Development of a Resonance Calculation Scheme Involving Exact Scattering Kernels

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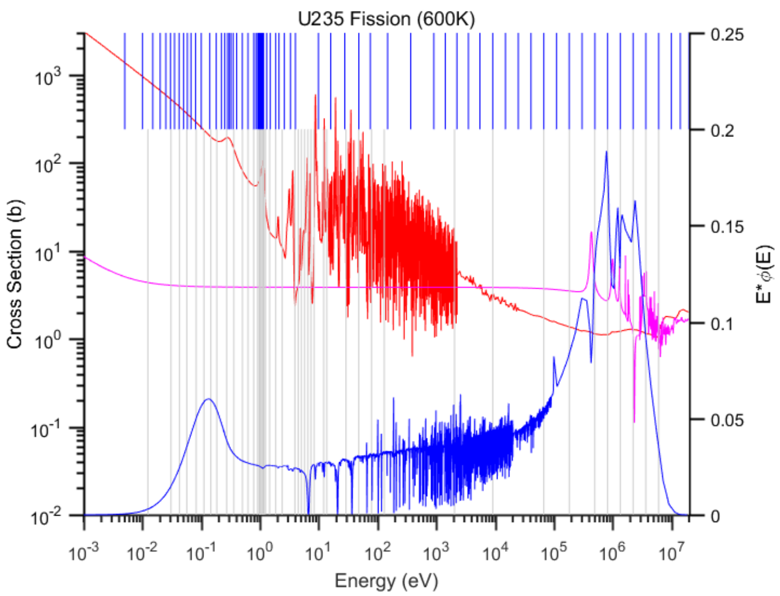
Contents

- **Resonance Calculation in Deterministic Methods**
  - **Resonance calculation is to address resonance self-shielding effects.**
    - To correct multi-group cross sections (XSs)
  - **The main concern is accurate estimation for the integration for effective XSs.**

$$\sigma_{eff,x,g}^{r} = \int_{E_g}^{E_{g-1}} dE \sigma_x^r(E)\phi(E) \Big/ \int_{E_g}^{E_{g-1}} dE \phi(E)$$



- **Conventional Resonance Calculation Methods**
  - **There are several methods for resonance calculation.**
    - Equivalence theory, the subgroup method, ultra-fine-group (UFG) methods
  - **Each method has its pros and cons due to its characteristic.**
    - (Equivalence theory) computing efficiency / limitation in its accuracy
    - (Subgroup) direct handling for spatial dependence / need for several correction techniques
    - (UFG) rigorous solution for energy dependence / approximation on geometry for computing efficiency

- **Slowing-Down Scattering Source**
  - **All of the resonance methods take slowing-down scattering sources.**

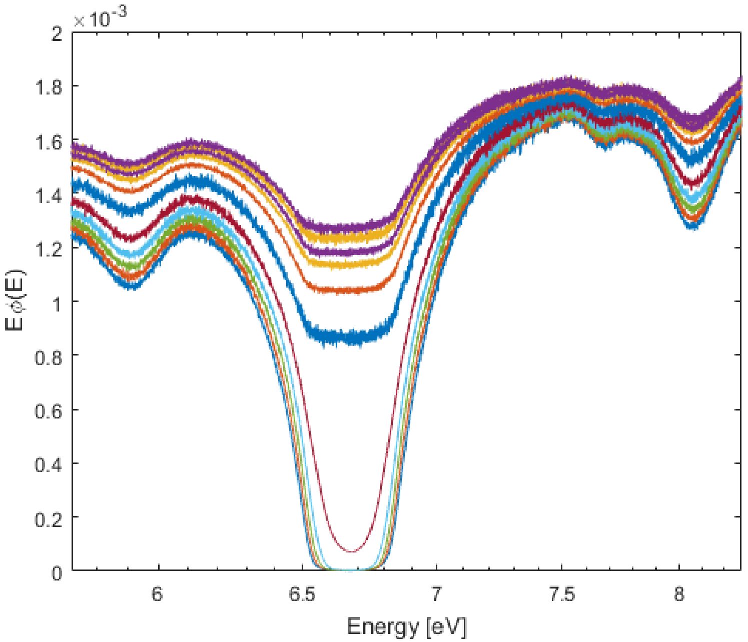
$$Q_{s\,sd}(E)=\sum_i N_i\int_E^{E/\alpha_i}\sigma_{s,i}(E')\phi(E')\frac{1}{1-\alpha_i}\frac{dE'}{E'}$$

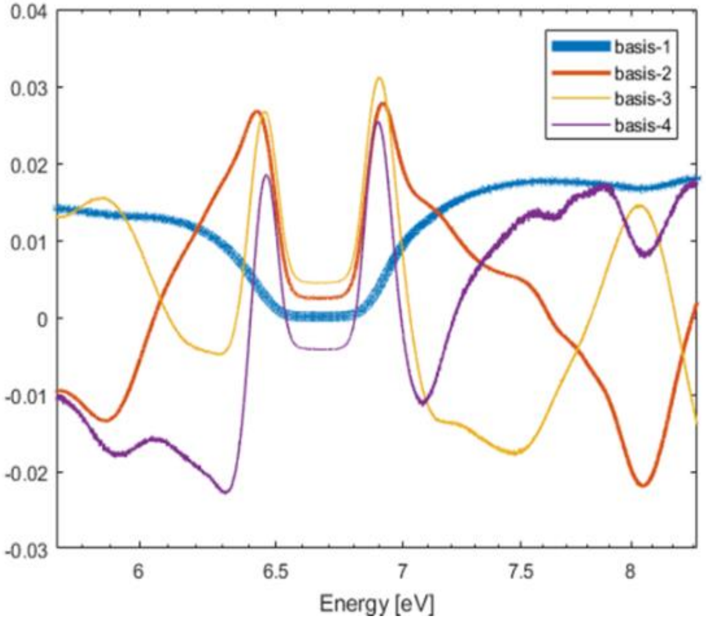
  - **Sometimes, it is further simplified by employing the intermediate resonance (IR) model.**

- **Problem of the Slowing-Down Scattering Source**
  - **However, there happens up-scattering in the epi-thermal energy domain.**
    - Due to the thermal motion of the target nucleus
    - Doppler broadening rejection correction (DBRC) method
  - **This makes a difference of about 10% in reactivities and fuel temperature coefficients (FTCs).**

- **Infeasibility of Addressing Up-Scattering Sources with Conventional Methods**
  - **Only UFG methods can address up-scattering effects directly.**
  - **However, it is almost impossible due to the tremendously large size of scattering matrices.**
    - The size is the square of the number of UFGs if stored in a dense matrix format.

- **Resonance calculation using energy Spectral Expansion (RSE) Method**
  - **The RSE method aims at reducing the complexity of UFG methods by applying the reduced order model (ROM).**
    - To handle heterogeneous core geometry directly, retaining the accuracy of UFG methods
  - **Basis expansion on UFG spectra is employed for the ROM.**
  - **Hence, the key of the RSE method is to extract a proper set of basis functions for flux spectra.**

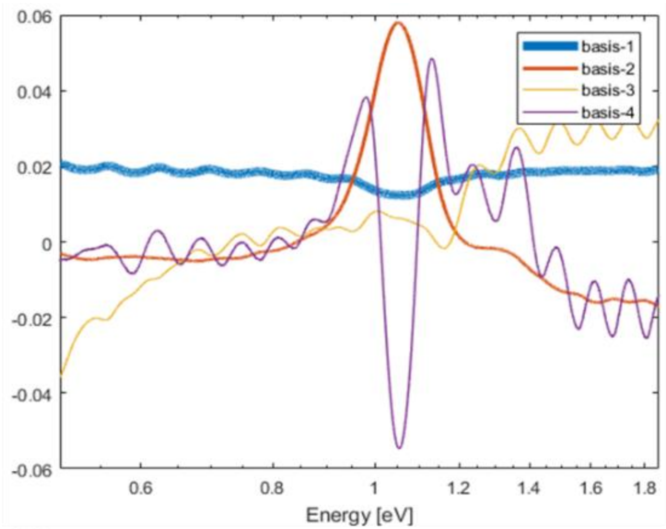


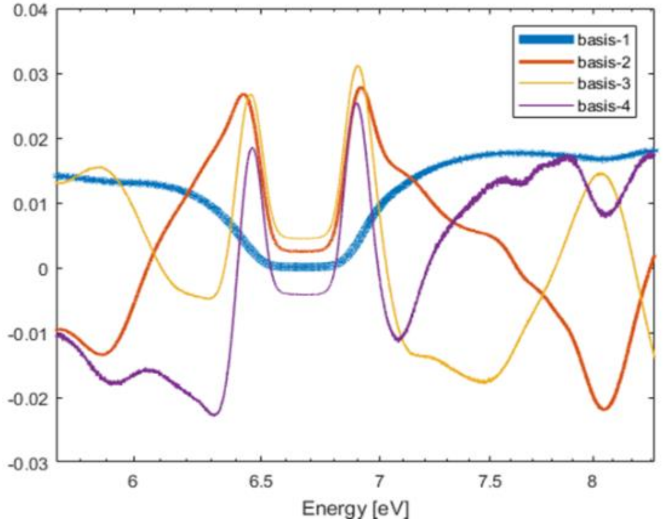


Determination of Basis Functions

- **Proper Orthogonal Decomposition (POD)**
  - **POD is a method for obtaining orthogonal functions to reduce complexity.**
  - **The size of a basis set from POD can be smaller than the other basis sets.**
  - **A basis set is extracted from the solutions of realistic single-pin problems.**
    - The basis functions are principal components of a physical field.
  - **In the POD method, singular value decomposition (SVD) is employed.**

- **Precedent Study on Basis Expansion for Resonance Calculation**
  - **One may consider traditional basis functions.**
    - Such as Legendre polynomials or Fourier series
  - **There was a trial to utilize Wavelet functions for resonance calculations.**
    - By W. Yang et al.[1] and W. Rooijen[2]
  - **However, the number of expansion functions becomes too large[2].**





1. W. Yang, H. Wu, and Y. Zheng, "Applications of Wavelets Scaling Function Expansion Method in Resonance Self-Shielding Calculation," *Ann. Nucl. Energy*, 37(5), 653 (2010).
2. W. Rooijen, "Feasibility of Wavelet Expansion Method to Treat the Energy Variable," *Proc. PHYSOR 2012*, Knoxvile, Tennessee, April 15-20 (2012).

- **Singular Value Decomposition (SVD)**
  - **A snapshot matrix is defined as the below.**

$$\mathbf{A} = \begin{pmatrix} \phi_1(E_1) & \phi_1(E_2) & \cdots & \phi_1(E_G) \\ \vdots & \vdots & \cdots & \vdots \\ \phi_n(E_1) & \phi_n(E_2) & \cdots & \phi_n(E_G) \end{pmatrix} \in \mathbb{R}^{N\times G}$$

  - **The products of the compact SVD are as follows.**
    - The rank of the matrix is r.

$$\mathbf{A} = \mathbf{U\Sigma V}^*,\ \mathbf{U} \in \mathbb{R}^{N\times r}, \mathbf{\Sigma} \in \mathbb{R}^{r\times r}, V \in \mathbb{R}^{G\times r}$$

$$\mathbf{U} = [\vec{u}_1 \quad \vec{u}_2 \quad \cdots \quad \vec{u}_r]$$

$$\mathbf{V} = [\vec{v}_1 \quad \vec{v}_2 \quad \cdots \quad \vec{v}_r]$$

$$\mathbf{\Sigma} = \begin{pmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \sigma_r \end{pmatrix}$$

- **Selection of a Basis Function Set**
  - **A subspace of the right singular vectors can be a basis set.**

$$(\mathbf{A})_{ij} = \sum_{k=1}^{r} u_{ik}\sigma_k v_{jk} \rightarrow \phi_i = \sum_{k=1}^{r} u_{ik}\sigma_k \vec{v}_k$$

  - **Finally, each basis can be obtained such that the set is orthonormal.**

$$f_k(E) = v_k(E) \text{ so that } \langle \vec{f}_k, \vec{f}_{k'} \rangle = \langle \vec{v}_k, \vec{v}_{k'} \rangle = \delta_{kk'} \text{ where } \mathbf{V}^*\mathbf{V} = \mathbf{I}_r \in \mathbb{R}^{r\times r} \text{(Semi-unitarity)}$$

Reproducibility of UFG Spectrum

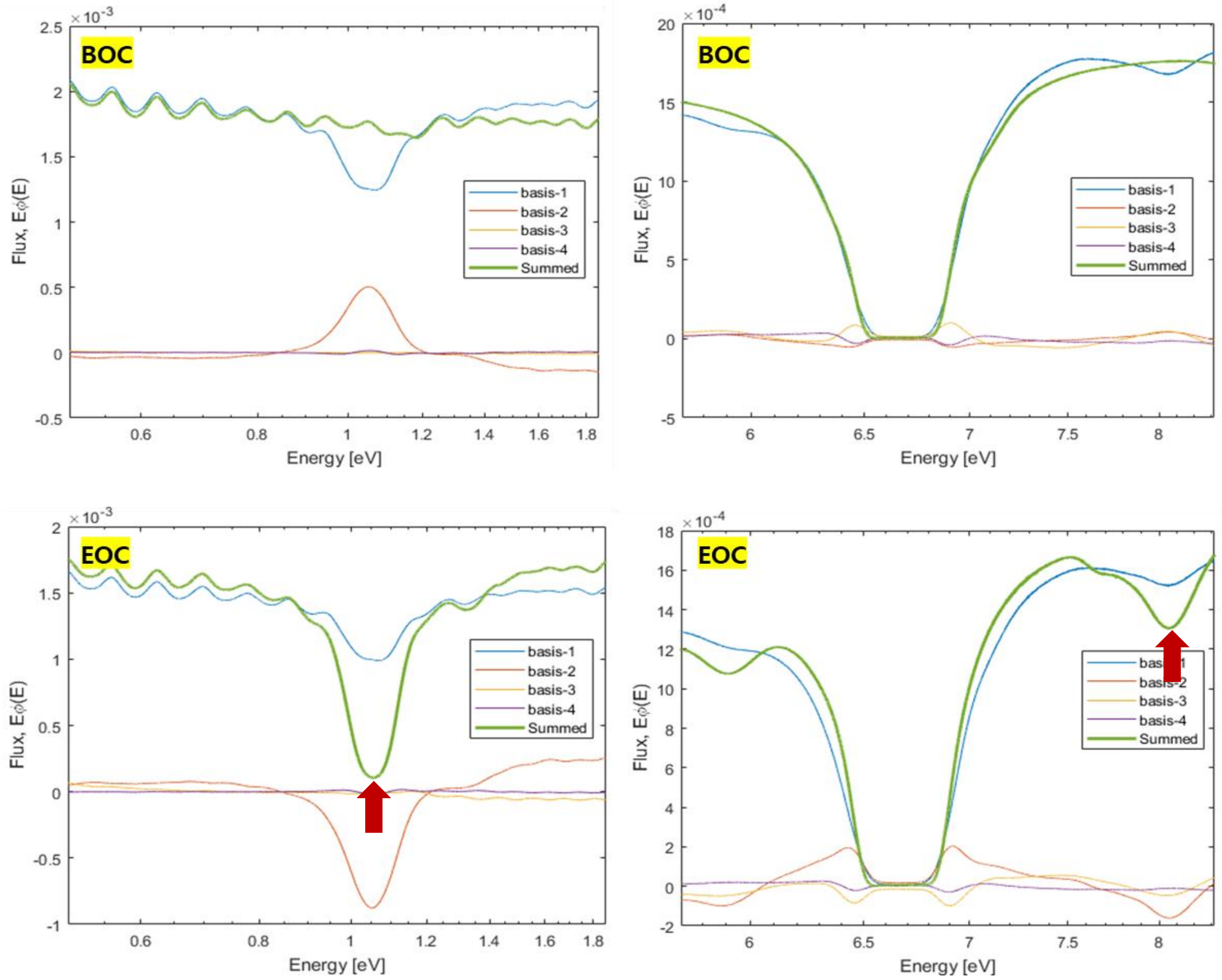
- **Reproduction of UFG Flux Spectrum**
  - **A UFG spectrum can be reproduced as follows:**

$$\phi_k = \int \phi^{ref}(E) f_k(E) dE \rightarrow \phi^{ref}(E) \simeq \sum_k \phi_k f_k(E).$$

  - **The contribution of a basis is as follows:**

$$\phi_k^{ref}(E) = \phi_k f_k(E)$$

- **Contributions of Bases to Different Spectra**
  - **The contributions are examined for two spectra from BOC and EOC states.**
    - Bold green lines are for the summed spectra.
    - The others are for contributions of the bases.
  - **The first basis determines the overall level.**
  - **High-order bases affect specific shapes.**
    - Shape changes from fuel depletion
    - Dip at 1 eV due to Pu-240
    - Dip at 8 eV due to Sm-152



Weak Formulation of the Transport Equation

- **Steady-state Neutron Transport Equation**

$$\mathbf{\Omega}\cdot\nabla\psi(E,\mathbf{\Omega},\mathbf{r})+\Sigma_t(E,\mathbf{r})\psi(E,\mathbf{\Omega},\mathbf{r}) = \frac{1}{4\pi}\int\Sigma_s(E'\rightarrow E)\phi(E',\mathbf{r})dE'+Q_{fix}(E,\mathbf{\Omega},\mathbf{r})$$

- **Basis Expansion of Flux**

$\psi(E,\mathbf{\Omega},\mathbf{r})\simeq\sum_k\varphi_k(\mathbf{\Omega},\mathbf{r})f_k(E)$, while the basis function satisfies, $\langle f_k, f_{k'}\rangle=\delta_{kk'}$ (orthonormality).

$$\rightarrow\phi(E,\mathbf{r})\simeq\sum_k\phi_k(\mathbf{r})f_k(E)$$

- **Weak Form Formulation of the NTE**

$$\int\left(\mathbf{\Omega}\cdot\nabla\psi(E,\mathbf{\Omega},\mathbf{r})+\Sigma_t(E,\mathbf{r})\psi(E,\mathbf{\Omega},\mathbf{r})\right)\cdot f_k(E)dE=\int\left(\frac{1}{4\pi}\int\Sigma_s(E'\rightarrow E)\phi(E',\mathbf{r})dE'+Q_{fix}(E,\mathbf{\Omega},\mathbf{r})\right)\cdot f_k(E)dE$$

$$\rightarrow\int\left(\mathbf{\Omega}\cdot\nabla+\Sigma_t(E,\mathbf{r})\right)\sum_{k'}\varphi_{k'}(\mathbf{\Omega},\mathbf{r})f_{k'}(E)\cdot f_k(E)dE=\int\left(\frac{1}{4\pi}\int\Sigma_s(E'\rightarrow E)\sum_{k'}\phi_{k'}(\mathbf{r})f_{k'}(E')dE'+Q_{fix}(E,\mathbf{\Omega},\mathbf{r})\right)\cdot f_k(E)dE$$

- **Steaming Term with Moments**

$$\int \mathbf{\Omega}\cdot\nabla\psi(E,\mathbf{\Omega},\mathbf{r})f_k(E)dE = \int \mathbf{\Omega}\cdot\sum_{k'}\nabla\varphi_{k'}(\mathbf{\Omega},\mathbf{r})f_{k'}(E)\cdot f_k(E)dE$$

$$=\sum_{k'}\mathbf{\Omega}\cdot\nabla\varphi_{k'}(\mathbf{\Omega},\mathbf{r})\int f_{k'}(E)\cdot f_k(E)dE = \mathbf{\Omega}\cdot\nabla\varphi_k(\mathbf{\Omega},\mathbf{r})$$

- **Collision Term with Moments**

$$\int \Sigma_t(E,\mathbf{r})\psi(E,\mathbf{\Omega},\mathbf{r})f_k(E)dE = \sum_{k'}\varphi_{k'}(\mathbf{\Omega},\mathbf{r})\int \Sigma_t(E,\mathbf{r})f_{k'}(E)f_k(E)dE$$

$$=\sum_{k'}\varphi_{k'}(\mathbf{\Omega},\mathbf{r})\Sigma_{t,kk'}(\mathbf{r})$$

- **Source Term with Moments**

$$\int \frac{1}{4\pi}\int \Sigma_s(E'\to E)\phi(E',\mathbf{r})dE' f_k(E)dE = \frac{1}{4\pi}\sum_{k'}\phi_{k'}(\mathbf{r})\iint \Sigma_s(E'\to E)f_{k'}(E')dE' f_k(E)dE$$

$$=\frac{1}{4\pi}\sum_{k'}\Sigma_{s,kk'}(\mathbf{r})\phi_{k'}(\mathbf{r})$$

- **Weak Form of the Equation of Fixed Source Problem**

$$\mathbf{\Omega}\cdot\nabla\varphi_k(\mathbf{\Omega},\mathbf{r}) + \sum_{k'}\Sigma_{t,kk'}(\mathbf{r})\varphi_k(\mathbf{\Omega},\mathbf{r}) = \frac{1}{4\pi}\sum_{k'}\Sigma_{s,kk'}(\mathbf{r})\phi_{k'}(\mathbf{r}) + q_{fix,k}(\mathbf{\Omega},\mathbf{r})$$

$$\to \mathbf{\Omega}\cdot\nabla\boldsymbol{\varphi}(\mathbf{\Omega},\mathbf{r}) + \mathbf{\Sigma}_t\boldsymbol{\varphi}(\mathbf{\Omega},\mathbf{r}) = \frac{1}{4\pi}\mathbf{\Sigma}_s\boldsymbol{\phi}(\mathbf{r}) + \mathbf{q}(\mathbf{\Omega},\mathbf{r}),$$

: Unknown

$$\Sigma_{t,kk'}(\mathbf{r}) \equiv \int f_k(E)\Sigma_t(E,\mathbf{r})f_{k'}(E)dE$$

$$\Sigma_{s,kk'}(\mathbf{r}) \equiv \iint f_k(E)\Sigma_s(E'\to E,\mathbf{r})f_{k'}(E')dE'dE$$

ENGINEERING

Sequence of the RSE Method

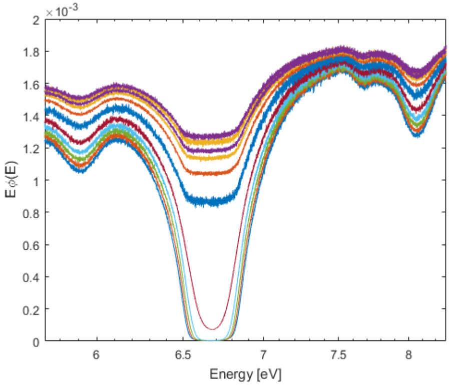
1. **Obtain Flux Spectra from UFG Solution**
   - **A set of single-pin problems are solved to get UFG spectra.**
     - For various conditions such as temperature or moderator density

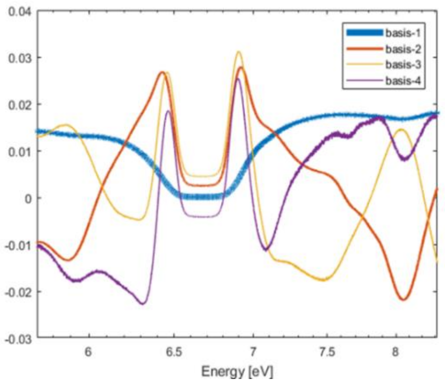
2. **Extract Basis Functions based on the POD Method**
   - **Composing a snapshot matrix, a basis set is obtained with POD.**

3. **Generation of XS Moments**
   - **XS moments are calculated with UFG XSs.**

4. **Solve the FSP to Obtain Flux Moments**
   - **A FSP system over a core is set with the XS moments.**
   - **Solving the FSP, the scalar flux moments are obtained.**

5. **Reconstruct UFG Flux Spectrum**
   - **UFG spectra are calculated with the flux moments and basis functions.**





$$\rightarrow f_k(E)$$

$$\Sigma_{t,kk'}(\mathbf{r}) \equiv \int f_k(E)\Sigma_t(E,\mathbf{r})f_{k'}(E)dE$$

$$\Sigma_{s,kk'}(\mathbf{r}) \equiv \iint f_k(E)\Sigma_s(E'\rightarrow E,\mathbf{r})f_{k'}(E')dE'dE$$

$$\downarrow$$

$$\boldsymbol{\Omega}\cdot\nabla\boldsymbol{\varphi}(\boldsymbol{\Omega},\mathbf{r})+\boldsymbol{\Sigma}_t\boldsymbol{\varphi}(\boldsymbol{\Omega},\mathbf{r})=\frac{1}{4\pi}\boldsymbol{\Sigma}_s\boldsymbol{\phi}(\mathbf{r})+\mathbf{q}(\boldsymbol{\Omega},\mathbf{r})$$

$$\rightarrow \phi_k(\mathbf{r})$$

$$\rightarrow \phi(E,\mathbf{r}) \simeq \sum_k \phi_k(\mathbf{r}) f_k(E)$$

Motivation for the Generalization of the RSE Method

- **Feasibility of Addressing Up-Scattering Sources**
  - **The reduction in the DOF is also advantageous to the size of scattering XSs.**

$$\Sigma_{s,kk'}(\mathbf{r}) \equiv \iint f_k(E)\Sigma_s(E' \to E) f_{k'}(E') dE' dE$$

  - **The size of the scattering matrix can be significantly reduced compared to UFG methods.**
    - The size of a matrix can reduce by the square of the reduction in the degrees of freedom.
  - **It becomes feasible to address up-scattering sources directly.**
  - **The feasibility is a powerful potential of the RSE method.**

- **Need for Practical Methods to Generate Exact XS Moments**
  - **Despite the potential, the conventional RSE method also applied the slowing-down approximation.**
  - **There are many obstacles when obtaining exact XS moments with UFG methods for numerical integration.**
    - Large memory requirement when employing UFG scattering XSs for $\Sigma_s(E' \to E)$
    - An enormous number of operations for every pair of basis functions, $\left(f_k(E), f_{k'}(E')\right)$
  - **A Monte Carlo method calculating XS moments is devised for efficiency.**

Generation of Cross Section Moments via Monte Carlo Method

- **Alternative Definitions of XS Moments**
  - **XS moments have to be defined differently to clarify their physical meaning.**
  - **Two rates are introduced for the alternative definitions.**

$$R_{t,k'}(E) \equiv \Sigma_t(E) f_{k'}(E) \qquad S_{k'}(E) \equiv \int \Sigma_s(E' \to E) f_{k'}(E') dE'$$

  - **They are the rates when the flux is given as a basis function.**
  - **Once the rates are obtained, XS moments are easily calculated.**

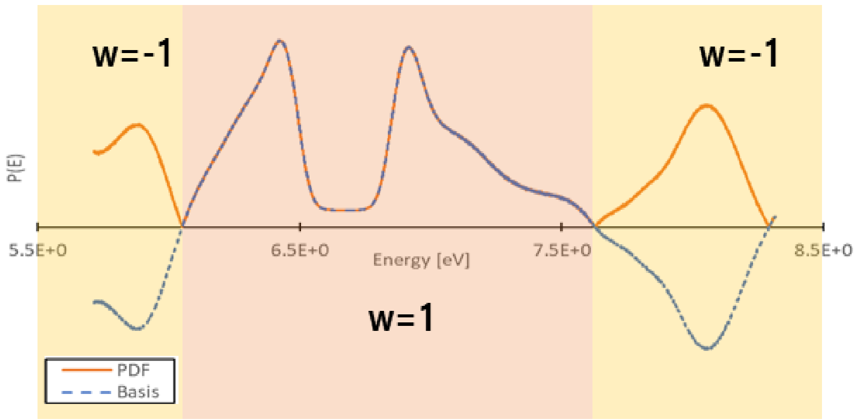
$$\Sigma_{t,kk'} = \int R_{t,k'}(E) f_k(E) dE \qquad \Sigma_{s,kk'} = \int S_{k'}(E) f_k(E) dE$$

$$\Sigma_{t,kk'} \equiv \int f_k(E) \Sigma_t(E) f_{k'}(E) dE$$

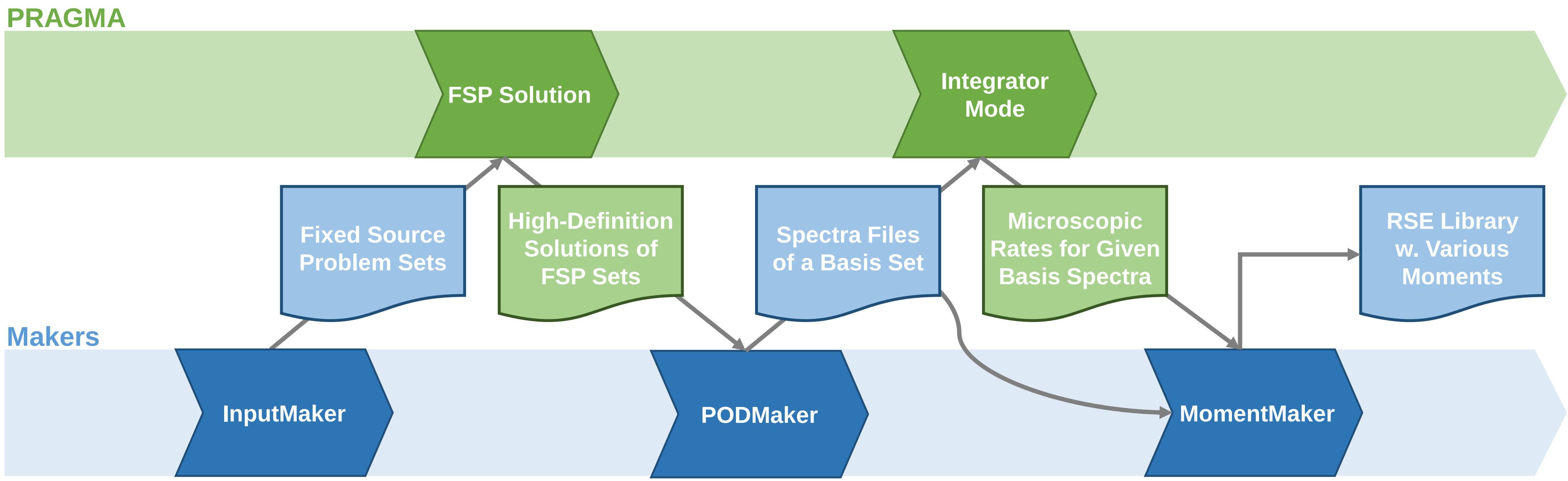
$$\Sigma_{s,kk'} \equiv \iint f_k(E) \Sigma_s(E' \to E) f_{k'}(E') dE' dE$$

- **Probability Density Function (PDF) for Basis Functions**
  - **Basis functions should be given as the energy distribution of samples.**
  - **They cannot be PDFs as they include negative values.**
  - **Thus, the PDF for a basis is defined as follows:**
    - PDF as the absolute of the basis function.
    - Weight of each sample as the sign of the function at the energy.

$$p(E) = |f(E)|, \; w(E) = f(E)/|f(E)|$$

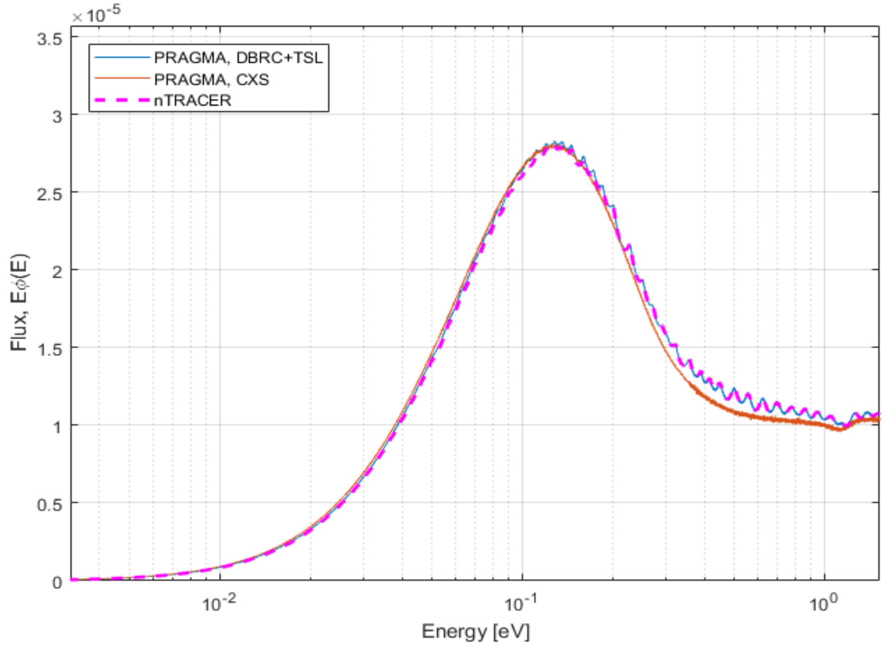


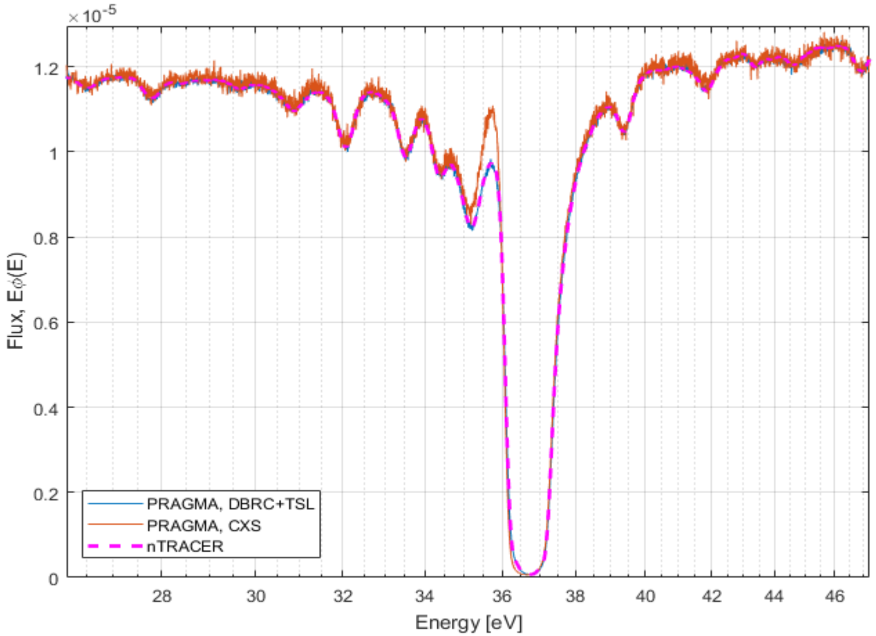
- **PRAGMA-Makers Library Generation System**
  - **PRAGMA and the three Makers scripts are employed to generate an RSE library.**
  - **A problem set is made by InputMaker to be solved by PRAGMA.**
  - **The basis set is given by PODMaker so that PRAGMA calculates various rates.**
  - **PRAGMA applies the DBRC model when solving problems and calculating the rates.**
  - **With the spectra of bases and the rates from PRAGMA, MomentMaker generates an RSE library.**



UFG Spectrum Reproducibility with Complex Scattering Effects

- **Spectrum Reproduction with the Consistent Cross Section Moments**
  - **It was possible to obtain a consistent spectrum to the Monte Carlo solutions with the exact XS moments.**
  - **The reproduced spectrum follows the spectrum with exact scattering models.**
    - The tiny waves in the thermal range from the thermal scattering law (TSL) of H_2O
    - The lower rebound due to up-scattering from DBRC
  - **The result shows good agreement to the spectrum with complicating scattering effects.**





OPR1000 FTC Verification Problems

- **The effect of non-uniform temperature profiles is an important issue in resonance calculations.**
  - Especially for direct whole-core calculations
- **The OPR1000-based single-pin problem set was tested to examine the non-uniform temperature profile.**
  - A benchmark problem from SNU
- **The compositions and temperature conditions are presented in the below table.**
- **Two different resonance scattering models, the DBRC and the constant XS (CXS), are compared.**

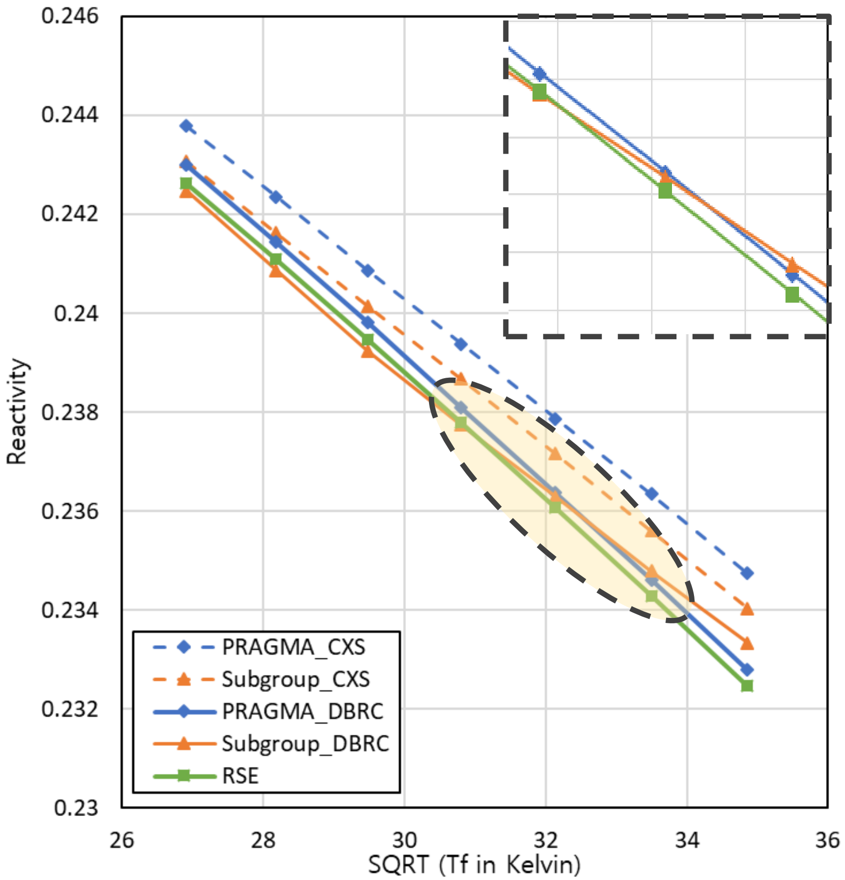
Region	Material	Radius (cm)	Temperature (K) for power level						
			50%	75%	100%	125%	150%	175%	200%
Fuel	UO_2 3.1w%	0.1846	790	902	1025	1158	1301	1454	1617
		0.2610	756	846	943	1047	1157	1274	1398
		0.3197	724	793	866	944	1025	1111	1200
		0.3692	693	744	797	852	909	967	1028
		0.4127	662	695	729	762	796	831	866
Gap	He	0.4203	630	645	661	676	691	707	722
Cladding	Nat. Zr	0.4862	606	611	615	618	622	625	629
Moderator	H_2O	1.2870 (pitch)	587	587	587	587	587	587	587

- **Multiplication Factors under Non-Uniform Temperature Profile**

	Reso. Scat. \ Power	50%	75%	100%	125%	150%	175%	200%
PRAGMA	DBRC	1.32100	1.31829	1.31548	1.31251	1.30956	1.30651	1.30344
	CXS	1.32237	1.31987	1.31730	1.31471	1.31212	1.30950	1.30675
nTRACER Subgroup	DBRC	1.32008 (-92)	1.31729 (-100)	1.31448 (-100)	1.3119 (-61)	1.30940 (-16)	1.30684 (+33)	1.30436 (+92)
	CXS	1.32112 (-125)	1.31860 (-127)	1.31605 (-125)	1.31349 (-122)	1.31089 (-123)	1.30823 (-127)	1.30555 (-120)
nTRACER RSE	DBRC	1.32034 (-66)	1.31770 (-59)	1.31487 (-61)	1.31198 (-53)	1.30902 (-54)	1.30596 (-55)	1.30289 (-55)

- **Superior Accuracy in Estimating FTCs**
  - **Physics in resonance scattering makes a change in the FTCs. (~ 10 %)**
  - **The estimation of the RSE method was better with the DBRC model.**
    - Despite the good agreement of the subgroup method with the CXS model

	CXS		DBRC		
	PRAGMA	Subgroup	PRAGMA	Subgroup	RSE
FTC [pcm/K]	- 1.834	- 1.833 (- 0.001)	- 2.078	- 1.847 (+ 0.231, 11 %)	- 2.068 (- 0.010, 0.5 %)



Conclusions and Future Plans

- **Development of a Resonance Method Directly Addressing Exact Scattering Sources**
  - **The generalized RSE method is developed to enable the direct handling of exact scattering sources.**
    - By eliminating the slowing-down approximation
  - **For practicality, the Monte Carlo method is devised to generate exact XS moments with PRAGMA.**
    - With the aid of the alternative definitions of XS moments and the PDFs for basis functions

- **High Accuracy in the Non-Uniform Temperature Profile Condition**
  - **The performance in the non-uniform temperature benchmark is examined.**
  - **Temperature dependence on reactivities with the DBRC model is accurately estimated.**
    - Under 1% error in the FTC estimation

- **Comprehensive Performance Examination for Realistic Cores**
  - **The accuracy is only tested for single-pin problems in this work.**
  - **A comprehensive examination is needed for realistic cores.**
    - In terms of the numerical and computational performance