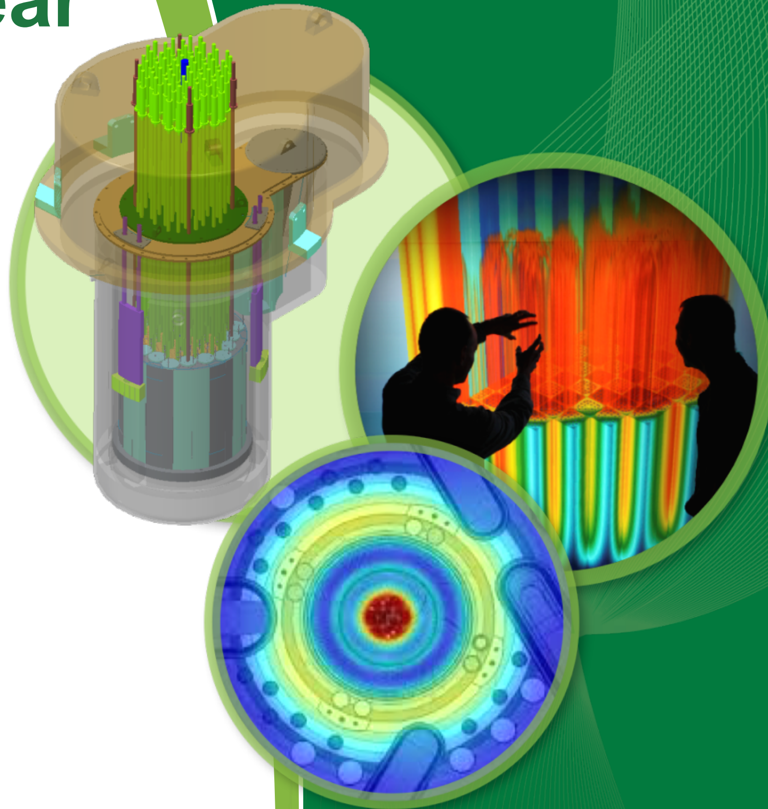
Advances in ORNL Nuclear Data Evaluation Methods



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Outline

- Motivation and background
- SAMMY modernization update
- Bayesian generalized data optimization method
- Phenomenological Dirac relativistic R-matrix formalism
- Thermal neutron scattering, $S(\alpha,\beta)$, evaluation framework
- Conclusions and outlook

Motivation and background

- DOE's programmatic pursuit of improved nuclear data (ND) and uncertainties (variances and covariances)
  - Nuclear Criticality Safety, Nuclear Engineering & Applications, Science
- SAMMY modernization approved by the US Nuclear Criticality Safety Program (NCSP)
  - Modernize the software quality assurance (SQA) programming framework (C++ APIs)
  - Modernize the evaluation methods
- Need for simultaneous, consistent evaluation of differential and integral benchmark experimental data
  - Revisit application of Bayes' Theorem to ND
  - Improve consistency between differential and integral uncertainties
  - Evaluated cross sections are now post-adjusted to fit integral data

SAMMY 8.1 released by RSICC April 2017:

- SAMINT: integral benchmark experiments inform research parameter evaluations (Implemented by Vlad Sobes)
- SAMMY integrated into SCALE SQA in AMPX footsteps
  - Automated cmake/ctest suite, revision control repository, FogBugz
  - Platforms supported Linux/gfortran, Mac/gfortran, Windows/ifort
- New detector resolution functions in collaboration with Rensselaer Polytechnic Institute (RPI)
- Updated physical constants; SAMMY and SAMRML compute consistently now
- Corrected a misplaced index that was causing incorrect matrix multiplication for non-diagonal data covariance matrix
- Implemented several other bug fixes
- Obtained license for distributing COULCWF with SAMMY/AMPX/SCALE

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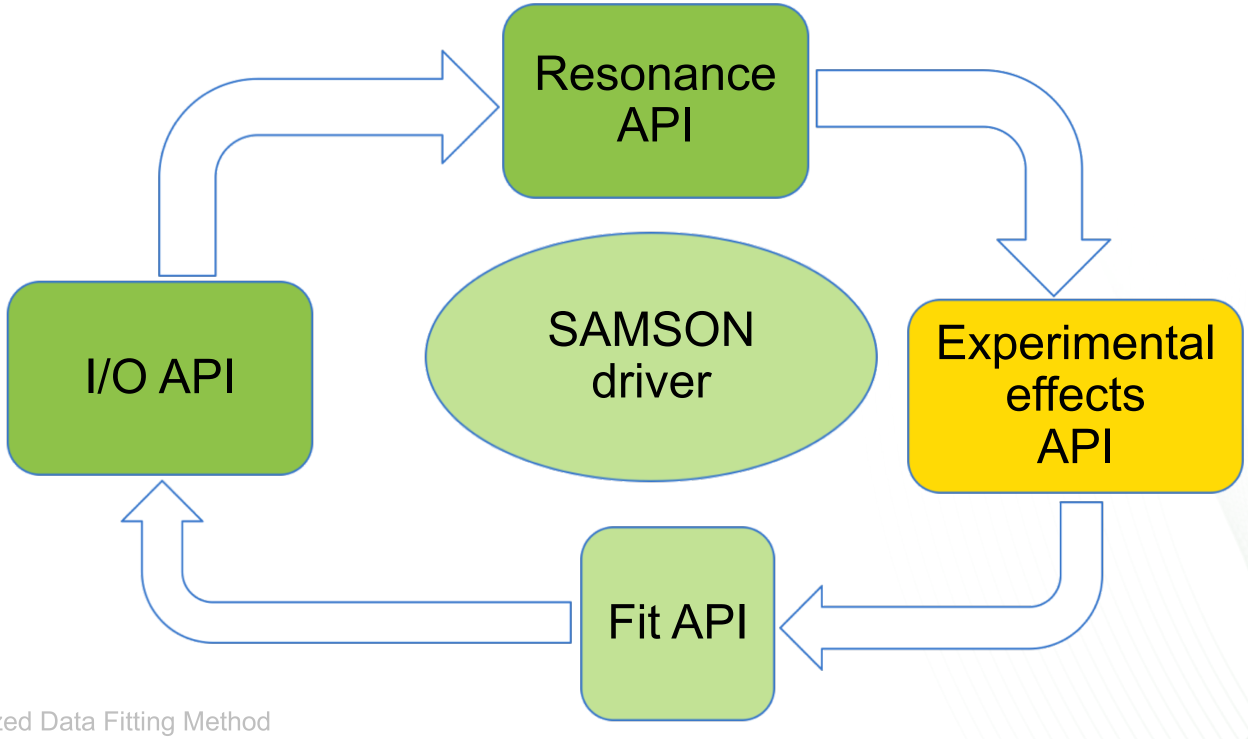
SAMSON high-level application programming interface (API) diagram

- Defines APIs before implementation
  - Enables variety of methods for each API
  - Leverages input/output (I/O) and Resonance API from C++ SAMRML
    - SAMMY PARameter and GND file reader/writer under development
    - To replace SAMMY I/O routines



Fit API: GLS, Bayesian Monte Carlo

GLS

Bayesian Monte Carlo

- Generalized least squares (GLS)
  - Nuclear Engineering Science Laboratory Synthesis (NESLS) summer intern Jinghua Feng implemented a prototype
  - Andrew Holcomb ported the prototype into the FitAPI
  - Compact expressions by Froehner were used (Sect. 2.2 of JEFF Report 18, 2000)
- Bayesian generalized data optimization method (CW2017)
  - NESLS summer intern Jinghua Feng implemented a prototype
  - Prototype avoids Peelle's Pertinent Puzzle (PPP) issue plaguing GLS of reduced data
- Fit differential and/or integral benchmark experiment data performed simultaneously instead of adjusting differential data retroactively

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Fit API: Preliminary interface

Interface
Fit
setData Set an instance of Data interface **initialize** After setting data object initialize internal data structures **execute** Do the actual fitting **finalize** Clean up any internal resources

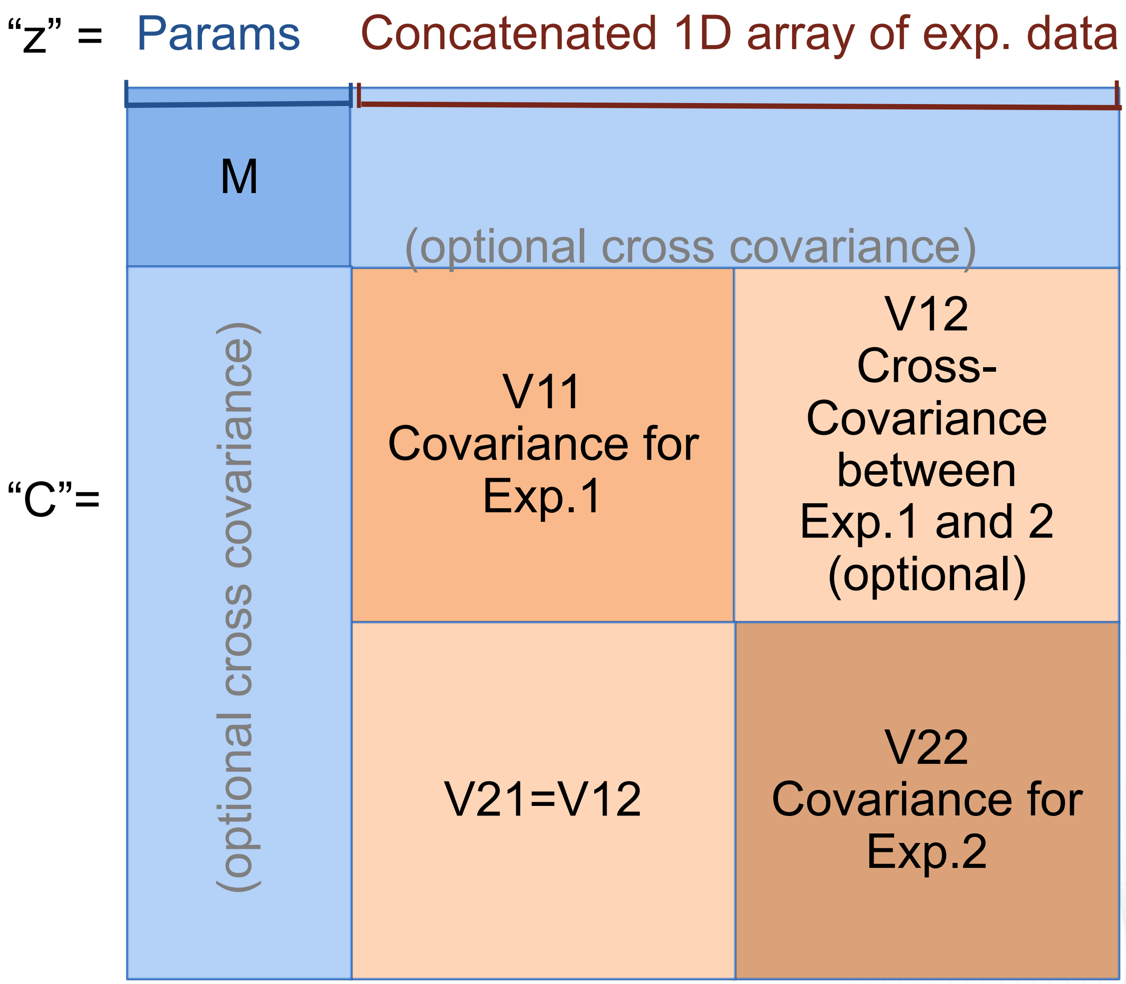
Interface
Array
getNumDim Get the number of dimensions **getSize(int dim)** Get the array size for dimension m **getValue(int i1, int i2, …)** Get the value for the indicated indices. In C++ we would pass in a vector of length getNumDim **setValue(int i1,int i2, …_** Set value

Interface
Data
getNumberParams Get the number of parameters **getNumData** Get the number of experimental data **getData** Get the list of experimental data (1-dim Array) **getParam** Get the list of initial params (1-dim Array) **getCovMatrix** Get the full covariance matrix (2-dim Array) **getTheory** Get theoretical values based on current parameters (1-dim Array) **setParam** Set the current parameters (1-dim Array) **setCovMatrix** Set the full covariance matrix (2-dim Array)

- Actual instances are instantiated by a factory class
- Data will have a method to obtain the derivatives (2-dim Array: getNumberParams x getNumData); there will be a function that computes derivatives numerically
- Fit calls setParams, getTheory, setCovMatrix repeatedly in the course of fitting the data

Fit API: GLS implementation

- Parameters and experimental data cast into 1D array by implementation of data
  - for generic use inside SCALE framework
  - Froehner's formulation and notation:



Fit API: GLS implementation

GLS

- Generalized least squares (GLS)
  - Compact expressions by Froehner (Sect. 2.2 of JEFF Report 18, 2000)

    (Warning: Nondiagonal data covariance matrix [DCM] may lead to PPP syndrome)

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \left[\mathbf{S}(\mathbf{x}_n)^\dagger \mathbf{C}^{-1} \mathbf{S}(\mathbf{x}_n)\right]^{-1} \mathbf{S}(\mathbf{x}_n)^\dagger \mathbf{C}^{-1} \left[\zeta - \mathbf{z}(\mathbf{x}_n)\right]$$

- Implementation uses *cpp-array* library (CPC **185**,1681, 2014)
  - Transparently parallelized via BLAS library (Intel MKL, cuBLAS, MAGMA)
  - Compact notation for matrix operations, e.g. parameter set update
  - P = P + inv(transpose(S) * inv(C) * S) * transpose(S) * inv(C) * (Π – T)
- BLAS advantages: drastically speeds up large matrix operations in SAMMY and shortens code (Arbanas, Dunn, Wiarda, M&C2011)

Experimental effects (EE) API

- Convolution of Doppler broadening, target, and detector effects, each one implenting the EE API:

Doppler broadening: FGM, DDXS, S(a,b) BROADEN/AMPX	Neutron transport: SHIFT API (DBRC, LH, multiple scatter.)	Resolution function via Monte Carlo N-Particle (MCNP) for example

- SHIFT API for on-the-fly neutron transport aspects
  - To enable fitting integral benchmark experiments (IBEs)
  - Developed for SCALE by Cihangir Celik (ORNL Nuclear Data and Criticality Safety) during FY2017
  - Message passaging interface (MPI) enabled
  - Could use MCNP input
- In principle, the entire experimental setup could be simulated
  - Fitting to raw data may be possible; varying opinions
  - Raw data may become publicly available (needed for Bayesian MC)

Relevant quotes from Edwin T. Jaynes (1922-1998)

- "… every Bayesian problem is open ended; no matter how much analysis you have completed, this only suggests still *other kinds of prior information* that you might have had, and therefore still more interesting calculations that need to be done to get still deeper insight into the problem."

⇨ *model defect* and its covariance introduced as priors

- "The *difficulties are never mathematical*; at no point do we encounter any mathematical problem that could not be dealt with by an undergraduate…"

⇨ Bayes' theorem is straightforward for given priors

from "Straight Line Fitting – a Bayesian Solution" (1999), which chronicles Bayesian straight line fitting during his lifetime (http://bayes.wustl.edu/etj/articles/leapz.pdf)

Principles and notation used in derivation

- Distinction is maintained between the variables' values and their *expectation* values for both *prior* **and** *posterior*
  - Prior generalized data expectation values $<z>=(<P>, <D>)$
  - PDF of a particular value $z=(P,D)$ is $p(z|<z>,C,T(.))$
  - Posterior expectation values denoted by a prime: $<z>'=(<P>', <D>')$
- *Symmetry* of any normal PDFs was enforced:

  $(z-<z>)^{+}C^{-1}(z-<z>)$, where $C=<(z-<z>)\,(z-<z>)^{+}>$
- The model, its defect, and defect covariance introduced as priors, which has important implications in the application of Bayes' theorem

$$T(\cdot), \langle\delta\rangle, \quad \mathbf{\Delta} \equiv \langle(\delta - \langle\delta\rangle)(\delta - \langle\delta\rangle)^{\mathsf{T}}\rangle$$

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Definitions used in derivation

- Generalized data, $z \equiv (P, D)$, and its covariance matrix $\mathbf{C}$

$$
\begin{aligned}
\mathbf{C} &\equiv \langle (z - \langle z \rangle)(z - \langle z \rangle)^{+} \rangle \\
&= \begin{pmatrix} \langle (P - \langle P \rangle)(P - \langle P \rangle)^{+} \rangle & \langle (P - \langle P \rangle)(D - \langle D \rangle)^{+} \rangle \\ \langle (D - \langle D \rangle)(P - \langle P \rangle)^{+} \rangle & \langle (D - \langle D \rangle)(D - \langle D \rangle)^{+} \rangle \end{pmatrix} \\
&\equiv \begin{pmatrix} \mathbf{M} & \mathbf{W} \\ \mathbf{W}^{+} & \mathbf{V} \end{pmatrix}
\end{aligned}
$$

- Generic Bayes' theorem:

$$p(\alpha|\beta\gamma) = p(\alpha|\gamma\beta) \propto p(\alpha|\gamma)p(\beta|\alpha\gamma)$$

- Generic Product Rule of Probability Theory:

$$p(\alpha\beta|\gamma) = p(\alpha|\beta\gamma)p(\beta|\gamma)$$

where α ,β and γ will be specified for each particular application

Direct derivation in generalized data notation

- Application of Bayes' theorem

$$p(\alpha|\beta\gamma) = p(\alpha|\gamma\beta) \propto p(\alpha|\gamma)p(\beta|\alpha\gamma)$$

with the following substitutions:

$$\alpha \to z$$

New prior: ⇨ $\beta \to T(\cdot), \langle\delta\rangle, \mathbf{\Delta}$ $\qquad \mathbf{\Delta} \equiv \langle(\delta - \langle\delta\rangle)(\delta - \langle\delta\rangle)^{\mathsf{T}}\rangle$

$$\gamma \to \langle z\rangle, \mathbf{C},$$

yields a posterior PDF for ***generalized*** data:

Posterior $\propto$ Prior $\times$ Likelihood

$$p(z|\langle z\rangle, \mathbf{C}, T(\cdot), \langle\delta\rangle, \mathbf{\Delta}) \propto p(z|\langle z\rangle, \mathbf{C}) \times p(T(\cdot), \langle\delta\rangle, \mathbf{\Delta}|z, \langle z\rangle, \mathbf{C})$$

(Normalized) generalized data posterior PDF

- Enables computation of arbitrary posterior expectation values:

$$\langle f(z)\rangle' = \int dz f(z) p(z|\langle z\rangle, \mathbf{C}, T(\cdot), \langle\delta\rangle, \mathbf{\Delta})$$

$$\langle z'\rangle \longrightarrow f(z') = z' = (P', D')$$

$$\mathbf{C}' \longrightarrow f(z') = (z' - \langle z'\rangle)(z' - \langle z'\rangle)^{+}$$

- Integration is over all posterior values of z'=*(P',D')*
  - Analogous to integrating out "nuisance parameters" (Jaynes 1999)
  - Posterior expectation values <z'>=(<P'>,<D'>) ≠ <z>=(<P>,<D>)
    - <D'>≠<D>; posterior experimental data are informed by the model
    - This appears to be an organic aspect of Bayes' theorem, not an adjustment
  - Evaluated model covariance matrix can be computed to ***all*** orders
  - Use *f(z')* below; *cf.* 1st order approximation (dT/dP')M'(dT/dP'), and V'

$$f(z') = (T(P') - \langle T(P')\rangle)(T(P') - \langle T(P')\rangle)^{+}$$

New Bayesian derivation outline

Bayes' Theorem

↓

Bayesian Generalized Data Fitting Method

↓

A Form Specialized for Normal PDFs

↓

Constrained Generalized Least Squares (CGLS)

↓

Generalized Least Squares (GLS)

The GLS in ND is at the bottom of this approximation hierarchy

Hierarchy of approximations I: posterior PDFs

- The most general posterior generalized data PDF is

$$p(z|\langle z\rangle, \mathbf{C}) \; \times \; p(T(\cdot), \langle\delta\rangle, \mathbf{\Delta}|z, \langle z\rangle, \mathbf{C})$$

- Assuming normal forms of PDFs, where $\tilde{\delta} \equiv T(P) - D$,

$$\mathcal{N}(z|\langle z\rangle, \mathbf{C}) \; \times \; \mathcal{N}(\tilde{\delta}|\langle\delta\rangle, \mathbf{\Delta})$$

- Taking the limit $\langle\delta\rangle \to 0$ and $\mathbf{\Delta} \to \mathbf{0}$

$$\mathcal{N}(z|\langle z\rangle, \mathbf{C}), \quad \text{constraint} \;\; T(P) = D$$

- Application of constraint into prior yields UMC-B w/o constraint

$$\mathcal{N}(z|\langle z\rangle, \mathbf{C}) \qquad z \equiv (P, D) \to (P, T(P))$$

Hierarchy of approximations II: cost functions

- The most general PDF in normal form, where $\tilde{\delta} \equiv T(P) - D$,

$$Q(z) \equiv (z - \langle z \rangle)^{\intercal} \mathbf{C}^{-1} (z - \langle z \rangle) + (\tilde{\delta} - \langle \delta \rangle)^{\intercal} \mathbf{\Delta}^{-1} (\tilde{\delta} - \langle \delta \rangle)$$

becomes CGLS in the limit $\langle \delta \rangle \to 0 \text{ and } \mathbf{\Delta} \to \mathbf{0}$

$$Q(z) \approx (z - \langle z \rangle)^{\intercal} \mathbf{C}^{-1} (z - \langle z \rangle), \quad \text{constraint } T(P) = D$$

- Application of constraint *before* cost minimization yields GLS

$$\begin{aligned} Q(z) \approx \quad & (P - \langle P \rangle)^{\intercal} \mathbf{M}^{-1} (P - \langle P \rangle) \\ & + (T(P) - \langle D \rangle)^{\intercal} \mathbf{V}^{-1} (T(P) - \langle D \rangle) \end{aligned}$$

Testing favors CGLS over GLS: χ^2 minimization

- CGLS has been used in high energy physics for 50+ years (APLCON; no PPP when used for systematic or data reduction parameters
- V. Blobel (U. Hamburg, DESY) compiled cases for which CGLS finds more reasonable fits than GLS or χ^2 minimization
  - http://www.desy.de/~blobel/apltalk.pdf
  - 2-D fitting with line, parabola, uncertainties in x- and y-dimensions
  - PPP appears in χ^2-min. but ***not*** in CGLS (p.17, 18)
  - Related to non-diagonal reduced DCM computed at experimental vs. theoretical values (N. Larson, SAMMY)

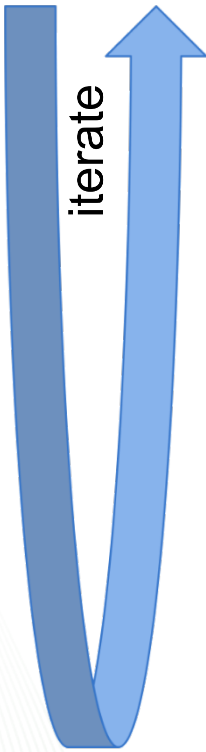
Constrained iterative Monte Carlo algorithm

- Iterate on posterior distribution until convergence is attained
  - "*k*," random sample label from posterior normal distribution $\mathcal{N}(\langle z'\rangle, \mathbf{C}')$
  - ω_k is the Monte Carlo weight for computing expectation values

$$\omega_k = \frac{p(z'_k|\langle z\rangle, \mathbf{C})}{p(z'_k|\langle z'\rangle, \mathbf{C}')} e^{-\frac{1}{2}(D'_k - T(P'_k))^+ \mathbf{X}'^{-1}(D'_k - T(P'_k))}$$

For constraint $\langle c(\cdot)\rangle = 0$

$$\langle z'\rangle = \sum_k \hat{\omega}_k z'_k \qquad \mathbf{C}' = \langle (z' - \langle z'\rangle)(z' - \langle z'\rangle)^+\rangle$$



- Resample using SVD of C':

$$z' = \langle P', T(P')\rangle + \mathcal{V}\mathcal{E}^{1/2}\mathcal{R} \qquad \text{where} \qquad \mathbf{C}' = \mathcal{V}\mathcal{E}\mathcal{V}^+$$

  - $\mathcal{R}$ is a *(#P + #D)* × *(#k)* matrix of $\mathcal{N}$(0,1) normal random numbers

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Conclusions and future applications

- Generalized data fitting method based on the Bayes' theorem
  - Accommodates model defect via constraint on expectation values
  - Implemented via iterative Monte Carlo method (J. Feng for SAMMY)
  - Its special cases:
    - Constrained [generalized] least squares (CLS) of V. Blobel in APLCON
    - Generalized linear least squares (GLLS) [constrained] TSURFER WHISPER
    - But NOT the $\chi^2 = (D-T(P'))V^{-1}(D-T(P'))$, which may yield different results (Blobel)
- Comparison of CLS/GLS to quantify accuracy of approximations
- Consideration of log normal random distributions (I. Kodeli)
- Enables multidimensional sampling such as cross sections *and* energies
- The new method could be used for consistent simultaneous optimization of differential and integral benchmark experiments
  - To simultaneously fit differential and integral parameters
  - To yield more complete and consistent evaluations

Phenomenological Dirac R-matrix formalism

- Originally derived for calculable R-matrix, but expressed in a form that could be used for phenomenological fitting
  - Ph.D. Thesis (2011): http://scholarworks.wmich.edu/dissertations/411
- Boundary condition is determined by the channel radius
- Compare to approximations and the non-relativistic R-matrix

J. Grineviciute and Dean Halderson PHYSICAL REVIEW C **85**, 054617 (2012)

$$R_{cc'} = \sum_{\mu} \gamma_{\mu c}\gamma_{\mu c'}/(E_\mu - E)$$

$$\mathbf{S} = \mathbf{v}^{1/2}(\mathbf{Fo} - \mathbf{RGo})^{-1}(\mathbf{F_I} - \mathbf{RG_I})\mathbf{v}^{-1/2} \qquad T_{cc'} = i(\delta_{cc'} - S_{cc'})/2$$

$$\langle f\rangle_{\alpha\sigma M_A,\alpha'\sigma' M'_A} = \frac{1}{k}\sum \sqrt{4\pi(2\ell+1)}C^{\ell 1/2 j}_{0\sigma m} C^{J_A j J_B}_{M_A m M_B} C^{J'_A j' J_B}_{M'_A m' M_B} C^{\ell' 1/2 j'}_{m'_\ell \sigma m'} \times i^{(\ell-\ell')} e^{i(\delta'_\kappa + \delta'_{\kappa'})} T_{\alpha J_A \ell j J_B, \alpha' J'_A \ell' j' J'_B} Y_{\ell' m'_\ell}(\mathbf{k}').$$

$$\frac{d\sigma}{d\Omega}(\theta) = \frac{1}{2(2J_A+1)} \sum_{\sigma\sigma' M'_A M'_A} \left| \langle f_c\rangle_{\sigma\sigma'}\delta_{J_A\alpha M_A, J'_A\alpha' M'_A} + \langle f\rangle_{\alpha\sigma M_A,\alpha'\sigma' M'_A}\right|^2$$

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ORNL S(a,b) evaluation framework overview

- The objective is to combine experimental double differential scattering data and model parameters to yield the best estimate of double differential cross section (DDCS) and *uncertainties*
- Data and simulation fit is achieved using the Unified Monte Carlo (UMC) [1] method
- Simulations are constrained by physical properties of material
- Framework tested on light water
  - Data collected from ORNL Spallation Neutron Source (SNS)
  - RPI collaboration
- Validated using benchmarks from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) handbook
- C. Chapman's Ph.D. https://smartech.gatech.edu/handle/1853/58693

Framework specifics: simulation

- Ran simulations of TIP4P/2005f [2] water in a box in the classical molecular dynamics (MD) code GROMACS [3]
- Computed density of states using trajectories from GROMACS
- Intermediate structure factor calculated using Gaussian approximation found in Abe and Tasaki [4]

$$F(q,t) = \exp\left[-\frac{q^2}{2}\frac{\hbar}{M}\int_0^\infty d\omega\,\frac{g(\omega)}{\omega}\left\{\coth\left(\frac{\hbar\omega}{2k_BT}\right)(1-\cos(\omega t)) - i\sin(\omega t)\right\}\right]$$

$$S(\alpha,\beta) = k_BTe^{\frac{-E}{2k_BT}}\big(S(q,E)\big) = k_BTe^{\frac{-E}{2k_BT}}\left(\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}F(q,t)e^{\frac{-iEt}{\hbar}}dt\right)$$

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Framework specifics: simulation

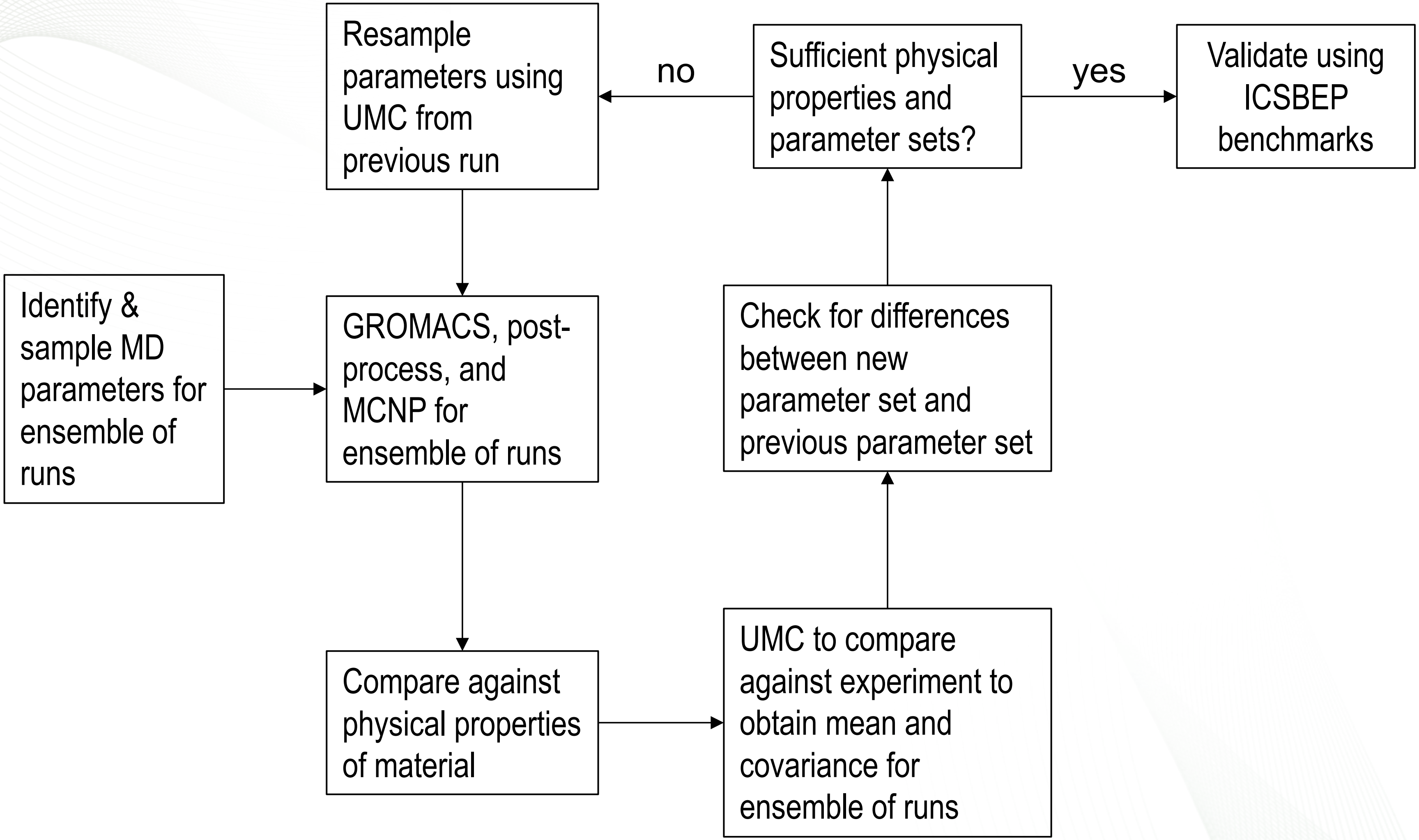
- Calculated scattering law using code developed for this project:

  Intermediate structure factor → dynamic structure factor → scattering law

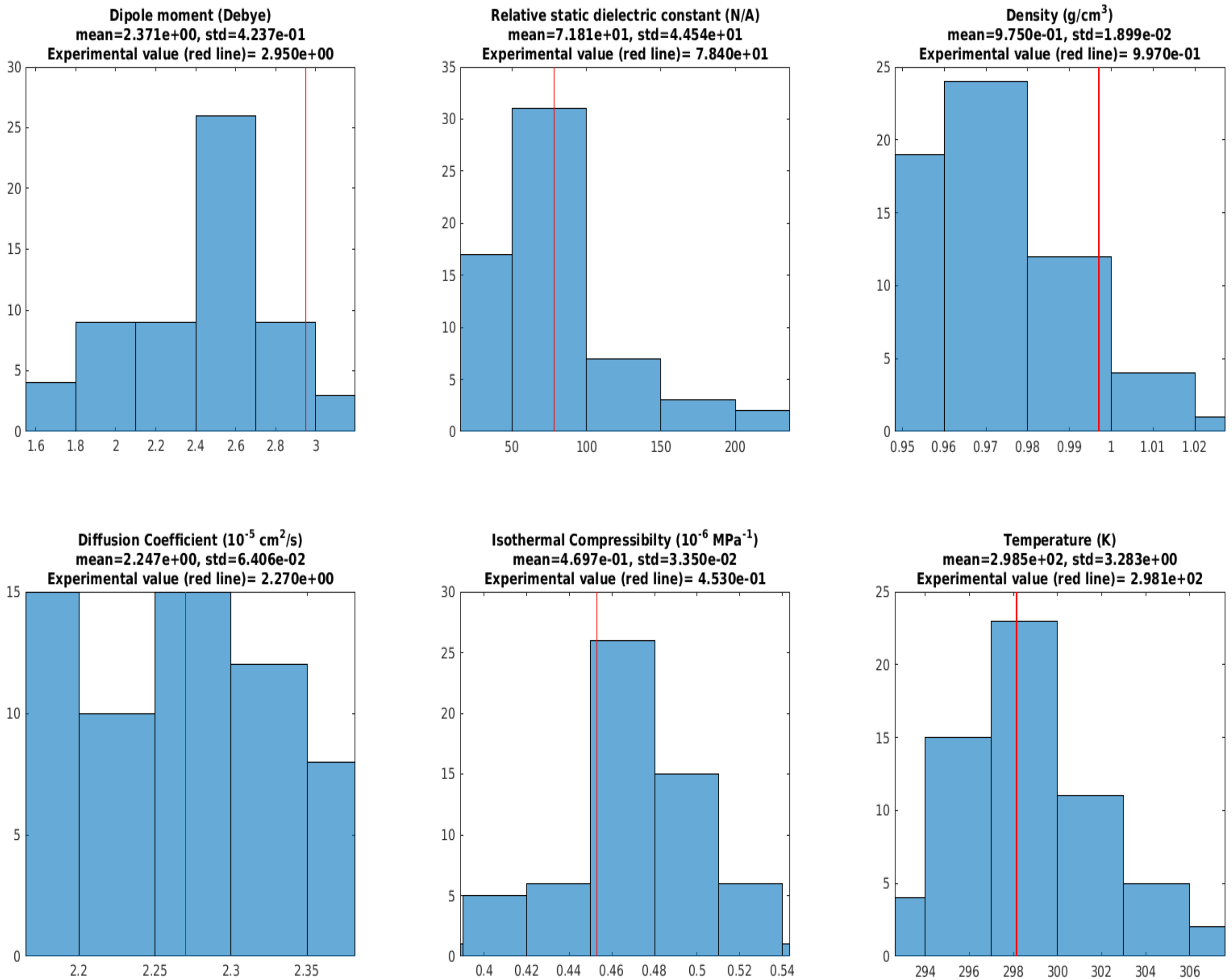
- Ran simplified MCNP code
- DDCS convoluted with SNS detector resolution function

$$\frac{d^2\sigma}{dE_f d\Omega} = \frac{\sigma_b}{4\pi k_B T}\sqrt{\frac{E_f}{E_i}}\, e^{\frac{-\beta}{2}} S(\alpha, \beta)$$

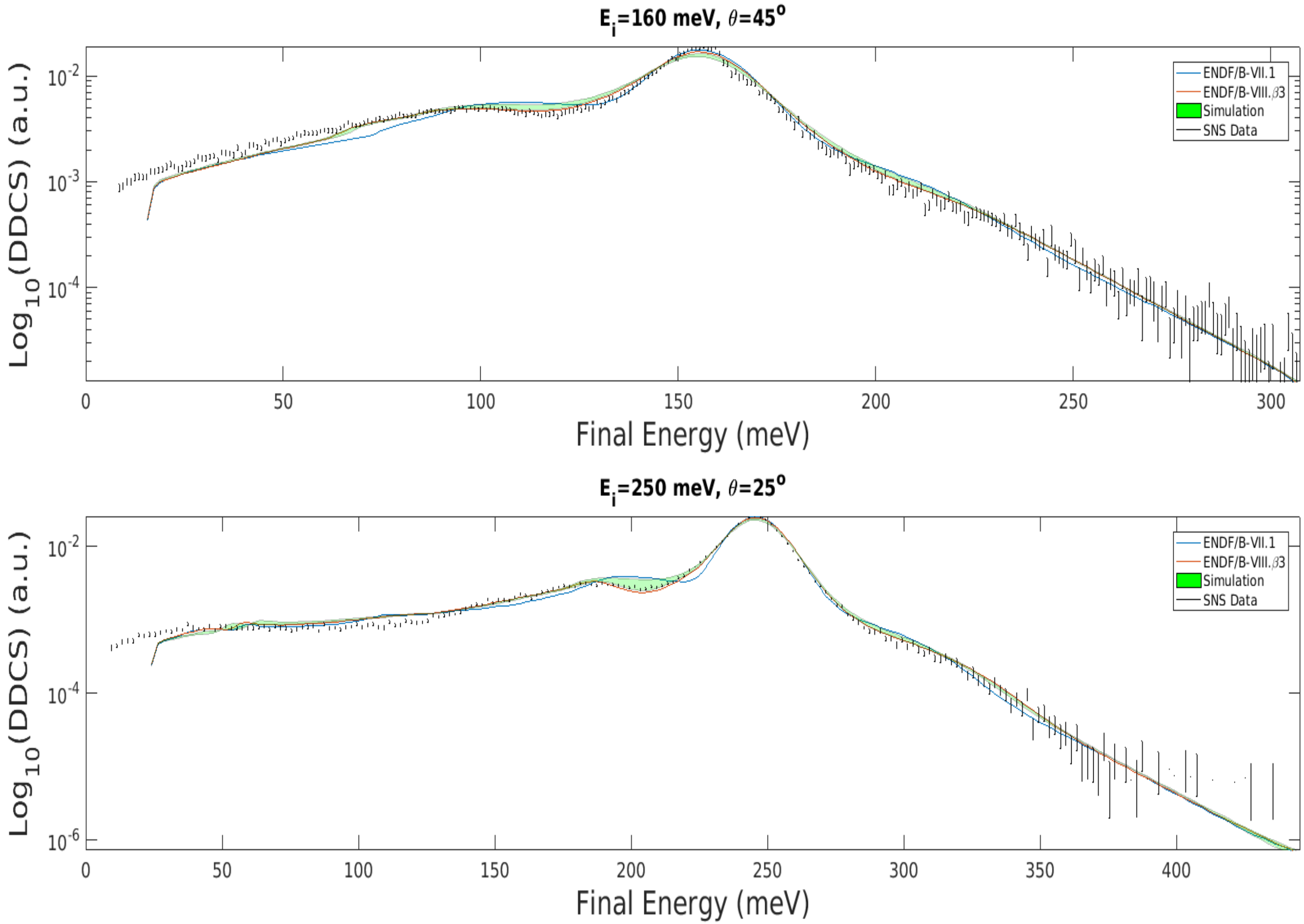
Framework outline



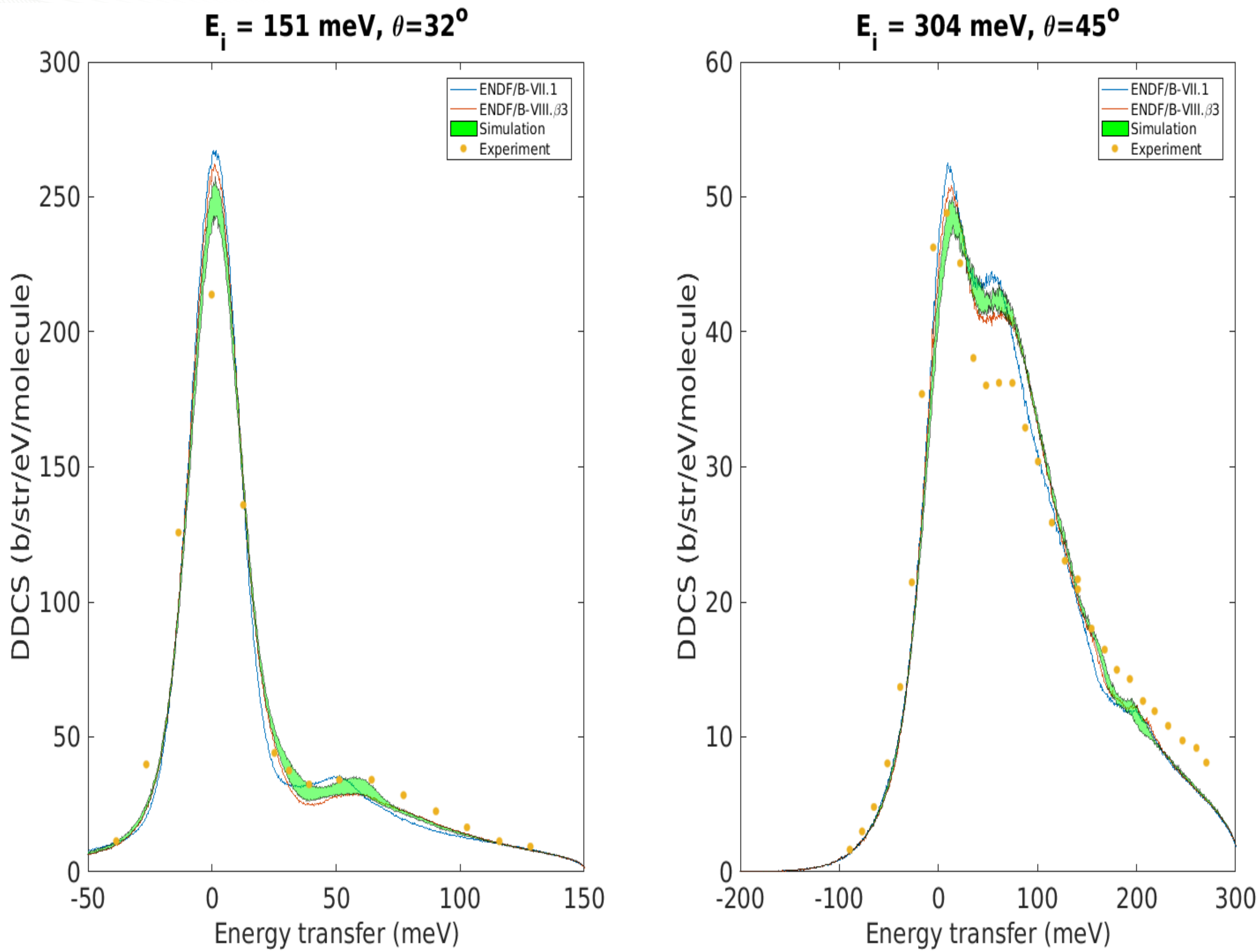
Results: properties of water



Results: DDCS – SNS



Results: DDCS – independent



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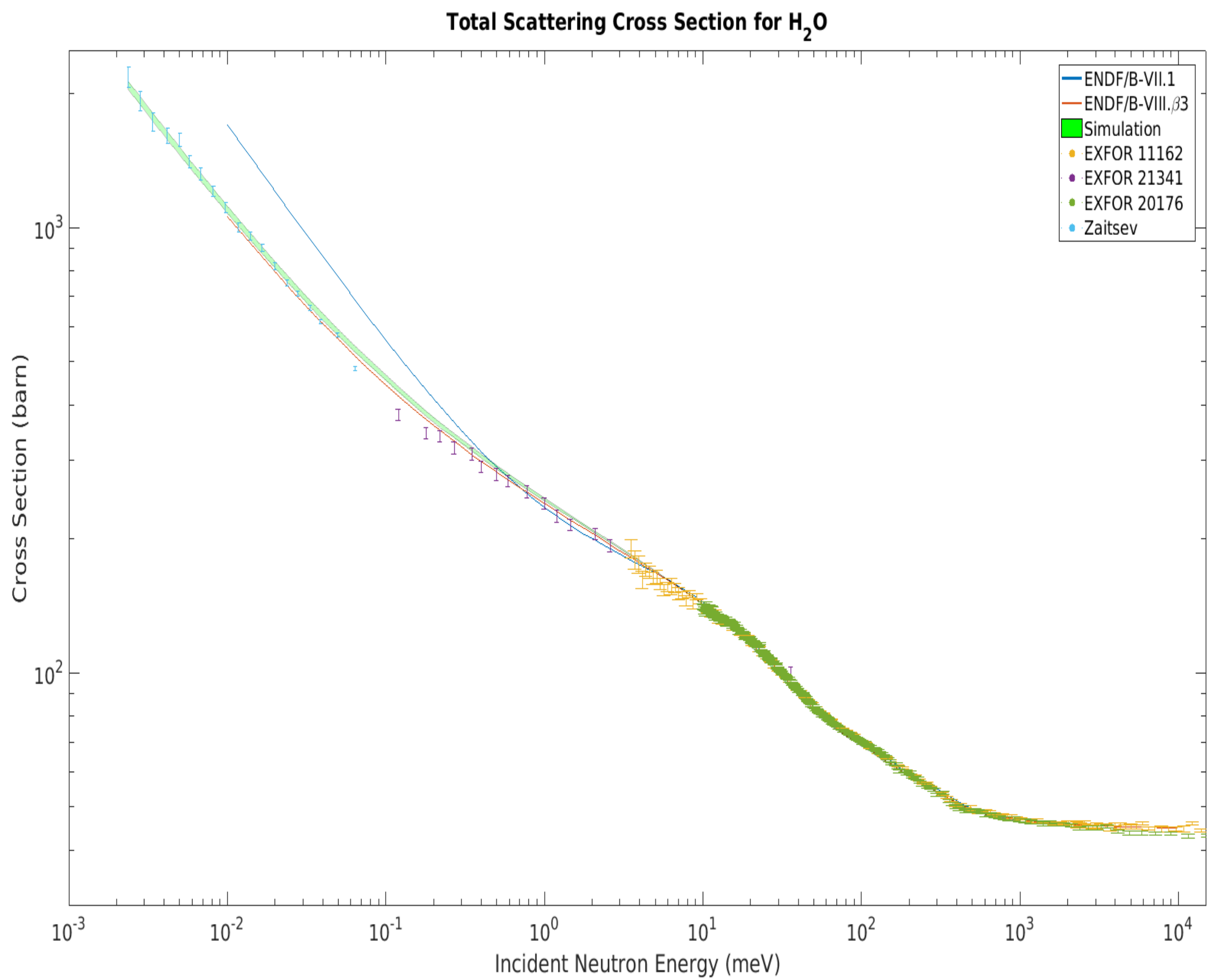
Results: total cross section

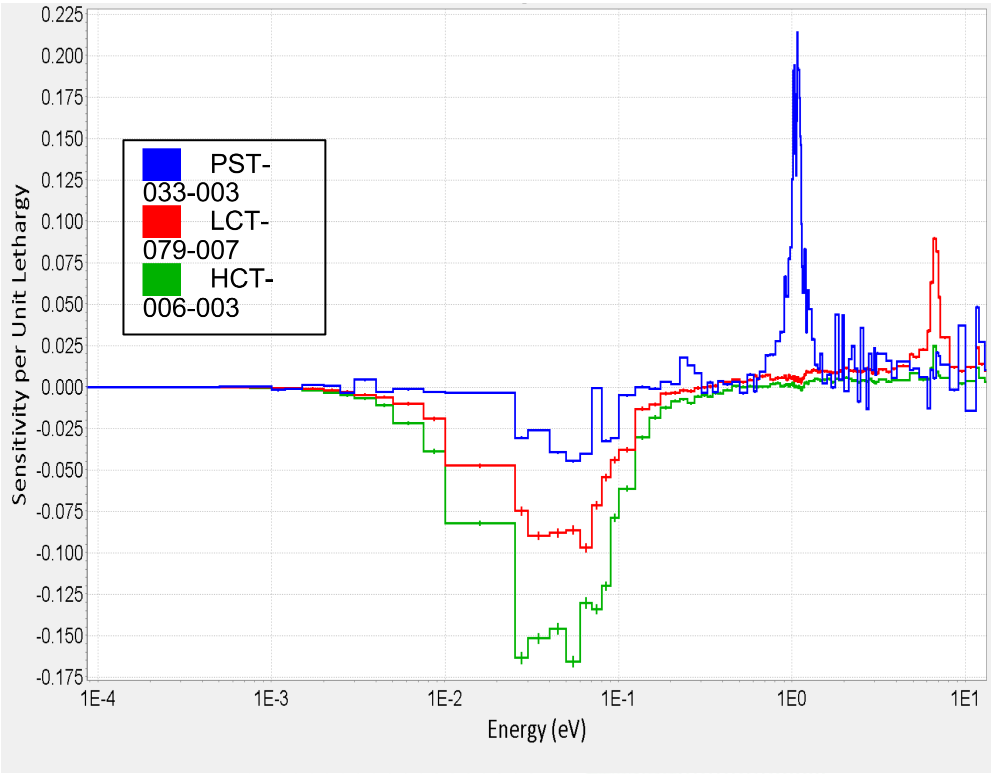


Results: ICSBEP benchmarks

Benchmarks

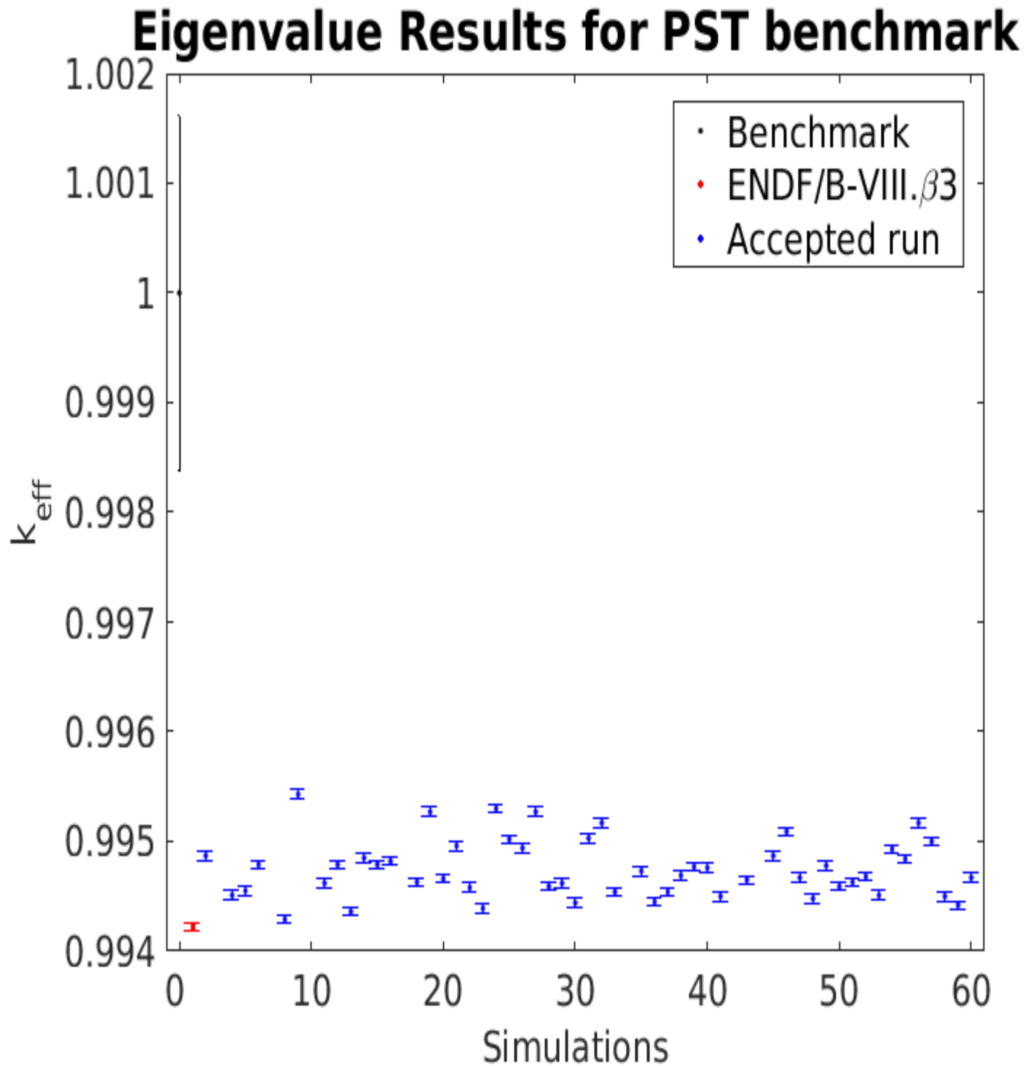
- PST-033-003: plutonium nitrate solution surrounded by water
- LCT-079-007: water moderated and reflected triangular pitched UO_2 fuel elements
- HCT-006-003: water moderated hexagonally pitched high enriched (80% ^{235}U) fuel rods

Sensitivity plot



Results: PST-033-003

ENDF Library	K_{eff}	St.Dev (pcm)	ΔK_{eff} (pcm)
Benchmark	1.00000	162	N/A
ENDF/B-VII.1	0.99349	4	651
ENDF/B-VIII.β3	0.99422	4	578
New XS	0.99483	4	517



- Noticeable improvement
- Issues may be caused by materials other than light water

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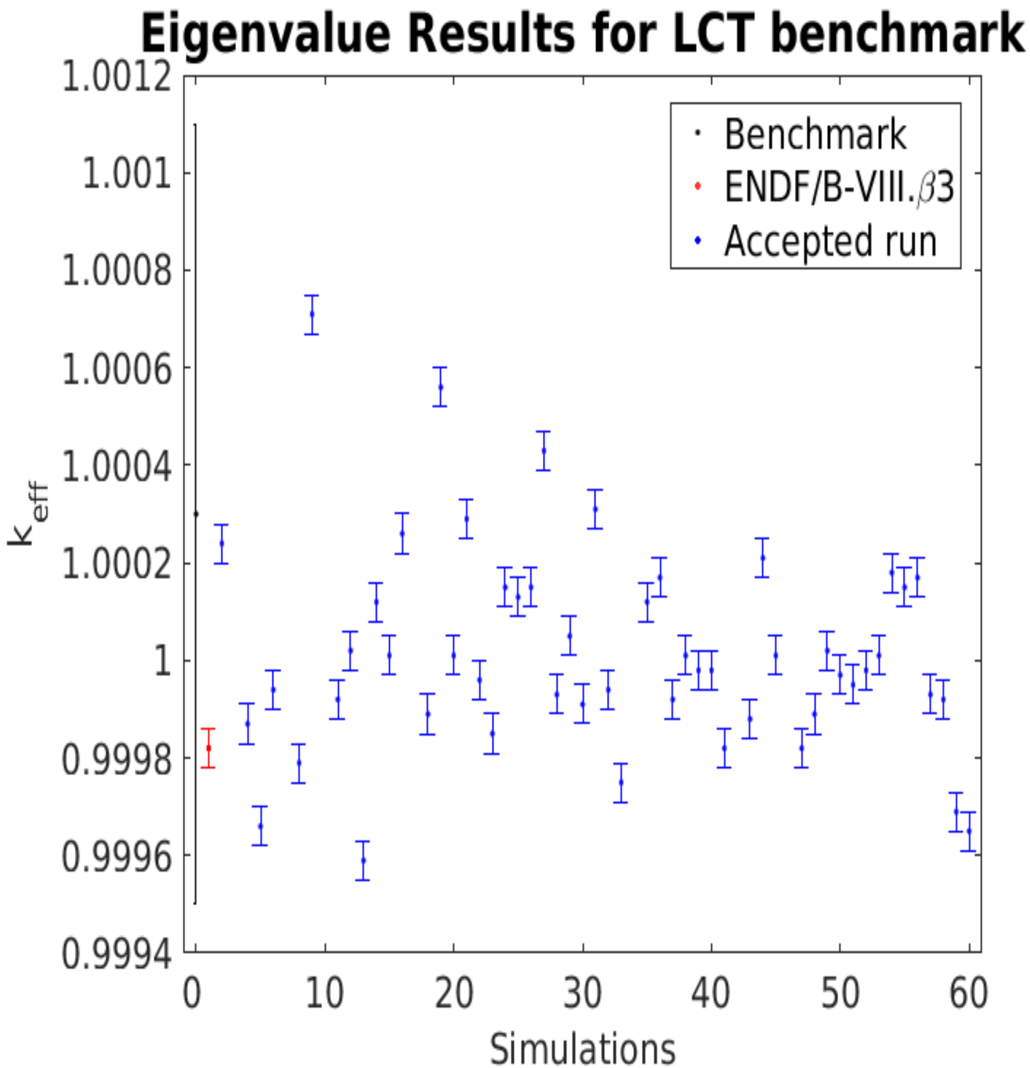
Results: LCT-079-007

ENDF Library	K_{eff}	St.Dev (pcm)	ΔK_{eff} (pcm)
Benchmark	1.00030	80	N/A
ENDF/B-VII.1	0.99933	4	97
ENDF/B-VIII.β3	0.99982	4	48
New XS	1.00006	4	24



- Inconclusive improvement
- Results within error bounds of experimental uncertainty

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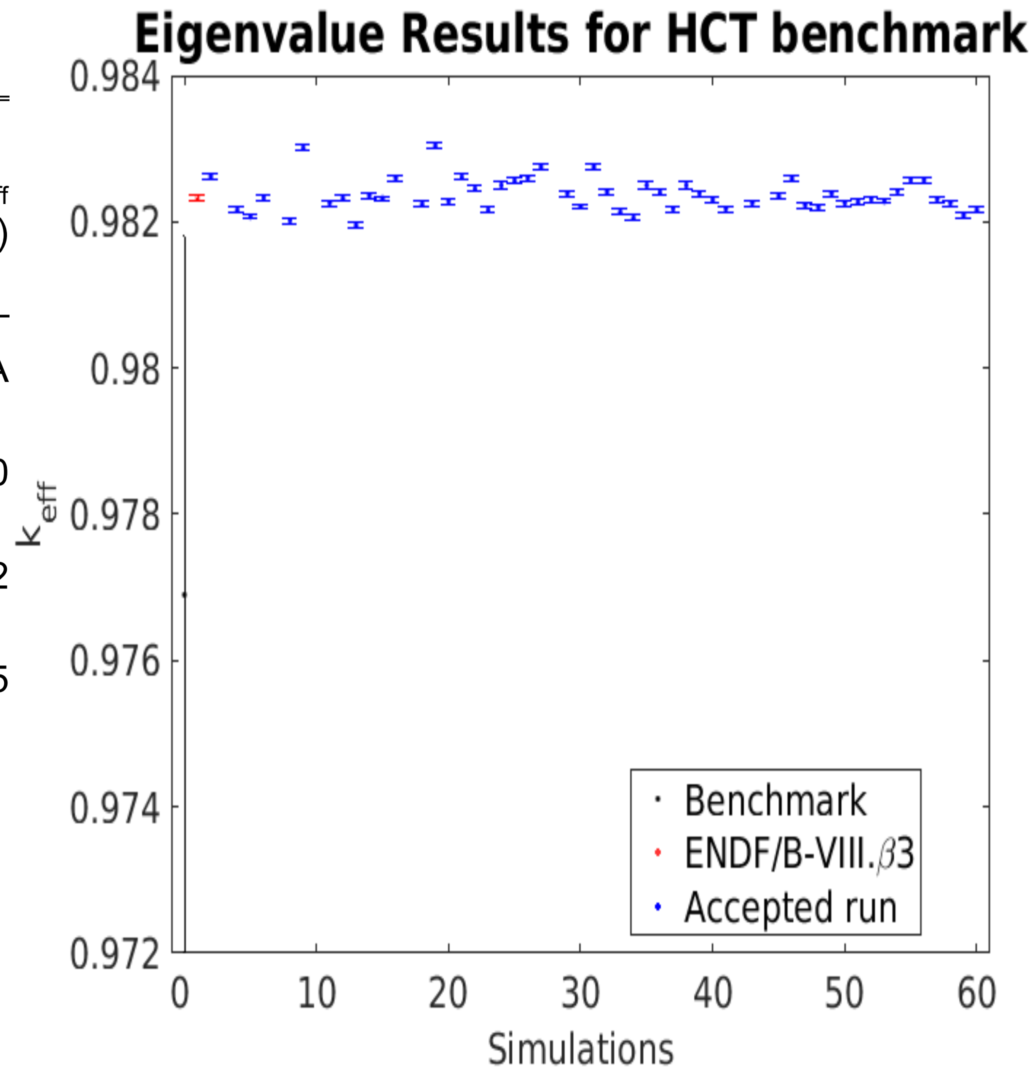
Results: HCT-006-003

ENDF Library	K_{eff}	St.Dev (pcm)	ΔK_{eff} (pcm)
Benchmark	0.97690	490	N/A
ENDF/B-VII.1	0.98190	4	-500
ENDF/B-VIII.β3	0.98232	4	-542
New XS	0.98245	4	-555



- Slightly worse results
- Still within 2 standard deviations of experiment

Conclusions

- Evaluation Framework was presented to generate thermal scattering law and uncertainties
- It showed sufficient agreement with the properties of light water
- It also showed good agreement with ENDF/B-VII.1 and ENDF/B-VIII.β3
- It has been validated against independent DDCS and ICSBEP benchmarks

Future work

- Other temperatures for light water: recent discussion about deficiencies at high temperatures
- Other models of light water
- Other materials
- Covariance generation and propagation
- ENDF format for $S(\alpha, \beta)$ covariance and uncertainties

S(a,b) Acknowledgments

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