A Novel Methodology for Generating Thermal Scattering Cross Sections and Uncertainties

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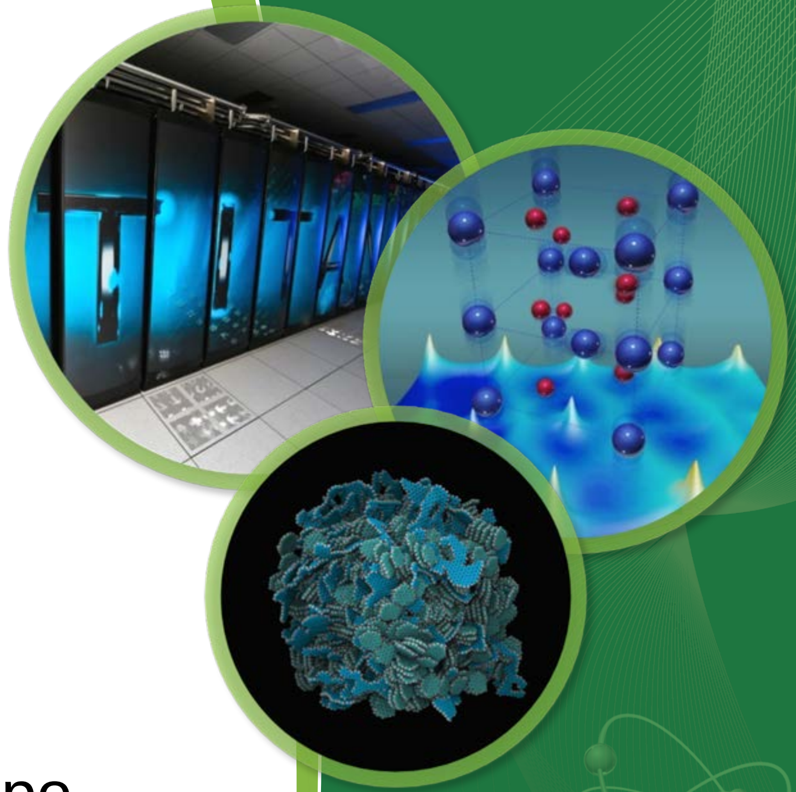

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Introduction

- Motivation
- Framework overview
- Framework specifics
- Results
- Conclusions

Framework motivation

- Thermal reactor systems are sensitive to thermal scattering
- New experimental double differential cross section (DDCS) data are becoming available
- There are no uncertainty or covariance data for thermal scattering materials
- Framework motivation is applicable for any method of generating double differential thermal scattering data

Framework overview

- The objective is to combine experimental double differential scattering data and model parameters to yield the best estimate of 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 Oak Ridge National Laboratory (ORNL) Spallation Neutron Source (SNS)
  - RPI collaboration
- Validated using benchmarks from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) handbook

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 & Tasaki [4]

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

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

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 specifics: Unified Monte Carlo

- Capable of handling non-linearities which may exist in analyses
  - Ratio data
  - Data with large uncertainties
- Based on Bayes Theorem & Principle of Maximum Entropy
- Prior and likelihood functions are assumed to be multivariate Gaussian functions
- Generates an ensemble of quantities used to calculate cross section and covariance values

Framework specifics: UMC-B

- UMC-B was chosen for this framework
- Simulations are assigned a weight that is used to calculate mean and covariance values

$$\omega_k = \exp\left\{-\frac{1}{2}\left[(\boldsymbol{y_k} - \boldsymbol{y_E})^T \cdot \boldsymbol{V_E}^{-1} \cdot (\boldsymbol{y_k} - \boldsymbol{y_E})\right]\right\}$$

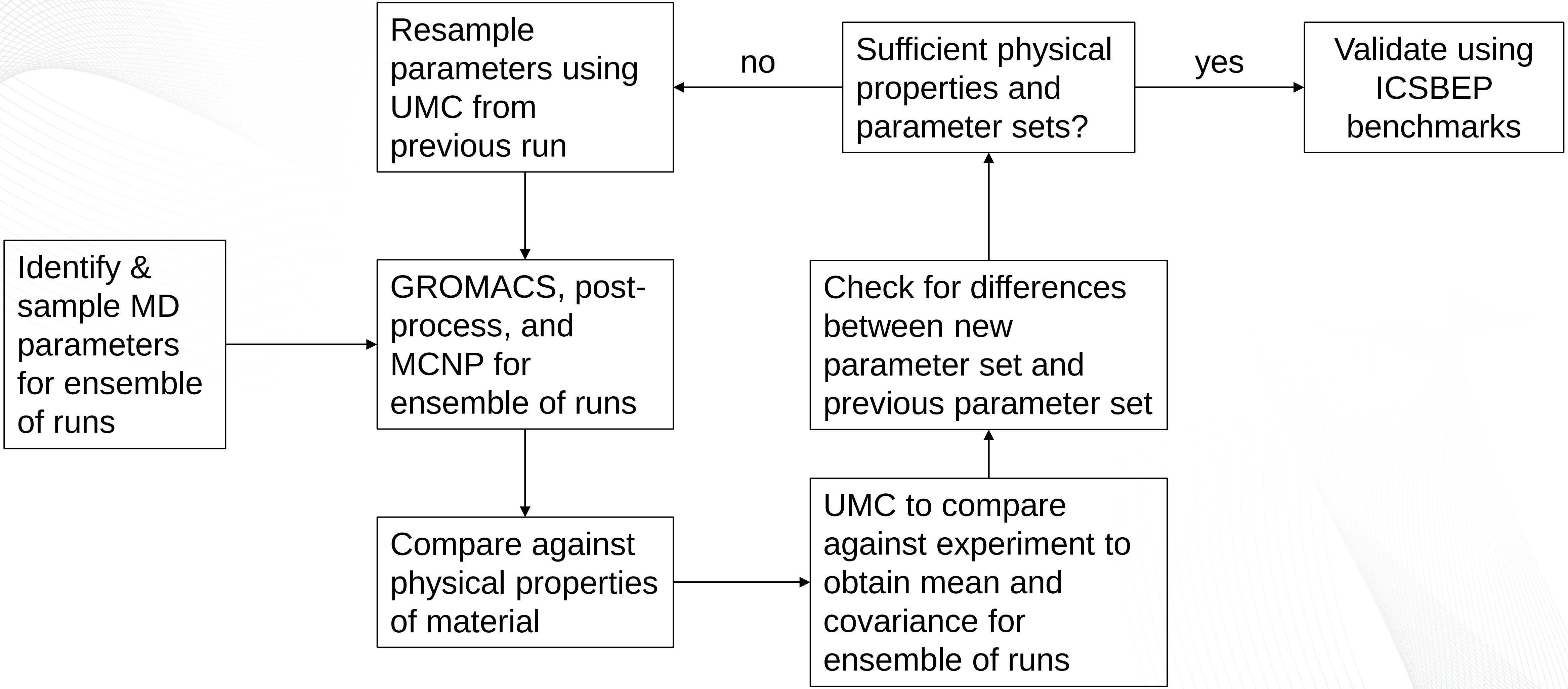
$$\langle x_i \rangle = \lim_{K\to\infty} \frac{\sum_{k=1}^{K} x_{ik}\omega_k}{\sum_{k=1}^{K} \omega_k}$$

$$\langle \boldsymbol{V} \rangle_{i,j} = \lim_{K\to\infty} \frac{\sum_{k=1}^{K} x_{ik}x_{jk}\omega_k}{\sum_{k=1}^{K} \omega_k} - \langle x_i \rangle \langle x_j \rangle$$

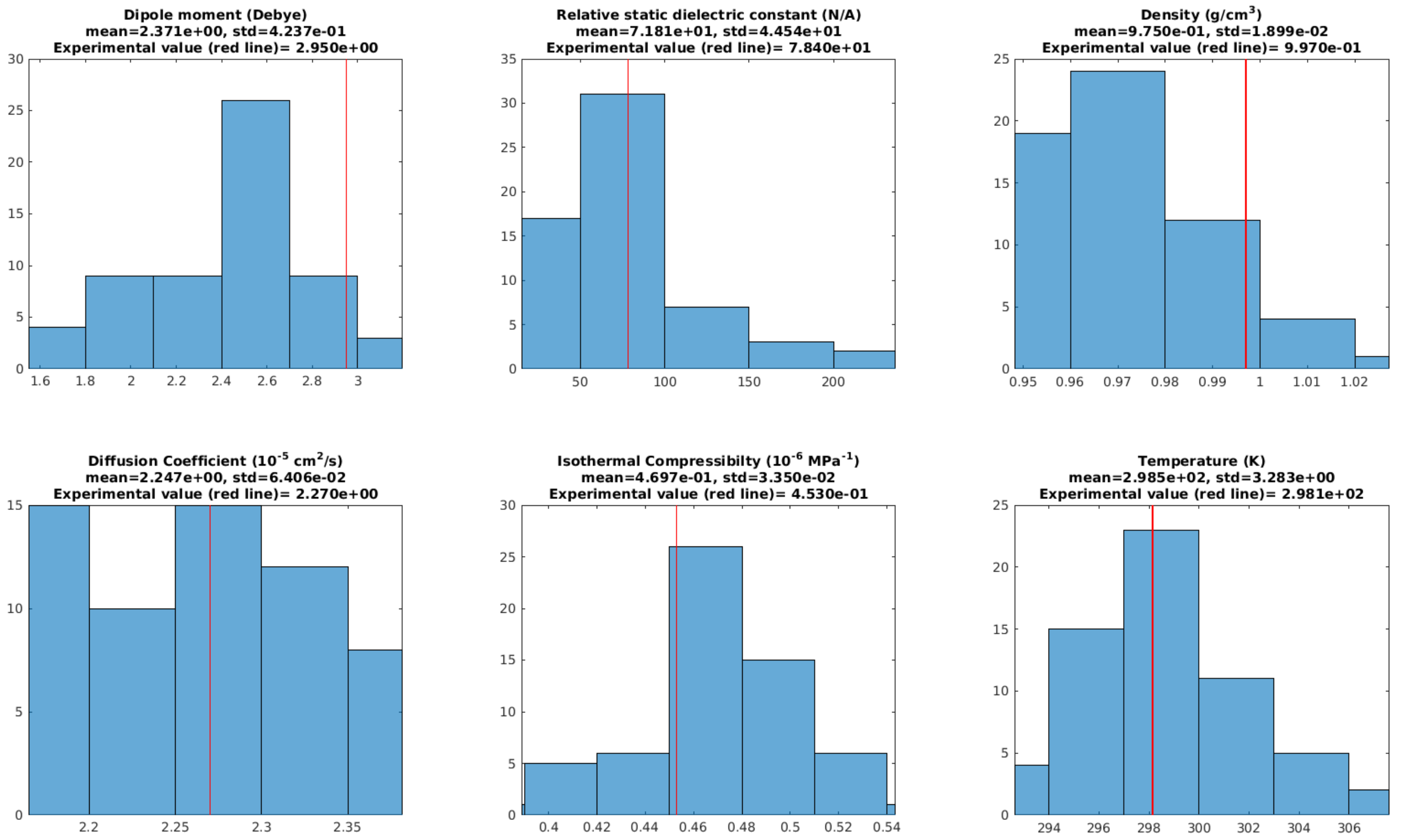
Framework specifics: validation

- Simulations are validated against the physical properties of water
- Cross sections are validated two ways
  - Against independent cross sections [5]
    - Double differential in scattering energy and angle
    - Single differential in scattering angle
    - Total scattering
  - Against experimental benchmark problems sensitive to hydrogen
    - From ICSBEP Handbook
    - Compared against benchmarks run with ENDF/B-VII.1 and ENDF/B-VIII.β3 data

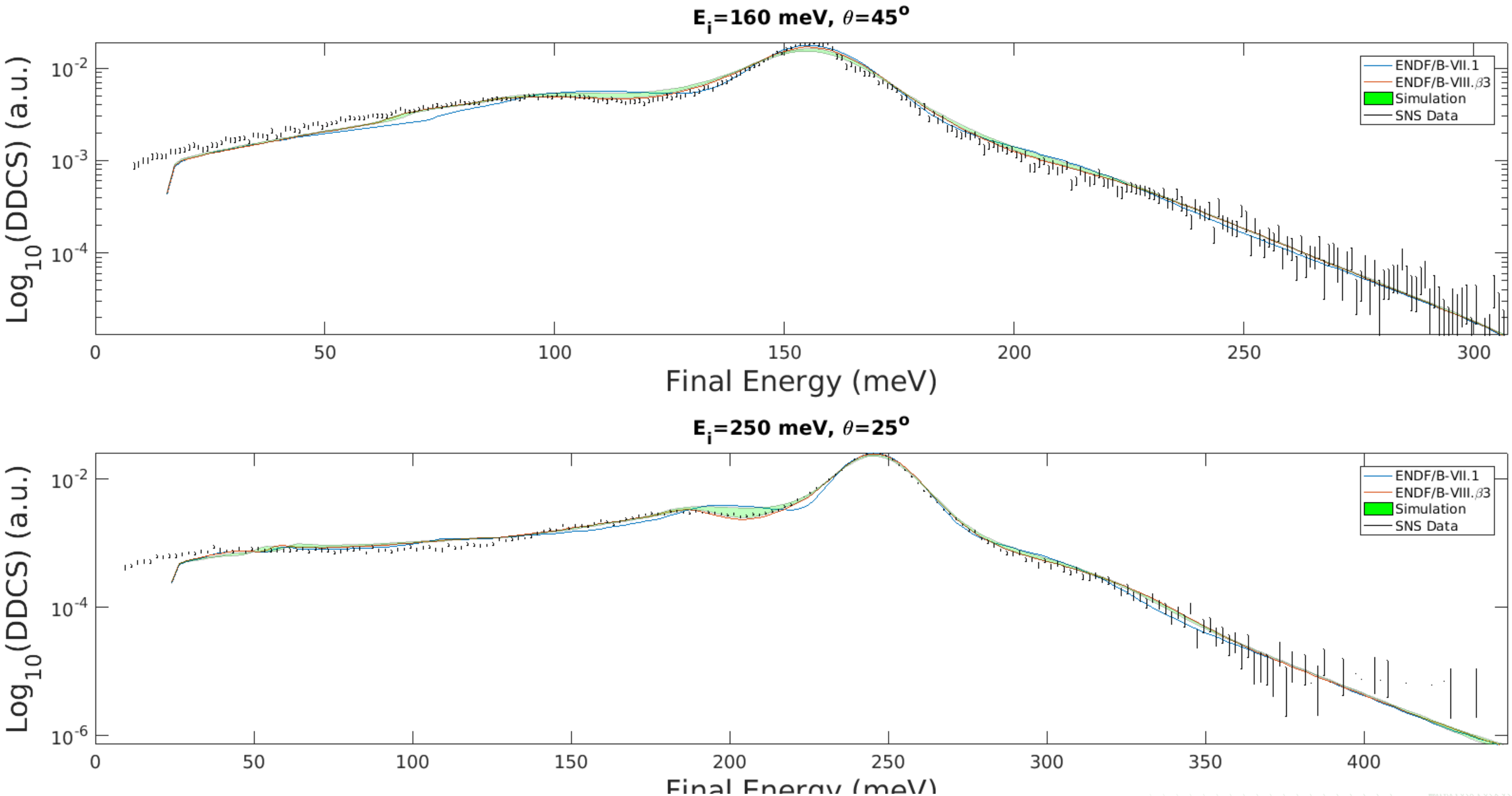
Framework outline



Results: properties of water



Results: DDCS – SNS



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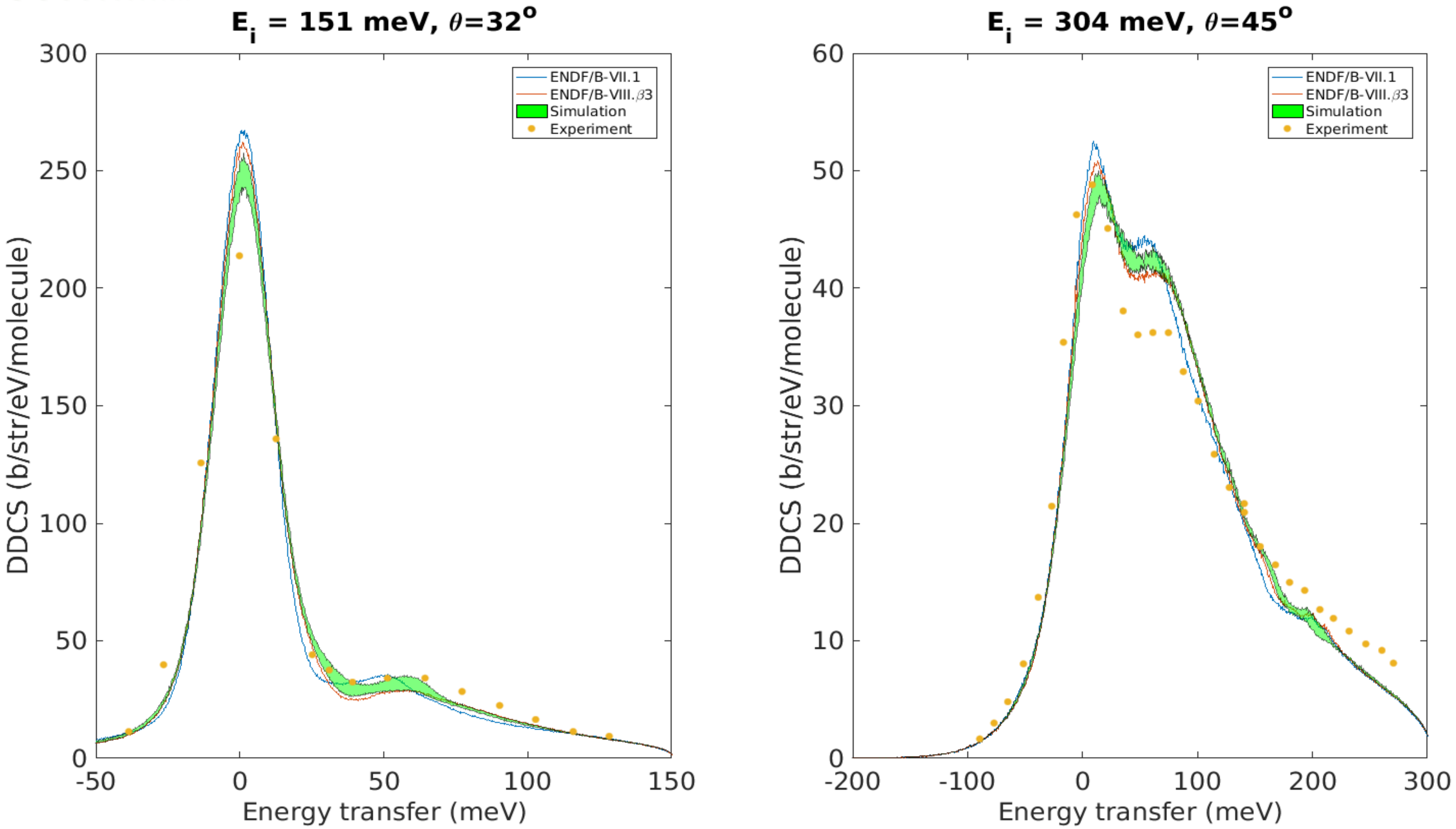
Results: DDCS – independent



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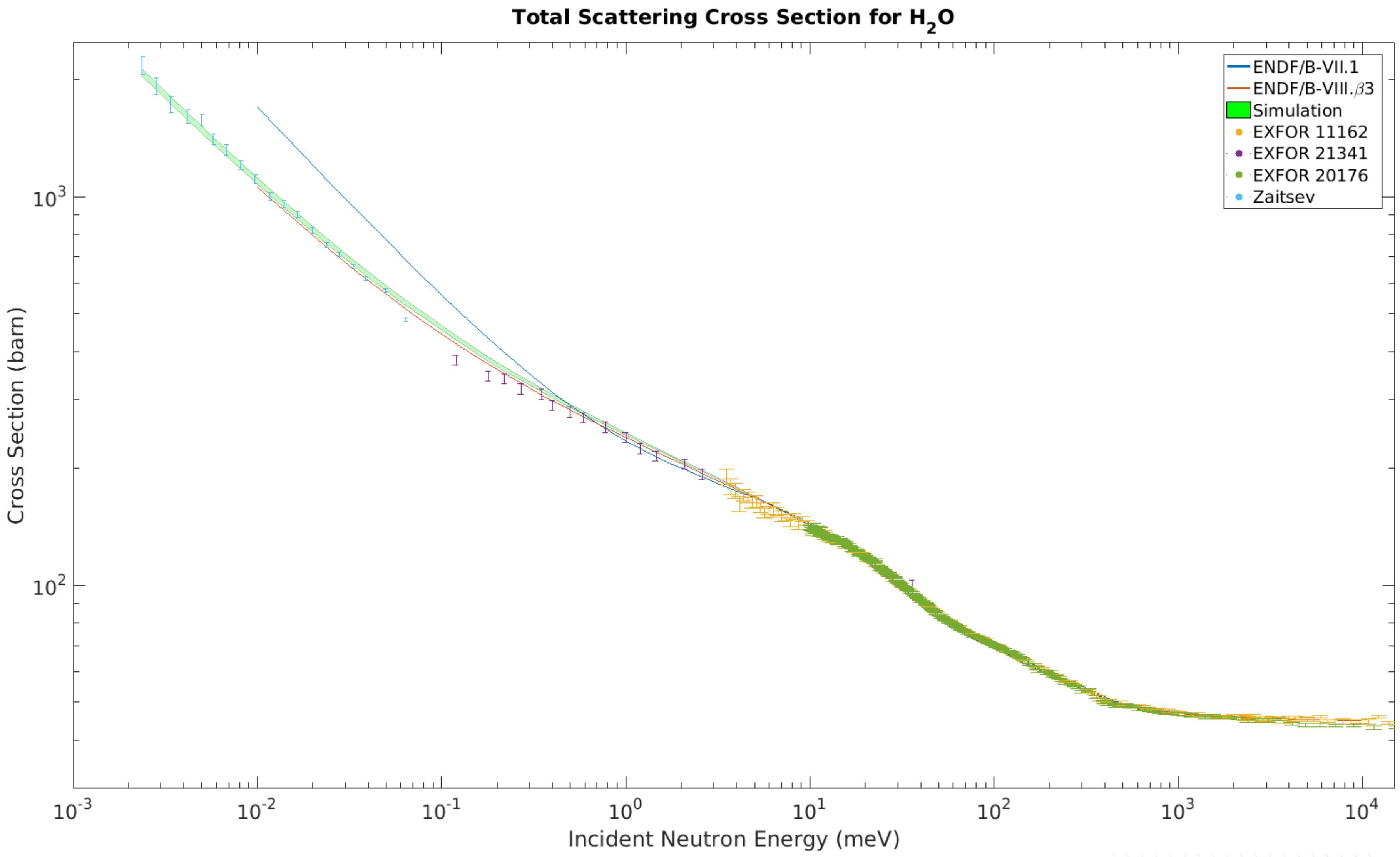
Results: total cross section

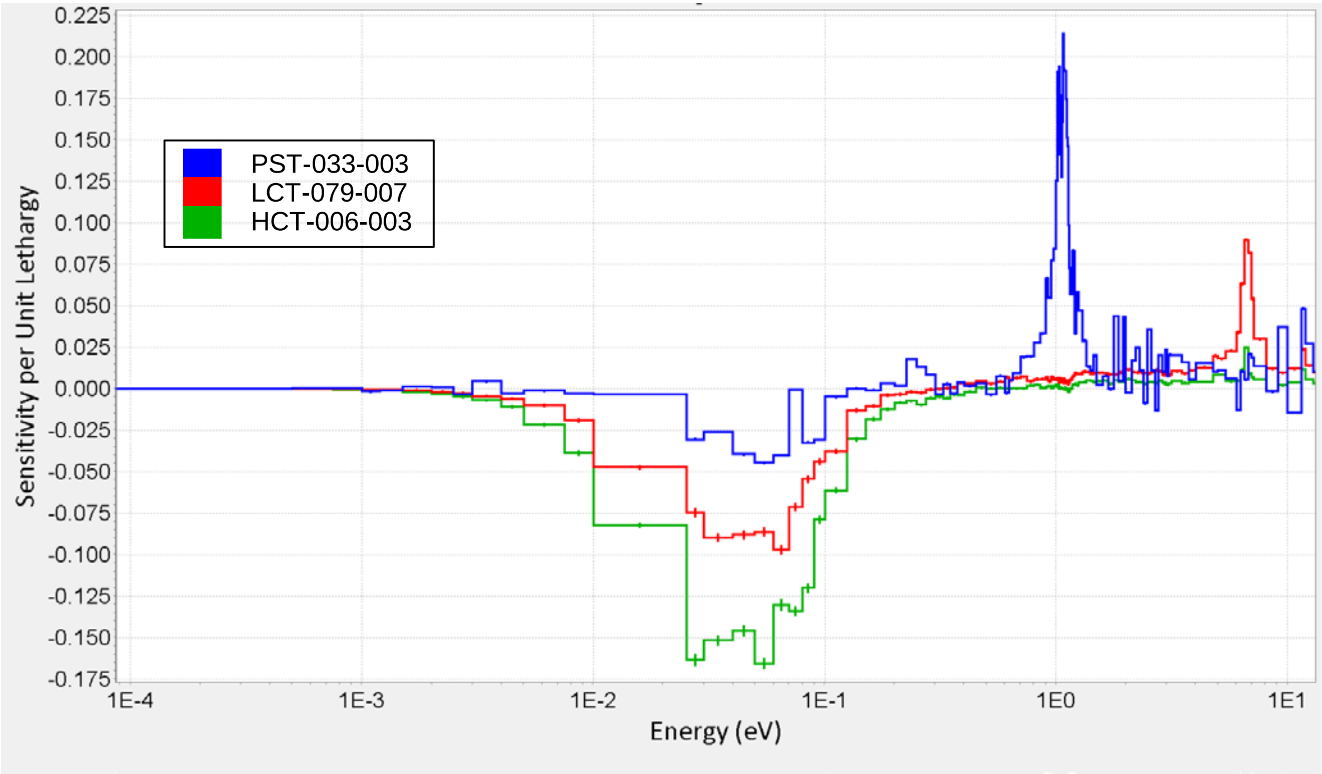


Results: ICSBEP benchmarks

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

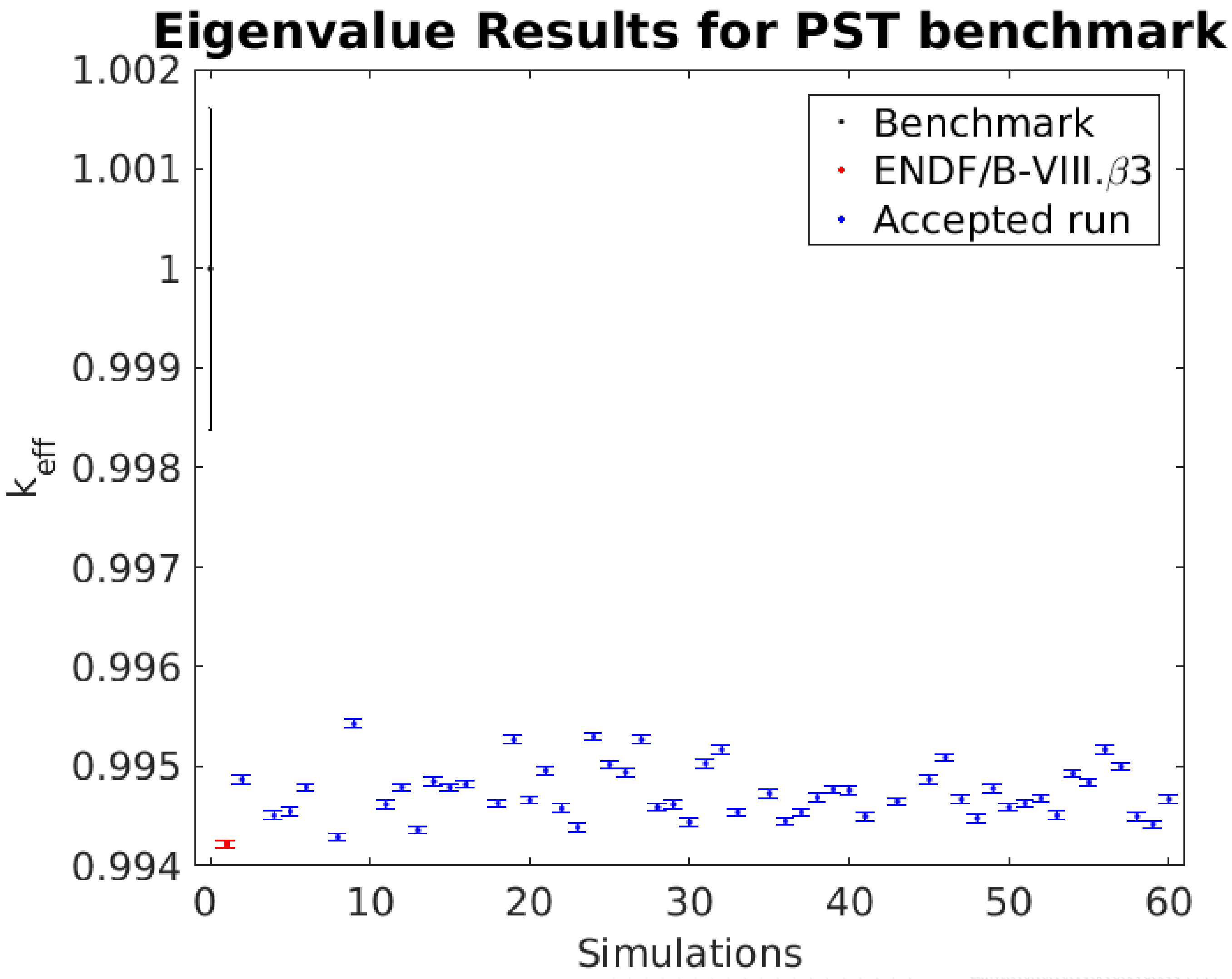
Sensitivity plot



Results: PST-033-003

ENDF Library	K_{eff}	St.Dev (pcm)	Δ K_{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

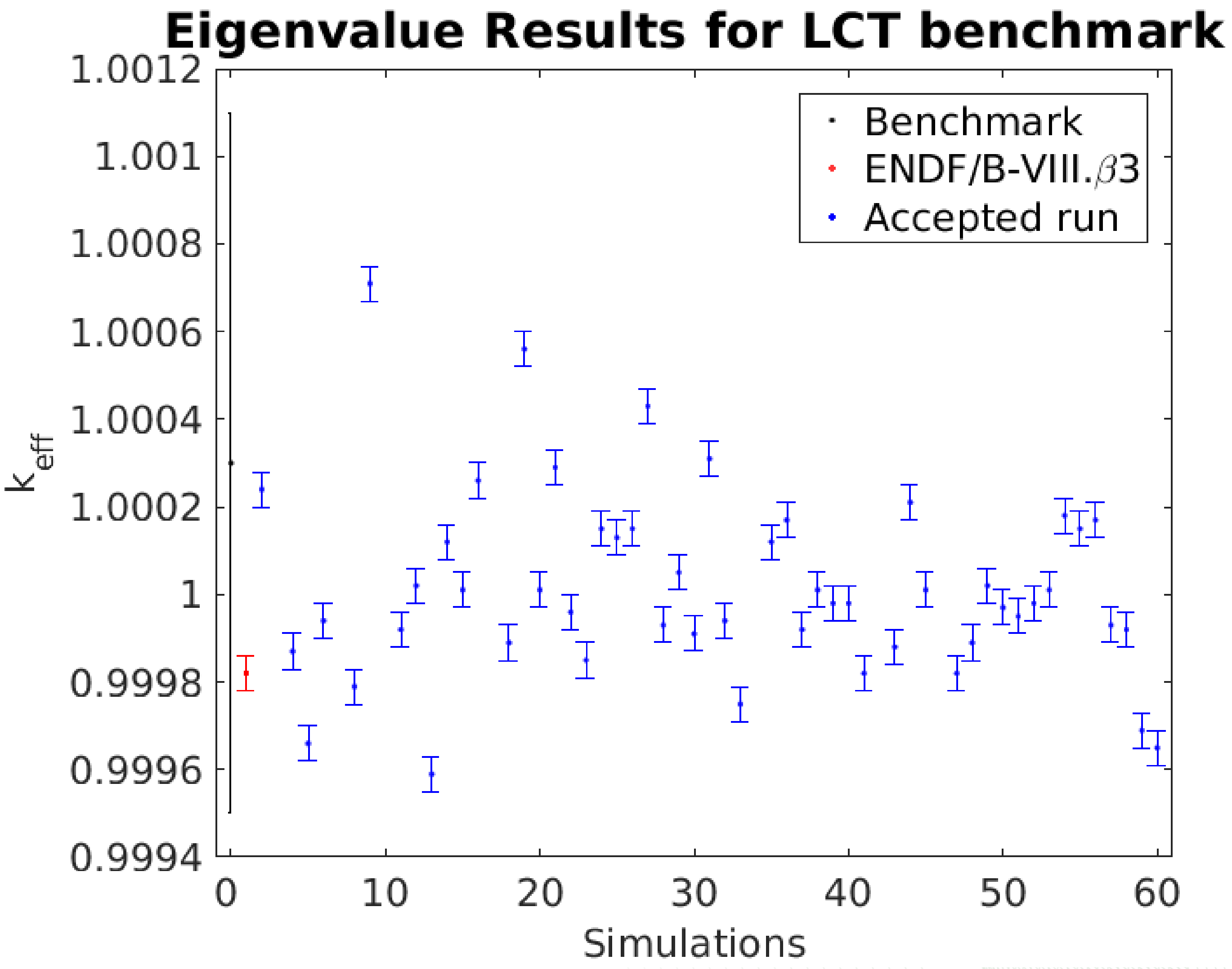
- Noticeable improvement
- Issues may be caused by materials other than light water



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

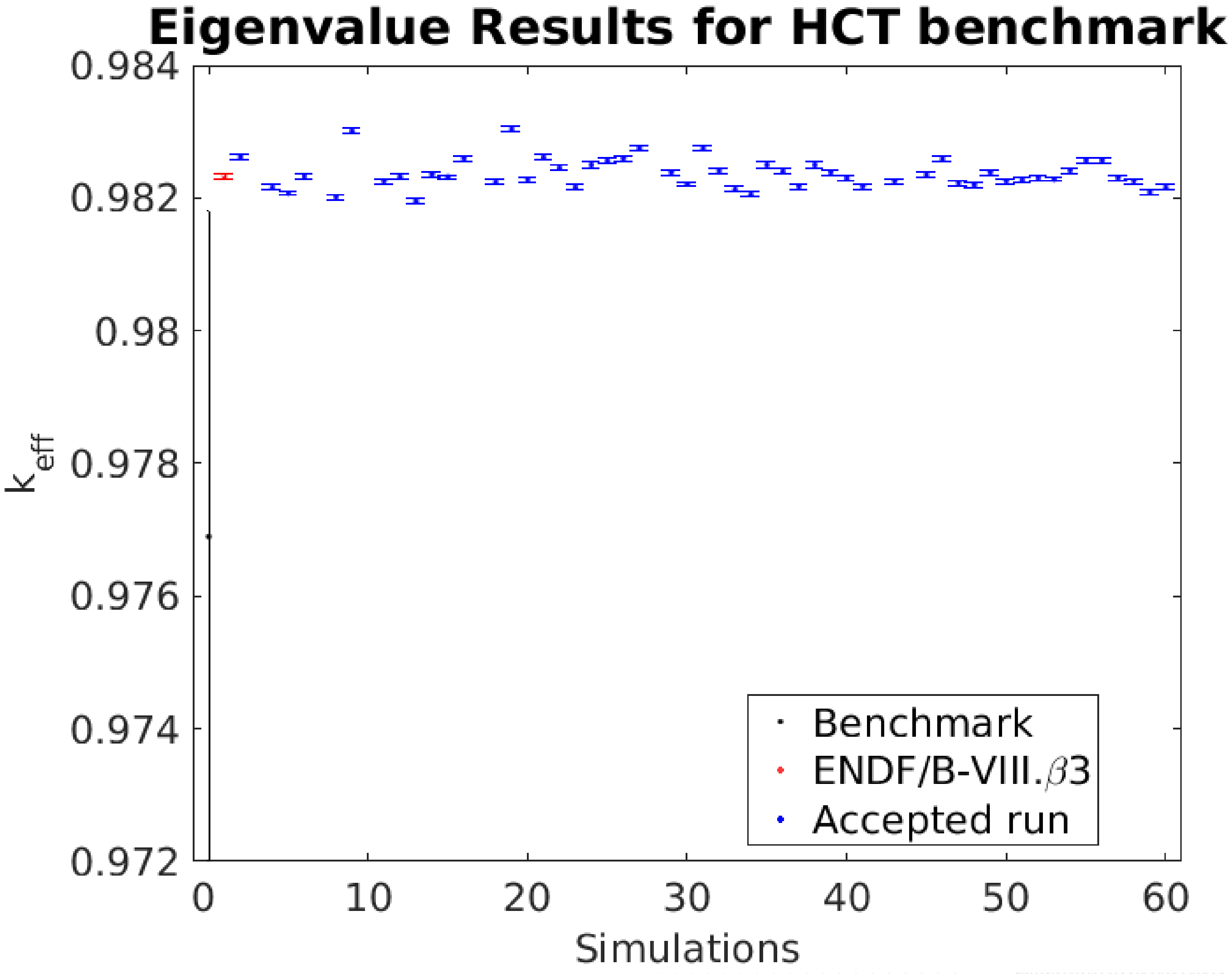
- Inconclusive improvement
- Results within error bounds of experimental uncertainty



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 is 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

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- NERSC

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- [2] M. Gonzalez and J. Agascal, "A flexible model for water based on TIP4P/2005," *The Journal of Chemical Physics,* vol. 135, 2011.
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