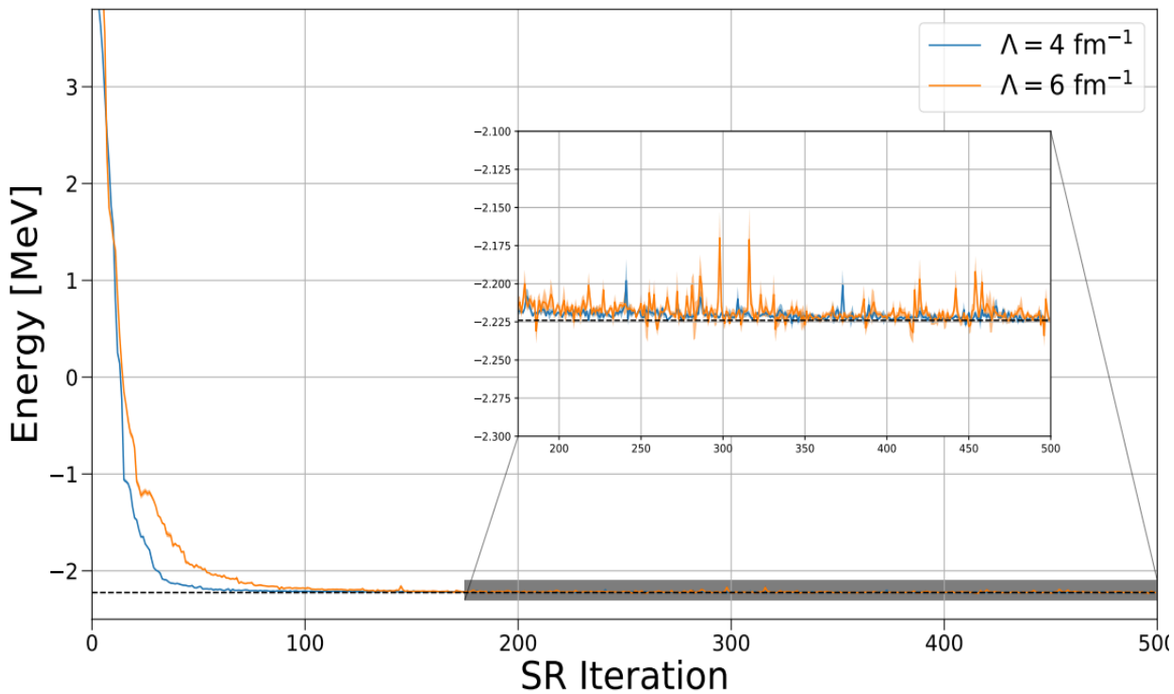
Variational Monte Carlo calculations with artificial neural-network correlators

U.S. DEPARTMENT OF ENERGY | Office of Science

NUCLEI Nuclear Computational Low-Energy Initiative



Convergence of the stochastic-reconfiguration training algorithm

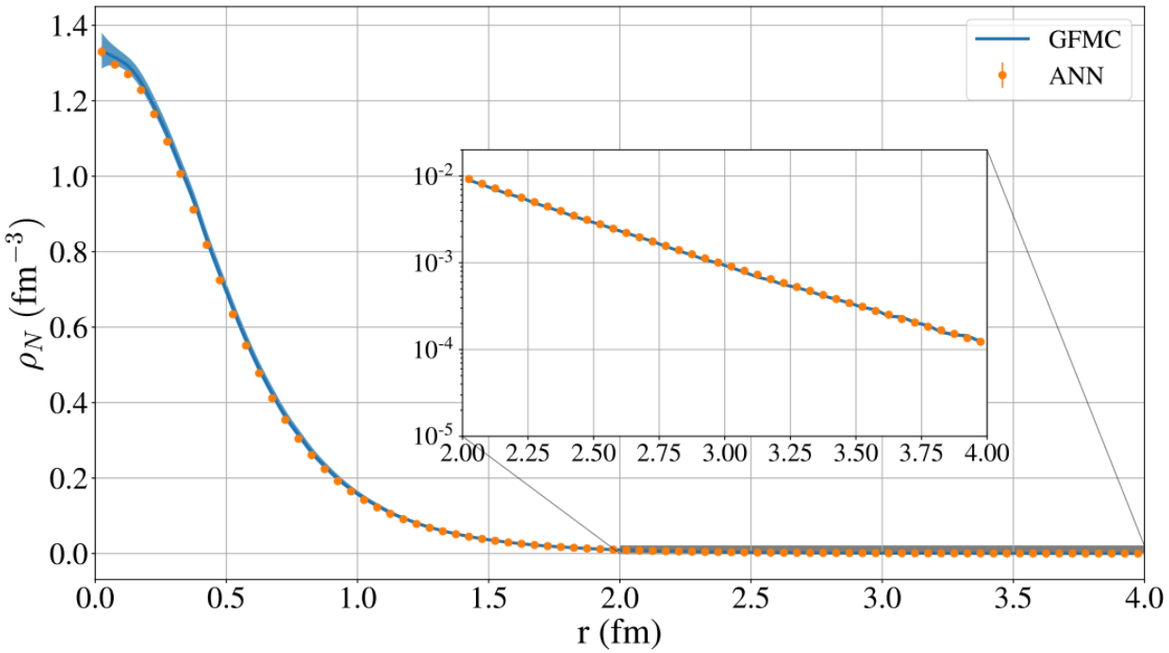


Figure: point-nucleon density of ^{3}H from the ANN and GFMC calculations;

Objectives

- Devise accurate nuclear wave functions suitable for quantum Monte Carlo calculations that do not scale exponentially with the number of nucleons;
- Generalize artificial-neural network representations used in condensed-matter systems to explicitly account for the spin-isospin dependence of the nuclear force;

Impact

- We used an artificial neural network to represent a nuclear correlation operator that takes as input the spatial and spin-isospin coordinates of the nucleons;
- We devised a dedicated stochastic reconfiguration algorithm to efficiently train the ANN;
- Using a LO pionless-EFT Hamiltonian, we proved that the ANN outperforms conventional Jastrow ansatz and perfectly reproduces the density profile of the nucleus, including the slow decaying tails;

Accomplishments

- C. Adams, G. Carleo, A. Lovato, N. Rocco, arXiv 2007.14282 (PRL in press)