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Adaptive-in-temperature method for fast on-the-fly sampling of thermal neutron scattering data in MCNP6

Wei Ji
Nuclear Engineering Program
Rensselaer Polytechnic Institute (RPI)

2022 Annual Nuclear Criticality Safety Program
Technical Program Review
February 15, 2022

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Team Members and Collaborators

- RPI Team Members
  - Wei Ji (PI, Professor, jiw2@rpi.edu)
  - Yaron Danon (Co-PI, Professor)
  - Camden Blake (PhD student)

- Collaborators
  - Forrest Brown (retired) – Los Alamos National Laboratory
  - Robert Little – Los Alamos National Laboratory

Acknowledgement

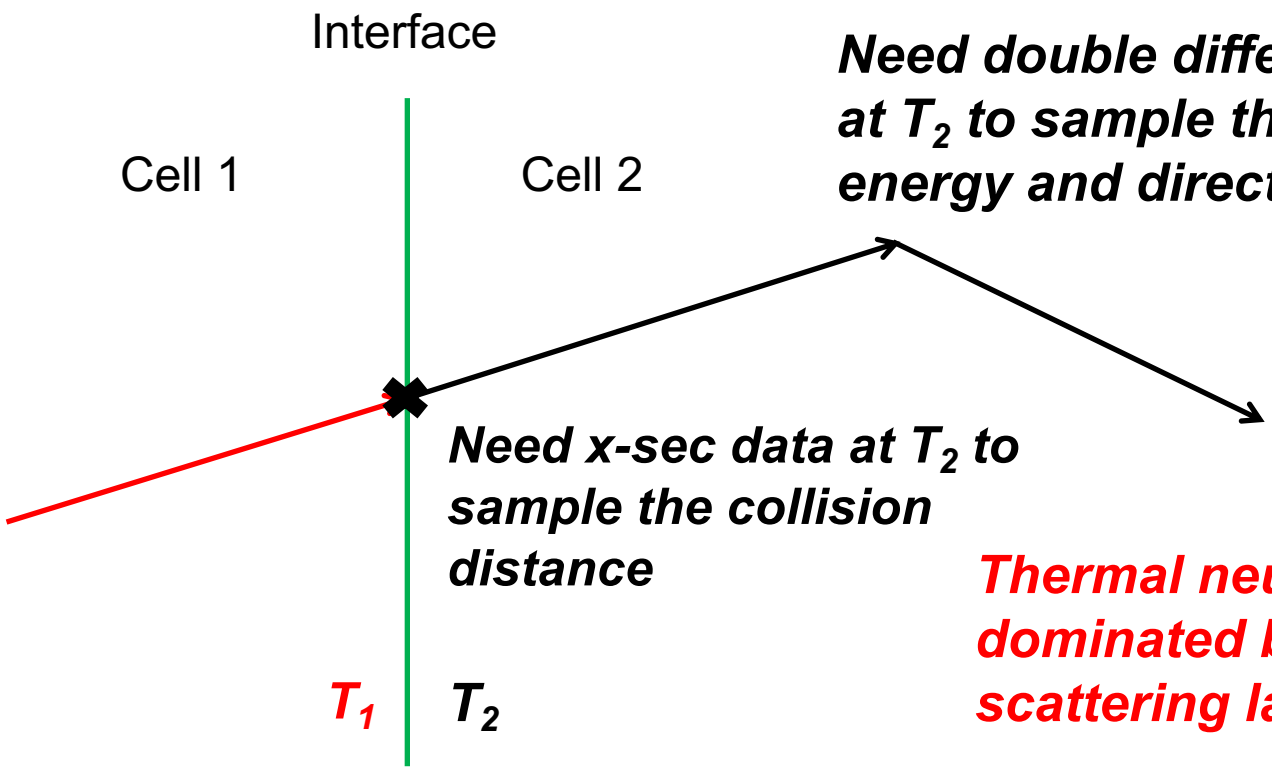
This work was supported by the Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the Department of Energy.

Project Objective and Motivation

- Develop thermal data libraries for selected isotopes in MCNP6 to support on-the-fly S(alpha, beta) sampling for temperature ranges applicable to nuclear criticality safety

Enhance the physics treatment in MCNP6 so that it can perform fast on-the-fly sampling of S(alpha, beta) data at arbitrary temperature

A General Random Walk Sampling in MCNP



Need double differential x-sec at T_2 to sample the outgoing energy and direction

Need x-sec data at T_2 to sample the collision distance

Thermal neutron scattering dominated by S(alpha, beta) scattering law

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

α: momentum transfer β: energy transfer

Current Data Storage Format for MCNP6

- NJOY is used to create correlated energy-angle distributions for inelastic scattering.
- These consist of two parts.
  - A set of equally probable final energy bins for each incident energy.
  - A set of equally probable cosine bins for each incoming and outgoing energy pair.
- This is done for each temperature.

Current Data Storage Format for MCNP6

T_1	CDF_1	...	CDF_n	...	CDF_N
E_1	$E'_{1,1}$		$E'_{1,n}$		$E'_{1,N}$
...					
E_m	$E'_{m,1}$		$E'_{m,n}$		$E'_{m,N}$
...					
E_M	$E'_{M,1}$		$E'_{M,n}$		$E'_{M,N}$

T_1	E'_1	...	E'_n	...	E'_N
E_1	$\mu'_{CDF,1,1}$		$\mu'_{CDF,1,n}$		$\mu'_{CDF,1,N}$
...					
E_i	$\mu'_{CDF,m,1}$		$\mu'_{CDF,m,n}$		$\mu'_{CDF,m,N}$
...					
E_M	$\mu'_{CDF,M,1}$		$\mu'_{CDF,M,n}$		$\mu'_{CDF,M,N}$

T_1		CDF_1	...	CDF_k	...	CDF_K
(E_1, E'_1)	$\mu'_{CDF,1,1}$	$\mu'_{1,1,1}$		$\mu'_{1,1,k}$		$\mu'_{1,1,K}$
...	...					
(E_m, E'_n)	$\mu'_{CDF,m,n}$	$\mu'_{m,n,1}$		$\mu'_{m,n,k}$		$\mu'_{m,n,K}$
...	...					
(E_M, E'_N)	$\mu'_{CDF,M,N}$	$\mu'_{M,N,1}$		$\mu'_{M,N,k}$		$\mu'_{M,N,K}$

Current Sampling Procedure in MCNP6

1. Determination of target's temperature (T).
2. Find data sets at nearest temperatures ($T_i<T<T_{i+1}$).
3. Sample outgoing energy based on T_i and T_{i+1} data sets, and then do interpolation to obtain outgoing energy at T.
4. Similar procedure to obtain outgoing angle at T.

T_i	CDF_1	...	CDF_n	CDF_{n+1}	...	CDF_N
E_1	$E'_{1,1}$		$E'_{1,n}$	$E'_{1,n+1}$		$E'_{1,N}$
:						
E_m	$E'_{m,1}$		$E'_{m,n}$	$E'_{m,n+1}$		$E'_{m,N}$
E_{m+1}	$E'_{m+1,1}$		$E'_{m+1,n}$	$E'_{m+1,n+1}$		$E'_{m+1,N}$
:						
E_M	$E'_{M,1}$		$E'_{M,n}$	$E'_{M,n+1}$		$E'_{M,N}$

T_{i+1}	CDF_1	...	CDF_n	CDF_{n+1}	...	CDF_N
E_1	$E'_{1,1}$		$E'_{1,n}$	$E'_{1,n+1}$		$E'_{1,N}$
:						
E_m	$E'_{m,1}$		$E'_{m,n}$	$E'_{m,n+1}$		$E'_{m,N}$
E_{m+1}	$E'_{m+1,1}$		$E'_{m+1,n}$	$E'_{m+1,n+1}$		$E'_{m+1,N}$
:						
E_M	$E'_{M,1}$		$E'_{M,n}$	$E'_{M,n+1}$		$E'_{M,N}$

Data Storage Requirements by MCNP6

- To be able to **sample** thermal scattering, MCNP stores all the thermal data directly.
- This leads to a large amount of data that is needed.
  - For example, in the thermal energy range: 24 MB per temperature for graphite or H in water
  - For a realistic reactor, 50-100 temperatures are needed

Material	File Size (MB)
Al	25
Be (Metal)	28
H in Benzene	69.5
Be in BeO	69.5
Fe	28.9
Graphite	24.2
D in D_2O	30
H in ZrH	116.3
H in H_2O	24.9
O_2 in UO_2	75.1
O in BeO	57.5
H in Polyethylene	19.6
Si in SiO_2	41.6
U in UO_2	50.5
Zr in ZrH	56.1

How to Decrease Data Storage for MCNP6?

- Any better way to improve the storage requirement (and associated sampling procedures)?

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

β: energy transfer

α: momentum transfer

$$E \rightarrow E', \text{ then } \left(E, E'\right) \rightarrow \mu$$

$$E \rightarrow \beta, \text{ then } \qquad \beta \rightarrow \alpha$$

Data Storage & Sampling Methods in MC21

- Sample momentum (α) and energy (β) transfer directly.
  - α and β can then be converted into E′ and μ

$$E' = E + \beta kT \qquad \mu = \frac{2E + kT(\beta - A\alpha)}{2\sqrt{E(E + \beta kT)}}$$

- MC21 implements this strategy.

Data Storage & Sampling Methods in MC21

- Coupled α and β distributions are created.
  - A table of incident energies versus CDF values that contain β values.
  - A table of α versus β mesh values that contain function values, which serve as a memory reduction technique where the function values are used to create α CDFs on-the-fly.
- This is done for each temperature.

Data Storage in MC21

T_1	CDF_1	…	CDF_j	…	CDF_N
E_1	$\beta_{1,1}$		$\beta_{1,n}$		$\beta_{1,N}$
…					
E_m	$\beta_{m,1}$		$\beta_{m,n}$		$\beta_{m,N}$
…					
E_M	$\beta_{M,1}$		$\beta_{M,n}$		$\beta_{M,N}$

T_1	β_1	…	β_N
α_1	$F(\alpha_1,\beta_1)$		$F(\alpha_1,\beta_N)$
…			
α_m	$F(\alpha_m,\beta_1)$		$F(\alpha_m,\beta_N)$
…			
α_M	$F(\alpha_M,\beta_1)$		$F(\alpha_M,\beta_N)$

$$F(\alpha_m,\beta_n) = \int_0^{\alpha_m} S(\alpha',\beta_n)e^{\beta_n/2}d\alpha'$$

$$\alpha_{max} = \frac{\sqrt{E}+\sqrt{E-\beta kT}}{AkT}$$

$$\alpha_{CDF}(\alpha|\beta_n,E) = \frac{F(\alpha,\beta_n)-F(\alpha_{min},\beta_n)}{F(\alpha_{max},\beta_n)-F(\alpha_{min},\beta_n)}$$

$$\alpha_{min} = \frac{\sqrt{E}-\sqrt{E-\beta kT}}{AkT}$$

C. T. Ballinger, "The Direct S(alpha, beta) Method for Thermal Neutron Scattering," Knolls Atomic Power Laboratory, Schenectady, NY, 1994.
T. M. Sutton, et al., "The MC21 Monte Carlo Transport Code (LM-06K144)," (M&C + SNA 2007), LaGrange Park, IL, 2007.

Sampling Procedure in MC21

1. Determination of target's temperature (T).
2. Find data sets at nearest temperatures ($T_i<T<T_{i+1}$).
3. Sample β based on T_i and T_{i+1} data sets, and then do interpolation to obtain β at T.
4. Similar procedure to obtain α at T.
5. Convert α and β to outgoing energy and scattering angle at T.

T_i	CDF_1	...	CDF_n	CDF_{n+1}	...	CDF_N
E_1	$\beta_{1,1}$		$\beta_{1,n}$	$\beta_{1,n+1}$		$\beta_{1,N}$
:						
E_m	$\beta_{m,1}$		$\beta_{m,n}$	$\beta_{m,n+1}$		$\beta_{m,N}$
E_{m+1}	$\beta_{m+1,1}$		$\beta_{m+1,n}$	$\beta_{m+1,n+1}$		$\beta_{m+1,N}$
:						
E_M	$\beta_{M,1}$		$\beta_{M,n}$	$\beta_{M,n+1}$		$\beta_{M,N}$

T_{i+1}	CDF_1	...	CDF_n	CDF_{n+1}	...	CDF_N
E_1	$\beta_{1,1}$		$\beta_{1,n}$	$\beta_{1,n+1}$		$\beta_{1,N}$
:						
E_m	$\beta_{m,1}$		$\beta_{m,n}$	$\beta_{m,n+1}$		$\beta_{m,N}$
E_{m+1}	$\beta_{m+1,1}$		$\beta_{m+1,n}$	$\beta_{m+1,n+1}$		$\beta_{m+1,N}$
:						
E_M	$\beta_{M,1}$		$\beta_{M,n}$	$\beta_{M,n+1}$		$\beta_{M,N}$

A Little Recap

T_1	CDF_1	...	CDF_n	...	CDF_N
E_1	$E'_{1,1}$		$E'_{1,n}$		$E'_{1,N}$
...					
E_m	$E'_{m,1}$		$E'_{m,n}$		$E'_{m,N}$
...					
E_M	$E'_{M,1}$		$E'_{M,n}$		$E'_{M,N}$

T_1	E'_1	...	E'_n	...	E'_N
E_1	$\mu'_{CDF,1,1}$		$\mu'_{CDF,1,n}$		$\mu'_{CDF,1,N}$
...					
E_i	$\mu'_{CDF,m,1}$		$\mu'_{CDF,m,n}$		$\mu'_{CDF,m,N}$
...					
E_M	$\mu'_{CDF,M,1}$		$\mu'_{CDF,M,n}$		$\mu'_{CDF,M,N}$

T_1		CDF_1	...	CDF_k	...	CDF_K
(E_1, E'_1)	$\mu'_{CDF,1,1}$	$\mu'_{1,1,1}$		$\mu'_{1,1,k}$		$\mu'_{1,1,K}$
...	...					
(E_m, E'_n)	$\mu'_{CDF,m,n}$	$\mu'_{m,n,1}$		$\mu'_{m,n,k}$		$\mu'_{m,n,K}$
...	...					
(E_M, E'_N)	$\mu'_{CDF,M,N}$	$\mu'_{M,N,1}$		$\mu'_{M,N,k}$		$\mu'_{M,N,K}$

T_1	CDF_1	...	CDF_j	...	CDF_N
E_1	$\beta_{1,1}$		$\beta_{1,n}$		$\beta_{1,N}$
...					
E_m	$\beta_{m,1}$		$\beta_{m,n}$		$\beta_{m,N}$
...					
E_M	$\beta_{M,1}$		$\beta_{M,n}$		$\beta_{M,N}$

T_1	β_1	...	β_N
α_1	$F(\alpha_1, \beta_1)$		$F(\alpha_1, \beta_N)$
...			
α_m	$F(\alpha_m, \beta_1)$		$F(\alpha_m, \beta_N)$
...			
α_M	$F(\alpha_M, \beta_1)$		$F(\alpha_M, \beta_N)$

$$F(\alpha_m, \beta_n) = \int_0^{\alpha_m} S(\alpha', \beta_n) e^{\beta_n/2} d\alpha'$$

Current Data Storage Techniques

- Key Points:
  - Both MCNP6 and MC21 interpolate scattering data in order to account for temperature effects.
  - Therein, a large amount of data is needed to ensure accuracy.
- Any further improvement to decrease data storage?
  - We (RPI) have (or had*) a solution!

* [1] A. T. Pavlou and W. Ji, "On-the-Fly Sampling of Temperature-Dependent Thermal Neutron Scattering Data for Monte Carlo Simulations," Annals of Nuclear Energy, 71, 411-426, 2014.
* [2] A. T. Pavlou, "An Adaptive-In-Temperature Method for On-The-Fly Sampling of Thermal Neutron Scattering Data in Continuous-Energy Monte Carlo Codes," Rensselaer Polytechnic Institute, Troy, NY, 2015.

From (E, E′, μ') Space to (α, β) Space

T_1	CDF_1	...	CDF_n	...	CDF_N
E_1	$E'_{1,1}$		$E'_{1,n}$		$E'_{1,N}$
...					
E_m	$E'_{m,1}$		$E'_{m,n}$		$E'_{m,N}$
...					
E_M	$E'_{M,1}$		$E'_{M,n}$		$E'_{M,N}$

T_1	E'_1	...	E'_n	...	E'_N
E_1	$\mu'_{CDF,1,1}$		$\mu'_{CDF,1,n}$		$\mu'_{CDF,1,N}$
...					
E_i	$\mu'_{CDF,m,1}$		$\mu'_{CDF,m,n}$		$\mu'_{CDF,m,N}$
...					
E_M	$\mu'_{CDF,M,1}$		$\mu'_{CDF,M,n}$		$\mu'_{CDF,M,N}$

T_1		CDF_1	...	CDF_k	...	CDF_K
(E_1, E'_1)	$\mu'_{CDF,1,1}$	$\mu'_{1,1,1}$		$\mu'_{1,1,k}$		$\mu'_{1,1,K}$
...	...					
(E_m, E'_n)	$\mu'_{CDF,m,n}$	$\mu'_{m,n,1}$		$\mu'_{m,n,k}$		$\mu'_{m,n,K}$
...	...					
(E_M, E'_N)	$\mu'_{CDF,M,N}$	$\mu'_{M,N,1}$		$\mu'_{M,N,k}$		$\mu'_{M,N,K}$

T_1	CDF_1	...	CDF_j	...	CDF_N
E_1	$\beta_{1,1}$		$\beta_{1,n}$		$\beta_{1,N}$
...					
E_m	$\beta_{m,1}$		$\beta_{m,n}$		$\beta_{m,N}$
...					
E_M	$\beta_{M,1}$		$\beta_{M,n}$		$\beta_{M,N}$

T_1	β_1	...	β_N
α_1	$F(\alpha_1, \beta_1)$		$F(\alpha_1, \beta_N)$
...			
α_m	$F(\alpha_m, \beta_1)$		$F(\alpha_m, \beta_N)$
...			
α_M	$F(\alpha_M, \beta_1)$		$F(\alpha_M, \beta_N)$

$$F(\alpha_m, \beta_n) = \int_0^{\alpha_m} S(\alpha', \beta_n) e^{\beta_n/2} d\alpha'$$

A Better Strategy Than MCNP6 & MC21

T_1	CDF_1	...	CDF_n	...	CDF_N
E_1	$E'_{1,1}$		$E'_{1,n}$		$E'_{1,N}$
...					
E_m	$E'_{m,1}$		$E'_{m,n}$		$E'_{m,N}$
...					
E_M	$E'_{M,1}$		$E'_{M,n}$		$E'_{M,N}$

T_1	E'_1	...	E'_n	...	E'_N
E_1	$\mu'_{CDF,1,1}$		$\mu'_{CDF,1,n}$		$\mu'_{CDF,1,N}$
...					
E_i	$\mu'_{CDF,m,1}$		$\mu'_{CDF,m,n}$		$\mu'_{CDF,m,N}$
...					
E_M	$\mu'_{CDF,M,1}$		$\mu'_{CDF,M,n}$		$\mu'_{CDF,M,N}$

T_1		CDF_1	...	CDF_k	...	CDF_K
(E_1, E'_1)	$\mu'_{CDF,1,1}$	$\mu'_{1,1,1}$		$\mu'_{1,1,k}$		$\mu'_{1,1,K}$
...	...					
(E_m, E'_n)	$\mu'_{CDF,m,n}$	$\mu'_{m,n,1}$		$\mu'_{m,n,k}$		$\mu'_{m,n,K}$
...	...					
(E_M, E'_N)	$\mu'_{CDF,M,N}$	$\mu'_{M,N,1}$		$\mu'_{M,N,k}$		$\mu'_{M,N,K}$

T_1	CDF_1	...	CDF_j	...	CDF_N
E_1	$\beta_{1,1}$		$\beta_{1,n}$		$\beta_{1,N}$
...					
E_m	$\beta_{m,1}$		$\beta_{m,n}$		$\beta_{m,N}$
...					
E_M	$\beta_{M,1}$		$\beta_{M,n}$		$\beta_{M,N}$

T_1	β_1	...	β_N
α_1	$F(\alpha_1, \beta_1)$		$F(\alpha_1, \beta_N)$
...			
α_m	$F(\alpha_m, \beta_1)$		$F(\alpha_m, \beta_N)$
...			
α_M	$F(\alpha_M, \beta_1)$		$F(\alpha_M, \beta_N)$

$$F(\alpha_m, \beta_n) = \int_0^{\alpha_m} S(\alpha', \beta_n) e^{\beta_n/2} d\alpha'$$

	CDF_1	...	CDF_n	...	CDF_N
E_1	$\beta(T)_{1,1}$		$\beta(T)_{1,n}$		$\beta(T)_{1,N}$
:					
E_m	$\beta(T)_{m,1}$		$\beta(T)_{m,n}$		$\beta(T)_{m,N}$
:					
E_M	$\beta(T)_{M,1}$		$\beta(T)_{M,n}$		$\beta(T)_{M,N}$

	CDF_1	...	CDF_N
β_1	$\alpha(T)_{1,1}$		$\alpha(T)_{1,N}$
:			
β_m	$\alpha(T)_{m,1}$		$\alpha(T)_{m,N}$
:			
β_M	$\alpha(T)_{M,1}$		$\alpha(T)_{M,N}$

A Better Strategy Than MCNP6 & MC21

- These $\boldsymbol{\beta}(T)_{m,n}$ and $\boldsymbol{\alpha}(T)_{m,n}$ enable "**on-the-fly**" treatment of temperature-dependence (vs. interpolation between temperatures).

	CDF_1	…	CDF_n	CDF_{n+1}	…	CDF_N
E_1	$\boldsymbol{\beta}(T)_{1,1}$		$\boldsymbol{\beta}(T)_{1,n}$	$\boldsymbol{\beta}(T)_{1,n+1}$		$\boldsymbol{\beta}(T)_{1,N}$
:						
E_m	$\boldsymbol{\beta}(T)_{m,1}$		$\boldsymbol{\beta}(T)_{m,n}$	$\boldsymbol{\beta}(T)_{m,n+1}$		$\boldsymbol{\beta}(T)_{m,N}$
E_{m+1}	$\boldsymbol{\beta}(T)_{m+1,1}$		$\boldsymbol{\beta}(T)_{m+1,n}$	$\boldsymbol{\beta}(T)_{m+1,n+1}$		$\boldsymbol{\beta}(T)_{m+1,N}$
:						
E_M	$\boldsymbol{\beta}(T)_{M,1}$		$\boldsymbol{\beta}(T)_{M,n}$	$\boldsymbol{\beta}(T)_{M,n+1}$		$\boldsymbol{\beta}(T)_{M,N}$

A Better Strategy Than MCNP6 & MC21

	CDF_1	…	CDF_n	…	CDF_N
E_1	$\beta(T)_{1,1}$		$\beta(T)_{1,n}$		$\beta(T)_{1,N}$
:					
E_m	$\beta(T)_{m,1}$		$\beta(T)_{m,n}$		$\beta(T)_{m,N}$
:					
E_M	$\beta(T)_{M,1}$		$\beta(T)_{M,n}$		$\beta(T)_{M,N}$

	CDF_1	…	CDF_N
β_1	$\alpha(T)_{1,1}$		$\alpha(T)_{1,N}$
:			
β_m	$\alpha(T)_{m,1}$		$\alpha(T)_{m,N}$
:			
β_M	$\alpha(T)_{M,1}$		$\alpha(T)_{M,N}$

- How do we define these $\boldsymbol{\beta}(T)_{m,n}$ and $\boldsymbol{\alpha}(T)_{m,n}$?
- This is where new research direction can jump in.
  - Data Analytics Methods?
  - Machine Learning Methods?

On-The-Fly Strategy Data Storage Format

	CDF_1	...	CDF_N
E_1	$[b_{1,1,1} \dots b_{1,1,K}]$		$[b_{1,N,1} \dots b_{1,N,J}]$
...			
E_m	$[b_{m,1,1} \dots b_{m,1,K}]$		$[b_{m,N,1} \dots b_{m,N,K}]$
...			
E_M	$[b_{M,1,1} \dots b_{M,1,K}]$		$[b_{M,N,1} \dots b_{M,N,K}]$

	CDF_1	...	CDF_N
β_1	$[a_{1,1,1} \dots a_{1,1,L}]$		$[a_{1,N,1} \dots a_{1,N,L}]$
...			
β_m	$[a_{m,1,1} \dots a_{m,1,L}]$		$[a_{m,N,1} \dots a_{m,N,L}]$
...			
β_M	$[a_{M,1,1} \dots a_{M,1,L}]$		$[a_{M,N,1} \dots a_{M,N,L}]$

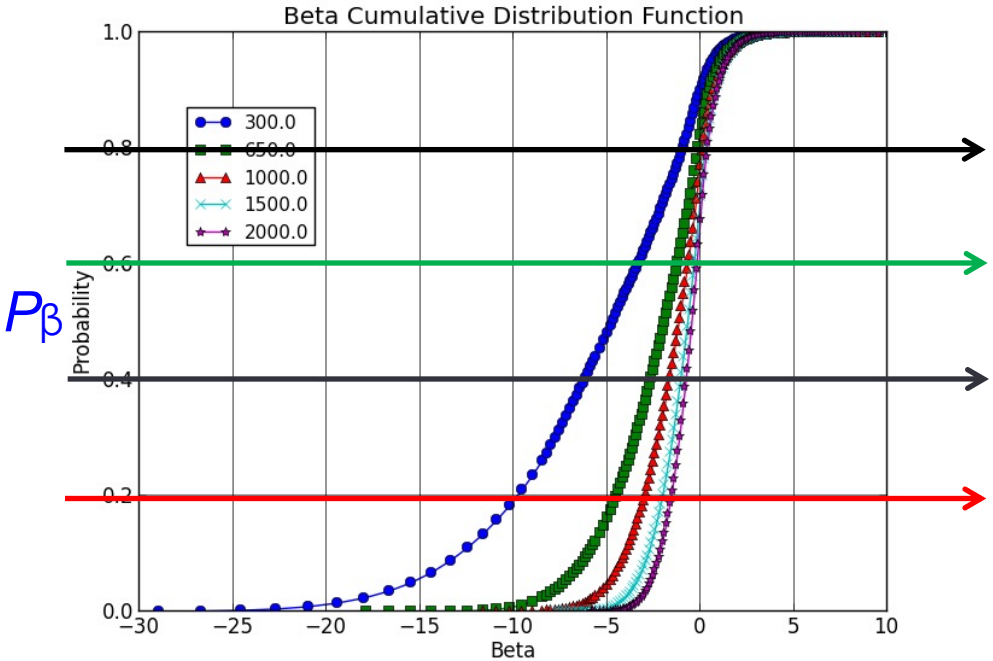
$$\beta(T)_{m,n} = \sum_{k=1}^{K} b_{m,n,k} X^k(T) + const.$$

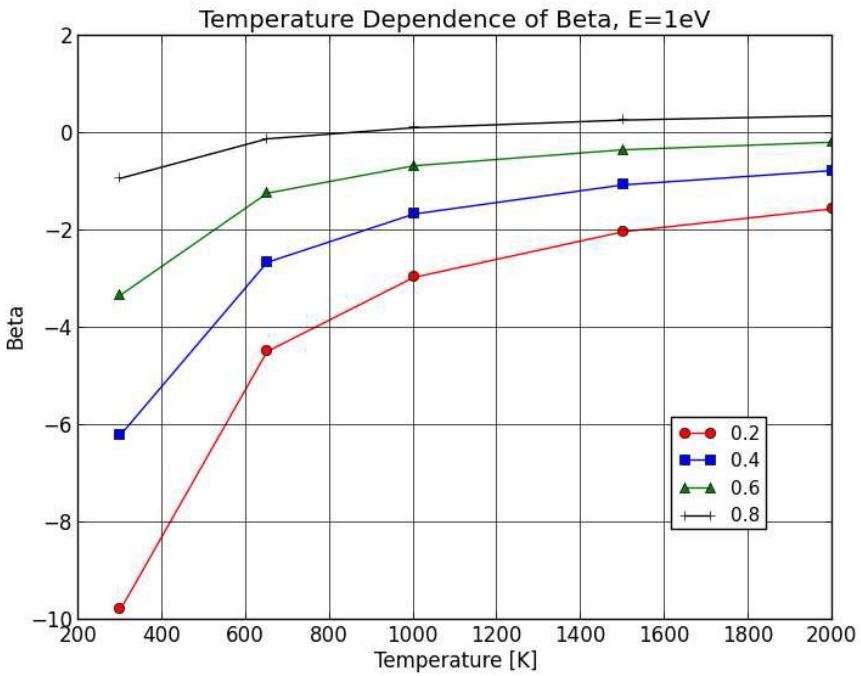
$$\alpha(T)_{m,n} = \sum_{l=1}^{L} a_{m,n,l} X^l(T) + const.$$

Where K and L are the orders of the fits.

One typical example: $\beta(T) \approx \sum_{n=0}^{N} b_n T^{-n}, \quad \alpha(T) \approx \sum_{m=0}^{M} a_m T^{-m}$

On-The-Fly Strategy Data Generation



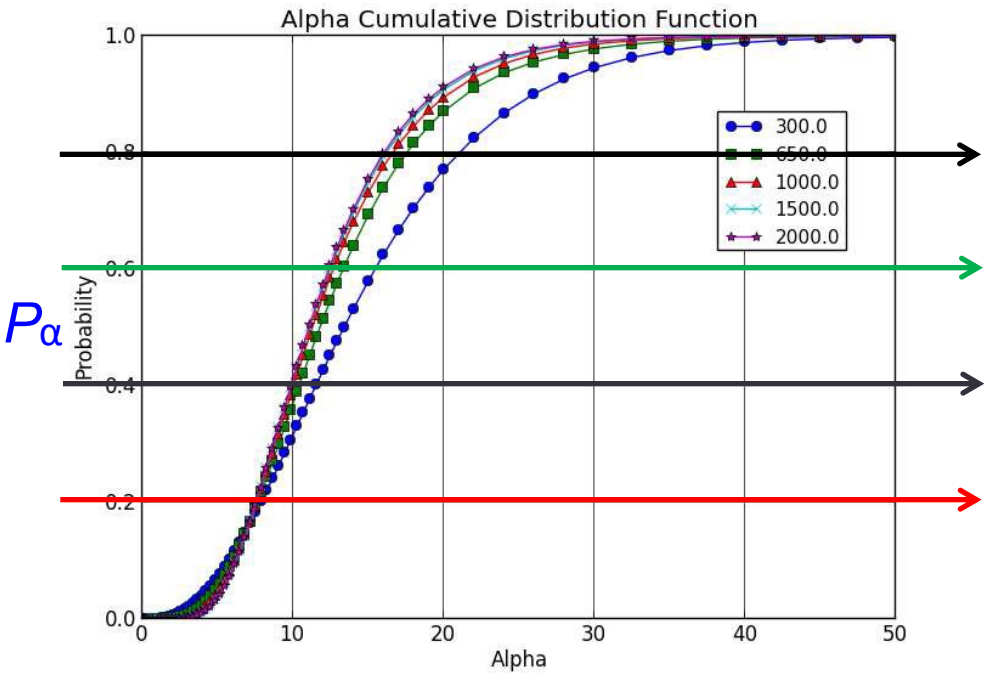


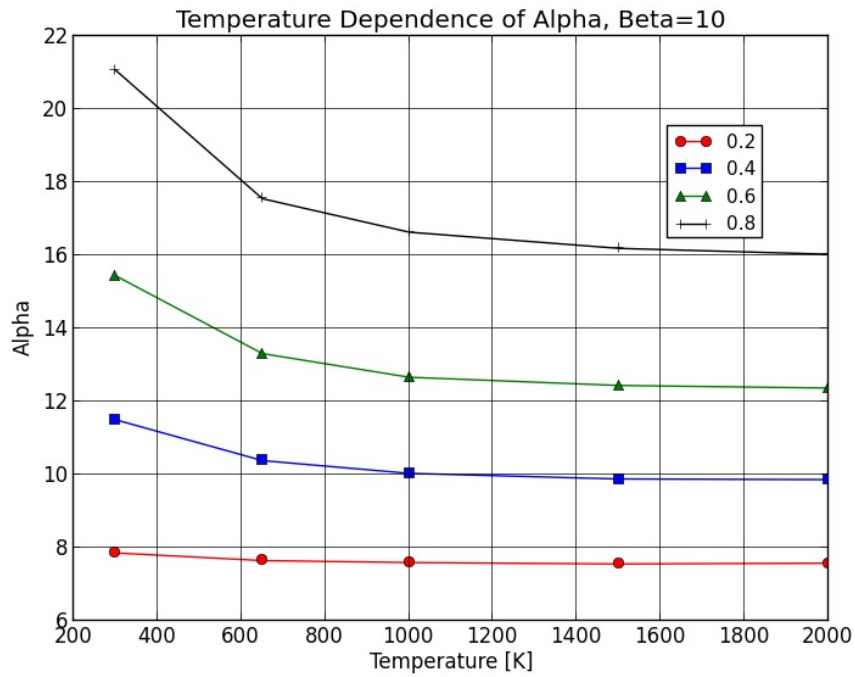
§ Beta PDFs for graphite at 1.0 eV and various temperatures

§ Beta CDFs for graphite at 1.0 eV and various temperatures

β temperature fit meshes: E, P_β

On-The-Fly Strategy Data Generation





§ Alpha PDFs for graphite at $\beta = 10$ and various temperatures

§ Alpha CDFs for graphite at $\beta = 10$ and various temperatures

α temperature fit meshes: β, P_α

Current and Future …

- Contract with LANL was finalized (delayed by a year) …
- On-the-fly strategy driven libraries are being developed based on ENDF/B-VIII.0.
- Will report more details on the next review meeting.
- Any questions?

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