Systematic Emulations of Nuclear Observables

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Problem: Solve the λ-dependent N-body Hamiltonian

$$H^\lambda = T + V^\lambda + W^\lambda + \cdots$$

Expensive many-body simulations (HFB, PGCM, ...) provide λ dependent observables.

Sensitivity Analysis

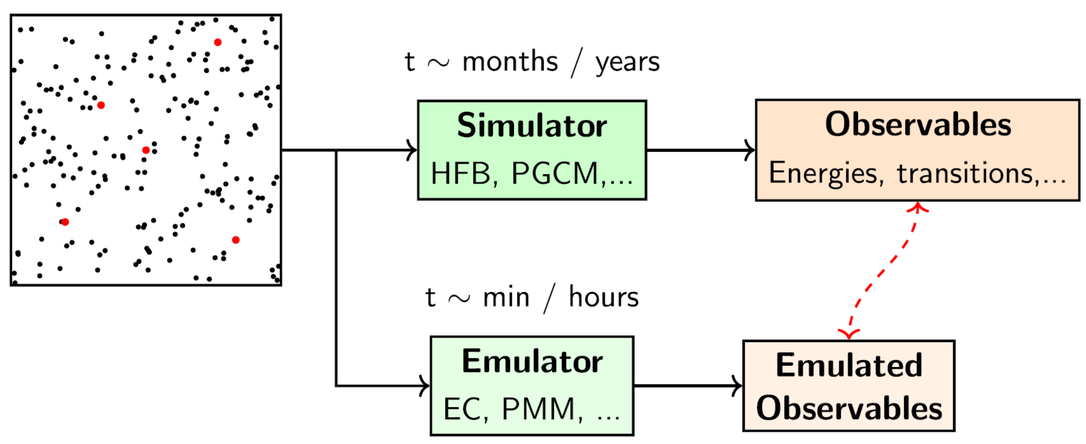
- Identify λ-sensitive observables
- Quantify sensitivity
- Propagate parameter uncertainties

Surrogate Model

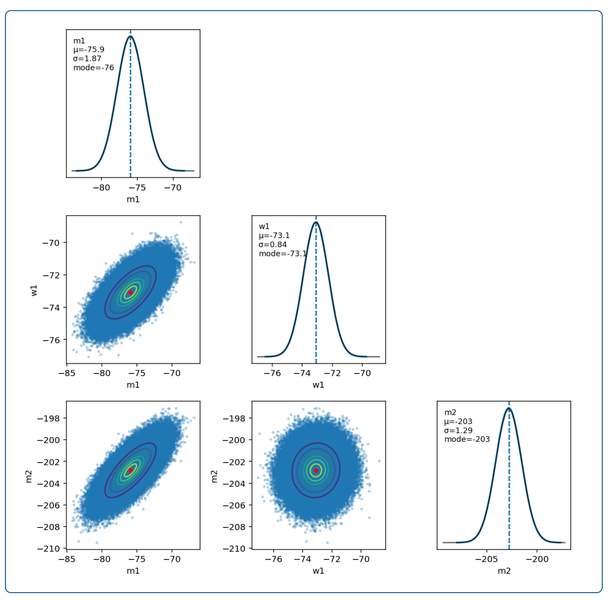
- Emulate the high-cost simulator
- Reduce computational cost
- Enable fast numerical fits

Challenge: Full simulations for each λ are computationally expensive.

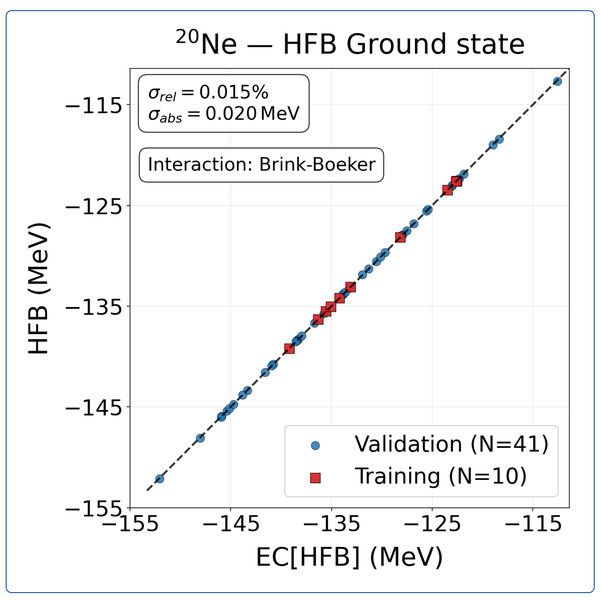
Goal: Fast and reliable exploration of the λ parameter space.



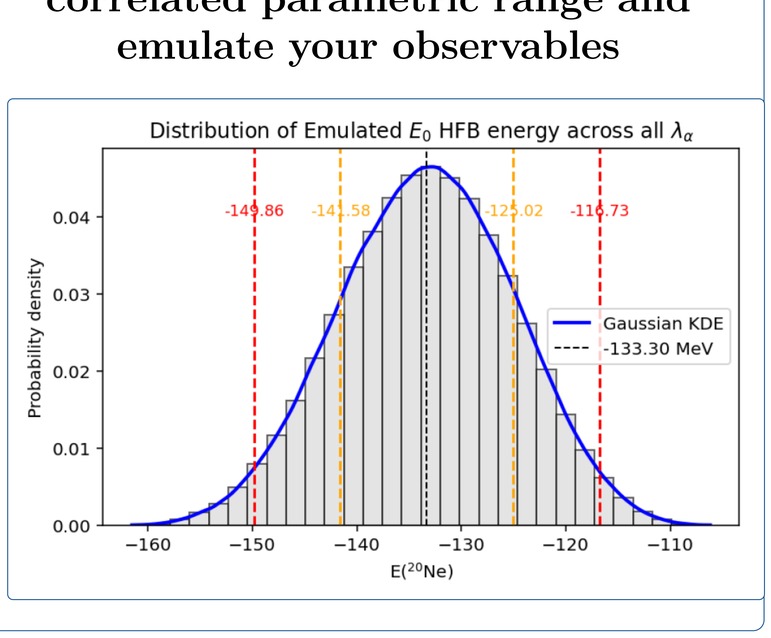
Step 1: Choose your interaction, Simulator, statistical model, and fit.



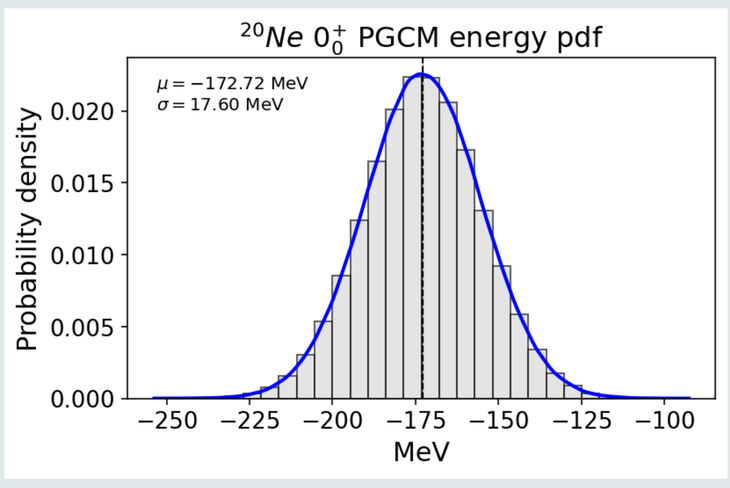
Step 2: Choose your emulator and optimize it against observables.

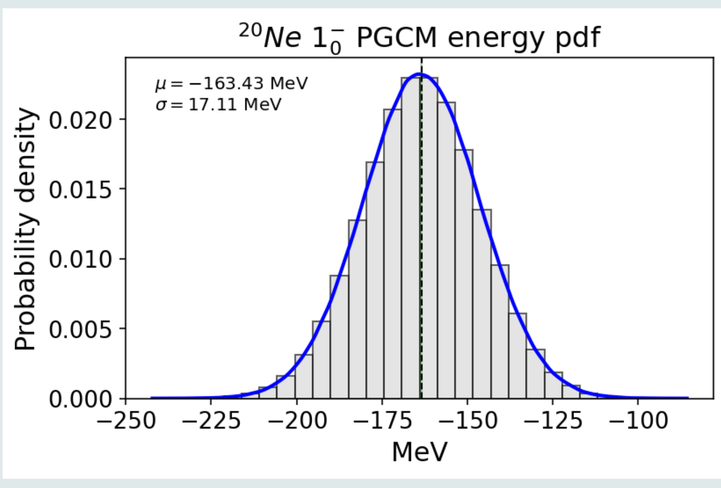


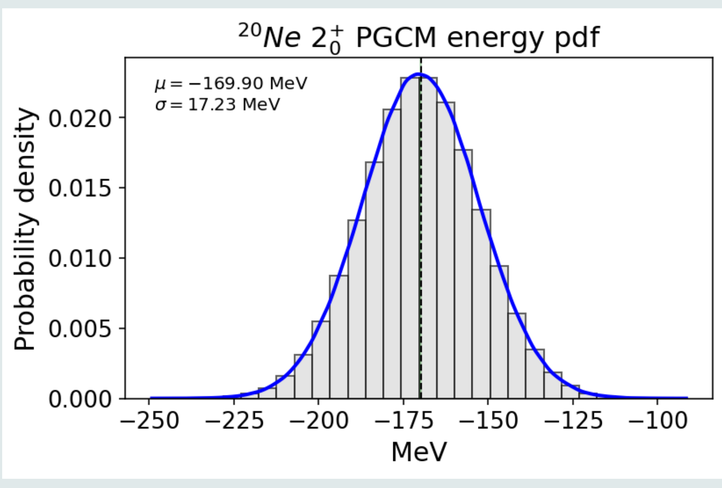
Step 3: Interpolate within the correlated parametric range and emulate your observables



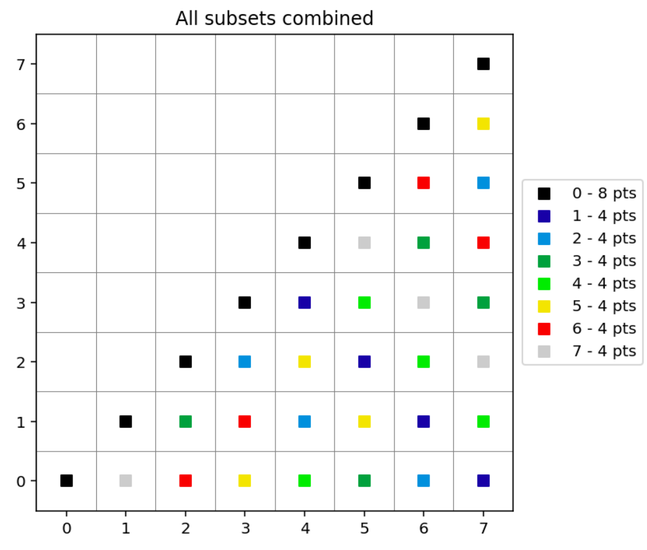
Ne20 PGCM-EC PRELIMINARY RESULTS







BONUS: Optimization of PGCM Kernel Computation: Constrained 1-Factorization of the Complete Graph



Reformulate the problem: For any parametrization λ_α and N_q collective coordinates q, we need to compute all kernels

$$\langle \Phi^{\lambda_\alpha}(q)|P^{\tilde{\sigma}}|\Phi^{\lambda_{\alpha'}}(q')\rangle \longleftrightarrow ((q,\alpha),(q',\alpha')) \longleftrightarrow (k,k'), \qquad k = a+\alpha N_q.$$

Goal: Partition all kernel pairs into disjoint batches

$$\mathcal{S} = \{(k,k')\} = \bigsqcup_{s=1}^{N_s} \mathcal{S}_s.$$

Constraints:

- **Matching:** in each $\mathcal{S}_s$, a state k appears in at most one pair (k,k').
- **Capacity:** each batch contains at most N_T pairs: $|\mathcal{S}_s| \leq N_T$, with N_T the number of available threads.

Objective:

- Minimize N_s,
- Maximize capacity utilization.

OUTLOOK

- Finalize the PGCM workflow for a single nucleus
- Extend the study to the nuclear chart
- Investigate more refined interactions, including chiral EFT
- Use the emulator to fit interactions at the PGCM level
- Benchmark the EC emulator against PMM and other emulator frameworks