Covariance Matrix of a Double-Differential Elastic Scattering Cross Section

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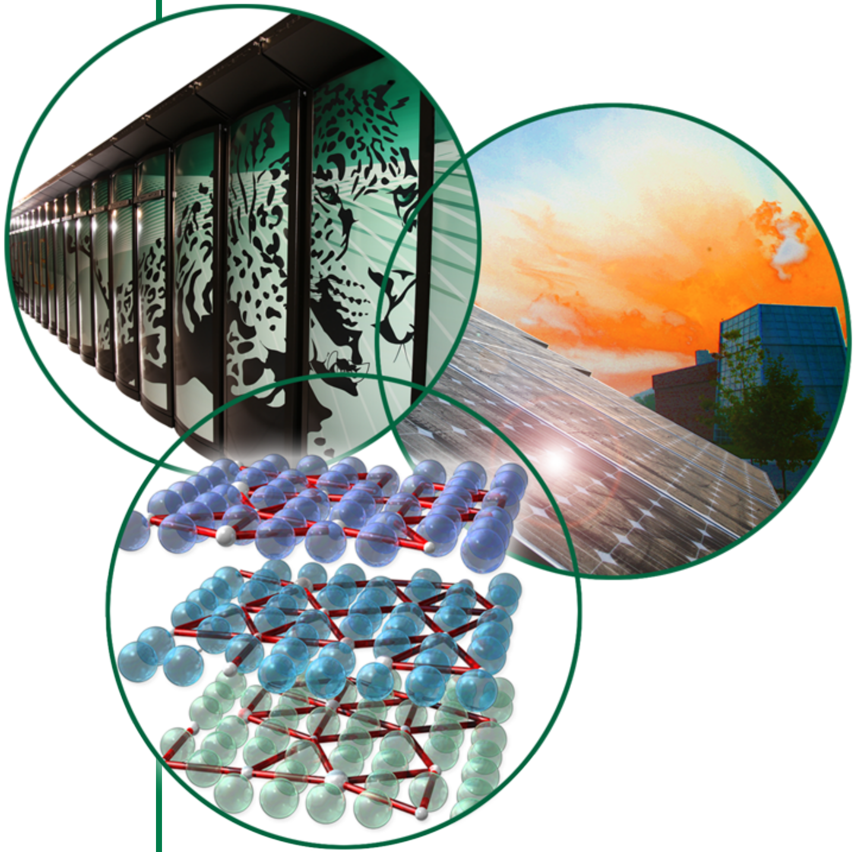

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T-dependent Legendre Moments

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

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

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

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

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

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

Later we will use Blatt-Biedenharn coefficients $\mathrm{B}_m(E_{\mathrm{CM}})$ for an anisotropic angular distribution of scattering XS.

- **Integration by parts is used evaluate the two inner integrals**
  - **Analytical integration by parts is automated in the program**

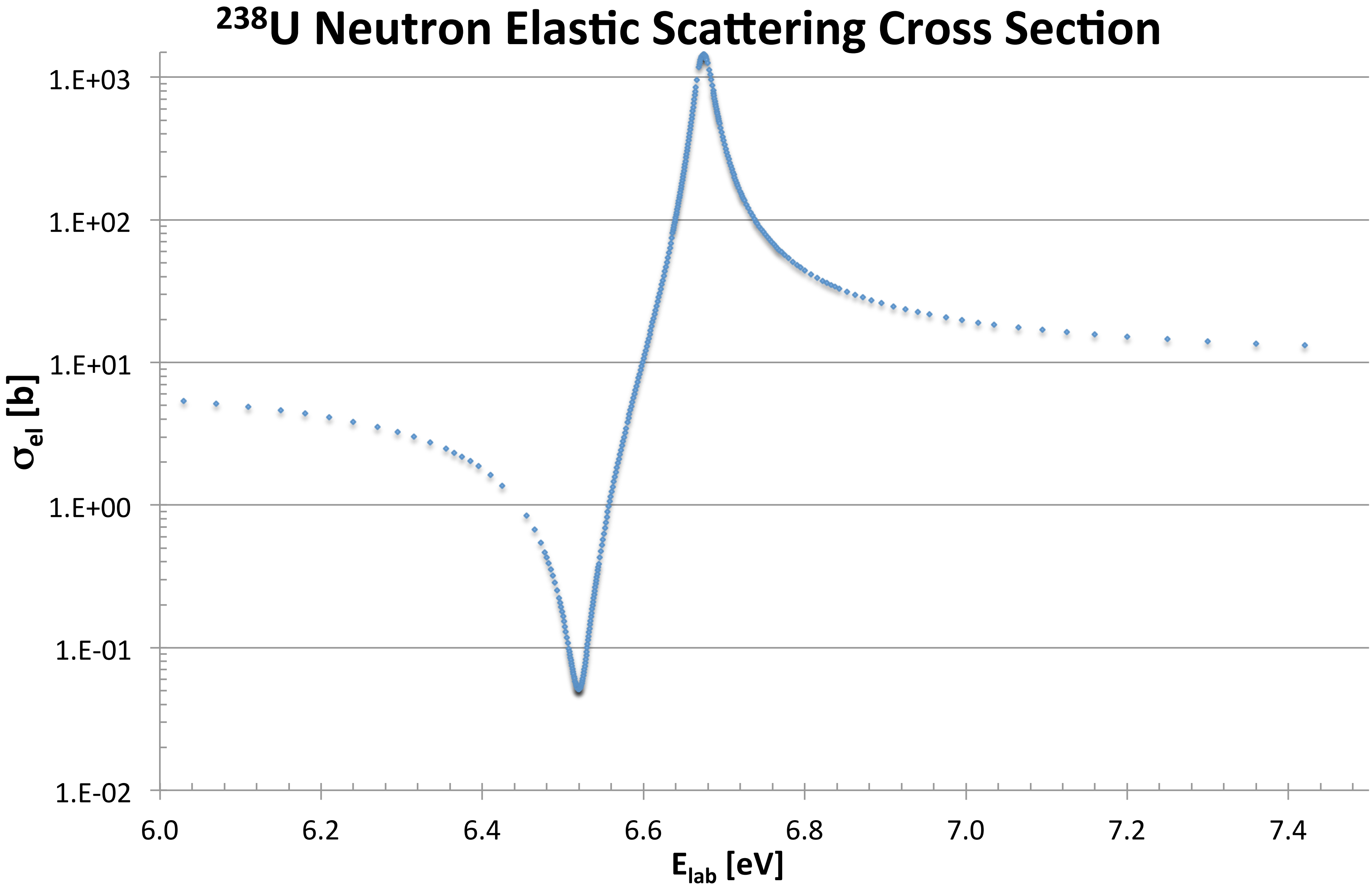
$$\sigma_n^T(E\rightarrow E') = \sum_{m\geq 0}\sigma_{nm}^T(E\rightarrow E')$$

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

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

G. Arbanas *et al.*, Proc. MC 2011, May 8-12, 2011, Rio de Janeiro, Brazil, ISBN 978- 85-63688-00-2, LAS/American Nuclear Society, (2011). [CD-ROM]

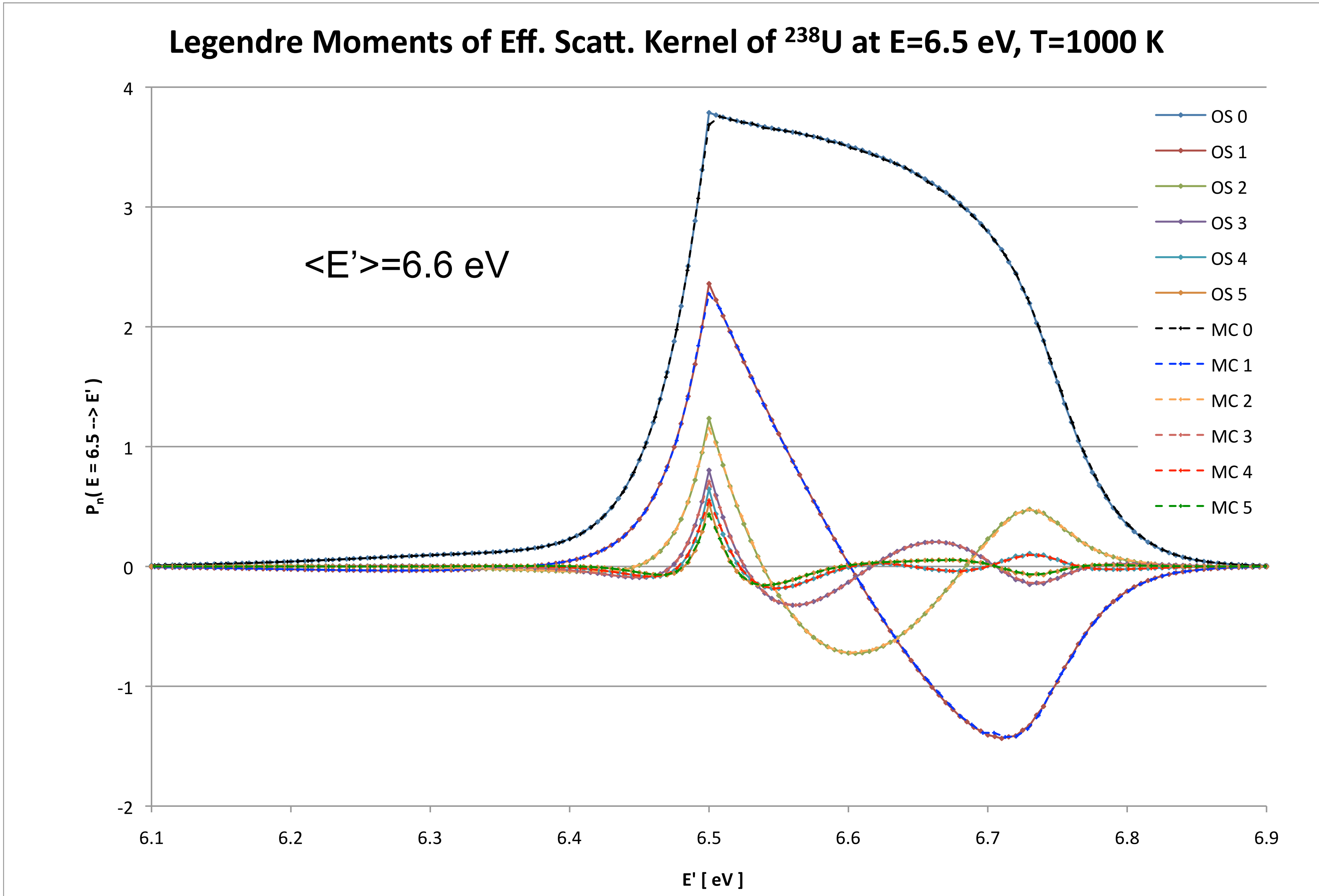
Elastic Scattering Cross Section



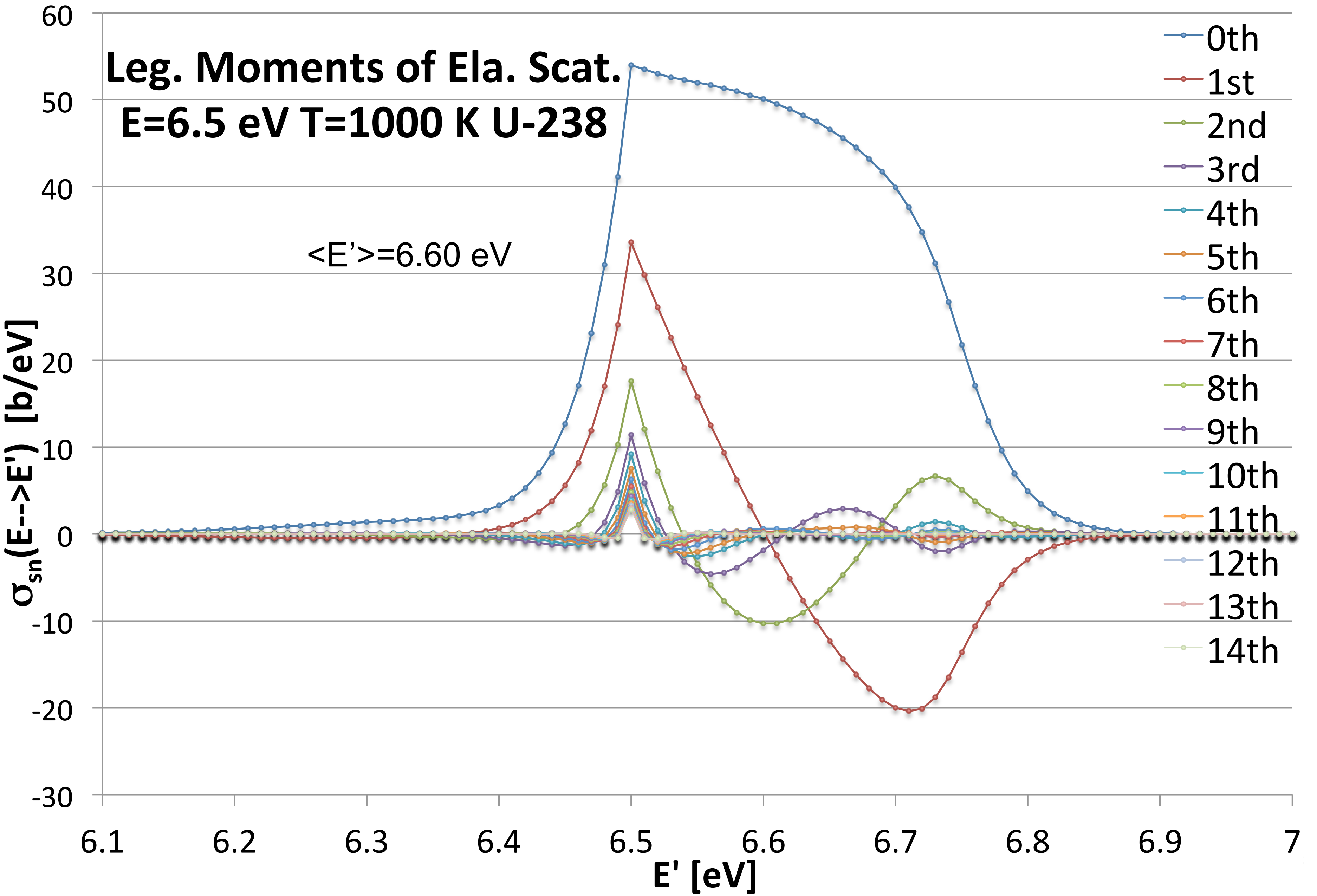
Test 3 a): isotropic scattering in CoM

- In the next slide we show the first six (0- to 5-th) Legendre moments computed by our method ("OS") and by the MC
  - A good agreement can be seen for all moments.
  - The incoming energy E=6.5 eV was intentionally chosen just below the 6.7 eV resonance energy to magnify the effect of up-scattering:
    - i.e., there is a large probability that the outgoing energy E' > E = 6.5 eV
      - Consider the area under the $P_0(E \rightarrow E')$ below E vs. above E on the next slide

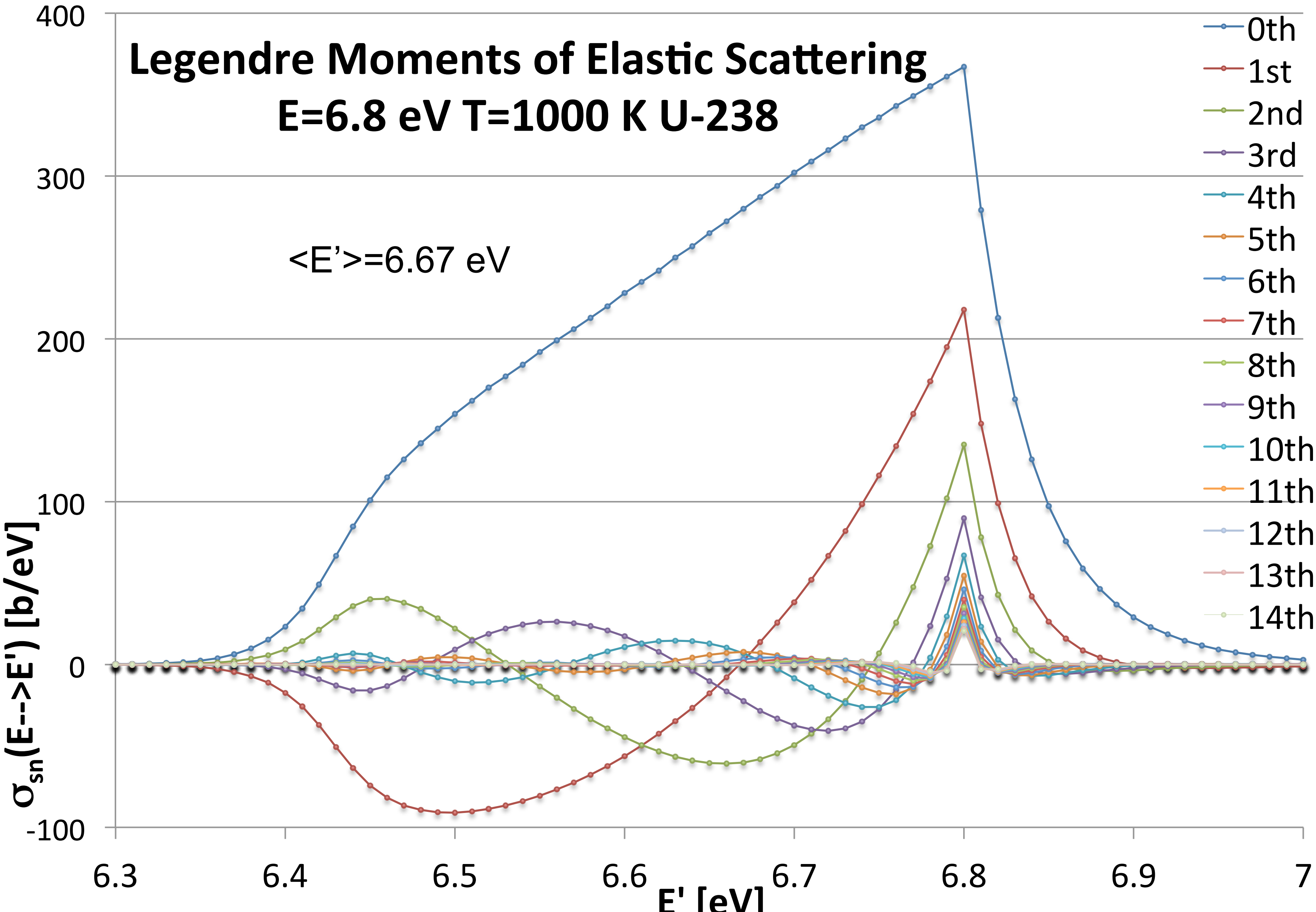
Consistency with Monte Carlo



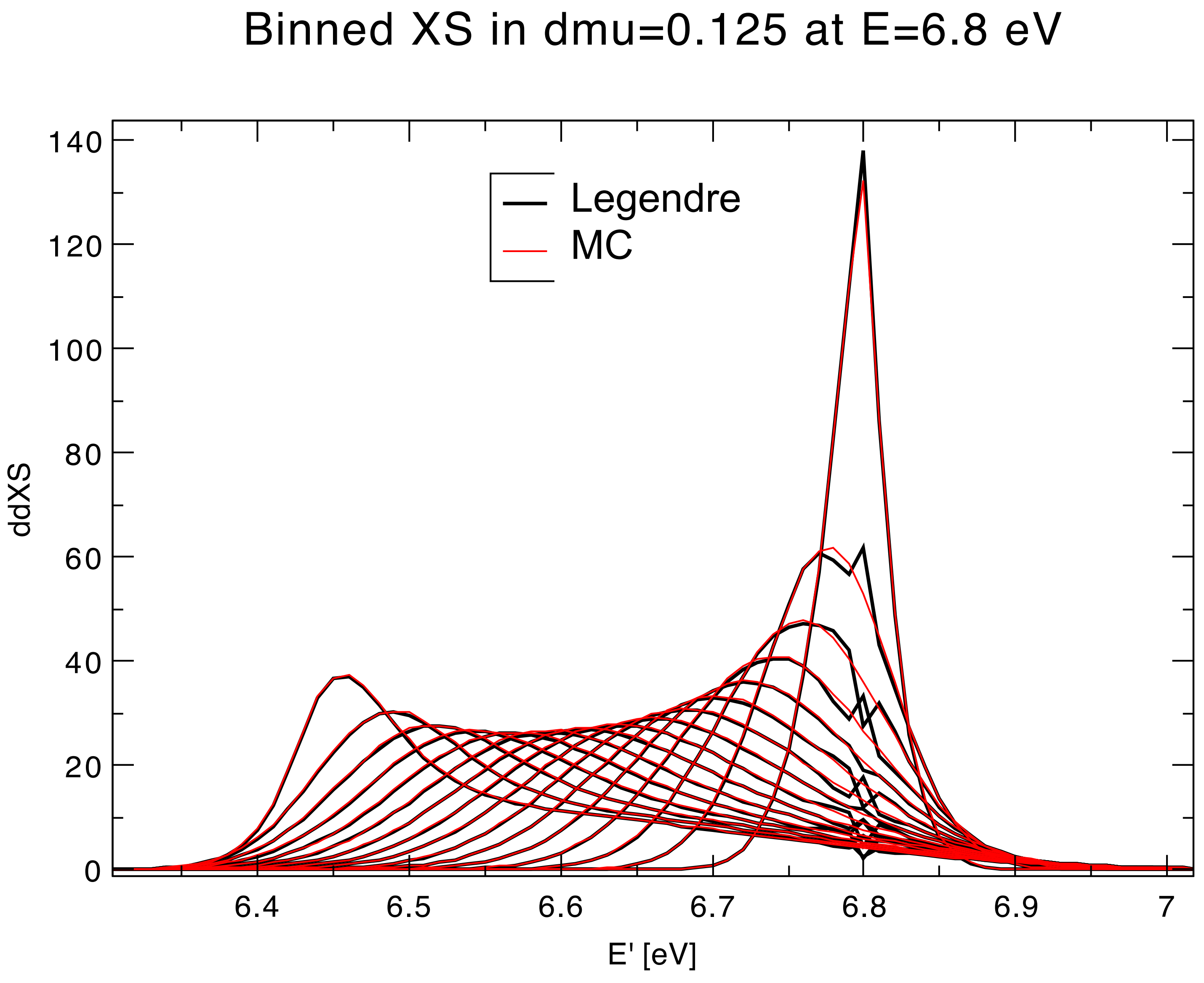
0-14th Legendre Moments E=6.5 eV



0-14th Legendre Moments E=6.8 eV

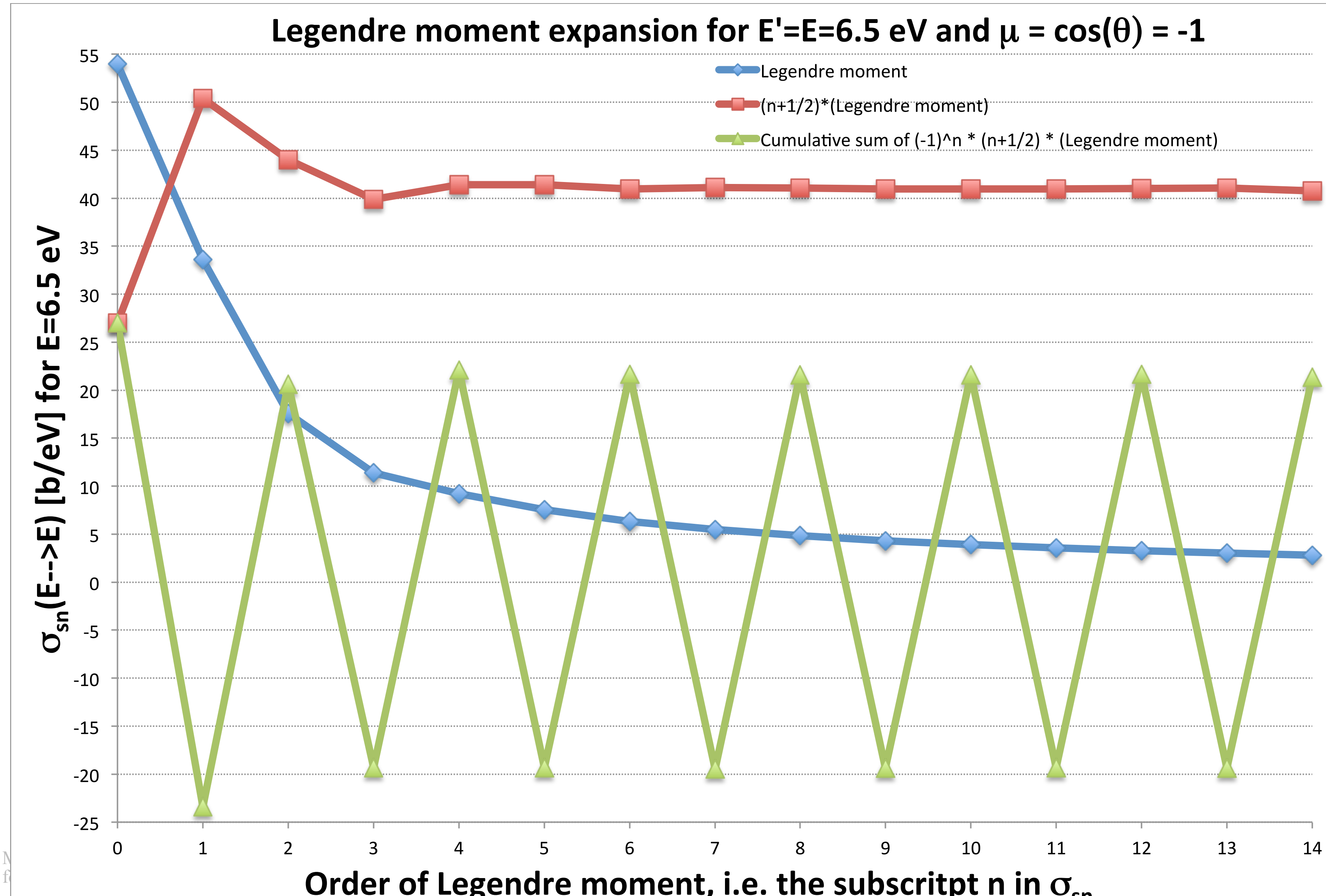


DD XS Legendre Expansion vs. MC



Legendre moments for E'=E

- This plot explains slow convergence of DD XS near E'=E



Variance of Legendre Moments

- The expressions for Legendre moments described above can be used to compute a variance-covariance of DD XS.
- Propagation of uncertainties of the scattering cross section yields expressions for variance-covariance of the Legendre Moments.
  - We write down the expressions on the next slide
  - Assumption:
    - All uncertainty arises from the variance-covariance of the 1D scattering cross section only.
- To appear in Proceedings of NCSC2, September 2011, Vienna

Covariance of Legendre Moments

- ***n*-th Legendre Moment could be written as**

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

  – **Where** $f_{nm}^T(E \to E', t)$ **contains all of the kinematic factors**

- **Using the above, a covariance of Legendre Moments is**

$$\langle \delta\sigma_n^T(E \to E')\delta\sigma_{n'}^T(E \to E') \rangle \propto \sum_{m,m' \ge 0} \int_0^\infty \int_0^\infty f_{nm}^T(E \to E', t) f_{n'm'}^T(E \to E', t')$$

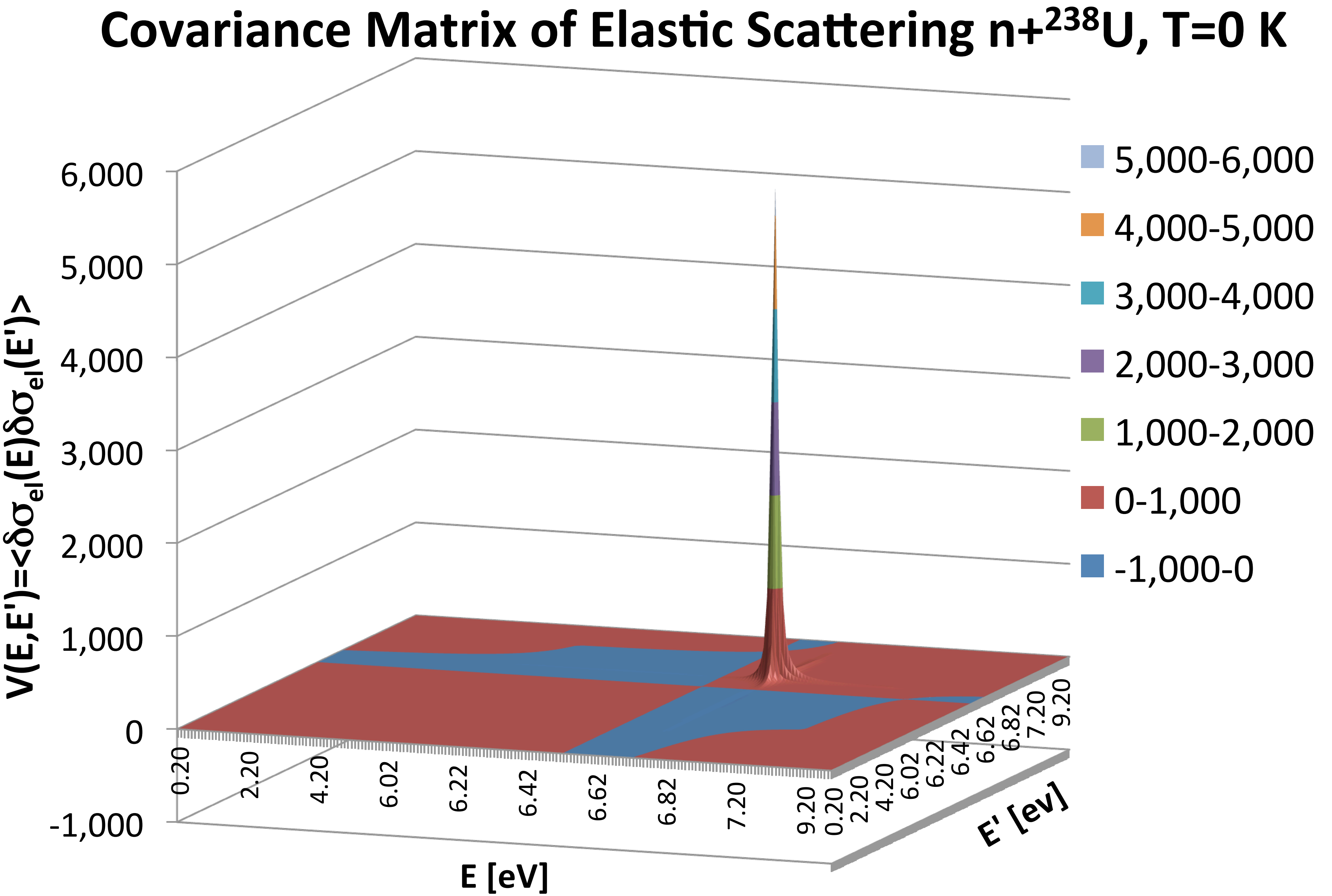
$$\langle \delta\sigma^{0K}(E_{\mathrm{CM}}(t))\delta\sigma^{0K}(E_{\mathrm{CM}}(t')) \rangle dt dt'$$

  – **Where** $\langle \delta\sigma^{0K}(E_{\mathrm{CM}}(t))\delta\sigma^{0K}(E_{\mathrm{CM}}(t')) \rangle$ **is the 0*K* scatt. XS covariance**

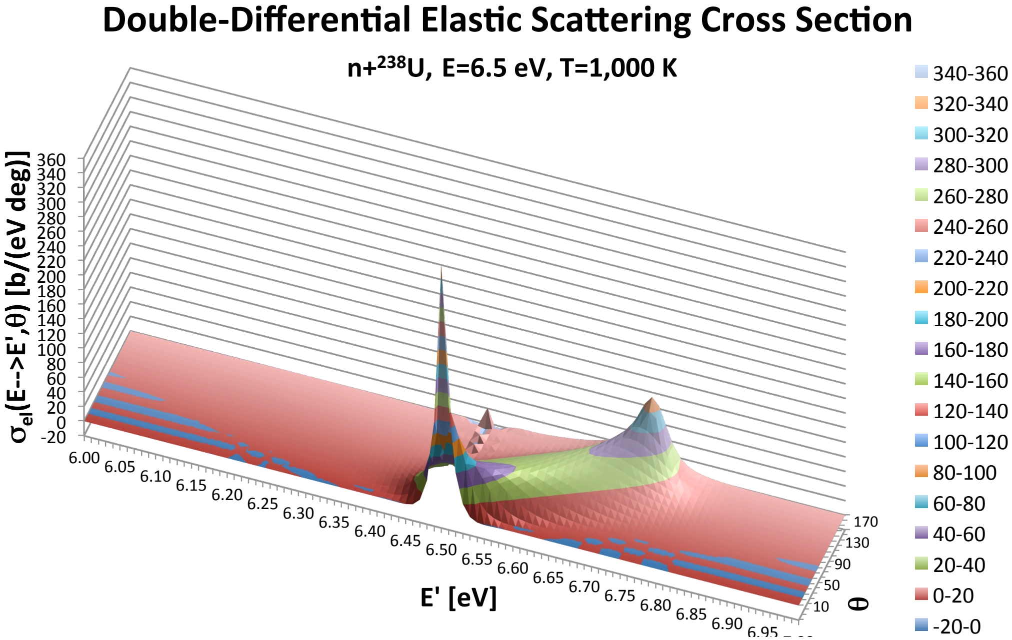
- **Using the above, a variance of double diff. scatt. XS is**

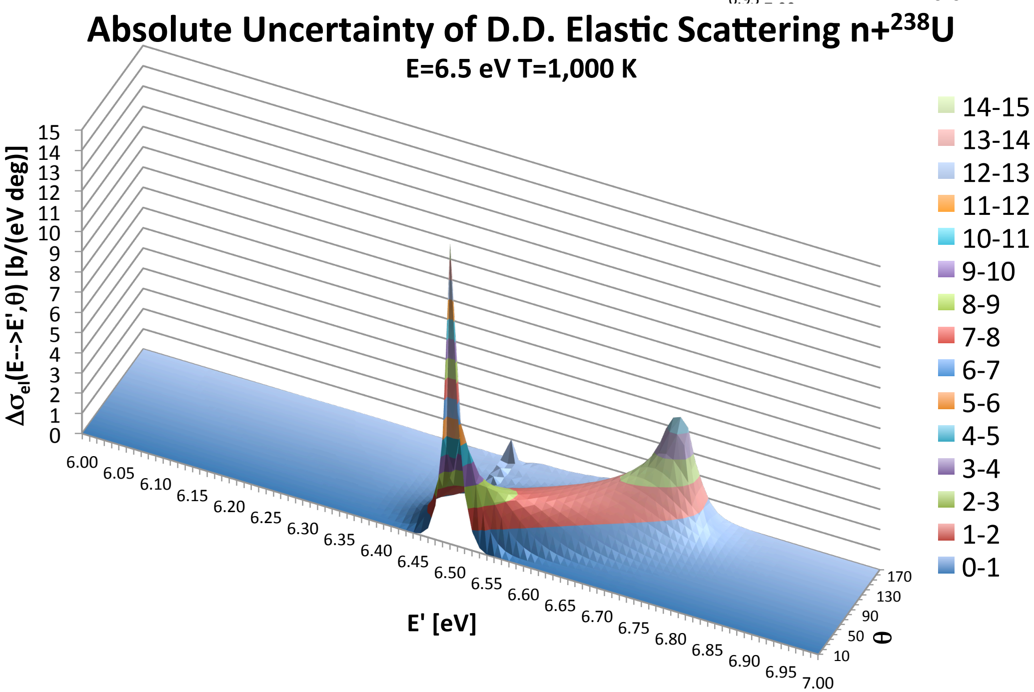
$$\langle (\delta\sigma_s^T(E \to E', \mu))^2 \rangle \propto \sum_{n,n' \ge 0} \frac{2n+1}{2} \frac{2n'+1}{2} P_n(\mu_{\mathrm{lab}}) P_{n'}(\mu_{\mathrm{lab}}) \langle \delta\sigma_n^T(E \to E')\delta\sigma_{n'}^T(E \to E') \rangle$$

Elastic Scattering Covariance Matrix



DD XS and its uncertainty: up-scattering





- **The two shapes are similar**
  - Their ratio is approx. equal to the uncertainty at the the peak of the 6.67 eV resonance, i.e. 5%
  - Also true at E=6.8 eV on the next slide
  - # neutrons / angle ≈ const.
    - But *not* their energy distribution
- **Slow convergence at E=E'**
  - Other methods considered:
    - Factor out $(n+1/2)\sigma_n(E\text{-->}E')$
    - Interpolate $E'=E-\Delta$ and $E'=E+\Delta$

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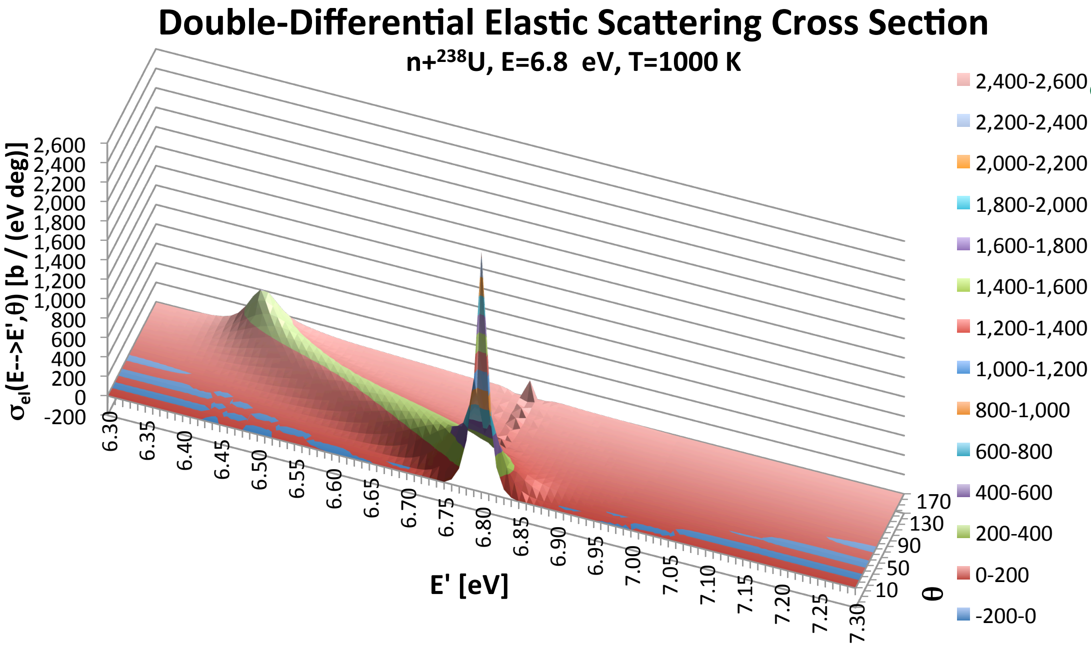
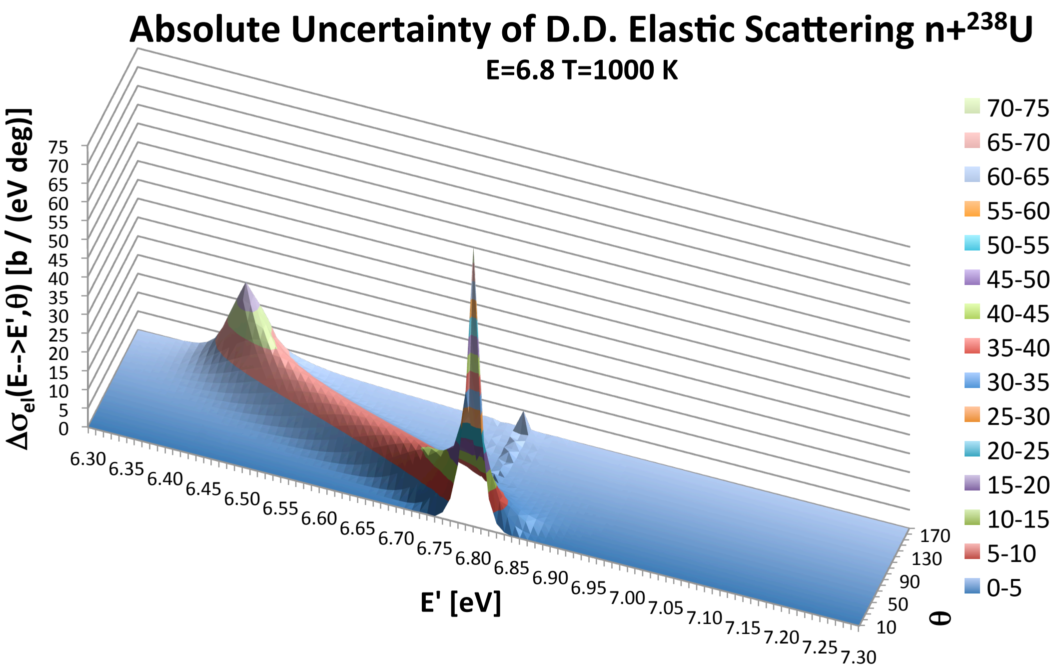
DD XS and its uncertainty: down-scattering





- The two shapes are similar
  - Their ratio is approx. equal to the uncertainty at the the peak of the 6.67 eV resonance, i.e. 5%
  - Also true at E=6.5 eV on the previous slide
- Slow convergence at E=E'
  - Other methods considered:
    - Factor out $(n+1/2)\sigma_n(E\text{-->}E')$
    - Interpolate E'=E-Δ and E'=E+Δ

Summary and Outlook

- Doppler broadened DD XS (or its Legendre moments)
  - Needed for resonances of heavy nuclei below few 100's eV
- Exact Legendre moments can now be computed up to 20th
  - The original triple-nested integral cast into a single integral
  - Effects of anisotropic scattering in the CoM frame computable
- Computed Variance-Covariance of DD XS (or its Leg. Mom.'s)
  - Study convergence of Legendre moments to DD XS (e.g. MC)
- Attempts to implement exact Legendre moments into CENTRM, a 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

Testing the method:

- In order of increasing difficulty the tests were:
  1. Compared to method used in SCALE that is valid for constant XS
  2. Compared integral DB XS to the integral of $P_0(E \rightarrow E')dE'$
  3. Compared the Legendre moments to those computed by MC (B. Becker) for
     a) isotropic angular scattering XS in the CoM
     b) anisotropic --------------------||------------------------
- All tests passed
- Results of various tests in 2. and 3 a) and 3 b) will be shown
- All plots in this presentation set T=1000 K
  – several other temperatures have been used

Test 2: Integrated DB scatt. XS

- **The integrated DB scatt. XS can be computed as**

$$\sigma^T_{\text{scatt.}}(E) = \int_0^\infty \sigma^T_0(E \to E')\, dE'$$

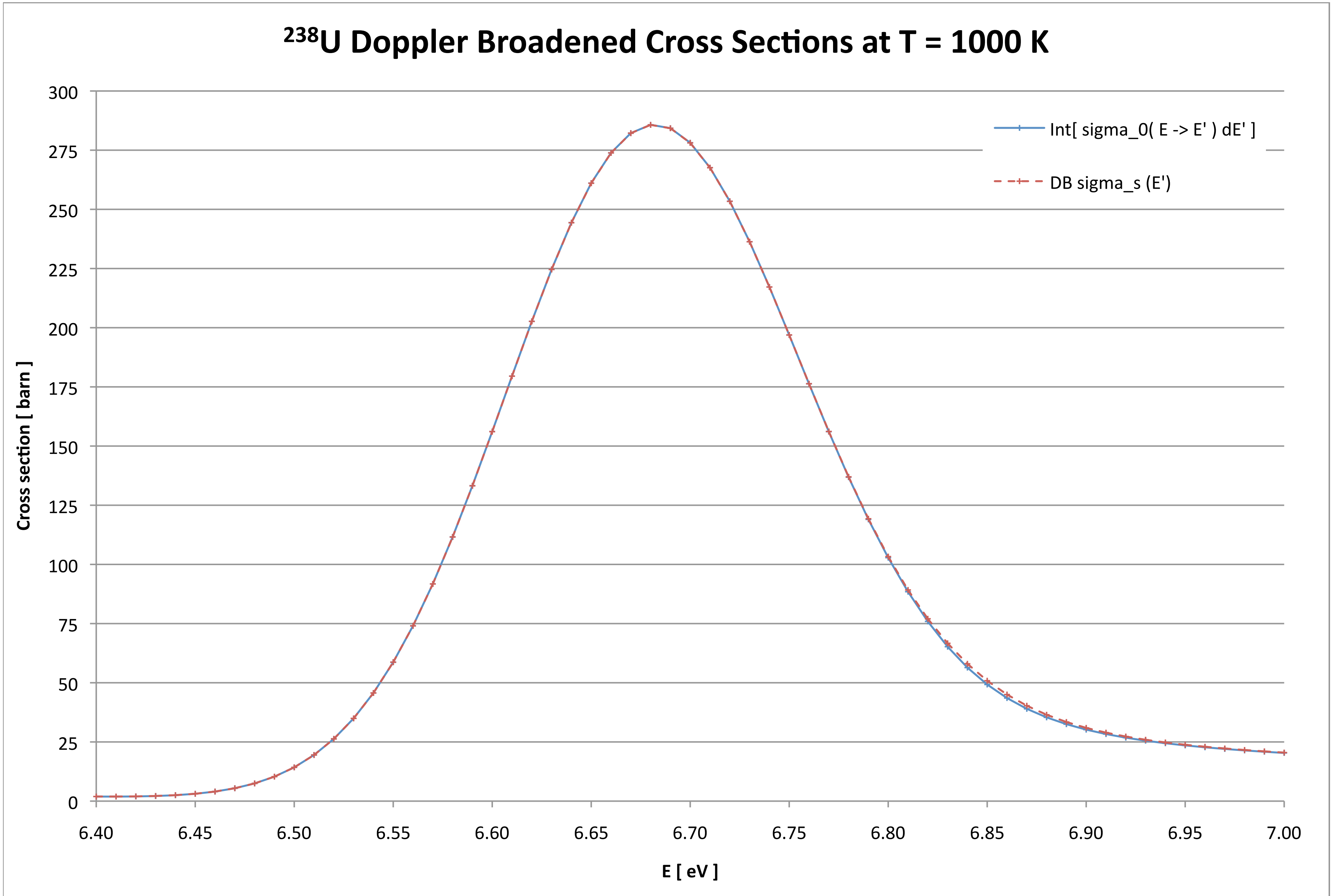
- **and also as (e.g. Sec. III.B.1 of the SAMMY Manual: http://www.ornl.gov/sci/nuclear_science_technology/nuclear_data/sammy/manual.html)**

$$\sigma^T_{\text{scatt.}}(E) = \frac{1}{\Delta_D \sqrt{\pi}} \int_0^\infty \left[e^{-4(E-\sqrt{EE'})^2/\Delta_D^2} - e^{-4(E+\sqrt{EE'})^2/\Delta_D^2} \right] \sigma^{T=0\,K}(E') \sqrt{E'/E}\, dE'$$

$$\Delta_D \equiv \sqrt{\frac{4 m_{\text{neutron}} E k T}{M_{\text{target}}}}$$

- **The next slides shows a good agreement between the two for energies E spanning the 6.7 eV ^{238}U resonance:**

Consistency check with integrated DB XS



Overview

- A history of various methods and approximations used to compute Doppler broadening of energy-dependent cross sections as a function of temp. *T* will be outlined
- A method to compute Legendre moments derived by Ouisloumen and Sanchez (OS) Nucl. Sci. Eng. 107, 189 (1991):
  - The original expression is a triple-nested integral
    - Practical only for computation of the 0th and the 1st Legendre moment and for isotropic angular distribution of of scattering cross section
  - A new method renders a triple-nested integral of OS into a single integral by virtue of systematic application of integration by parts
    - Arbitrary order of Legendre moments are computable
    - Arbitrary angular distribution of the scatt. XS in the CoM can be handled
- This method is then applied to computation of covariances of DD XS near the 6.67 eV resonance of U-238

Brief review of *T*-dependent methods

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

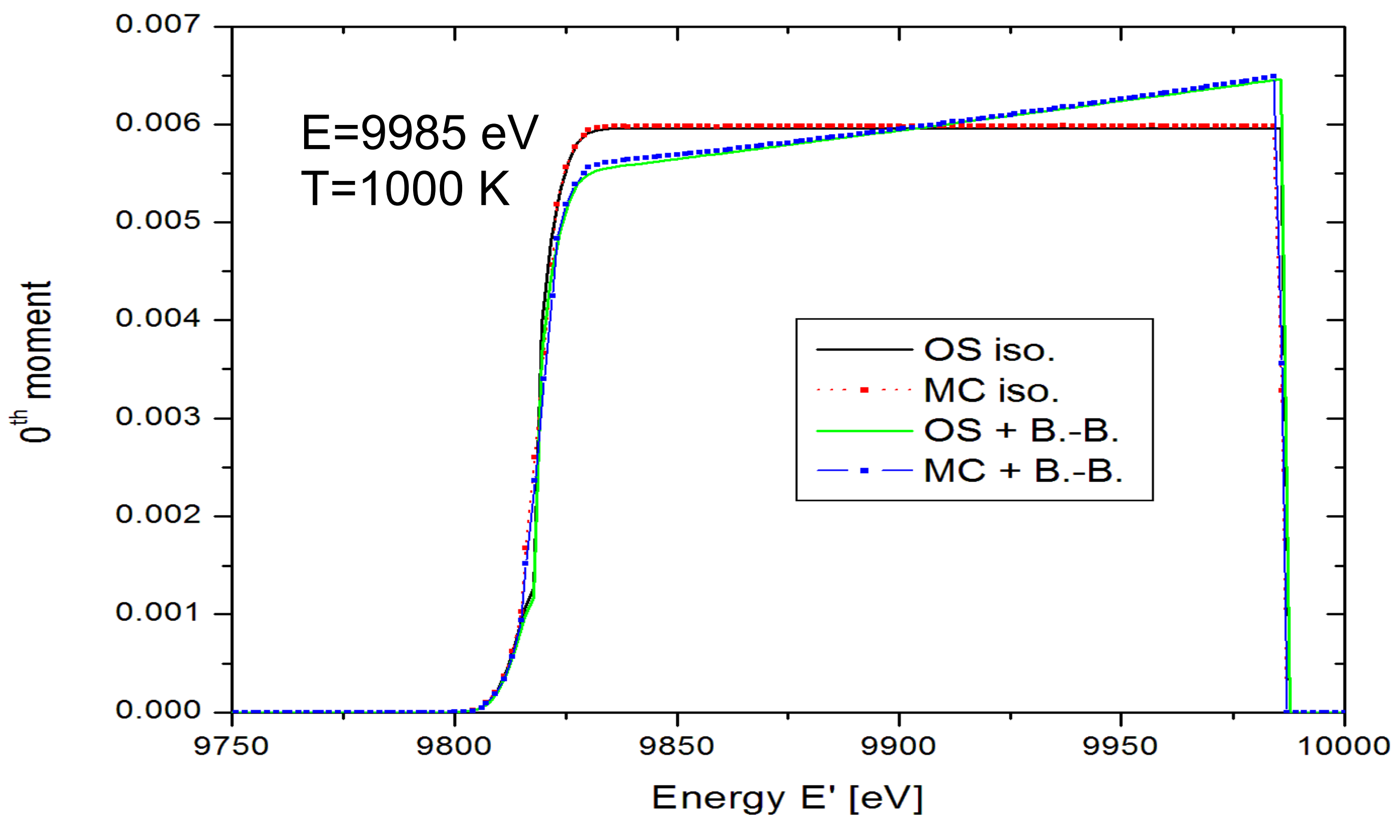
- Wigner and Wilkins (1954)
  - P_0 for a constant isotropic XS
- Blackshaw and Murray (1967)
  - P_0 and P_1 of *E*-dependent (e.g. resonant) isotropic XS
- Ouisloumen and Sanchez (1991)
  - All Legendre moments of *E*-dependent *ani*sotropic XS
  - only P_0 computed; P_1, etc. involve a three-fold 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 an experimental version of NJOY
- This Work
  - All Leg. Moments, Ang. Dist. In CM, via a single integral

Anisotropic Ang. Scattering in the CoM

- Conventional Blatt-Biedenharn (BB) coefficients are used to introduce anisotropic angular distribution into the CoM
- Our computation is compared with the Monte-Carlo (MC)
- Anisotropy introduced by the BB coeff's increases with E
  - Consequently, deviations between Legendre moments for the BB anisotropic ang. dist. and the respective moments for the isotropic ang. dist. increase with incoming energy E. The following deviations were computed for temperature T = 1000 K
    - ~ 0.01% at 6 eV
    - ~ 2% at 2 keV
    - ~ 10% at 10 keV
- To magnify the deviations, the incoming energy E is set relatively high, E = 9985 eV and T = 1000 K.

$P_0(E \rightarrow E')$ isotropic vs. anisotropic (BB)

- The isotropic and anisotropic 0-th Legendre moments computed by:
  - our method (labeled “OS” for Ouisloumen-Sanchez)
  - Monte-Carlo (“MC”)
- Relatively good agreement between OS and MC everywhere
  - But, our computation displays odd behavior at E’=9820 for isotropic and anisotropic, to be resolved



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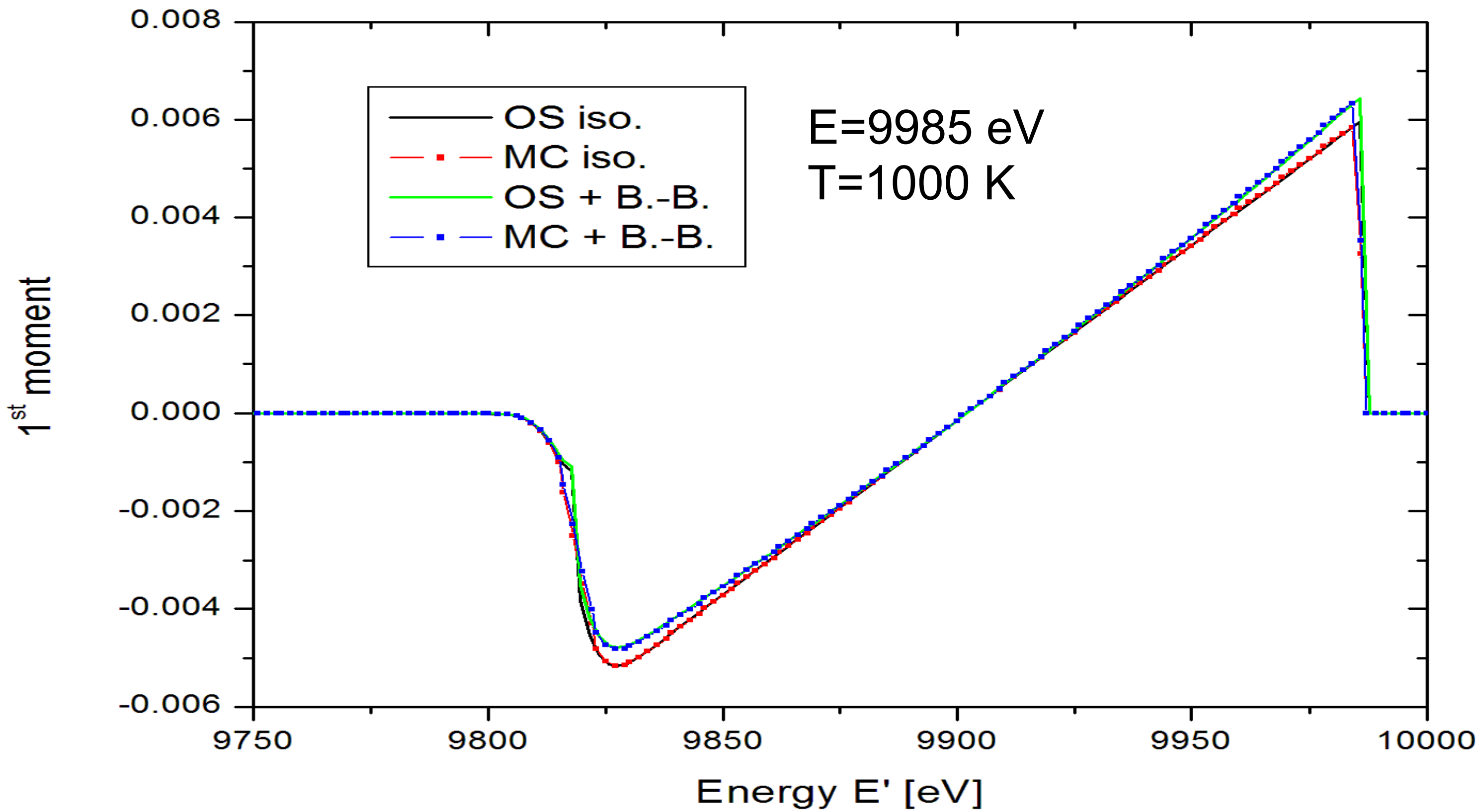
P_1(E→E') isotropic vs. anisotropic (BB)

- The isotropic and anisotropic 1-th Legendre moments computed by:
  - our method (labeled "OS" for Ouisloumen-Sanchez)
  - Monte-Carlo ("MC")
- Relatively good agreement between OS and MC everywhere
  - But, our computation displays odd behavior at E'=9820 for isotropic and anisotropic, to be resolved



P_2(E→E') isotropic vs. anisotropic (BB)

- The isotropic and anisotropic 2-th Legendre moments computed by:
  - our method (labeled "OS" for Ouisloumen-Sanchez)
  - Monte-Carlo ("MC")
- Relatively good agreement between OS and MC everywhere
  - But, our computation displays odd behavior at E'=9820 for isotropic and anisotropic, to be resolved