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Potential Energy Surface Emulation and Impact on Fission Trajectories

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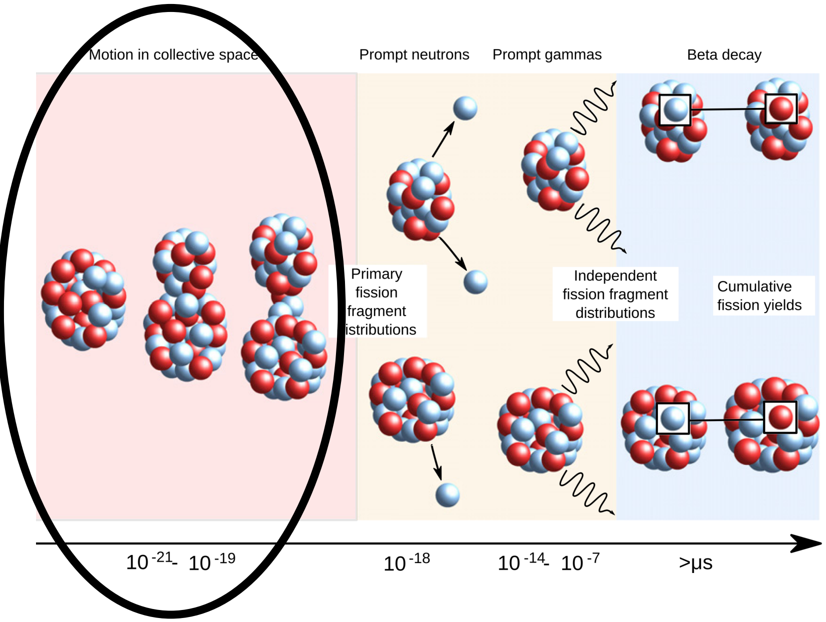
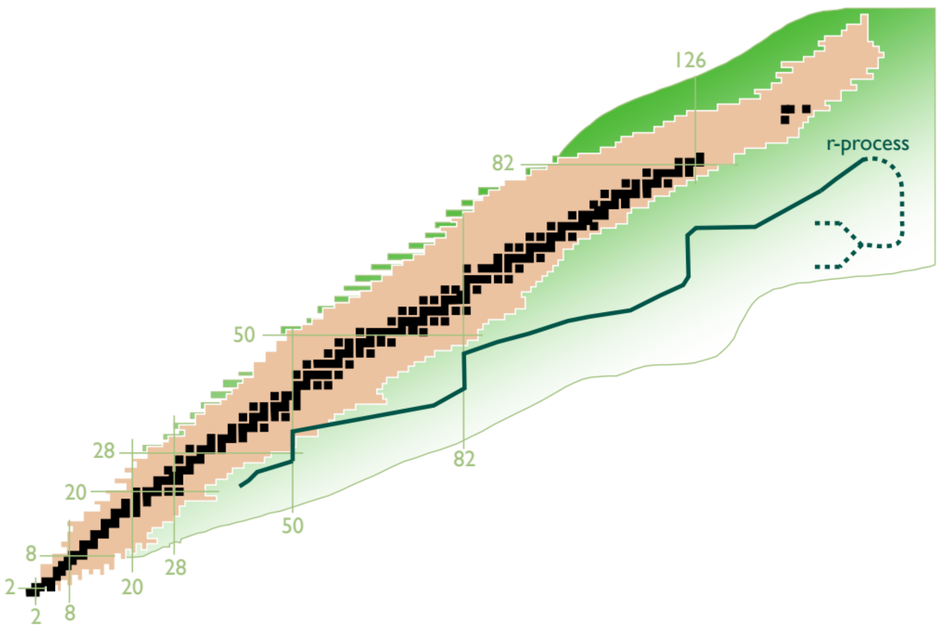
Outline

- Physics overview
  - Nuclear fission
  - Density functional theory
  - WKB approach to tunneling
- Neural network overview
- Results

Nuclear Fission

- Splitting of heavy nucleus into lighter fragments
- Important for understanding *r*-process nucleosynthesis, through fission cycling

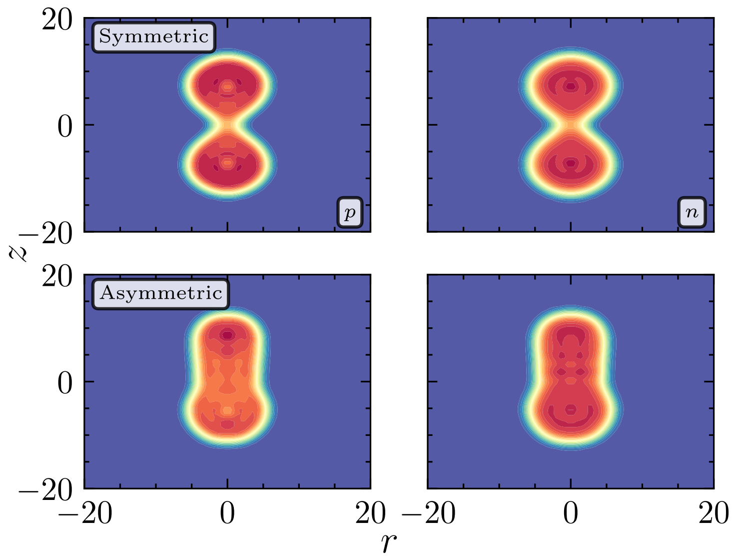




Left: M. Bender, et al. "Future of nuclear fission theory." J. Phys. G Nucl. Part. Phys. 47.11 (2020): 113002.
Right: https://cococubed.com/pix_pages/nuclide_chart.shtml

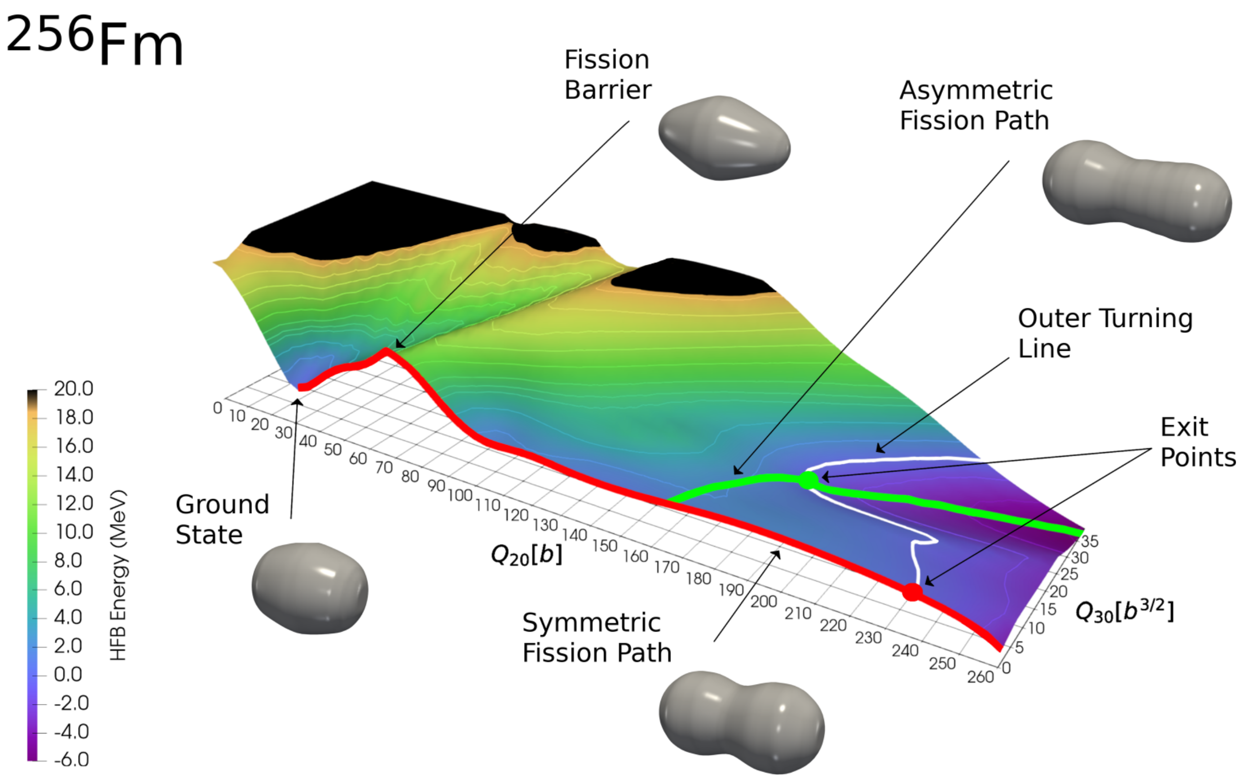
Density Functional Theory (DFT)

- Solve Hartree-Fock-Boguliubov (HFB) equations with a density-dependent energy density functional
  - Nucleons move in a self-consistent mean field
  - Describes collective motion well
  - Static description of the nucleus
- Use constrained HFB equations to examine nuclear shape



DFT and Fission

- For grid of deformations, compute:
  - HFB energy, for potential energy surface (PES)
  - Collective inertia tensor $M_{\mu\nu}$

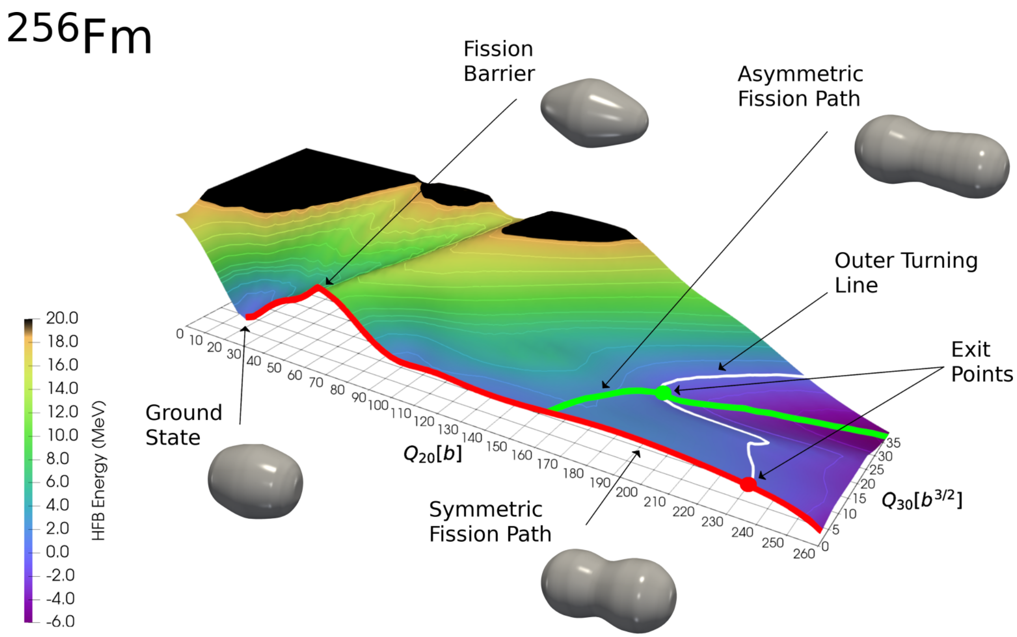


DFT and Fission

- Fission described as tunneling through a barrier
  - Solve in WKB approximation

$$L(s) = \int_{s_0}^{s_1} ds \sqrt{2V_{\text{eff}}(s)M_{\mu\nu}(s)\dot{q}_\mu \dot{q}_\nu}$$

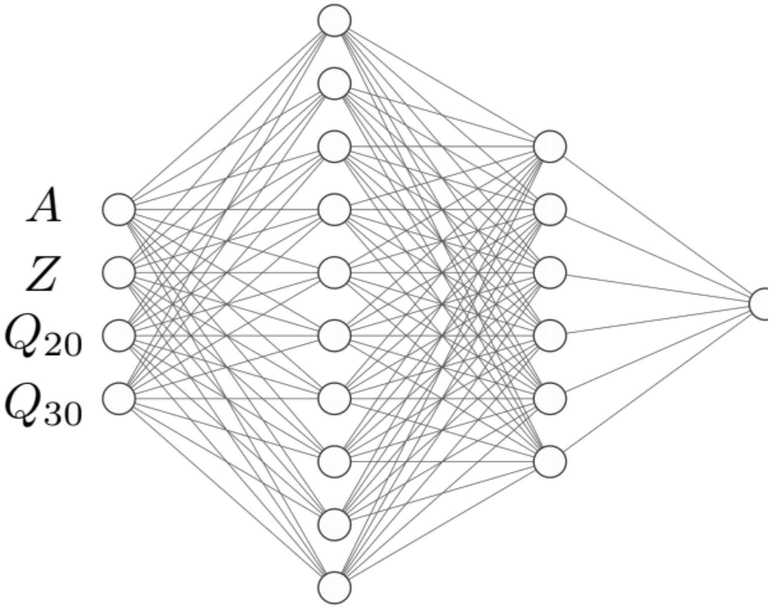
  - Fragment yields determined by exit point location [1]



[1] J. Sadhukhan et. al., Phys. Rev. C 101, 065803 (2020)

Neural Network Emulator

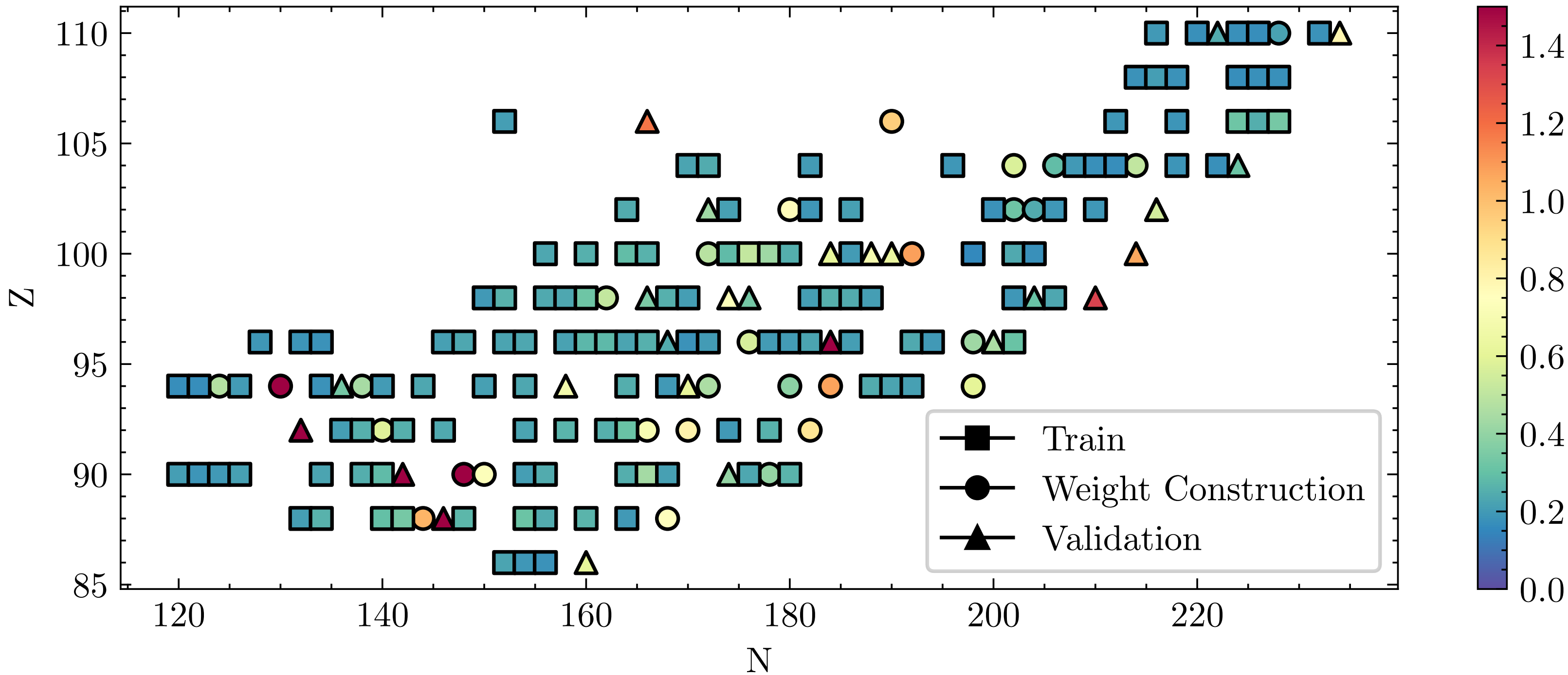
- Use committee of neural networks (NNs) to emulate PES and collective inertia across the nuclear chart, similar to [1]
- Collective inertia must be positive semi-definite matrix
  - Emulate eigenvalue decomposition of inertia
  - Components vary on multiple scales, so emulate log of values
- Dataset is 200 nuclei, with ~700 points per nucleus
  - From D1S Gogny interaction [2]
- Vary depth of NN



[1] R.-D. Lasseri et. al., Phys. Rev. Lett. 124, 162502 (2020)
[2] J. Berger et. al., Nucl. Phys. A 428, 23 (1984)

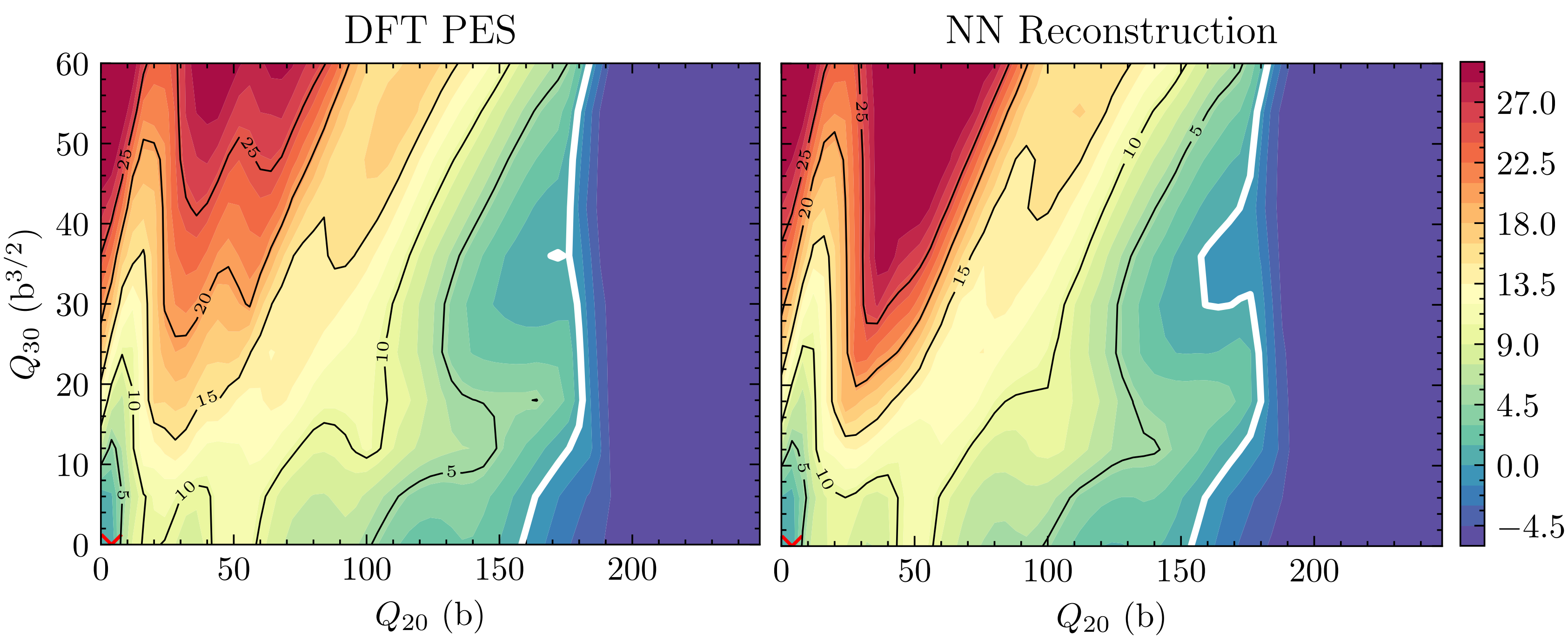
Results: PES Quality

- Root-mean-squared error across all nuclei considered
  - PES varies on order of 10 MeV
- PES of most nuclei reproduced well
  - Order of 400 keV RMSE



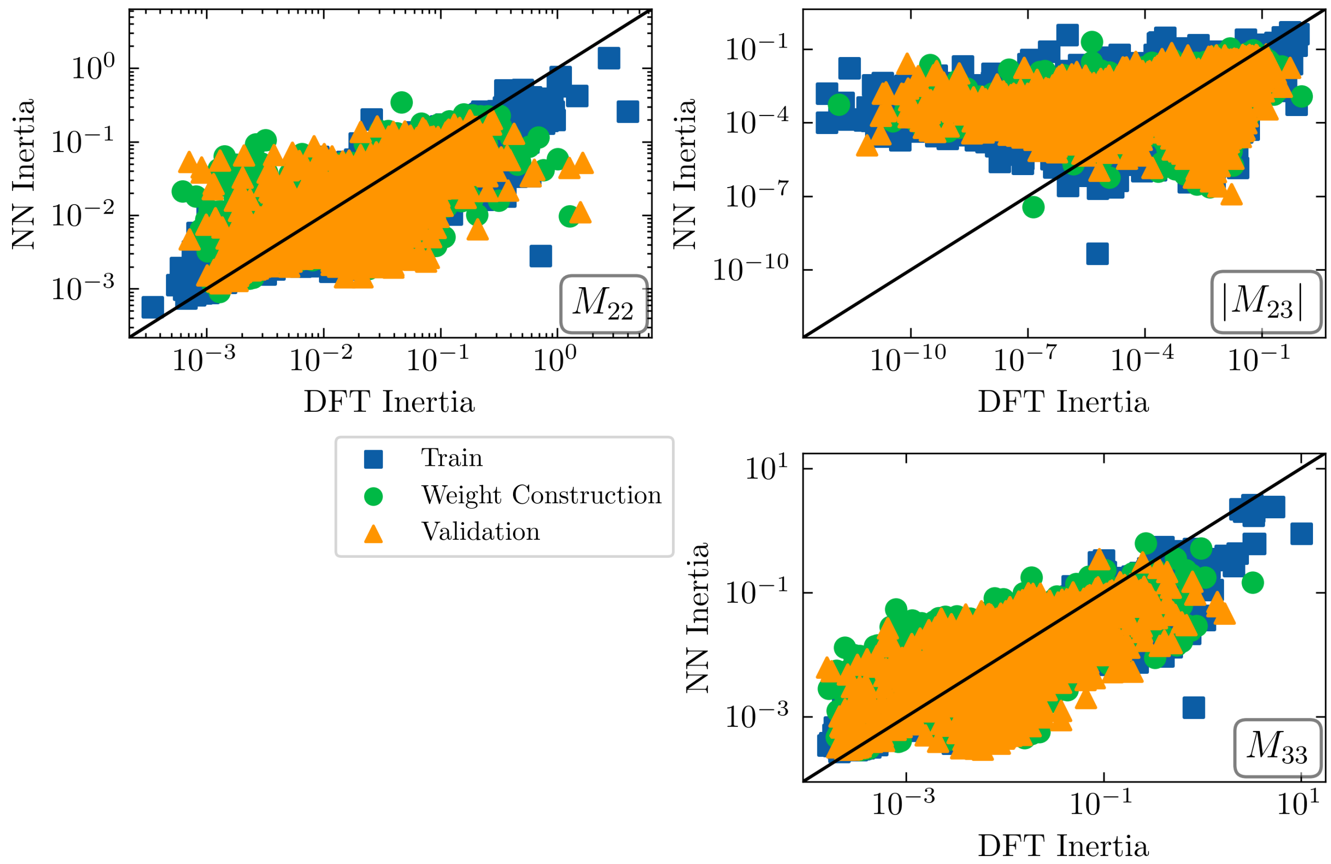
Results: PES Quality

- ^{280}Cm has largest RMSE, at 2 MeV
- Qualitative features reproduced
  - Ground state and outer turning line locations
- Non-accessible regions are dominant source of error



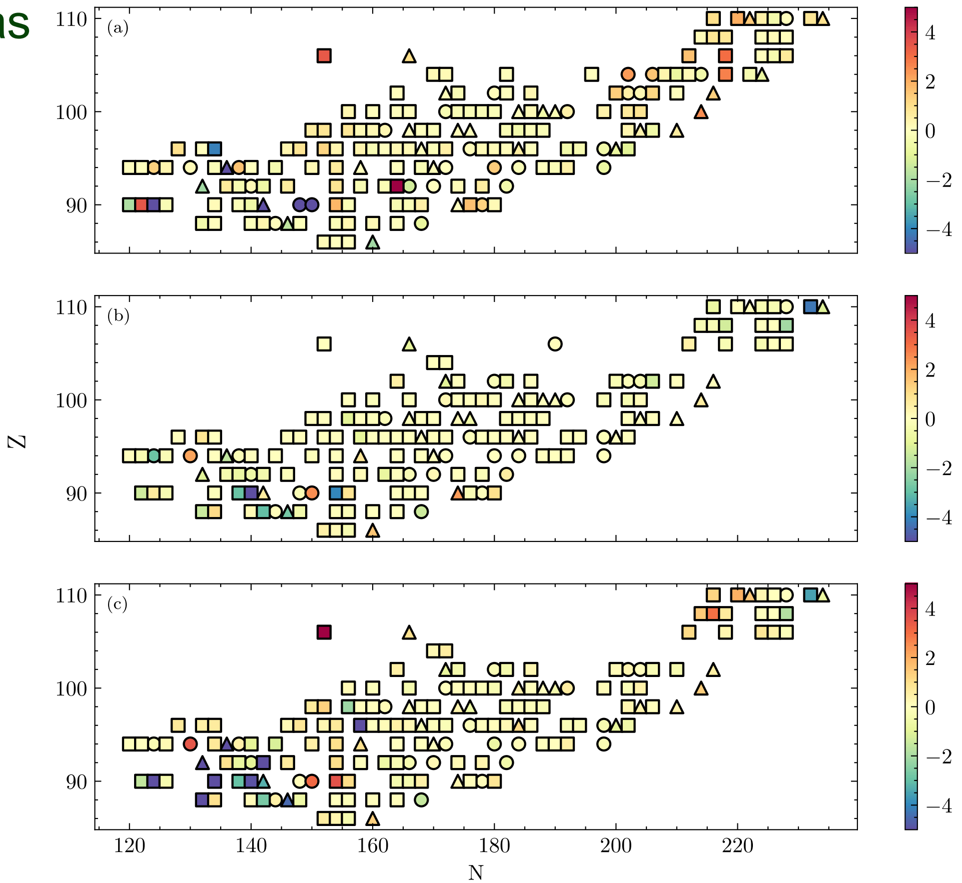
Results: Collective Inertia

- NN captures diagonal components well across multiple orders of magnitude
- Small off-diagonal components usually overestimated



Results: Exit Points

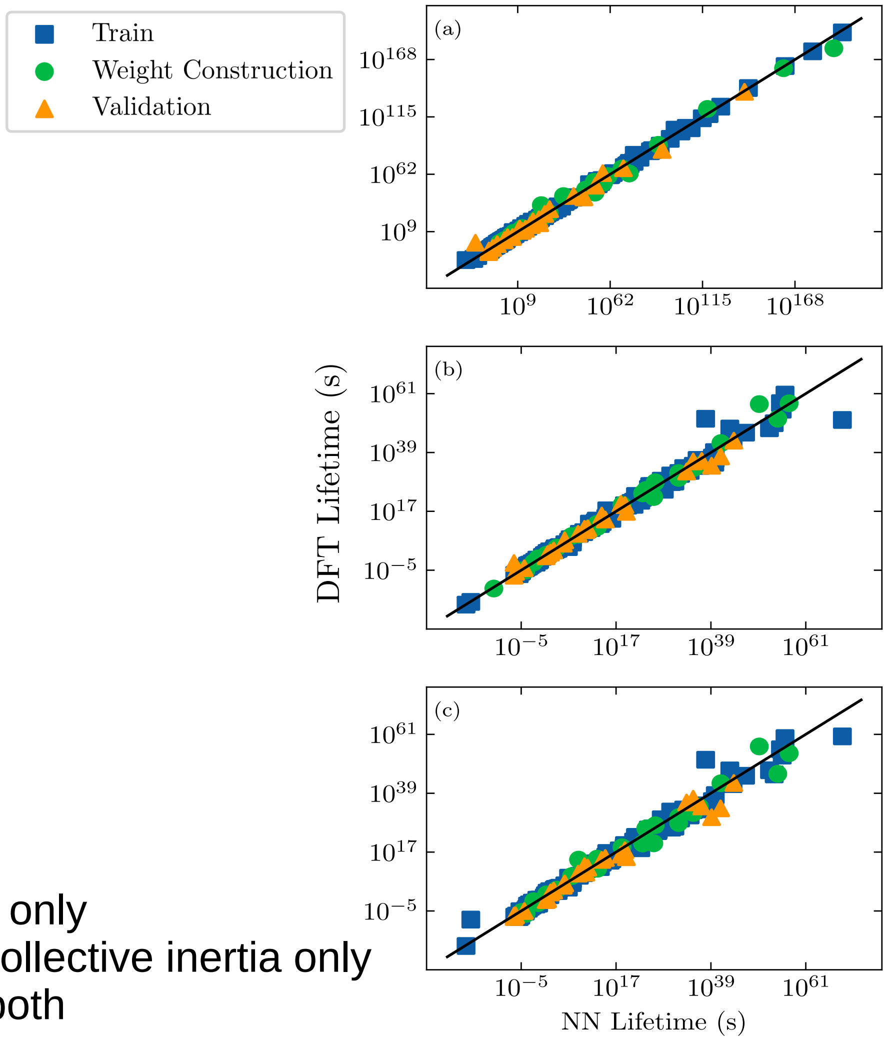
- Octupole moment of exit point shown as proxy for fragment yields
  - Quadrupole moment behaves similarly
  - Take weighted average over different fission modes
- Both PES and inertia emulated well enough to accurately predict fragment yields
  - Most important to emulate PES correctly
  - ^{280}Cm reproduced almost exactly



(top): impact of PES only
(middle): impact of collective inertia only
(bottom): impact of both

Results: Lifetimes

- Show lifetime ratio
  - Lifetimes systematically incorrect in current space of collective coordinates
- DFT lifetimes typically reproduced by NNs within 1-3 orders of magnitude
  - Collective inertia critically important
- Nuclei with long spontaneous fission lifetime have larger error
  - Expected, and not problematic



(top): impact of PES only
(middle): impact of collective inertia only
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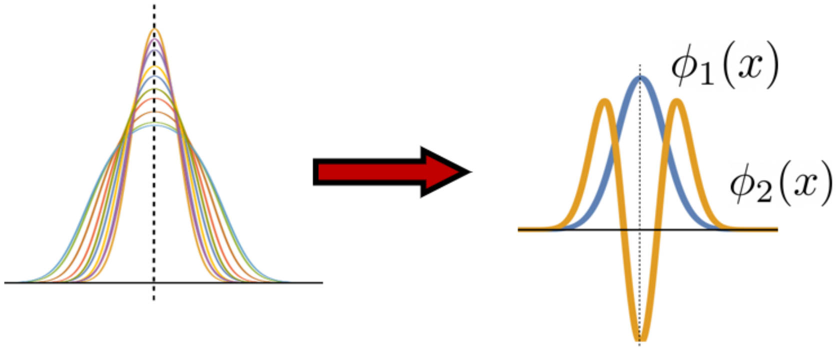
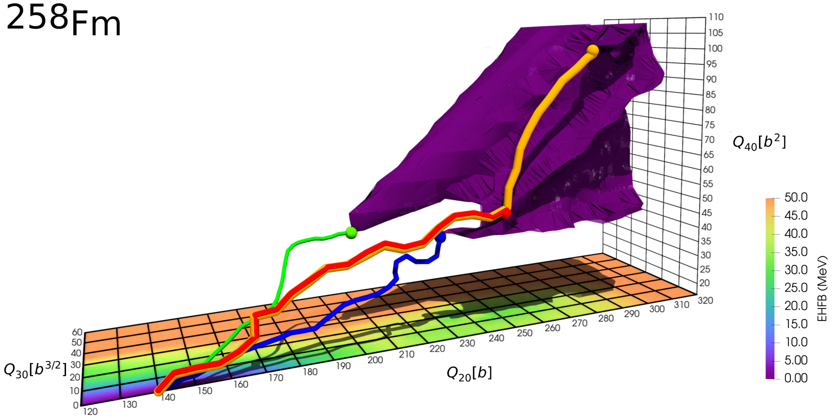
Future Directions

- Other emulation methods
  - Reduced basis methods
  - Gaussian processes
- Expansion to more collective coordinates
  - Dynamic pairing fluctuations, higher multipole moments
- Large-scale predictions and model calibration



^{258}Fm



Questions?