Ex fissio ad astra:
Extending optical models to the fission fragment region

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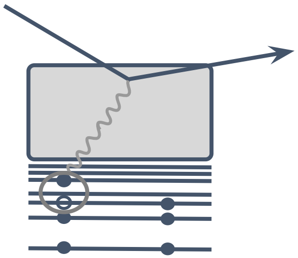
NUCLEAR ENGINEERING &
RADIOLOGICAL SCIENCES
UNIVERSITY OF MICHIGAN

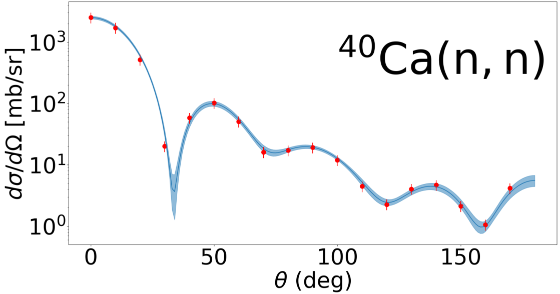
Workflow for phenomenology of compound nucleus reactions

1. measure $\mathcal{D}^{\text{direct}} = \{\frac{d\sigma_\alpha}{d\theta}, \sigma_{\text{el}}, \sigma_t\}$

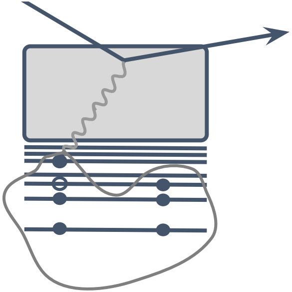


$$\frac{d\sigma_\alpha}{d\theta} \propto |\langle \alpha \,|\, \mathcal{T} \,|\, \alpha \rangle|^2$$

1. measure $\mathcal{D}^{\text{direct}} = \{ \frac{d\sigma_\alpha}{d\theta}, \sigma_{\text{el}}, \sigma_t \}$
2. calibrate optical model potential $V(r, E, A, Z; \boldsymbol{\zeta})$ to maximize posterior likelihood $p(\boldsymbol{\zeta} | \mathcal{D}^{\text{direct}})$



Courtesy of Pablo Giuliani and Daniel Odell



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Workflow for phenomenology of compound nucleus reactions

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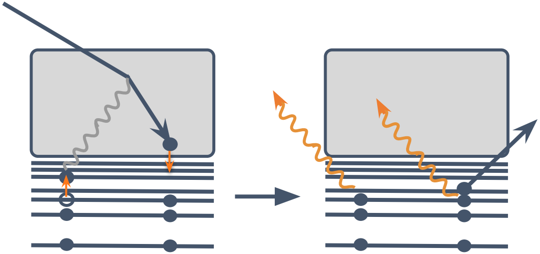
2. calibrate optical model potential $V(r, E, A, Z; \boldsymbol{\zeta})$ to maximize posterior likelihood $p(\boldsymbol{\zeta}|\mathcal{D}^{\text{direct}})$
3. apply optical model to generate transmission coefficients for compound-nucleus reactions

Using Hauser-Feshbach formalism de-excitation of compound nucleus is Markovian process:

$$p_{cc'}(\alpha) = \frac{|\langle\alpha|\mathcal{T}_{cc'}|\alpha\rangle|^2 \rho(E_{c'})}{\sum_{c''} |\langle\alpha|\mathcal{T}_{cc''}|\alpha\rangle|^2 \rho(E_{c''})}$$

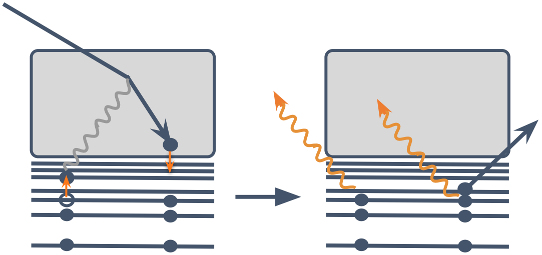


$$\sigma_{cc'} \propto |\langle\alpha\,|\,\mathcal{T}_{cc'}\,|\,\alpha\rangle|^2\, \rho(E_{cc'})$$

Often requires significant **extrapolation** of OMP away $A, Z \in \mathcal{D}^{\text{direct}}$

Can we globally optimize to both direct and compound reactions?

1. measure $\mathcal{D}^{\text{direct}} = \{\frac{d\sigma_\alpha}{d\theta}, \sigma_{\text{el}}, \sigma_t\}$
2. measure $\mathcal{D}^{\text{compound}} = \{\sigma_{cc'}\}$
3. calibrate optical model potential $V(r, E, A, Z; \boldsymbol{\zeta})$ to **both direct and compound observables** by maximizing posterior likelihood $p(\boldsymbol{\zeta}|\mathcal{D}^{\text{direct}}, \mathcal{D}^{\text{compound}})$



$$\sigma_{cc'} \propto |\langle \alpha \,|\, \mathcal{T}_{cc'} \,|\, \alpha \rangle|^2 \rho(E_{cc'})$$

Challenges:

- computational cost of evaluating posterior likelihood
- high-dimensional parameter and observable space

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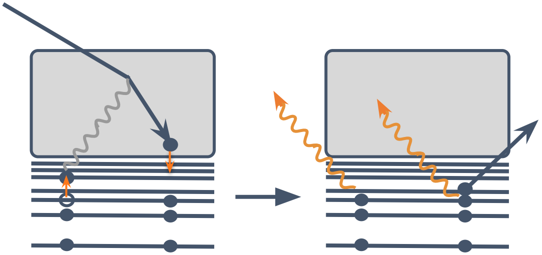


$$\sigma_{cc'} \propto |\langle\alpha|\mathcal{T}_{cc'}|\alpha\rangle|^2 \rho(E_{c'})$$

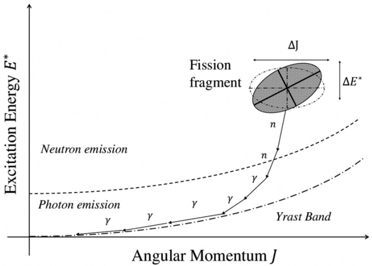
Challenges:

- computational cost of evaluating posterior likelihood $\rightarrow$ **emulators**
- high-dimensional parameter and observable space $\rightarrow$ **MCMC**

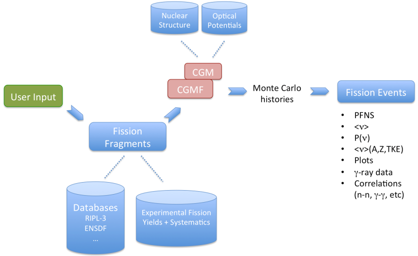
Fission as case study for fitting to compound nucleus reactions

Why do we care about fission fragments?

- **predictive fission modeling**: [Lovell and Neudecker, 2021]
- **cross sections for fission fragments**: nuclear non-proliferation, forensics and safeguards [Hebborn et al., 2022]
- **cross sections for r-process nuclei**: neutron capture processes in supernovae and compact-object mergers sensitive to isovector terms in optical potentials [Goriely and Delaroche, 2007]



[Marin et al., 2021] arXiv:2104.06166



Goal: Globally optimize OMP to observables including prompt neutron-fragment correlations with github.com/beykyle/cgmf [Talou et al., 2021]

But first, are fission observables even sensitive to the optical model?

- Propagate predictive posterior distribution of 3 OMPs through CGMF to fission observables
- Brute force approach - 40K cpu-hours
- `Python` bindings added to `CGMF` for massively parallel UQ using `mpi4py`
- replace scattering kernel with OMPLib

Uncertainty-quantified OMPs - potential priors for global fitting:

Phenomenological models fit to $\mathcal{D}^{\text{direct}}$ [Pruitt et al., 2020]:

- KDUQ
- CHUQ

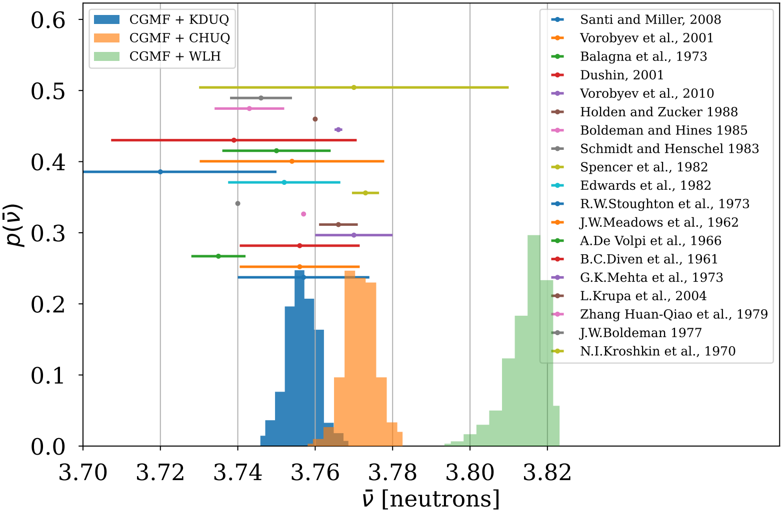
Microscopic model derived from N3LO χEFT forces in nuclear matter folder to nuclear density distributions

- WLH [Whitehead et al., 2021]

There are many observables we can use from $\mathcal{D}^{\text{fission}}$, all are noisy, convolved and depend on assumptions unrelated to OMP to model. Experiments are difficult, uncertainties may be missing/under-reported.

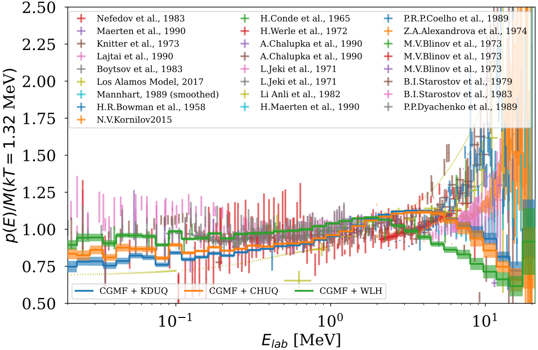
Are neutron yields sensitive to the optical model?

Posteriors propagated through to average neutron multiplicity per fission event in ^{252}Cf(sf)

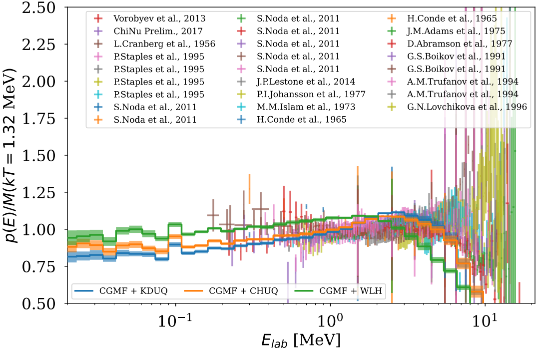


Are neutron energies sensitive to the optical model?

Credible intervals for Prompt Fission Neutron (energy) Spectrum (PFNS)



^{252}Cf(sf)

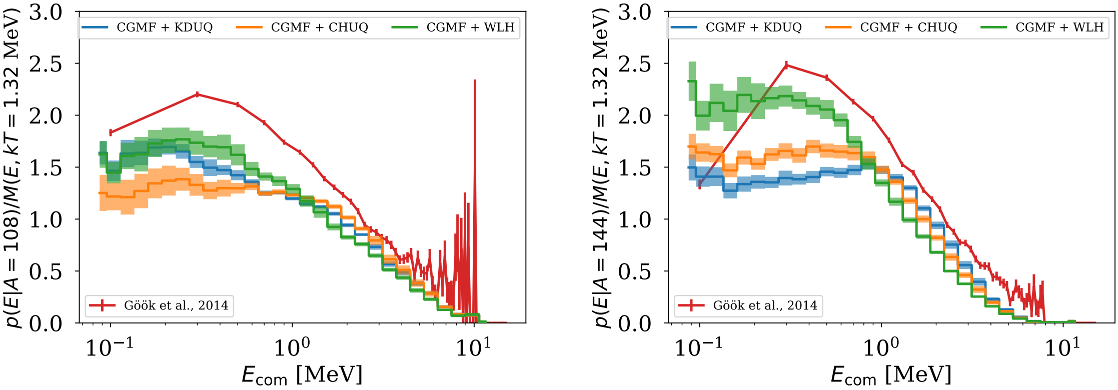


^{235}U(nth,f)

All OMPs are too soft, microscopic especially so. Finite size effects important at low energy; neglected in nuclear matter approach?

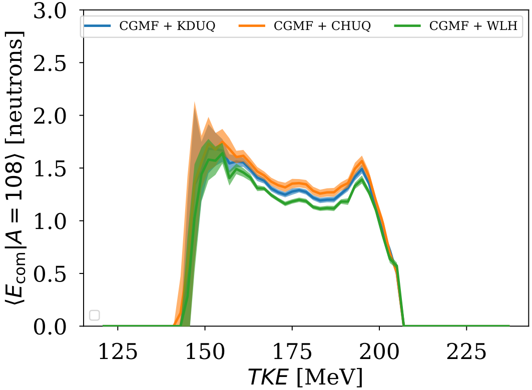
Are neutron energies conditional on A sensitive to the optical model?

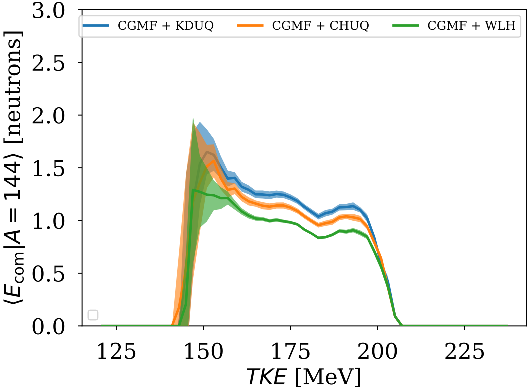
Credible intervals in $p(E_{\text{com}}|A)$ in ^{252}Cf(sf)



CHUQ and KDUQ disagree on A, E dependence away from stability - but both reproduce $\mathcal{D}^{\text{direct}}$. Issues with WLH limited to heavy fragment region.

Are neutron energies conditional on A & TKE sensitive to the optical model?

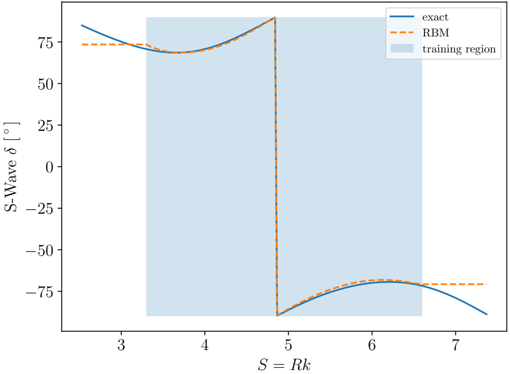




This can be measured with current experiments, and extracted event-by-event from past experiments

MCMC $\times$ MCHF $=$ MC^2!

- 1000x speedup for test problem - big implications for Monte Carlo Hauser-Feshbach
- intrusive nature allows us to emulate history-by-history correlations
- empirical interpolation to “affinize” potential: big speedup but hurts extrapolation
- embedding emulator in production code `CGMF`
- Stick around for Daniel Odell’s talk next
- (python note)book: nuclear-rbm



RBM emulator of S-wave phase shift δ_0 of the Woods-Saxon potential as width S is perturbed

Path forward

Conclusion:

- we can constrain reaction models away from stability by studying fission, but it requires emulation and careful Bayesian calibration

Path forward:

- incorporate RBM emulators into `CGMF`
- calibrate OMP to cross sections in FF region ($\mathcal{D}^{\text{direct}}$), and n-fragment correlations ($\mathcal{D}^{\text{fission}}$)
- include excitation energy sharing at scission in parameter space?
- treat deformations in (emulated) coupled channels approach?
- utilize Green's function formalism to understand Hauser-Feshbach better?
- handle unreported experimental error/covariances robustly?

Some lessons learned from ISNET-9:

- history-by-history (rather than histogram) treatment of observables $\mathcal{D}$
- Bayesian model mixing - let the model learn A, Z dependence?
- benefit of interacting with diverse multi-disciplinary community

Thanks for your time!

Thank you to the organizers, as well as to Pablo Giuliani, Kyle Godbey and Daniel Odell for teaching me emulators!

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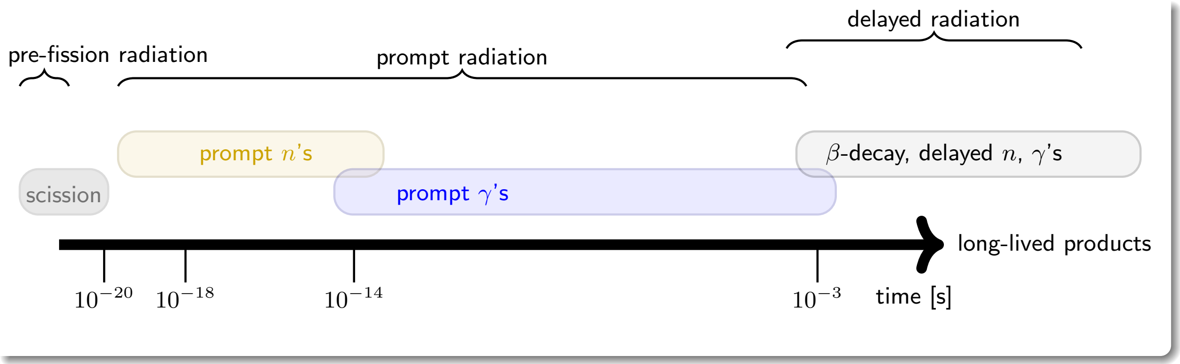
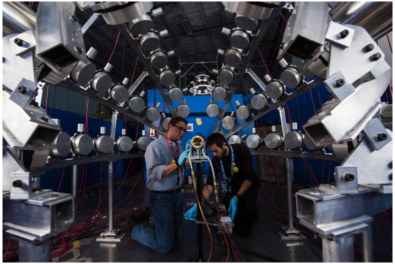
Backup slides

Fission and its observables



Goal: learn properties of neutron-rich nuclei by studying **prompt n's**, **prompt γ's**, & **fragments** from fission

Fission and its observables



Chi-Nu experimental array at LANSCE (courtesy of M. Devlin)

n-fragment correlations:

- [Göök et al., 2014] ^{252}Cf
- [Göök et al., 2018] ^{235}U

γ-fragment correlations:

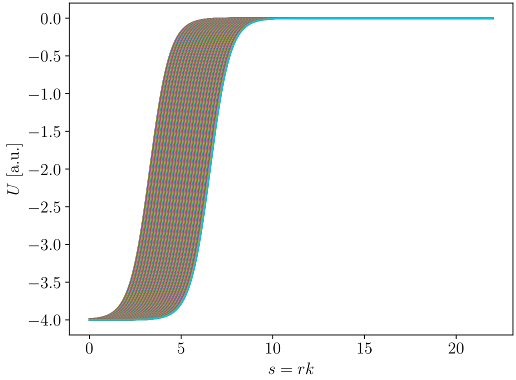
- [Travar et al., 2021] ^{252}Cf
- [Giha et al., 2023] ^{239}Pu
- [Wilson et al., 2021] ^{252}Cf, ^{238}U, ^{232}Th

n-γ-fragment correlations?

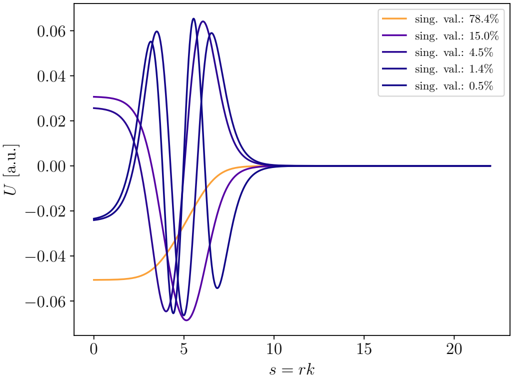
- Giha et al., ongoing at Gammasphere

Ideally, we would like an n-γ-fragment correlated measurement with $\sim$amu isotopic resolution

Affine-decomposition of a Woods-Saxon potential with Empirical Interpolation Method

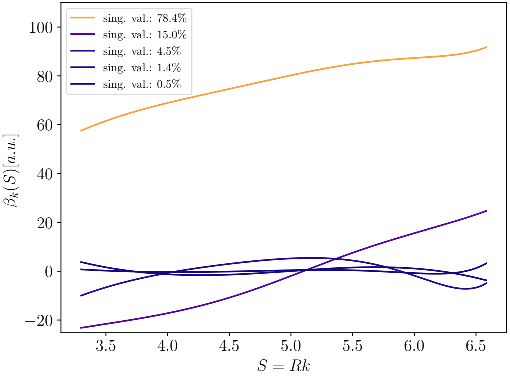


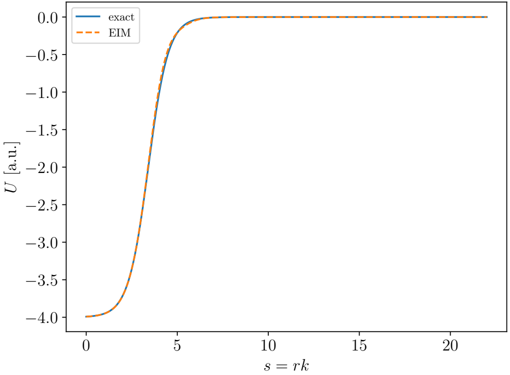
N training potentials $U(s, S_i)$ for $S \in T = \{S_i\}_{i=1}^N$



$M = 5$ principal components of the training set; $\{U_\kappa(s)\}_{\kappa=1}^M$

Affine-decomposition of a Woods-Saxon potential with Empirical Interpolation Method

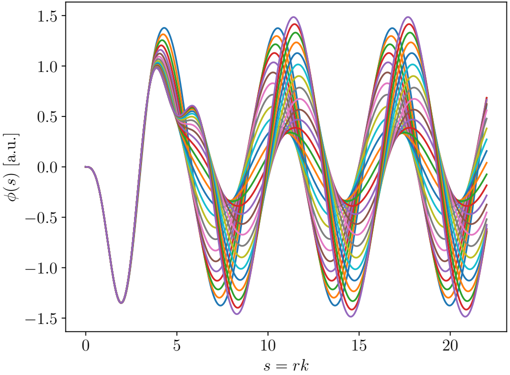




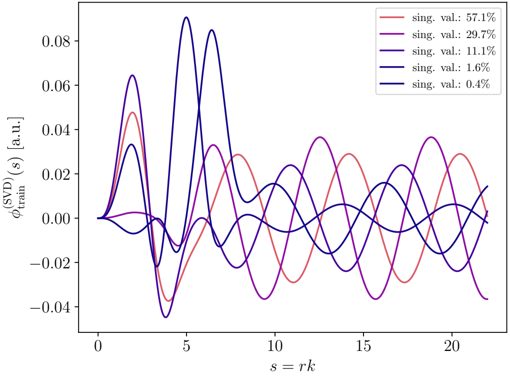
$$\beta_\kappa(S) = \sum_{j=1}^{M} \left(U_\kappa(s_j)\right)^{-1} U(s_j, S)$$

$$R = 3.1 \text{ fm}, \ k \approx 1.09 \text{ fm}^{-1}; \ S \approx 3.41$$
$$\{S_i\} \subset [3.29, 6.59]$$

Building a reduced basis for our scattering problem

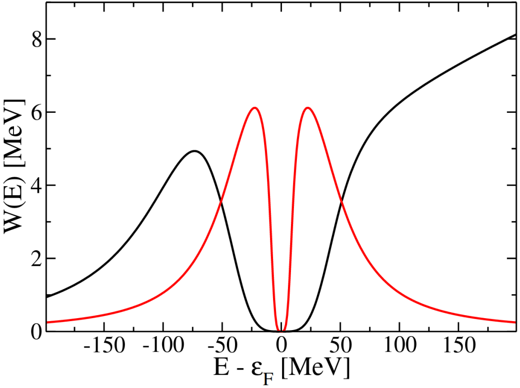


N high-fidelity training solutions with free solution subtracted $\{\psi_i(s) - \phi_0\}_{i=1}^{N}$



$P = 5$ principal components of the training set $\{\phi_j\}_{j=1}^{P}$

Long-range correlations at low energy



Energy dependence of imaginary **volume** and **surface** terms in a phenomenological DOM [Waldecker, 2011]. **Surface** term dominates at low energy due to LRCs!