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Review of Challenges to Achieving Nuclear Data Sensitivity and Uncertainty Analysis for Fusion

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Outline

- Sensitivity analysis and uncertainty quantification
- Nuclear analysis workflows
- Nuclear data uncertainty analysis of gamma heating rates
  - JAEA FNS Clean Benchmark Experiments (V, W, Cu, Fe, C)
- Nuclear data uncertainty analysis of shutdown dose rates
  - ITER Equatorial Port Plug

Sensitivity & Uncertainty Analyses

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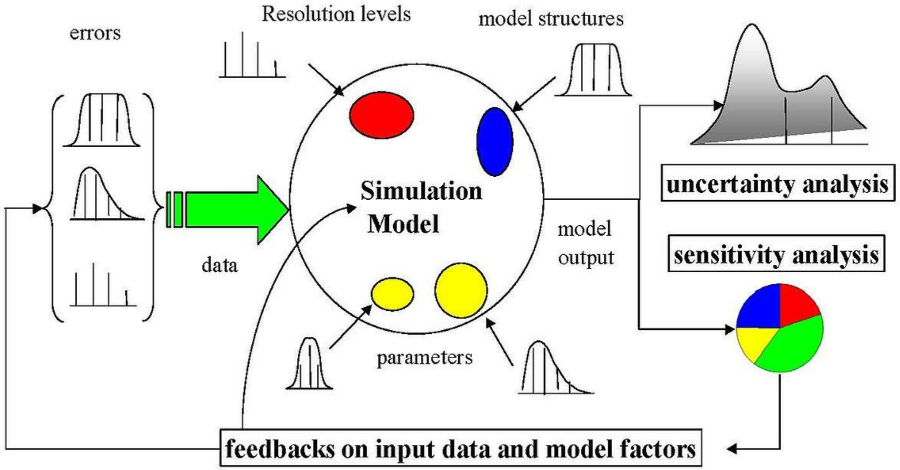
- Response uncertainty is caused by **uncertain input parameters**
- Propagation of input parameter uncertainties through code calculations is necessary:
- To breakdown response uncertainty into input parameter contributions
- To identify important input parameters (isotopes, reactions, energy ranges) contributing the most to the response uncertainty



Ref: Wikipedia "sensitivity analysis"

Motivation for Uncertainty Analysis

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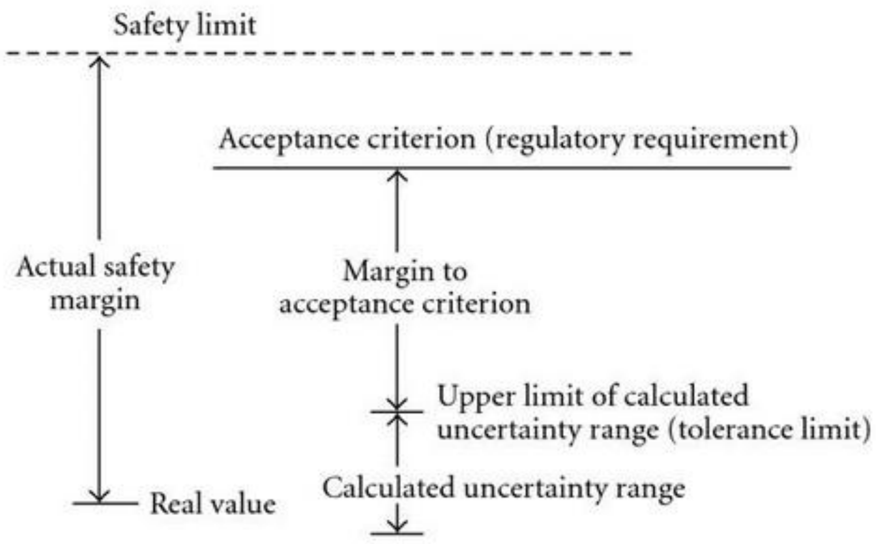
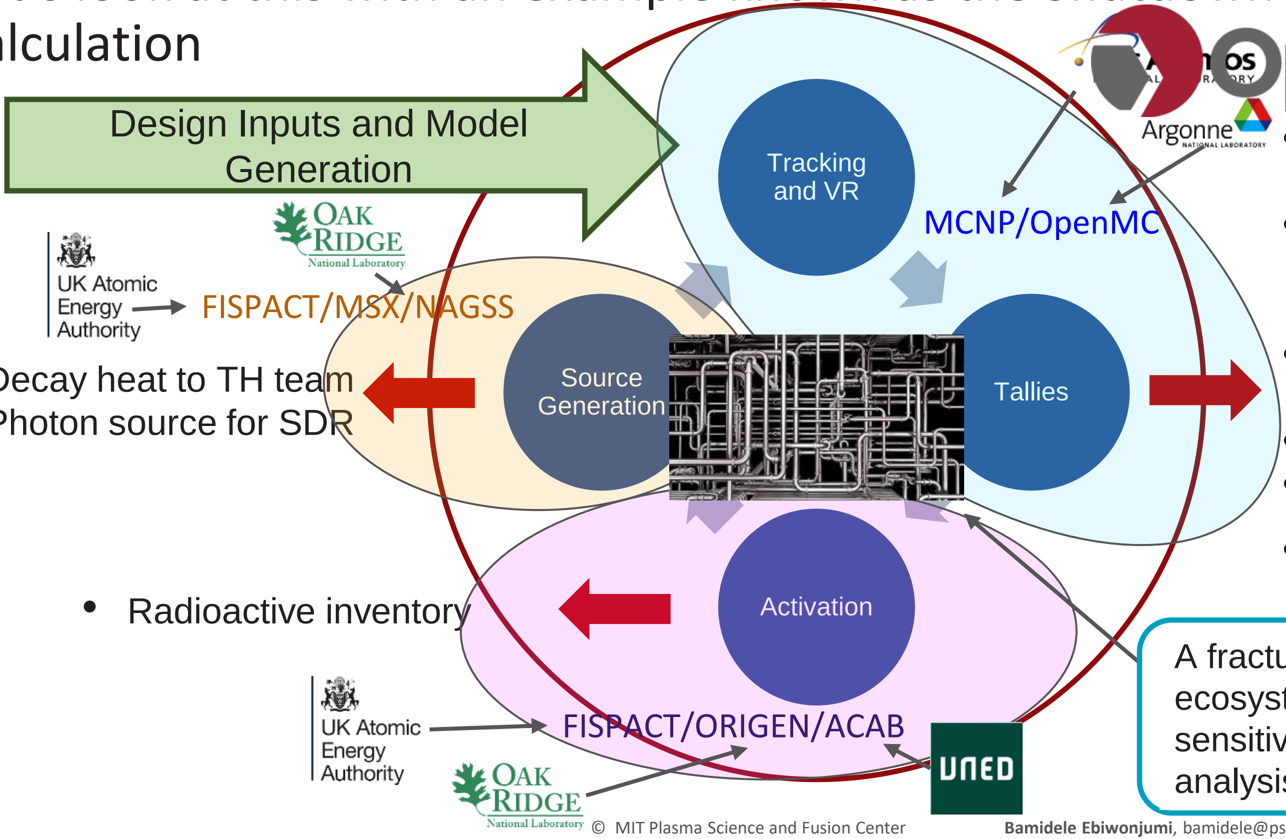
- Confidence in calculated quantities demand the uncertainty analysis of simulation responses
- Regulatory requirement: safety parameters must lie within acceptable criteria
- Conservatism in safety margins (traditional approach to safety analyses) has been minimized
- Current approach: Best Estimate Plus Uncertainty (BEPU) – best estimate acceptable if accompanied by uncertainty evaluation.



Glaeser, Horst, GRS Method for Uncertainty and Sensitivity Evaluation of Code Results and Applications, *Science and Technology of Nuclear Installations*, 2008, 798901

Nuclear analysis for fusion reactors

Let's look at this with an example known as the Shutdown Dose Rate (SDR) calculation



- Decay heat to TH team
- Photon source for SDR

- Radioactive inventory

- Nuclear heating to PFC, VV, and Magnet teams
- DPA / light atom production to structural teams
- Direct dose during operation
- TBR calculations
- Synthetic diagnostic info
- **Shutdown dose rate for maintenance**

A fractured simulation ecosystem complicates sensitivity and uncertainty analysis

Fusion Modeling S/U Analysis Software Ecosystem

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Nuclear data sampling	Transport, Activation, S/U Analysis
SANDY (SCK-CEN)	OpenMC (MIT, ANL)
FRENDY (JAEA)	MCNP (LANL) PERT card (differential operator sampling) FSEN (version 6.4)
TALYS (NRG)	SERPENT 2.2.1 (VTT)
	MCSEN (local update, MCNP patch)
	SUS3D (IJS) (adjoint flux: PARTISN, TORT, DENOVO, ATTILLA) (+ sensitivity analysis due to gamma cross-sections)
SAMPLER (ORNL)	SCALE (ORNL) DENOVO ORIGEN MONACO

Rigorous 2-Step & Direct 1-Step SDR Workflows

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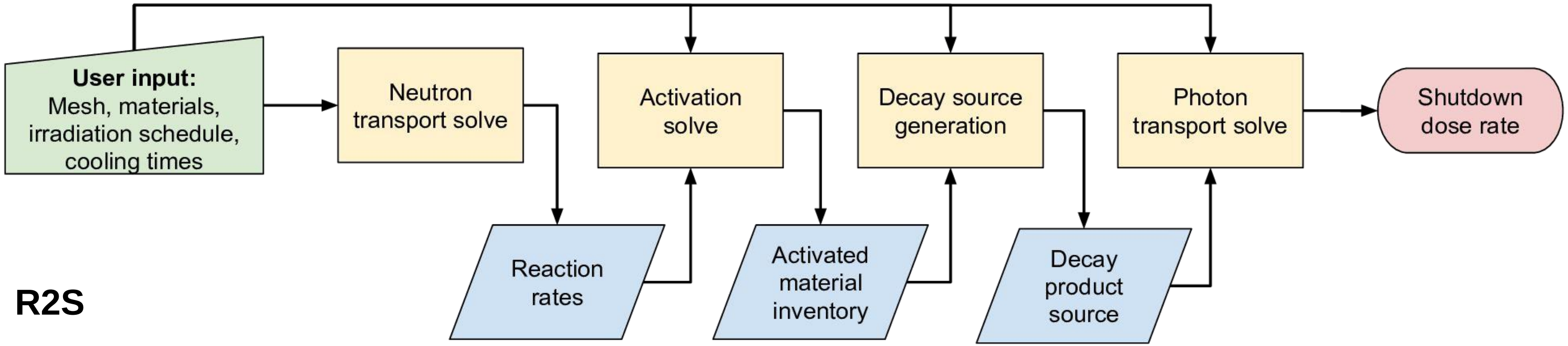
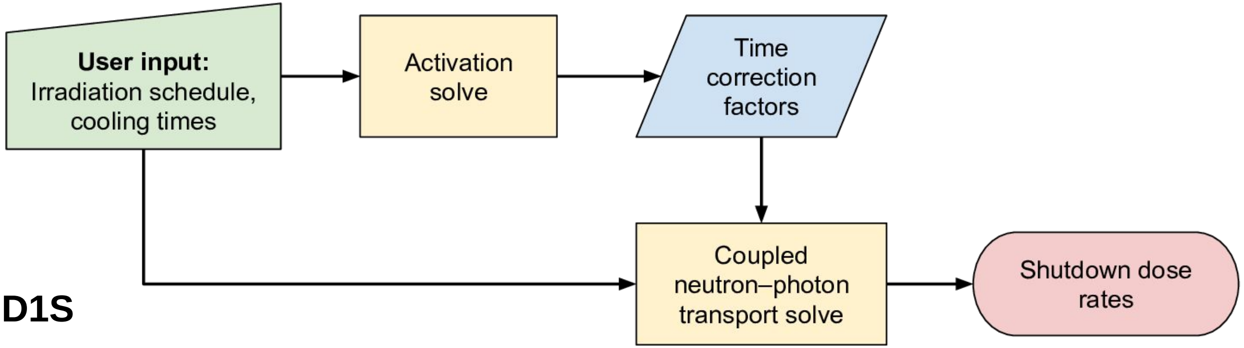


R2S

Peterson et al., Development and validation of fully open-source R2S shutdown dose rate capabilities in OpenMC, Nucl. Fusion 64 (2024) 056011



D1S

Romano et al., Initial implementation of the D1S methodology for shutdown dose rate calculations in the OpenMC Monte Carlo particle transport code. 26th Technology of Fusion Energy (TOFE) 2024, July 21 – 25, Madison, Wisconsin, USA.

Uncertain Input Parameters

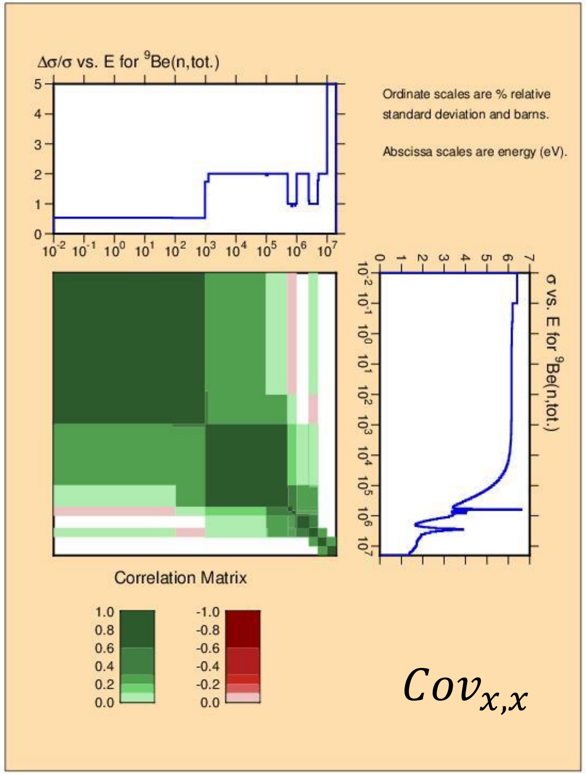
- Nuclear data
  - Activation data
  - Neutron cross-sections
  - Secondary particles:
    - energy distribution
    - angular distribution
  - Photo-atomic interaction data
  - Damage/displacement cross-sections
  - KERMA
  - ~~Fission product yield~~
  - Decay data (Q-values, half-lives)
    - Small effect on k_{eff}, inventory, decay heat
- Non-nuclear data
  - Material compositions, Design specifications
  - Operating conditions, Statistical errors

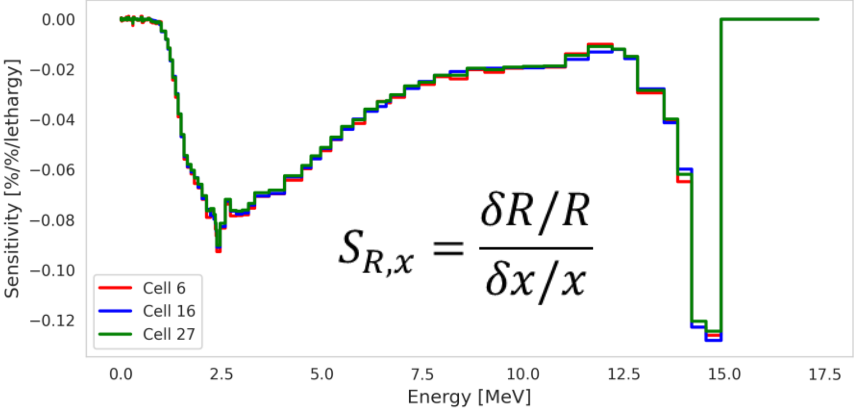
Library	Number of nuclides w/covariance
ENDF/B-VIII.0	182
JENDL-5	105
JEFF3.3	447
FENDL-3.1	58
TENDL	2,850
CENDL-3.2	70 (fission products)

Photo-atomic cross-section data
no covariance in ENDF/B library (NJOY)
Covariance location exist in GNDS (FUDGE)

KERMA/Displacement/Damage cross-section
no covariance in ENDF/B library (NJOY)

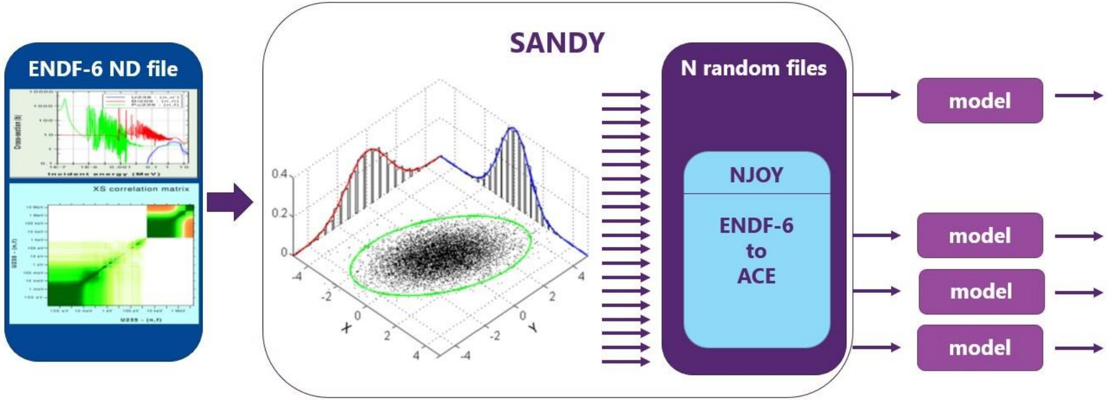
Nuclear Data Uncertainty Propagation





Sandwich Rule

$$\sigma_R^2 = S_{R,x} Cov_{x,x} S_{R,x}^T$$



E. Belfiore, Sensitivity and uncertainty analysis for nuclear data of relevance in spent nuclear fuel characterization, MSc Thesis, Politecnico di Torino, 2023.

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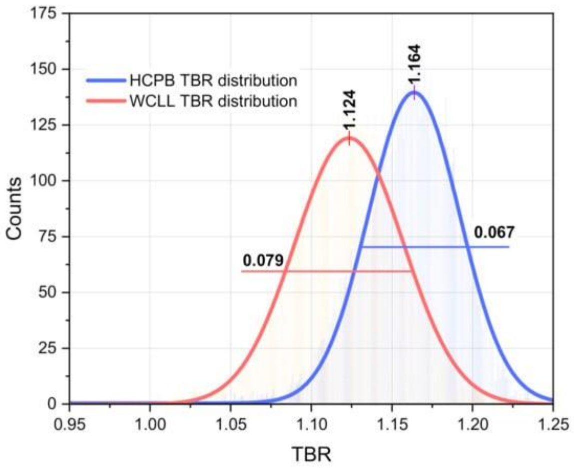
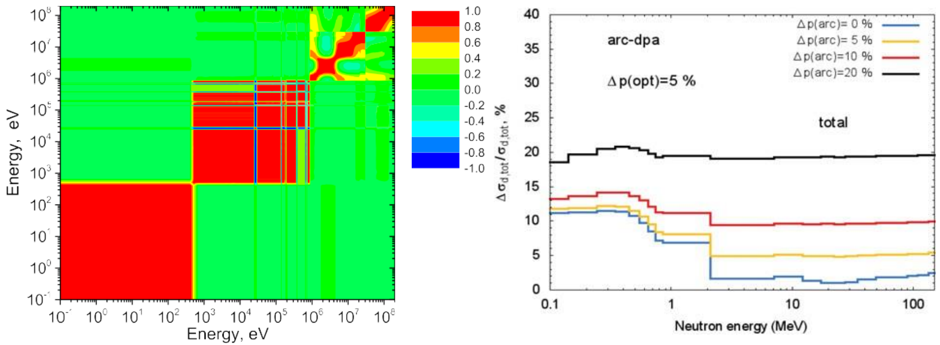
Nuclear Data S/U Analyses

- FNG Helium Cooled Pebble Bed (HCPB)
- Helium cooled lithium lead (HCLL) Test Blanket Module
- Water Cooled Lithium Lead (WCLL) DEMO blanket
- MIT ARC reactor design
- Karlsruhe spherical experiment (KANT)
- FNS/JAERI time-of-flight experiment (TOF)
- Oktavian, FNS and LLNL Pulsed Sphere expts.
- Non-existing and limited uncertainty analysis
  - Radiation damage, displacement cross-section
  - Nuclear heating
  - Shutdown dose rates



Park, et al., Statistical analysis of tritium breeding ratio deviations in the DEMO due to nuclear data uncertainties, Appl. Sci. 2021, 11(11), 5234.



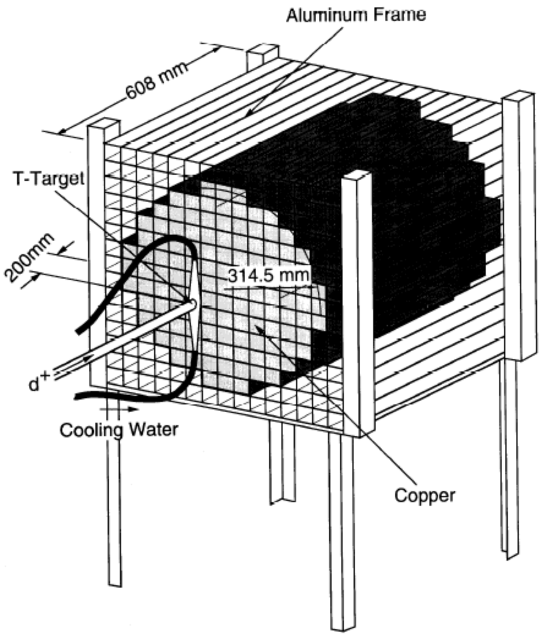
Simakov et al., Iron NRT- and arc-displacement cross sections and their covariances, Nucl Mat. Ene., 15 (2018).

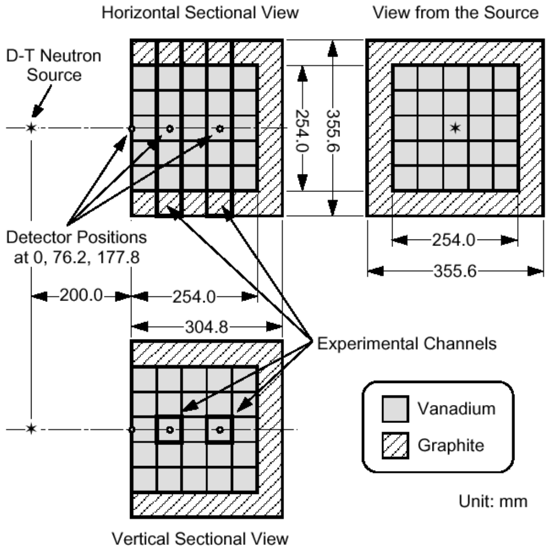
Uncertainty Analyses of Gamma Heating

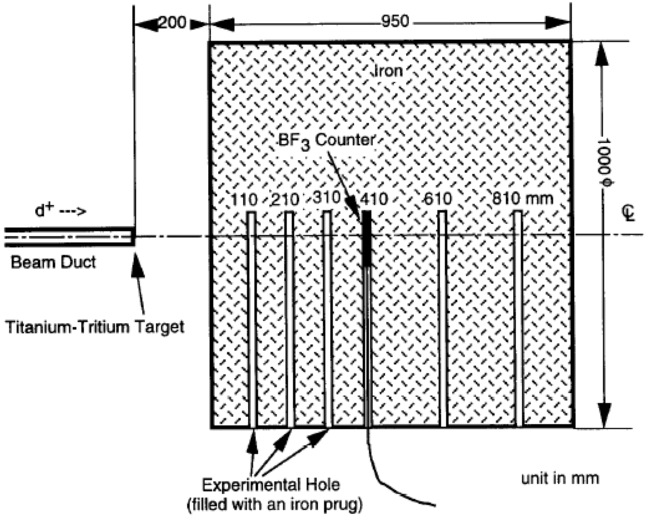
- JAEA FNS Clean Benchmark Experiments
  - Fe Cylinder, quasi-cylinder (W, Cu, C), V cube

Table 2 Nuclear heating rates and their required accuracy at various position for neutron wall loading of 1MW/m² in typical experimental fusion reactor.

positions	maximum nuclear heating rate	required accuracy
the first wall	~15 W/cm³	~20 %
inside blanket	~10 W/cm³	10~20 %
surface of divertor	~5 W/cm³	~20 %
vacuum vessel	~0.1 W/cm³	~50 %
toroidal coil	~0.001 W/cm³	~30 %

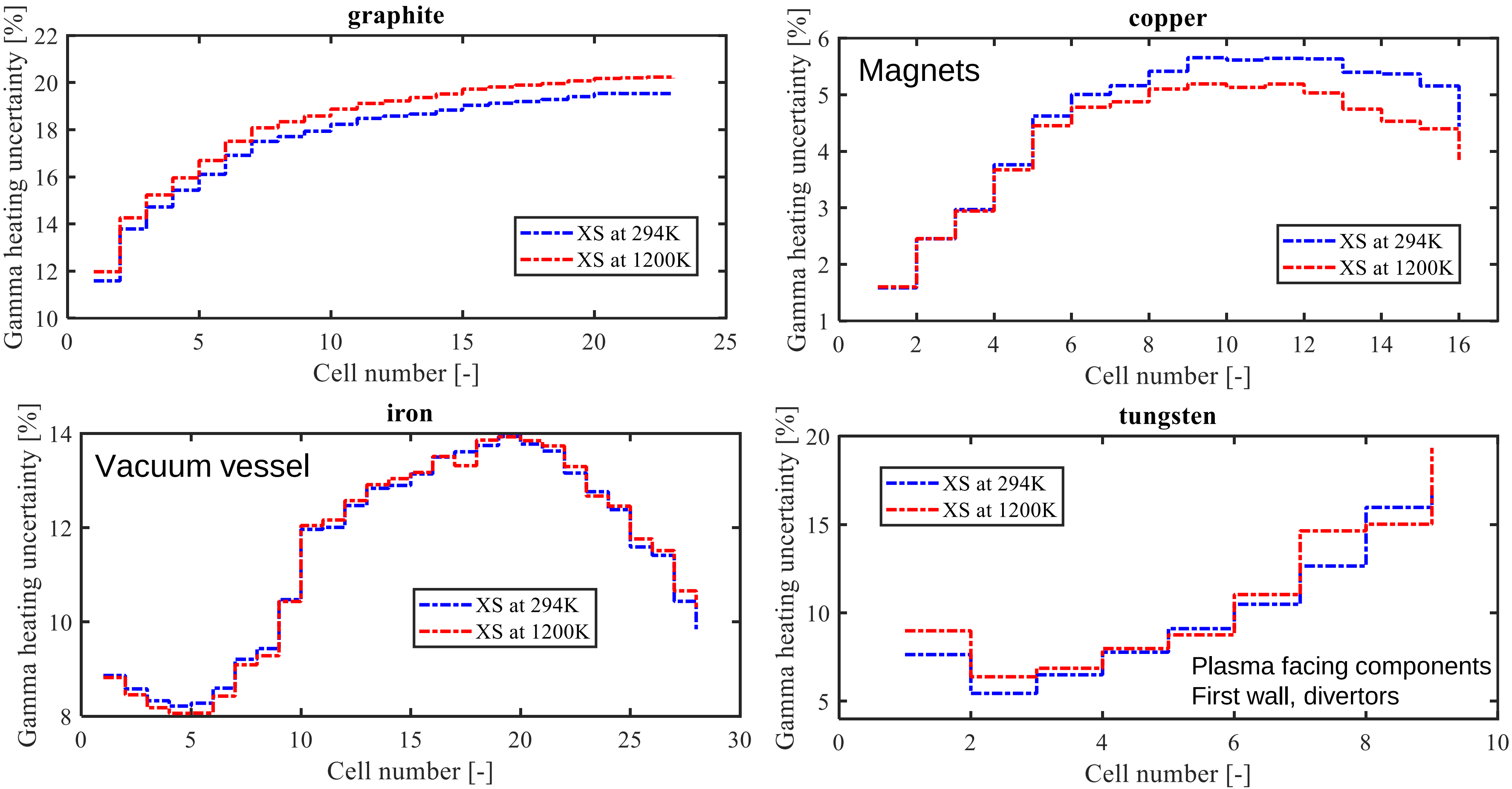






F. Maekawa, et al., Data collection of fusion neutronics benchmark experiment conducted at FNS/JAERI. JAERI-Data/Code 98-021, Japan Atomic Energy Research Institute, 1998.

Nuclear Data Uncertainty Analyses of Gamma Heating



Uncertainty Analyses of Shutdown Dose Rate

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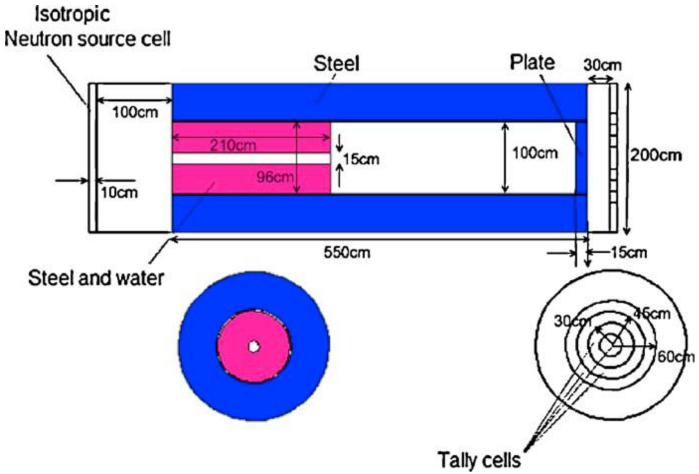
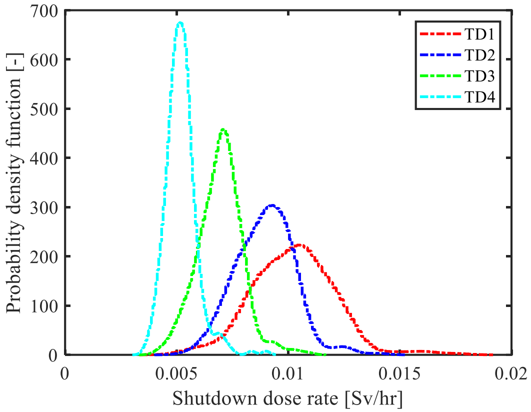
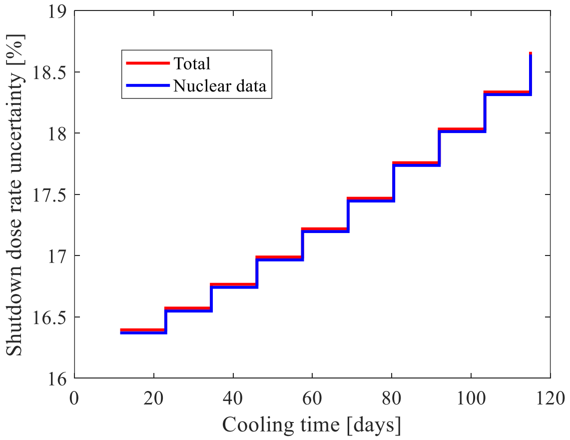


SRC, n/s	Duration	Repetitions
1.07E17	2 years	1
8.25E17	10 years	1
0.0	0.667 years	1
1.66E18	2 years	1
0.0	3920 s	17
2.00E19	400 s	
0.0	3920 s	4
2.80E19	400 s	



Ref: M. J. Loughlin, Conclusions of Shutdown Dose Rate Benchmark Study, IDM Number: 6593RF v1.0, 6th ITER Neutronics Meeting, Hefei, China, June 19-24, 2011

TD1	Stat. Err. [%]	NXS Uncer. [%]	Time
OpenMC/1	10.50	14.29	3 weeks
OpenMC/2	0.89	16.37	12 hours



Random cross-sections from SANDY
All reaction cross-sections with covariances perturbed
300 simulations performed

Challenges: ND Uncertainty Analysis

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Nuclides	Covariance library
^{54}Cr, ^{62}Ni, ^{58}Fe, W, V, Cu, $^{39,40,41}K$, $^{122,124}Sn$, $^{32,33,34,36}S$, ^{31}P, ^{93}Nb	JEFF3.3
$^{61,64}Ni$, ^{55}Mn, $^{112,114,115,116,117,118,119,120}Sn$, ^{181}Ta	TENDL-2019
$^{1,2}H$, $^{10,11}B$, ^{15}N, $^{46,47,48,49,50}Ti$, ^{59}Co, $^{90,91,92,94,96}Zr$, $^{92,94,95,96,97,98,100}Mo$, $^{206,207,208}Pb$, ^{209}Bi	ENDF/B-VII.1
^{12}C	ENDF/B-VIII.0
^{14}N	JENDL-5

Library	Number of nuclides
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KERMA/Displacement/Damage cross-section
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Summary

- Uncertainty propagation through fusion workflows is limited due to workflow complexities, nuclear data and availability of computational tools
- Gaps in nuclear data, coupling different codes, and lack of single platform makes S/U analysis challenging in fusion
- For responses with limited and incomplete uncertainty analysis
  - Radiation damage/dpa (cross-section uncertainties N/A)
  - Shutdown dose rates (photo-atomic cross-section uncertainties N/A)
  - Nuclear heating (photo-atomic cross-section & KERMA uncertainties N/A)
  - Randomly sample model parameters (TALYS)
    - Calculate cross-sections from random model parameters (NJOY HEATR/GAMINR)
    - Obtain statistical moments, propagate uncertainties through code

Thank you!

This work is supported by
Commonwealth Fusion Systems

Backup Slides

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- No nuclear data random sampling code can sample photo atomic cross-section data, KERMA, damage/displacement cross-sections, using their covariances
- TALYS can produce random samples of the nuclear data mentioned above for the TENDL library
- Nuclear data random sampling codes mostly have been developed for neutron cross-section data
- Complete sensitivity analysis isn't possible currently for nuclear heating and shutdown dose rate calculations
- Only P_1 terms in MF34 (covariance of secondary angular distribution) can be typically processed
- Currently, uncertainty quantification isn't a priority in FENDL, will be in future.
- Comprehensive assessment of target accuracy of fusion reactor responses is pending
- In evaluated file 'A', taking data from evaluated file 'B' for some specific utilization, destroys consistency among data.