

# Introduction to Resonance Self-Shielding Methods in SCALE :: XSPROC and ESSM

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# What is Multigroup Resonance Self-Shielding Effect?

#### **Boltzmann neutron transport equation**

Continuous energy

$$\hat{\Omega} \cdot \nabla \psi + \Sigma_t(\vec{r}, E)\psi(\vec{r}, E, \hat{\Omega}) = \int_{4\pi} d\Omega' \int_0^\infty dE \Sigma_s(\vec{r}, E' \to E, \hat{\Omega}' \cdot \hat{\Omega})\psi(\vec{r}, E', \hat{\Omega}') + q(\vec{r}, E, \hat{\Omega})$$

Multigroup

 $\geq$ 

$$\hat{\Omega} \cdot \nabla \psi_g + \Sigma_{l,g}(\vec{r})\psi_g(\vec{r},\hat{\Omega}) = \sum_{g'} \int_{4\pi} \sum_l \frac{2l+1}{4\pi} P_l(\hat{\Omega} \cdot \hat{\Omega}') \Sigma_{s,g'g}^l \psi_{g'}(\vec{r},\hat{\Omega}') d\hat{\Omega}' + \frac{1}{k_{eff}} \chi_g \sum_{g'} v_g \Sigma_{f,g'} \phi_{0,g'}$$

- Multigroup resonance self-shielding effect
  - Somewhat different from physical resonance, but mostly from it.
  - Composition  $\geq$





# **Representative Resonance Self-Shielding Methods**

#### Bondarenko approach

- Procedure
  - Prepare resonance cross section tables
    - $\sigma_{x,g}$  vs. background cross sections (XS)
    - High order calculation for flux weighting
      - Narrow resonance approximation
      - Homogeneous slowing down calculation
      - o Heterogeneous slowing down calculation
      - o Continuous energy Monte Carlo calculation
    - Estimate background XS
      - Dancoff factor, fixed source calculation ...
    - Read/interpolate self-shielded XS tables
  - Calculate resonance interference effect
    - Bondarenko iteration, Resonance interference table
- Application
  - Methods
    - Embedding Self-Shielding method: Polaris, MPACT
    - Subgroup method: MPACT, HELIOS, DeCART
    - Dancoff method: SCALE-BONAMI, CASMO
  - Drawbacks

**CAK RIDGE** 

- Fast but less accurate
- Fine energy groups
- Reactor specific XS libraries

- PW Slowing down calculation
  - Procedure
    - Divide whole domain into constituent cells
    - Global Dancoff factor
    - MCDancoff in SCALE
    - Adjust cell pitch for each cell
    - Global Dancoff factors
    - Perform pointwise slowing down calculations
      - Heterogeneous cells
    - Obtain self-shielded MG XSs & scatt. matrices
      - Flux weighting
  - Application
    - **SCALE-XSProc**, MC<sup>2</sup>-3
    - Drawbacks
      - Accurate but very time consuming
      - Poor global effect

### Hybrid method

- Bondarenko + Slowing down methods
  - SCALE-BONAMI+CENTRM
  - MPACT ESSM-X

# **SCALE-XSPROC**



# **SCALE-XSPROC Cross Section Processing Procedure**

#### Standard procedure





### **SCALE-XSPROC BONAMI Based Bondarenko Procedure**

#### BONAMI methods

- Background cross sections for homogeneous media
  - Narrow resonance approximation

$$\sigma_{0,g}^r = \frac{1}{N^r} \sum_{i \neq r} N^i \sigma_{t,g}^i$$

> Intermediate resonance approximation without resonance interference

$$\sigma_{0,g}^{r} = \frac{1}{N^{r}} \sum_{i \neq r} N^{i} \lambda_{g}^{i} \sigma_{p}^{i}$$

> Intermediate resonance approximation with resonance interference

$$\sigma_{0,g}^{r} = \frac{1}{N^{r}} \sum_{i \neq r} N^{i} (\sigma_{a,g}^{i} + \lambda_{g}^{i} \sigma_{p}^{i})$$

- Background cross sections for heterogeneous media
  - Equivalence theory between homogeneous and heterogeneous systems

$$\hat{\Omega} \cdot \nabla \psi_{g} + \sum_{i} (\Sigma_{a,g}^{i} + \lambda_{g}^{i} \Sigma_{p}^{i}) \psi_{g}(\hat{\Omega}) = \sum_{i} \lambda_{g}^{i} \Sigma_{p}^{i} \longleftrightarrow \left[ \sum_{i} (\Sigma_{a,g}^{i} + \lambda_{g}^{i} \Sigma_{p}^{i}) + \Sigma_{e} \right] \phi_{g}(\hat{\Omega}) = \sum_{i} \lambda_{g}^{i} \Sigma_{p}^{i} + \Sigma_{e}$$

$$\sigma_{0,g}^{r} = \frac{1}{N^{r}} \left[ \sum_{i \neq r} N^{i} (\sigma_{a,g}^{i} + \lambda_{g}^{i} \sigma_{p}^{i}) + \Sigma_{e} \right]$$

$$\sigma_{e}^{r} = \frac{\Sigma_{e}}{N^{r}}$$



# SCALE-XSPROC BONAMI Based Bondarenko Procedure

#### BONAMI methods

- How to obtain equivalence (or escape) cross sections
  - Internal Dancoff method

$$\Sigma_e = \frac{(1-c)A}{\overline{\ell}[1+(A-1)c]}$$

- $\overline{\ell}$  = Average chord length = 4\*volume / Surface area
- A = Bell factor to improve the accuracy of the Wigner rational approximation Otter: as a function of  $\Sigma_t \overline{\ell}$ Leslie as a function Dancoff factor
- c = Dancoff factor

\*Probability that a neutron from an absorber reaches other absorber without a collision

#### External Dancoff method

- Dancoff factors are obtained from MCDancoff
- Input for SCALE



# SCALE-XSPROC BONAMI Based Bondarenko Procedure

#### BONAMI methods

- Spatially dependent self-shielding method (SCALE-6.3)
  - Multiple fuel zones with non-uniform temperature distribution
  - > Dancoff factor obtained by internal 1-D cylindrical CPM solver
  - Newly developed extended Stoker-Weiss method



т	<u>lm</u>	$F_m$
1	$l_1(\rho_k) = \frac{2R}{\pi} (\sqrt{1 - \rho_k^2} + \frac{\sin^{-1} \rho_k}{\rho_k} + \frac{\pi}{2} \rho_k)$	$\frac{s_0 \rho_k l_1(\rho_k)}{4V_k}$
2	$l_2(\rho_k) = \frac{2R}{\pi} (\sqrt{1 - \rho_k^2} + \frac{\sin^{-1} \rho_k}{\rho_k} - \frac{\pi}{2} \rho_k)$	$-\frac{s_0\rho_k l_2(\rho_k)}{4V_k}$
3	$l_{3}(\rho_{k-1}) = \frac{2R}{\pi} \left( \sqrt{1 - \rho_{k-1}^{2}} + \frac{\sin^{-1} \rho_{k-1}}{\rho_{k-1}} + \frac{\pi}{2} \rho_{k-1} \right)$	$-\frac{s_0 \rho_{k-1} l_3(\rho_{k-1})}{4 V_k}$
4	$l_4(\rho_{k-1}) = \frac{2R}{\pi} \left( \sqrt{1 - \rho_{k-1}^2} + \frac{\sin^{-1} \rho_{k-1}}{\rho_{k-1}} - \frac{\pi}{2} \rho_{k-1} \right)$	$\frac{s_0 \rho_{k-1} l_4(\rho_{k-1})}{4 V_k}$



Nonuniform temperature :: Fission density



Temperature	# of fuel		BONAMI	56-group	BONAMI 2	252-group	CENTRM		
distribution	zones	CE-KENO	SCALE-6.2	SCALE-6.3	SCALE-6.2	SCALE-6.3	56-g	252-g	
Uniform	1	1.38340	1.37562	-	1.38015	-	1.38137	1.38066	
Uniform	3	1.38340	1.30303	1.38090	1.32919	1.38438	1.38120	1.38086	
Nonuniform	3	1.38416	1.30407	1.38281	1.33015	1.38575	1.38216	1.38171	



# **SCALE-XSPROC CENTRM Based Slowing Down Calculation I**

#### Pointwise slowing down calculation (CENTRM)

- Nuclear data
  - CRAWDAD
    - Pointwise cross sections
    - S(α,β) thermal scattering kernel data
  - > BONAMI
    - Self-shielded multigroup cross sections and scattering matrices
    - Problem dependent AMPX working library
- Pointwise + Multigroup hybrid
  - ➢ Upper multigroup range: ≥ DEMAX (default=20 keV)
    - Multigroup cross sections are determined by BONAMI
    - Convert multigroup data into pointwise data
  - Pointwise range: DEMIN-DEMAX (default=0.001 eV 20 keV)
    - Pure pointwise slowing down calculation

$$\begin{aligned} \hat{\Omega} \cdot \nabla \psi + \Sigma_t(\vec{r}, u)\psi(\vec{r}, u, \hat{\Omega}) &= \int_{4\pi} d\Omega' \int_0^\infty du' \Sigma_s(\vec{r}, u' \to u, \hat{\Omega}' \cdot \hat{\Omega})\psi(\vec{r}, u', \hat{\Omega}') + q(\vec{r}, u, \hat{\Omega}) \\ \int_{4\pi} d\Omega' \int_0^\infty du' \Sigma_s(\vec{r}, u' \to u, \hat{\Omega}' \cdot \hat{\Omega})\psi(\vec{r}, u', \hat{\Omega}') &= \sum_i \sum_{\ell=0}^L \sum_{k=0}^\ell \frac{2\ell+1}{2} Y_{\ell k}(\hat{\Omega}) \Sigma_\ell^i(u' \to u, )\Phi_{\ell k}(u') \end{aligned}$$

- ➢ Lower multigroup range: ≤ DEMIN (default=0.001 eV)
  - Multigroup cross sections are determined by BONAMI
  - Convert multigroup data into pointwise data





# **SCALE-XSPROC CENTRM Based Slowing Down Calculation II**

#### Pointwise slowing down calculation (continued)

#### Scattering physics

- > Epithermal elastic scatter
  - S-wave approximation assuming isotropic scattering in CM system
  - $\geq$  thermal cutoff energy (for example, 5 eV)
  - Discussion
    - o Not true actually
    - Cause some issue at epithermal neutron spectra
    - $\circ$   $\,$  Can be resolved by optimizing group structure
- > Epithermal inelastic scatter
  - DEMAX ≤ inelastic threshold
    - o Multigroup inelastic scattering matrices
  - DEMAX ≥ inelastic threshold
    - Discrete-level inelastic reaction: two-body interaction
    - High energy: discrete → continuum
- > Thermal scatter
  - ≤ thermal cutoff energy (for example, 5 eV)

$$\sigma_{\ell}(E' \to E, T) = \frac{\sigma_b}{T} \sqrt{\frac{E}{E'}} e^{-\frac{\beta(E' \to E)}{2}} \int P_{\ell}(\mu_0) S(\alpha, \beta, T) d\mu_0$$

- Free gas thermal kernel for  $S(\alpha,\beta)$ : internal analytic formula
- Bound thermal scatter
  - ENDF/B data processed by AMPX
  - Prepared by CRAWDAD



# SCALE-XSPROC CENTRM Based Slowing Down Calculation III

#### Pointwise slowing down calculation (continued)

- Slowing down transport solvers
  - O-dimensional slowing down
  - $\succ$  1-dimensional discrete ordinates (S<sub>N</sub>)
    - Slab and Wigner-Seitz cylinder and sphere
  - 2-dimensional method of characteristics (MOC)
    - 2D square with cylindrical fuels
  - > Two-region collision probability
- Double-heterogeneity treatment
  - Consecutive two PW slowing down calculation
    - Perform the 1<sup>st</sup> slowing down calculation for infinite TRISO array
    - Homogenize TRISO and matrix using the PW flux moments
       → disadvantage factors
    - Perform the 2<sup>nd</sup> slowing down calculation
    - Collapse PW into MG
    - Slab, cylinder and sphere

#### SCALE-6.3 improvement

- Use a Dancoff factor to adjust TRISO pitch to consider neutron leakage effect
- Dancoff factor can be a user input and obtained using MCDancoff
- TRISO pitch can be adjusted to have same Dancoff with input using internal 1D spherical CPM
- Nuclide dependent temperatures and PW data can be at the 2<sup>nd</sup> slowing down calculation over the homogenized TRISO and matrix region





# **SCALE-XSPROC CENTRM Based Slowing Down Calculation IV**

#### Energy group collapsing: Pointwise → Multigroup

- Equivalence relation between PW and MG
  - > Angle dependent total cross section + High order flux moment weighted scattering matrices

$$\hat{\Omega}_{m} \cdot \nabla \psi_{m,g} + \Sigma_{t,g} \psi_{m,g}(\vec{r}) = \sum_{\ell} (2\ell+1) P_{\ell}(\mu_{m}) \sum_{s,\ell,g'g} \Sigma_{s,\ell,g'g} \phi_{\ell,g'}(\vec{r}) + q_{g}(\vec{r})$$

$$\Sigma_{t,m,G} = \frac{\sum_{g \in G} \Sigma_{t,g} \psi_{m,g}(\vec{r})}{\sum_{g \in G} \psi_{m,g}(\vec{r})} \qquad \Sigma_{s,\ell,G'G} = \frac{\sum_{g' \in G', g \in G'} \Sigma_{s,\ell,g'g}^{g'} \phi_{\ell,g'}(\vec{r})}{\sum_{g' \in G'} \phi_{\ell,g'}(\vec{r})} \qquad q_{G}(\vec{r}) = \sum_{g \in G} q_{g}(\vec{r})$$

- Energy group collapsing: PMC, MIXMACRO
  - > Cross sections  $\sigma_{x,g,j}^{i} = \frac{\int_{\Delta E_{g}} dE \sigma_{x,g}^{i} \phi_{g,j}(E)}{\int_{\Delta E_{g}} dE \phi_{g,j}(E)}$
  - > Scattering matrices: various options

$$n2d = 0: \quad \sigma_{s,\ell,g'g}^{new} = \frac{\sigma_{s,0,g'}^{new}}{\sigma_{s,0,g'}^{orig}} \sigma_{s,\ell,g'g}^{orig} \quad for \ all \ groups$$
$$n2d = -1: \quad \sigma_{s,0,gg}^{new} = recompute \ using \ S - wave \ scatter \ for \ge thermal \ cutoff$$

$$n2d = 1: \quad \sigma_{s,l,g'g}^{new} = \int_{\Delta E_g} dE \int_{\Delta E_{g'}} dE' \sigma_{s,\ell}(E' \to E) \phi_{\ell}(E') / \int_{\Delta E_{g'}} dE' \phi_{\ell}(E') \quad \text{for } \ge \text{thermal cutoff}$$
  
$$\sigma_{s,l,g'g}^{new} = \int_{\Delta E_g} dE \int_{\Delta E_{g'}} dE' \sigma_{s,\ell}(E' \to E) \phi_0(E') / \int_{\Delta E_{g'}} dE' \phi_0(E') \quad \text{for } \le \text{thermal cutoff}$$

$$n2d = 2: \quad \sigma_{s,l,gg}^{new} = \sigma_{s,l,gg}^{orig} + \sigma_{t,g} - \sigma_{s,l,g}, \quad 0 < \ell < isct \quad for \ge thermal \ cutoff$$

$$n2d = -2: \quad n2d = 2 + n2d = -1 \quad for \ge thermal \ cutoff$$



# **EMBEDDED SELF-SHIELDING METHOD**



# **AMPX MG Resonance Cross Section Table Generation**

#### Multigroup resonance cross section tables

- Resolved self-shielded resonance data
  - > Narrow resonance approximation

$$\sigma_{i,g}(T,\sigma_0) = \frac{\int_g \sigma_i(T,E)\phi(T,E)dE}{\int_g \phi(T,E)dE}, \quad \phi(T,E) = \frac{\sigma_0}{\sigma_t(T,E) + \sigma_0}$$

- Intermediate resonance parameters (LAMBDA)
  - Probability to penetrate resonances of resonance nuclide by scattering with target nuclide
  - Mixture: <sup>1</sup>H + <sup>238</sup>U + target nuclide

$$\lambda_{g}^{x} = \frac{\sigma_{g,b}^{238} N^{238} - N^{238} \lambda_{g}^{238} \sigma_{p}^{238} - N^{1} \lambda_{g}^{1} \sigma_{p}^{1}}{N^{x} \sigma_{p}^{x}}$$

Homogeneous/heterogeneous resonance data (Roux)

PW slowing down calculation using CENTRM  

$$\hat{\Omega} \cdot \nabla \psi + \Sigma_{t}(\vec{r}, u)\psi(\vec{r}, u, \hat{\Omega}) = \int_{4\pi} d\Omega' \int_{0}^{\infty} du' \Sigma_{s}(u' \to u, \hat{\Omega}' \cdot \hat{\Omega})\psi(\vec{r}, u', \hat{\Omega}') + q(\vec{r}, u, \hat{\Omega})$$

$$\sigma_{x,g} = \int_{\Delta u_{g}} \sigma_{x}(u)\varphi(u)du / \int_{\Delta u_{g}} \varphi(u)du$$

• Background cross sections using ESSM

$$\hat{\Omega} \cdot \nabla \psi_{g,k} + \sum_{i} (\Sigma_{i,g,a}^{k} + \lambda_{i,g} \Sigma_{i,p}^{k}) \psi_{g,k}(\hat{\Omega}) = \sum_{i} \lambda_{i,g} \Sigma_{i,p}^{k}$$
$$\sigma_{R,b,g} = \frac{\sum_{i} N_{i} \lambda_{i} \sigma_{i,p,g} + \Sigma_{e,g}}{N_{R}} = \frac{\sigma_{a,g} \phi_{g}}{1 - \phi_{g}}$$



Case		1	2	3	4	5	б	7	8	9	10	11	12	13	14	15	16	17	18	19
Volume	Fuel	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	Clad	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	Mod	1	1	1	1	1	2	5	5	5	5	5	5	5	5	5	5	5	5	5
Fuel	235U	1	1	1	1	1	1	1	2-1	2-2	2-3	2-4	2-5	10-2	10-2	10-2	10-2	10-2	10-2	10-2
	<sup>238</sup> U	1	1	1	1	1	1	1	2-1	2-2	2-3	2-4	2-5	10-2	3·10 <sup>-3</sup>	10-3	10-4	10-5	10-7	10-8
	<sup>16</sup> O	1	1	1	1	1	1	1	2-1	2-2	2-3	2-4	2-5	10-2	10-2	10-2	10-2	10-2	10-2	10-2
H <sub>2</sub> O	$^{1}\mathrm{H}$	0.1	0.2	0.5	0.75	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	<sup>16</sup> O	0.1	0.2	0.5	0.75	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1



# **AMPX MG Resonance Cross Section Table Generation**

- Multigroup resonance cross section tables (continued)
  - Unresolved self-shielded resonance data
    - Probability table method with NR approximation

$$\sigma_{x,g,i} = \frac{\int_{g} \sum_{m} p_{i}^{m} \sigma_{x,i}^{m}(E) \phi^{m}(E) dE}{\int_{g} \sum_{m} p_{i}^{m} \phi^{m}(E) dE}$$

$$\phi^{m}(E) = \frac{W(E)}{N_{i}\sigma^{m}_{t,i}(E) + \sum_{j \neq i} N_{j}\sigma_{t,j}(E) + \Sigma_{e}(E)}$$

$$\sigma_{x,g,i} = \frac{\sum_{m} \frac{p_i^m \sigma_{x,i,g}^m}{\sigma_{t,i,g}^m + \sigma_{0,i,g}}}{\sum_{m} \frac{p_i^m}{\sigma_{t,i,g}^m + \sigma_{0,i,g}}}$$

- $\sigma_x^m$  $p^m$ = a cross section level *m* of reaction *x* in the URR probability table,
  - = a probability of the level *m*,
- = a self-shielded cross section of reaction x  $\sigma_{x,q}$



# **Embedded Self-Shielding Method**

#### Direct use of resonance self-shielded XS table

- Consistency between resonance data generation and use
  - Similar with the subgroup method
  - Primary method for SCALE-Polaris
- Procedure
  - a. Assume initial background cross section

$$\sigma_{b,g}^{r(n)} = \frac{1}{N^r} \sum_{i \neq r} N^i \lambda_g^i \sigma_p^i$$

b. Obtain corresponding absorption cross sections for all nuclides by reading and interpolation

$$\sigma^{i(n)}_{b,g} o \sigma^{i(n)}_{a,g}$$

c. Solve fixed source transport (ESSM) equation using transport solver (MOC)

$$\hat{\Omega} \cdot \nabla \psi_g^{(n+1)} + \sum_i N_i (\sigma_{g,a}^{i,(n)} + \lambda_g^i \Sigma_p^i) \psi_g^{(n+1)}(\hat{\Omega}) = \sum_i \lambda_g^i \Sigma_p^i$$

d. Update background cross sections using

$$\sigma_{b,g}^{r,(n+1)} = \frac{1}{N^r} \frac{\sum_{i} N^i \sigma_{g,a}^{i,(n)} \phi_g^{(n+1)}}{1 - \phi_g^{(n+1)}} - \lambda_g^r \sigma_p^r$$

- e. Convergence check for background cross sections
- f. Repeat b-e until converged



# **Recent and on-going Improvements**

#### Underlined improvements for SCALE-6.3

#### XSPROC

- > Thermal scattering kernel data reconstruction (CENTRM)
- Neutron leakage consideration for double-het fuels (CENTRM)
- > Spatially dependent resonance self-shielding method for nonuniform temperature (BONAMI)
- Improvement for nonuniform temperatures in TRISO (CENTRM)
- Explicit thermal scattering matrix reconstruction (PMC, MIXMACRO)
- Improve the drawback of S-wave approximation (AMPX)

### On-going & planned improvements

- SCALE-XSPROC
  - User defined thermal cutoff energy for free gas model
  - Consistent energy group collapsing to conserve reaction rate
    - Super-homogenization method (SPH)
- AMPX for ESSM
  - Extend within-group resonance data to thermal
  - Improve the SPH method for ROUX
- SCALE-Polaris ESSM
  - Dancoff based fast mode ESSM
  - > Spatially dependent ESSM for multiple fuel rings with non-uniform temperature distribution
  - On-the-fly energy group collapsing

