Multigroup Data Libraries for SCALE Applications

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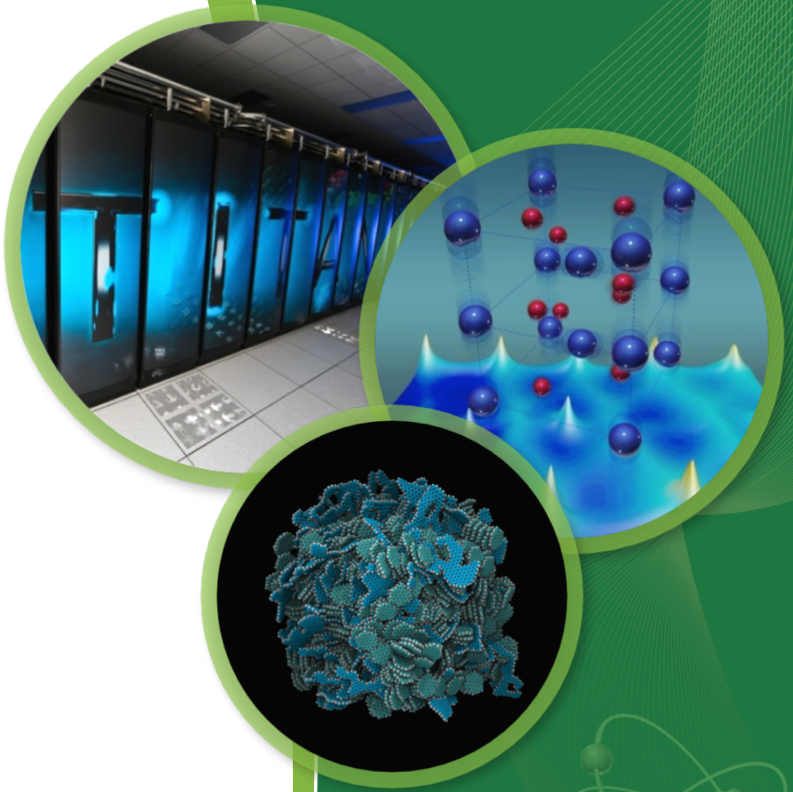
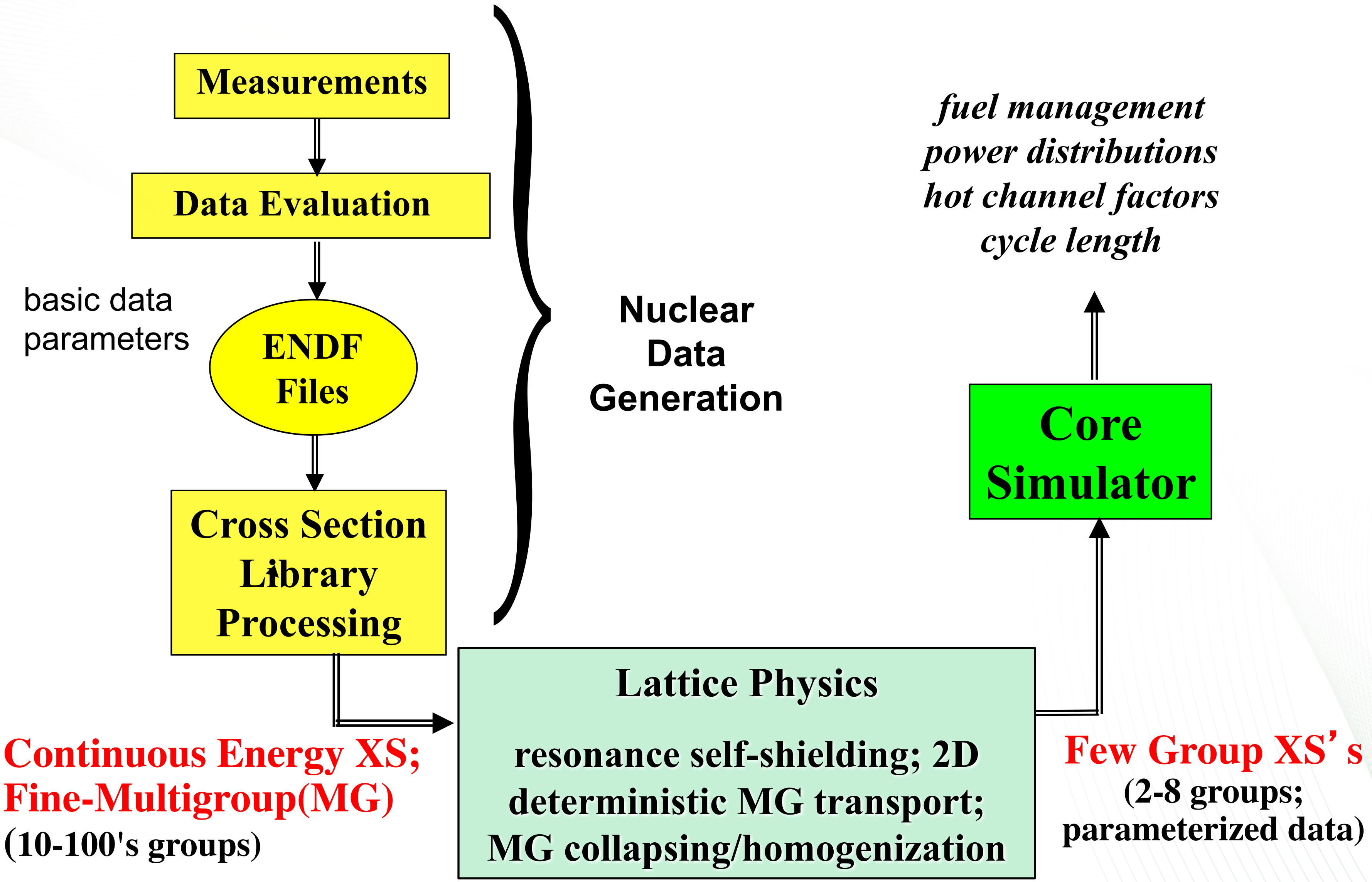


SCALE Users' Group Workshop

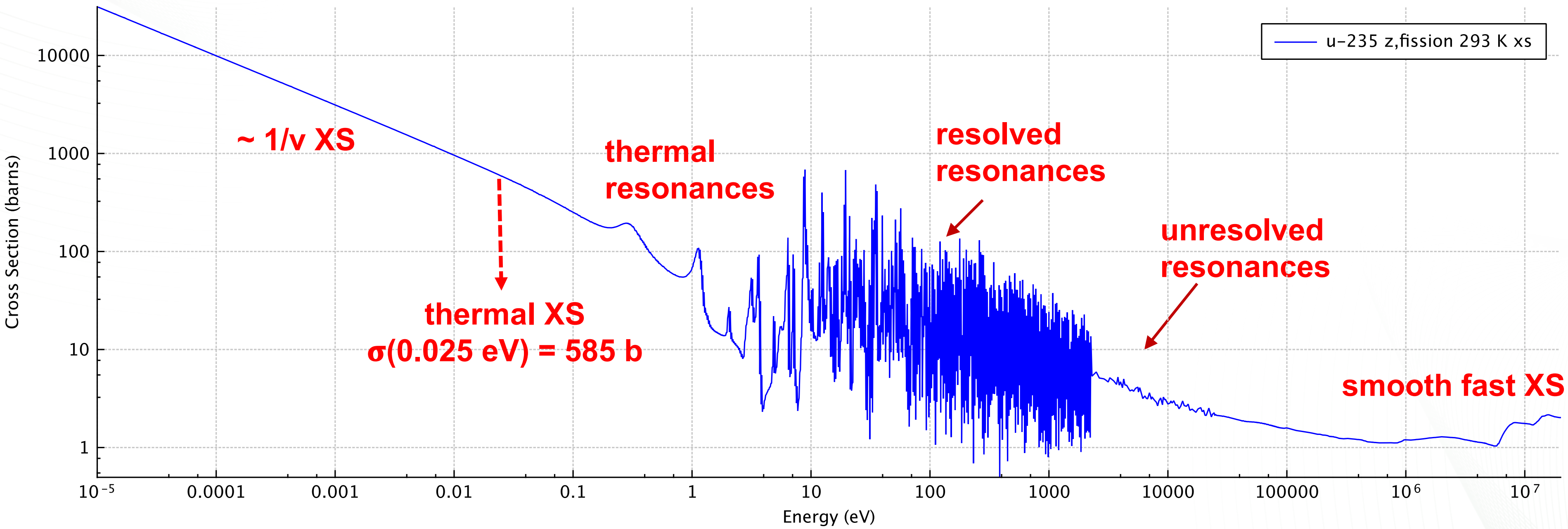
Oak Ridge, TN.

Sept. 27, 2017

Cross-Section Generation

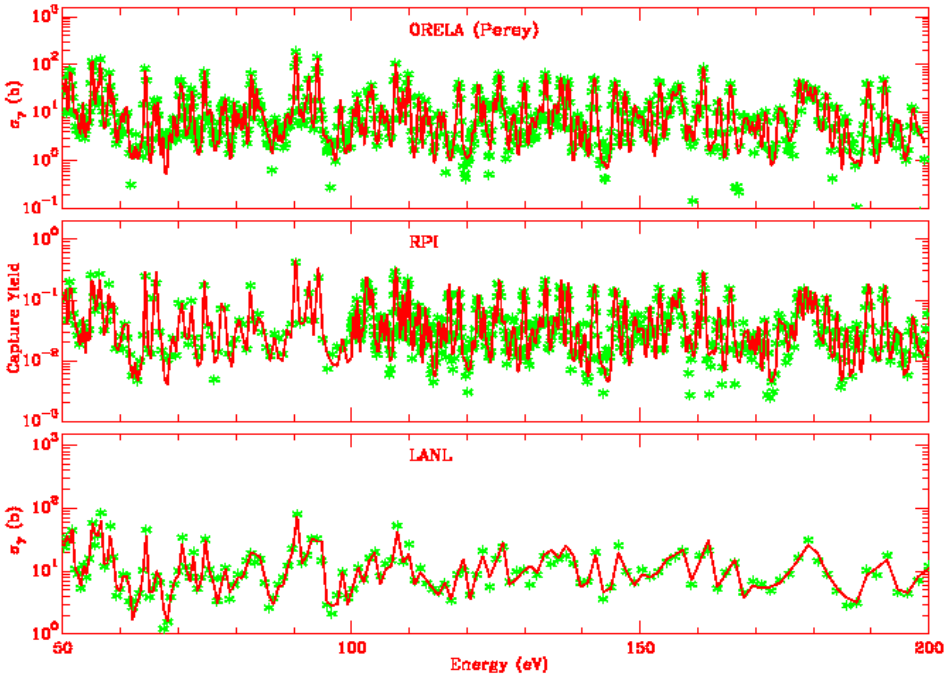


U235 Fission Cross Section



Evaluated Nuclear Data

- Experimental measurements provide interaction probabilities [$\sigma(E)$] vs. neutron energies
- Theoretical expressions $\sigma(E)$ can be derived from quantum mechanics
- Regression of parameters in nuclear physics models performed to best fit measured values
- Evaluated parameters and $\sigma(E)$ stored in ENDF/B files



ORNL Evaluation of U-235 Capture Data 50 – 200 (eV)

Measurements

↓ ***σ vs. E distributions***

Data Evaluation

↓ ***nuclear data parameters***

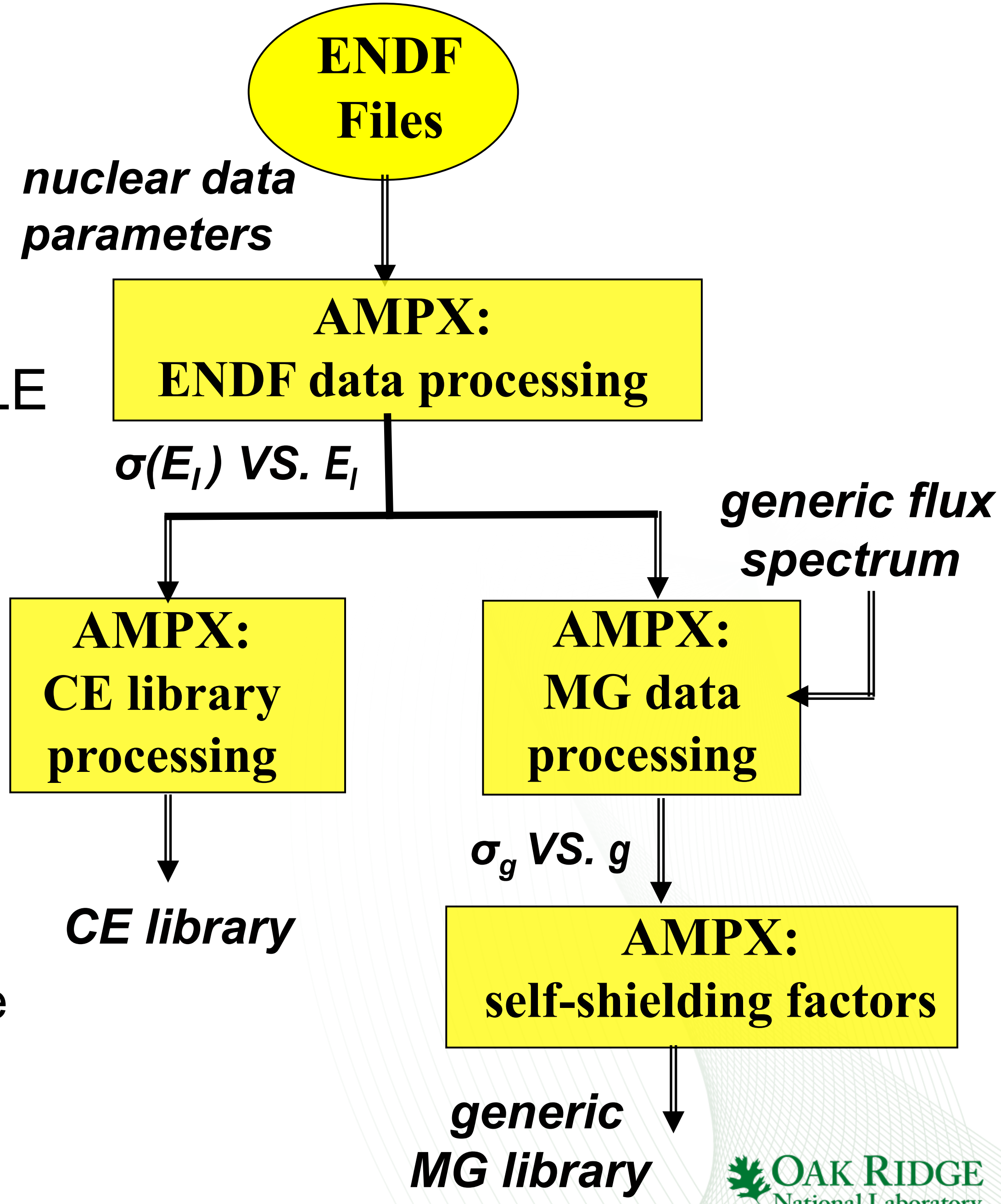
ENDF Files

ENDF/B-VII.1 Contains Evaluated Nuclear Data for 423 Nuclides

File	Description	File	Description
1	**General Information**	10	Cross Sections for the Production of Radioactive Nuclides
2	**Resonance Parameters**	11	General Comments of Photon Production
3	**Neutron Cross Sections**	12	Photon Production and Multiplicities and Transition Probability Arrays
4	**Angular Dist. of Secondary Particles**	13	Photon Production Cross Sections
5	**Energy Dist. of Secondary Particles**	14	Photon Angular Distributions
6	**Coupled Energy-Angle Dist. of Secondary Particles**	15	Continuous Photon Energy Spectra
7	**S(α, β) Scattering Law Data**	23	Photon Interaction Cross Sections
8	Radioactive Decay and Fission Product Data	27	Atomic Form Factors or Scattering Functions
9	Multiplicities for Production of Radioactive Nuclides	30 – 40	Data Covariance Files

Nuclear Data Processing For SCALE

- **AMPX** code system reads ENDF/B files and processes data to *continuous energy* (CE) or *multigroup* (MG) libraries distributed with SCALE
- **CE data library processing**
  - Converts ENDF data to linearized “point data” $\sigma(E_l)$ VS. E_l and energy-angle distributions
  - Convert point data to probability distributions for Monte Carlo
- **MG data library processing**
  - Determine MG energy structure
  - Average CE data over specified group structure using ”generic” energy spectrum
  - Compute resonance self-shielding data



SCALE MG Libraries Contain Generic Cross Sections and Self-Shielding Data

$$\sigma_g \equiv \frac{\int_g \phi(E)\sigma(E)dE}{\int_g \phi(E)dE}$$

- $\sigma(E)$ = energy-dependent CE data processed from ENDF/B
- $\Phi(E)$ = weight-function representing the energy spectrum

- *Problem-Independent MG Data (Generic, Infinitely Dilute)*

  $\Phi \rightarrow \Phi_\infty(E)$, "generic" function defined as the asymptotic flux in the limit of negligible resonance absorption. Does not depend on specific composition or geometry.

- *Problem-Dependent MG Data (Self-Shielded)*

  $\Phi \rightarrow \Phi_{sys}(E)$, the flux spectrum for the actual system of interest, accounting for resonance absorption effects. Depends on the actual absorber/moderator concentrations and geometry.

resonance absorption corrections are made to the generic library when used for a particular application.

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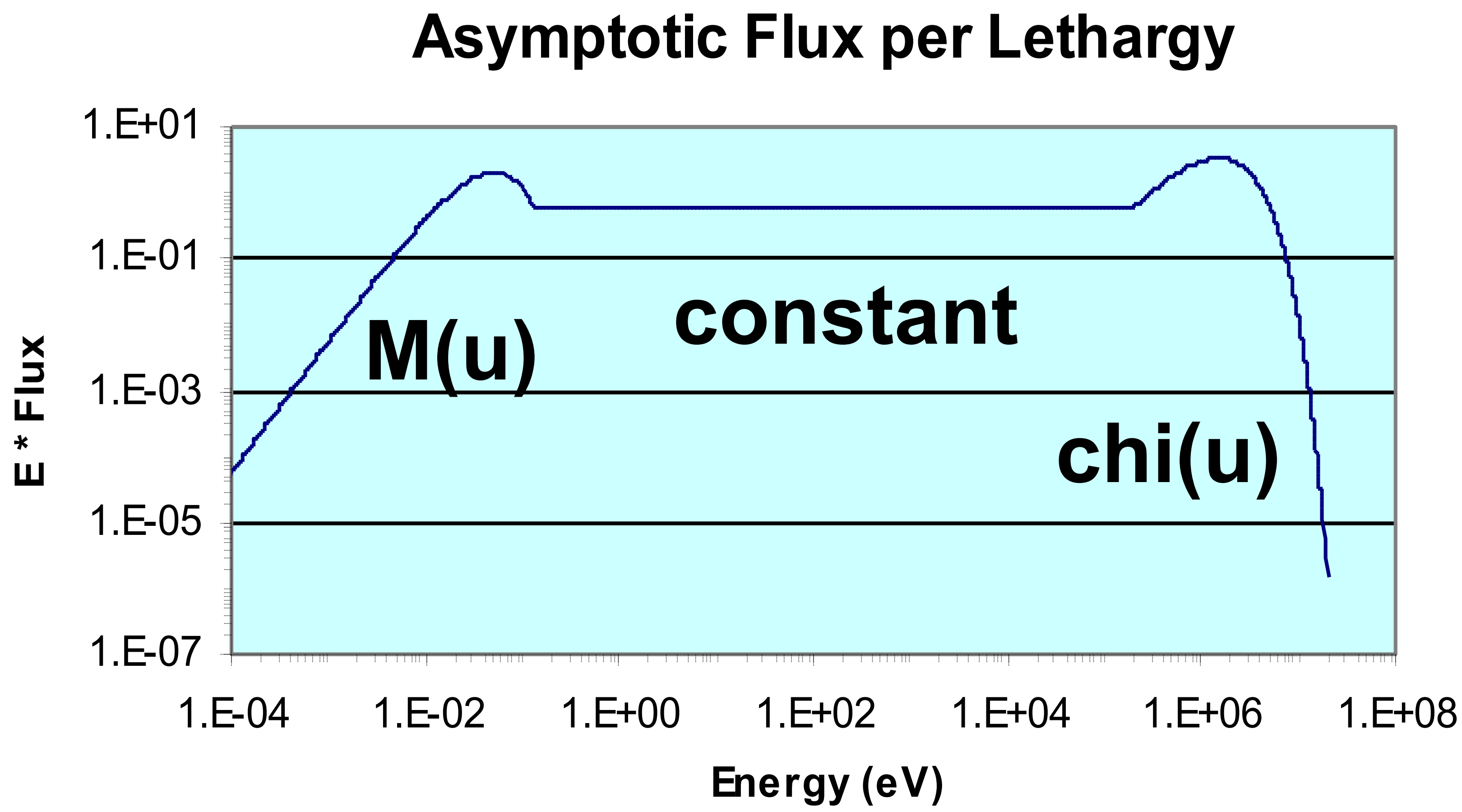
"Generic" Neutron Spectrum:
Fission Source in a Moderator
(Infinitely Dilute Resonance Absorbers)



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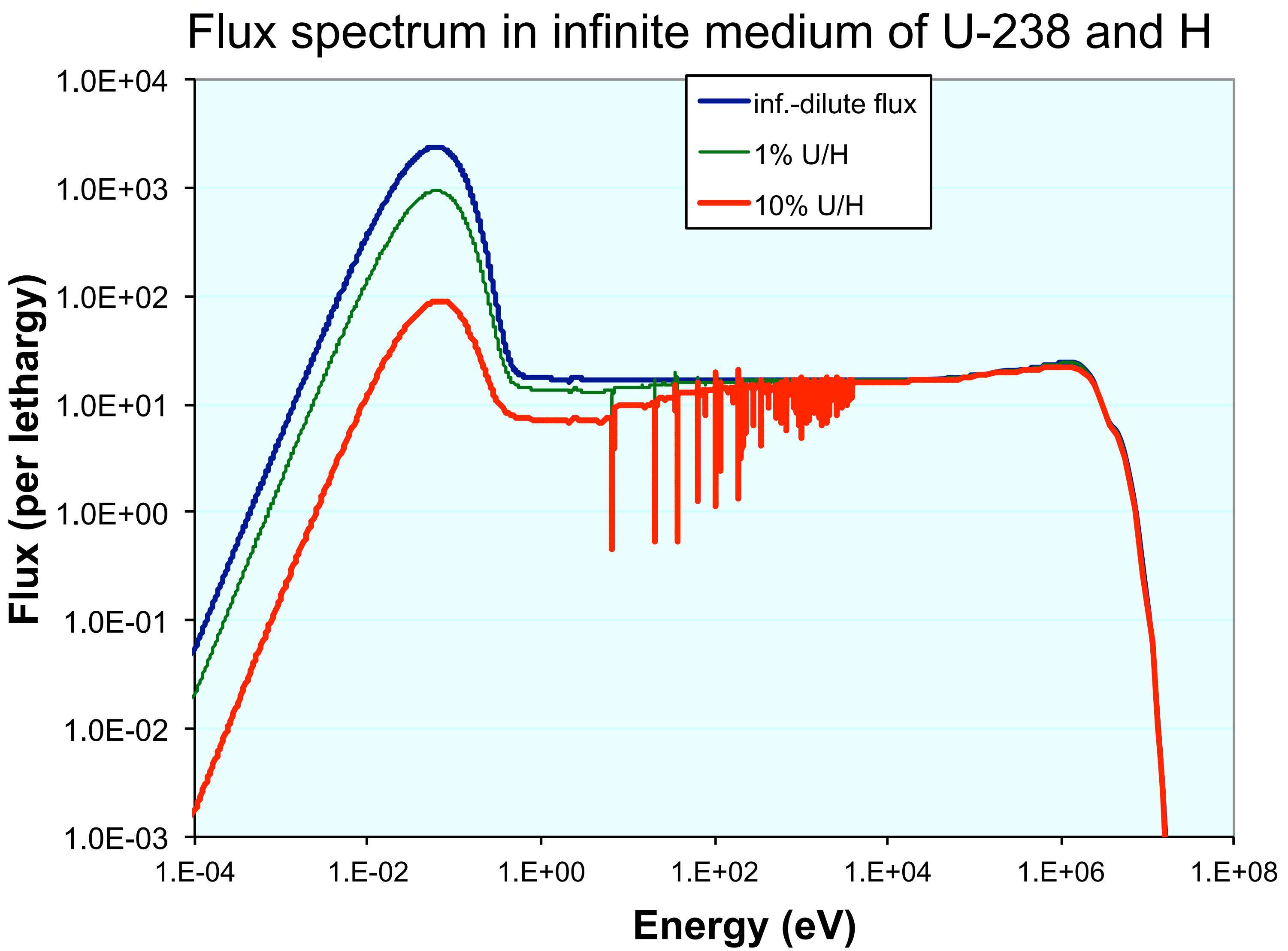
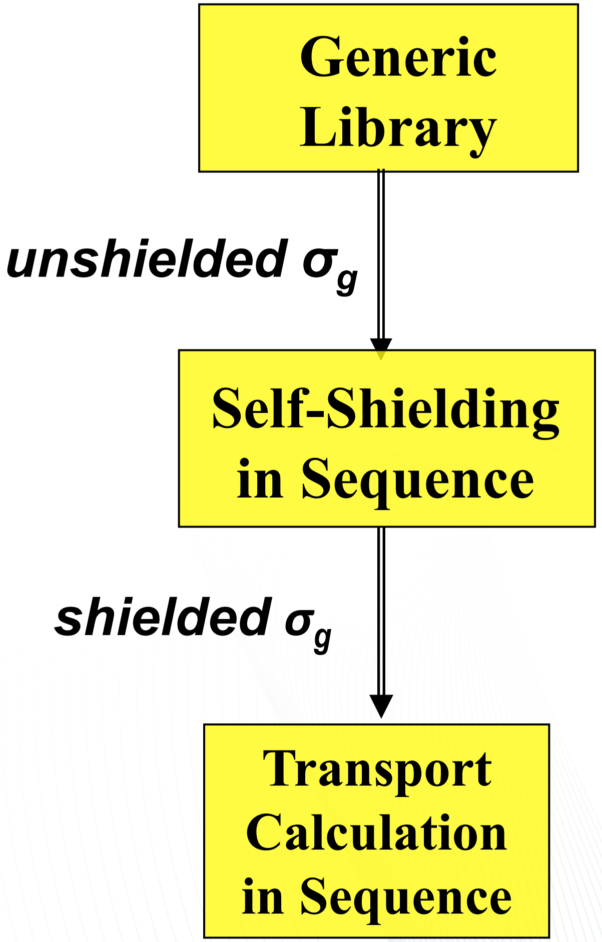
Impact of Resonance Absorption on Neutron Spectrum



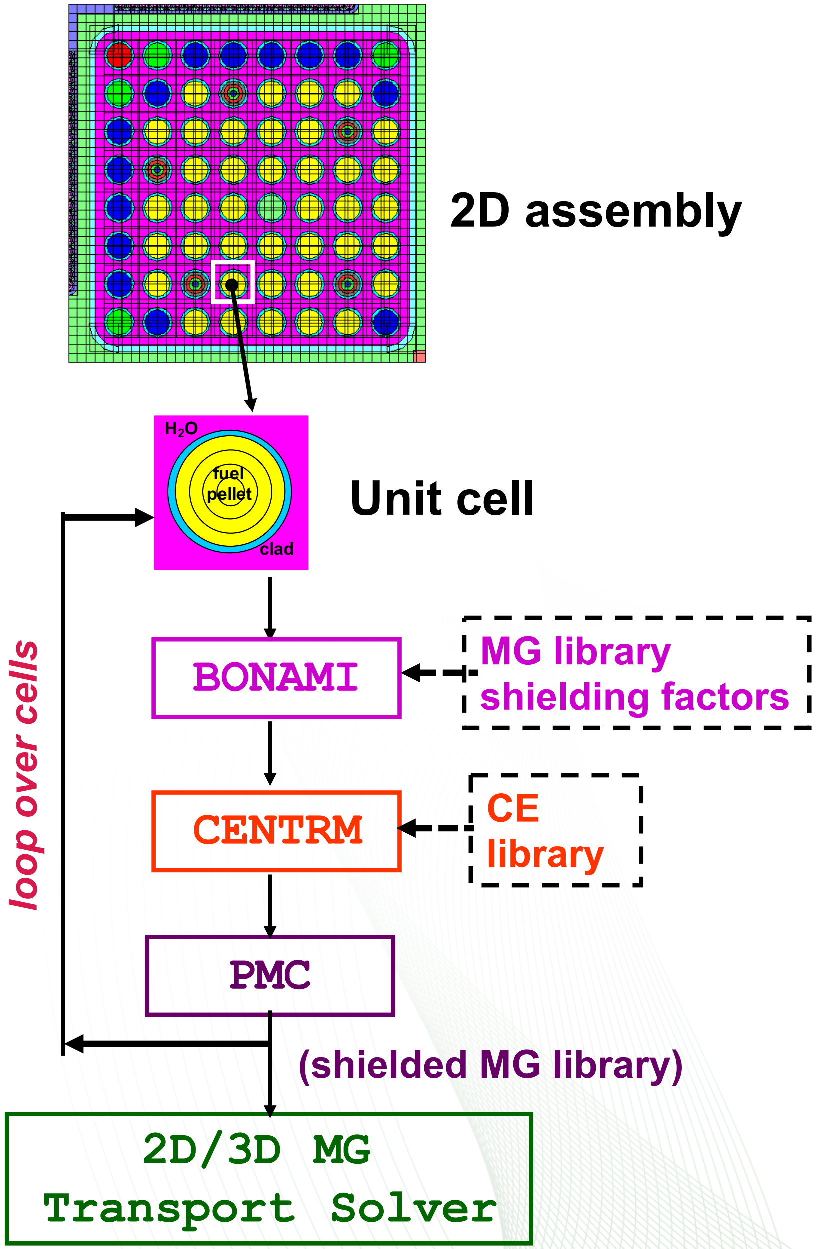
Conversion of Generic Library Cross Sections to Problem-Specific Self-Shielded Data

- Self-shielded data for transport calculations are computed during execution of SCALE sequences
- SCALE has two different methods for self-shielding
  - XSProc procedure default for CSAS and TRITON sequences
  - Bondarenko method default for Mavric and Polaris

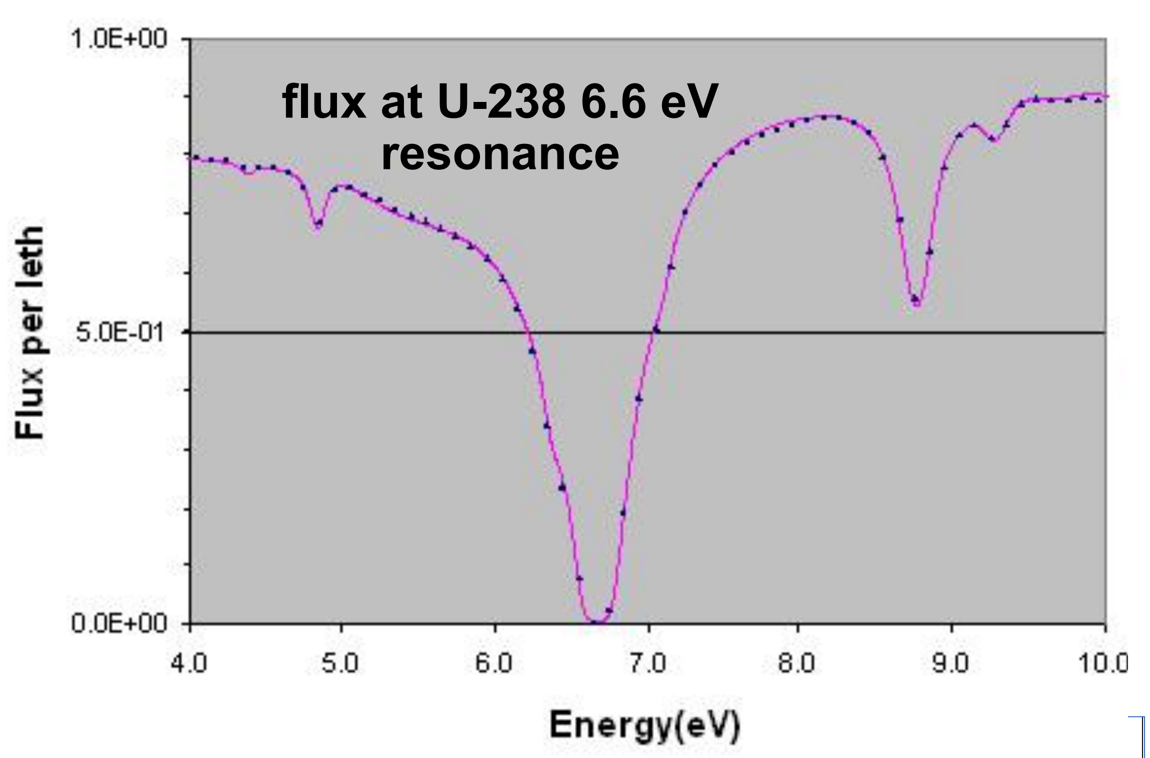


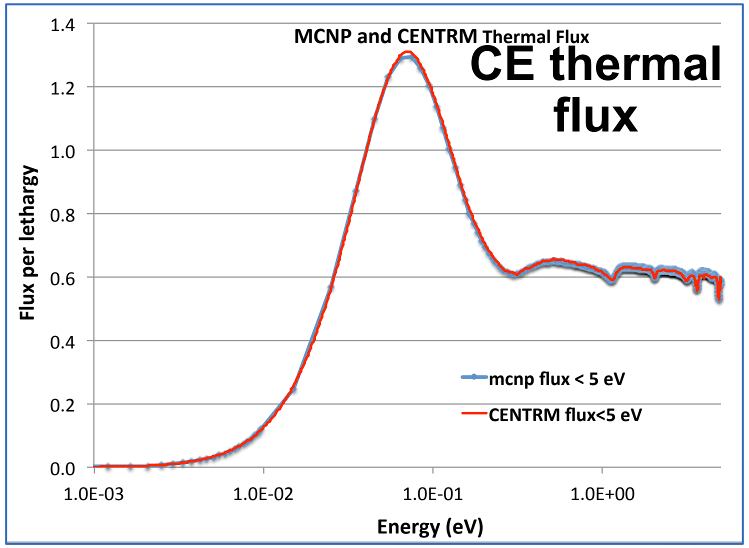
SCALE Resonance Self-Shielding with XSProc Module

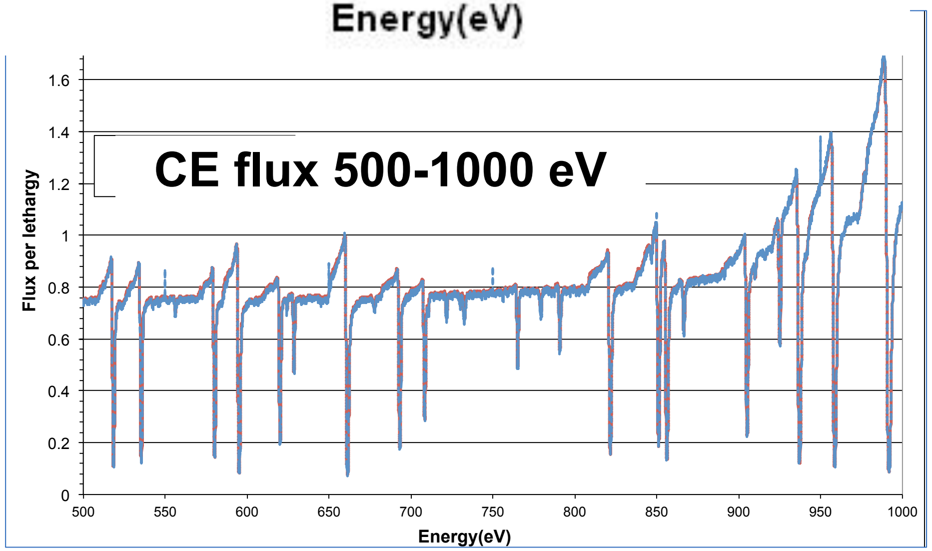
- XSProc is default method for CSAS (criticality), TRITON (general lattice physics)
  - BONAMI
    - Uses Bondarenko method with pre-computed self-shielded data stored in library
    - Interpolates library data to obtain shielded data in unresolved and fast range (and optionally in resolved range)
  - CENTRM/PMC
    - Generates "on-the-fly" shielded data using problem-specific spectra from CE deterministic calculations in resolved range

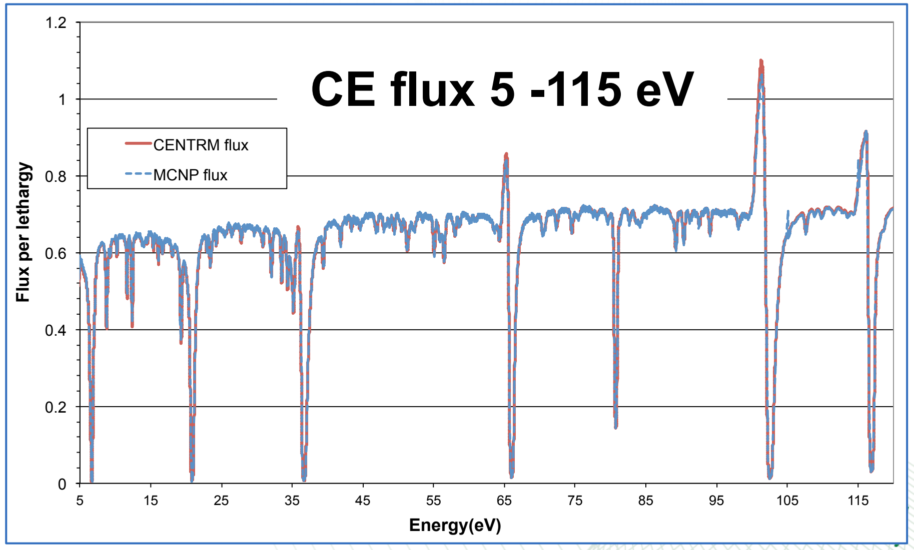


CENTRTM and MCNP Flux Spectra for PWR Lattice



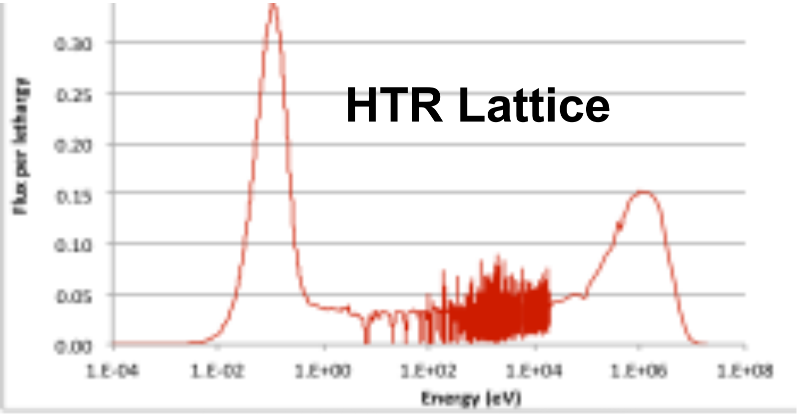


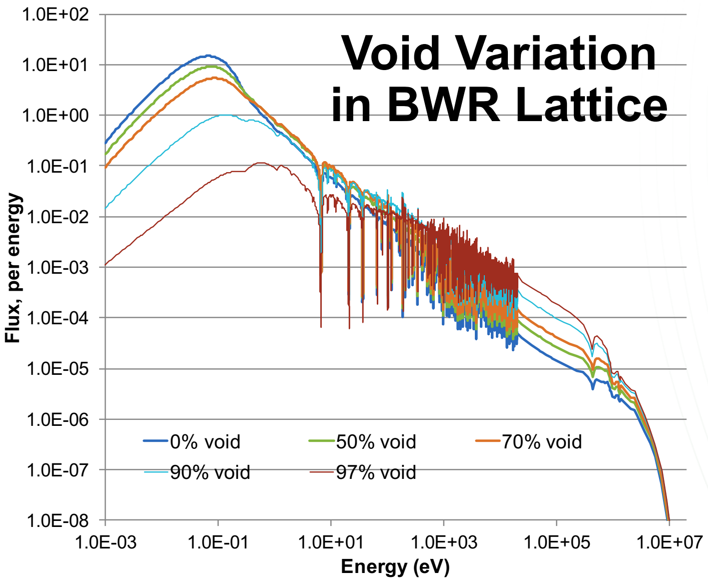


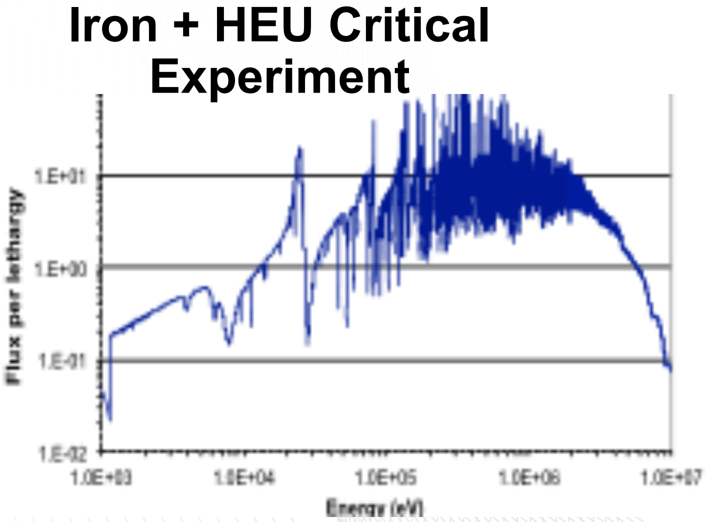


CENTRM/PMC Provides Capability to Address Resonance Effects Using First Principles

- Performs deterministic MoC or SN transport with CE library point data (70,000-100,00 energy points)
- Provides problem-specific CE weighting function to process MG data on-the-fly
- Explicit resonance overlap/interference
- Inherent space-dependent self-shielding
- Self-shielded elastic removal
- Includes impact of thermal scatter on self-shielding

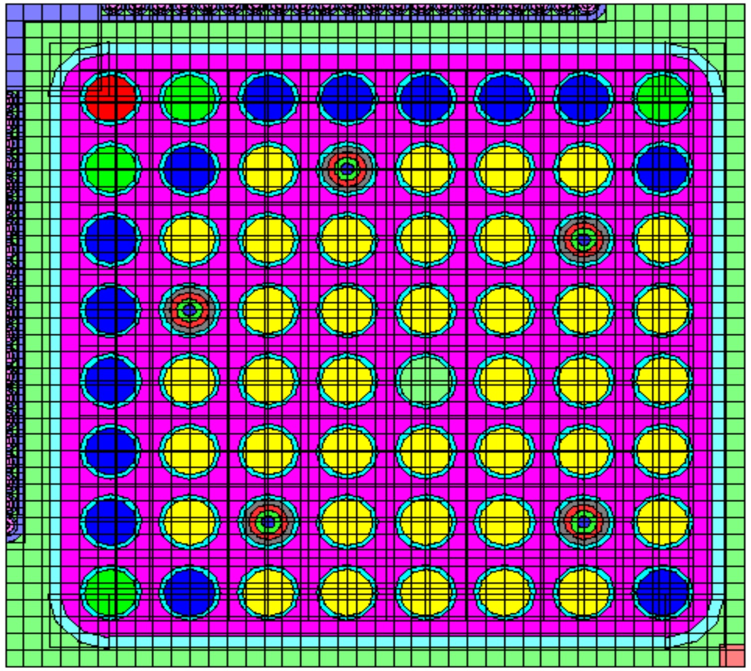






Bondarenko Methods Use ***Pre-computed*** Shielded Data Spanning Range of Self-Shielding Conditions

- Bondarenko is more approximate but faster than on-the-fly CENTRM/PMC
- Factors impacting self-shielding in lattices
  - Concentration of resonance nuclide(N_r)
  - Concentration of admixed moderators (Σ_m)
  - Composition of external moderators (Σ_{M^*})
  - Dimension/shape of fuel pins (e.g., *fuel radius*= R_f)
  - Arrangement of fuel pins (e.g., *pitch*=*P*)
  - Temperatures=T



$$\sigma_{g(\text{shielded})} = \sigma_g(N_r, \Sigma_m, \Sigma_{M^*}, R_f, P, T_F)$$

- "Equivalence theory" background cross section: $\sigma_0 \rightarrow (N_r, \Sigma_m, \Sigma_{M^*}, R_f, P, T_F)$

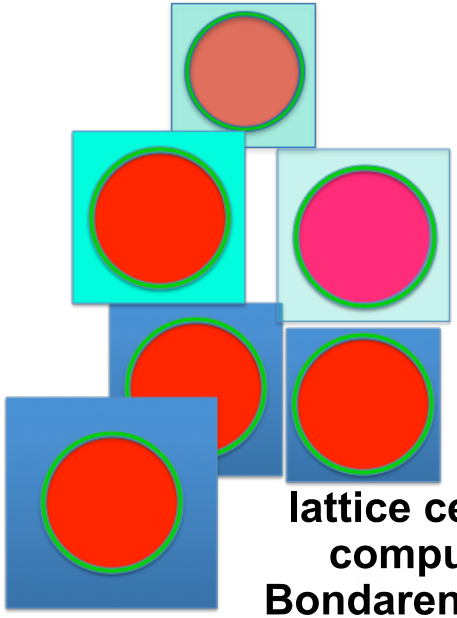
AMPX Calculation of Bondarenko Shielding Data with CENTRM/PMC (IRFfactor module)

- CENTRM/PMC calculate range of shielded cross sections for library by varying self-shielding conditions

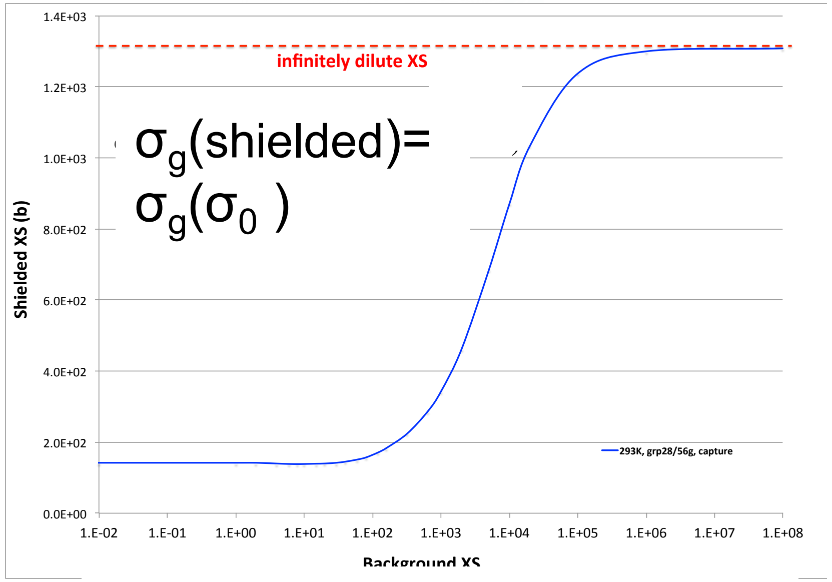
- *Heterogeneous lattice* models used for U, Pu, Gd, Zr
  - Vary lattice parameters $(N_r, \Sigma_m, \Sigma_{M^*}, R_f, P, T_F) \rightarrow \sigma_0$
  - Compute self-shielded data with CENTRM/PM for all σ_0

- Bondarenko data for other nuclides computed from *homogeneous media* models
  - Vary absorber/moderator number densities $(N_r, \Sigma_m) \rightarrow \sigma_0$

- Problem-dependent, self-shielded cross sections for lattice physics:
  - determine value of σ_0 $(N_r, \Sigma_m, \Sigma_{M^*}, R_f, P)$ for system
  - interpolate tabulated library values to obtain $\sigma_g(\sigma_0)$



lattice cells for computing Bondarenko data

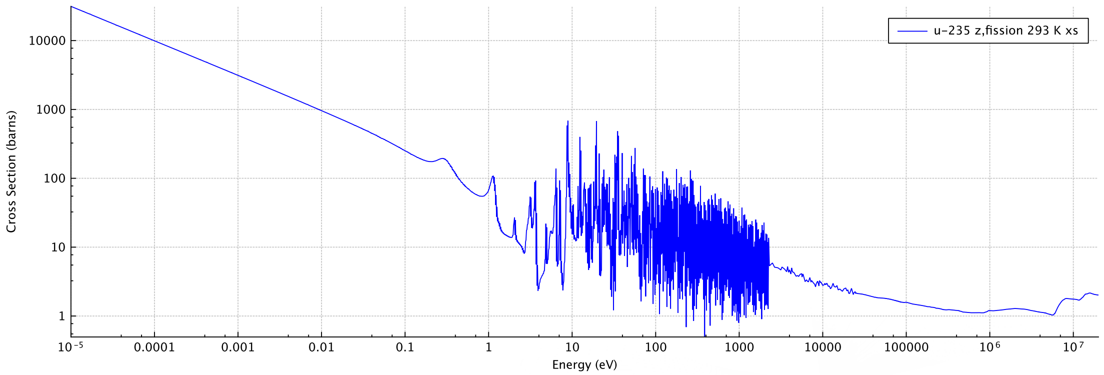


U-238 capture vs. σ_0
(group 121/252)

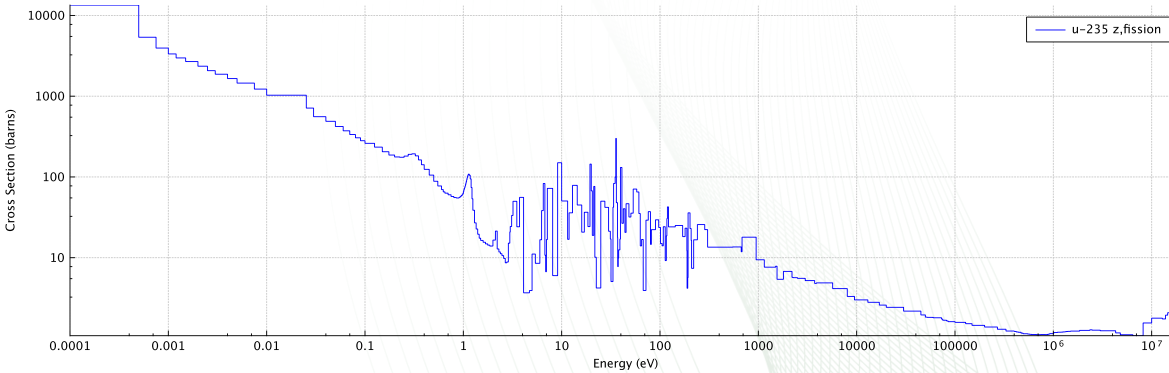
ENDF/B-VII.1 and VII.0 Nuclear Data Libraries in SCALE

- CE neutron/gamma library for Monte Carlo
  - general applications
- 252 fine-group
  - general reactor physics
  - criticality Safety
- 56 broad-group
  - LWR reactor physics
- 200 neutron/47 gamma coupled fine-group
  - shielding
  - fast-reactor analysis
- 28 neutron/19 gamma coupled broad-group
  - shielding

U235 Fission XS



CE data



252 MG data

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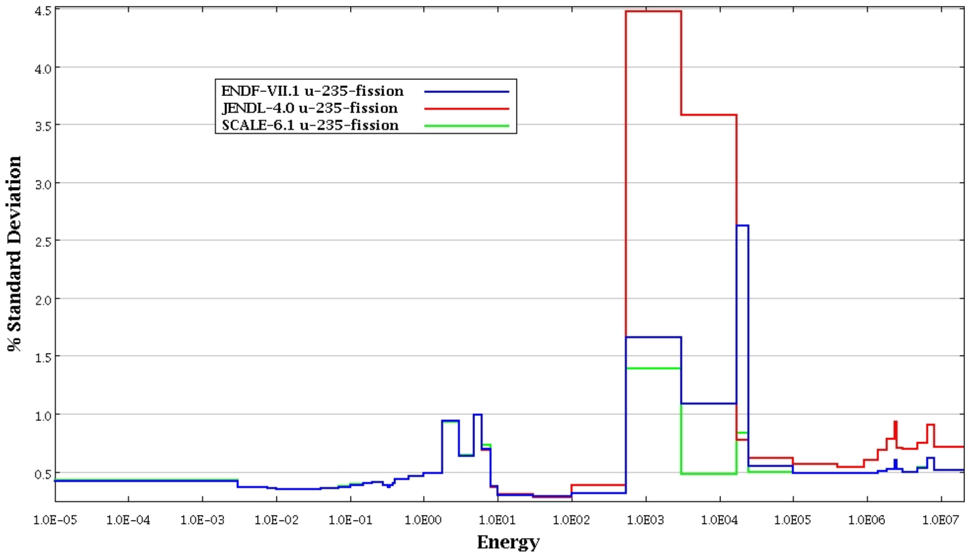
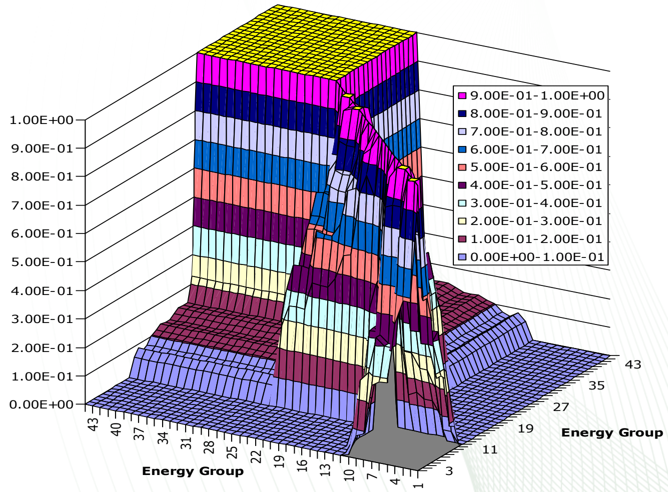
SCALE MG Covariance Libraries

- Evaluated nuclear data have uncertainties from uncertainties in measurements and evaluation techniques
- Uncertainties are described by covariance data
  – Standard deviations
  – Correlation matrices
- SCALE includes 252 and 56-group covariance libraries generated from several sources
  – Covariance data for 187 nuclides from ENDF/B VII.1
  – Covariances for ~215 nuclides from other sources
- SCALE modules TSUNAMI and Sampler compute uncertainty in results using covariance libraries



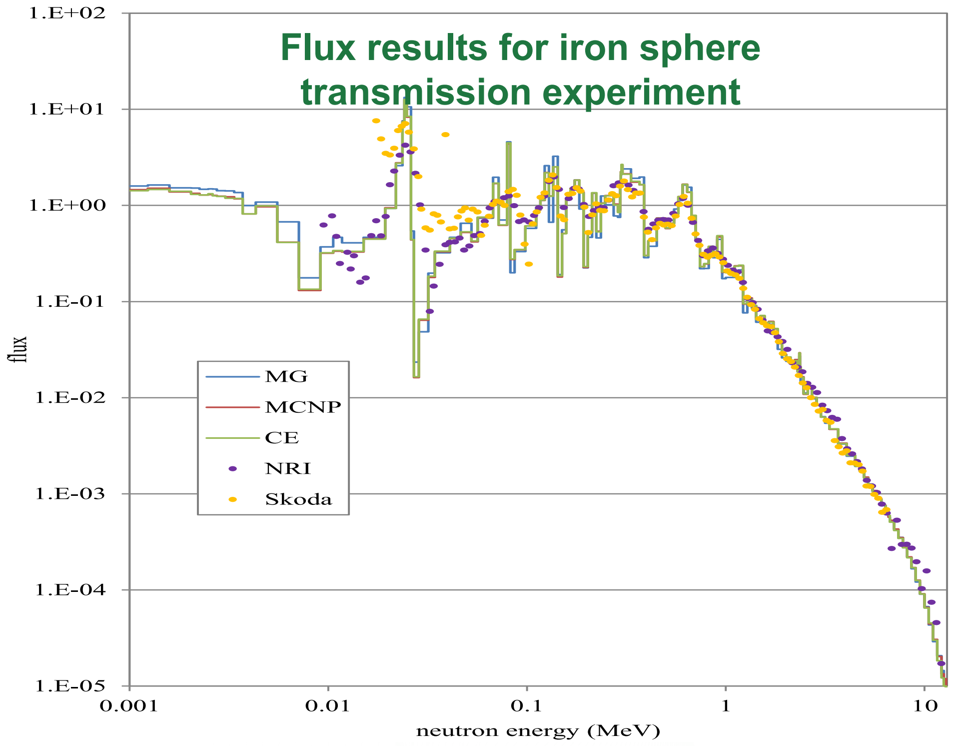
standard deviation In U-235 fission

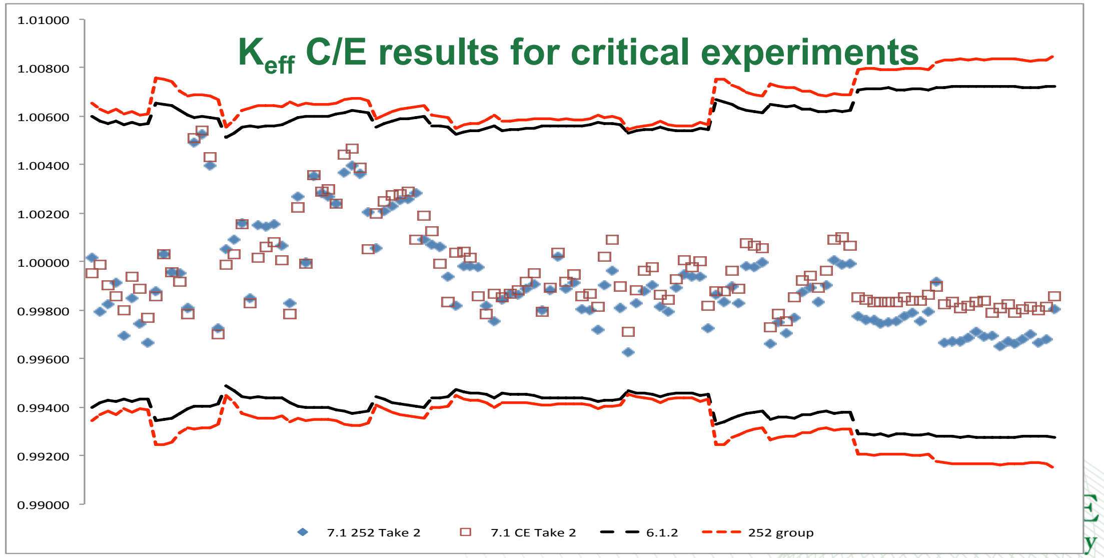


U-235 fission correlations

Validation and Nuclear Data Testing

- >5000 infinite medium k_{inf} tests
  - Every nuclide, differing moderation
- >7000 fixed-source transmission tests for neutron/gamma spectral data
  - Every nuclide/element at multiple energies
- 400 criticality benchmarks
  - HEU and LEU solutions
  - Pu solutions
  - LEU and Mox lattices
  - U and Pu metal fuels
- Shielding benchmarks
  - Fission and 14 MeV sources





SUMMARY

- AMPX code system processes ENDF/B-VII into SCALE CE and MG nuclear data
- SCALE-6.2 includes CE libraries for Monte Carlo codes Keno and Monaco, and for CENTRM/PMC
- "Generic" fine and broad MG libraries are available for lattice physics, criticality safety, and shielding applications
- Generic MG data is converted into problem-specific data using self-shielding modules in SCALE
  - On-the-fly CENTRM/PMC is default for Triton, CSAS sequences
  - Bondarenko method is default for Mavric and Polaris sequences
- MG libraries include Bondarenko self-shielding data pre-computed with CENTRM/PMC
- Extensive testing of SCALE CE and MG libraries was performed for thousands of verification tests and for ~ 400 critical benchmark experiments