SAMMY

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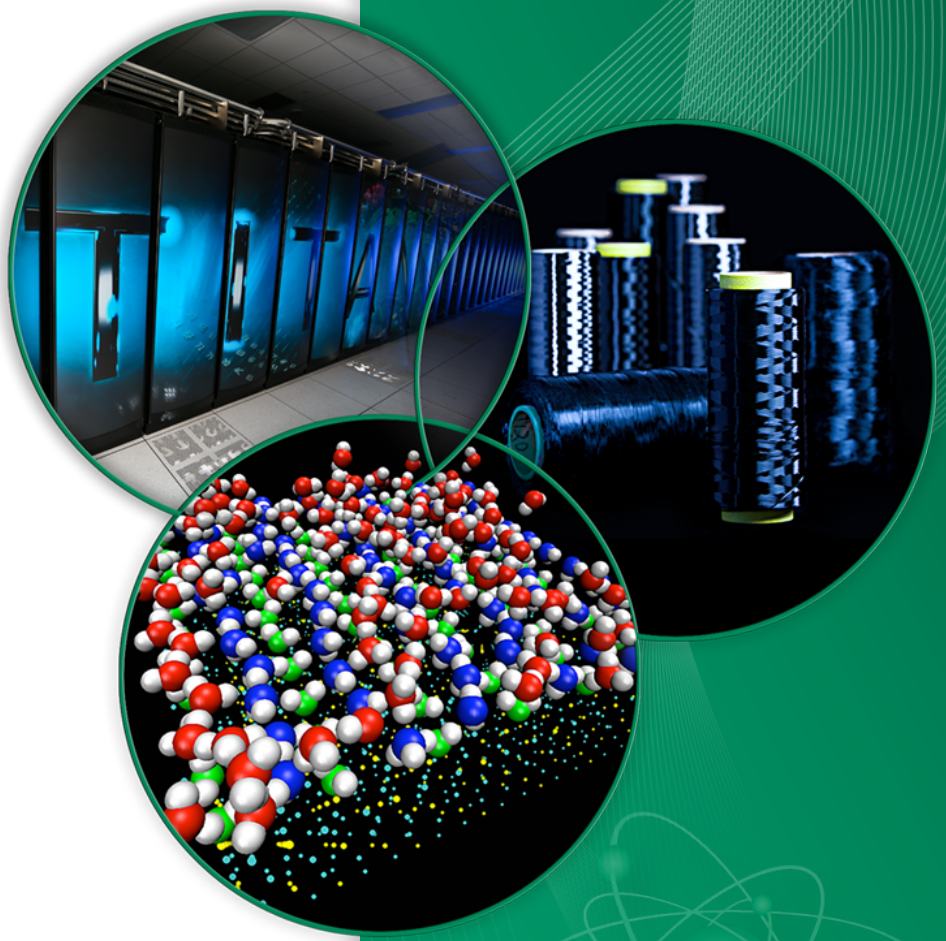


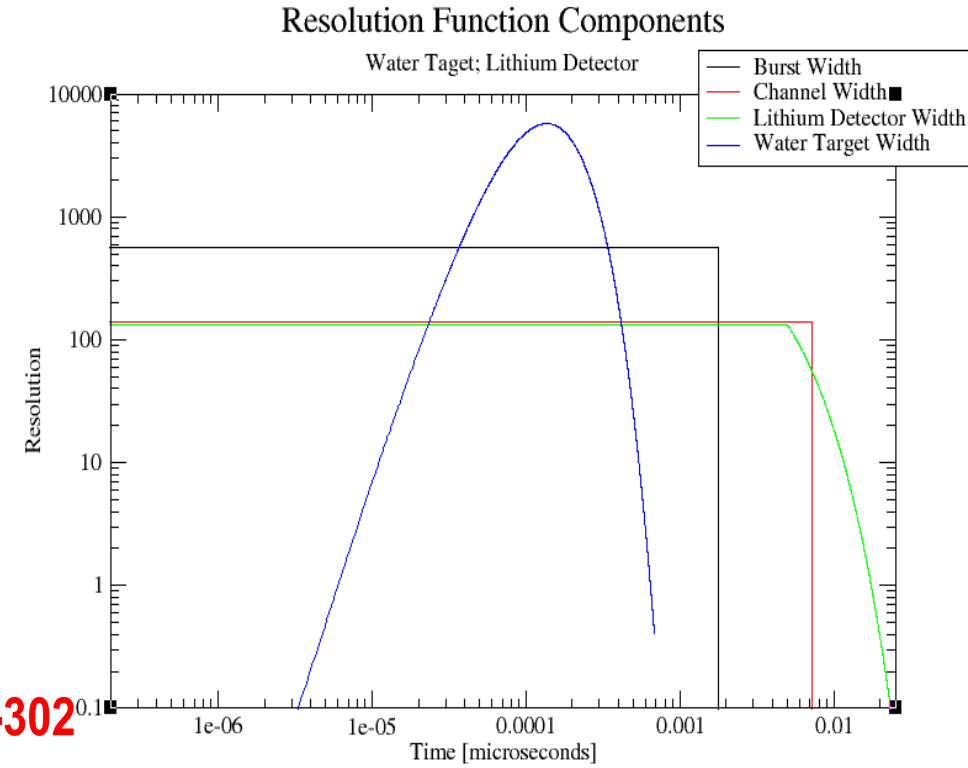
Nuclear Data Week, Brookhaven National Laboratory, Nov. 3-7, 2014

Overview

- New SAMMY Resolution Functions for RPI neutron detectors
  1. Lithium glass neutron detector array
  2. Liquid scintillator proton recoil neutron detector
- SAMMY Modernization Plan
- S(a,b) project update

Total SAMMY Resolution Function

- Convolution of four components:
  1. Burst width
  2. Neutron Sources:
     - Tantalum Target
     - Water Moderator
  3. time-of-flight channel width,
  4. Neutron Detector:
     - **Lithium Glass Neutron Detector**
     - **Liquid Scintillator Proton Recoil EJ-302**



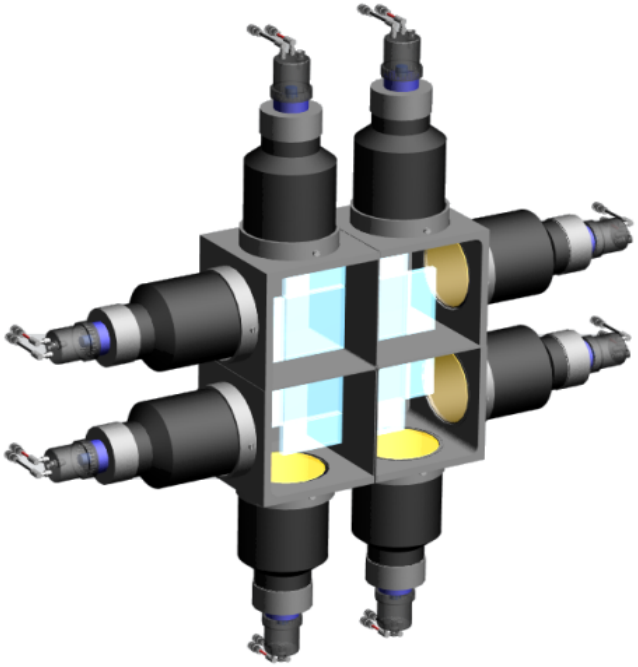
$$\bar{\sigma}(t) = \int I(t-t')\sigma(t')dt'$$

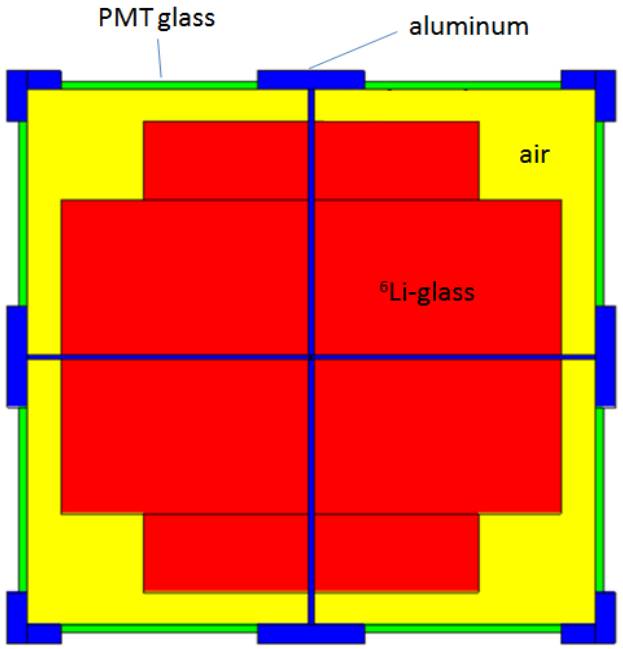
$$E = \frac{1}{2}mv^2 = \frac{1}{2}m\frac{L^2}{t^2}$$

$$I(t-t') = \int I_1(t-t_1)dt_1 \int I_2(t_1-t_2)dt_2 \int I_3(t_2-t_3)dt_3 \;\; I_4(t_3-t')$$

^{6}Li Glass Detector Array MELINDA

- MCNP simulated the detector and the time distribution of neutrons, tallying ^{6}Li (n,α) reactions





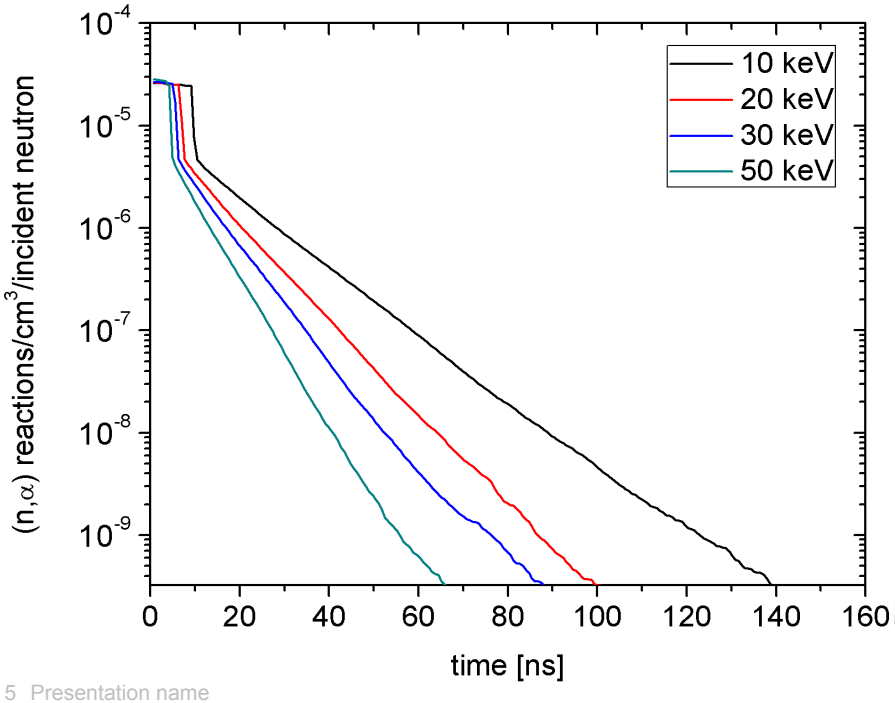
- [1] R. Bahran et al. "A New High Energy Resolution Neutron Transmission Detector System at the Gaerttner LINAC Laboratory" *Proceedings of The Tenth International Topical Meeting on Nuclear Applications and Utilization of Accelerators AccApp'11*, Knoxville, TN, 2011.
- [2] A. Youmans et. al. "Using Simulations To Determine The Energy Resolution Function Of Neutron Time-Of-Flight Experiments" *Proceedings of the 2013 Annual ANS Meeting, Washington, D.C. 2013*

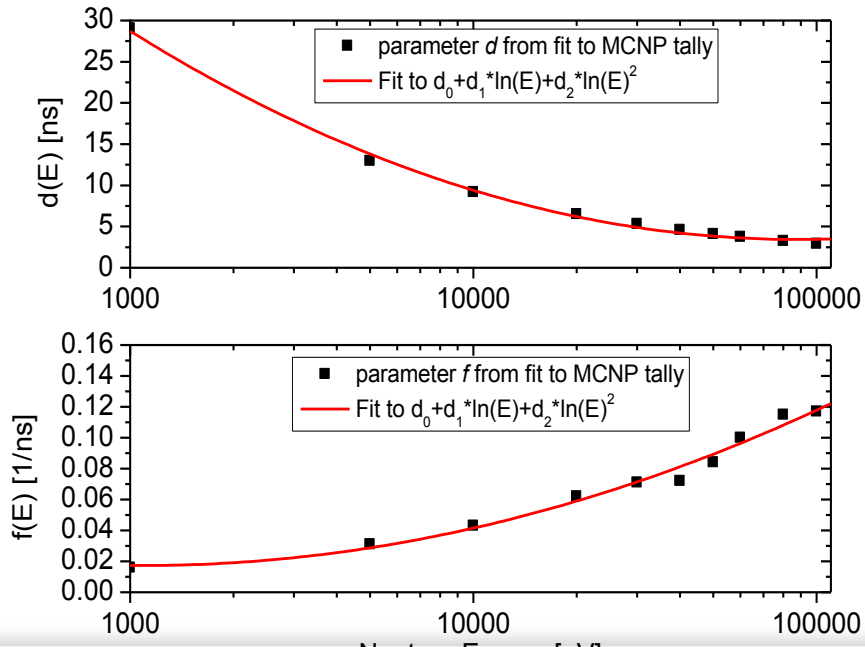
^{6}Li Glass Detector Array MELINDA cont'd.

- From MCNP simulation the RPI resolution function was implemented by making parameters of the SAMMY ORR, d and f, energy-dependent:

$$I_{4b}(l) = \begin{cases} Dg & \text{for } 0 < t < d \\ D\exp\left(-f\left(t-d\right)\right) & \text{for } d < t \end{cases}$$

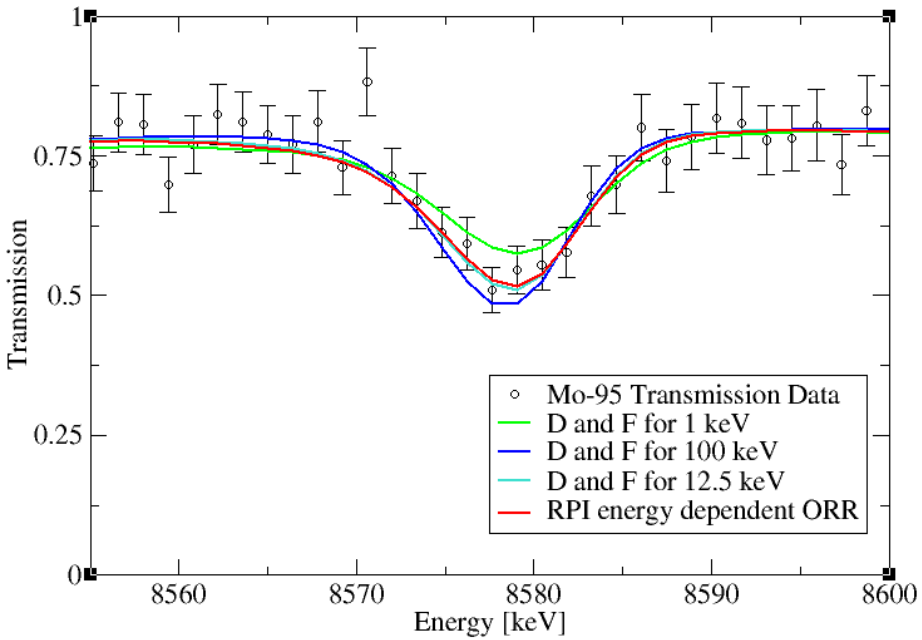
Caveat: d0, d1, d2, f0, f1, f2, should not be fitted because constant values for d and f have been hardwired into SAMMY resolution function.



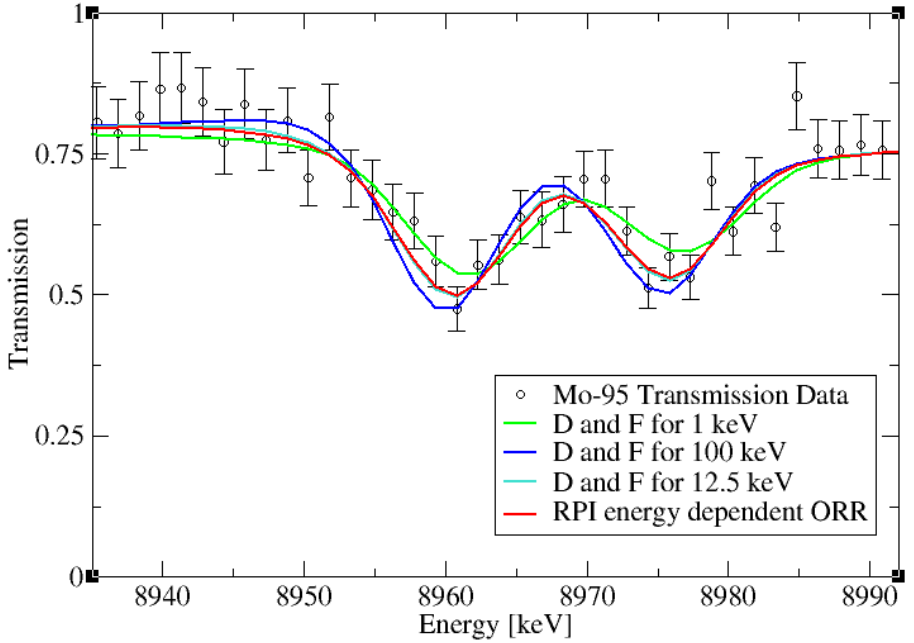


Results: Li-glass detector

- Sample comparison on RPI Mo-95 transmission data
  - *E*-dependent vs. constant *d* and *f*
  - We choose three constant values of *d* and *f* for comparison



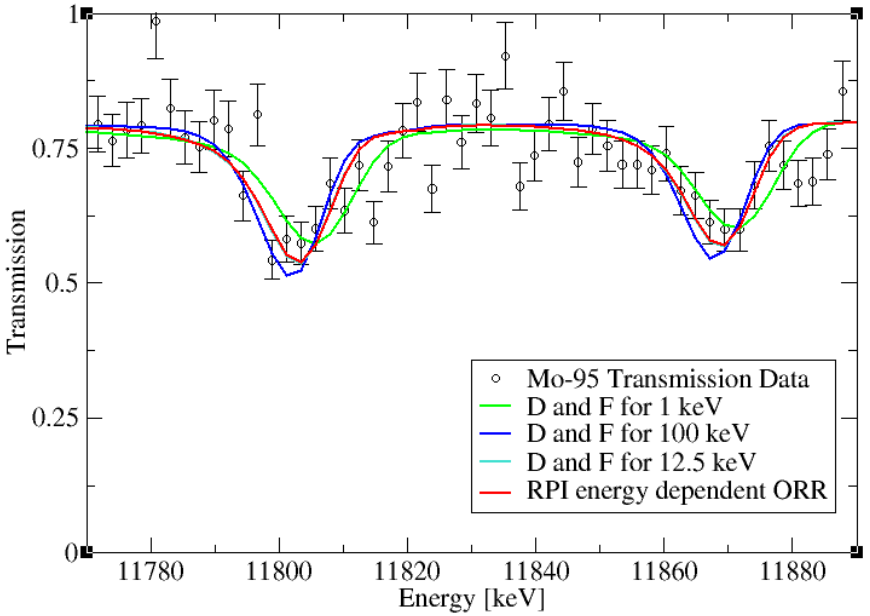
Comparing the original SAMMY detector resolution function to the modified function with Mo-95 data



Comparing the original SAMMY detector resolution function to the modified function with Mo-95 data

Results: Li-glass resolution function

- E-dependent Li-glass detector resolution function reduces χ^2

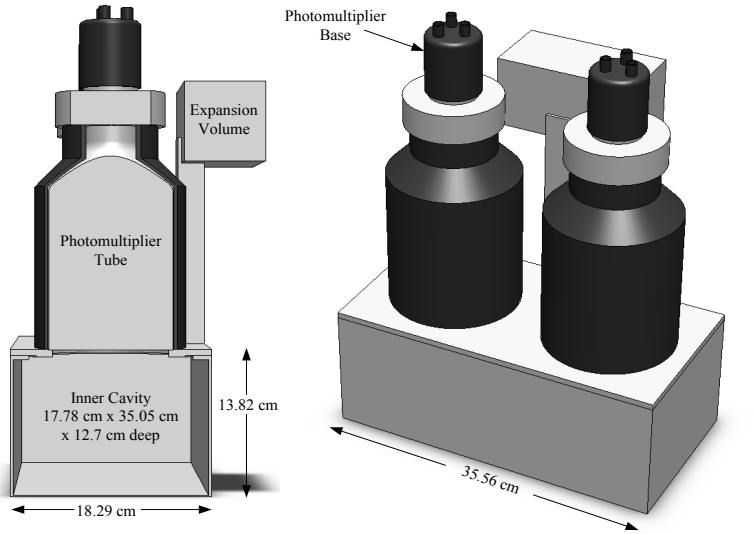


Comparing the original SAMMY detector resolution function to the modified function with Mo-95 data

Trial	Chi-Squared divided by N
d(E) and *f(E)*	1.38422
d, *f* constant, E=1 keV	1.67559
d, *f* const. E=12.5 keV	1.42627
d, *f* const. E=100 keV	1.55281

EJ-301 Liquid Scintillator

- (MCNP) was used to simulate the detector and the time distribution of neutrons as they react with the detector material, tallying elastic scattering with hydrogen in the proton recoil detector.
- Six modules shown below, each contains liquid $CH_{1.212}$. Neutrons scatter off of hydrogen, ejecting a proton. The proton deposits its energy through charged particle interactions into the scintillation material → pulse



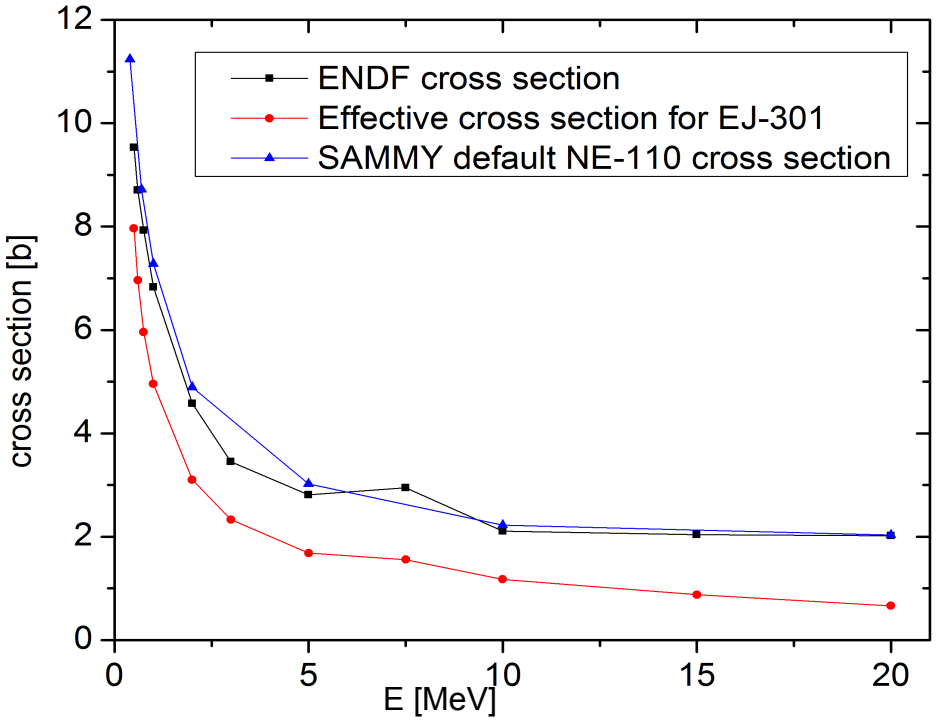
[3] M. Rapp, "Design and construction of a large area detector system and neutron total cross section measurements in the energy range 0.4 to 20 MeV," Ph.D. dissertation, Mech. Aero. Nucl. Eng. Dept., RPI, Troy, NY, 2011

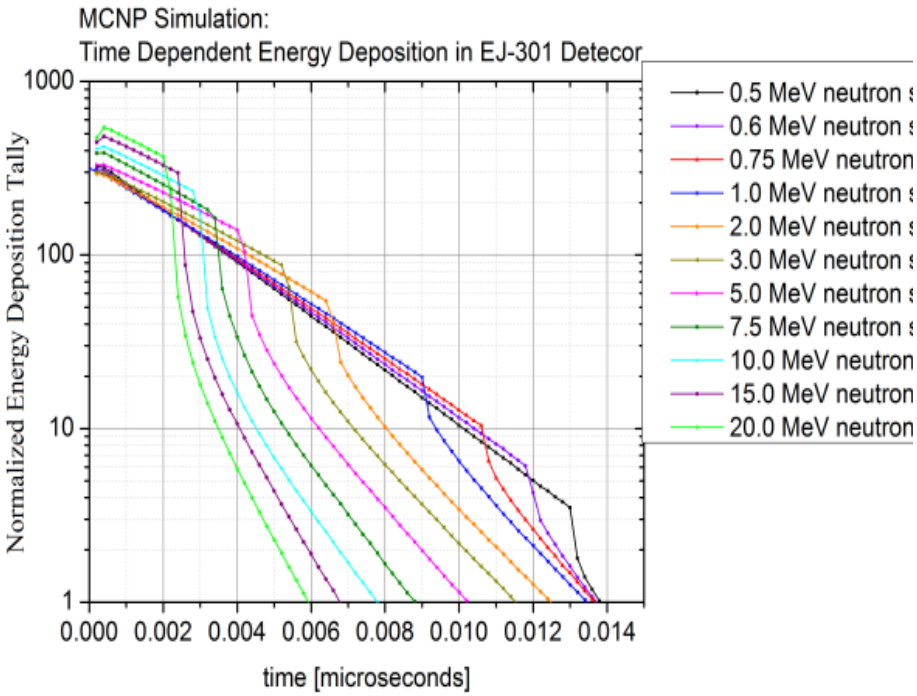
EJ-301 Liquid Scintillator cont.'d

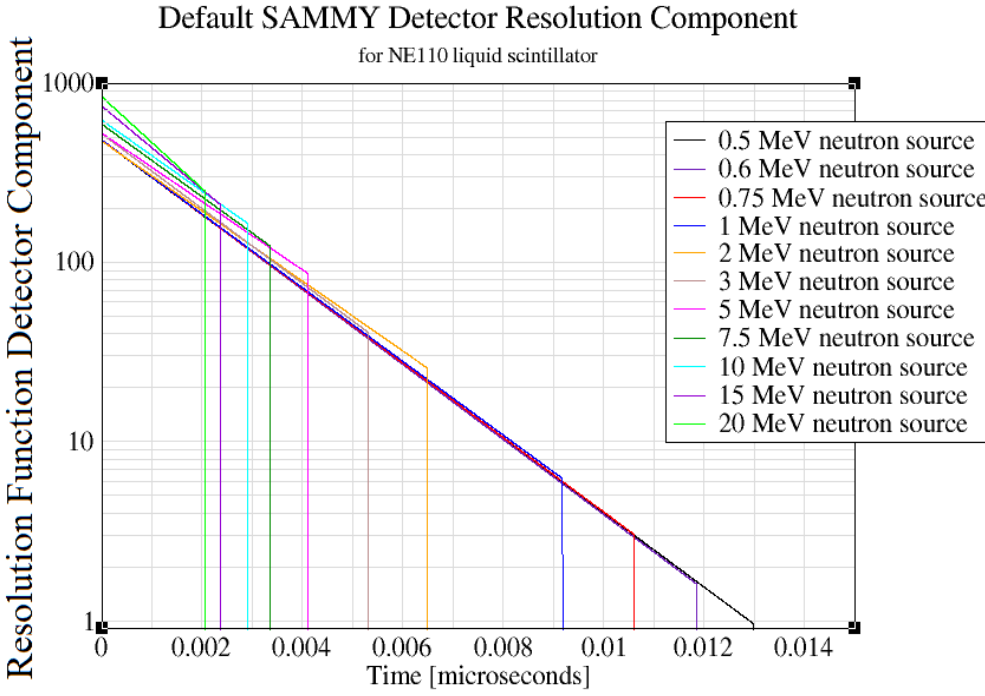
$$I'_{4a}(l) = \begin{cases} \Delta \exp(-\lambda\sigma l) & \text{for } 0 < l < \delta \\ 0 & \text{otherwise} \end{cases}$$

$$E = \frac{1}{2}mv^2 = \frac{1}{2}m\frac{L^2}{t^2}$$

Multiple scattering yields tapering below:





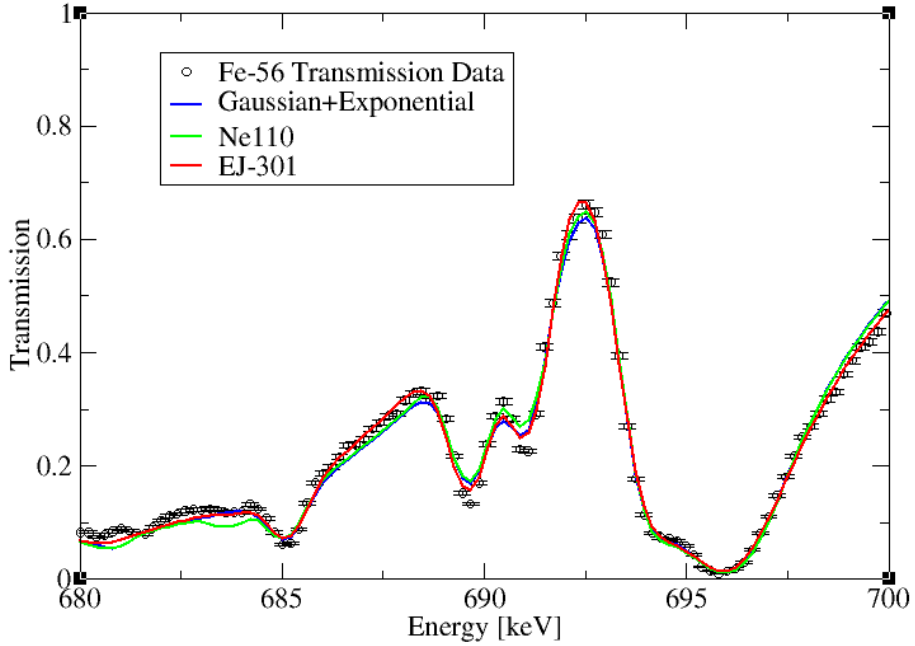


Results: Liq. Scintil. (EJ-301)

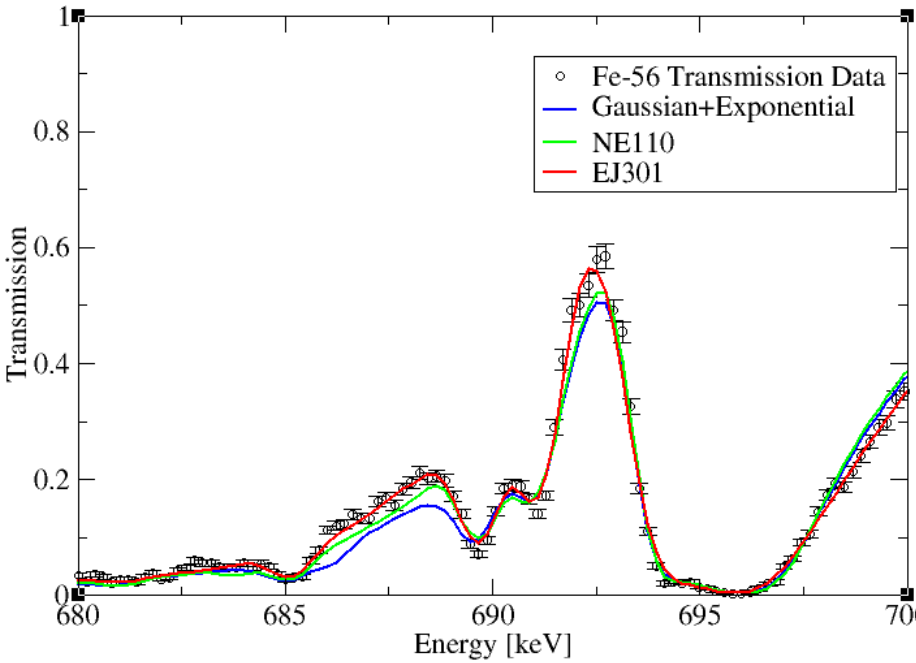
- EJ-301 resolution func. reduces χ^2

(everything else being the same)

Chi squared divided by N			
Resolution Function	**Thin Fe56 Sample**	**Medium Fe56**	**Thick Fe56**
Gauss.+Exp.	13.65	21.42	5.89
Ne-110	12.74	17.31	4.97
EJ-301	6.41	8.26	2.77



Comparison of different detector resolution functions with data from the medium Fe-56 sample at RPI.



Comparison of different detector resolution function with data from the thick Fe-56 sample at RPI.

SAMMY Modernization Plan

- Use Libraries to simplify programming and parallelization:
  - BLAS, LAPACK, Trillinos (?)
    - Abstractions: e.g. Armadillo library to write matrix product as A*B; good for R-matrix
  - Complex numbers, derivatives, etc.
- Implement in C++ (most likely)
  - ORNL SCALE development, build, Q&A framework
- Now is the time to think about connecting to URR, HE, IBEs, etc.
  - Synergies with AMPX
- Separate Bayesian fitting modules from R-matrix computations
  - A generic Bayesian fitting module could also be used for S(a,b) evaluations
- Feedback from community more than welcome

S(a,b) methods update

- S(a,b) evaluations via MD appear possible
  - Perform MD simulation
  - For liquids:
    - Compute Intermediate structure function (simpler than dyn. struct. funct.)
    - From it, compute dynamical structure function S(k,w)
  - For solids: one could use LAMMPS/PHANA to get phonon spectrum
  - ORNL Spallation Neutron Source data: S(k,w) and its covariance
    - compare and iterate, GLLS will yield interaction parameters and their covariance
  - Compute sensitivities from an adjoint MD simul, not numerical variations
- Applied for and received NERSC Startup Allocation: only 50K but:
  - All MD and DFT codes (including *ab initio* ones) available at NERSC
  - Will enable a prototype evaluation that could lead to other applications
- Promising collaborations here and with ORNL's MD experts
  - Will apply for ORNL's OLCF Director's Discretionary supercomp. alloc.

Third-party codes failing for water MD

This works

Additional slides

Overview

- Goal: Develop methods for generating covariance data of S(a,b)
  - In anticipation of the RPI data for H_20 and $Si0_2$ (Si), polyethylene; SNS
- General approach:
  1. Define model T as a function of some parameters P
  2. Fit model T to data to obtain covariance matrix M of parameters P
  3. Construct covariance of S(a,b) from M as C = S M S
     - Where $S = \partial T(P) / \partial P$ is the sensitivity matrix of model T
- Various models T being considered:
  - Addressing various levels of physical models
    - Various approximations: from DFT to MD to free gas,
    - Some assumptions revisited (e.g. form of the scattering w.f.)
  - *Ab intio* models more computationally intensive
- MADNESS Computational framework (R&D 100, SciDAC)
  - May provide novel computational approaches and insights

General consideration

- The form of the scattering function assumed
  - Plane wave + scattered wave
  - Can we estimate the magnitude of ensuing error? (assumed to be small)
- The low-energy (< 5 eV) neutron-nucleus scattering determined by the scattering length
- First-order Born approximation
  - Does not require a delta-function interaction;
    - Woods-Saxon is more realistic
    - But delta-function is likely a good approximation since size(nuclei) << size(atoms)
- This leads to expressions for S(k,w) or S(a,b) in terms of pair-wise correlation functions
  - Delineates neutron-scattering from material properties PCF
  - →PCF could be computed by e.g. MD
- What is an efficient path to S(a,b) covariance?

0. Single molecule scattering

- The motion of hydrogen atoms in water in terms of the H20 molecule as the basic dynamical unit.
  - Mark Nelkin, Phys. Rev. 119, **741** (1960)
- We could fit parameters of the S(a,b) expression to data
  - Parameters of water vibrations, torsional oscillations, etc.
  - From covariance/correlation of fitted parameters get covariance of S(a,b)
- We could also fit *neutron-nucleus* potential parameters

1. Molecular Dynamics (MD)

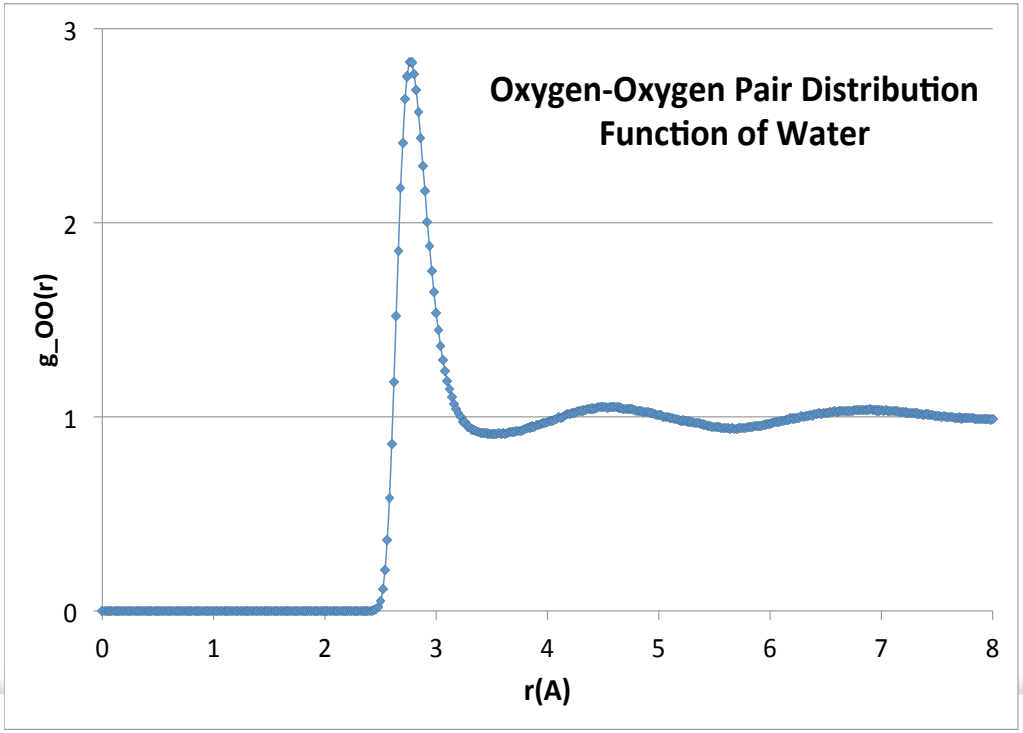
- MD Method:
  - assumes a parameterized interaction potential (e.g. Lennard-Jones)
  - Uses Newton's equation to evolve the many-body system
  - Then computes PCFs to get S(a,b) and structure factors
  - Faster but less accurate than more *ab initio* methods like DFT
  - Interaction parameters fitted to (usually) structure factors S(k)
  - The S(k) is the 0-th moment of S(q,w)
  - But parameter uncertainty or covariance is generally not provided
- Several established MD codes available
  - GROMACS, LAMMPS, NAMD
  - http://en.wikipedia.org/wiki/List_of_software_for_molecular_mechanics_modeling
  - Output molecular/atomic trajectories in time

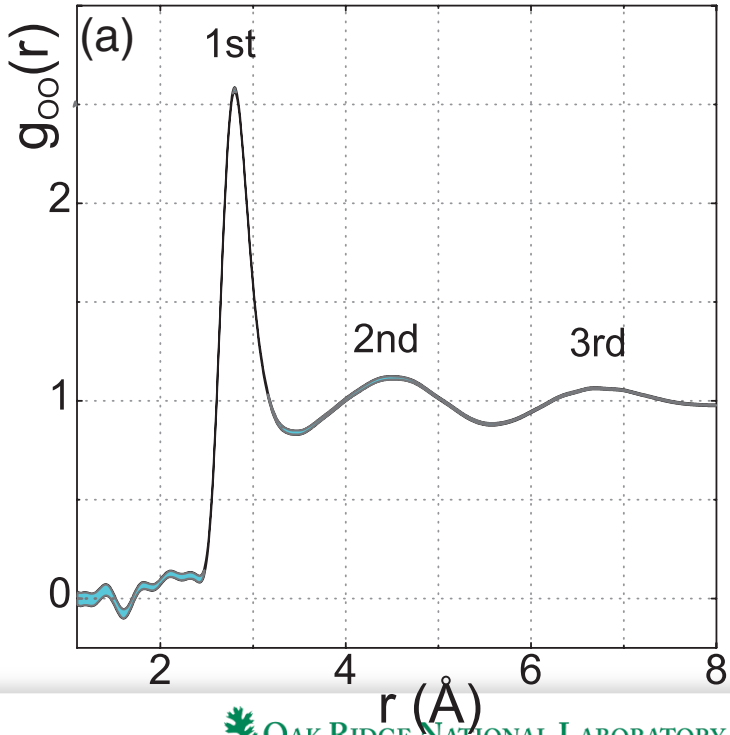
1. Molecular Dynamics (MD) cont'd.

- Trajectories processed to compute G(r,t), I(k,t), S(k,w)
  - Using dynsf: can take days to complete, prone to crashing
- Multi-atomic molecules like H_20 require computations S(k,w) for all possible different pairs:
  - O-O, H-H, O-H
  - The total S(k,w) is the weighted average of the the partial S(k,w)
    - Weights are: (scattering lengths) * (elemental fractions)
- Currently computing pairwise S(k,w) using dynsf
  - may need to develop a faster version
  - Cf. LAMMPS MD simulation takes a couple of hours on 32 processors
- Computed polyethylene, and SiO_2 phonon spectrum using LAMMPS
  - Also PE phonon spectrum has been extracted from SEQUOIA data
  - Data fitting and covariances are on the horizon

Gromacs Example Run Water

- O-O radial distribution function g(r)
  - Classical pair correlation function G(r,t) would give S(k,w)
  - https://github.com/cfinch/GROMACS_Examples/tree/master/water
  - Must use third party code e.g. dynsf to compute G(r,t) from the trajectories





2. Density Functional Theory

- Codes:
  - VASP, QuantumEspresso, BigDFT, MADNESS (more later)
  - http://en.wikipedia.org/wiki/List_of_quantum_chemistry_and_solid_state_physics_software
- Water is still not fully understood
  - Discrepancies between data an theory persist
    - structure factor, pairwise correlation function
  - Several recent Ph.D. thesis on water (active field)
- ~1,000's of atoms/molecules
- More accurate than MD
- DFT computations are used to fit MD interaction parameters
- A candidate framework for S(a,b) covariances

3. Total Montel Carlo

- By Koning and Rochman
- Could compute *covariance* of existing S(a,b) evaluations
  - For which covaraiance data does not exist
  - This method yields covariance by averaging large random ensembles
- Could be compared to new evaluations

4. SNS SEQUOIA Data reduction

Horace platform:

- One of the two preferred methods for data reduction and analysis
  - at the SNS SEQUOIA
  - double diff. (angle, energy) cross section is reduced to $S(\mathbf{q},\omega)$
  - Built-in function for parameter fitting to reduced data $S(\mathbf{q},\omega)$
    - Returns model parameters, their uncertainties, and the correlation matrix
    - One can compute the model covariance matrix of the $S(\mathbf{q},\omega)$
- An established platform
  - Works with MATLAB out of the box
  - Used in multitude of advanced papers
  - Downloadable from http://horace.isis.rl.ac.uk

Also DAVE: http://www.ncnr.nist.gov/dave/

Double-Differential Cross Section

- Ouisloumen and Sanchez (1991) cf. Rothenstein/Dagan/Becker
- Arbanas *et al.* M&C 2011, NCSC2 2012, PHYSOR 2012

$$\sigma_s^T(E \to E', \mu_{\rm lab}) = \sum_{n\geq 0}(n+\tfrac{1}{2})\sigma_{sn}^T(E \to E')P_n(\mu_{\rm lab})$$

$$\sigma_{sn}^T(E \to E') = \frac{\beta^{5/2}}{4E}e^{E/kT}\int_0^\infty t\sigma_s^{\rm tab}(E''(t))e^{-t^2/A}\psi_n(t)\mathrm{d}t,$$

$$\sigma_{sn}(\mathbf{x}) = \hat{O}_n(\mathbf{x})[\sigma_s^{\rm tab}]. \qquad \mathbf{x} \equiv (T, E, E'),$$

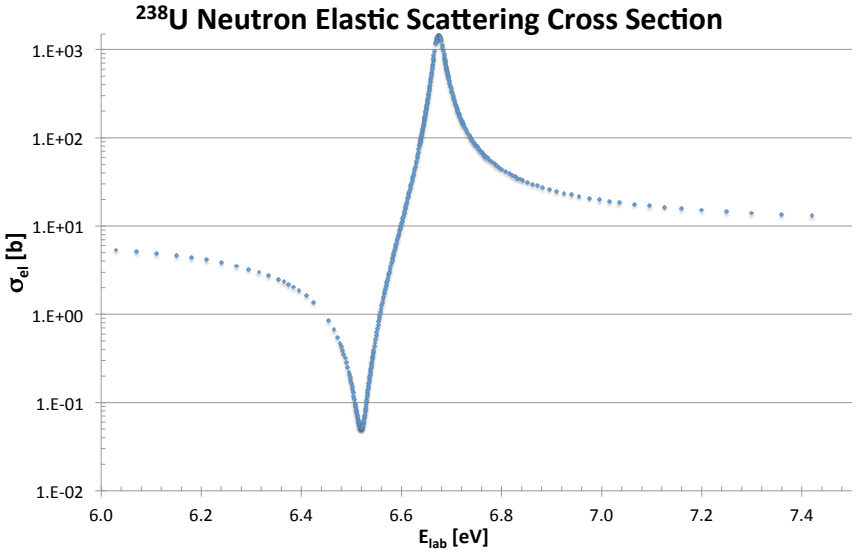
$$M_{nn'}(\mathbf{x},\mathbf{y}) \equiv \langle \delta\sigma_{sn}(\mathbf{x})\delta\sigma_{sn'}(\mathbf{y})\rangle = \hat{O}_n(\mathbf{x})\hat{O}_{n'}(\mathbf{y})[V_s]$$

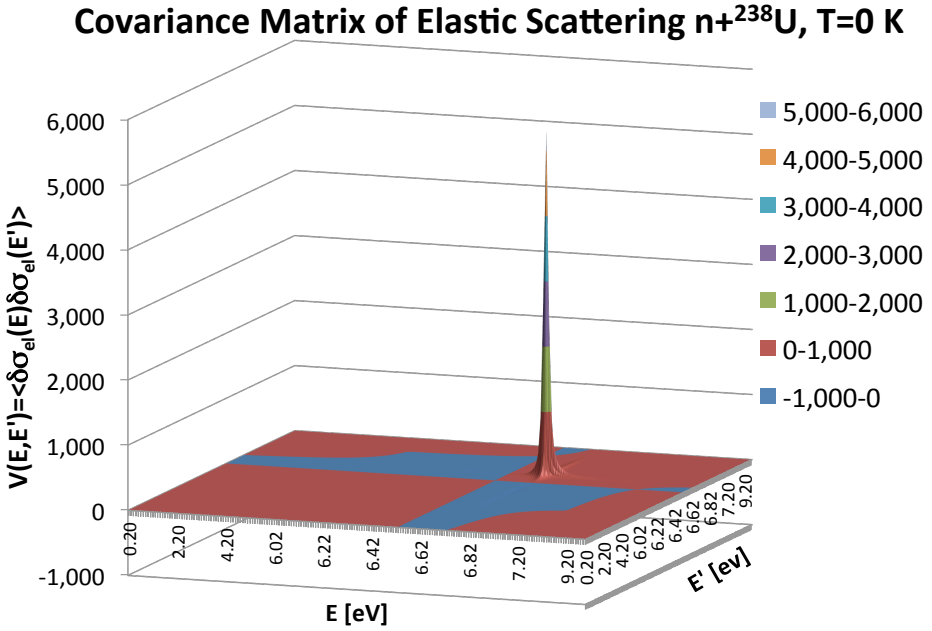
$$V_s(E,E') \equiv \langle \delta\sigma_s^{\rm tab}(E)\delta\sigma_s^{\rm tab}(E')\rangle$$

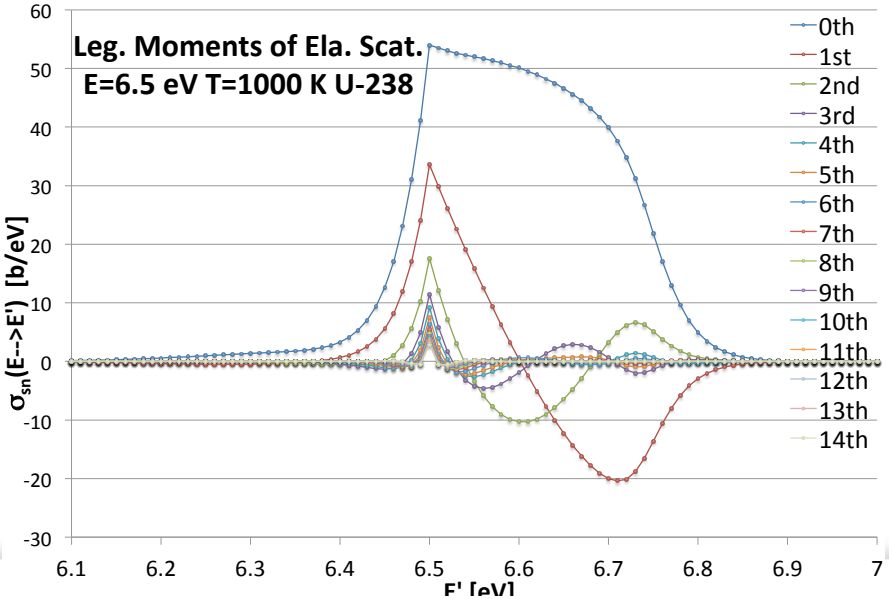
$$\langle \delta\sigma_s(\mathbf{x},\mu_{\rm lab})\delta\sigma_s(\mathbf{y},\mu'_{\rm lab})\rangle = \sum_{n,n'}(n+\tfrac{1}{2})(n'+\tfrac{1}{2}) \times P_n(\mu_{\rm lab})P_{n'}(\mu'_{\rm lab})M_{nn'}(\mathbf{x},\mathbf{y})$$

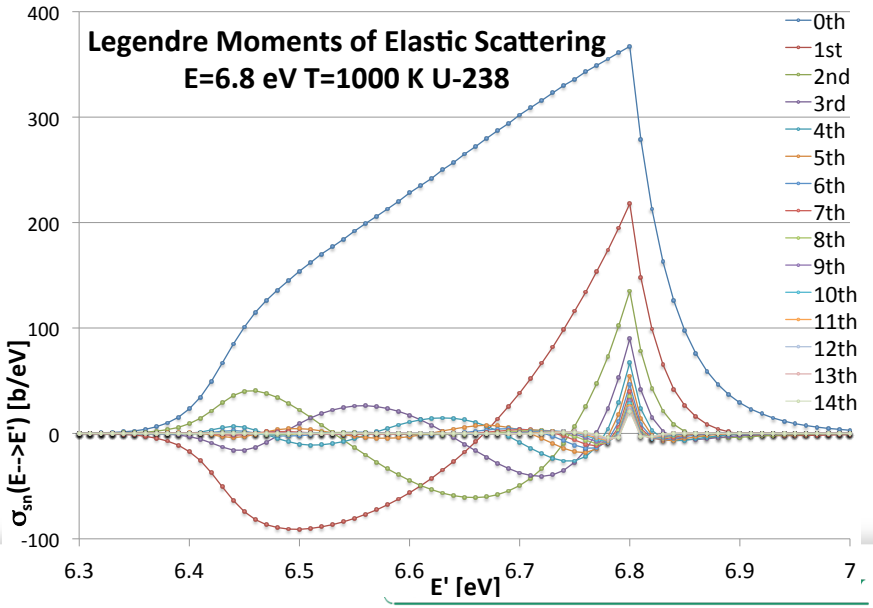
- The above could be used to connect to the thermal S(a,b)

Doppler Broadened Legendre Moments









Double-Differential Cross Section