TSL Style Covariances

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Mini-CSEWG meeting – 14 August 2024

Goal

- What this is
  - Discussion points to consider over the next few months regarding the storage, processing, and usage of a TSL covariance
- What this is **not**
  - A final decision on any sort of format or procedure
  - A discussion about how to produce the covariance

Broad questions to answer

- What to store the covariance of?
  - Implied that processing codes will be able to process this covariance to an eventual covariance of DDXS
- How to handle temperature dependence?
  - TSL temperature dependence is not necessarily analytical as other forms of nuclear data
- How will transport codes use this covariance?
  - Sampling? Sensitivity calculations?

What to store covariance of

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

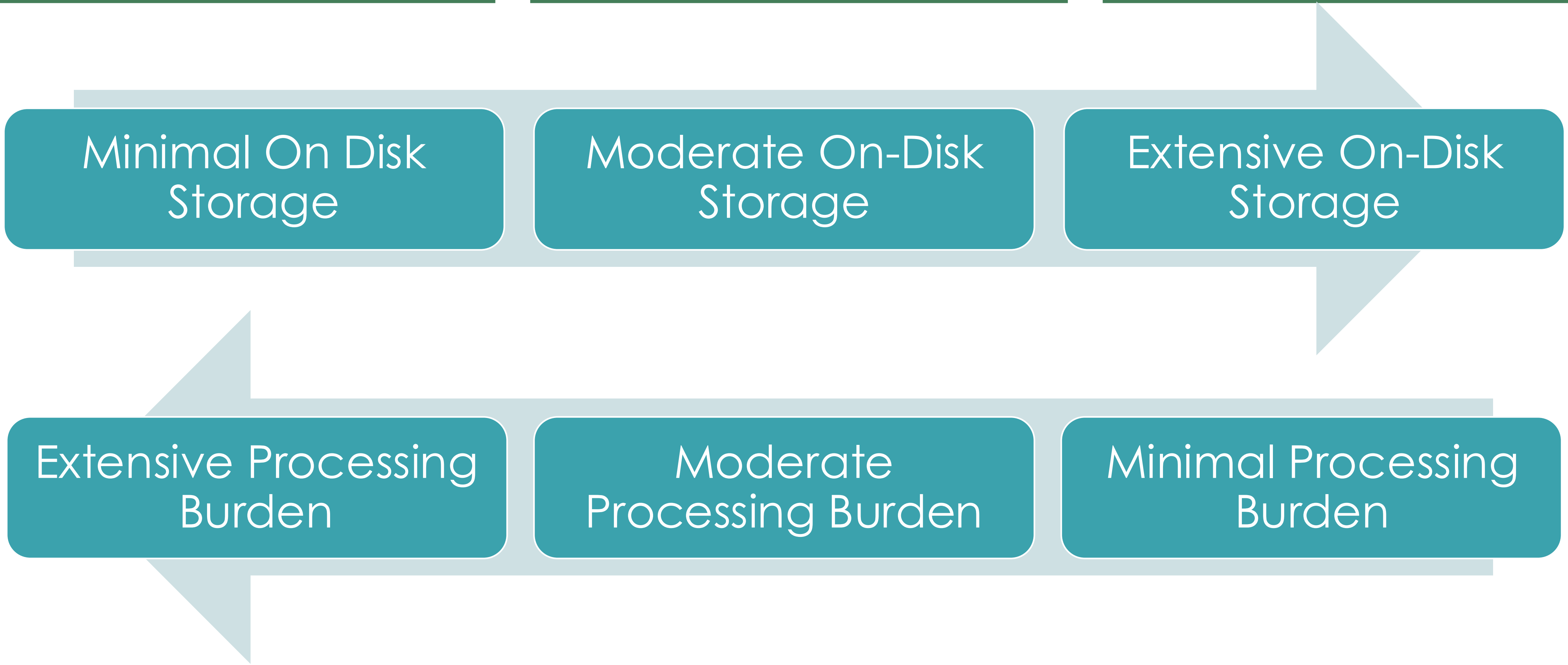
- Pros
  - Intuitive for users to comprehend
  - Relatively few parameters to store
  - Easier to account for temperature dependence
- Cons
  - Code-dependent (some of which are not publicly available)
  - Difficult to analytically propagate uncertainties through to cross section (**but not impossible**)

$S(\alpha,\beta)$

- 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 to store covariance of (cont.)

MD/DFT Parameters	LEAPR/NCrystal/FLASSH/etc. Input Parameters	$S(\alpha,\beta)$



How will transport codes use this covariance?

- Stochastic Sampling
  - Might not necessarily require a DDXS covariance
  - Could work for either CE or MG calculations
- Deterministic Calculations
  - Will require a DDXS covariance for sensitivity calculations
  - Could work for MG; CE would be difficult (if even possible)

Discussion

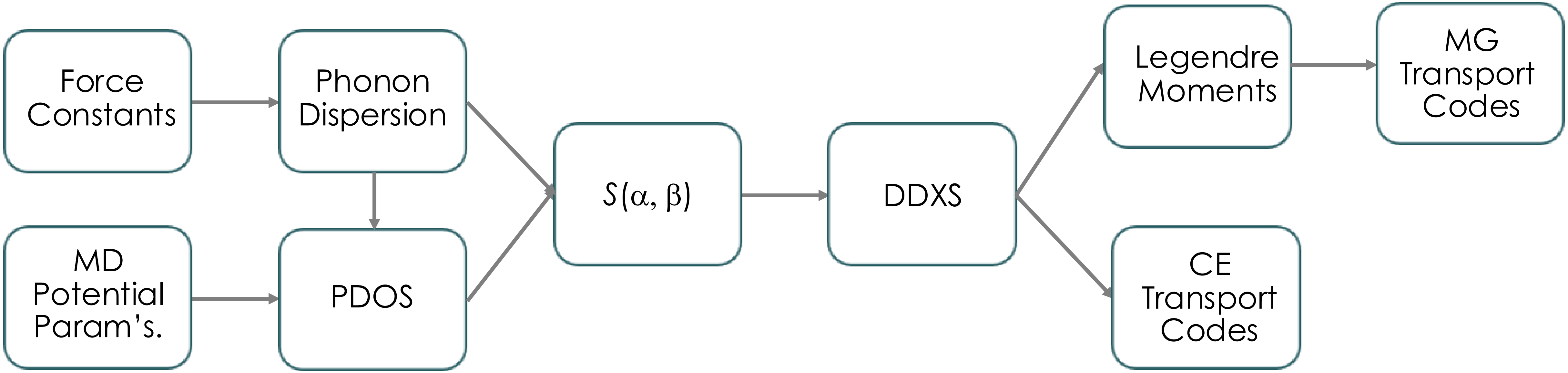
- What do we as a community need to do over the next few months?
  - Methods improvements?
  - Develop benchmark(s) to test efficacy of covariance methodology?
- Who outside of the CSEWG community do we need to reach out to?
- Do we need to simultaneously consider how covariances are generated?

Acknowledgements

Extra Slides – What we've done @ ORNL

- DNCSH funded task
- Start with covariance matrix created by Chapman in 2017
  - Known flaws with covariance methodology, but currently better than nothing
- Focus on two different methodologies:
  - Covariance of LEAPR input parameters (most notably PDOS & bound scattering cross section)
  - Matrix decomposition of $S(\alpha,\beta)$ covariance matrix

Extra Slides – TSL Covariance Propagation



$$\mathrm{cov}(y,y) = \frac{\delta y}{\delta x}\mathrm{cov}(x,x)\left(\frac{\delta y}{\delta x}\right)^{\mathsf{T}}$$

$$y = y(x)$$

Extra Slides – Cunningham's Law

- "If you want to get the right answer, don't ask a question, post the wrong answer"
- So…

Extra Slides – My proposal

- Store N largest diagonal & off-diagonal values of $S(\alpha,\beta)$
  - bogosort, of course
- LCOMP=2
- Store 1 temperature; use linear interpolation to other temperatures