# Legendre Moments of Doppler-broadened Resonance Elastic Scattering


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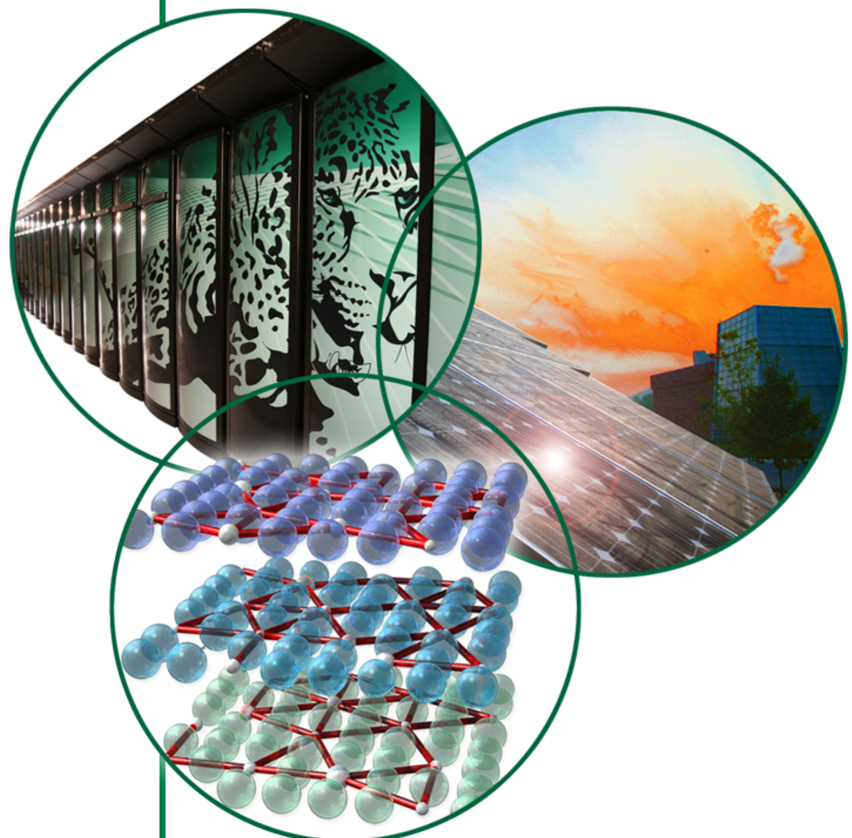

CSEWG Meeting
Santa Fe, NM,
11/3/2010


U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
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# 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 *ani*sotropic 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

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

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

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

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

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

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

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

# Integration by parts of nested integrals

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

$$P(E_{\mathrm{CM}},\mu_{\mathrm{CM}}) = \tfrac{1}{4\pi}\sum_{m\geq 0} \mathrm{B}_m(E_{\mathrm{CM}})P_m(\mu_{\mathrm{CM}})$$

- Integration by parts used evaluate the innermost integrals

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

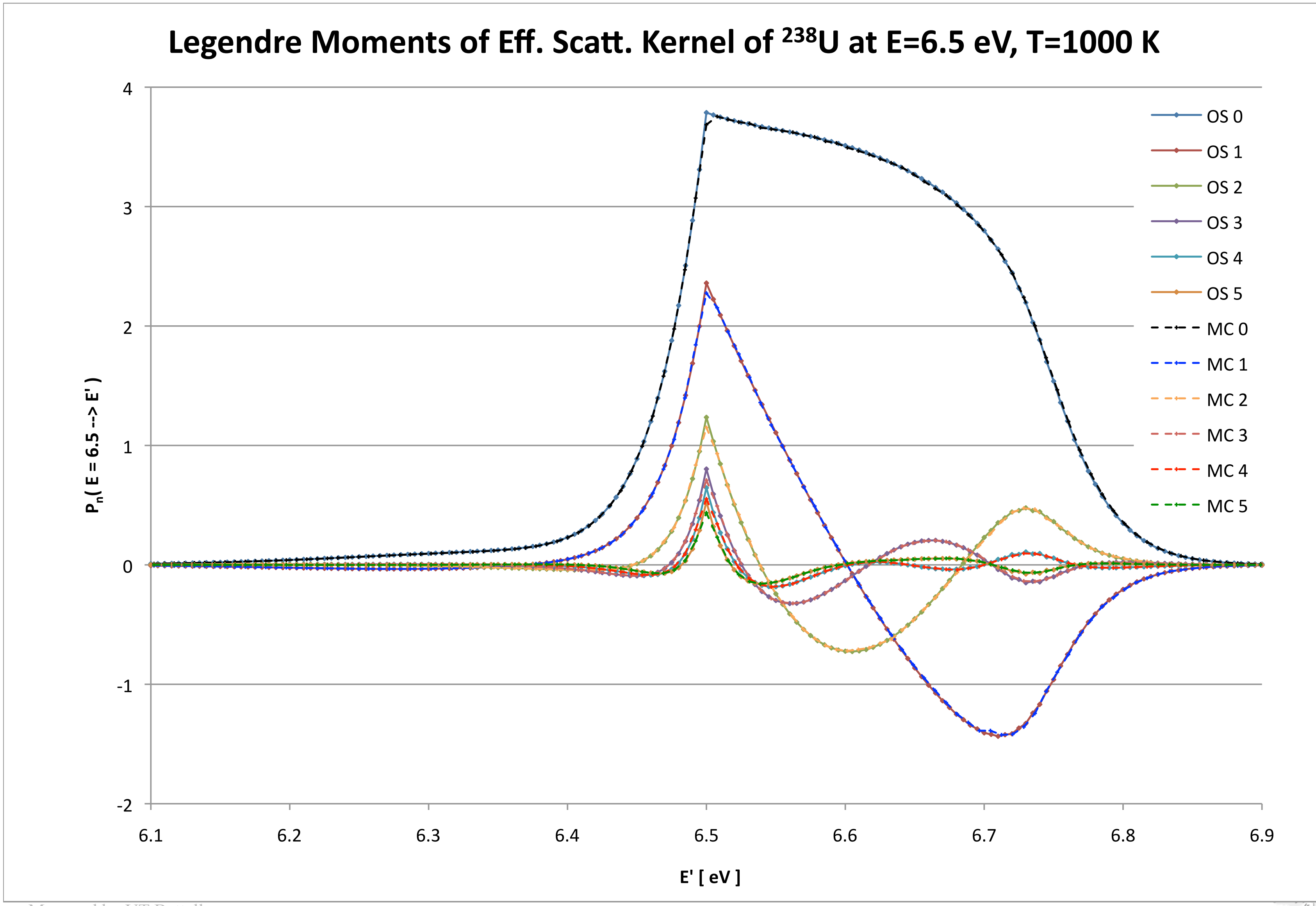
$$\sigma_{nm}^T(E\rightarrow E') \propto \int_0^\infty t\mathrm{B}_m(E_{\mathrm{CM}})\sigma^{0K}(E_{\mathrm{CM}})e^{-t^2/A}\psi_{nm}(t)dt$$

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

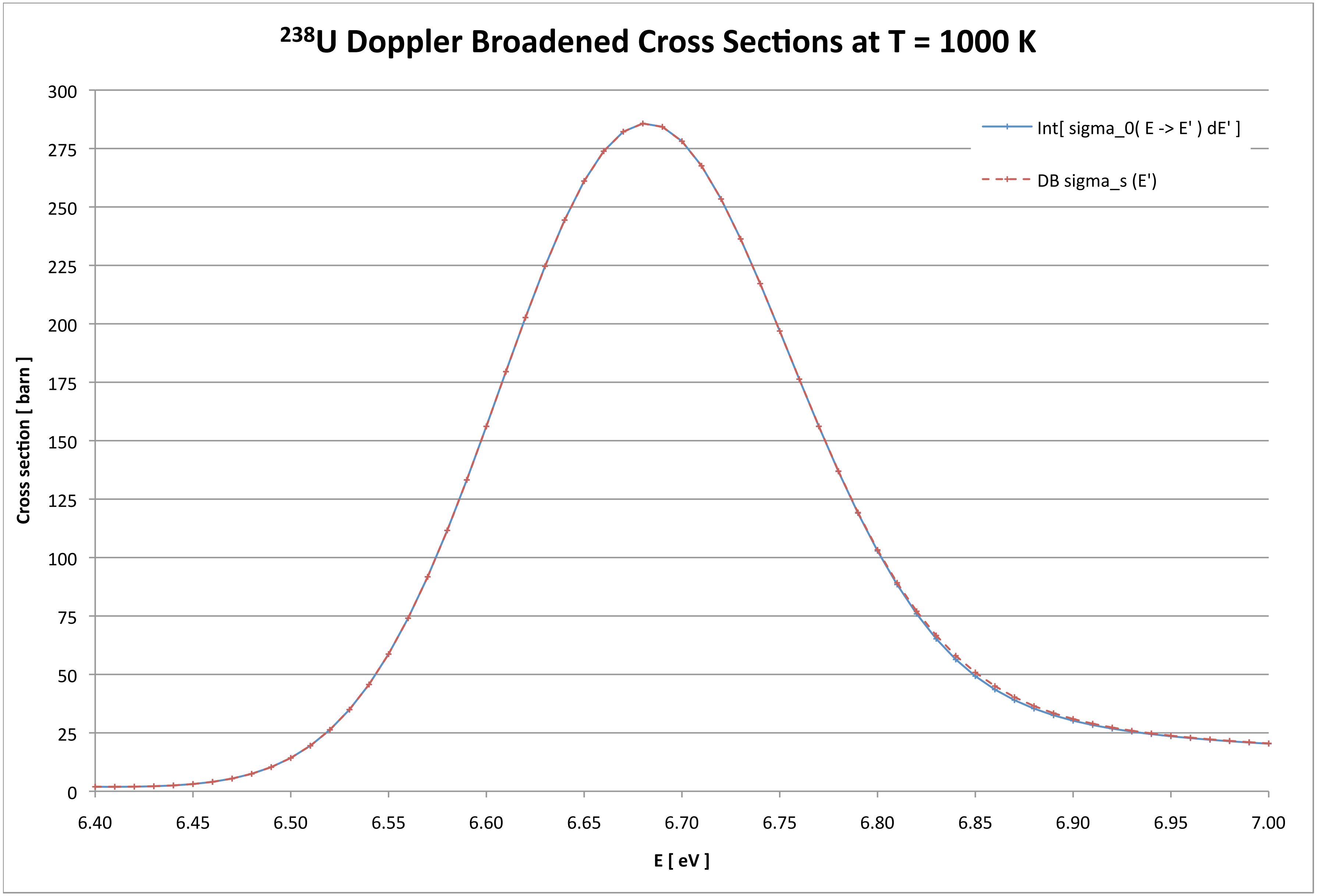
# Validation of computed kernels

- 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



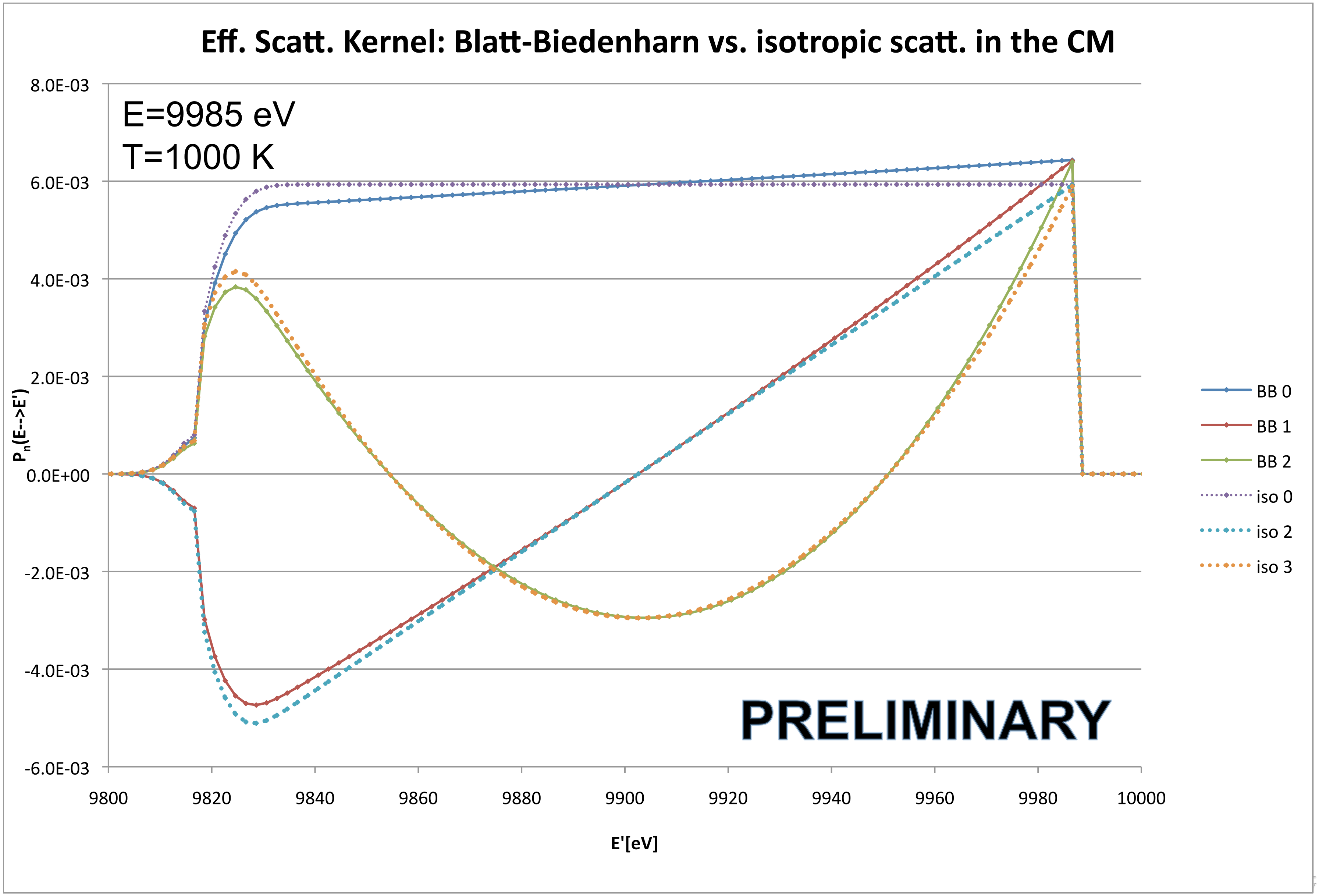
# Consistency check with integral XS



# 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)

# Effect of Blatt-Biedenharn on Legendre m.



# Uncertainties of DD XS (preliminary)

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

$$\sigma_n^T(E \to E') \propto \sum_{m \geq 0} \int_0^\infty f_{nm}^T(E \to E', t)\, \sigma^{0K}(E_{\mathrm{CM}}(t))\, dt$$

a "functional"

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

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

# 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)

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

- Caused by thermal agitation → 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 (CENTRM)

# Status of MC and deterministic codes

- MCNP computes accurate scattering kernels
  – DBRC implemented in MCNP by 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
  – NJOY uses DD XS kernel of Rothenstein and Dagan (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

# $T$-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.) |