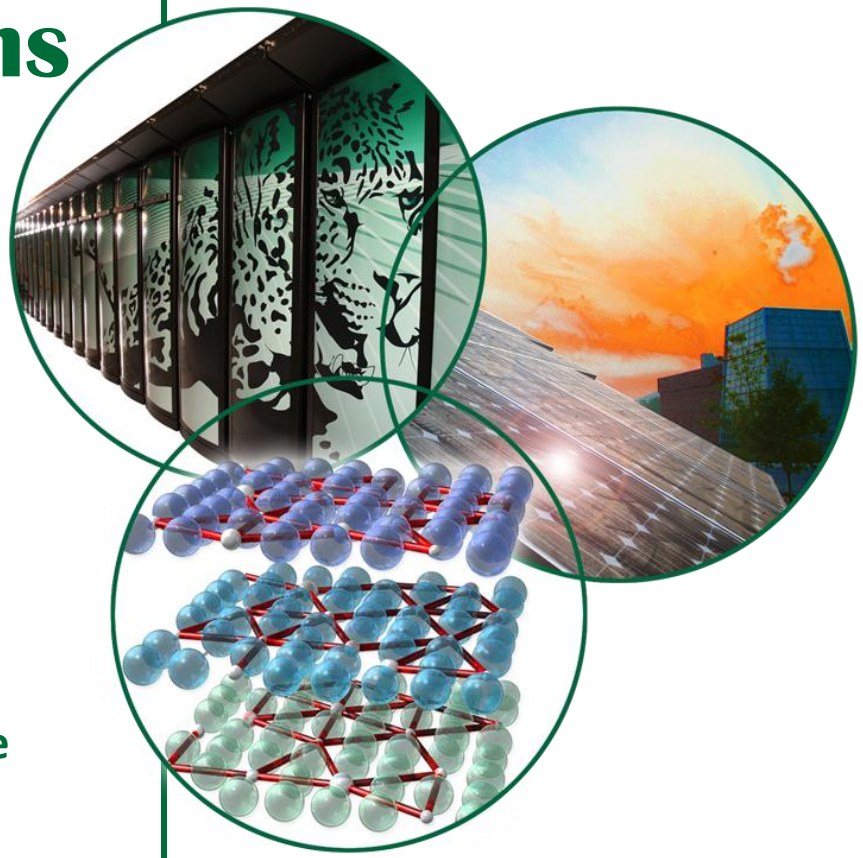
Nuclear Data Error Propagation in Fusion Benchmark Calculations



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Motivation

- Uncertainty quantification for a one-dimensional fixed-source geometry using ORNL's Scale Code System
  - *Determine the uncertainty in the calculated total flux outside of a spherical system*
    - *Uncertainty in the calculated response comes from two sources*
      - *Uncertainty in nuclear data (i.e. cross sections)*
      - *Uncertainty in the fixed source*
- An example problem from the SINBAD fusion database will be used to illustrate fixed-source S/U analysis.

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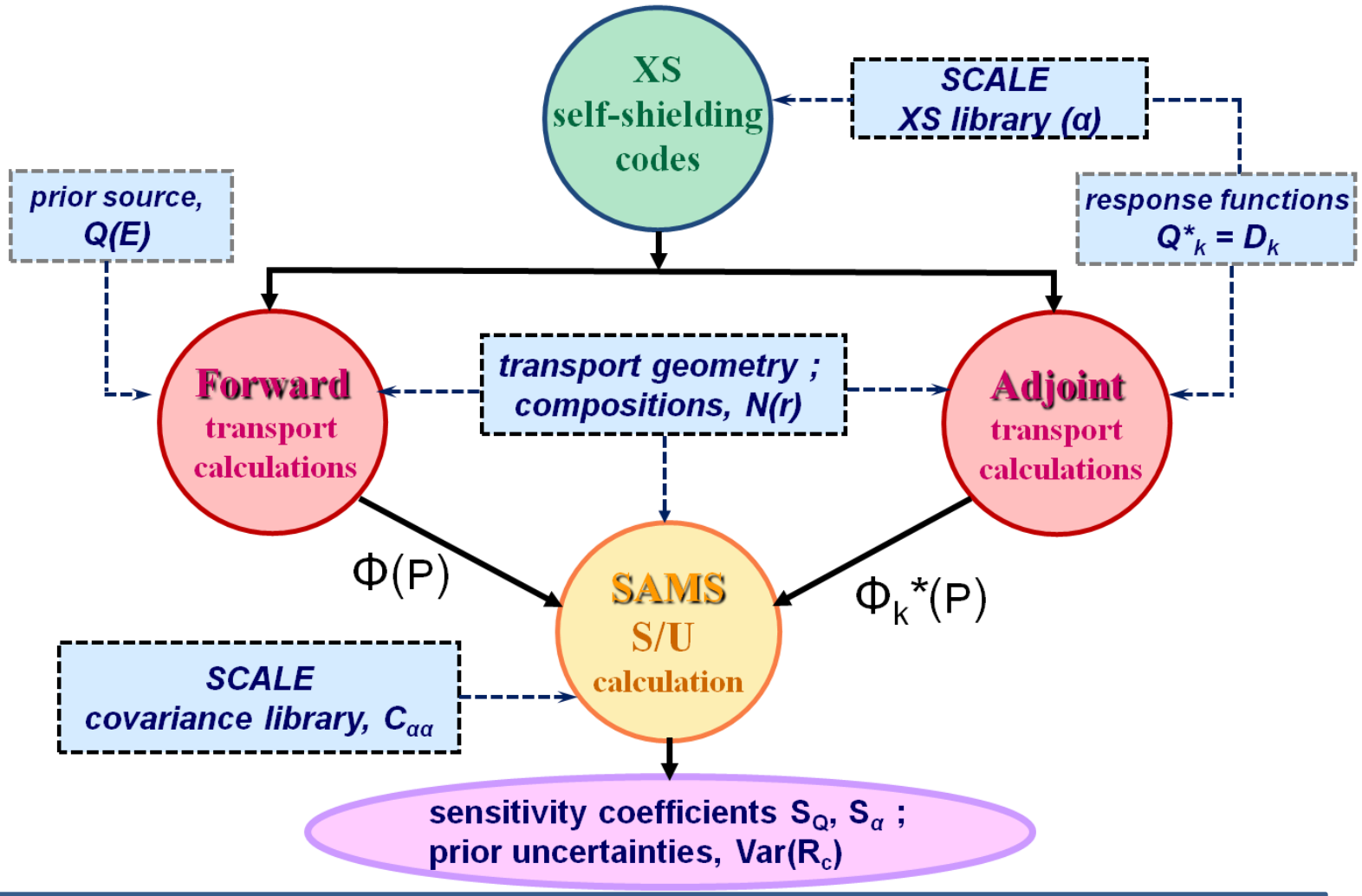
TSUNAMI Computation Sequence



SAMS was previously capable of S/U analysis for eigenvalue problems only. It was recently updated for fixed-source S/U analysis.

Sensitivity to Nuclear Data

- The sensitivity of a given response to the cross section data is given by

$$S_{x,i} = \frac{\sigma_x}{R_i}\frac{dR_i}{d\sigma_x}$$

where σ_x is the cross section for reaction x and R_i is the function of interest

- Scale calculates sensitivity to a large variety of cross sections:

  Total, elastic and inelastic scattering, capture, fission, (n,α) , (n,γ), (n,2n), etc

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Sensitivity to Fixed Source

- The sensitivity of a given response to the cross section data is given by

$$S_{q_n,i} = \frac{q_n}{R_i}\frac{dR_i}{dq_n}$$

where q_n is the fixed source of interest and R_i is the response function of interest

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Calculation of Sensitivity Coefficients Using Adjoint-Based Perturbation Theory

- Adjoint-Based Perturbation Theory calculation of sensitivity of a response to the total cross section

$$\frac{dR_i}{d\sigma_t} = \int dV \int d\Omega \int dE\ \psi^*(\mathbf{r}, E, \mathbf{\Omega})\sigma_t \psi(\mathbf{r}, E, \mathbf{\Omega})$$

- Adjoint-Based Perturbation Theory calculation of sensitivity of a response to the fixed source

$$\frac{dR_i}{dq_n} = \int dV \int d\Omega \int dE\ \psi^*(\mathbf{r}, E, \mathbf{\Omega}) q_n$$

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Propagation of Uncertainty

- The uncertainty in a given response as a function of sensitivity coefficient is given by

$$\delta_{R_i} = SCS^T$$

S: sensitivity coefficients for a given cross section or source

C: matrix of covariances between nuclear data or source energy groups

- Covariance Data:
  - Cross Sections: Scale has covariance data for > 300 materials
  - Fixed Source: Covariance is assumed to be =1 between all energy groups for the fusion benchmark problems (data assumed to be fully correlated)

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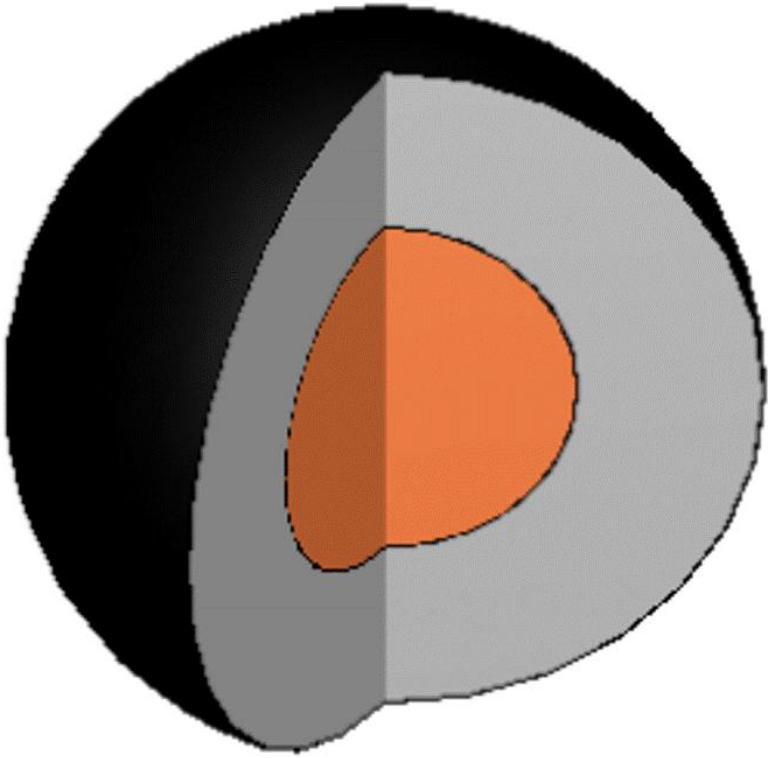
Test Geometry



Source region (Air)
0.0 -10.0 cm

Aluminum Shield Region
(10.2 -19.75 cm)

Casing Regions
(Chromium, Nickel, Iron) –
0.2 cm thick

- 14 MeV Neutrons are created by D-T fusion in the air region
- The VitaminB7 200 energy group neutron library is used in the simulations
- neutrons/cm^3·s are measured in a 0.5 cm thick region of void surrounding the outer casing region - the adjoint source is a volumetric source of 1.0 in each energy group throughout this region

Geometry and source information are taken from the Oktavian Program fusion experiment studies

Source Information

Lower Energy (MeV)	Upper Energy (MeV)	Source ($n/cm^3 \cdot s$)	Variance ($n/cm^3 \cdot s$)
17.333	20.000	0.000044	0.000029
15.683	17.333	0.180111	0.000384
14.550	15.683	0.451046	0.000797
13.840	14.550	0.631132	0.000983
12.840	13.840	0.181859	0.000395
10.000	12.840	0.006069	0.000099
8.187	10.000	0.00106	0.000055
6.434	8.187	0.00069	0.000047
4.800	6.434	0.00055	0.000046
4.304	4.800	0.00051	0.000045
3.000	4.304	0.00047	0.000044
2.479	3.000	0.00062	0.000044

Sensitivity Analysis

Sensitivity of calculated response to material cross sections (% change in response due to a 1% change in cross section)

Material	Total Scatter	Capture	Total	Direct Perturbation (Total)	Percent Difference
Aluminum	0.214642	-0.189360	0.02528	0.02521	0.278
Chromium	0.007321	-0.000533	0.00678	0.00662	2.42
Nickel	0.004293	-0.001191	0.00302	0.00303	-0.330
Iron	0.025954	-0.003174	0.02278	0.02264	0.618

Sensitivity of calculated response to fixed source for 2 selected energy groups

Energy Group	Sensitivity	Direct Perturbation	Percent Difference
13.84-14.55 MeV	0.424178	0.424967	-0.186
12.84-13.84 MeV	0.121054	0.121291	-0.195

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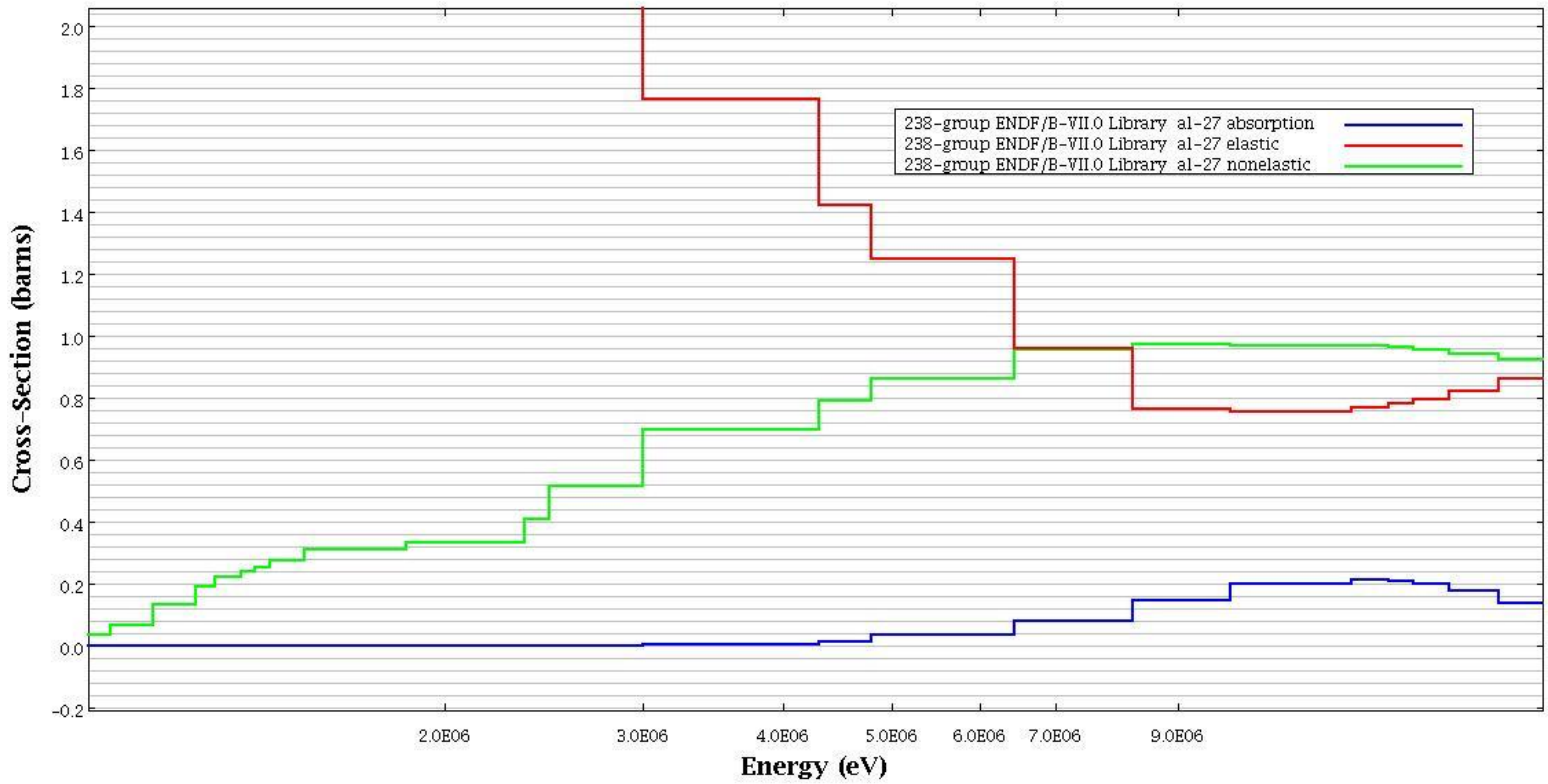
Why Positive Total Sensitivities to Shield Materials?



Absorption in ^{27}Al drops to near zero around 6 MeV. Increased number density in the shielding material yields more scattering into lower energies – meaning less absorption and more neutron leakage

Uncertainty of Calculated Responses

- Uncertainty in calculated response due to uncertainties in cross section data: 0.9969%
  - Top contributors to nuclear data uncertainty:

Nuclide-Reaction	Nuclide-Reaction	Uncertainty Contribution
^{27}Al (n,2n)	^{27}Al (n,2n)	0.6672
^{27}Al (n,p)	^{27}Al (n,p)	0.4484
^{27}Al (n,n')	^{27}Al (n,n')	0.4186
^{56}Fe (n,2n)	^{56}Fe(n,2n)	0.3060
^{27}Al (n,α)	^{27}Al (n,α)	0.2985
^{27}Al elastic	^{27}Al (n,n')	-0.2792

- Uncertainty in calculated response due to uncertainties in fixed-source: 0.6876%
- Calculated Response: 366.475 ± 1.211%

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Summary and Conclusions

- The TSUNAMI-1D Sequence in Scale has been modified to do fixed-source uncertainty analysis
  - *Capable of handling sensitivity of a response to both the material cross sections and the fixed source itself*
- An example problem from the SINBAD fusion database was used to illustrate this new capability
  - *Variances and covariances for cross section data were taken from cross section libraries*
  - *Variances in the fixed source were taken from the original benchmark publication, covariances between energy groups in the source were assumed to be =1*

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Summary and Conclusions (cont'd)

- A calculated response uncertainty that accounted for both sources of uncertainty was computed, yielding the following results:

Response: 366.475 ± 4.438 n/cm^{3}s
Total Uncertainty: 1.211%
Uncertainty due to uncertainty in nuclear data: 0.9969%
Uncertainty due to uncertainty in fixed source: 0.6867%

- Propagation of fixed source uncertainty shows that uncertainty in the scalar flux response due to uncertainty in the source is an order of magnitude larger than the uncertainty in the strongest source groups (the groups near 14MeV)

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