Deep learning nuclear cross sections

How deep is deep, really?

P(ND)^2-3
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Nicolas Schunck | NACS

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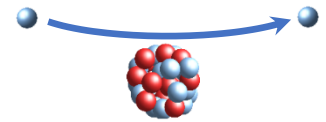
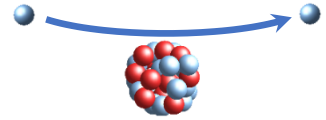
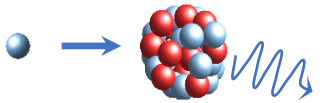
Nuclear cross sections encode the probability that a reaction takes place as a function of the energy of the projectile



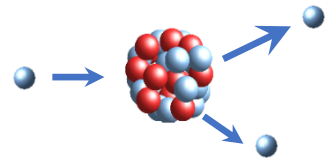
Elastic: X(n,el)



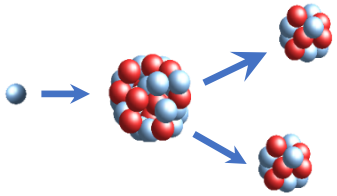
Inelastic: X(n,n')



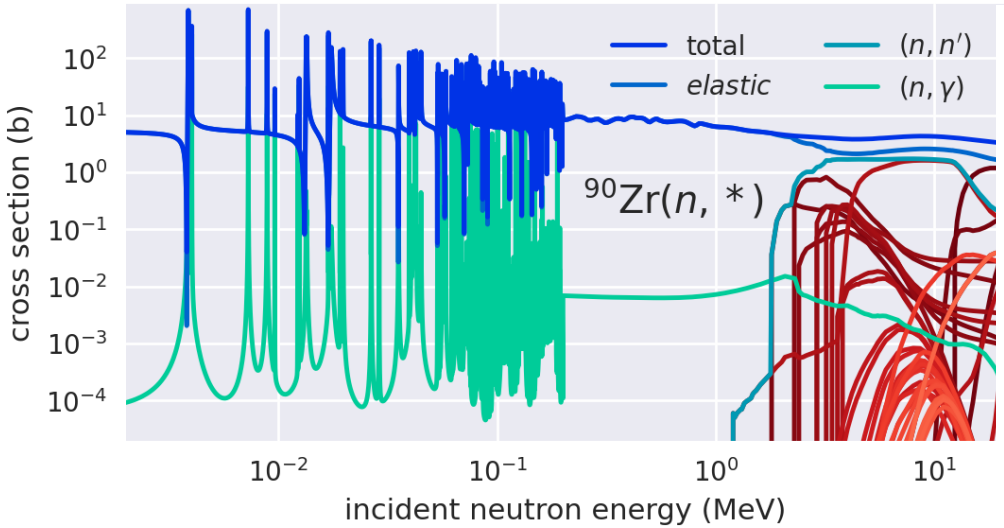
X(n,γ)

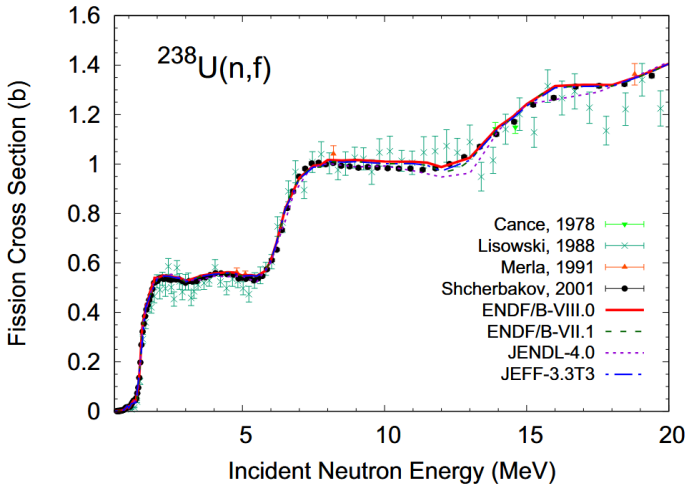


X(n,2n)



Fission: X(n,f)

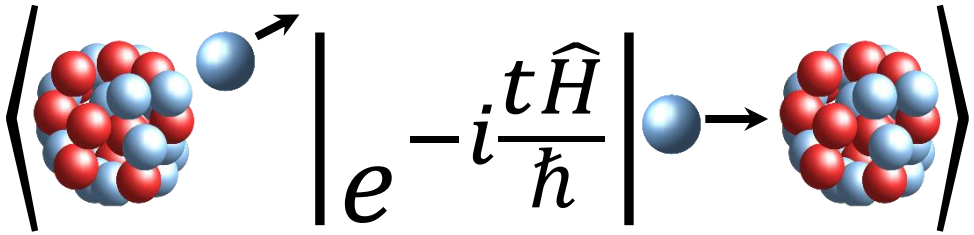




- Reaction cross section are often extremely hard to measure and have large uncertainties
- Discrepant measurements are common
- Theoretical predictions require blending nuclear structure with reaction theory

Data should emerge from a single quantum-mechanical theory of nuclei not a patchwork of independent calibrated models

Utopia



- Nuclear many-body problem is not solvable exactly
- Nuclear Hamiltonian is not that well known

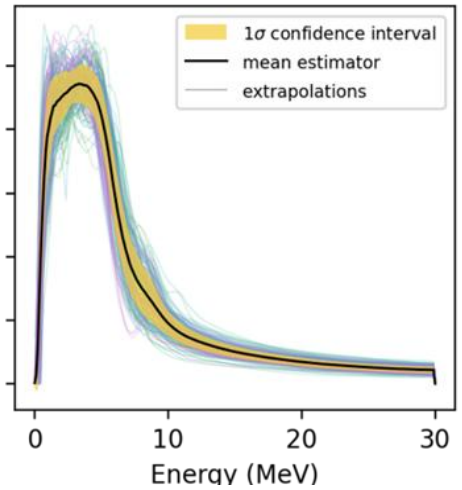
Real World

A. Optical Model 2845
1. Functional form 2847
2. Spherical dispersive OMP 2848
3. Coupled channels and direct reactions 2849
4. Semi-microscopic optical model (JLM) 2851
5. Complex particles 2853
6. Parameter uncertainties 2854
B. Level Density 2854
1. Constant temperature model 2854
2. Backshifted Fermi gas model 2856
3. Generalized superfluid model 2856
4. Collective effects in the level density 2857
5. Microscopic level densities 2858
6. Parameter uncertainties 2858
C. Gamma-ray Strength Functions 2859
1. Models for gamma-ray strength functions 2859
2. Renormalization of gamma-ray strength functions 2860
3. Photoabsorption cross section 2860
4. Parameter uncertainties 2860
D. Fission 2861
1. Fission transmission coefficients 2861
2. Fission barrier parameters 2863
3. Parameter uncertainties 2863
E. Compound Nucleus Reactions 2863
F. Pre-equilibrium Model 2866
1. Two-component exciton model 2866
2. Photon exciton model 2867
3. Continuum stripping, pick-up, break-up and knock-out reactions 2868
4. Pre-equilibrium angular distributions 2869
5. Parameter uncertainties 2870
G. Multiple Emission 2870
1. Multiple Hauser-Feshbach decay 2870
2. Multiple pre-equilibrium emission 2872
H. Nuclear Structure and Model Parameters 2872
I. Astrophysical Reaction Rates 2873

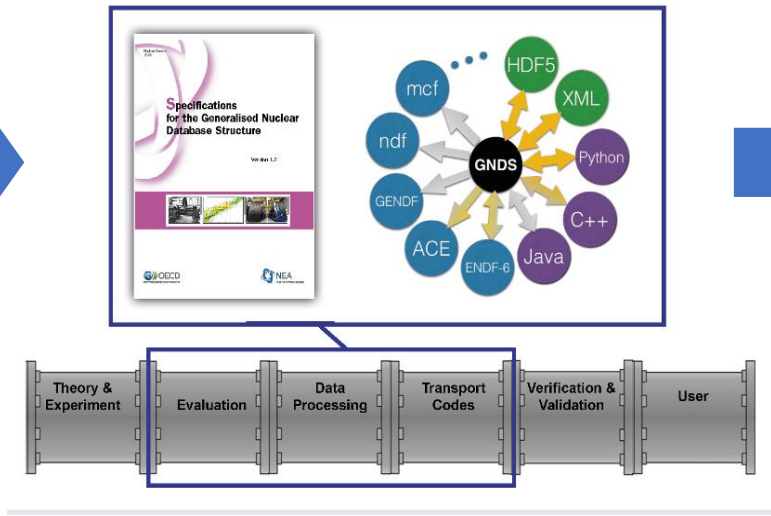
Uncertainties of nuclear cross section data ("covariances") are just about as important as data themselves

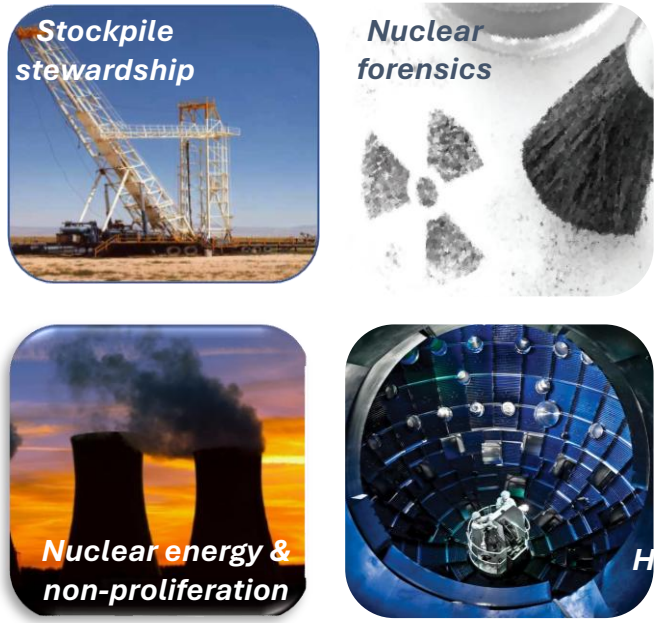
- There are always uncertainties in nuclear data: application users need to know them to propagate them in applications
- Users work directly with a full, processed library – not individual cross sections

Random realizations of cross sections

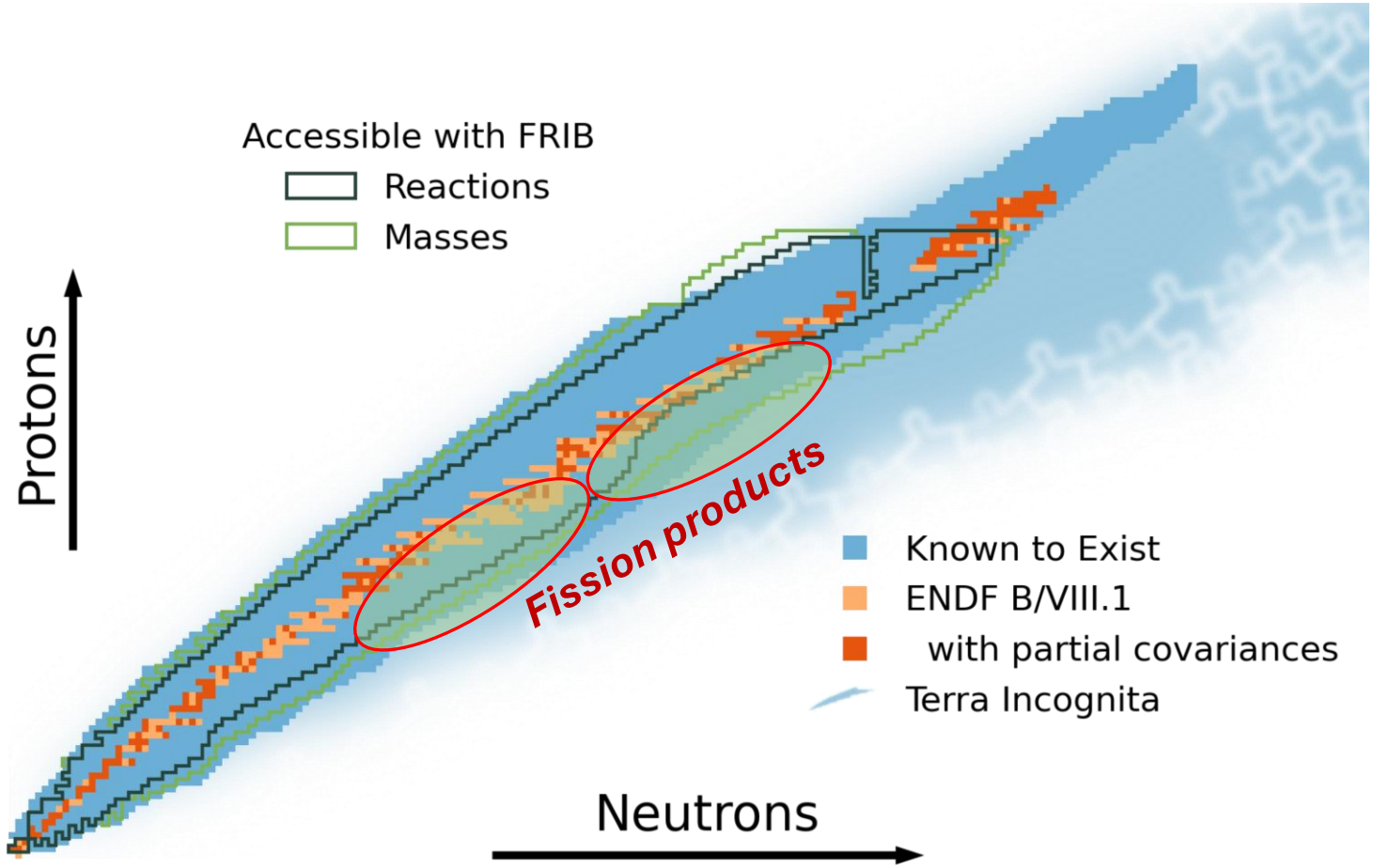


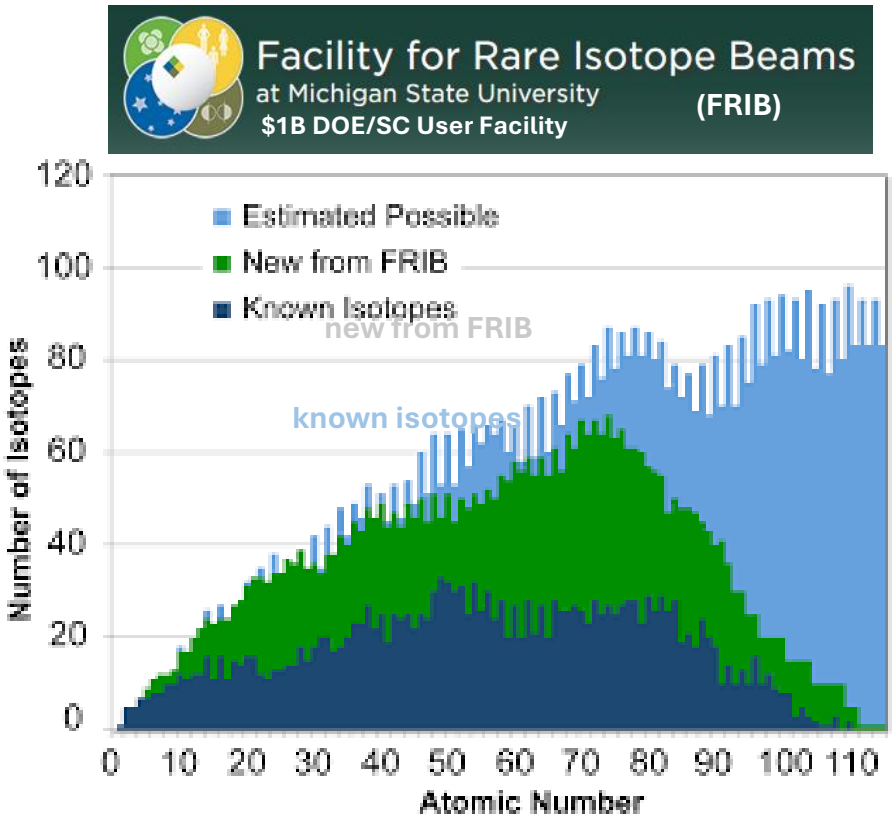
New sets of full libraries (additional processing)





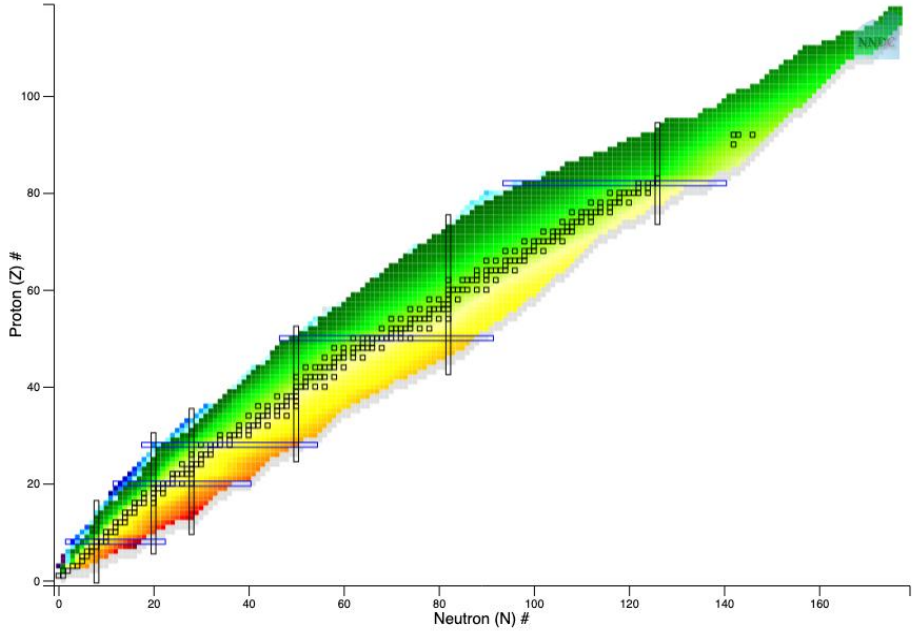
Only a tiny subset of data in current libraries contain covariances – cross-material covariances are nonexistent

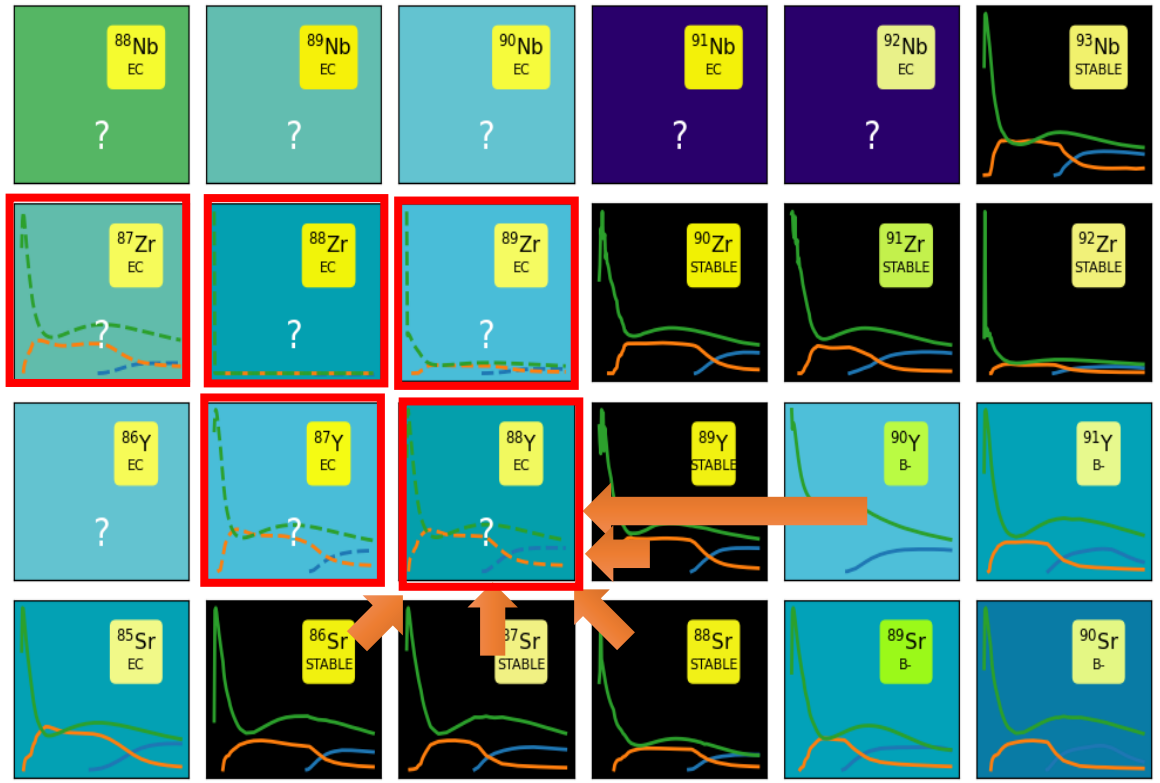




Reaction networks involve many radioactive nuclei that are largely inaccessible to experiments

Many nuclear properties exhibit clear, simple patterns across the nuclear chart – this is AI/ML territory



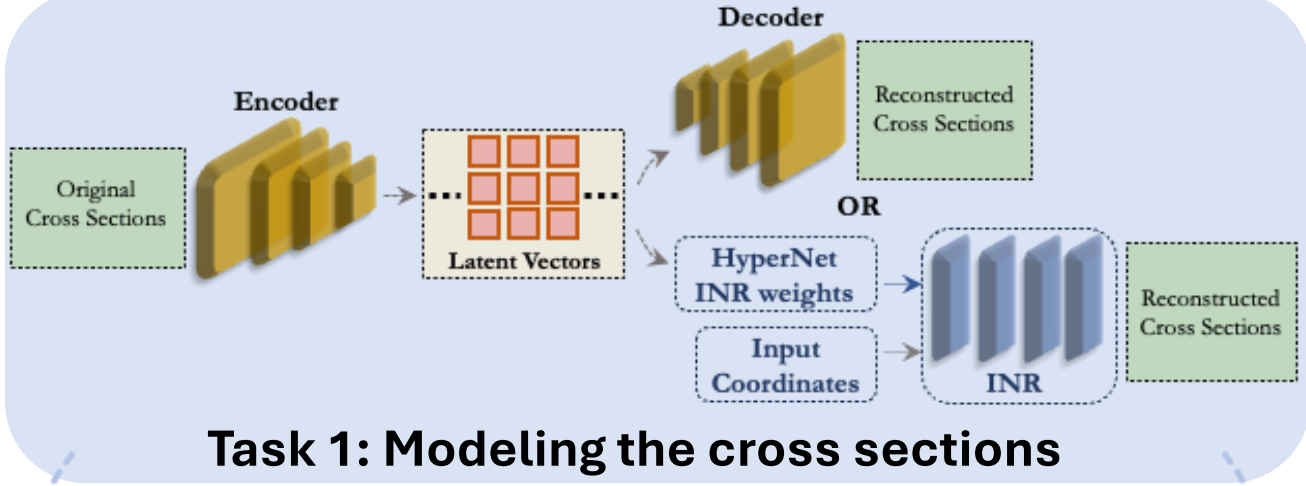


- Current nuclear theory cannot capture most of the correlations between nuclear data

Can an AI/ML model learn how cross sections transform as we add or remove nucleons?

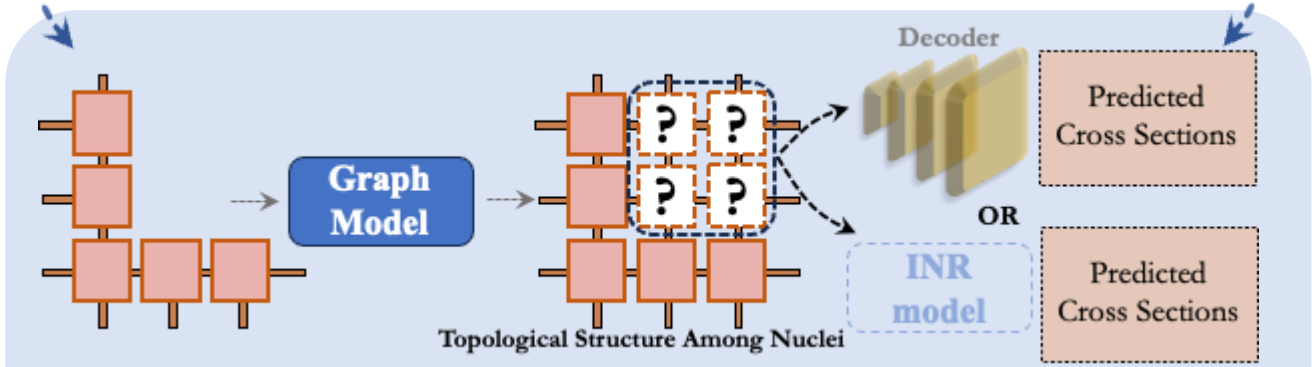
Our deep learning approach combines dimensionality reduction with predictions to enable uncertainty

Standard/INR-based Representation learning

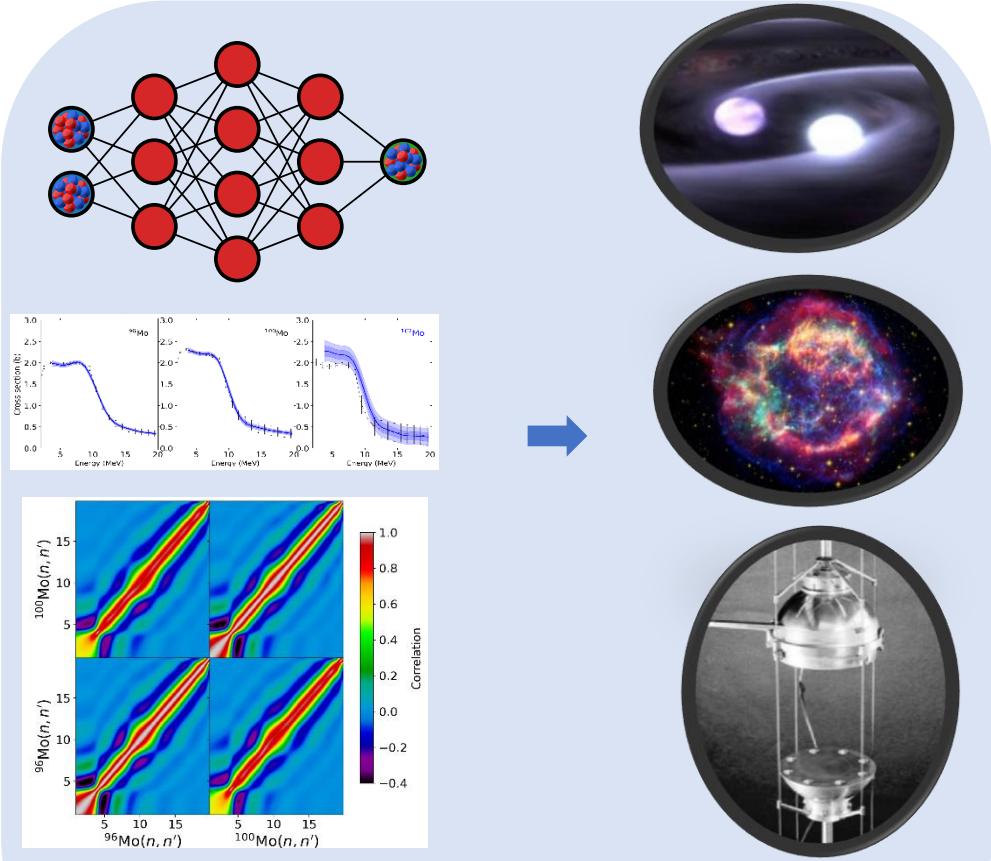


Task 1: Modeling the cross sections

Graph Neural Network Imputation



Task 2: Predicting unknown cross sections



Task 3: Uncertainty quantification and propagation

Variational autoencoders (VAE) compress information while allowing to generate new realizations

- Dataset = TENDL library
- Data size: N=1024
  - Cross sections = vectors of length 256 (values at energy points)
  - 4 cross sections simultaneously
- Latent space: dimension p=32
- 2151 original training samples
- Data augmentation: make linear combinations of existing cross sections to increase number of samples

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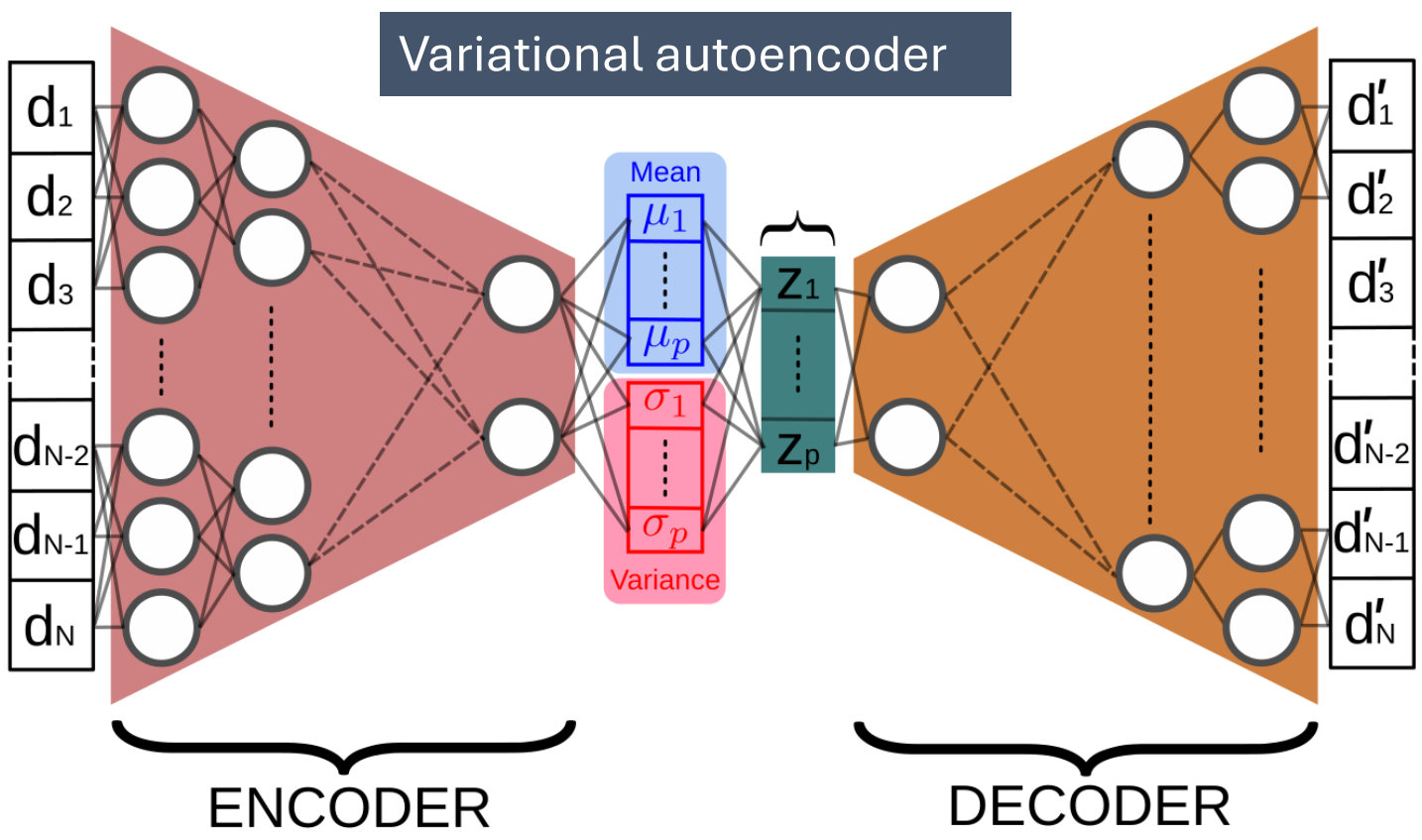
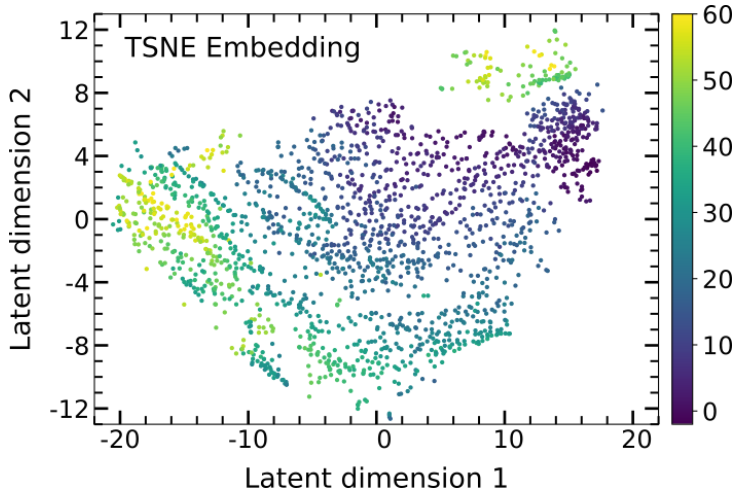
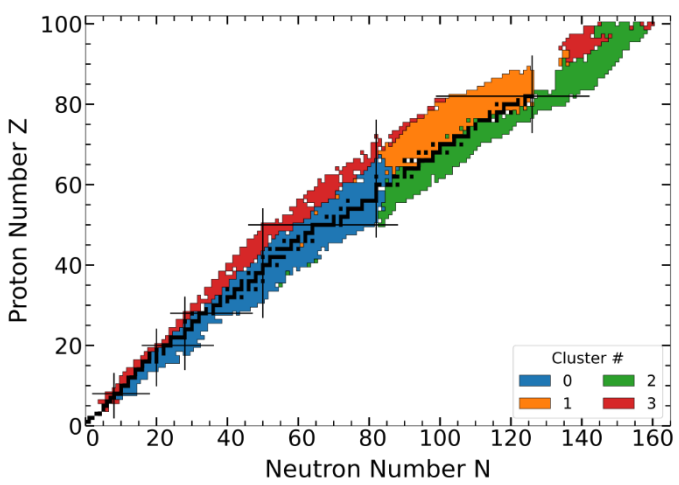
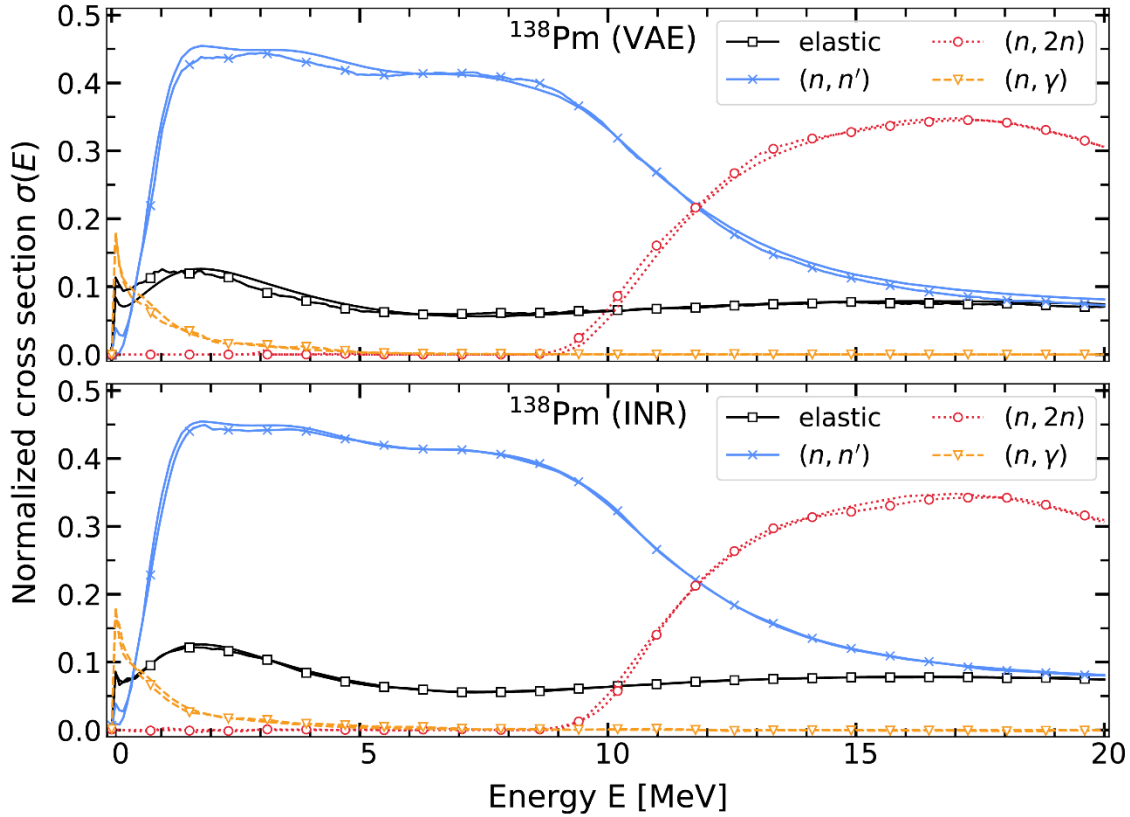


VAE excel at learning the space of cross sections and can already "discover" some physics

- Simultaneous encoding of 4 different channels with factor ~30x compression
- AI/ML can learn physical properties from encoding alone!



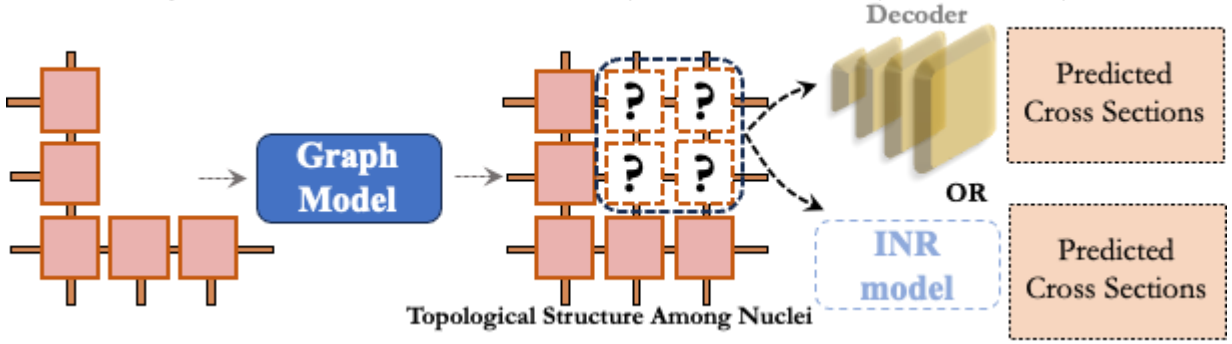




Precision of reconstruction is superior to typical experimental/model uncertainties

Graph neural network can learn the relationships between cross sections in different nuclei

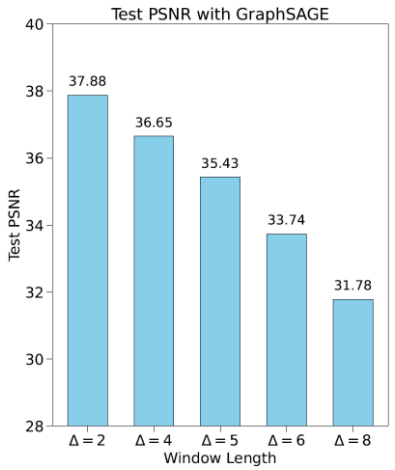
- Cross sections live on a 2D finite-size grid indexed by neutron and proton number
- Nuclear properties in “neighboring” nuclei are strongly correlated
- Finding missing nodes: the entire nuclear chart is modeled as a graph
  - Nodes = nuclei (N,Z) with cross-section data
  - Edges = local relationship based on proximity

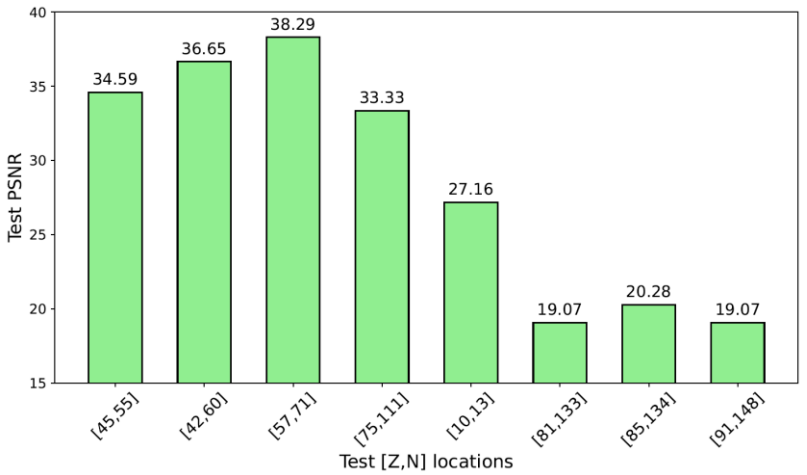


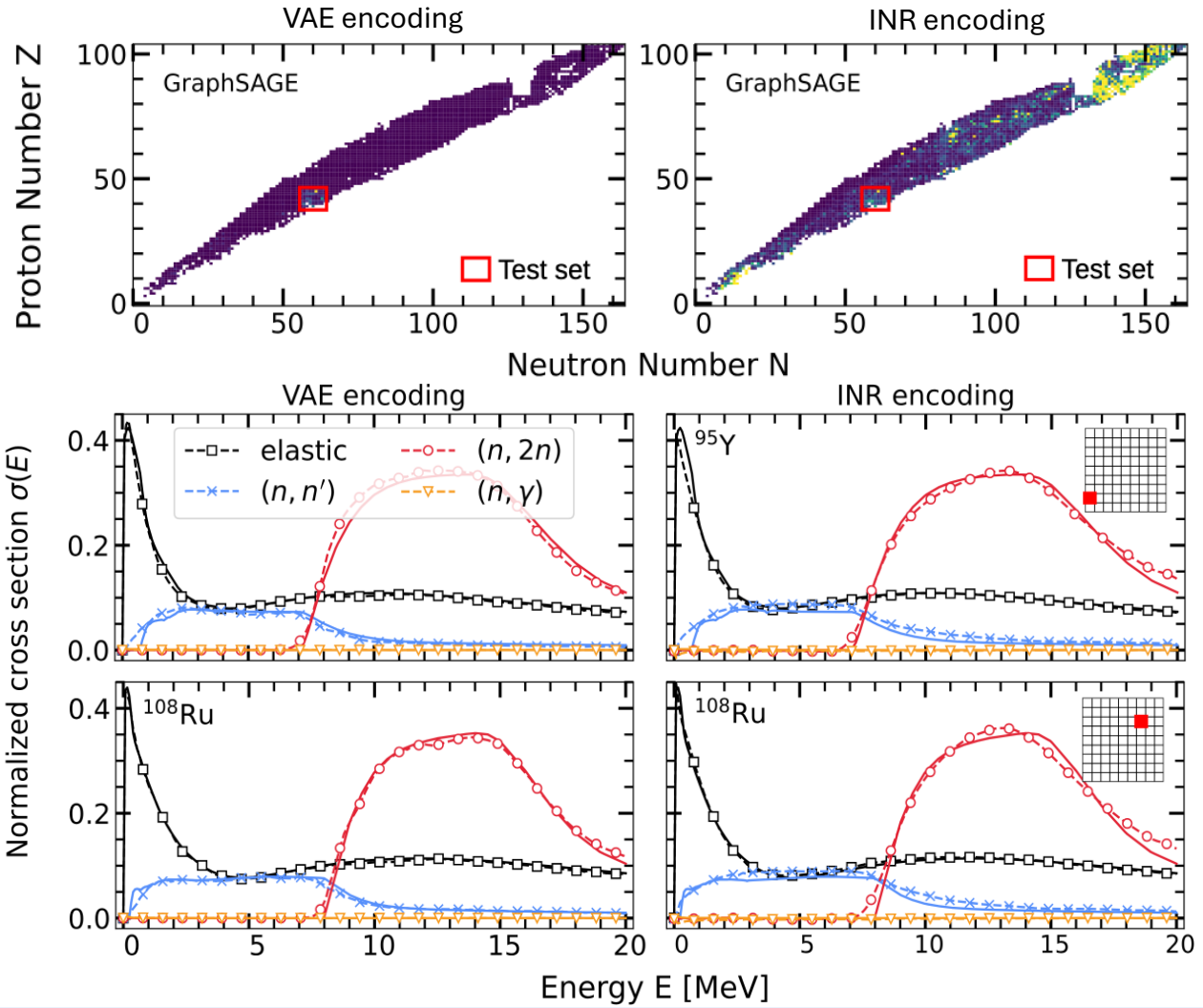
Aspect	Transductive Setting	Inductive Setting
Graph Access	Full graph (including test nodes) available during training	Test nodes are completely unseen during training
Test Region	Nodes are masked but part of the graph	Nodes are excluded from training input
Generalization Target	Learn to predict missing info within the same graph	Learn patterns that transfer to entirely new, unseen graph regions
Difficulty	Easier – Exploit full graph structure	Harder – Requires strong generalization beyond training distribution
Use Case	Imputation within a known domain	Deployment to new, unseen domains

Average error of GNN predictions across both training and testing set is very small

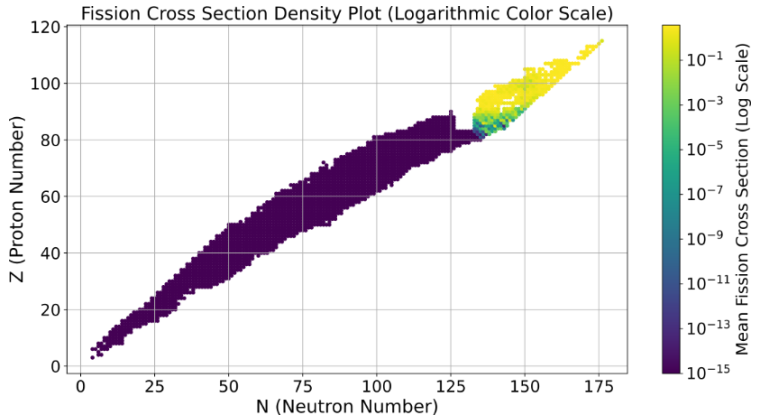
- Testing data ~ 3% of entire dataset
- Random masking of fraction of training set at each epoch (20% of training set)
- Predictions in ^{102}Mo = 5 neutrons and protons away from the training region





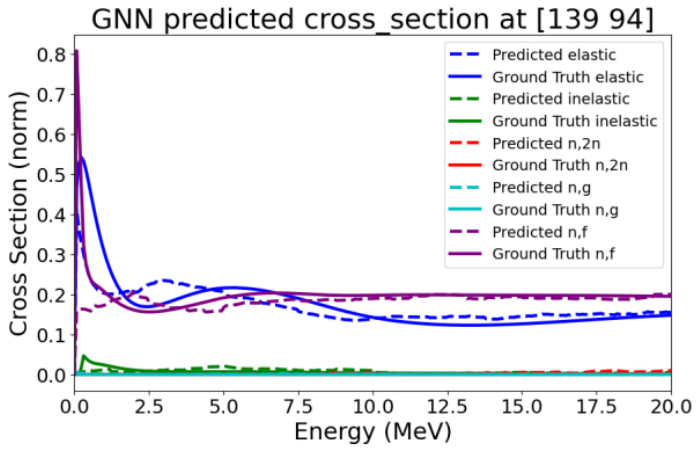


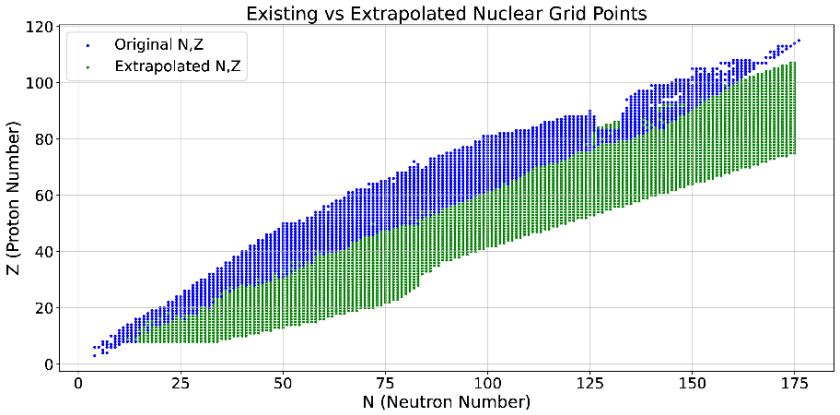
Adding fission cross sections or predicting far from training data quickly leads to problems

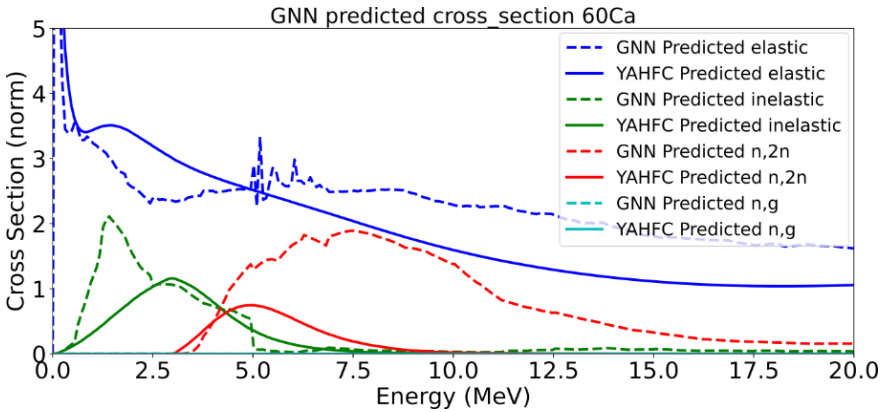


- Fission cross section only available for a small number of nuclei: how do we learn trends?
- How can we believe our training set also contains the physics of, say neutron-rich nuclei?

Work by **Manuel Catacorarios**







Exclusive data-driven deep-learning seems to have limited predictive power

Conclusion

- Demonstration of direct prediction of small set of neutron-induced cross section with AI/ML techniques
  - Fast regime is doable, resonance region would be a different story
  - It is possible to learn the joint latent space of several cross sections
- AI/ML provides an improvable ‘meta-model’ of cross sections that can quickly incorporate the effect of new data
- Predictive power remains inferior to physics-based models far outside training region
  - Small datasets are trademark of (nuclear) physics
  - Accuracy and precision requirements are significant challenges

Should AI/ML really be a substitute to nuclear theory or a tool to augment it?