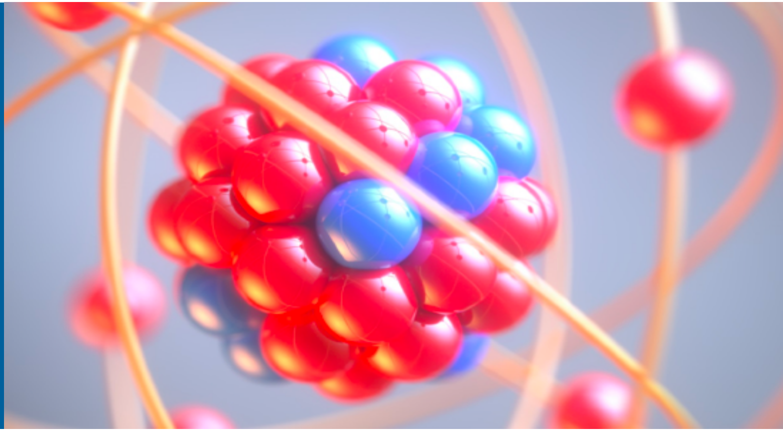
SOLVING THE QUANTUM MANY-BODY PROBLEM WITH NEURAL NETWORK QUANTUM STATES



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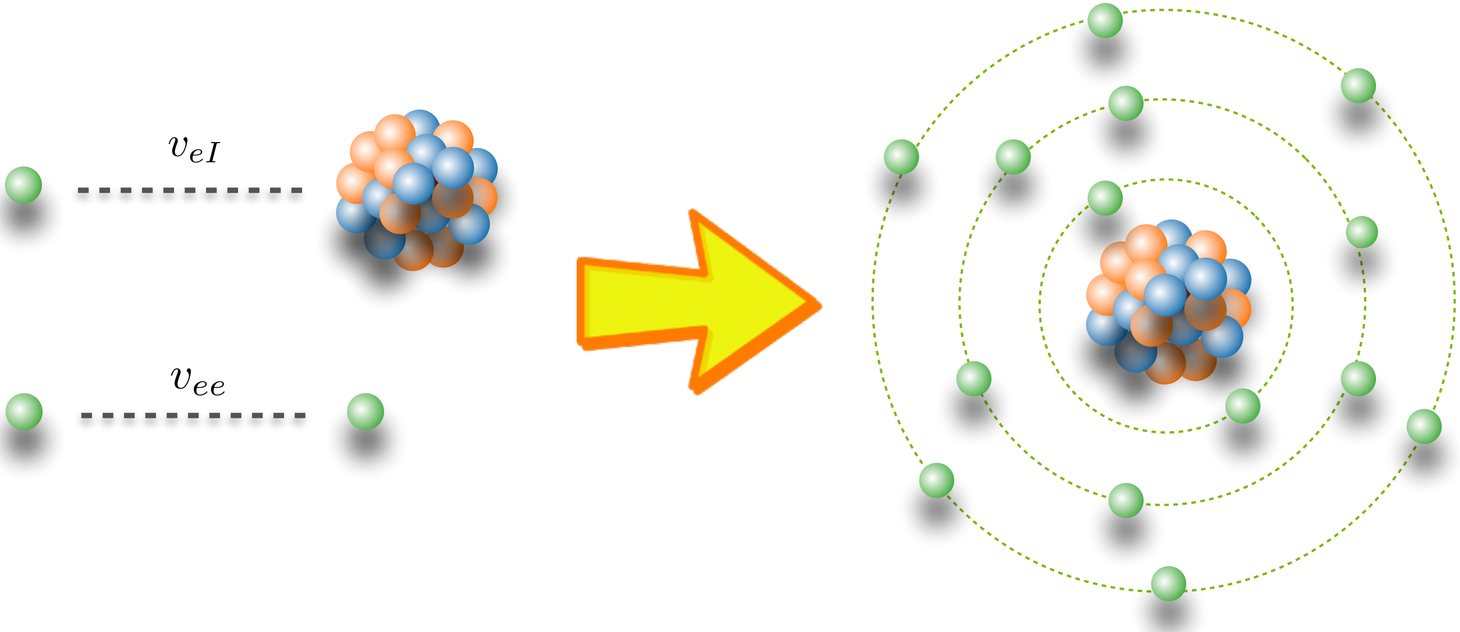
Argonne NATIONAL LABORATORY

Data-Intensive Computing & AI/ML Applications at Scale
17 August, 2023

THE QUANTUM MANY-BODY PROBLEM

Goal: predict the properties of systems made of several quantum particles from the first principles of quantum mechanics.



Multidisciplinary impact: nuclear physics (and high-energy physics), quantum chemistry, condensed matter physics, materials science..

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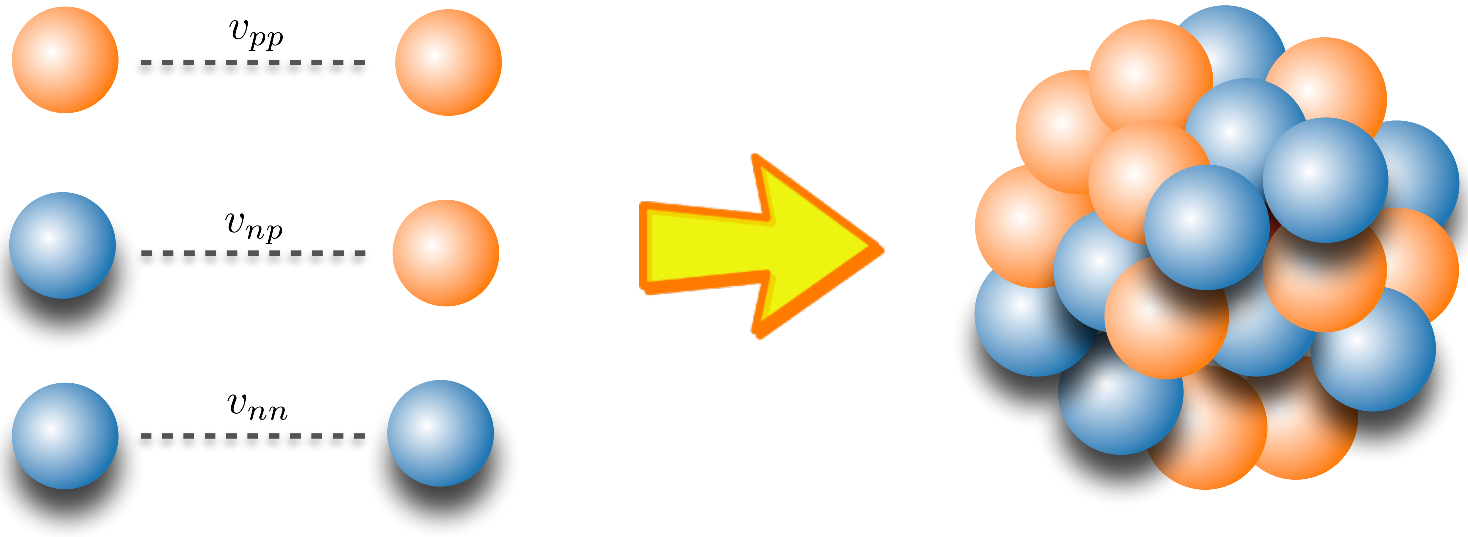

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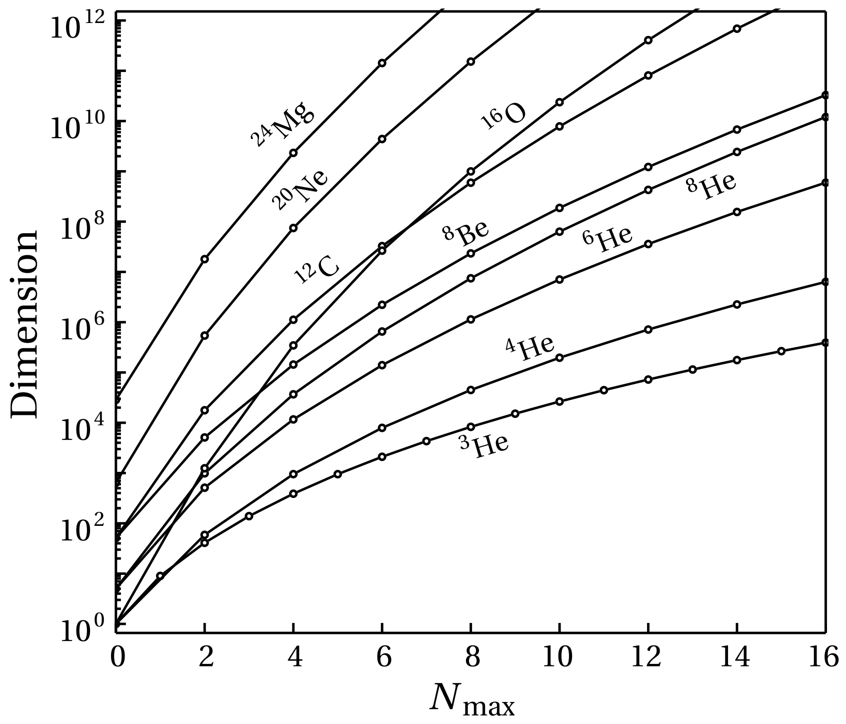
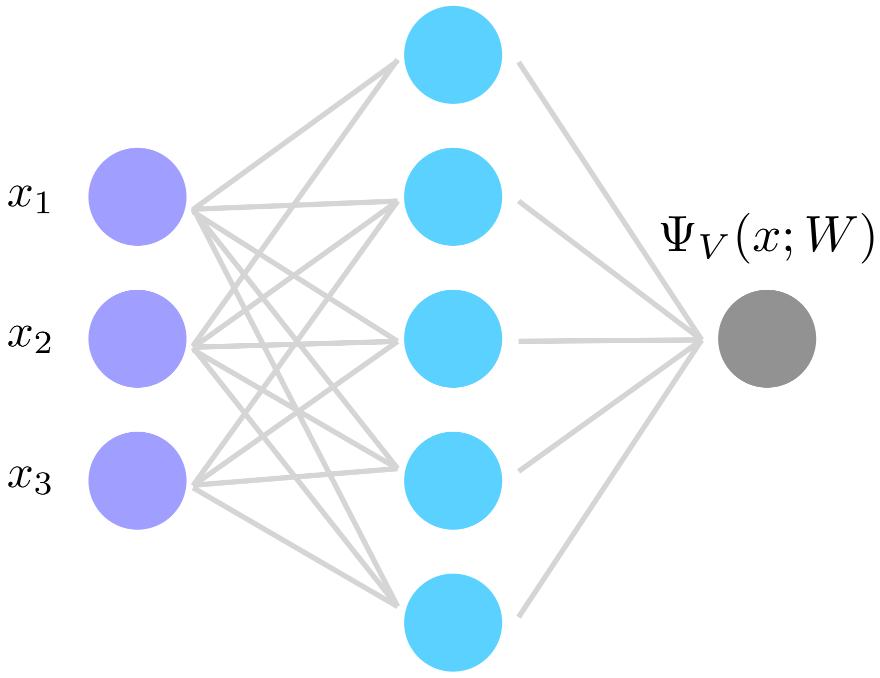
CURSE OF DIMENSIONALITY AND NQS

$$H\Psi_0(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N) = E_0\Psi_0(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N)$$

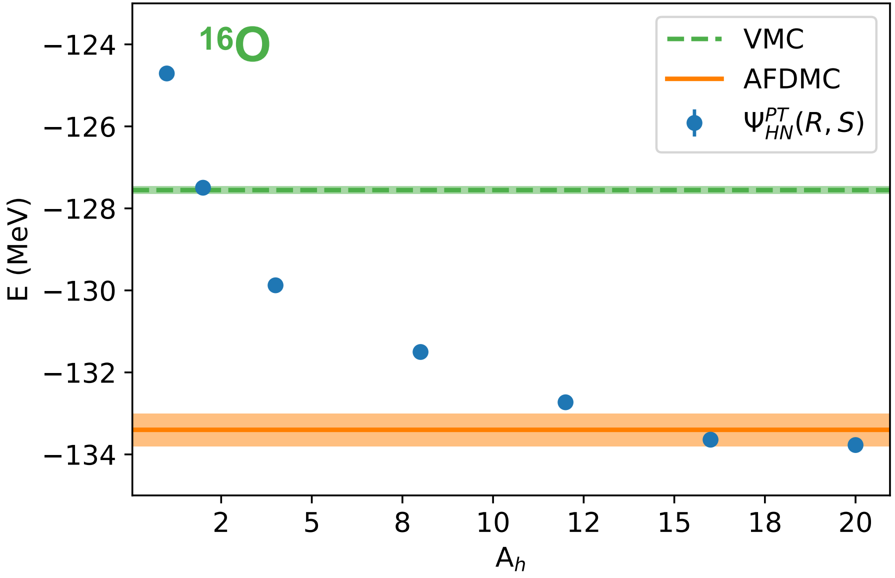


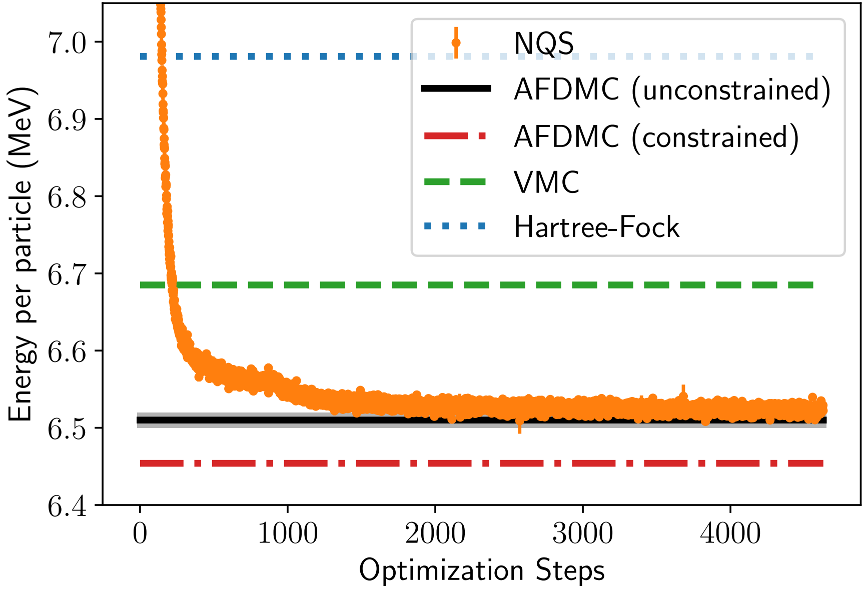


$$E_V \equiv \frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} > E_0$$

NUCLEAR PHYSICS APPLICATIONS

We developed NQS to solve the many-body problem for nuclei and neutron-star matter





C. Adams, AL, et al., Phys. Rev. Lett. ***127****, 022502 (2021)*

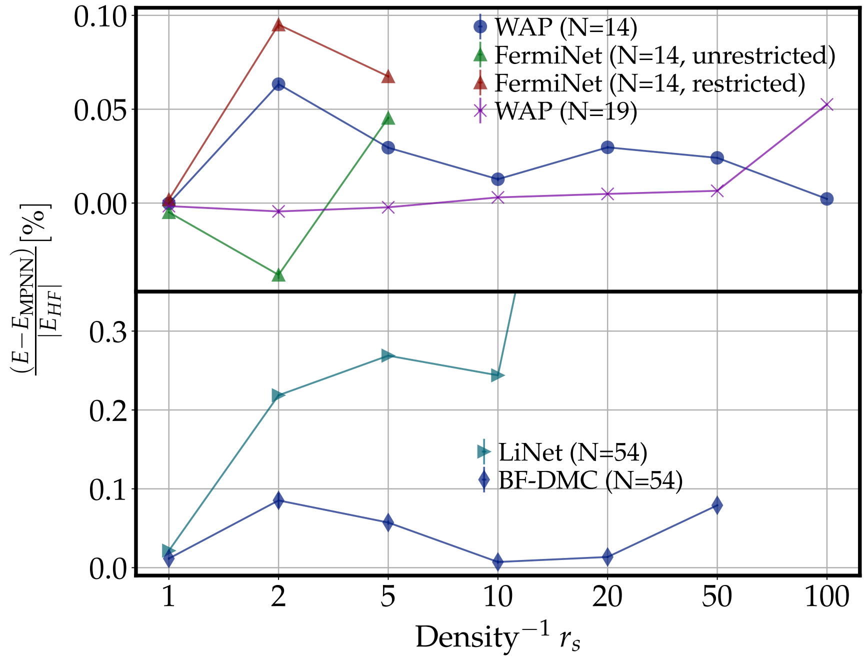
AL, et al., Phys. Rev. Res. ***4****, 043178 (2022)*

A. Gnech, AL, et al, Few Body Syst. ***63****, 1 (2022)*

B. Fore, AL et al., Phys. Rev. Res. ***5****, 033062 (2023)*

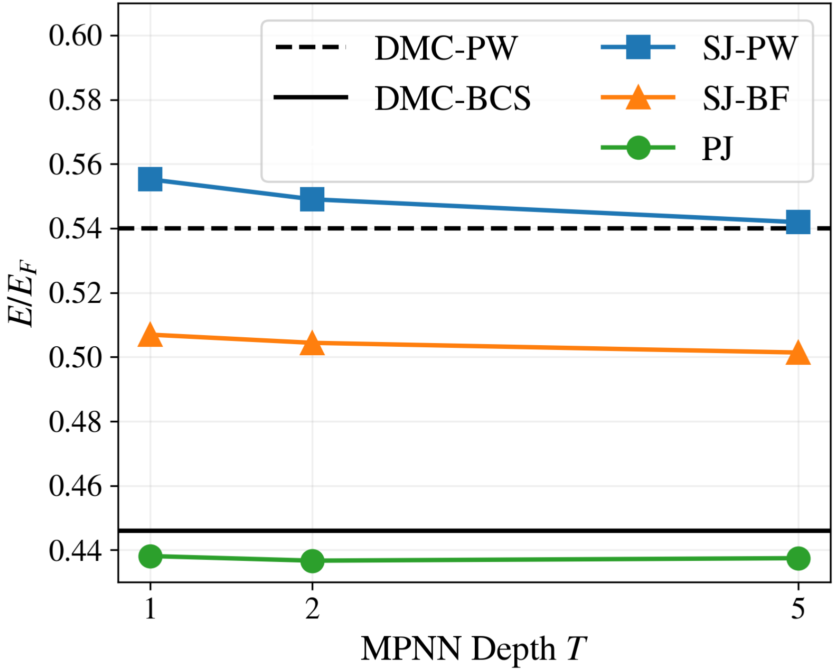
CONDENSED MATTER APPLICATIONS

We ventured into condensed-matter problems with NQS based on message-passing graph networks



G. Pescia, AL, et al., Phys. Rev. Res. **4** (2022) 023138

G. Pescia, AL, et al., 2305.08831 [cond-mat.quant-gas]



J. Kim, AL, et al. arXiv:2305.08831

PATH FORWARD WITH AURORA

Now (Swing, Theta-GPU, Polaris):

- Quantum systems with up to ~50 particles on full Polaris with almost ideal scaling;

Aurora:

- Heavy nuclei, (up to Uranium!); relevant for FRIB (@MSU), ATLAS (@Argonne);
- Isospin-asymmetric nuclear matter; direct impact on astrophysical observations;
- Spin-imbalanced Fermi gas closer to the thermodynamic limit;
- Molecules, benchmark with state-of-the-art diffusion Monte Carlo and coupled cluster methods
- Real-time quantum dynamics: Electron and neutrino-nucleus scattering, neutron-star cooling, nuclear fission and fusion, responses of condensed-matter systems;

Ongoing and potential synergies

- Multidisciplinary, ideal for CPS: Corey Adams, Yury Alexeev, Anouar Benali, Noemi Rocco;

Funding:

- DOE Early Career Award,
- DOE-NP-SciDAC, DOE-HEP-SciDAC,
- Argonne LDRD