

Temperature- dependent Scattering Kernels for non- Thermal Moderators

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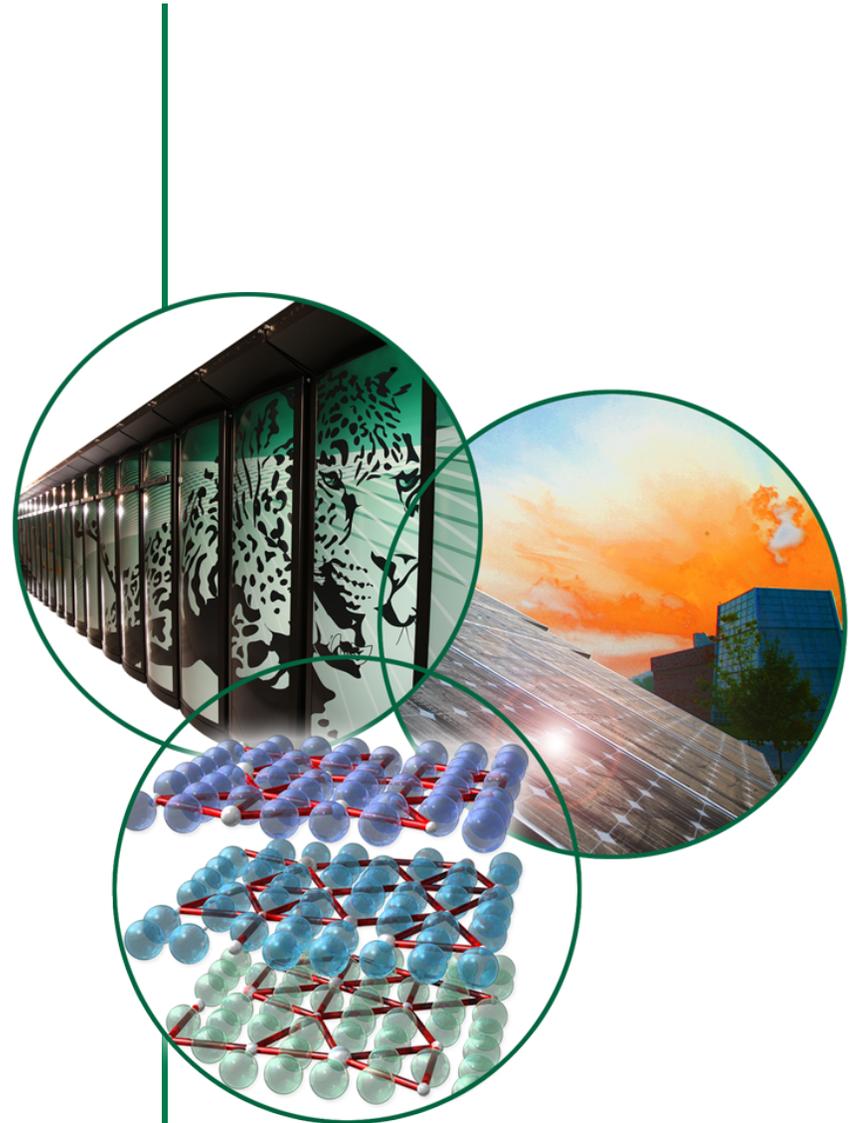
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Origin and Relevance of $\sigma^T(E \rightarrow E', \mu)$

- **Caused by thermal agitation \rightarrow Doppler broadening**
- **Documented and advocated by Rothenstein, Dagan et al.**
 - Rothenstein and Dagan, Ann. Nucl. En. 25, 209, (1998); NDST2007
 - Becker, Dagan, Lohnert, Ann. Nucl. En. 36, 470 (2009) ; etc.
- **Asymptotic, or approximate kernels are not sufficient because:**
 - Integral XS is Doppler broadened, but differential XS is NOT, T set to 0
 - Resonant cross section is approximated by a constant
 - Does not account for enhanced up- (down-) scattering for $E < E_r$ ($E > E_r$)
- **Corrected computation yield:**
 - Pu239 production increased by 2% after 50 MWD/Kg
 - <440 PCM decrease in criticality of LWR fuel cell at 1200 K
- **Legendre moments used in deterministic codes (e.g. CENTRM)**

Status of MC and deterministic codes

- **MC codes can implement accurate scattering kernels**
 - DBRC tried and works in MCNP; B. Becker *et al.*, Ann. Nucl. En. 36 (2009) 470
 - CE Keno: DBRC method tried and works (Doro Wiarda's AMPX Status Report).
- **Deterministic codes**
 - Dagan modified NJOY for DD XS of Rothenstein (Dagan et al, NDST 2007)
 - Direct computation of exact Leg. Mom.'s of scatt. kernel is missing
 - e.g. CENTRM uses Legendre moments for a constant XS
- **An algorithm for direct computation of Leg. mom.'s of scatt. Kernel presented in a later talk**
 - A paper being prepared for the M&C 2011

Stored v. Computed *T*-dep Scatt Kernel

- **Stored in ENDF:**
 - **Pros:**
 - save time to some users
 - Legendre moments require less storage than DD XS:
 - $(E \times E' \times L_{\max})$ vs $(E \times E' \times N_{\text{angle}})$
 - **Cons:**
 - May not be at the right *T* or $(E \rightarrow E')$ grid for an app.
 - More work for evaluators
- **Computed by processing codes:**
 - **Pros:**
 - Arbitrary *T*, or $(E \rightarrow E')$ -grid
 - Uniquely determined by EL XS
 - Less work for evaluators
 - **Cons:**
 - Computed by users via processing codes; requires more time

Brief review of T -dependent methods

- **Wigner and Wilkins (1954)**
 - P_0 for a constant isotropic XS
- **Blackshaw and Murray (1967)**
 - P_0 and P_1 of E -dependent (e.g. resonant) isotropic XS
- **Ouisloumen and Sanchez (1991)**
 - All Legendre moments of E -dependent *anisotropic* XS
 - only P_0 computed; P_1 , etc. involve a three-fold nested integral
- **Rothenstein and Dagan (1998, 2004)**
 - Double differential scattering XS (two-fold nested integral)
 - It reproduces Legendre moments of Ouisloumen and Sanchez
 - Implemented in NJOY
- **This Work**
 - All Leg. Moments, Ang. Dist. In CM, via a single(*) integral

T-dependent Legendre Moments

$$\sigma^T(E \rightarrow E', \mu_{\text{lab}}) = \sum_{n \geq 0} \frac{2n+1}{2} \sigma_n^T(E \rightarrow E') P_n(\mu_{\text{lab}})$$

- Legendre moments of Ouisloumen and Sanchez (Nucl. Sci. Eng. 107, 189, (1991)) are three-fold nested integrals
 → computable in principle, but CPU-time consuming

$$\sigma_n^T(E \rightarrow E') \propto \int_0^\infty t \sigma_s^{0K}(E_{\text{CM}}(t)) e^{-t^2/A} \psi_n(t) dt \quad \mathbf{1}$$

$$\psi_n(t) = \left[H(t - t_-) H(t_+ - t) \int_{\epsilon_{\text{max}} - t}^{\epsilon_{\text{min}} + t} + H(t - t_+) \int_{\epsilon_{\text{max}} - t}^{\epsilon_{\text{min}} + t} \right] \quad \mathbf{2}$$

$$\times e^{-x^2} \int_0^{2\pi} P_n(\mu_{\text{lab}}) P(\mu_{\text{CM}}) d\phi dx \quad \mathbf{3}$$

$$\mu_{\text{lab}} = \mu_{\text{lab}}(x, t, E, E'), \quad \mu_{\text{CM}} = \mu_{\text{CM}}(x, t, E, E')$$

$$t = kTu/A, \quad x = kTc/A$$

Integration by parts of nested integrals

- If the ang. dist. prob. in the CM is a Legendre expansion

$$P(E_{\text{CM}}, \mu_{\text{CM}}) = \frac{1}{4\pi} \sum_{m \geq 0} B_m(E_{\text{CM}}) P_m(\mu_{\text{CM}})$$

- Integration by parts used evaluate the innermost integrals

$$\sigma_n^T(E \rightarrow E') = \sum_{m \geq 0} \sigma_{nm}^T(E \rightarrow E')$$

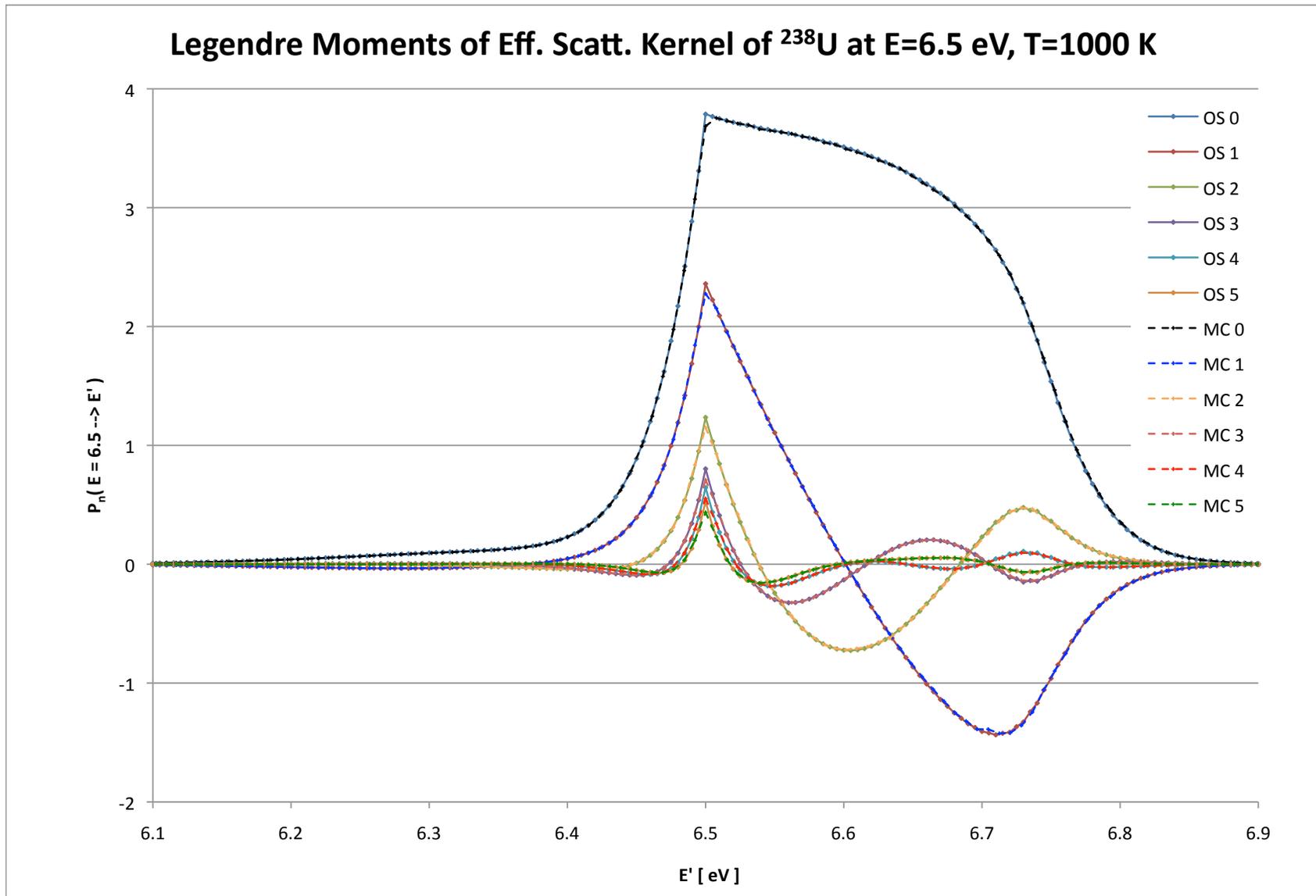
$$\sigma_{nm}^T(E \rightarrow E') \propto \int_0^\infty t B_m(E_{\text{CM}}) \sigma^{0K}(E_{\text{CM}}) e^{-t^2/A} \psi_{nm}(t) dt$$

- $\psi_{nm}(t)$ in terms of erf(); derivation in a M&C 2011 paper

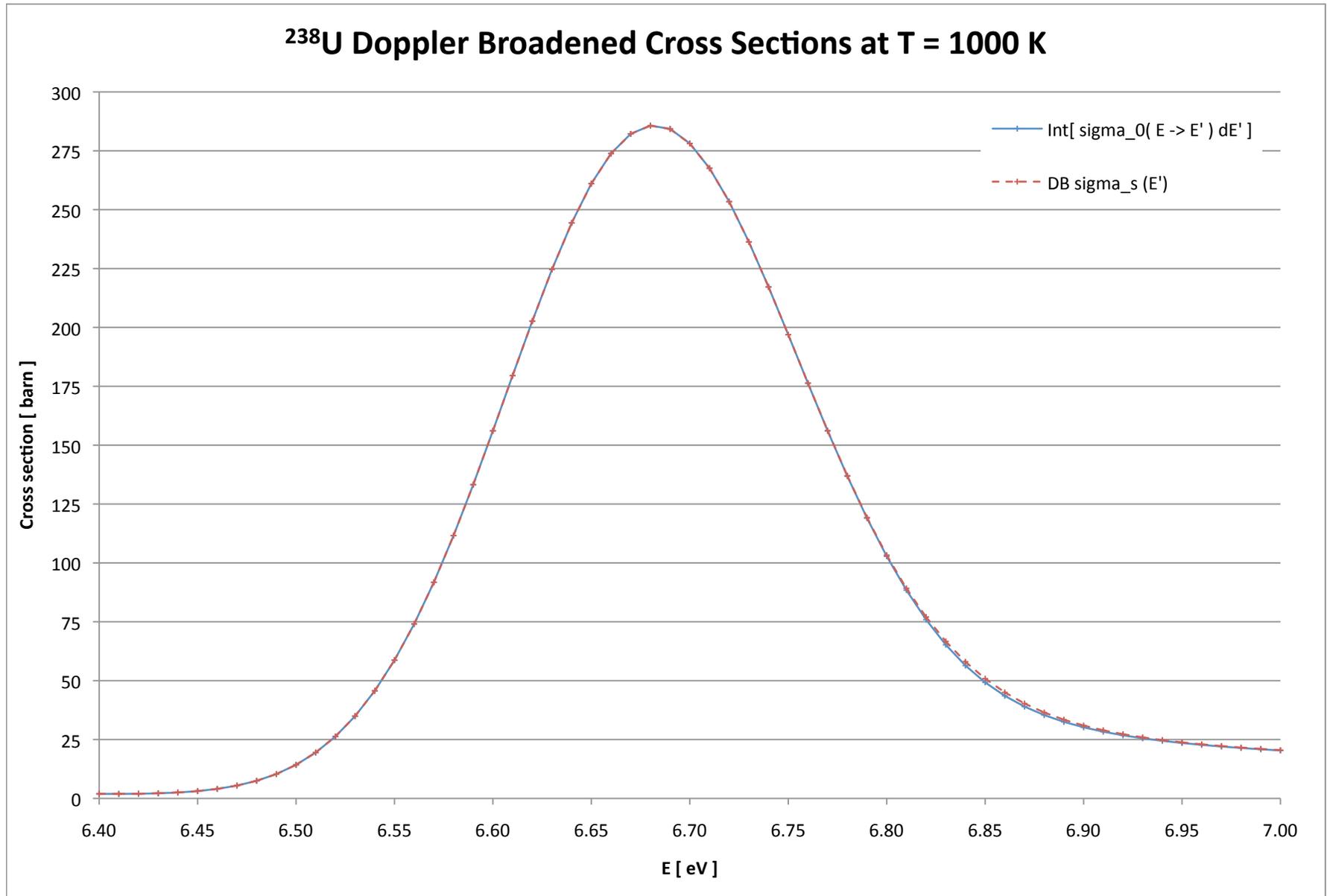
Validation of computed kernels

- Compared to MC kernels by B. Becker for isotropic XS
- Compared integral DB XS to the integral of $P_0(E \rightarrow E')dE'$
- Compared to FLANGE method for a constant XS
- TO DO: compare *anisotropic* in the CM to MC for the same

Deterministic vs. Monte Carlo



Consistency check with integral XS



Angular distribution: Blatt-Biedenharn

- Our first try for anisotropic angular dist. in the CM
- At 6 eV ~0.01% effect
- At 2 keV ~2% effect
- At 10 keV ~10% effect (show plot)

Uncertainties of DD XS (preliminary)

- Assuming all uncertainties come from the el. scatt. XS

$$\sigma_n^T(E \rightarrow E') \propto \sum_{m \geq 0} \int_0^\infty f_{nm}^T(E \rightarrow E', t) \sigma^{0K}(E_{\text{CM}}(t)) dt \quad \text{a "functional"}$$

$$\langle \delta\sigma_n^T(E \rightarrow E') \delta\sigma_{n'}^T(E \rightarrow E') \rangle \propto \sum_{m, m' \geq 0} \int_0^\infty \int_0^\infty f_{nm}^T(E \rightarrow E', t) f_{n'm'}^T(E \rightarrow E', t') \langle \delta\sigma^{0K}(E_{\text{CM}}(t)) \delta\sigma^{0K}(E_{\text{CM}}(t')) \rangle dt dt'$$

$$\langle (\delta\sigma_s^T(E \rightarrow E', \mu))^2 \rangle \propto \sum_{n, n' \geq 0} \frac{2n+1}{2} \frac{2n'+1}{2} P_n(\mu_{\text{lab}}) P_{n'}(\mu_{\text{lab}}) \langle \delta\sigma_n^T(E \rightarrow E') \delta\sigma_{n'}^T(E \rightarrow E') \rangle$$

Summary and Outlook

- **Doppler broadened DD XS, or its Leg. mom.'s, is needed**
 - Important for resonances of heavy nuclei below few 100's eV
- **Exact Legendre moments can now be computed**
 - The original triple-nested integral cast into a single integral
 - Effects of anisotropic scattering in the CM computable
- **CENTRM: deterministic CE 1-dim discrete ordinates**
 - Solving Boltzmann Eq. on a *fine* energy mesh, typically 70,000 pts.
 - Using the scattering kernel in the scattering source computation
- **Implementation into SAMMY considered (w/ N.M. Larson)**

T-Dep. Scatt. Kernels $P^T(E \rightarrow E', m)$; history

	Wigner Wilkin	Blackshaw Murray	Ouisloumen Sanchez	Rothenstein Dagan	This work
Year	1954	1967	1991	1998, 2004	2010
Comments		Legendre moments	Legendre moments	d.d. XS a two- fold nested integral	Legendre moments
E-dep. XS	No	Yes	Yes	Yes	Yes
P0	Yes	Yes	Yes (computed)	Yes (via d.d. XS)	Yes
P1	No	Yes (not comp.)	Yes (not comp.)	Yes (via d.d. XS)	Yes
Pn n>1	No	No	Yes (three-fold nested integral)	Yes (via d.d. XS)	Yes (single integral)
Ang. dist. CM	No	No	Yes (in principle)	Isotropic	Yes (Leg. mom.)