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# On-The-Fly Sampling for Inelastic Incoherent Thermal Neutron Scattering for Monte Carlo Codes

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# Team Members and Collaborators

- RPI Team Members
  - Camden Blake (PhD Student)
  - Wei Ji (PI)
  - Yaron Danon (Co-PI)
- Collaborators
  - Forrest Brown (retired) – LANL
  - Robert Little - LANL

# Acknowledgment

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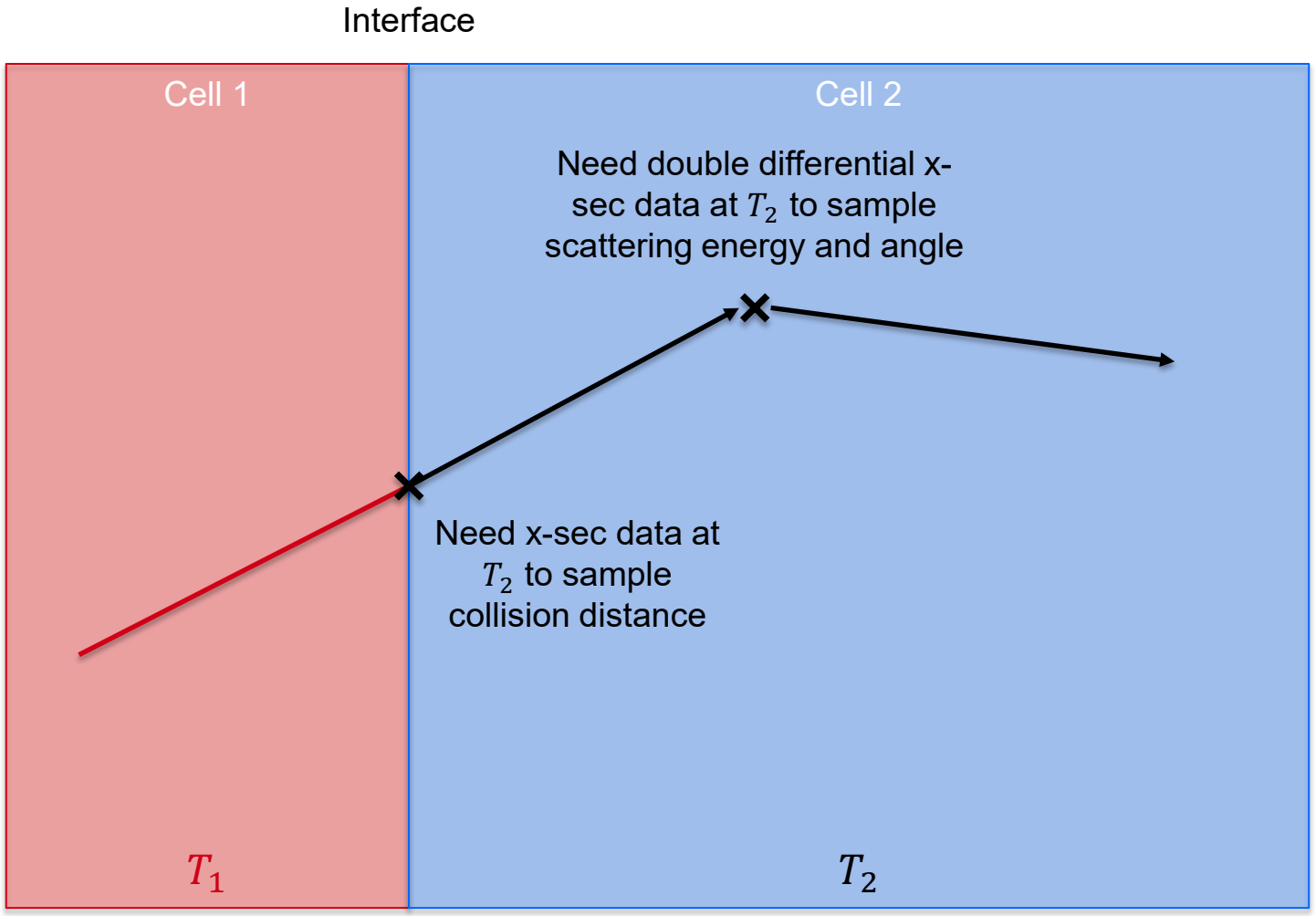
# Project Motivation




## $S(\alpha,\beta)$ scattering law dominates thermal neutron scattering

$$\sigma(E \to E', \mu, T) = \frac{\sigma_b}{2kT}\sqrt{\frac{E'}{E}}e^{\left(-\frac{\beta}{2}\right)}S(\alpha,\beta,T)$$

$\alpha$: momentum transfer $\beta$: energy transfer

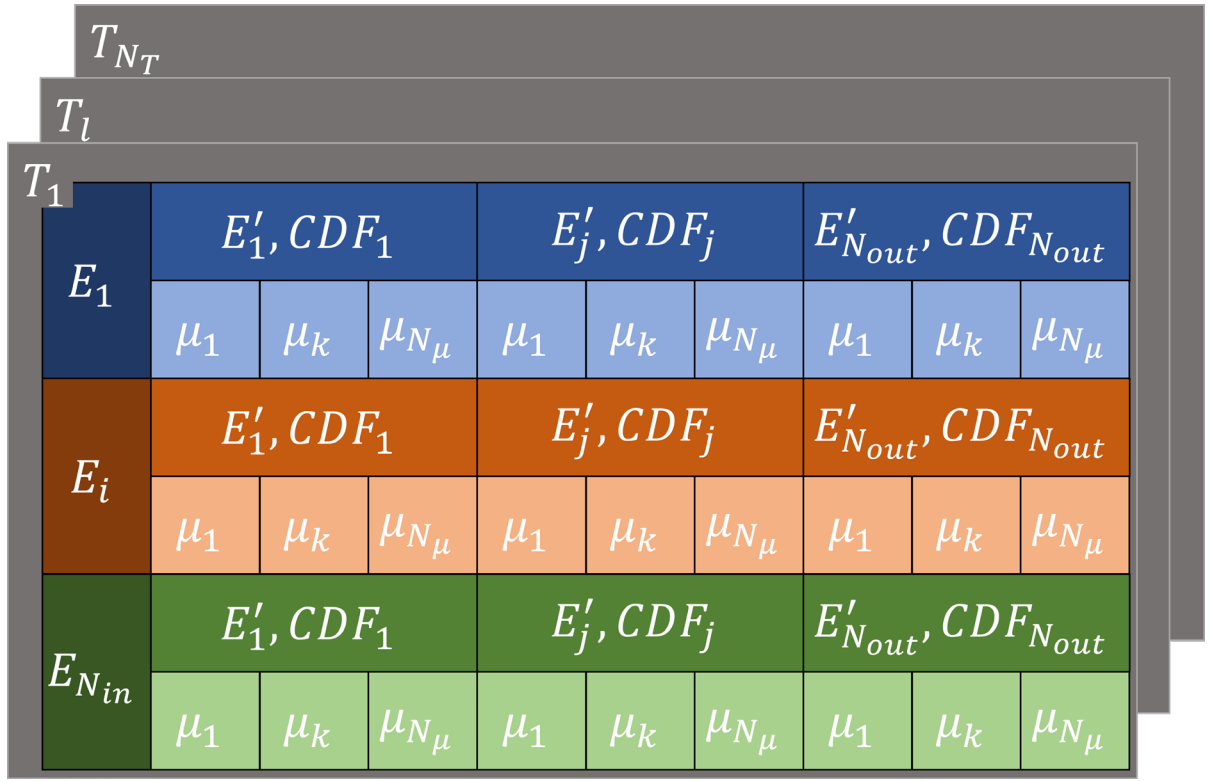
$$\alpha = \frac{E + E' - 2\mu\sqrt{EE'}}{A_0 kT} \qquad \beta = \frac{E' - E}{kT}$$

# Project Motivation

- Current thermal libraries store inelastic incoherent scattering distributions as functions of incident energy, outgoing energy, scattering angle, and temperature $(E, E', \mu, T)$.
- Makes MCNP ACE thermal library very large
- Unwieldy for HPC simulations

# Project Motivation

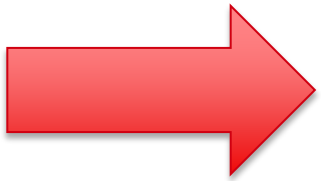
| Material | Temperature Range [K] | # Files | Total Size [MB] |
|---|---|---|---|
| be-beo | 293.6 - 1200 | 8 | 339.34 |
| o-beo | 293.6 - 1200 | 8 | 280.24 |
| grph | 296 - 2000 | 10 | 393.99 |
| grph10 | 296 - 2000 | 10 | 328.88 |
| grph30 | 296 - 2000 | 10 | 312.08 |
| h-h2o | 283.6 - 800 | 18 | 536.1 |




- ACE Files(ENDF80SaB2): 33 Materials for a total of 9.41 GB

# Project Objective

- Create a method to generate a small thermal library
- Adaptive in temperature
- Retains sampling accuracy
- Minimizes computational burden



**Single file for a material**

**Works for any temperature**

**Only 20-30 MB**

# Approach to Produce the OTF Library

1. Evaluate the Thermal Scattering Law (TSL) for the material of interest → $S(\alpha, \beta, T)$.
2. Calculate sampling probability distributions (PDFs and CDFs) over the applicable temperature range.
3. Apply a regression model to remove the temperature dependence from the data.

# Approach – Step 1

- Obtain input leapr data from ENDF/B-VIII.0
- Contains:
  - Material specific model parameters
  - Phonon spectrum
  - Alpha and Beta calculation grids
  - Temperature range for the material

# Approach – Step 1

- Use leapr to generate ‘high fidelity’ $S(\alpha, \beta, T)$ data
  - Investigating to see if the default alpha and beta grids are enough to linearize sampling distributions
  - A fine temperature grid is chosen, typically using 5K increments

# Approach – Step 2

- Creation of the sampling distributions needed for sampling.

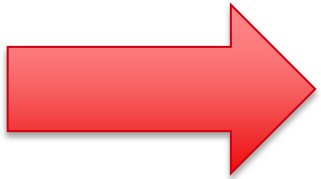
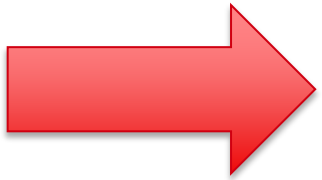
PDFs

$$g(\beta|E,T) = \frac{exp\left(-\frac{\beta}{2}\right)\int_{\alpha_-}^{\alpha_+} S(\alpha,\beta,T)d\alpha}{\int_{\beta_-}^{\beta_+}\int_{\alpha_-}^{\alpha_+} exp\left(-\frac{\beta}{2}\right) S(\alpha,\beta,T)d\alpha d\beta} \qquad \hat{h}(\alpha|\beta,T) = \frac{S(\alpha,\beta,T)}{\int_0^{\infty} S(\alpha,\beta,T)d\alpha}$$

CDFs

$$G(\beta|E,T) = \int_{\beta_-}^{\beta} g(\beta'|E,T)d\beta' \qquad \hat{H}(\alpha|\beta,T) = \int_0^{\alpha} \hat{h}(\alpha|\beta,T)d\alpha'$$

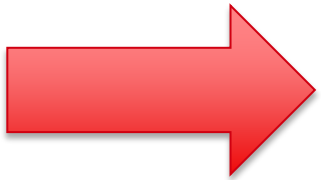
# Approach – Step 3

- CDF sampling distributions are fixed to set CDF values and repeated for every temperature.
- $E_i, \beta_j \rightarrow CDF_{i,j}$  $\mathrm{E_i}, CDF_j \rightarrow \beta_{i,j}$
- $\beta_i, \alpha_j \rightarrow CDF_{i,j}$  $\beta_i, CDF_j \rightarrow \alpha_{i,j}$
- Polynomial regression is then performed on the $\beta_{i,j}$ and $\alpha_{i,j}$ as functions of temperature.

# Approach – Step 3

- This yields a set of coefficients that can be used to recover the alpha and beta value at any temperature OTF.

| $T_m$ | $\beta_1$ | $\beta_j$ | $\beta_J$ |
|---|---|---|---|
| $E_1$ | $CDF_{m,1,1}$ | $CDF_{m,1,j}$ | $CDF_{m,1,J}$ |
| $E_i$ | $CDF_{m,i,1}$ | $CDF_{m,i,j}$ | $CDF_{m,i,J}$ |
| $E_I$ | $CDF_{m,I,1}$ | $CDF_{m,I,j}$ | $CDF_{m,I,J}$ |



| | $CDF_1$ | $CDF_j$ | $CDF_J$ |
|---|---|---|---|
| $E_1$ | $B(T)_{1,1}$ | $B(T)_{1,j}$ | $B(T)_{1,J}$ |
| $E_i$ | $B(T)_{i,1}$ | $B(T)_{i,j}$ | $B(T)_{i,J}$ |
| $E_I$ | $B(T)_{I,1}$ | $B(T)_{I,j}$ | $B(T)_{I,J}$ |

# Approach - Result

- Single file for each material
- Small size
- Used for any temperature
- Maintains accuracy
- Not computationally expensive*

| | $CDF_1$ | | $CDF_j$ | | $CDF_{N_P}$ | |
|---|---|---|---|---|---|---|
| $E_1$ | $B_1$ | $B_{N_C}$ | $B_1$ | $B_{N_C}$ | $B_1$ | $B_{N_C}$ |
| $E_i$ | $B_1$ | $B_{N_C}$ | $B_1$ | $B_{N_C}$ | $B_1$ | $B_{N_C}$ |
| $E_{N_{in}}$ | $B_1$ | $B_{N_C}$ | $B_1$ | $B_{N_C}$ | $B_1$ | $B_{N_C}$ |

$$\beta = \sum_{l}^{N_C} B_l * X_\beta(T)$$

| | $CDF_1$ | | $CDF_j$ | | $CDF_{N_P}$ | |
|---|---|---|---|---|---|---|
| $\beta_1$ | $A_1$ | $A_{N_C}$ | $A_1$ | $A_{N_C}$ | $A_1$ | $A_{N_C}$ |
| $\beta_i$ | $A_1$ | $A_{N_C}$ | $A_1$ | $A_{N_C}$ | $A_1$ | $A_{N_C}$ |
| $\beta_{N_F}$ | $A_1$ | $A_{N_C}$ | $A_1$ | $A_{N_C}$ | $A_1$ | $A_{N_C}$ |

$$\alpha = \sum_{l}^{N_C} A_l * X_\alpha(T)$$

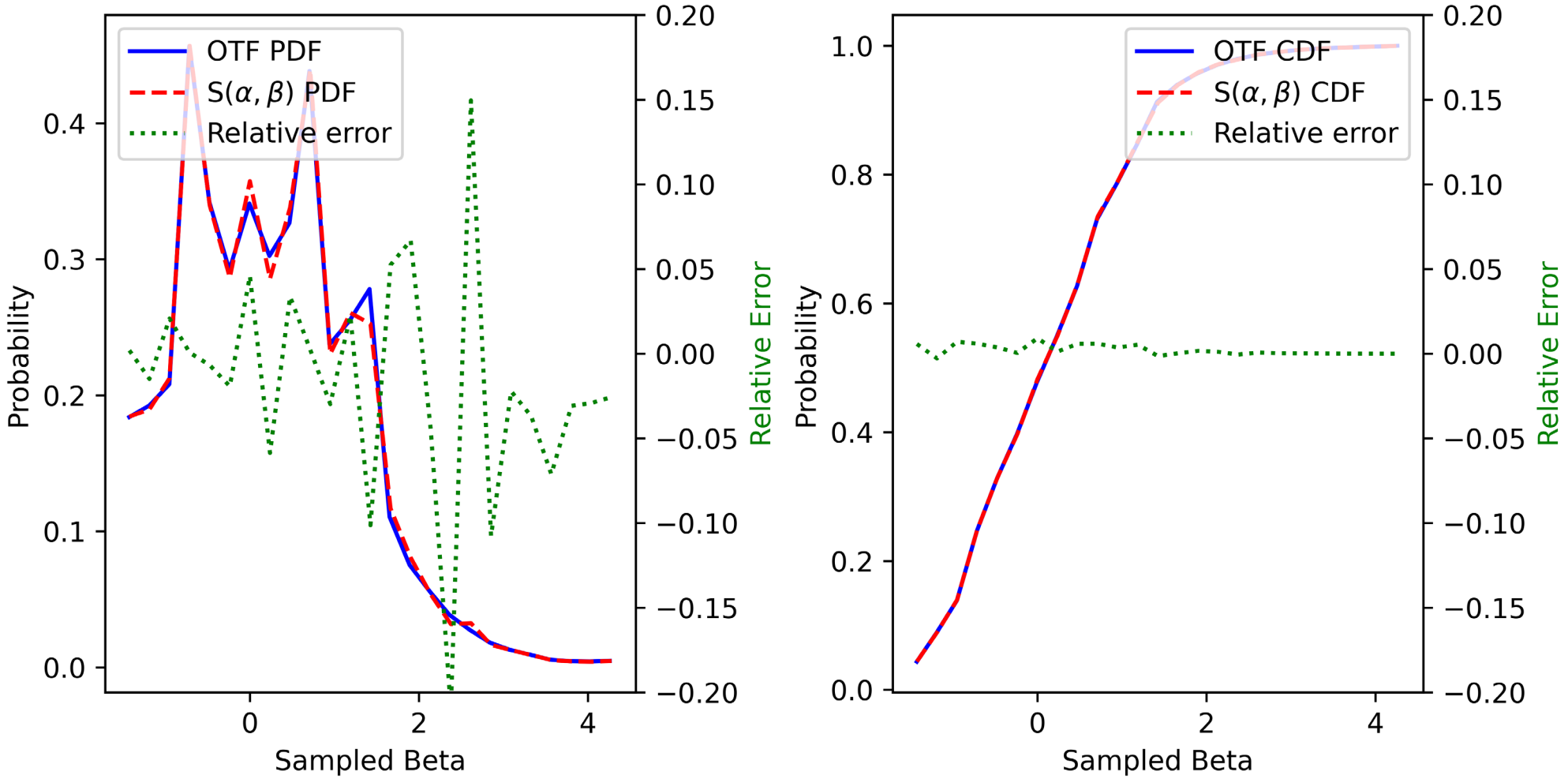
# Results

- Currently have 24 materials being treated in this manner
- 9 materials are not being treated
  - Materials with only one temperature:
    - L-CH4, S-CH4, and HinC5O2H8
  - Materials with problems in leapr input
    - Ortho/Para H and D, SiO2-alpha, and SiO2-beta

# Results – Small Size

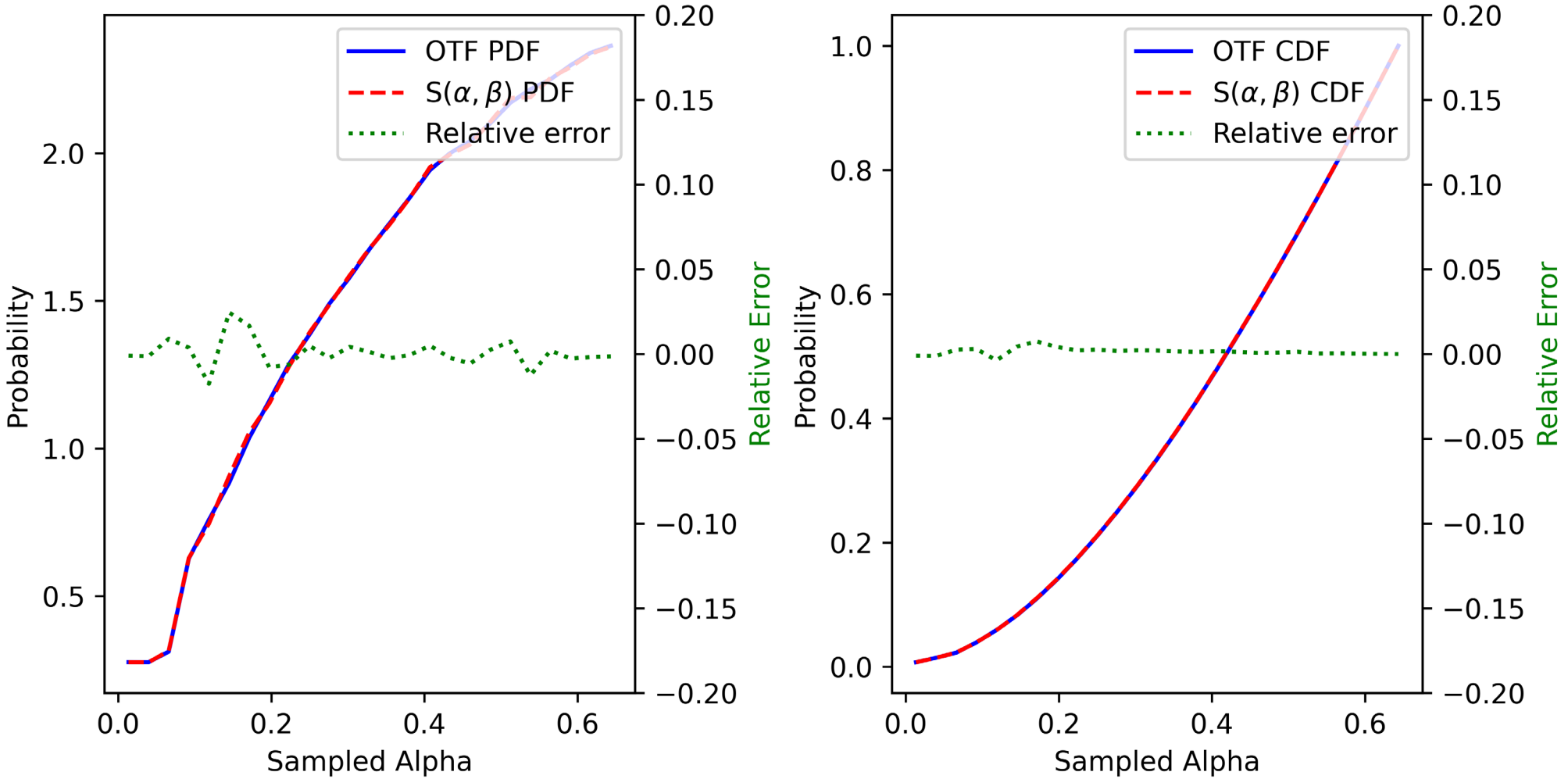
| Material | OTF Storage [MB] | Material | OTF Storage [MB] |
|---|---|---|---|
| 013-Al-027 | 5.5 | HinIcelh | 17.6 |
| 026-Fe-056 | 5.7 | OinIcelh | 12.6 |
| crystalline-graphite | 12.7 | OinD2O | 12.6 |
| reactor-graphite-10P | 12.7 | DinD2O | 12.6 |
| reactor-graphite-30P | 12.7 | OinUO2 | 7.1 |
| Be-metal | 7.1 | UinUO2 | 7.1 |
| OinBeO | 9.9 | NinUN | 12.7 |
| BeinBeO | 9.9 | UinUN | 12.7 |
| HinH2O | 10.4 | HinYH2 | 12.7 |
| HinCH2 | 12.7 | YinYH2 | 7.6 |
| CinSiC | 9.9 | HinZrH | 7.1 |
| SiinSiC | 9.9 | ZrinZrH | 4.8 |

# Results – Maintains Accuracy



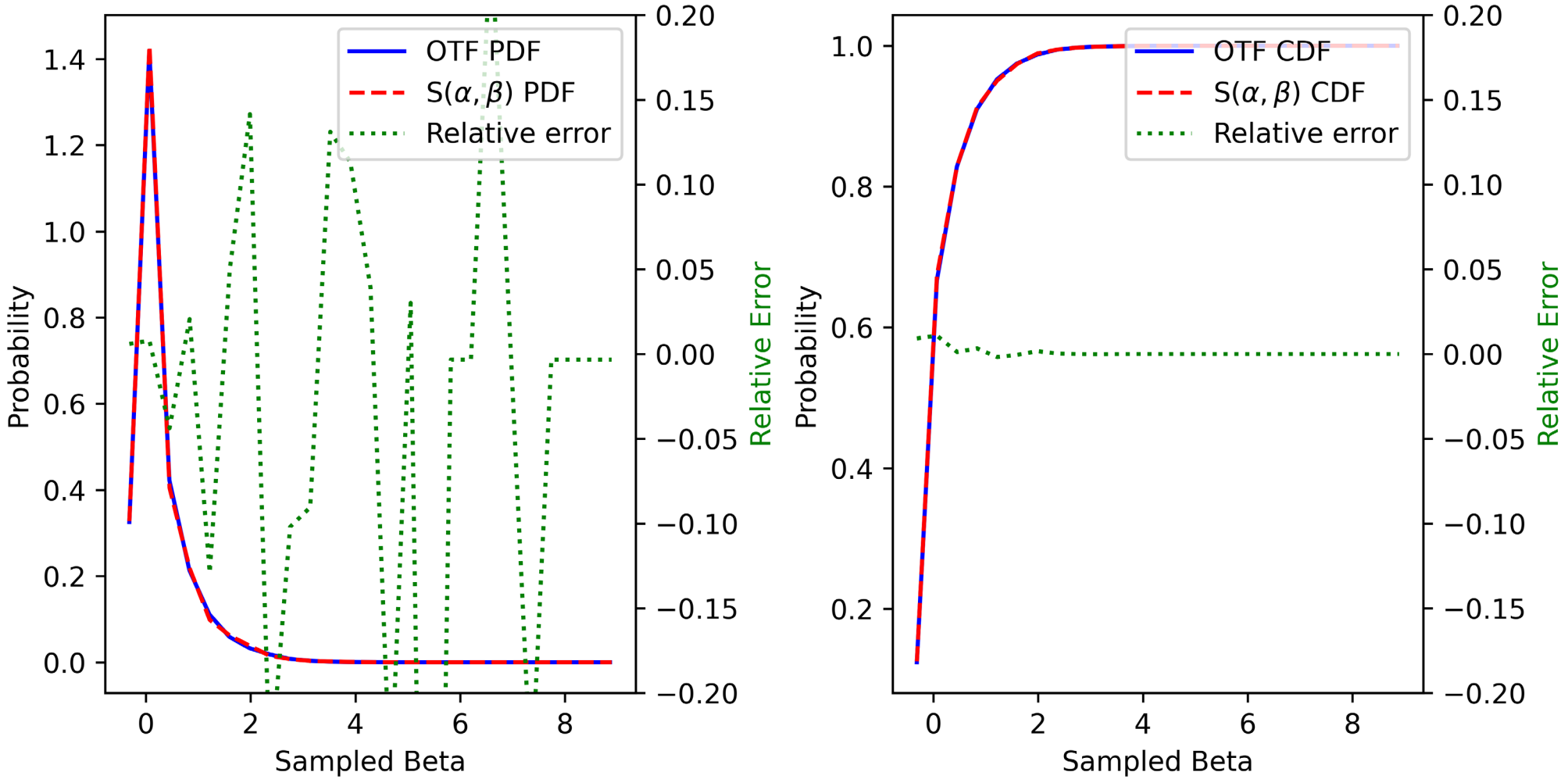

**Sampled $\beta$ PDF and CDF distributions and associated errors for Be in BeO at 751K and with an incident energy of 0.1 eV.**

# Results – Maintains Accuracy



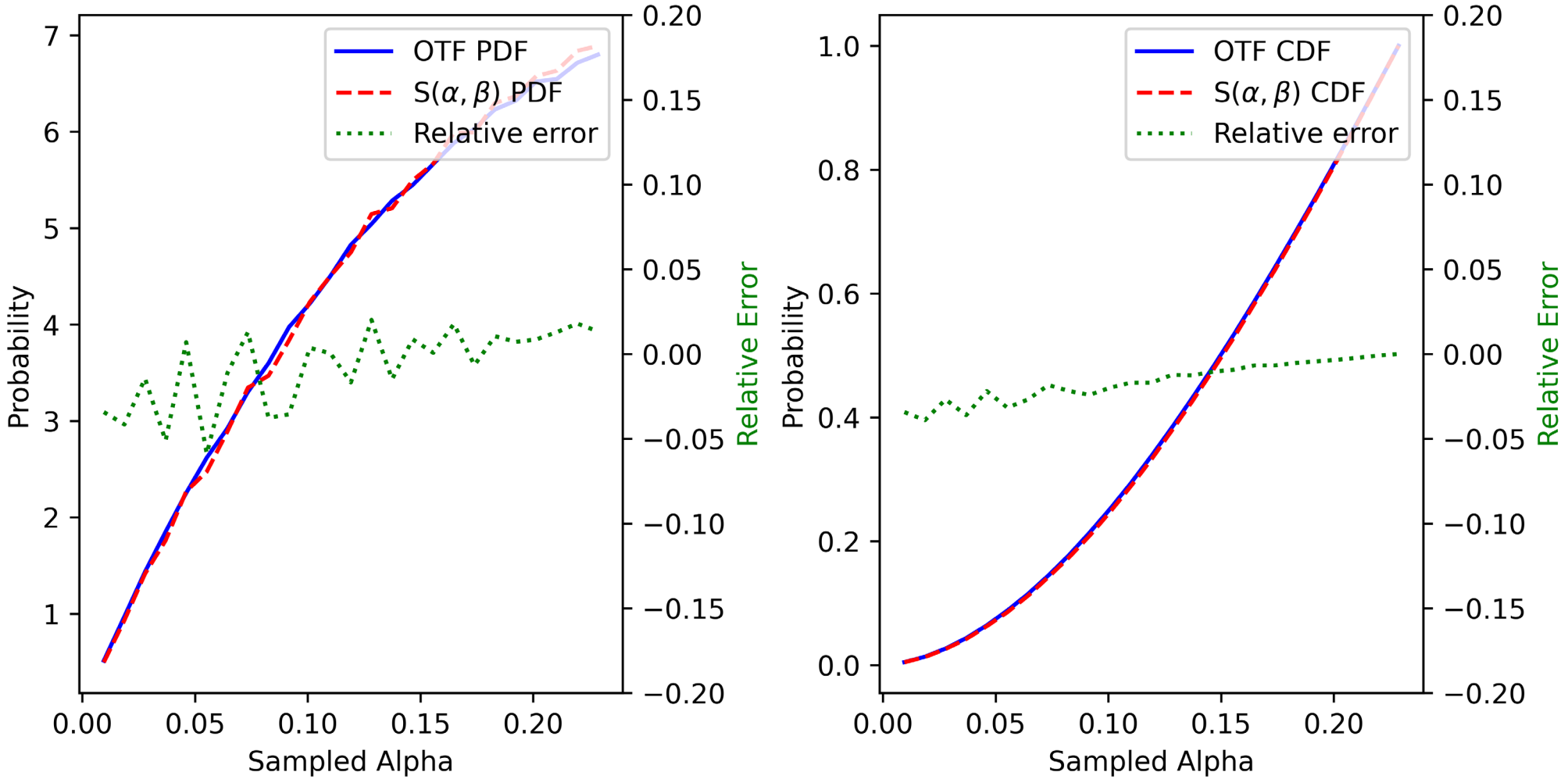

**Sampled $\alpha$ PDF and CDF distributions and associated errors for Be in BeO at 751K and with an incident energy of 0.1 eV and scattering energy of 0.09 eV.**

# Results – Maintains Accuracy




**Sampled $\beta$ PDF and CDF distributions and associated errors for graphite at 1146K and with an incident energy of 0.05 eV.**

# Results – Maintains Accuracy




**Sampled $\alpha$ PDF and CDF distributions and associated errors for graphite at 1146K and with an incident energy of 0.05 eV and scattering energy of 0.09 eV.**

# Results – Sampling Times

| Material | $S(\alpha,\beta)$ [s] | OTF [s] | Ratio | Material | $S(\alpha,\beta)$ [s] | OTF [s] | Ratio |
|---|---|---|---|---|---|---|---|
| **013-Al-027** | 0.119 | 0.446 | 3.758 | **HinIcelh** | 0.127 | 0.305 | 2.403 |
| **026-Fe-056** | 0.114 | 0.362 | 3.168 | **OinIcelh** | 0.120 | 0.420 | 3.484 |
| **graphite** | 0.127 | 0.533 | 4.182 | **OinD2O** | 0.126 | 0.471 | 3.730 |
| **graphite-10P** | 0.125 | 0.472 | 3.766 | **DinD2O** | 0.131 | 0.334 | 2.555 |
| **graphite-30P** | 0.135 | 0.590 | 4.382 | **OinUO2** | 0.126 | 0.479 | 3.805 |
| **Be-metal** | 0.124 | 0.485 | 3.898 | **UinUO2** | 0.126 | 0.561 | 4.608 |
| **OinBeO** | 0.127 | 0.499 | 3.930 | **NinUN** | 0.120 | 0.486 | 4.067 |
| **BeinBeO** | 0.124 | 0.485 | 3.917 | **UinUN** | 0.122 | 0.475 | 4.065 |
| **HinH2O** | 0.132 | 0.488 | 3.704 | **HinYH2** | 0.151 | 0.525 | 3.485 |
| **HinCH2** | 0.127 | 0.462 | 3.649 | **YinYH2** | 0.117 | 0.494 | 4.239 |
| **CinSiC** | 0.123 | 0.492 | 3.988 | **HinZrH** | 0.125 | 0.370 | 2.968 |
| **SiinSiC** | 0.120 | 0.530 | 4.397 | **ZrinZrH** | 0.116 | 0.468 | 4.016 |

## Current and Future

- OTF sampling treatment has been applied to 24 materials in the ENDF/B-VIII.0 library.
- A Fortran based sampling paradigm has been developed
- Updating to ENDF/B-VIII.1 when released
- Implementation into MCNP
- Linearization optimization of the OTF treatment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