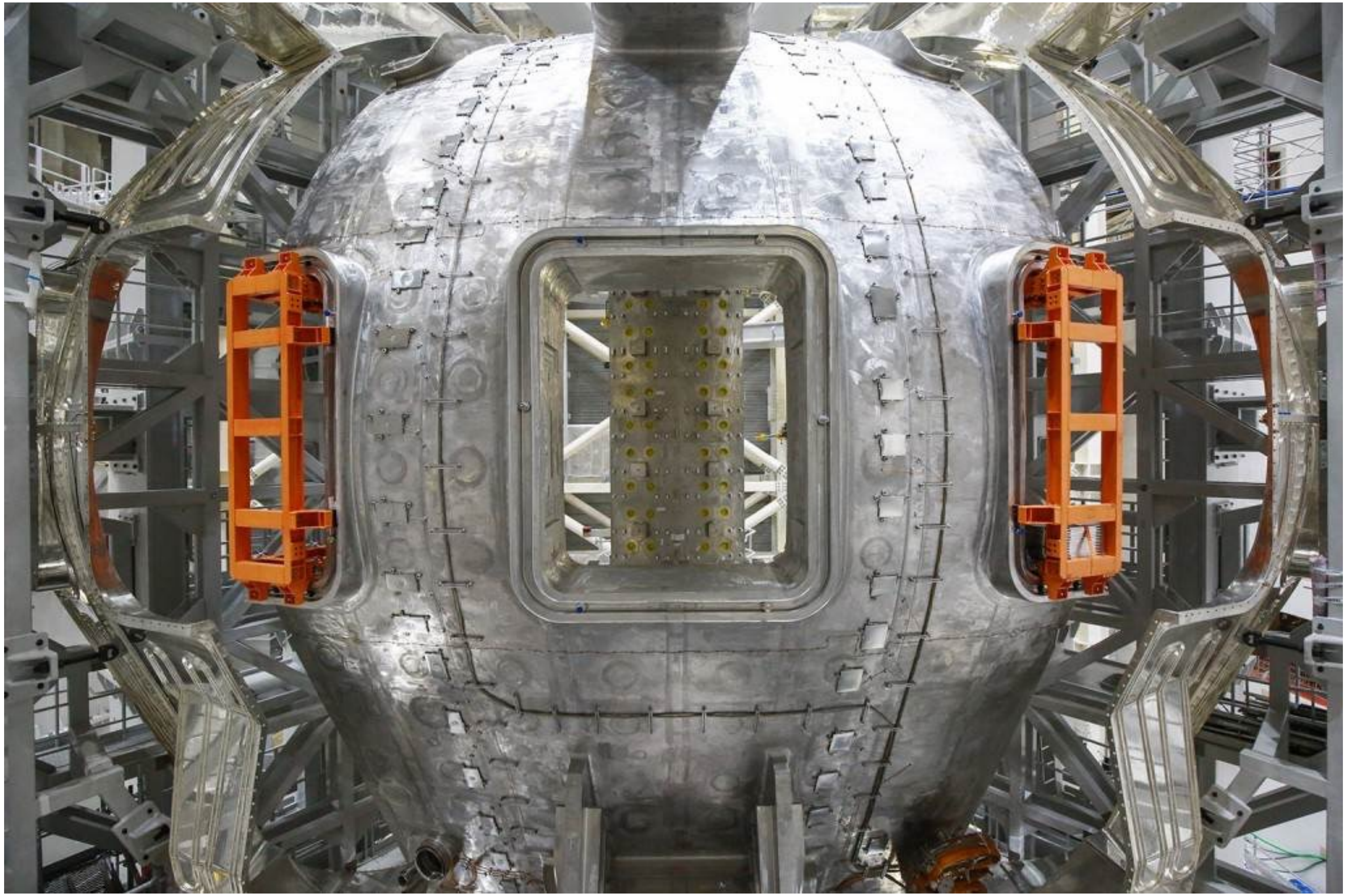
Outline

- Motivation
- Computational benchmarks
  - Fluid activation, large scale streaming, skyshine, variance reduction, homogenization, shutdown dose rate etc.
  - Identify both the issues with workflows and nuclear data
  - ITER SDDR benchmark v2
- Experimental benchmarks
  - Update existing SINBAD experiments
  - Uncertainty quantification
- Tools and workflows at ORNL
- Previous contributions to CoNDERC

Motivation

The ITER machine





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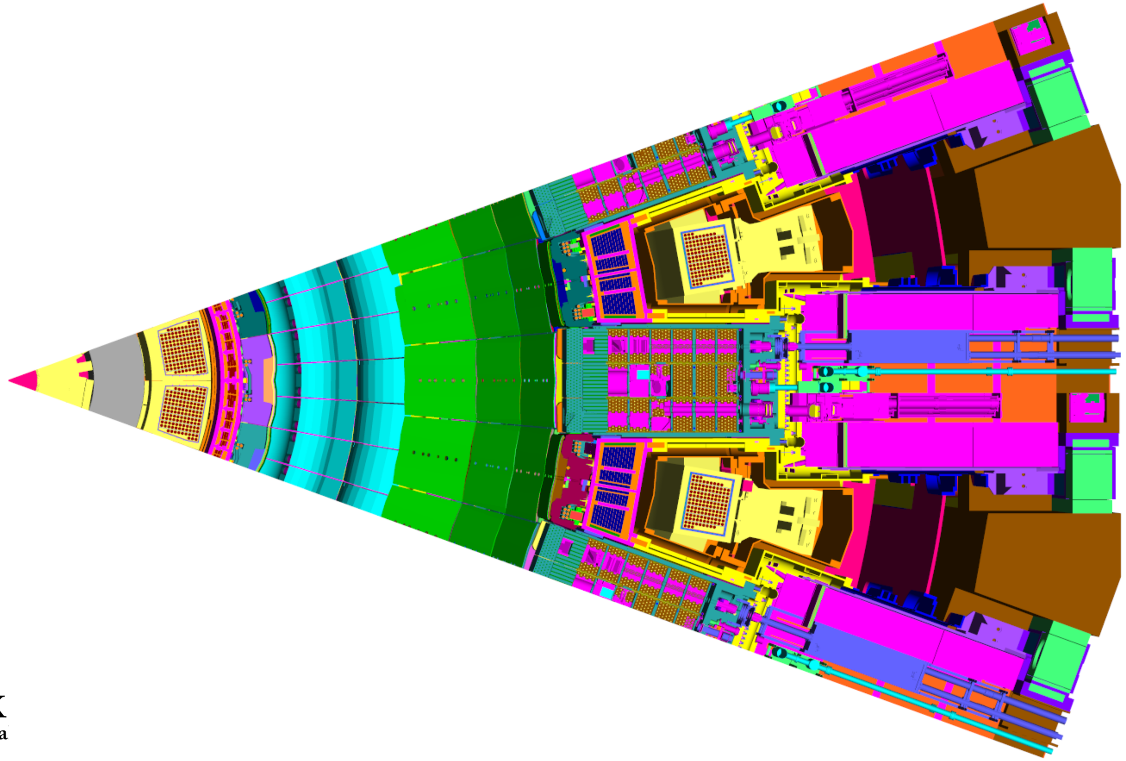
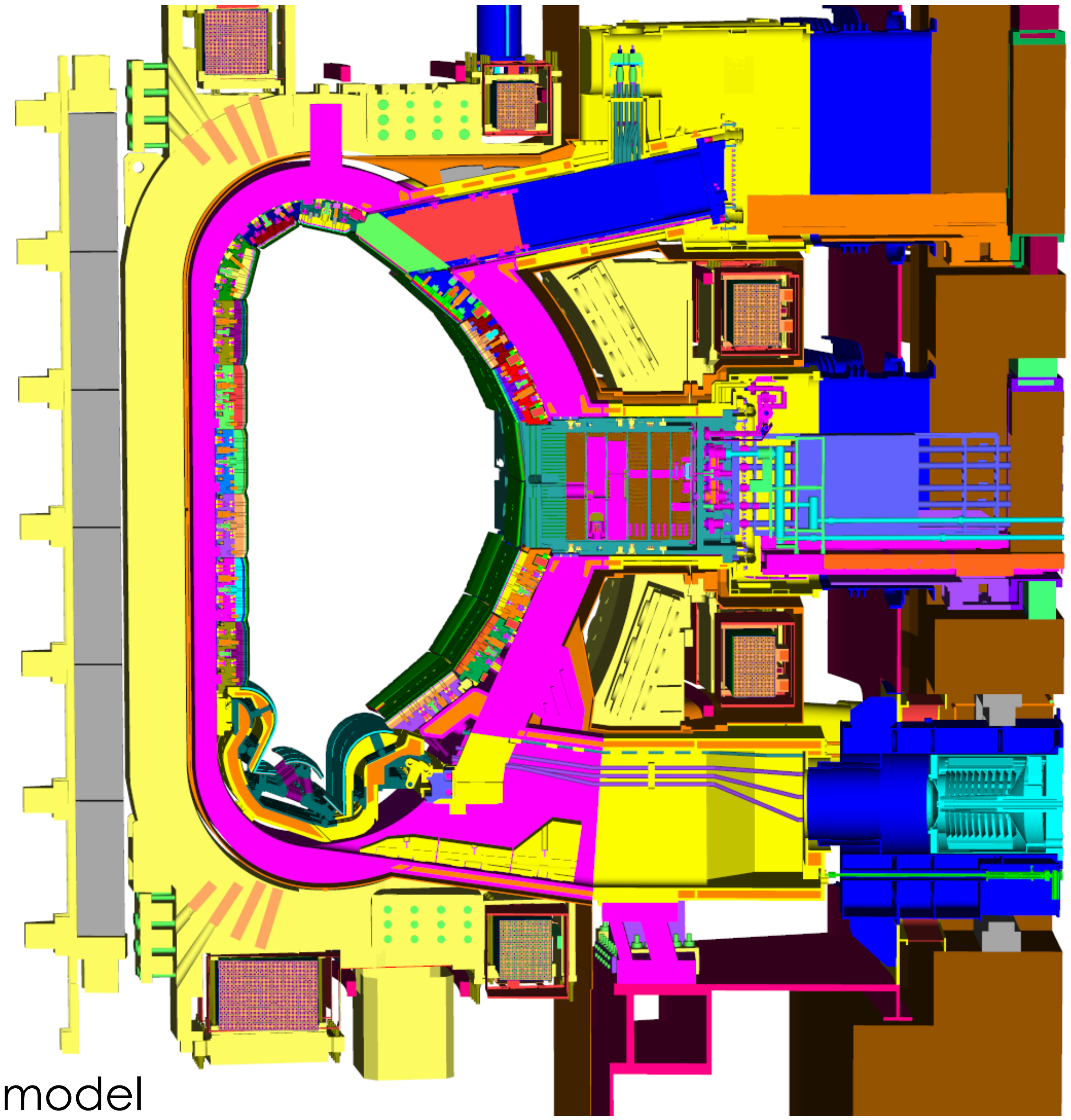
ITER MCNP models

- C-model (40°)
  - 108K surfaces, 70K cells
- CB-model (40° + full building model)
  - 166K surfaces, 107K cells
- E-lite model (360° up to bioshield)
  - ~0.5 million surfaces, ~0.33 million cells

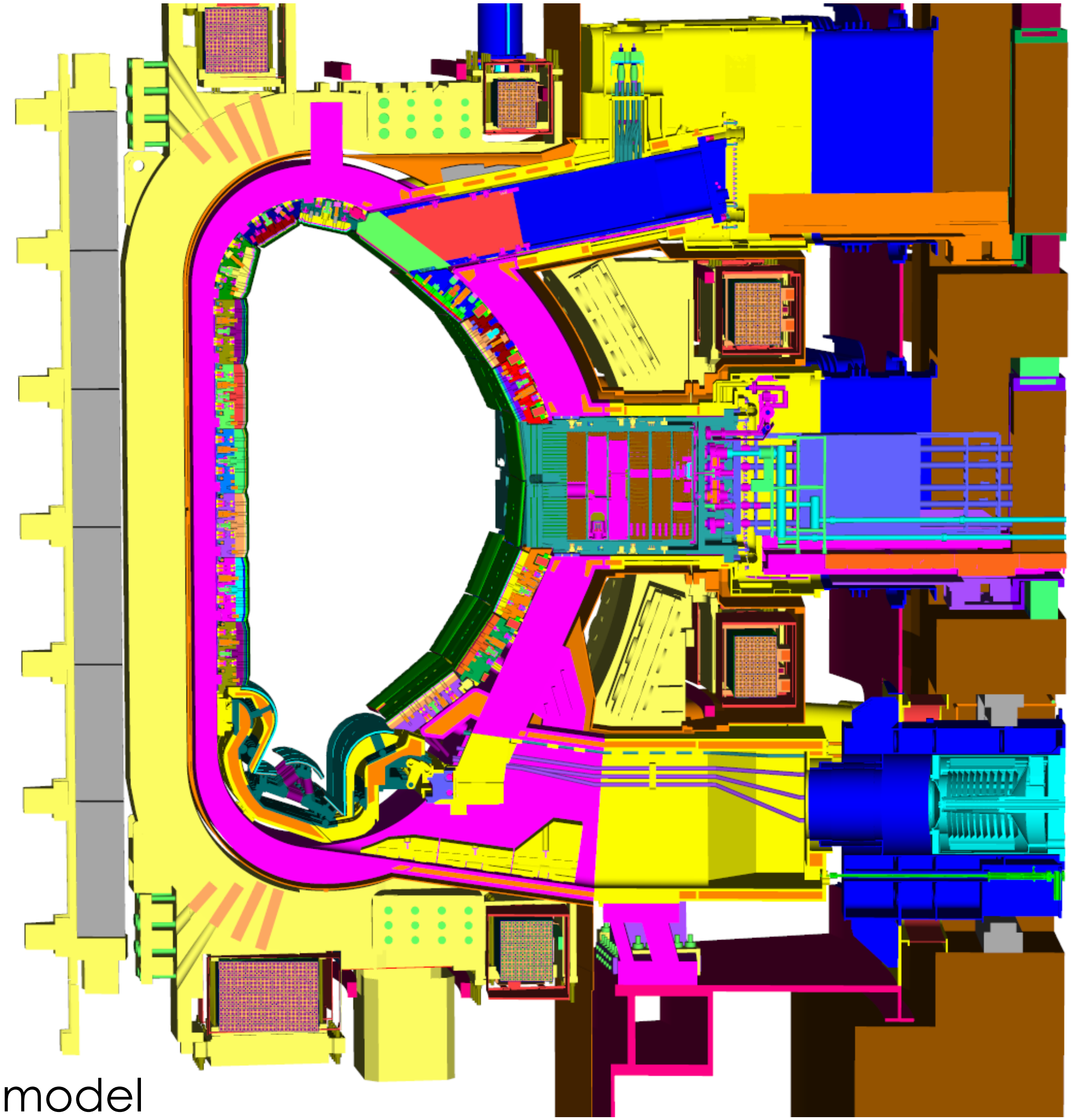




C-model

ITER quantities of interest

- Flux/fluence (neutron, gamma)
- Total nuclear heating (neutron + gamma)
- Tritium production (neutron)
- DPA (neutron)
- Helium production (neutron)
- Dose - ambient, silicon, polyethylene (neutron, gamma)
- Activation



C-model

Interest from private companies

- Fusion startups
  - Commonwealth Fusion Systems (USA)
  - TAE Technologies (USA)
  - Helion Energy (USA)
  - General Fusion (Canada)
  - Zap energy (USA)
  - Tokamak Energy (UK)
  - First Light Fusion (UK)
  - HB11 (Australia)
  - Kyoto Fusioneering (Japan)
  - Focused Energy (USA)
  - Etc.

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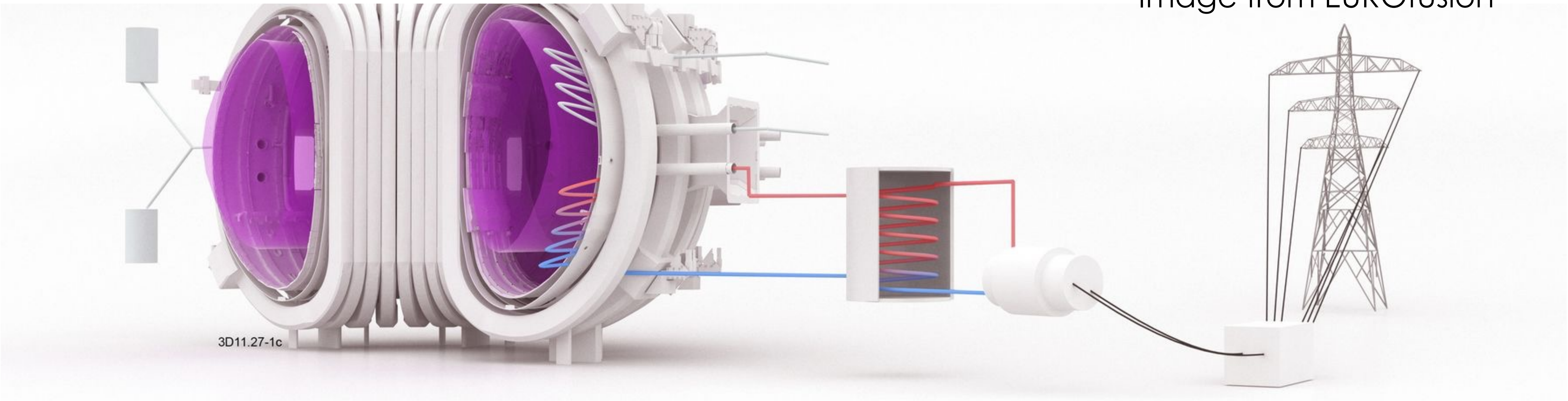
  - Focused Energy (USA)
  - Etc.

- They want to use their tools
- Often a lack of know-how
- A clear need for benchmarks and guidelines/handbooks

Fusion beyond experimental reactors

- European DEMO
- US Fusion Pilot Plant
- China Fusion Engineering Test Reactor
- JApanese DEMO

Image from EUROfusion



Two prong approach to help this emerging industry

- Computational benchmarks
  - Identify gaps in methodologies and nuclear data
  - Assess uncertainties
  - Reduce safety margins
- Experimental benchmarks
  - Validate methodologies
  - New experiments based on lessons learned
  - Improve nuclear data

Two prong approach to help this emerging industry

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Provide recommendations and guidelines in a form of a fusion neutronics handbook

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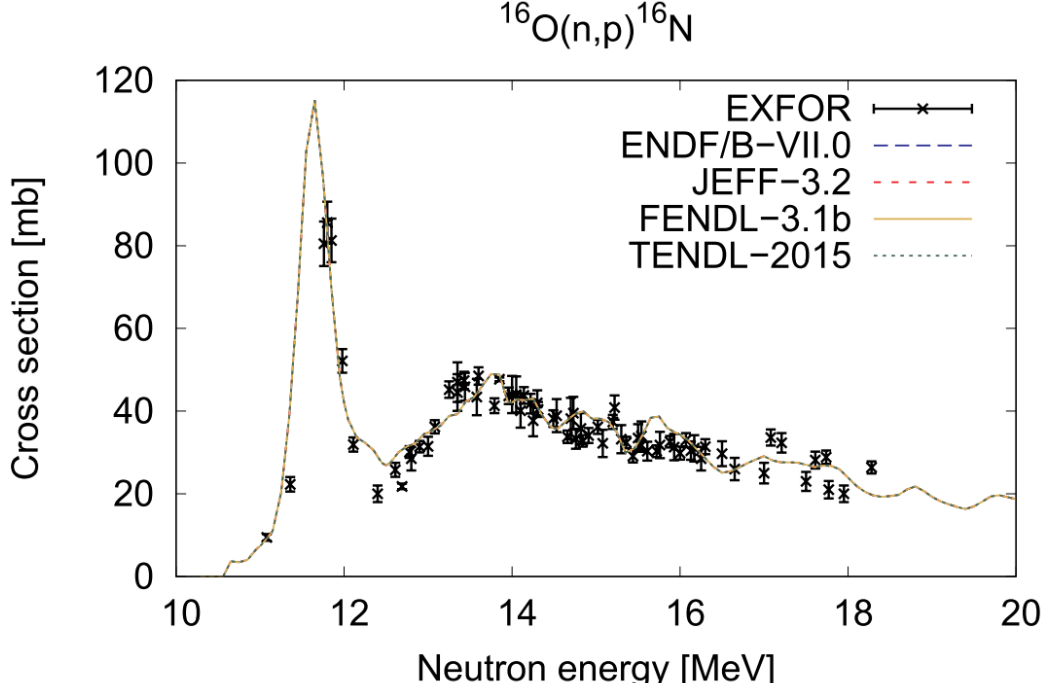
Computational benchmarks

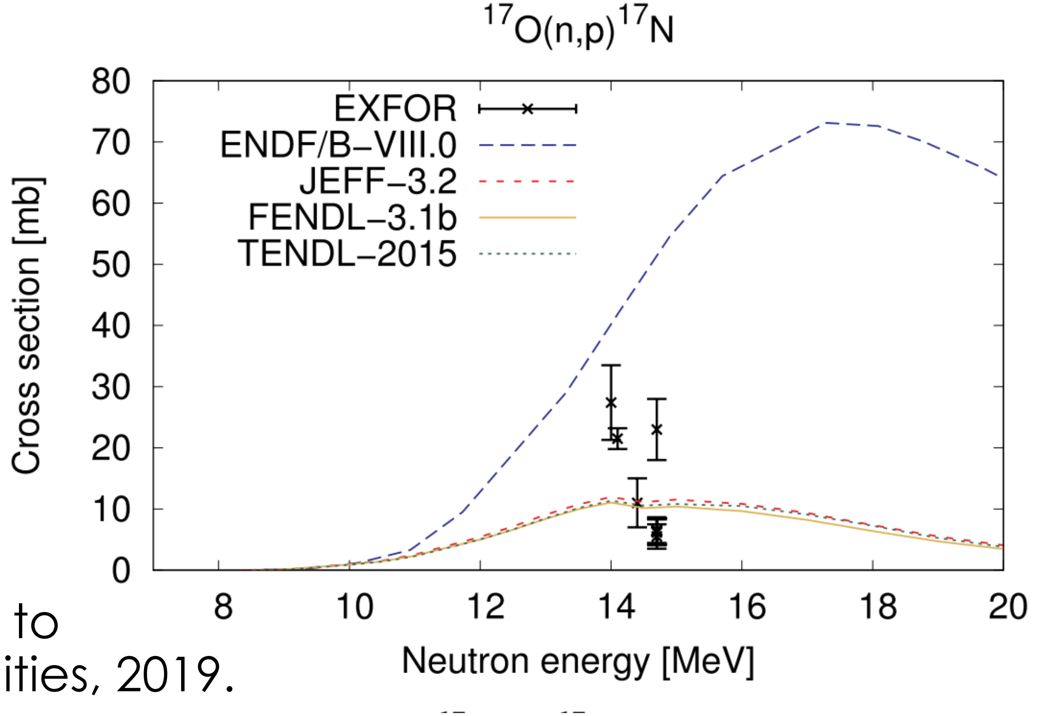
Computational benchmarks

- Fluid activation
  - Corrosion products
  - Coupling CFD and neutronics
  - Nuclear data
- Analysis of large-scale models and skyshine
  - Nuclear data and methodologies
- Variance reduction
  - Stochastic vs deterministic
  - Biasing
  - Over splitting etc.
- Homogenization
  - Where is it acceptable
- Shutdown dose rate
  - Methodologies (inventory codes)
  - Effect of assumptions (D1S vs R2S)
  - Meshing (material mixing)
  - Energy binning (neutron and gamma transport, activation, decay)
  - Nuclear Data

Fluid activation

- Water activation
  - Lacking nuclear data
  - Experimental setups in progress: JSI and JET
- Activated corrosion products
  - Code development needed
  - Lessons learned from the fission field



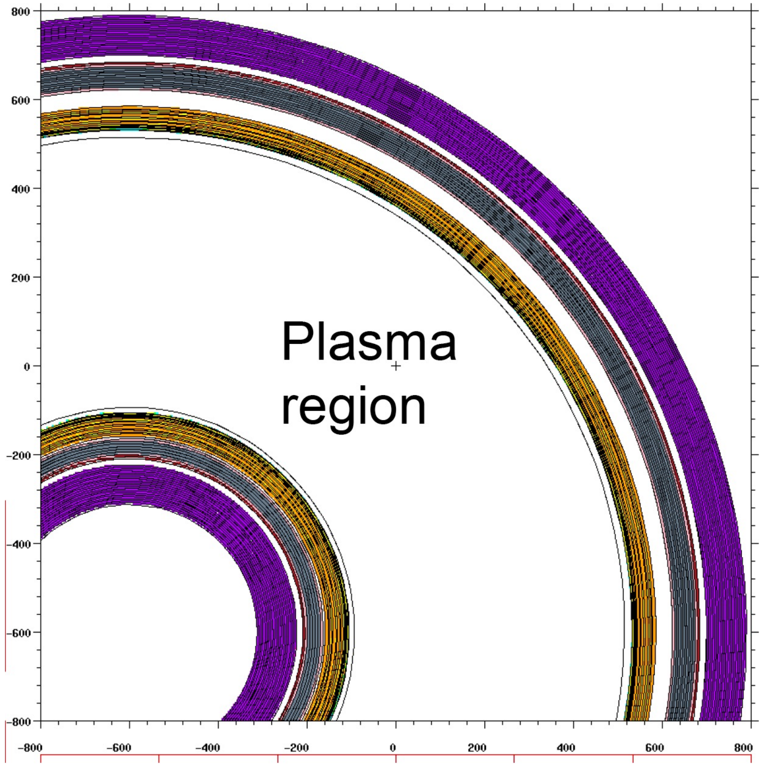


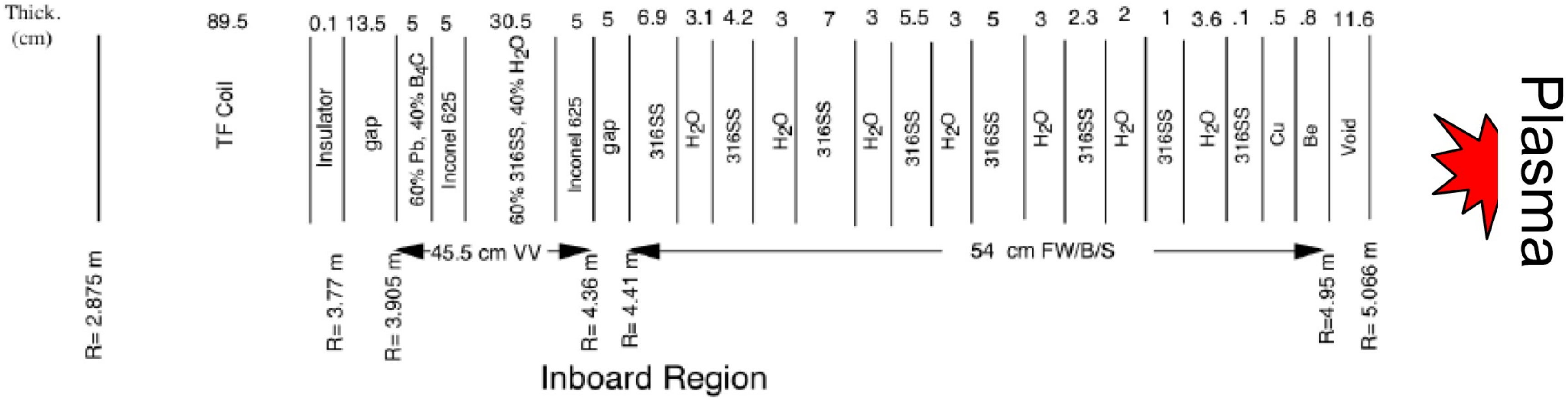
A. Žohar, L. Snoj: On the dose fields due to activated cooling water in nuclear facilities, 2019.

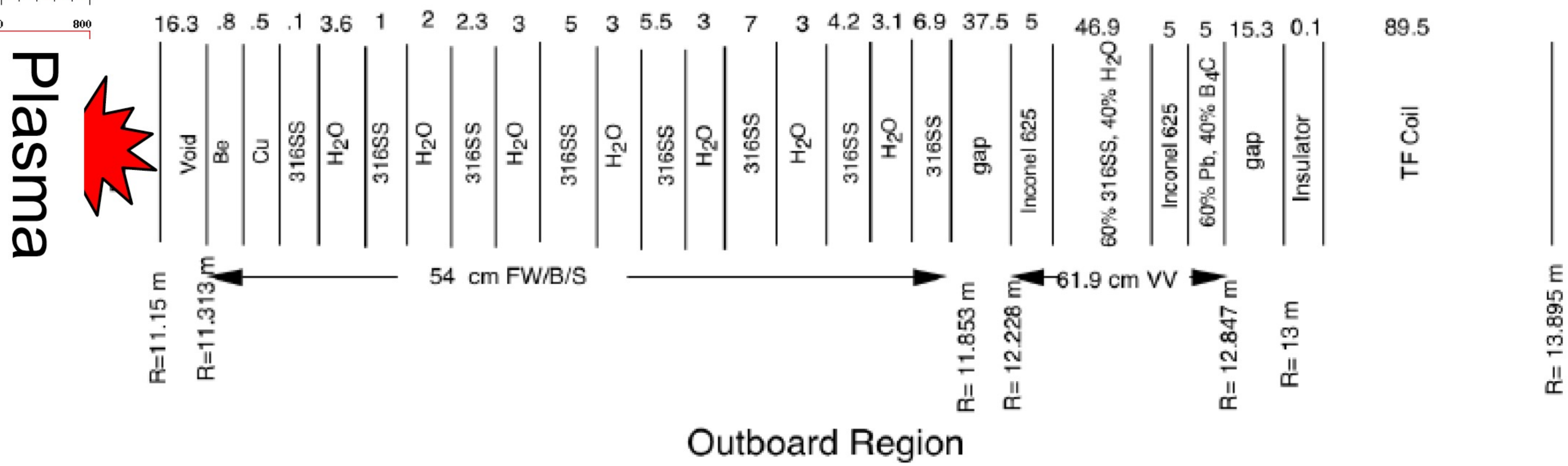
Shutdown dose rate

- D1S vs R2S
  - Both have advantages and drawbacks
  - Assumptions are made a-priori which might impact the results
  - Most code systems are internally developed and not available to the general public
  - Not enough experiments for validation/verification
- Nuclear data
  - Combination of transport and activation data
  - Lackluster or nonexistent propagation of uncertainties between steps
- Comprehensive validation and verification absolutely necessary to reduce safety margins

ITER 1-D cylindrical calculation benchmark – update!







Authored by Tim Bohm, University of Wisconsin, Madison. Pictures from: FENDL meeting 2020

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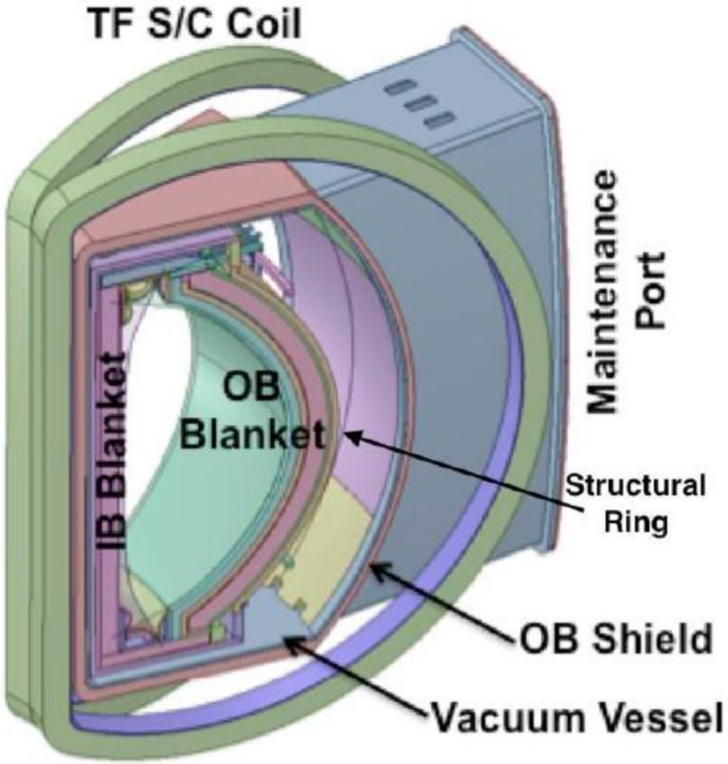
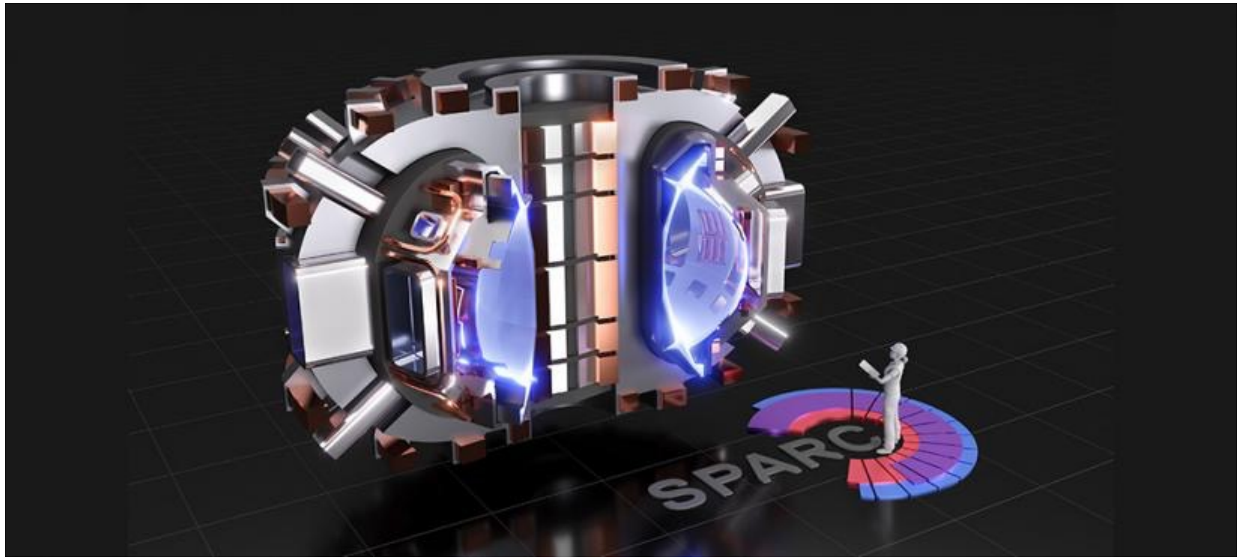
Simplified 3-D model

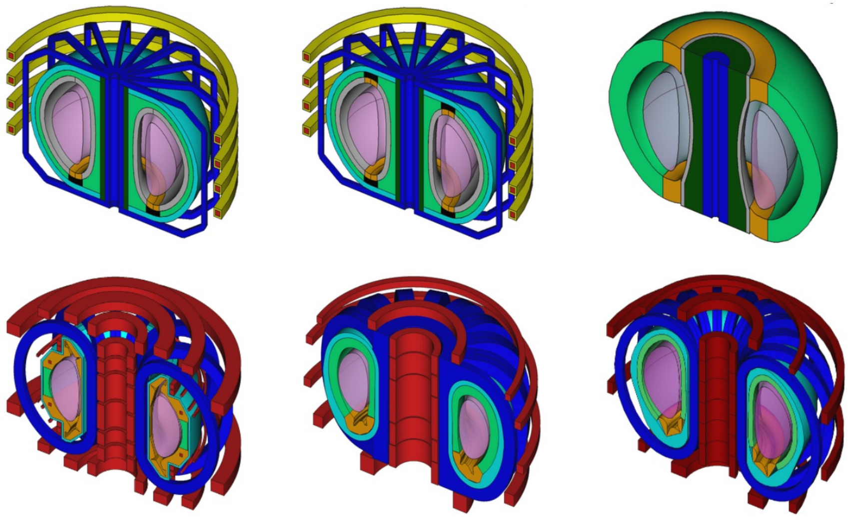
U.S. Fusion Nuclear Science facility (step to FPP)



Picture from:
T. Bohm, FENDL meeting 2020

SPARC or ARC
CAD rendering by T. Henderson, CFS/MIT-PSFC



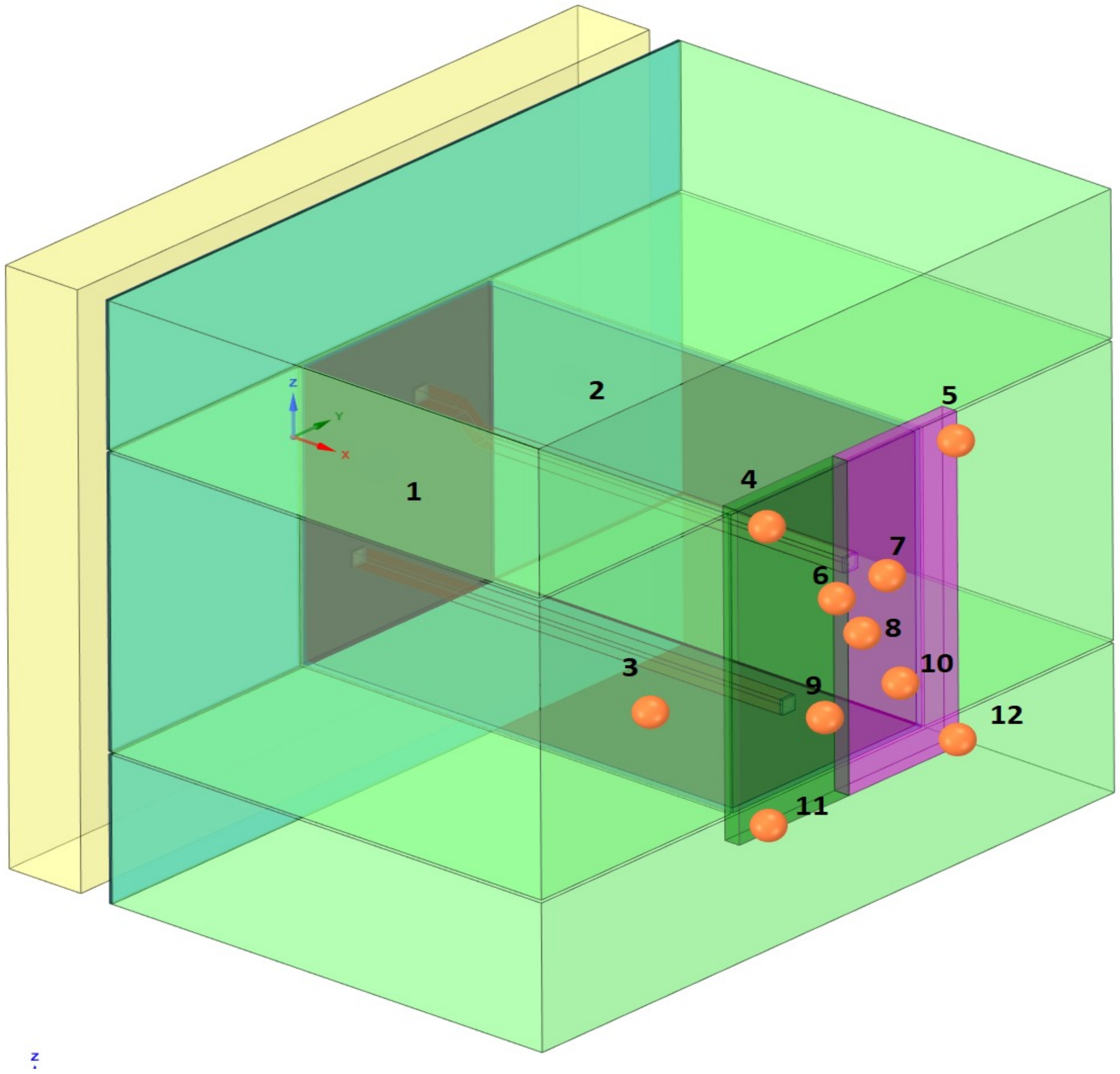


Generic model created using Paramak (https://paramak.readthedocs.io/en/main/)

ITER SDDR benchmark v2

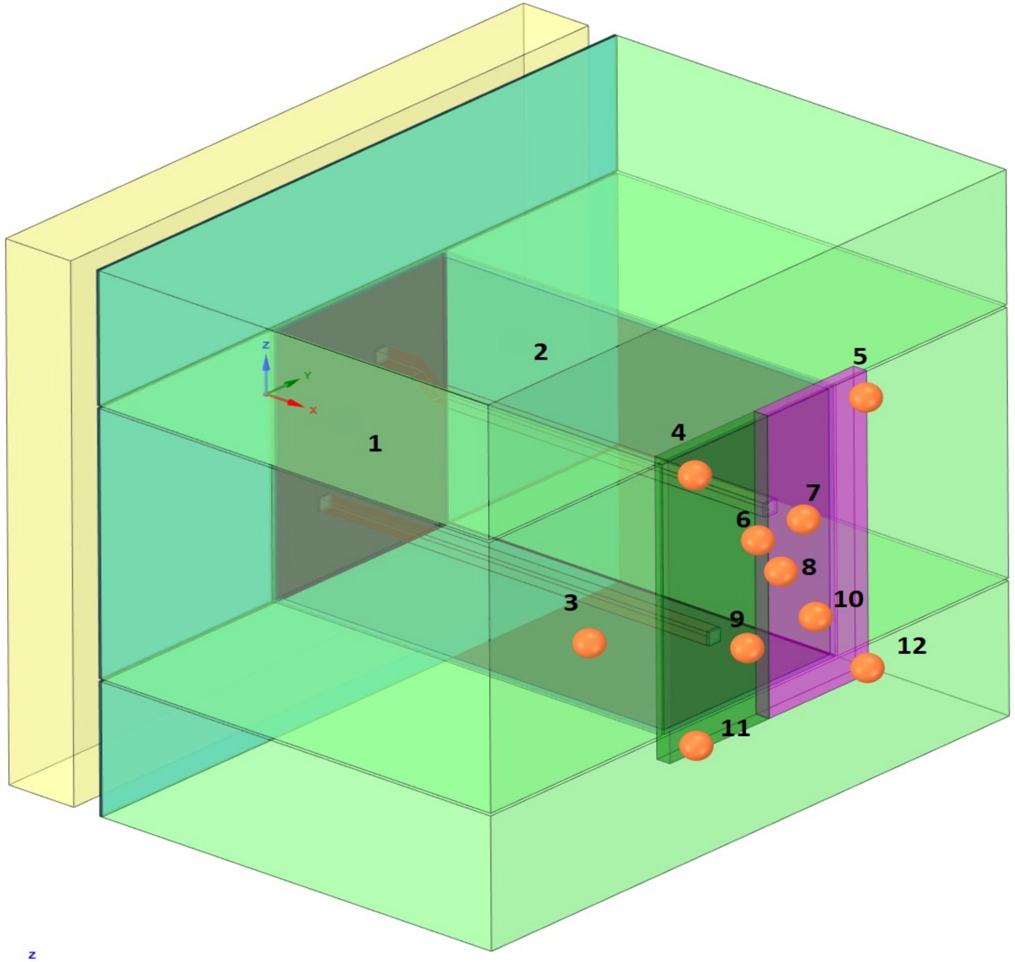
Why?

- Previous shutdown dose rate benchmark showed significant differences between results from different research groups
- It has been used, cited ~30 times, for validation of SDDR code systems
- Updated model, geometry and materials, based on current ITER design
- Simple enough to run on a workstation – can be used to attract new students to fusion neutronics



ITER SDDR benchmark v2 – blind test

- Quantities of interest
  - SDDR (1s, 6h, 10^6s)
  - Gamma spectra
- Target audience
  - Fusion neutronics labs and universities
- Distribution
  - CAD model
  - Material and source description
  - Irradiation scenario
- Release date
  - End of 2022



Experimental benchmarks

Experimental benchmarks

- SINBAD
  - Re-evaluate and prepare for modern code systems
  - CAD
  - Uncertainty quantification
- New experiments
  - Fill in the gaps
  - Address the lack of data in operational regimes outside of the currently operating machines

Re-evaluate for modern code systems

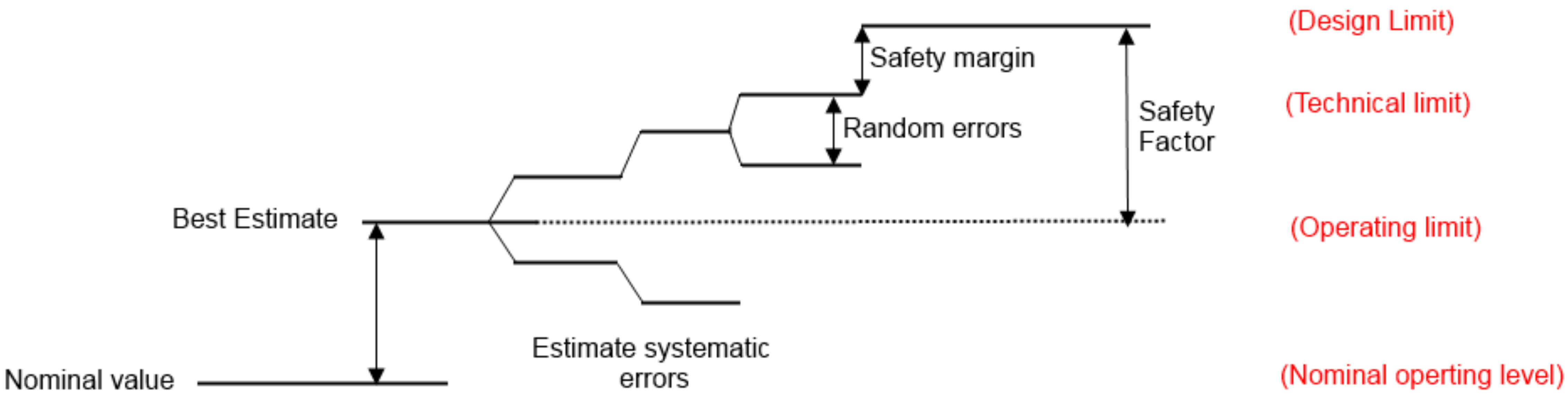
- Fusion benchmarks from SINBAD to the standards of ICSBEP
  - Based on the new “level” methodology proposed by the SINBAD task force
- Evaluate with modern codes and data
- Create CAD models as a starting point
- Perform sensitivity analysis on all relevant parameters
  - Data, material composition and impurities, geometry description including gaps etc.
- Priority list as we see it in collaboration with CFS:
  - Skyshine, FNG-SS, -Dose, -Copper, -W, -Streaming, FNS-Dogleg

CAD

- CAD should be the new starting point for every benchmark evaluation
- Establish a Q&A procedure for CAD models
  - Interferences, water tightness, bad surfaces etc.
- Common format – stp or STEP (Standard for the Exchange of Product Data)
  - One step file per material
- Metadata in json files
  - Material, source, tally response function etc.

Comprehensive uncertainty analysis to determine safety factor

- Methodology for Determination of Safety Factor for Nuclear Analysis, M. Loughlin, ITER IO



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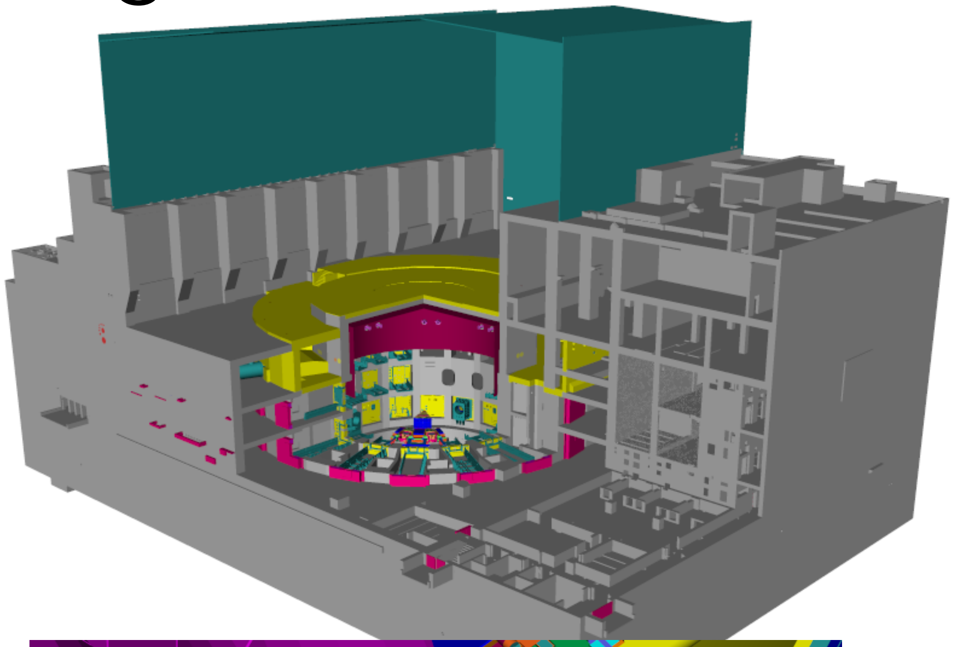
Tools and workflows at ORNL

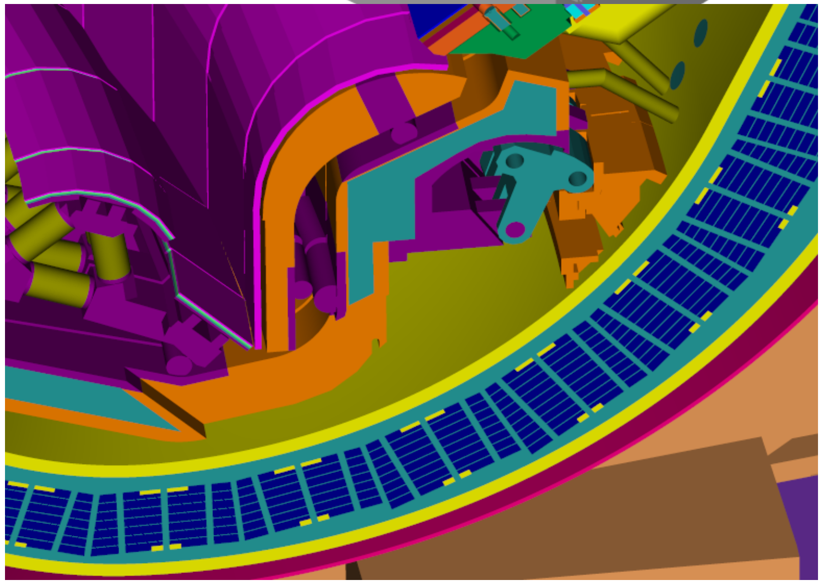
ORNL developed tools and methodologies

- ADVANTG (AutomateD VAriaNce reducTion Generator)
  - (FW-, MS-)CADIS workflow for variance reduction determination
- Denovo
  - 3D discrete ordinates, parallel, transport solver
- Shift
  - Massively parallelizable Monte Carlo transport code
- ORNL-TN (ORNL Transformative Neutronics)
  - Expanded and improved version of MCNP5v1.6

ORNL developed tools and methodologies

- Lava
  - MCNP runtpe file interrogation
  - LavaMint - Stochastic volume calculation.
  - Complement detector
- Python parser
  - Used to renumber cells, surfaces, universes and materials
- Radiant, Omnibus raytracer
  - 3D and 2D visualization of MCNP models.





MS-CADIS computational steps (ORNL R2S Code Suite)

1) Determination of variance reduction parameters for initial neutron transport using MS-CADIS
   a. Generate transition matrices
   b. Fold the transition matrices with the gamma adjoint transport solution
   c. Run ADVANTG in CADIS mode with the adjoint neutron source to determine VR parameters.
2) Neutron transport simulation
3) Activation calculation
4) Biased (CADIS) sampling the decay gamma source
5) Gamma transport simulation

Previous contributions to CoNDERC

Previous contributions to CoNDERC

- MCNP input decks created for TIARA shielding experiment
  - Concrete and iron (polyethylene remains)
  - 43 MeV and 68 MeV sources
  - Liquid scintillator (spectra), Bonner spheres and fission chambers
  - Variance reduction provided
  - Experimental data in readable form provided
  - Calculations with TENDL-2019, JEFF-3.3, JENDL-4.0, ENDF/B-VII.1 and ENDF/B-VIII.0
  - CAD models available but not distributed
- ASPIS Iron 88
  - Similarly to TIARA (Al, Au, In, Rh, S) inputs and variance reduction provided

Conclusion

Conclusion

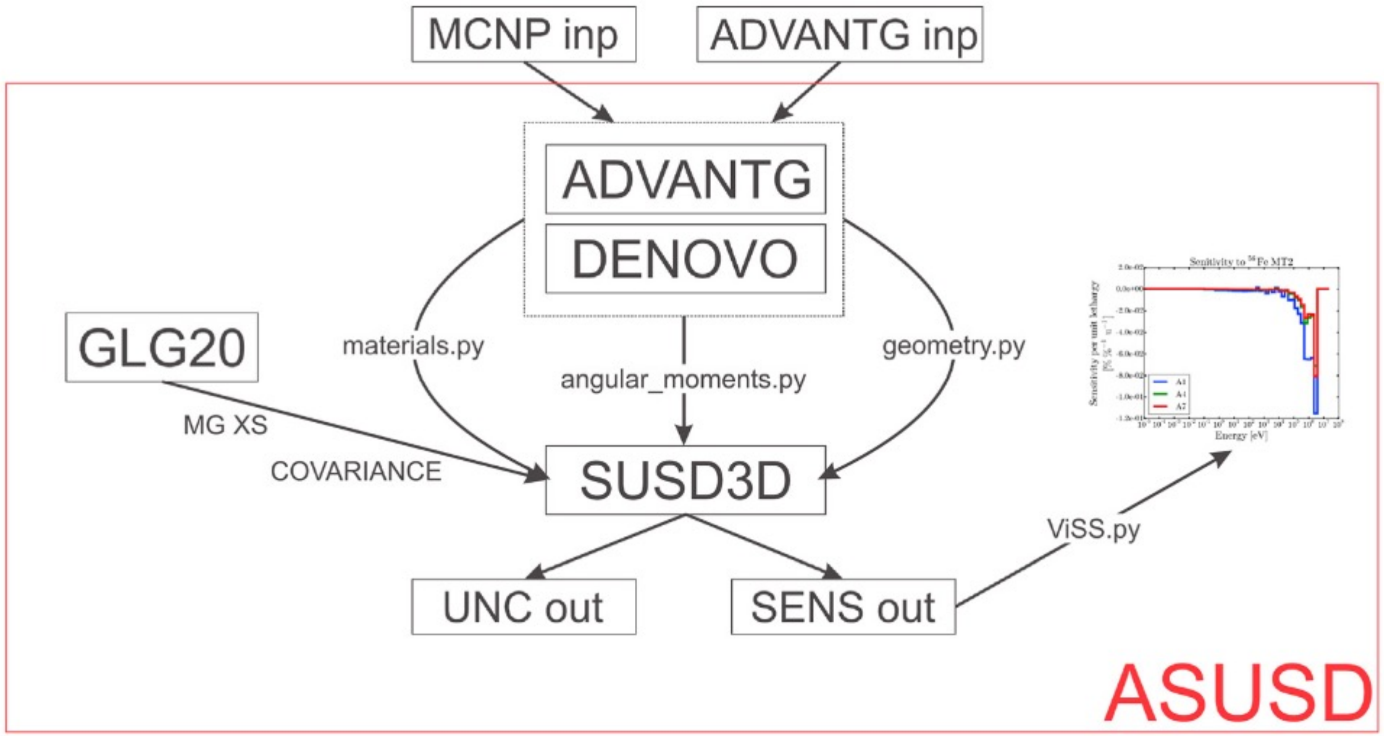
- Fusion is an emerging industry – neutronics must be an integral part of the design process
  - Tools, methodologies and workflows must be easily and comprehensively V&Ved
- Lack of user-accessible benchmarking tools for fusion neutronics
  - Computational benchmarks
  - Experimental benchmarks
  - Comprehensive uncertainty quantification
- ITER SDDR v2 blind test
- ORNL developed tools and methodologies
  - ADVANTG, Shift, ORNL-TN, Origen
- Previous contributions to CoNDERC

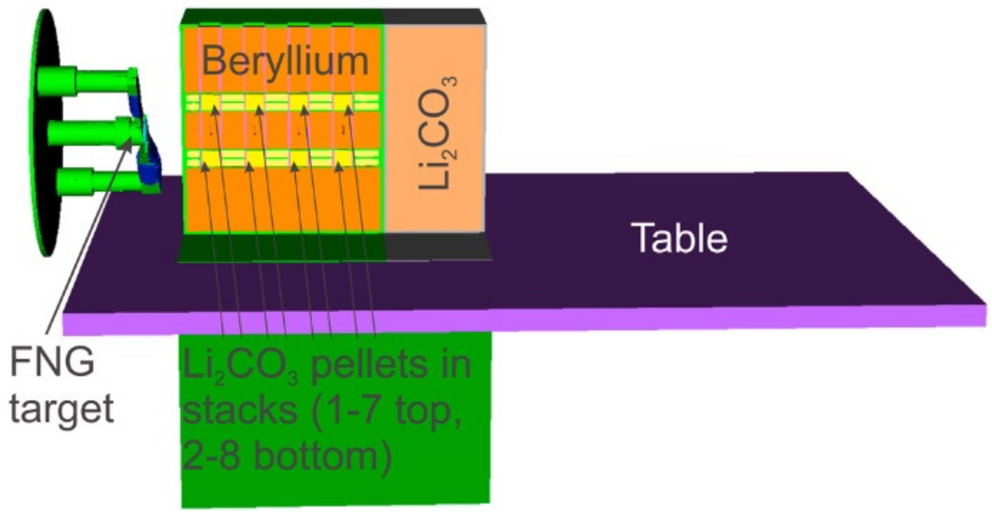
Additional slides

Nuclear data uncertainty propagation

- SUSD3D and ASUSD
  - Perturbation based nuclear data sensitivity and uncertainty analysis of criticality and fixed source problems
  - SUSD3D developed by I. Kodeli and coupled with several deterministic solvers
  - ASUSD, couples SUSD3D and ADVANTG. Applicable to larger models from MCNP. PhD thesis for fusion applications.
- SANDY
  - Random sampling of nuclear data developed by L. Fiorito
  - Independent of nuclear data evaluation (ENDF-6 format files)

ASUSD verification on FNG HCPB





Relative uncertainties of tritium production rate on ^{6}Li (MT105) in regard to MT2, MT16 and all partial reaction cross section (Total) uncertainty because of ^{9}Be. Calculated using SANDY and ASUSD.

	Stack 1 [%]		Stack 3 [%]	Stack 5 [%]	Stack 7 [%]	
	ASUSD	SANDY	ASUSD	ASUSD	ASUSD	SANDY
Total	2.7	2.8	2.6	2.3	2.0	2.0
MT16	1.2	1.4	1.1	1.1	1.0	1.2
MT2	2.4	N.C.	2.4	2.0	1.7	N.C.

Methodology and computation tools

- Variance reduction using ADVANTG
  - Prompt responses: CADIS or FW-CADIS

$$\sigma_{d\ FW-CADIS} = q_n^{\dagger}(\vec{r}, E_n) = \frac{1}{R_1}\sigma_{d,1} + \frac{1}{R_2}\sigma_{d,2} + \cdots + \frac{1}{R_N}\sigma_{d,N}$$

  - Delayed responses - SDDR: MS-CADIS

$$\sigma_{d\ MS-CADIS} = q_n^{\dagger}(\vec{r}, E_n) = \int K(\vec{r}, E_n \rightarrow E_p)\phi_p^{\dagger}(\vec{r}, E_p)dE_p$$