TSL Covariance Format – Preliminary Proposal

Chris W. Chapman, Goran Arbanas, Jordan McDonnell, Doro Wiarda

Oak Ridge National Laboratory

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From mini-CSEWG: Quantities to Store in a Covariance

MD/DFT Parameters

- Pros
  - Most faithful representation of physics
  - Relatively few parameters to store
- Cons
  - Difficult to analytically propagate uncertainties through to cross section (maybe impossible)
  - Code-dependent (some of which are proprietary)
  - Confusing to users
  - Special care needed to include nuclear reaction contribution

LEAPR/NCrystal/FLASSH/etc. Input Parameters

- Pros
  - Intuitive for users to comprehend
  - Relatively few parameters to store
  - Easier to account for temperature dependence
- Cons
  - Code-dependent (some of which are not publicly available)
  - Difficult to analytically propagate uncertainties through to cross section (**but not impossible**)

$S(\alpha,\beta)$

- Pros
  - Intuitive for users to comprehend
  - Analytical link to double differential scattering cross section
- Cons
  - Very large (~40 GB for 1 temperature of ENDF8.0 light water), so compression algorithm required
  - Even with compression algorithm, temperature dependence difficult

What do we want in an eventual TSL covariance?

- Ability to analytically calculate covariance of double differential scattering cross section
  - Rules out MD/DFT parameters
- Code-agnostic
  - Complicates “Input parameters” covariance
- Small file size
  - Complicates $S(\alpha,\beta)$ covariance

Basic Idea

- Start with equation for DDXS $\sigma(E, E', \mu)$

$$\sigma(E, E', \mu) = \frac{\sigma_b}{2k_BT}\sqrt{\frac{E'}{E}}\, e^{-\beta/2} S(\alpha, \beta) = s_b(E, E') S(\alpha, \beta)$$

- Equation for covariance of DDXS:

$$\langle \hat{\sigma}(E_1, E_1', \mu_1) \hat{\sigma}(E_2, E_2', \mu_2) \rangle = s_b(E_1, E_1') \langle \hat{S}(\alpha_1, \beta_1) \hat{S}(\alpha_2, \beta_2) \rangle s_b(E_2, E_2')$$

$$\hat{\sigma}(E, E', \mu) \equiv \sigma(E, E', \mu) - \langle \sigma(E, E', \mu) \rangle$$

- Roadblock: how to transform covariance of two variables (α, β) into covariance of three variables (E, E', μ)?

Basic Idea – continued

- Approximate DDXS into Legendre Coefficients

$$\sigma(E,E',\mu) \approx \sum_{n=0}^{N} \left(n+\frac{1}{2}\right) \sigma_n(E,E') P_n(\mu)$$

$$\sigma_n(E,E') = \int_{-1}^{1} \sigma(E,E',\mu) P_n(\mu) d\mu = s_B(E,E') \int_{-1}^{1} S(\alpha,\beta) P_n(\mu) d\mu$$

- Substitute back into previous equations

$$\langle \hat{\sigma}(E_1,E_1',\mu_1) \hat{\sigma}(E_2,E_2',\mu_2) \rangle \approx \sum_{n,m}^{N} \left(n+\frac{1}{2}\right)\left(m+\frac{1}{2}\right) \langle \hat{\sigma}_n(E_1,E_1') \hat{\sigma}_m(E_2,E_2') \rangle P_n(\mu_1) P_m(\mu_2)$$

$$\langle \hat{\sigma}_n(E_1,E_1') \hat{\sigma}_m(E_2,E_2') \rangle = s_b(E_1,E_1') s_b(E_2,E_2') \int \int_{-1}^{1} \left\langle \hat{S}(\alpha_1,\beta_1) \hat{S}(\alpha_2,\beta_2) \right\rangle P_n(\mu_1) P_m(\mu_2)\, d\mu_1 d\mu_2$$

PRELIMINARY Idea 1: $S(\alpha, \beta)$ covariance

- Store covariance of reduced $\sigma_b S(\alpha, \beta)$
  - $S(\alpha, \beta)$ for the "TSL" effects
  - σ_b to ensure the covariance is a covariance of cross section
- Reduced how?
  - Coarse (α, β) grid?
  - Matrix decomposition?
  - Remove intractably small values of covariance?
  - Some combination of the above?

Preliminary Idea 2: Functional of phonon density of states (PDOS)

- It is possible to approximate $S(\alpha,\beta)$ as a function of the PDOS $\rho(\beta)$

$$S(\alpha,\beta) \approx \langle S(\alpha,\beta)\rangle + \int \left.\frac{\delta S(\alpha,\beta)}{\delta\rho(\beta')}\right|_{\langle\rho(\cdot)\rangle} (\rho(\beta') - \langle\rho(\beta')\rangle)d\beta'$$

- Where

$$\left.\frac{\delta S(\alpha,\beta)}{\delta\rho(\beta')}\right|_{\langle\rho(\cdot)\rangle} = \alpha g(\beta')\Sigma(\alpha,\beta,\beta') \qquad g(\beta) \equiv \frac{e^{-\frac{\beta}{2}}}{2\beta\, sinh\frac{\beta}{2}} \quad \& \quad \Sigma(\alpha,\beta,\beta') \equiv S(\alpha,\beta-\beta') - S(\alpha,\beta)$$

- Therefore

$$\left\langle \hat{S}(\alpha_1,\beta_1)\hat{S}(\alpha_2,\beta_2)\right\rangle \approx \alpha_1\alpha_2 \int\int g(\beta_1')\,\Sigma(\alpha_1,\beta_1,\beta_1')\langle\rho(\beta_1')\rho(\beta_2')\rangle\Sigma(\alpha_2,\beta_2,\beta_2')g(\beta_2')d\beta_1'd\beta_2'$$

Questions for the Audience

- Is there any preference between the two?
  - Could allow for both with a flag denoting which format to store
- Do we want this to be in ENDF format or GNDS format?
  - Existing format in GNDS for $S(\alpha, \beta)$ covariance on user-defined (α, β) grid, would only require a slight adjustment for inclusion of σ_b
- How could/should we test the efficacy of these formats?

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