Accelerating HFB Simulations for Nuclear Structure and Dynamics

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International School of Nuclear Physics
45th Course
Nuclei in the Laboratory and in Stars

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Outline

- Motivation: self-consistent mean-field (SCFM) theory needs quantified uncertainties
- Emulators for toy model show 100x speedup over high-fidelity solver
- Emulators for UNEDF1 functional show 10x speedup, with 10 keV error or less
- Many future directions to pursue!

Self-Consistent Mean Field Theory

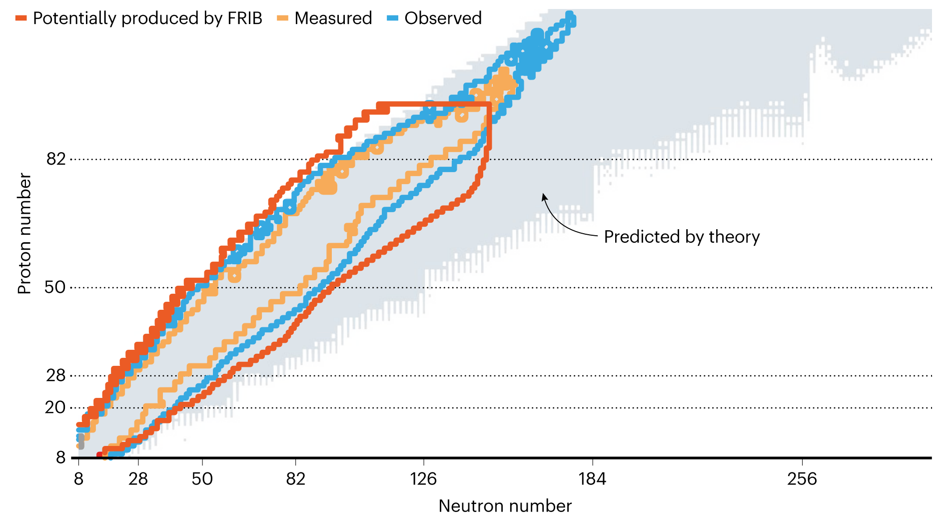
- Nucleons feel mean-field potential generated by other nucleons

$$h[\psi]\psi_i = \epsilon_i\psi_i$$

  - Solve for nucleonic wavefunctions self-consistently by iterative diagonalization
- Useful for (super-)heavy nuclei
  - Out of range of ab-initio models
  - Nuclear structure, fission (see talk by Eric Flynn)
- Energy density functional (EDF) described phenomenologically
  - Model parameters must be fit!
- Think Hartree-Fock(-Boguliubov) theory

Uncertainty Quantification

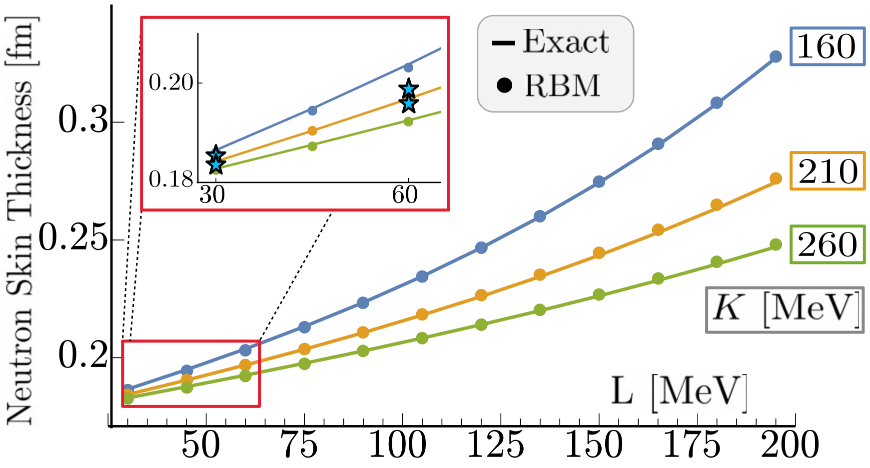
- Theoretical predictions need quantified uncertainties
  - Understand model sensitivities
  - Extrapolate away from valley of stability
  - Quantified inputs to nuclear astrophysics studies
- Want to understand in Bayesian framework
  - Sample $>10^6$ sets of model parameters
- Computational challenge: how to reduce cost of individual calculations?
  - Answer: emulators!



https://www.nature.com/articles/d41586-022-00711-5

Intrusive Emulators

- Examples:
  - Reduced basis method, eigenvector continuation, etc.
  - Contrast with neural networks, Gaussian processes
- Needs less training data
- Able to control emulation error
  - Trade-off between accuracy and runtime
- Straightforward interpretation
- Implementation requires understanding the model!



Neutron skin thickness of ^{48}Ca using reduced basis method. From E. Bonilla et. al., Phys. Rev. C 106, 054322 (2022)

A Toy Model

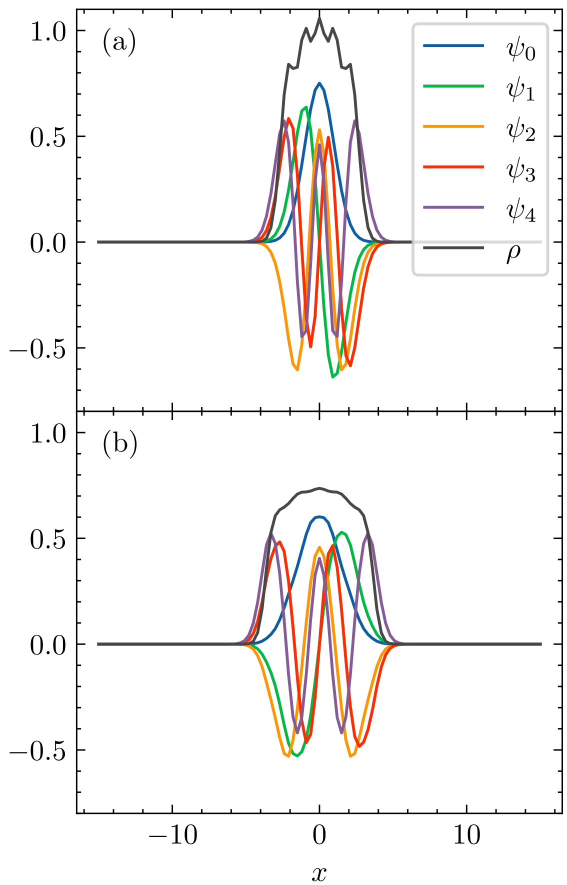
- A modified Gross-Pitaevskii (GP) model

$$h[\psi] = h_{\mathrm{HO}} + q\rho^{\sigma}(x),$$

$$\rho(x) = \sum_{i=1}^{N} |\psi_i(x)|^2$$

  - Prototypical Skyrme EDF

- How to solve the real problem?
  - Guess ρ_{in}
  - Expand Hamiltonian in basis $\{\phi_a\}$ (typically harmonic oscillator states)
  - Diagonalize and compute ρ_{out}
  - Repeat until $\rho_{\mathrm{out}} = \rho_{\mathrm{in}}$



(a): Wavefunctions and density for harmonic oscillator
(b): Same for GP

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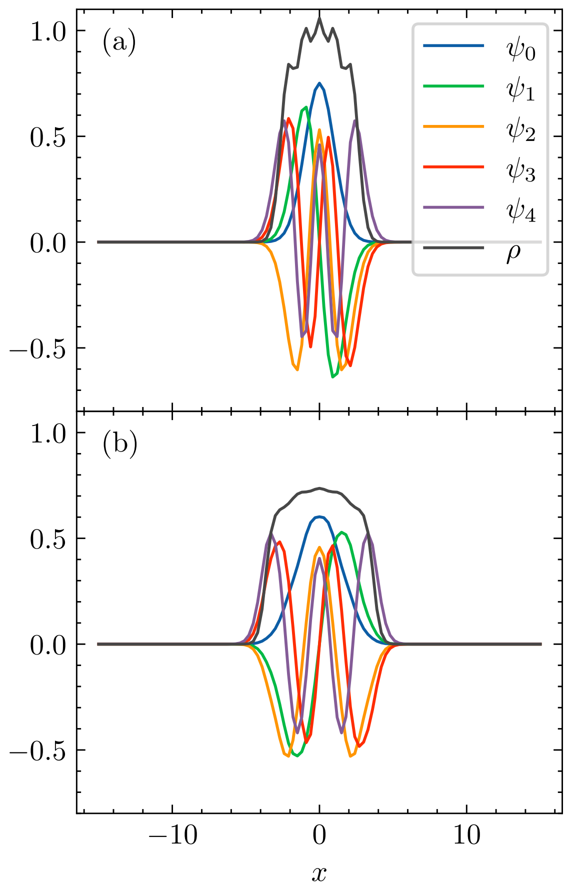
- Non-affine parameter dependence!



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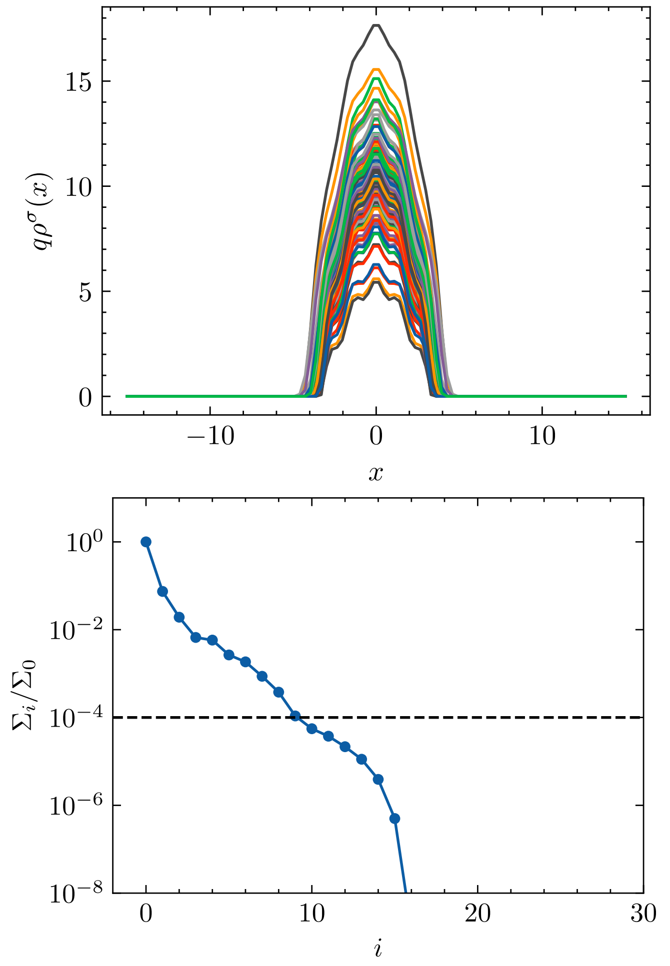
A Toy Model

- Bottleneck is transforming to basis, so emulate the field

$$f(x;q,\sigma) = q\rho^\sigma(x) \approx \sum_i a_i(q,\sigma) f_i(x)$$

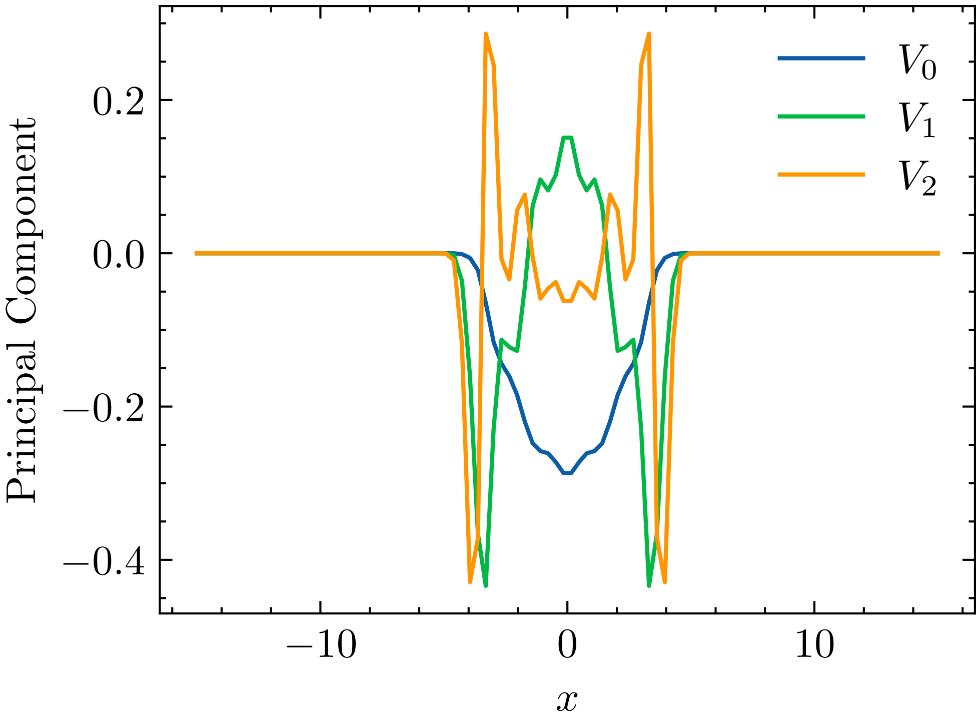
  - Called “empirical interpolation” (EI)
  - Precompute integrals $\langle \phi_a | f_i(x) | \phi_b \rangle$
- Fields are qualitatively similar
  - Take singular value decomposition to find $f_i(x)$
  - Decay of singular values tells us how many $f_i(x)$ we need
- Determine coefficients by constructing field at specific x values



Top: sample fields
Bottom: singular values from SVD of fields

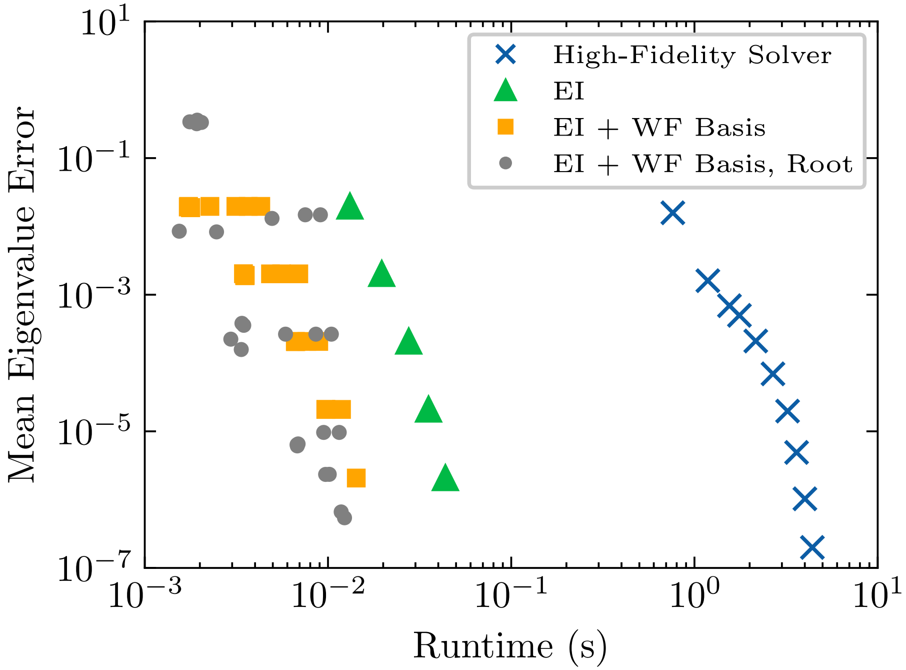
Principal Components

- Principal components are interpretable
  - First component is overall shape
  - Additional components are corrections



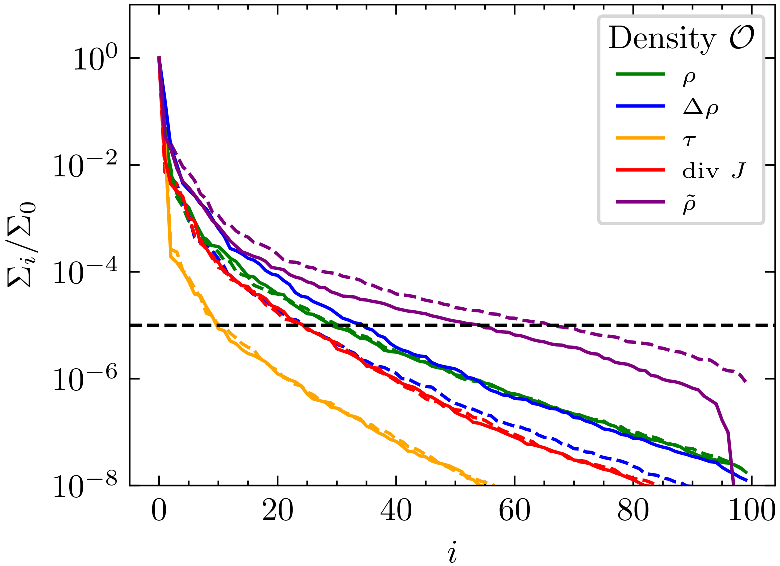
A Toy Model: Results

- Compare to original solver by plotting accuracy vs runtime
  - Ground truth is solver with very high tolerance
- Approximately 100x speedup with minimal accuracy loss!
- Further speedups available:
  - Emulating wavefunctions adds an additional factor speedup, due to diagonalizing smaller Hamiltonian
  - Rewriting problem to use a gradient-based root finding method can give additional speedup*



Skyrme HFB

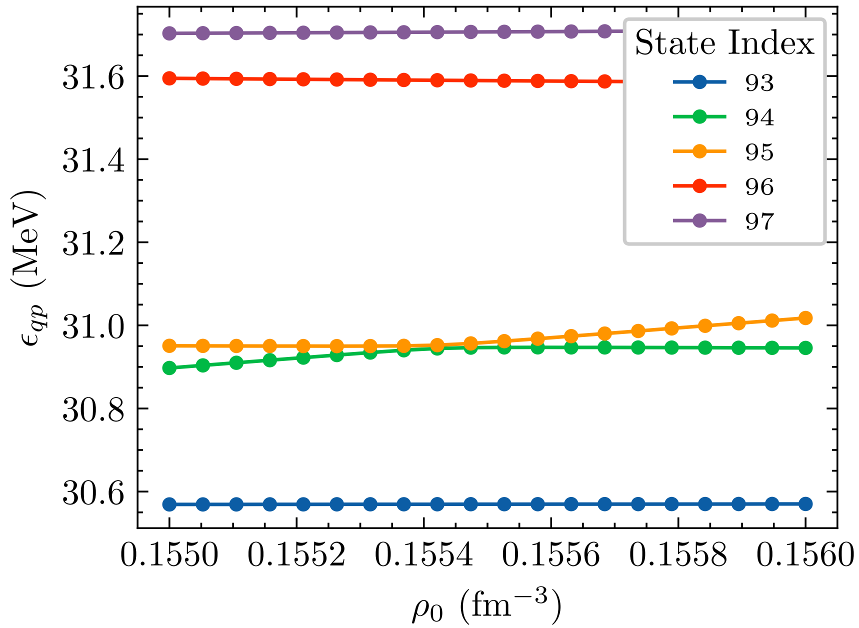
- Skyrme form of EDF used widely in realistic calculations
  - Use EDF parameters samples from posterior of UNEDF1 calibration (J. D. McDonnell et. al., Phys. Rev. Lett. 114, 122501 (2015))
  - 12-dimensional parameter space
  - Consider ground state of ^{254}Fm
  - Enforce axial, time-reversal symmetry (no parity!) using HFBTHO
    - 25 oscillator shells
- Want to use empirical interpolation on the fields $\frac{\delta E}{\delta \mathcal{O}}$
  - SVD suggests that empirical interpolation should work



Proton (neutron) shown in solid (dashed) lines

Skyrme HFB

- Can other steps be emulated?
  - Hard to emulate individual wave functions, due to level crossings
    - Instead can emulate all wave functions at once
  - Computing expansion coefficients requires reconstructing fields on entire mesh grid
    - Due to Coulomb potential
    - Can truncate grid with negligible accuracy cost



Skyrme HFB

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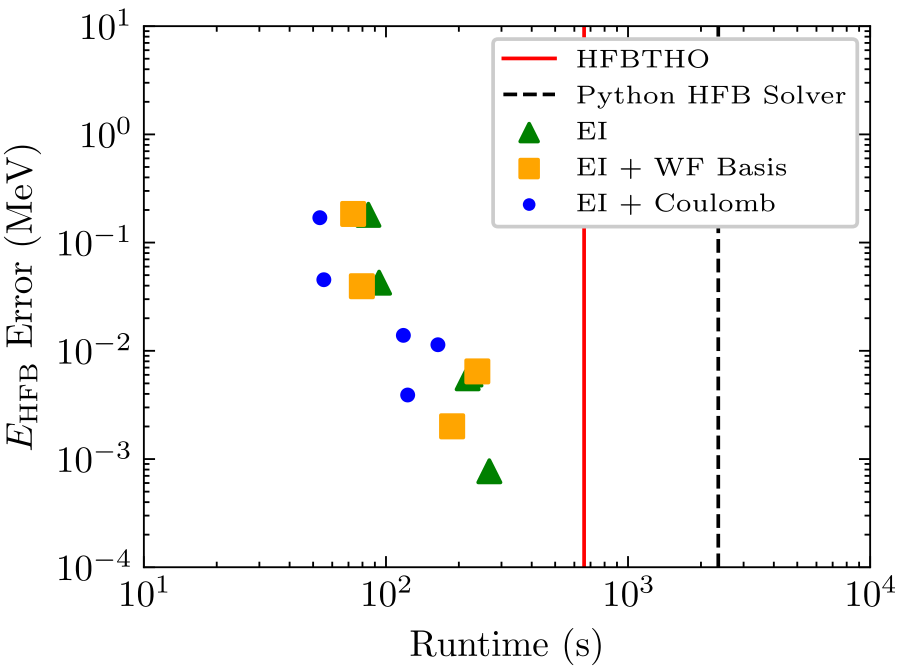
- **Python emulator is 10x faster than Fortran code HFBTHO**
  - Fortran emulator likely faster



Takeaways

- Basis expansion codes amenable to empirical interpolation
- SVD useful diagnostic tool for emulator development
- Rephrasing the problem in a novel way can (sometimes) help
- Intrusive emulators are worth exploring!

Future Directions

- Evaluate performance on fission isomer and constrained HFB calculations
  - Hope to enable UQ for fission yields (see Eric's talk)
- Incorporate emulator into high-fidelity solver
  - Use empirical interpolation when solver nears convergence
- Explore use in calculations across the nuclear chart
  - Use basis from one nucleus to study another
- Interest in generalizations
  - Nonlinear embedding (replace PCA to find basis)
  - Similar techniques for coordinate-space solvers?

Questions?

- Thanks to collaborators!
  - Pablo Giuliani
  - Kyle Godbey
  - Witek Nazarewicz

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