Ex fissio ad astra: extending nuclear phenomenology to the fission fragment region

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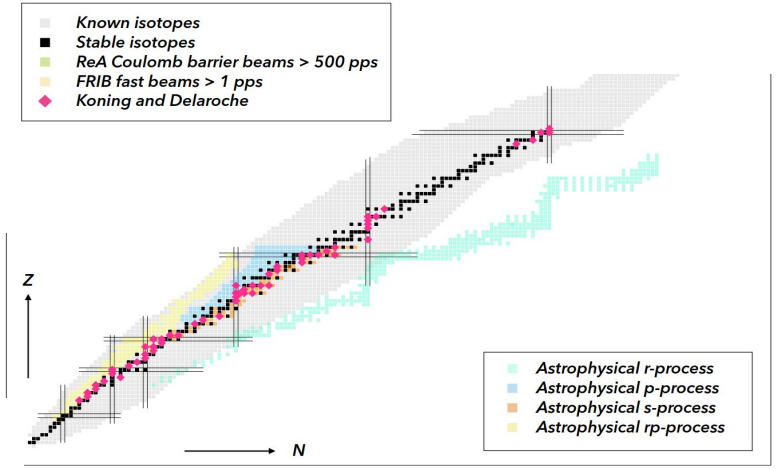
Mission Relevance: why do we care about fission fragments?

- **fission modeling** (e.g. CGMF): energy, open physics q's, data evaluation [Lovell and Neudecker, 2021]
- **cross sections for fission fragments**: spent nuclear fuel, accelerator driven and fast breeder reactors, non-proliferation, forensics [Hebborn et al., 2022]
- **cosmology:** neutron capture processes in supernovae and compact-object mergers
  - sensitive to isovector terms in optical model [Goriely and Delaroche, 2007]

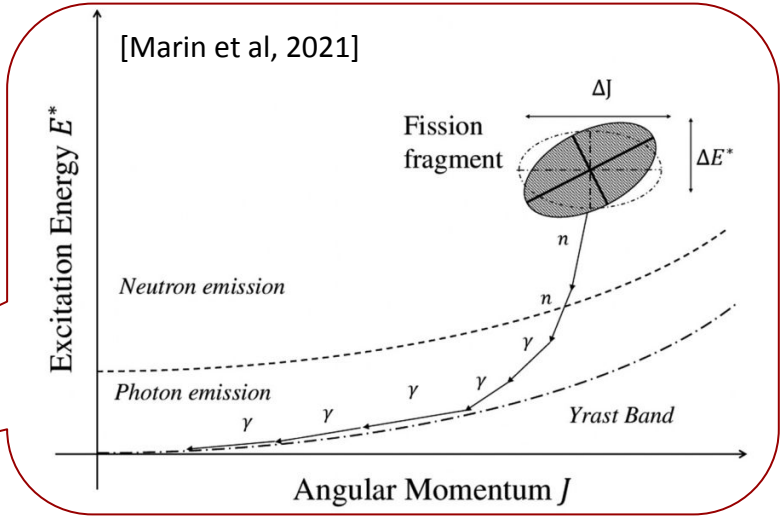


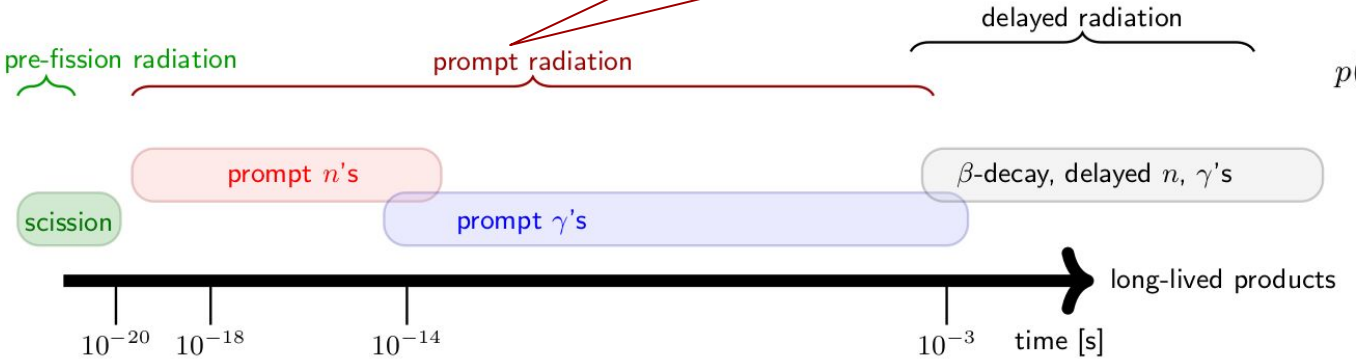
[Hebborn, et al, 2022]

Goal: construct the first Dispersive Optical Model (DOM) fit to fission observables

Fission fragment de-excitation

Experimental fission observables give us information about the behavior of neutron-rich isotopes



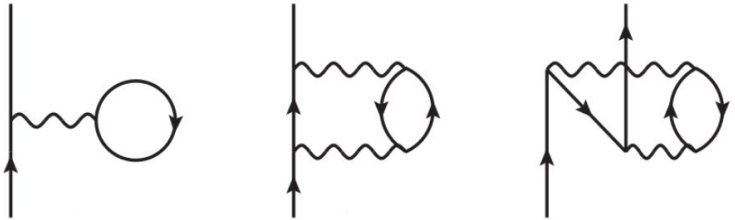


$$p(\alpha \to \beta) = \frac{|\langle \alpha|\mathcal{T}|\beta\rangle|^2 \rho(\beta)}{\sum_\gamma |\langle \alpha|\mathcal{T}|\gamma\rangle|^2 \rho(\gamma)}$$

Hauser-Feshbach picture

The Dispersive Self-Energy (DSE): like a complex “index of refraction” for nuclear media

- complex, energy dependent, non-local potential that a particle feels due to correlations with a medium:



1st (Hartree-Fock) and 2nd (1p1h) order contributions to the DSE

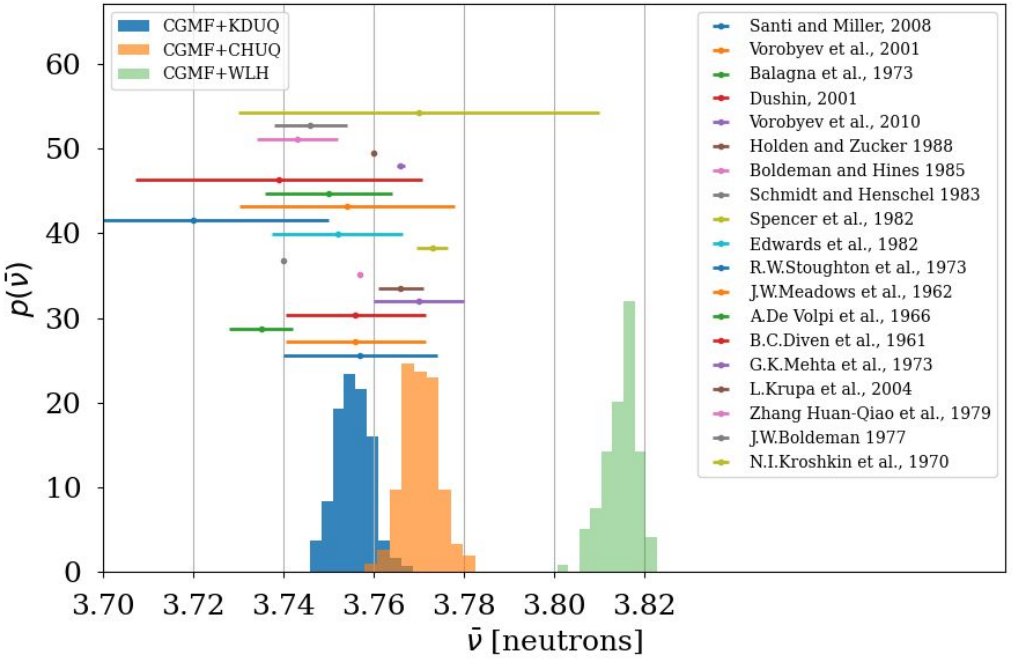
- phenomenological; can be fit to reaction and structure observables
  - function of (r,r’,E,A,Z)
  - 10-50 parameters

- Optical Model (OM) refers to simplified DSE models
- fit to reaction observables only (elastic xs)

Question: are fission observables even sensitive to the OM?

Method: Propagation of uncertainty of 3 optical models in CGMF to fission observables using Monte Carlo Hauser-Feshbach:

- phenomenological: **Koning-Delaroche**, **Chapel-Hill 89**
- microscopic: **Whitehead-Lim-Holt**



Answer: yes!

C. D. Pruitt, et al, 2023: arxiv.org/abs/2211.07741
T. R. Whitehead, et al, 2021: arxiv.org/abs/2009.08436

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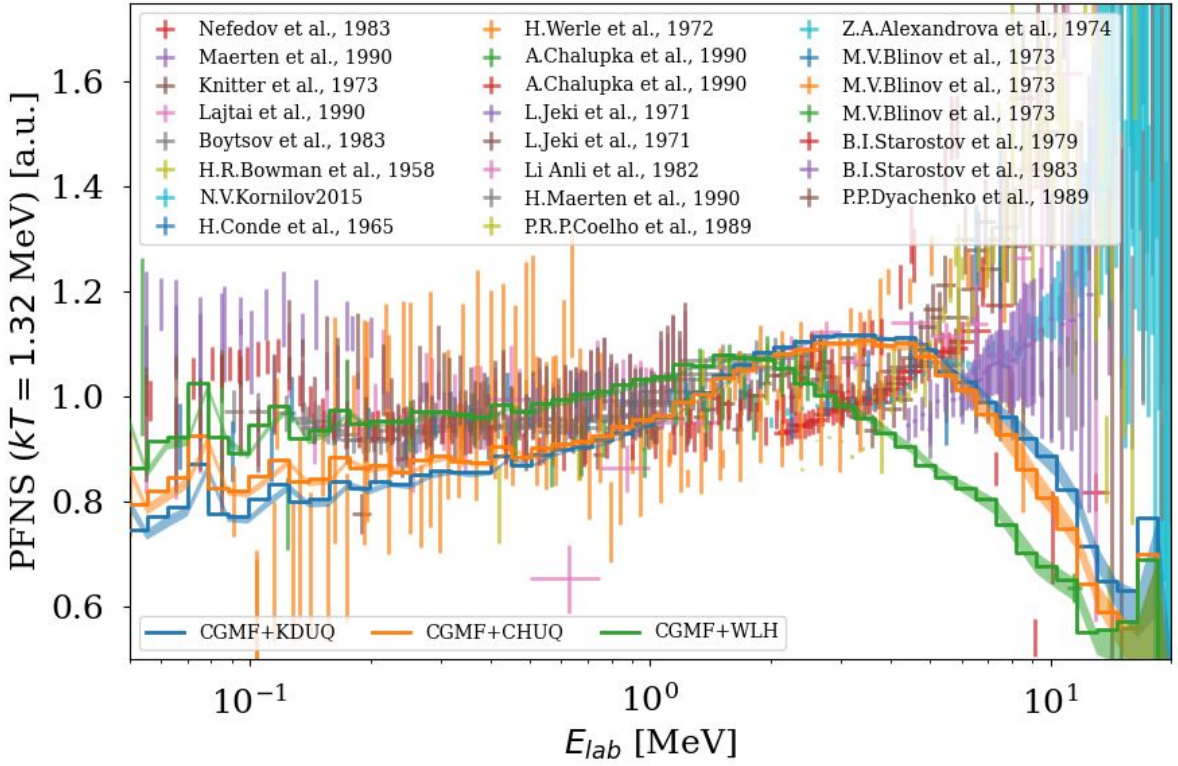
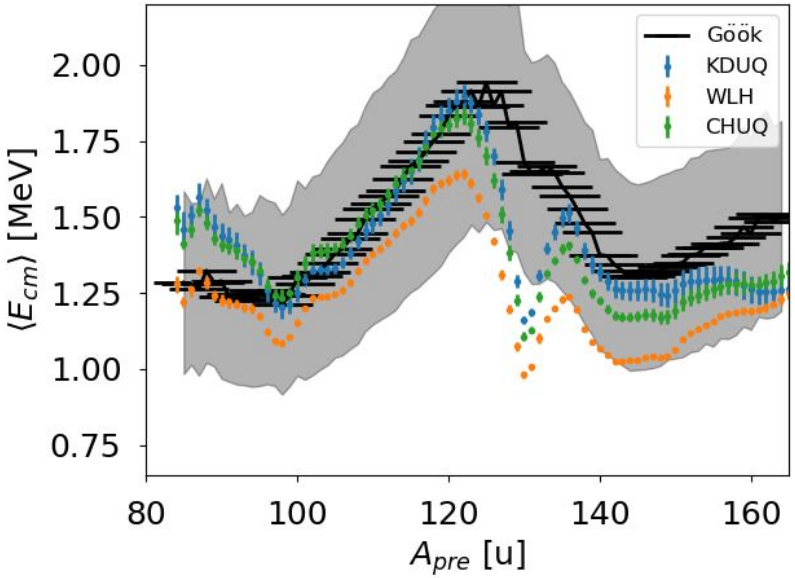
Question: are fission observables even sensitive to the OM?



Answer: sorta?

Question: are fission observables even sensitive to the OM?



Answer: yes!

- **key experiments: fragment-correlated neutron spectroscopy**
- **microscopic nuclear matter approach unsuitable?**

We can (and need to) speed things up by training a Reduced Basis Method (RBM) reaction emulator

- MCHF × MCMC? That's Monte-Carlo^2!
- the Reduced Basis Method (RBM) can be used to emulate a high-fidelity solver of the Schrödinger equation; quickly generate scattering solutions as a parameter is perturbed

Offline:

1. **Construct training space with high-fidelity solver**
2. **Compress with Proper Orthogonal Decomposition (POD)**

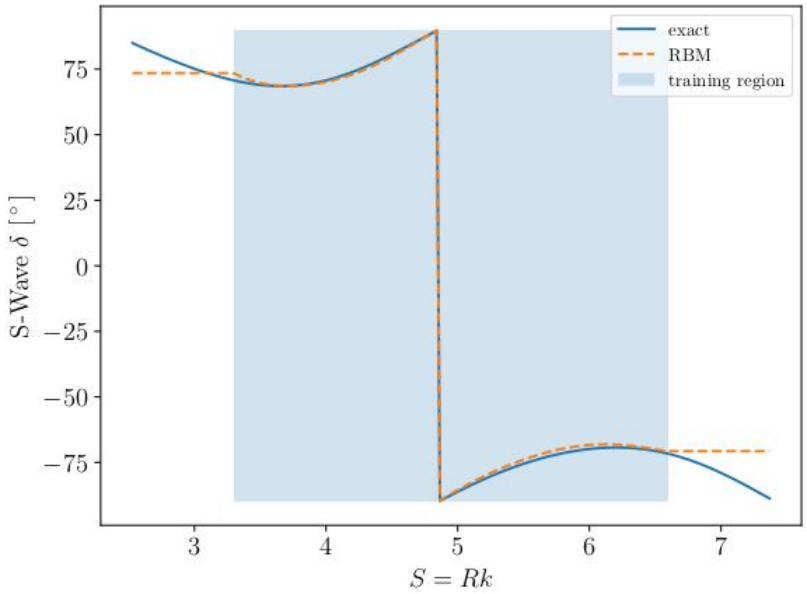
Online:

3. **Solve reduced system projecting onto principal components**

We can speed things up by training a Reduced Basis Method (RBM) reaction emulator

Test problem: scattering on a Woods-Saxon potential with varying width:

- **1000x speedup!**
- online stage: inverting 5x5 matrix
- non-affine in width parameter; requires Empirical Interpolation Method (EIM)
- github.com/kylegodbey/nuclear-rbm



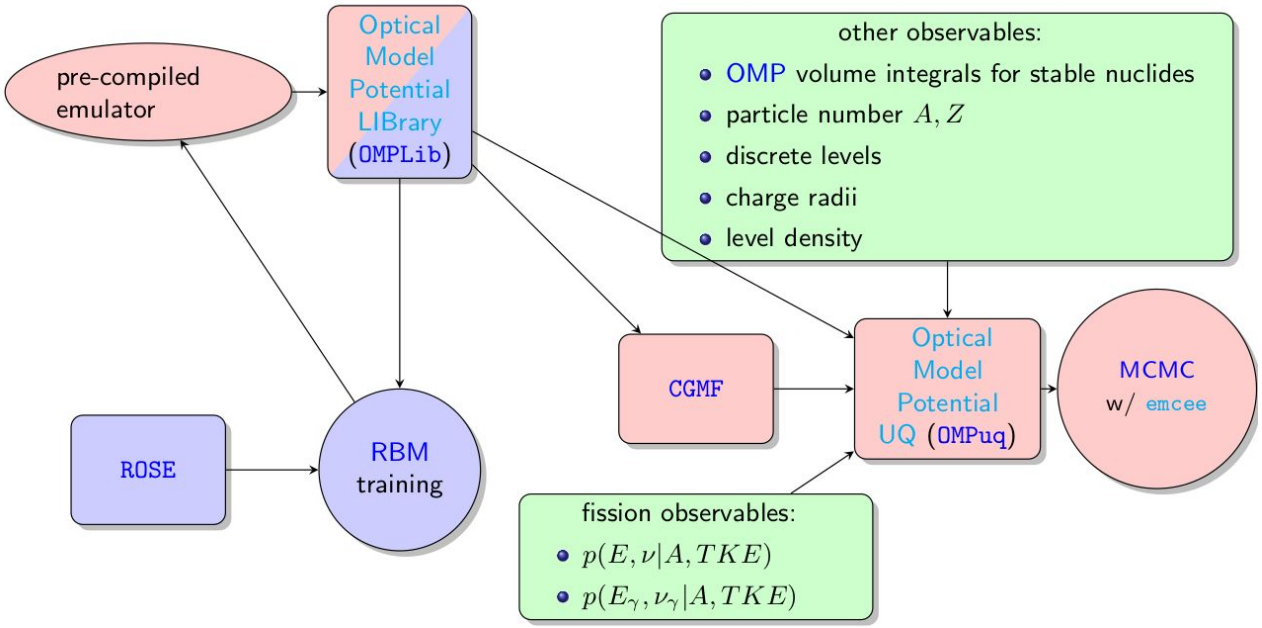
To do: put it all together and fit an optical model to fission

Novel Hauser-Feshbach approach using only ingredients from the DSE:

1. Determine off-shell T-matrix by solving the Dyson equation in Lagrange-Legendre basis
2. Determine single-particle propagator in momentum space from T-Matrix
3. Extract spectral density from imaginary part of propagator

No longer need external level density model!

$$p(\alpha \to \beta) = \frac{|\langle\alpha|\mathcal{T}|\beta\rangle|^2 \rho(\beta)}{\sum_\gamma |\langle\alpha|\mathcal{T}|\gamma\rangle|^2 \rho(\gamma)}$$



Conclusions:

- fission observables are sensitive to the optical model
- microscopic models from nuclear matter folding approach may be unsuitable to describe low energy scale of fission
- emulators based on the RBM show great promise to accelerate Monte Carlo Hauser-Feshbach simulations

Remaining tasks:

- integrate RBM emulator into Hauser-Feshbach
- perform MCMC fitting

Expected Impact:

- Better understanding of nuclear reaction and structure away from stability
- Improved modeling of systems with fission fragments
  - Breeder reactors, non-proliferation scenarios, etc.
- Optimization, uncertainty-quantification, significant (1E2-3x) speedup, to CGMF

MTV Impact:

- Collaboration with Cole Pruitt; LLNL Nuclear Data & Theory (NDT) group
- Fall 22 on-site visit and collaboration with Amy Lovell; LANL Nuclear Data Group (T-2)
- Collaboration with FRIB-TA/BAND via MSU & OU: github.com/kylegodbey/nuclear-rbm
- Calculable R-matrix code with library of optical potentials: github.com/beykyle/omplib
- Modified version of CGMF: github.com/beykyle/cgmf

Acknowledgements





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