



Advancing Nuclear Data Uncertainty Quantification: EMU and Machine Learning

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Evaluations with Means and Uncertainties

EMU is a tool to generate realizations of evaluated data in GNDS format by sampling from a covariance matrix

Realizations can be input into any application that uses GNDS to propagate uncertainties

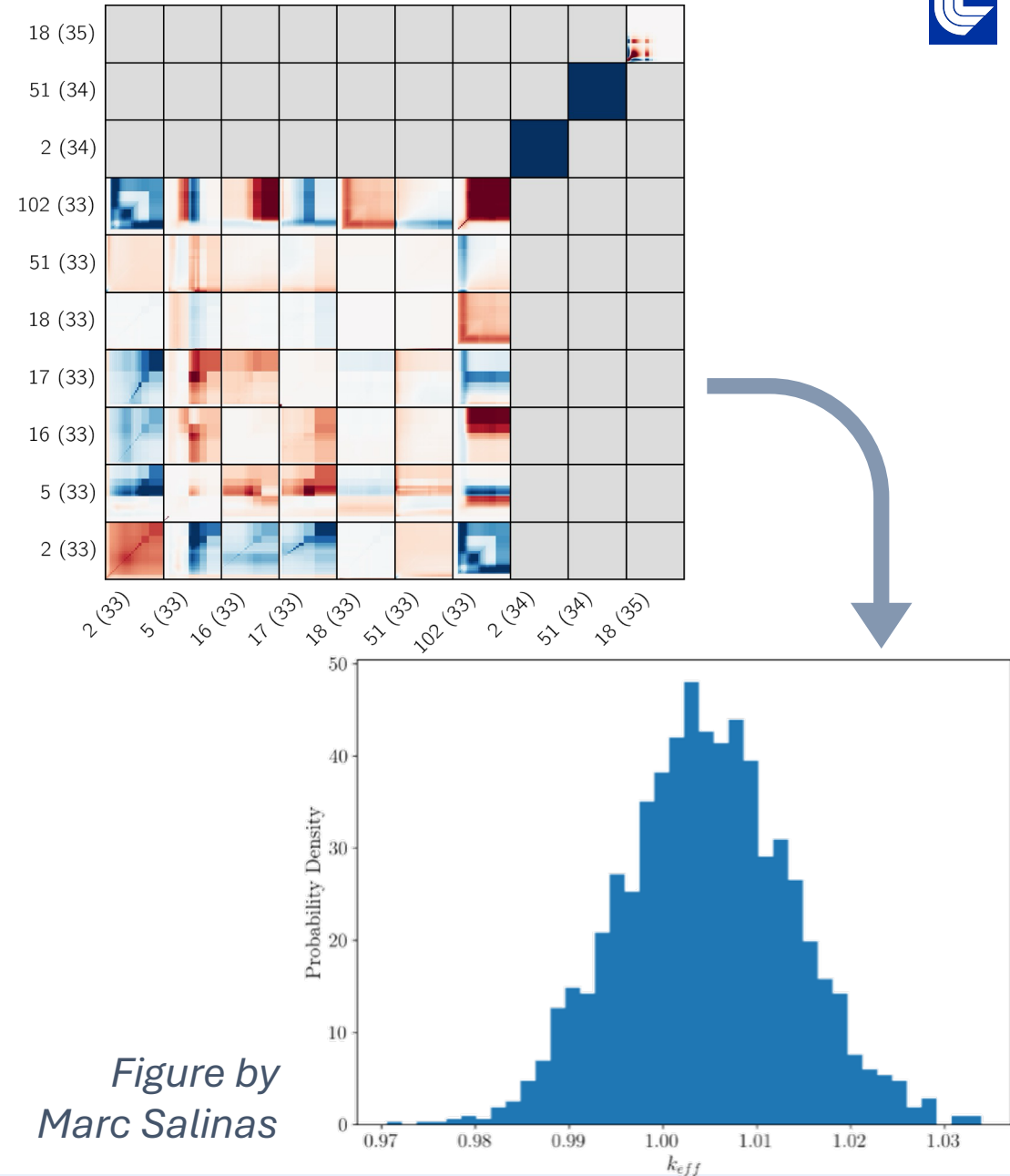


Figure by Marc Salinas

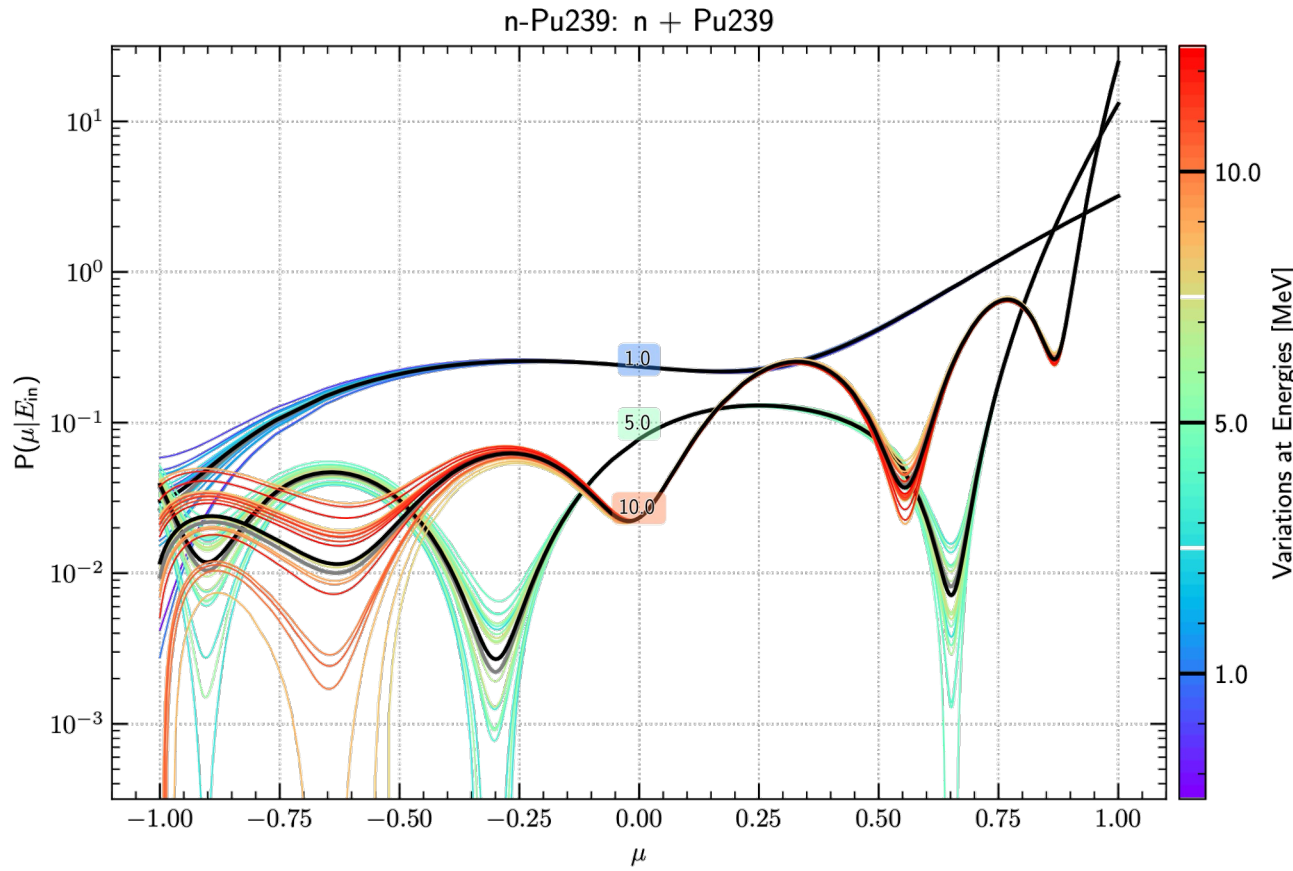


EMU can sample from all available data within a GNDs covariance suite

- Cross sections
- Angular distributions
- Resolved resonance parameters
- Prompt fission neutron spectra
- Neutron multiplicities



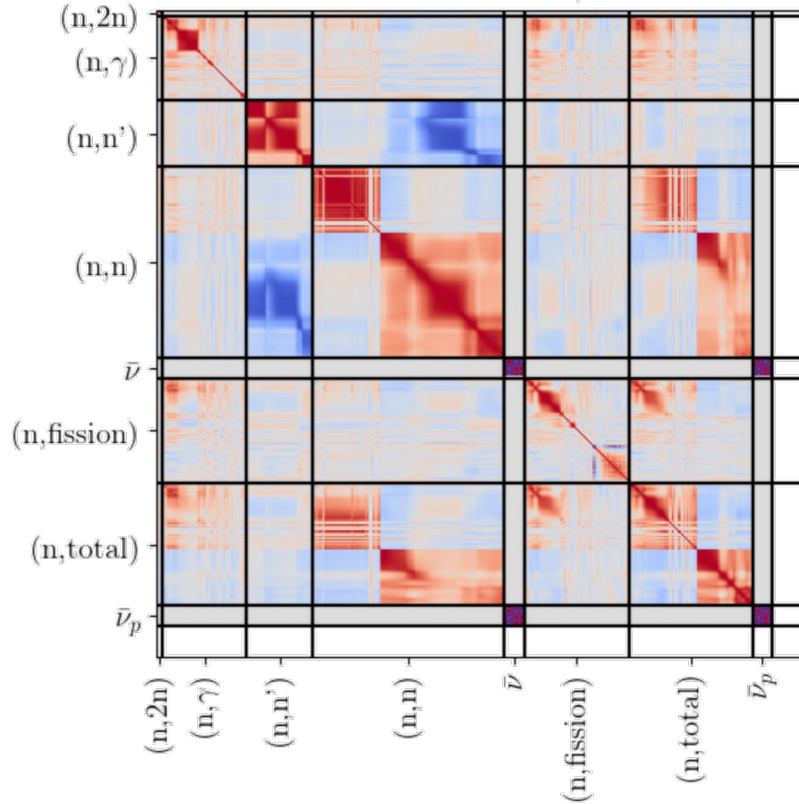
Give me a covariance matrix large enough, and a machine on which to sample it, and I will uncertainty-quantify the world



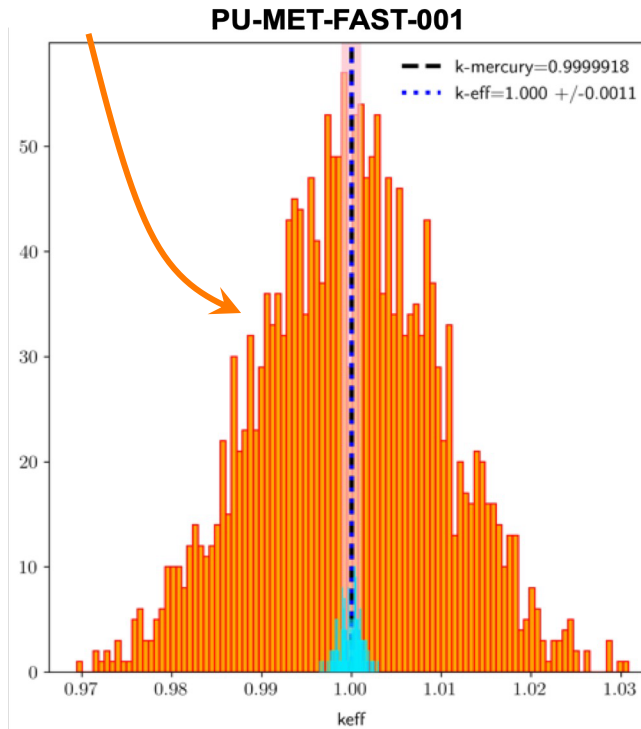
Constraining covariances with critical assembly data

prior
correlation matrix

Correlation Matrix: $n+^{239}\text{Pu}$



all EMU samples

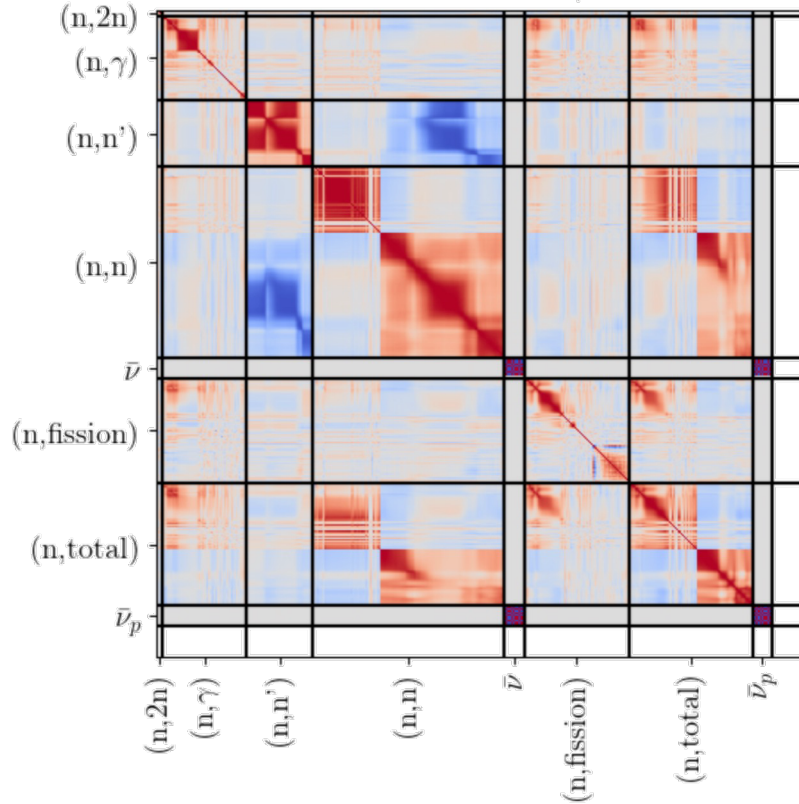


Figures by Marc Salinas and Maria Anastasiou

Constraining covariances with critical assembly data

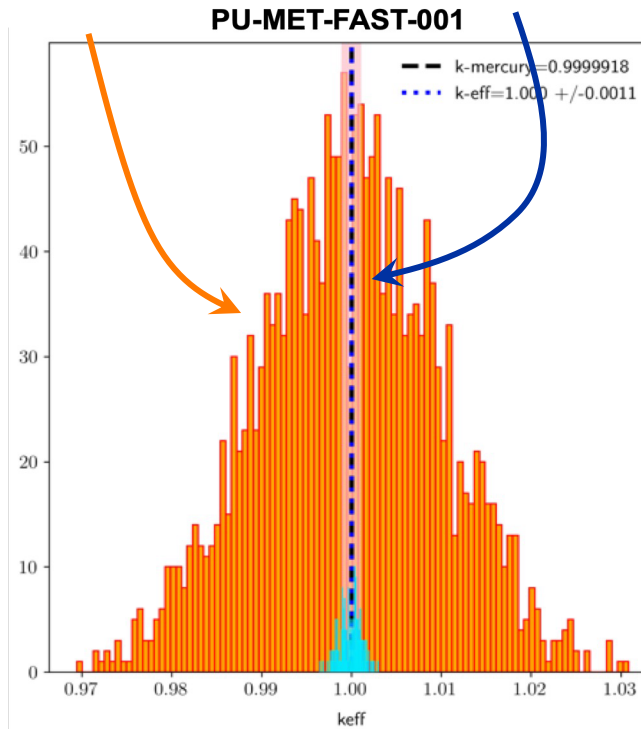
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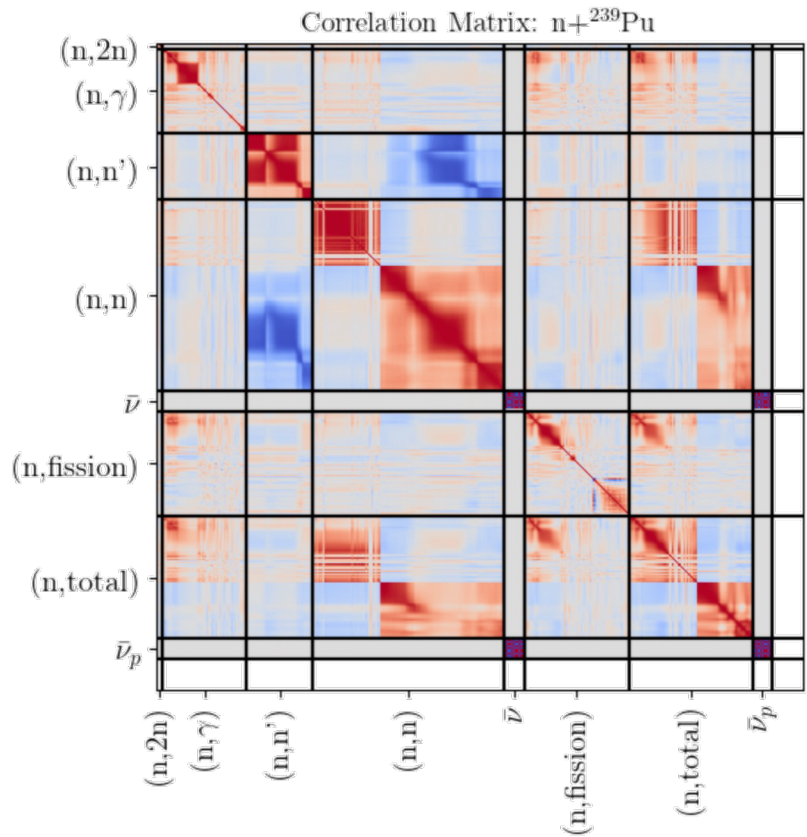
experimental k_{eff}



Figures by Marc Salinas and Maria Anastasiou

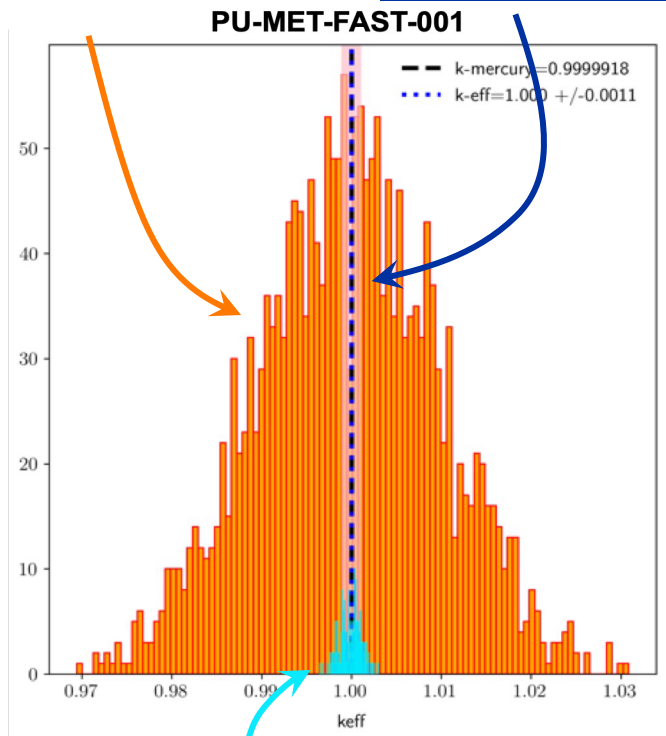
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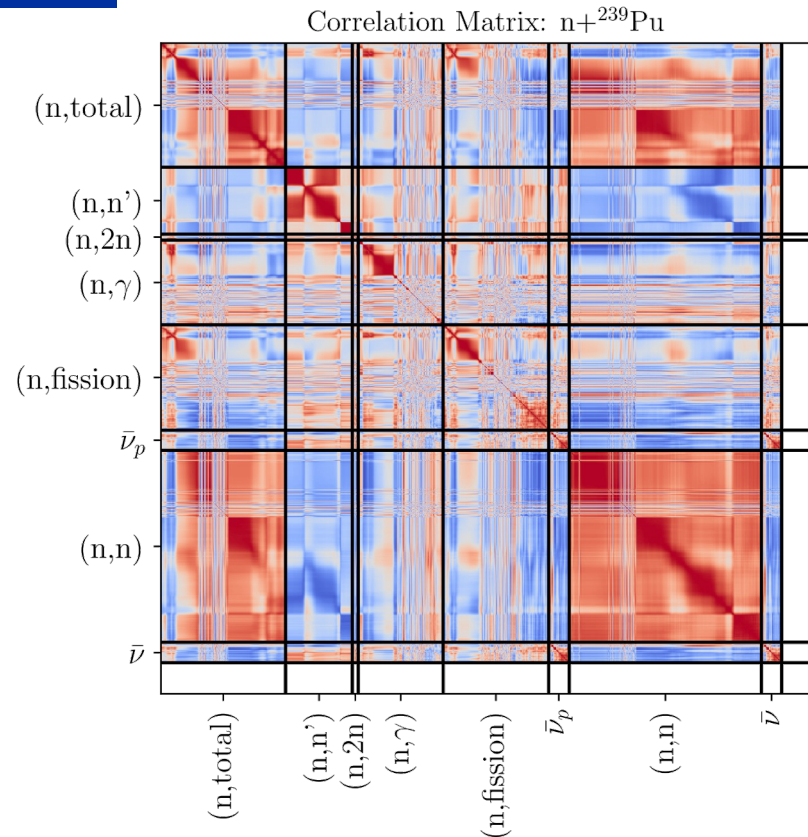
all EMU samples

experimental k_{eff}



down-selected samples

posterior correlation matrix

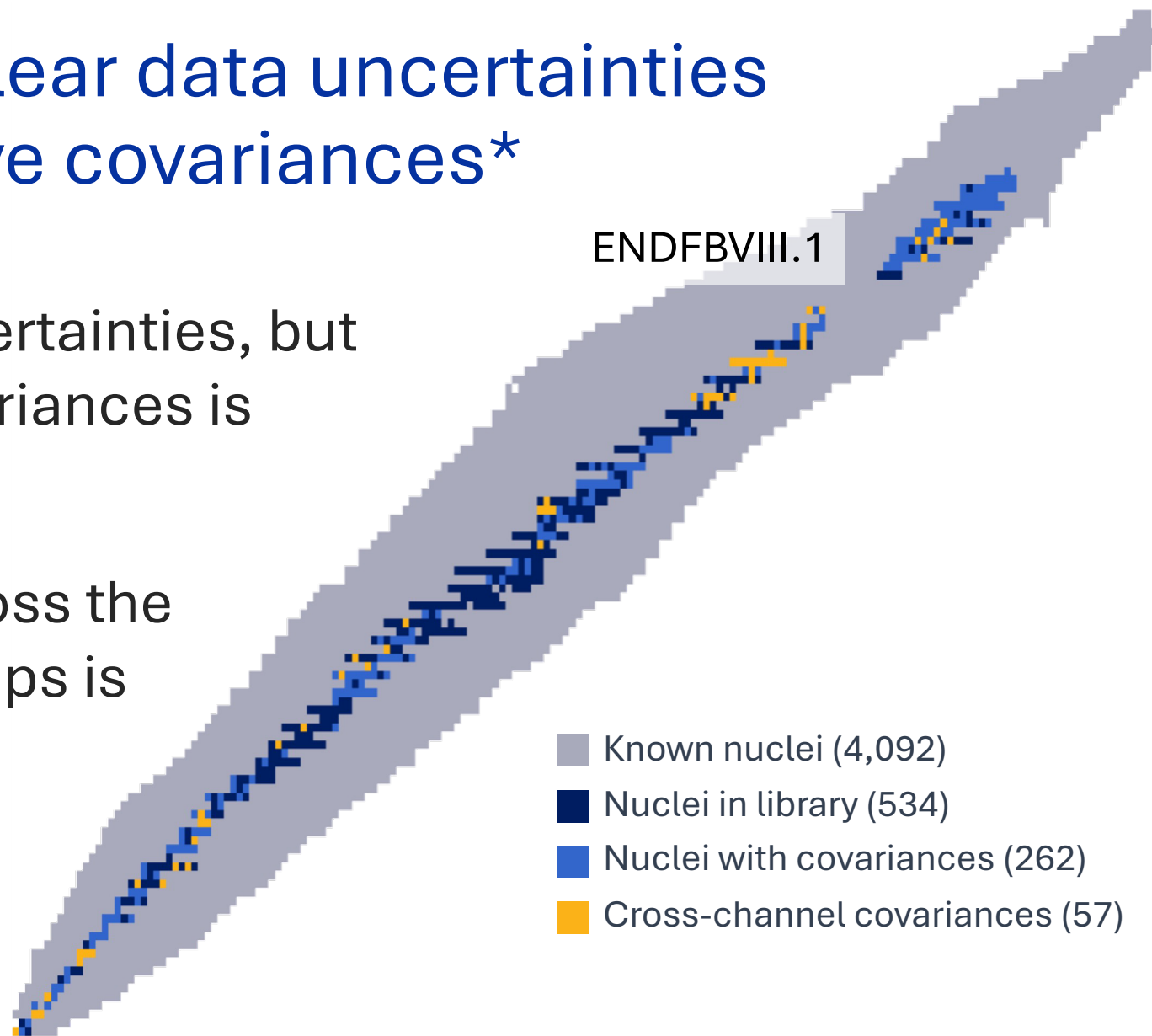


Figures by Marc Salinas and Maria Anastasiou

We can't propagate nuclear data uncertainties with EMU if we don't have covariances*

EMU is ready to propagate uncertainties, but the coverage of evaluated covariances is sparse and uneven

Rigorous theory-based UQ across the chart of nuclides to fill these gaps is possible, but computationally expensive

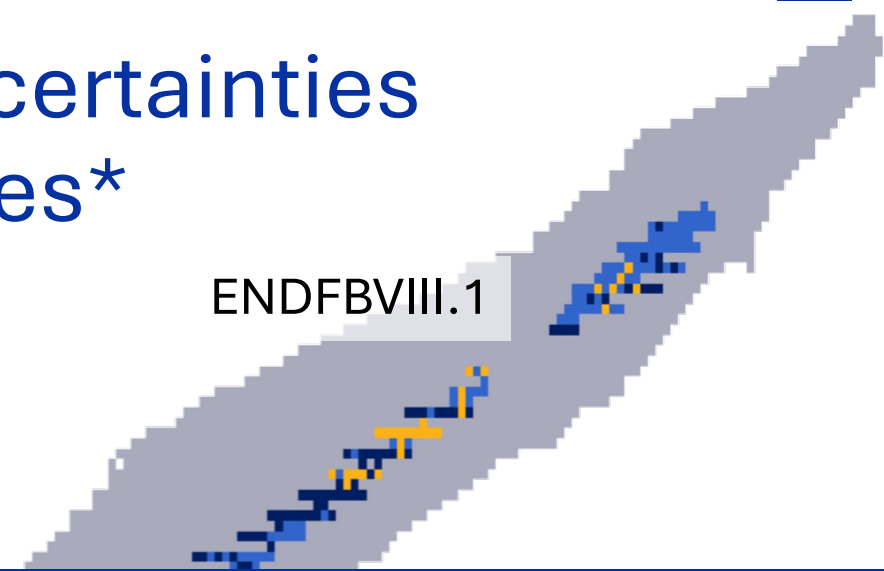


*technically EMU *can* sample without covariances



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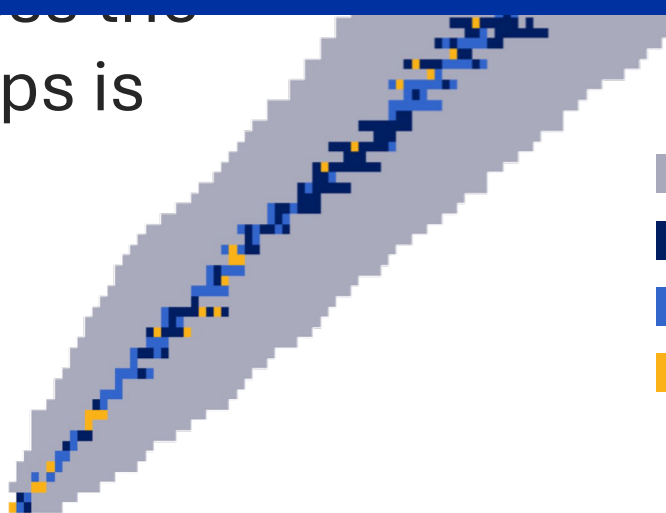
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Can AI/ML help?

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- Known nuclei (4,092)
- Nuclei in library (534)
- Nuclei with covariances (262)
- Cross-channel covariances (57)



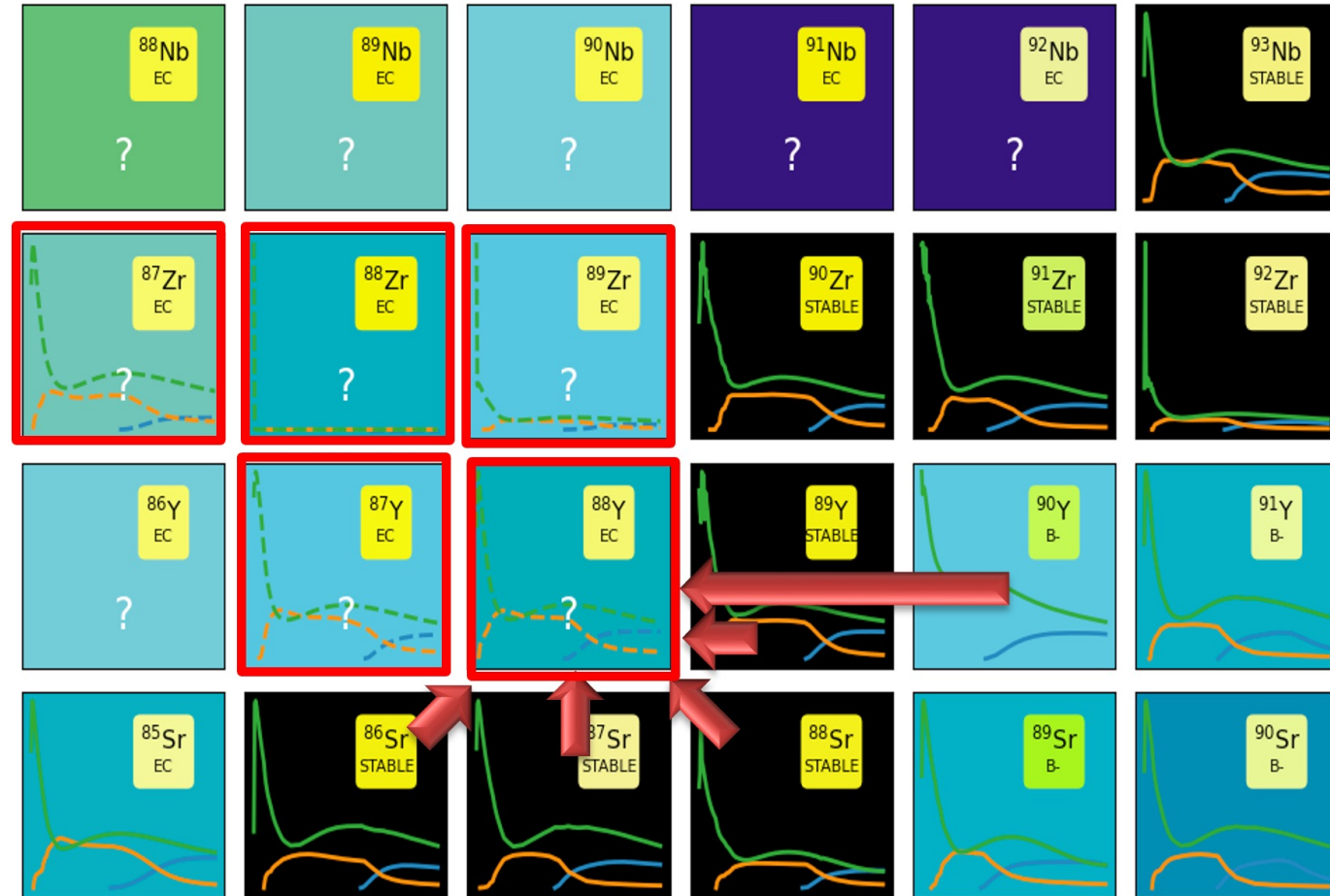
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Cross sections evolve systematically

Can this be learned with ML methods?

Goal: predict n-induced cross sections off stability

- elastic
- inelastic
- capture
- (n,2n)



Effectively, machine-learning *cross-material-channel* covariances



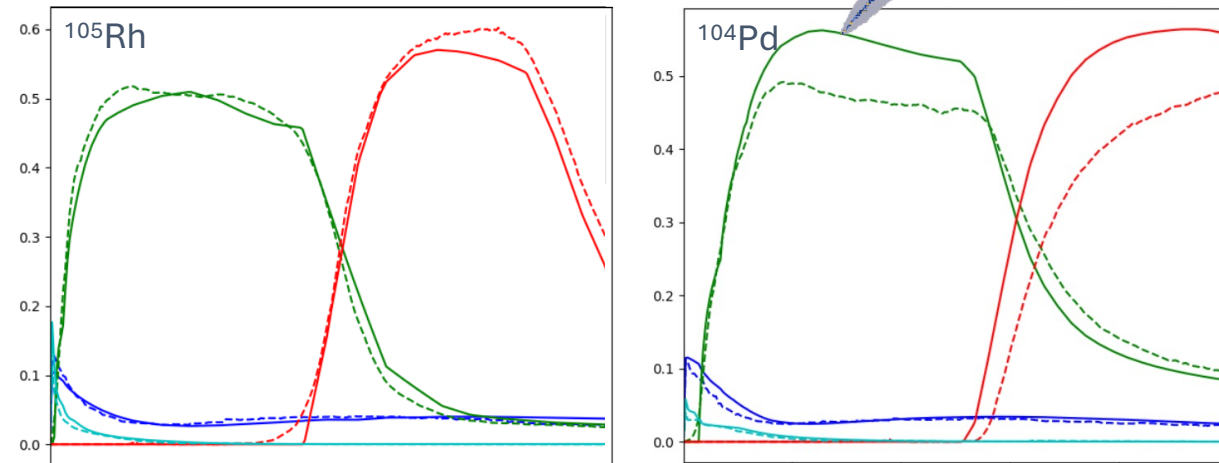
ML cross-sections show early success

Graph neural networks to predict how neutron-induced cross sections evolve with \pm nucleons

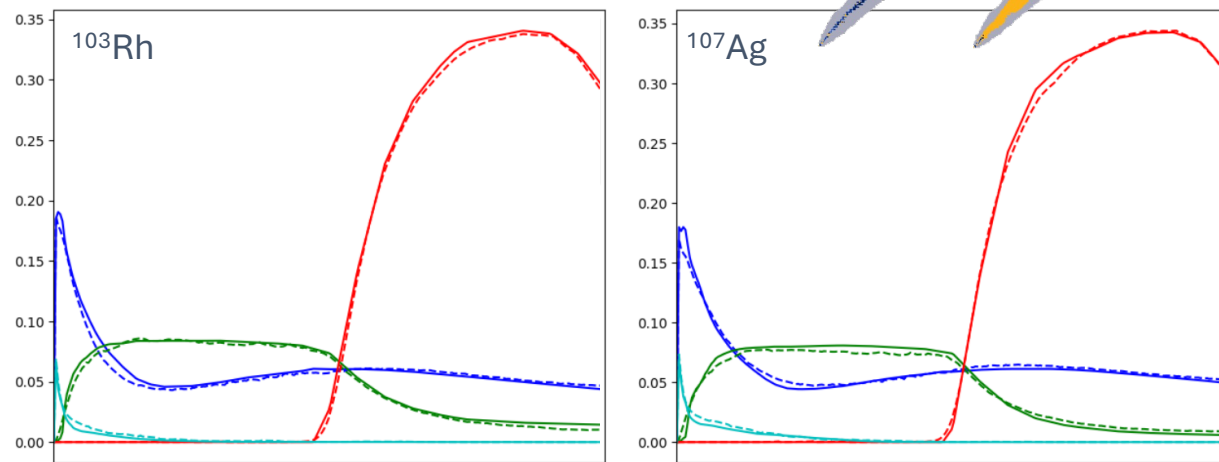
Simultaneous entire-library prediction

More training data (in this case, from theory) yielded more accurate ML predictions

trained on ENDF only



ENDF + TENDL (theory)



— truth - - - - prediction

Figure by Hongjun Choi (see also [Choi+ 2025](#))



We have also worked towards using ML to predict *covariances* for those cross sections

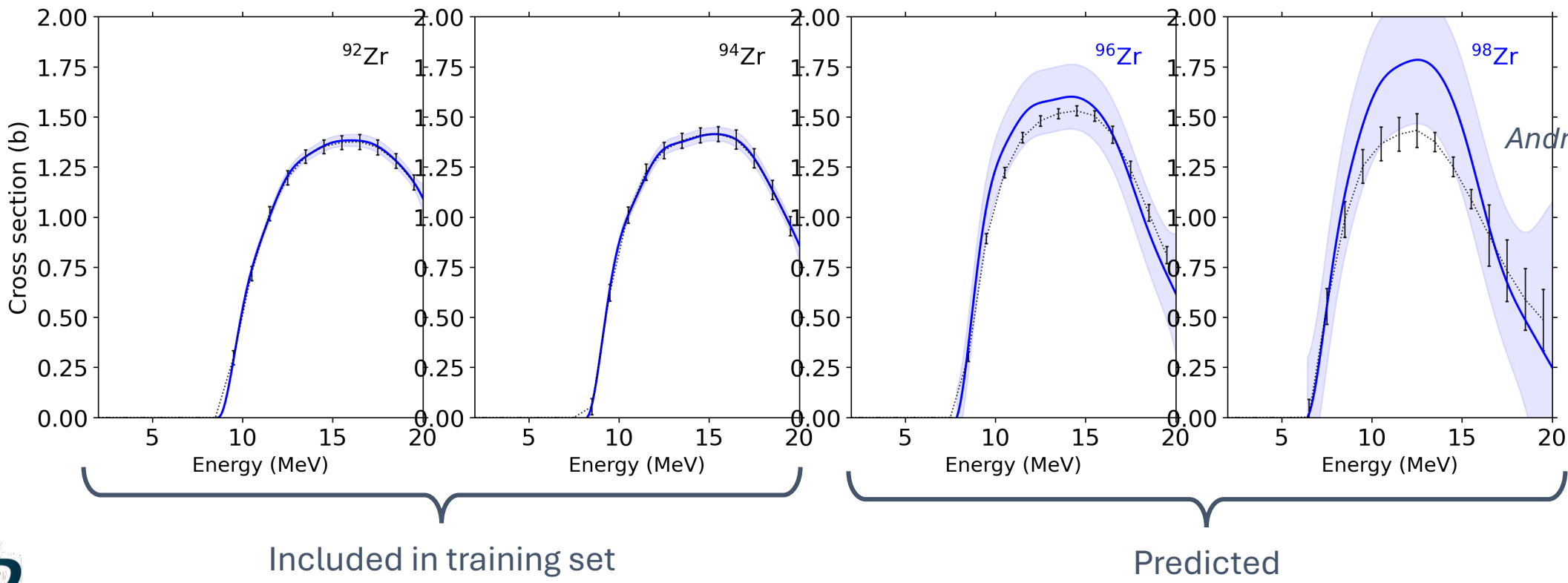


Figure by Andre Sieverding



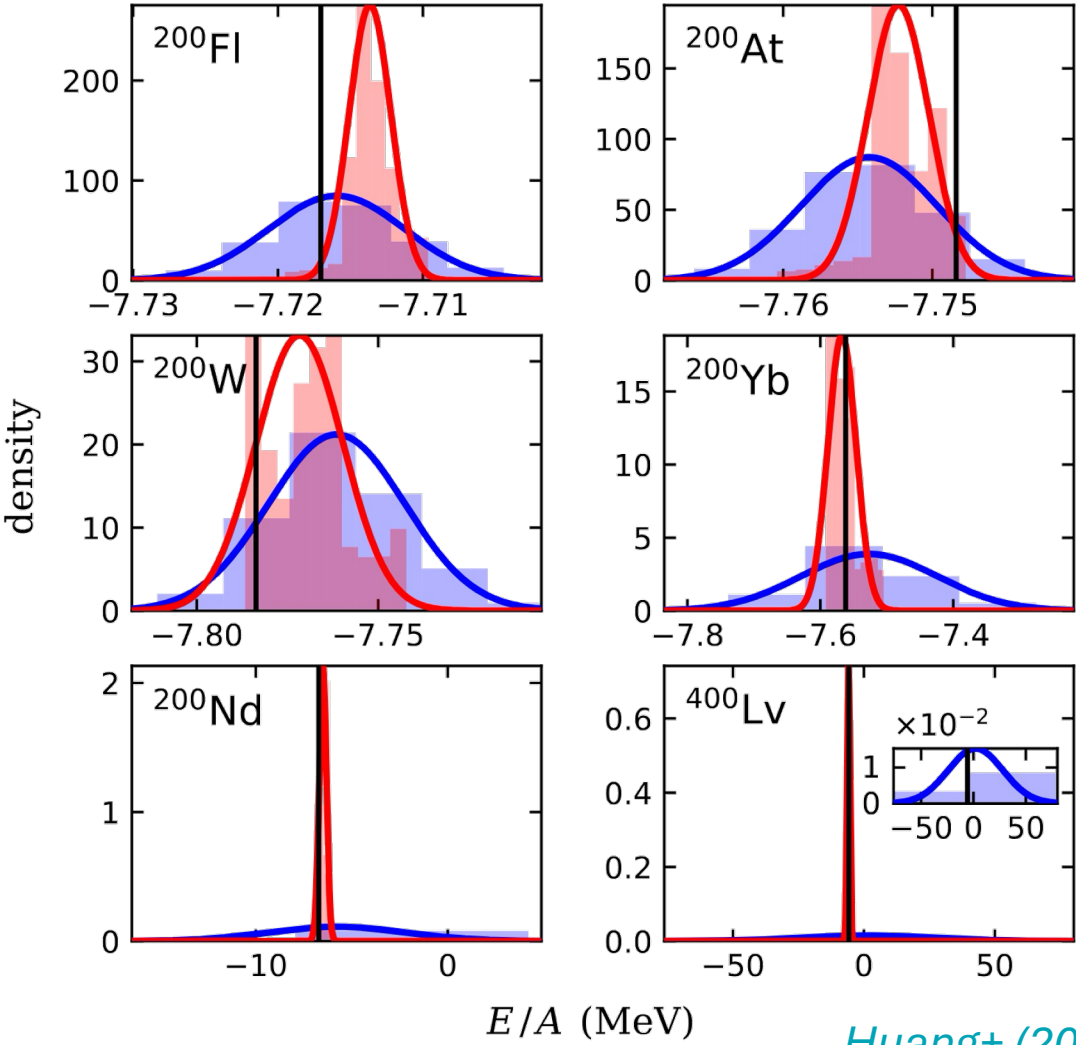
The uncertainties predicted away from stability are very conservative



Additional efforts to quantify uncertainty in the ML model

An example study: quantifying neutral network models trained on DFT predictions of nuclear masses

This approach enables rapid, data-driven UQ to directly link input parameter uncertainties to output



Huang+ (2025)

Useful for a meta-UQ analysis of the ML prediction!



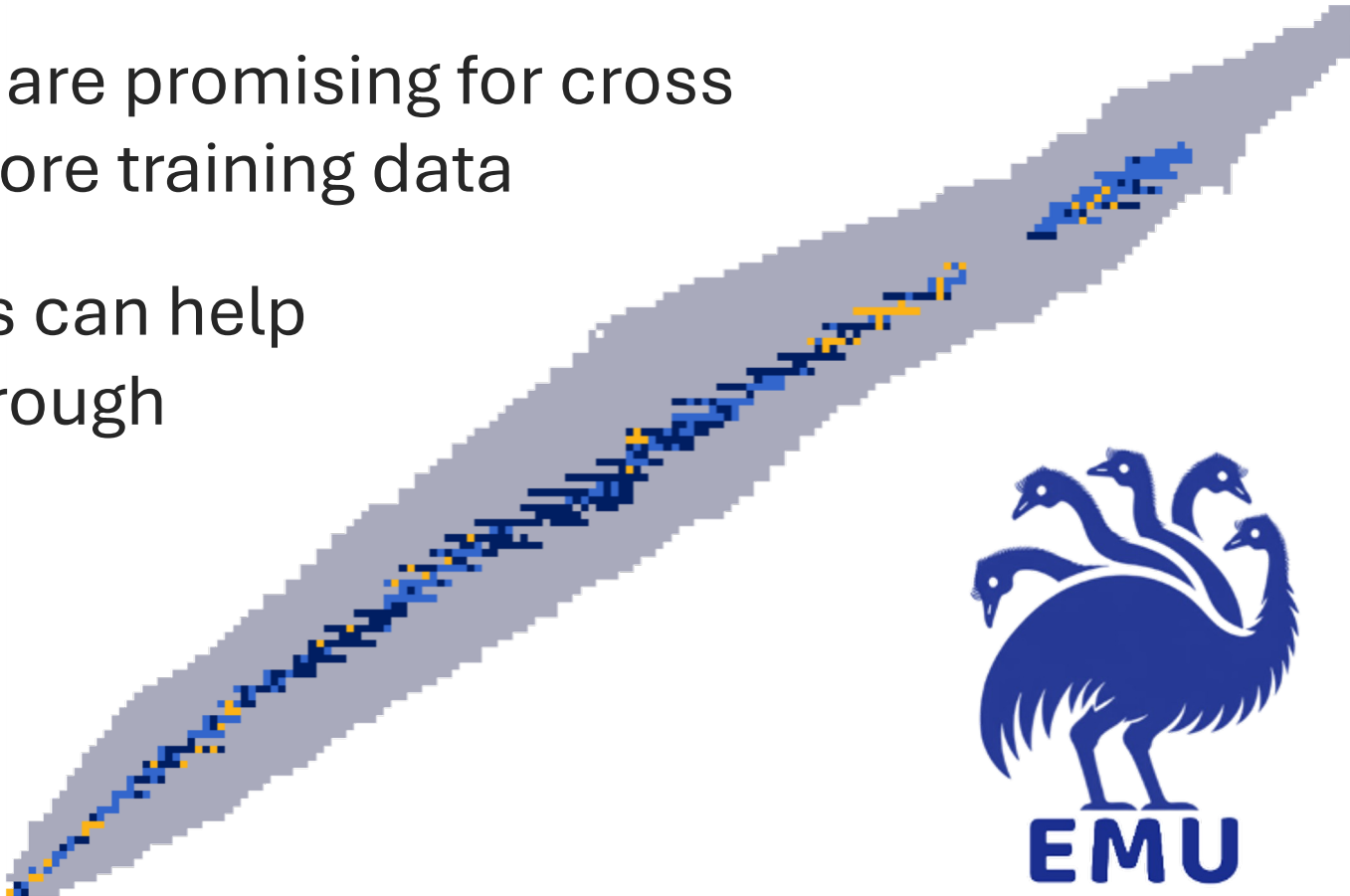


More complete covariances across the chart of nuclides will expand the capacity of EMU

Machine learning techniques are promising for cross sections and benefits from more training data

Theory efforts on key isotopes can help guide ML predictions, e.g., through reinforcement learning

Is there another way to get more data?



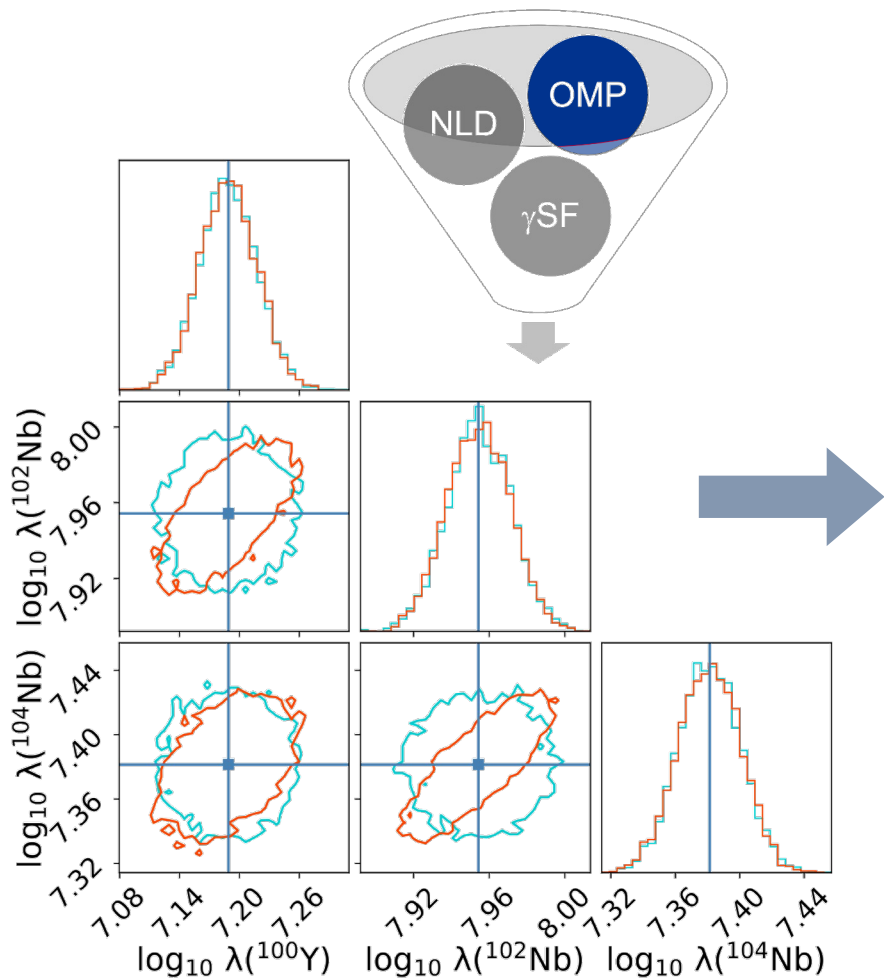


Genesis Mission

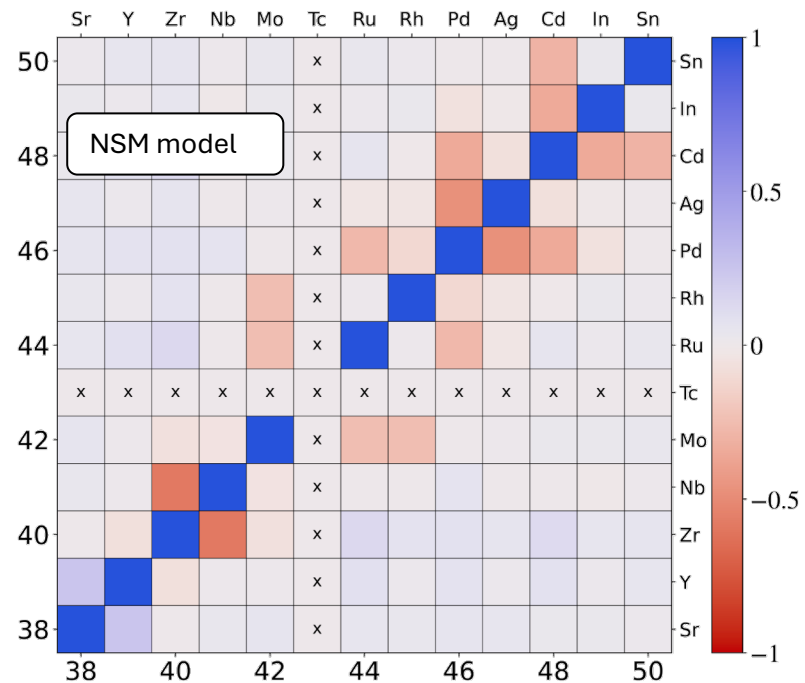


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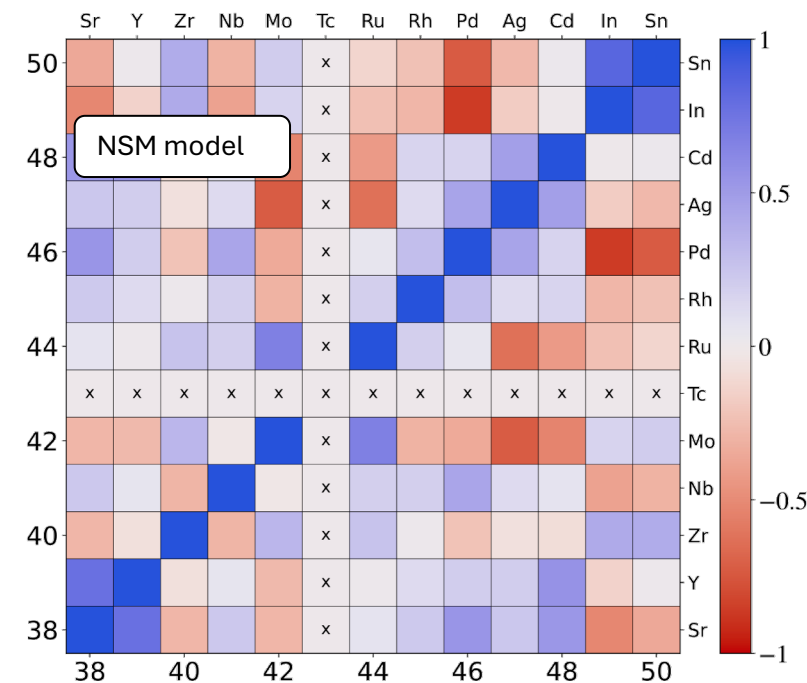
Correlations between astrophysical (n,γ) rates informed by reaction theory → correlations between observed elements



without OMP-based correlations

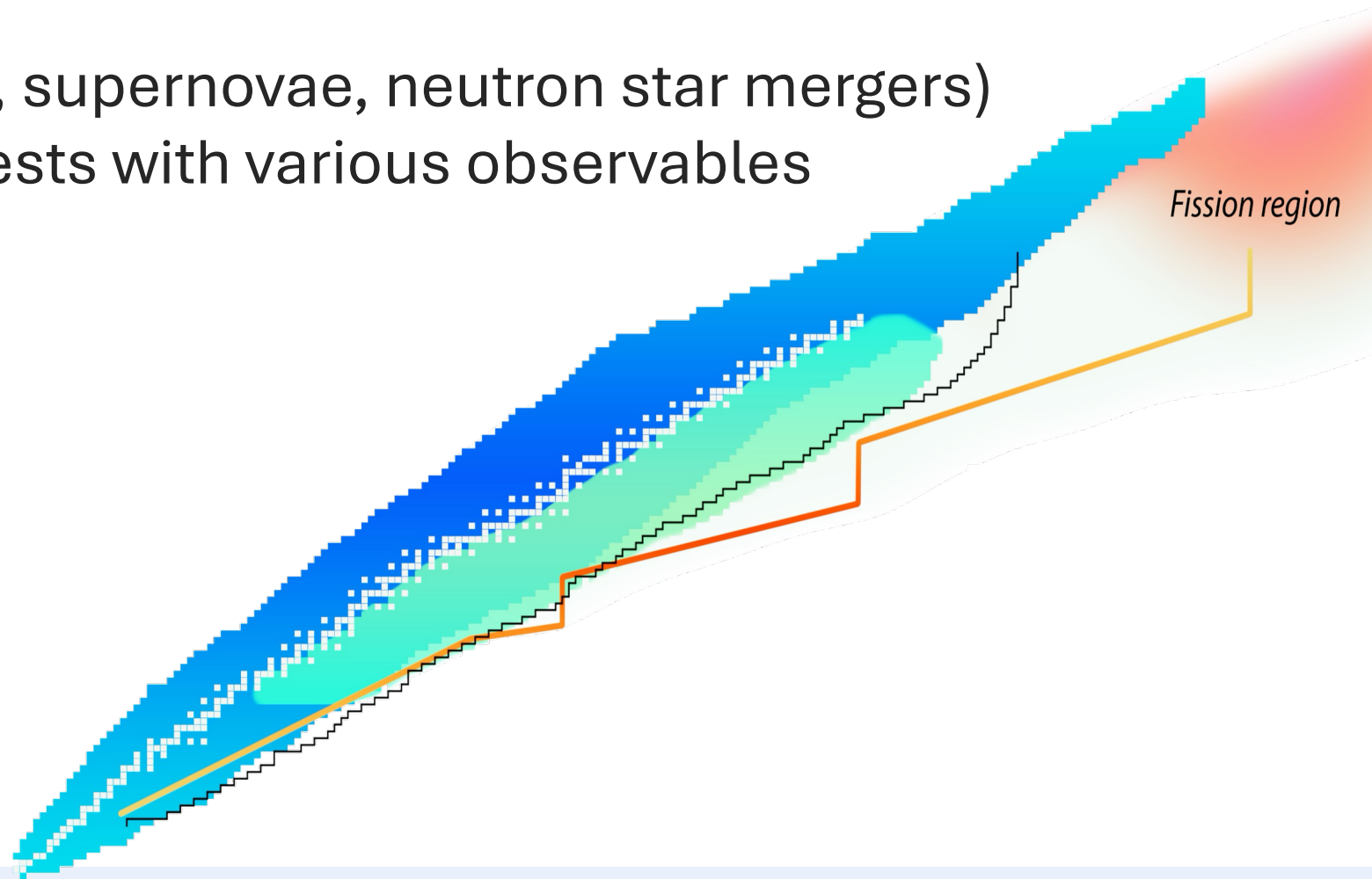


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Perspective: astrophysics to enable building cross-material covariances for neutron-rich nuclei?

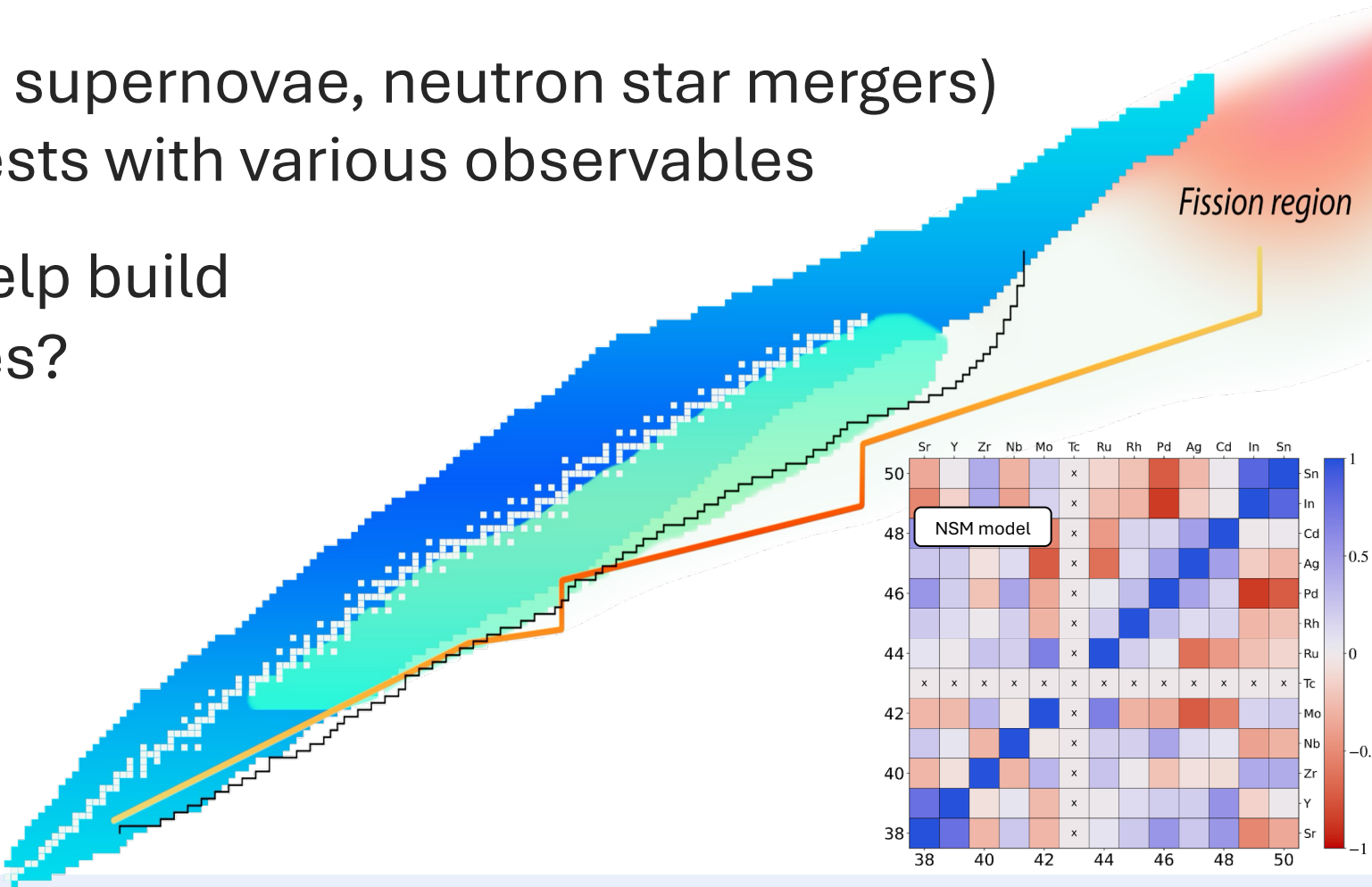
Astronomical events (e.g., supernovae, neutron star mergers) are the ultimate Integral tests with various observables



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Rich dataset: can AI/ML help build cross-material covariances?

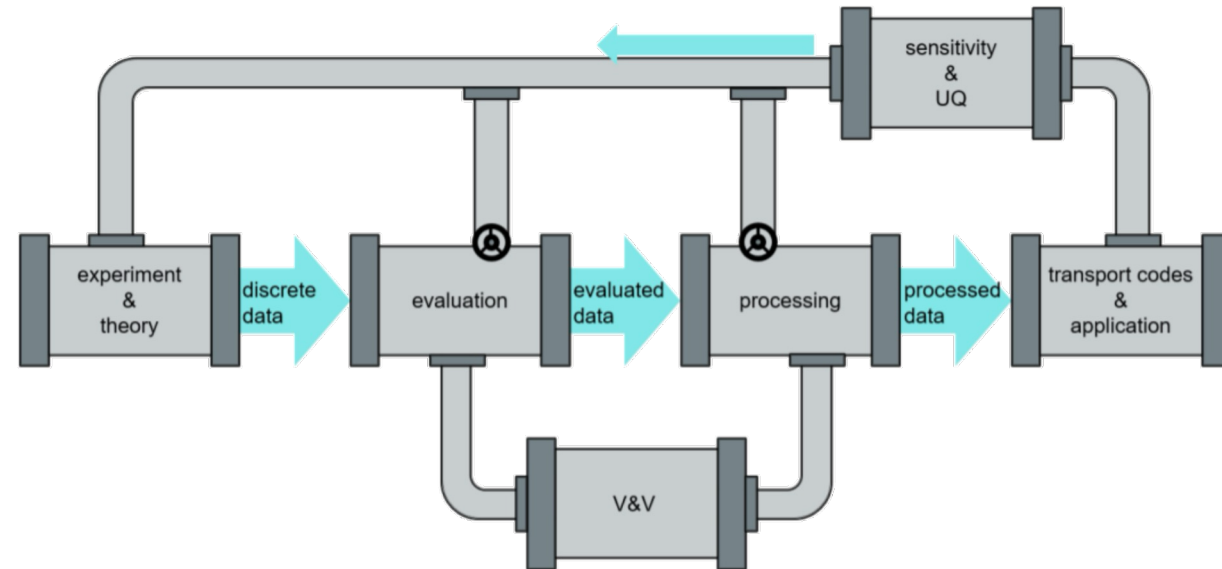


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Combined with iterative UQ (EMU), room for astro in the evaluation pipeline to constrain nuclear data/covariances?

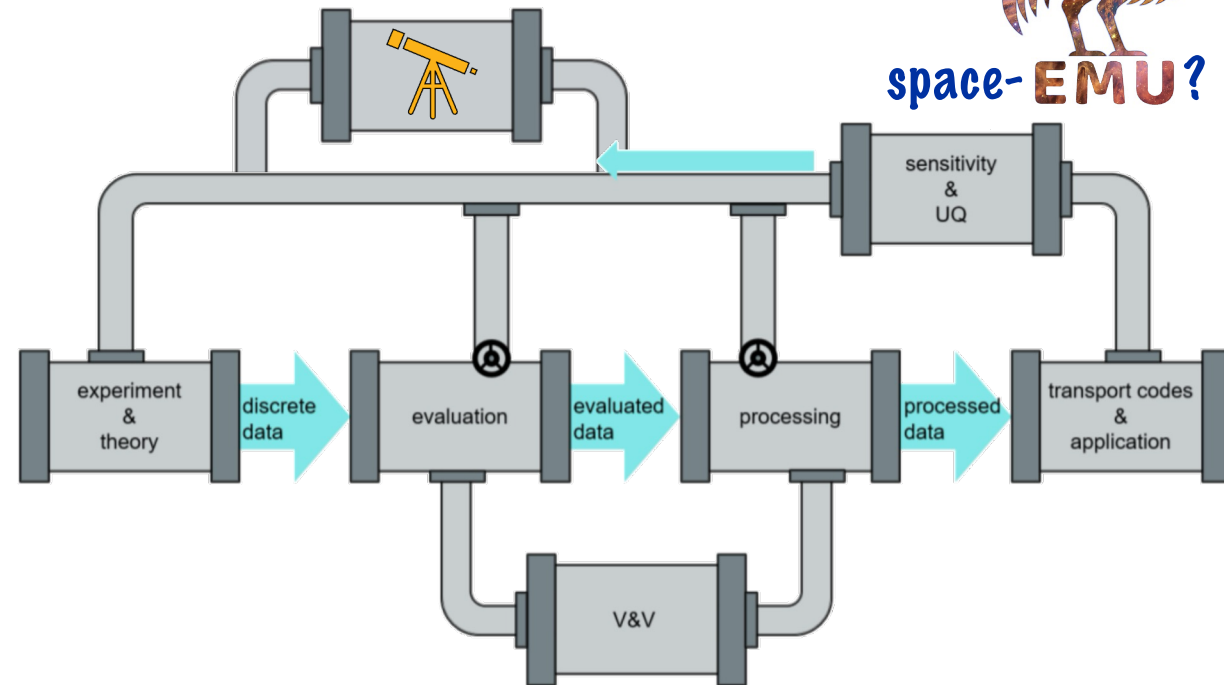


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Thanks!



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H. Choi



A. Sharma



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M. Salinas



M. Anastasiou



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