Understand potential of machine learning (ML) algorithms for calibrating computationally expensive energy density functionals using parallel computing resources given:

- Available training/experimental data (100s) much smaller than flagship ML uses (millions+)
- Derivatives are not available

Reveals that targeted optimization methods typically outperform zeroth-order ML methods when little data are available for training computationally expensive nuclear physics models

Provides actionable guidelines and directions for future research for leveraging parallel physics simulations in an energy-efficient manner

Excellent results when applied to calibration of Fayans energy density functionals

Performance of best-tuned variants on an instance of calibrating the Fayans energy density functional. Solid lines indicate median performance; transparent bands indicate 25th-75th quantile performance. Best solutions are found in the allotted budget by POUNDERS; randomized methods achieve early reductions.

**Objectives**

**Impact**

**Accomplishments**