OAK RIDGE National Laboratory

Progress on Light Water TSL Covariance

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Previously

- Generated covariance of H-H_2O $S(\alpha, \beta)$ using Unified Monte Carlo (UMC) method
  - Pre-generated 4000 samples of $S(\alpha, \beta)$ from multivariate Gaussian [1]
  - Fit to double differential & total scattering cross sections
  - Linear weights used to calculate mean value & covariance of quantities of interest (phonon DOS, $S(\alpha, \beta)$, etc.)
- Mathematical / computational implementation in neutron transport codes underway

Previously

- Storing covariance of 3 quantities:
  - $S(\alpha, \beta)$
  - Bound scattering XS
  - Effective temperature
- Total size: 70376 parameters
  - 37 GB file size full covariance
  - 17 GB ‘realistic’ (zeros removed) full covariance
  - 8.5 GB realistic upper triangular

How to Reduce File Size

- Need to reduce file size
  - Community consensus
  - Covariance should be usable by users on semi-modern laptops
- Multiple ways to do this:
  - Matrix decomposition
    - Difficult due to wide ranging values of covariance (1e8 - 1e-60)
    - Not obvious *a priori* which values are or aren't important to keep
  - Group-structuring
    - Difficult to group (α, β) components together since there's potential for overlap
  - Manual entry removal

How to Reduce File Size

- Remove rows/columns if variance is less than threshold value
- Slightly 'nudge' covariance to make it positive-definite (fixes numerical roundoff issues) [2]
  - Does not change values of diagonal, variance remains unchanged

Threshold	Stored Parameters	Theoretical File Size [MB]
Evaluated	70376	18894
1e-33	32570	4047
1e-15	21136	1704
1e-13	18771	1344
1e-11	15220	884
1e-9	12046	554
1e-7	8198	256
1e-5	4398	74
1e-3	2152	18
1e-1	1060	4

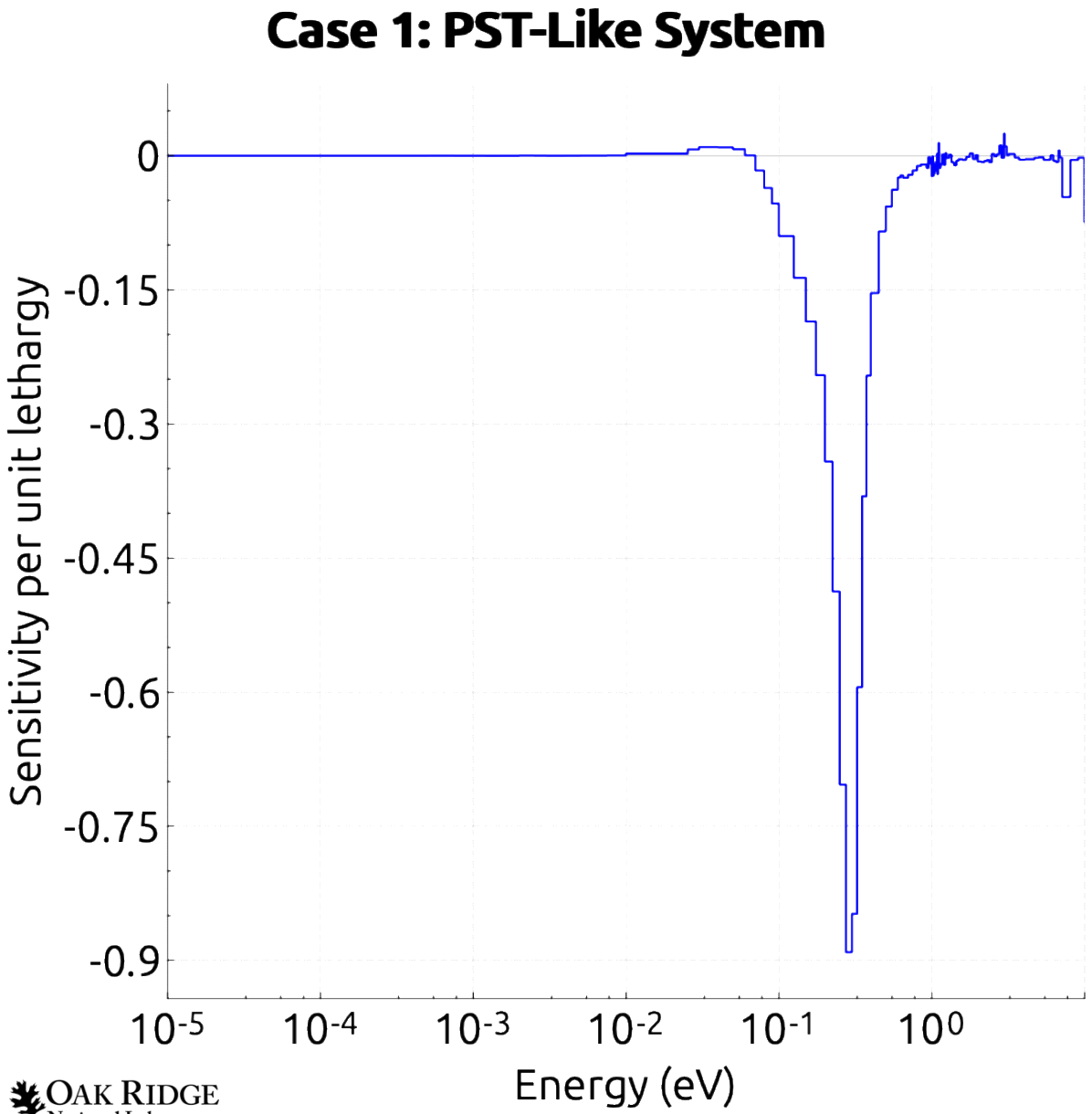
How to test efficacy of new covariance

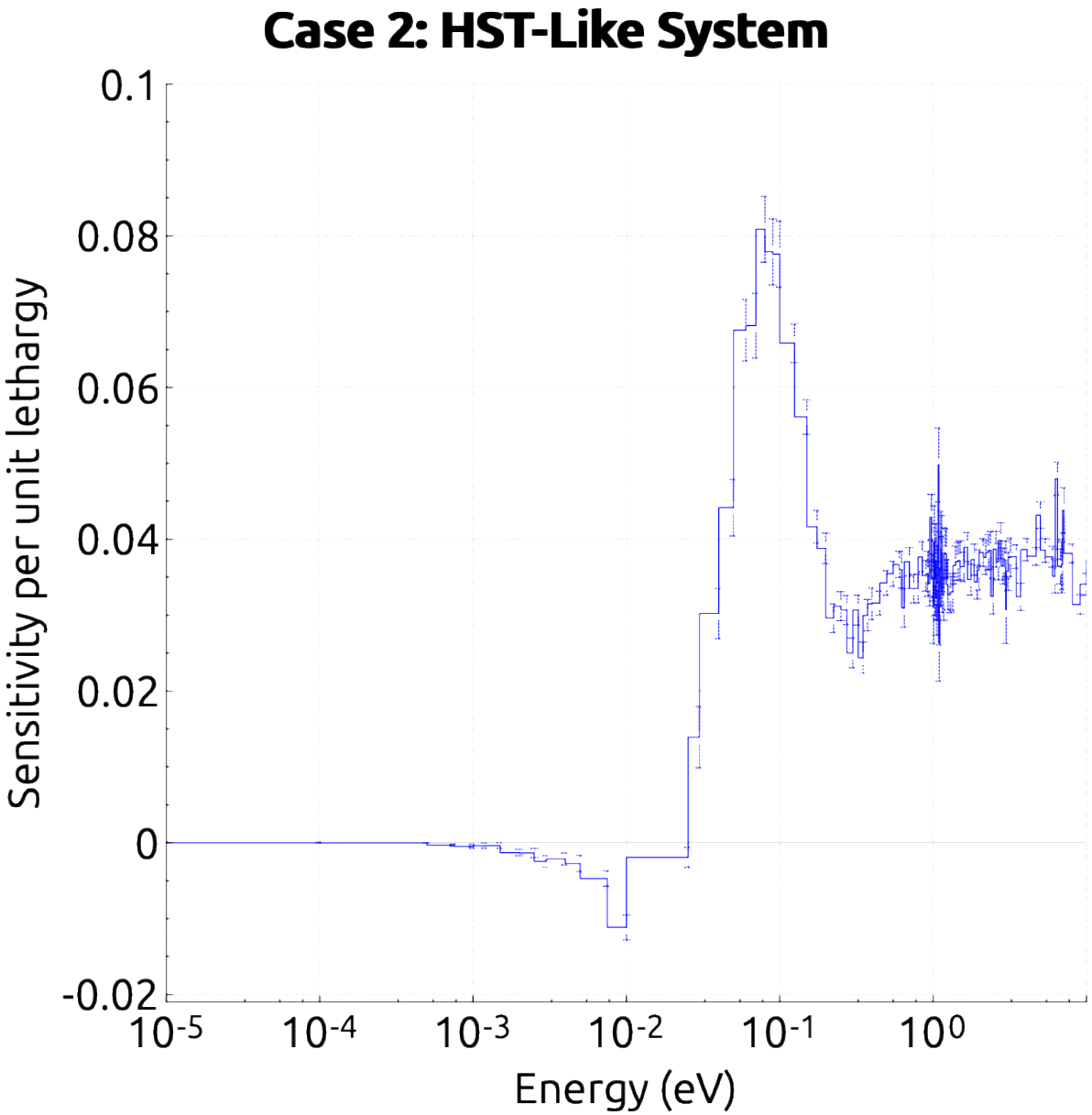
- Compare covariance
  - Directly compare covariance with original covariance
  - Mathematical models not built for large dimensionality matrices
- Compare sampled cross sections
  - Generate ensemble of sampled cross sections; compare mean value & covariance against evaluated cross section
  - Only applicable in multigroup case; difficult to determine importance in DDXS range
- Compare effect of sampled cross sections on applications
  - Most robust & straightforward
  - Need to ensure applications cover full range of applicability for covariance

Two simple cases

- Create systems with significant sensitivity to H-H2O scattering below 10 eV
  - Loosely modeled as Plutonium & HEU solution systems
- Evaluated case:
  - Run simulation from 4000 input $S(\alpha, \beta)$
  - Use UMC-calculated linear weights to calculate mean value & variance in simulated results
- Reduced cases:
  - Generate 1000 realizations of $S(\alpha, \beta)$ for each reduced file size
  - Run simulations on realizations, calculate mean value & variance

Two simple cases





Results & Analysis

- Simulations run with CE cross sections in SCALE with statistical uncertainty 5 pcm
- Two findings:
  - No significant changes in mean value as a function of threshold
  - Change in spread in k_{eff} not identical between models
- Unclear if this is unexpected or unusual; more testing required

Threshold	Case 1 (PST-esque)			Case 2 (HST-esque)		
	Mean k_{eff}	Spread of k_{eff} [pcm]	Δk_{eff}	Mean k_{eff}	Spread of k_{eff} [pcm]	Δk_{eff}
Evaluated	0.22445	385		0.55628	241	
1E-33	0.22461	391	6	0.55624	238	-2
1E-15	0.22446	370	-15	0.55631	235	-6
1E-13	0.22435	364	-21	0.55629	244	3
1E-11	0.22437	345	-40	0.55624	241	0
1E-09	0.22455	309	-76	0.55616	241	0
1E-07	0.22442	276	-109	0.55621	235	-6
1E-05	0.22424	270	-115	0.55634	241	0
1E-03	0.22439	259	-126	0.55627	265	24
1E-01	0.22440	256	-129	0.55625	269	28

Conclusions & Future Work

- Preliminary testing of reduced file size performed
- More testing needed to answer questions of differing spread in k_{eff} results:
  - CE vs MG
  - Realistic systems (ICSBEP benchmarks / reactors) vs. toy models presented here
  - $S(\alpha, \beta)$ vs. PDOS covariance

Acknowledgements

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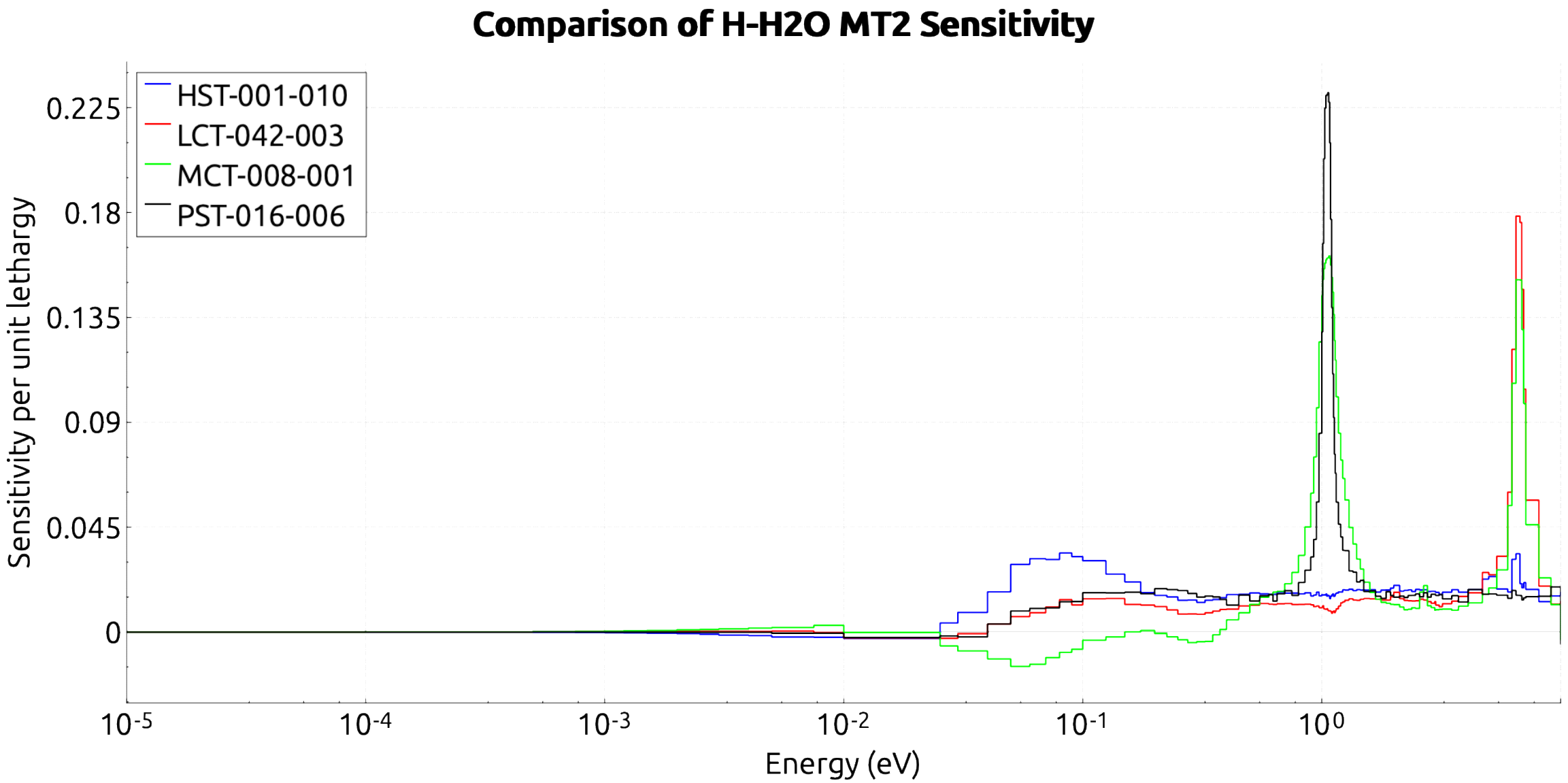
References

- [1] Lance Maul, José Ignacio Márquez Damián, George Braoudakis, Mark Ho, Guan Heng Yeoh, "Perturbation scheme for estimating uncertainties in thermal scattering cross sections of water", *Annals of Nuclear Energy*, **121**, (232-249) 2018 https://doi.org/10.1016/j.anucene.2018.07.020
- [2] https://www.statsmodels.org/stable/generated/statsmodels.stats.correlation_tools.cov_nearest

Questions?

Extra slide – VALID benchmarks sensitive to H-H_2O



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