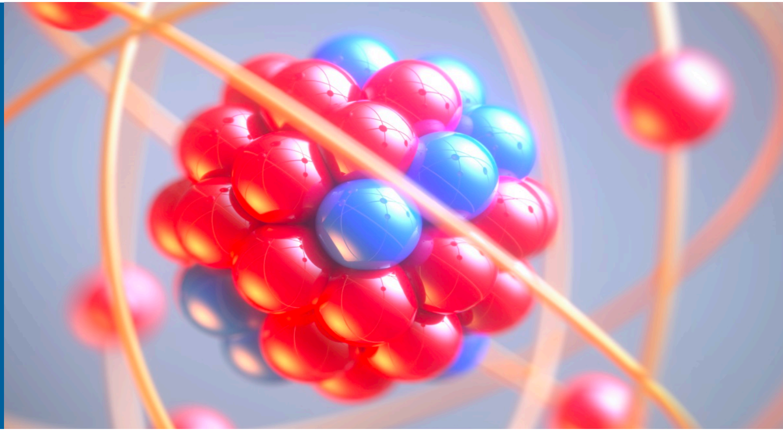
VARIATIONAL LEARNING QUANTUM WAVE FUNCTIONS



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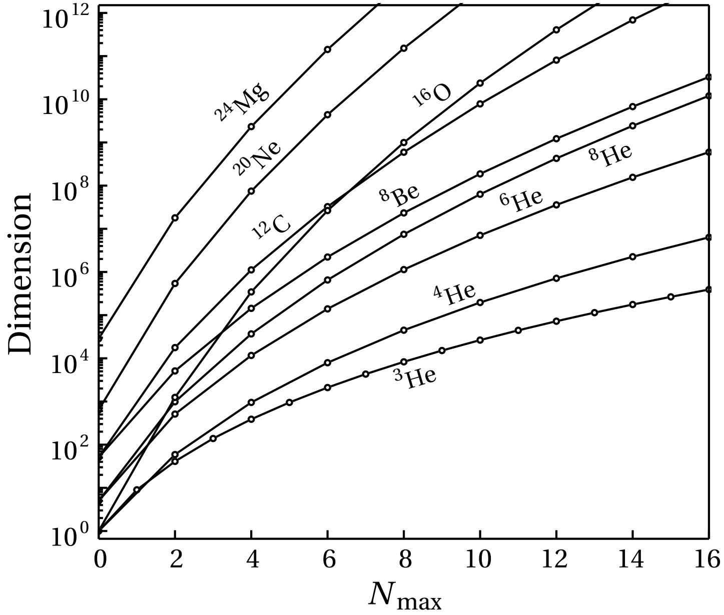
MONSTRE Collaboration Meeting

12 Maggio, 2023

COURSE OF DIMENSIONALITY

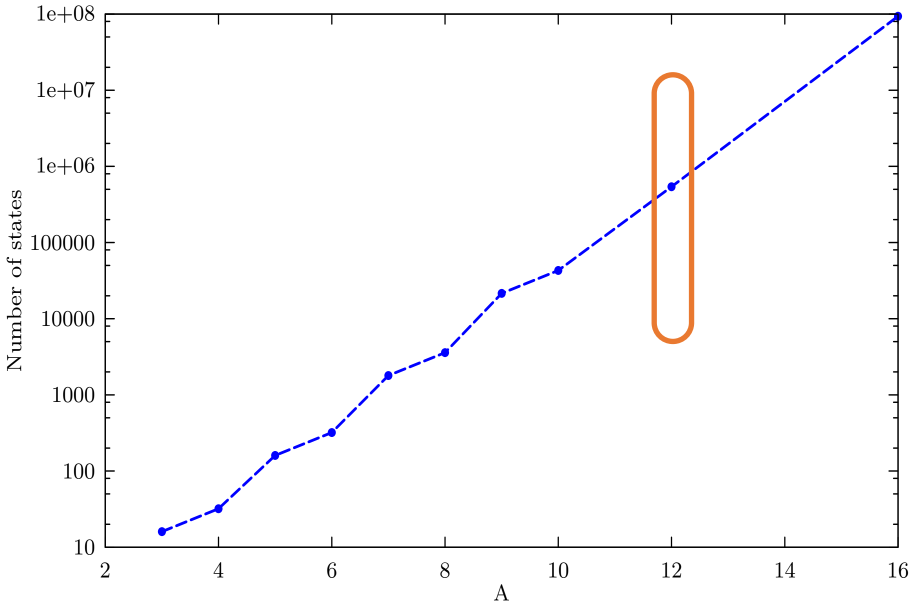
Configuration-Interaction

$$\Psi_0(x_1,\ldots,x_A) = \sum_n c_n \Phi_n(x_1,\ldots,x_A)$$



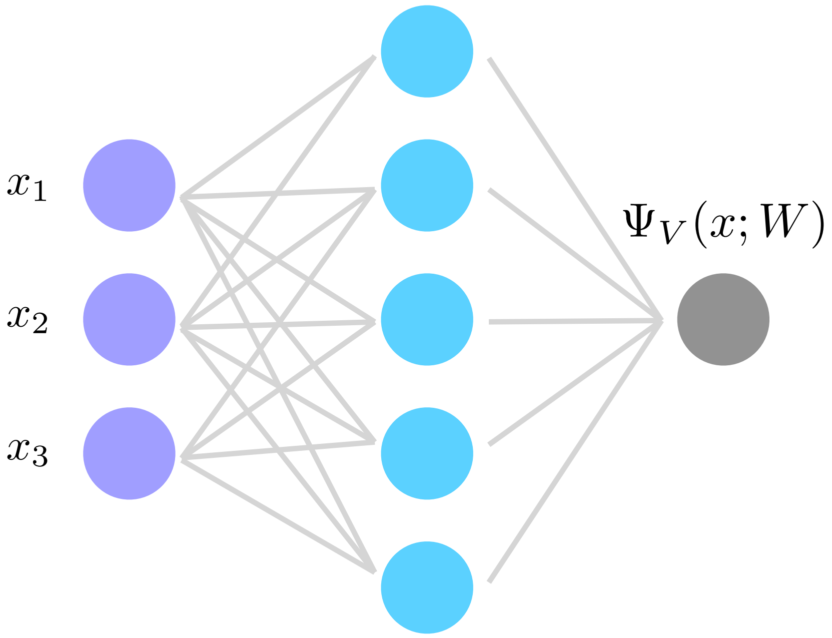
Green's function Monte Carlo

$$\lim_{\tau\to\infty} e^{-(H-E_0)\tau}|\Psi_T\rangle = c_0|\Psi_0\rangle$$



NEURAL-NETWORK QUANTUM STATES

Originally introduced by Carleo and Troyer for spin systems, NQS are now widely and successfully applied to study condensed-matter systems

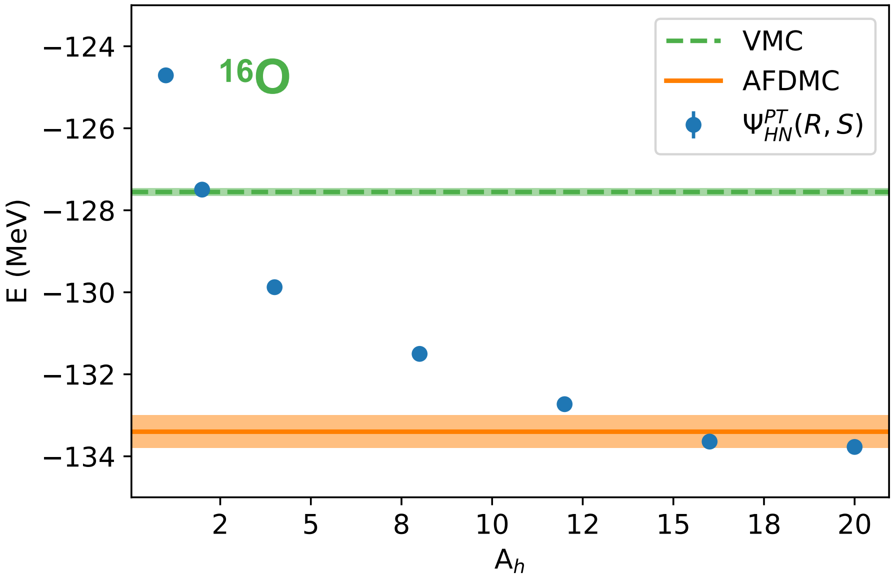


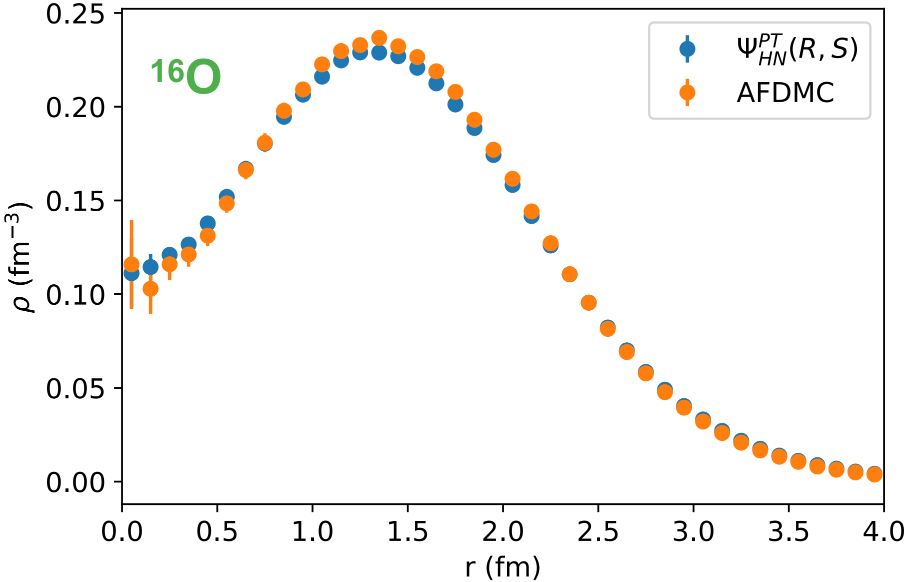
$$E_V \equiv \frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} > E_0$$

$$E_V \simeq \frac{1}{N} \sum_{X \in |\Psi_V(X)|^2} \frac{\langle X | H | \Psi_V \rangle}{\langle X | \Psi_V \rangle}$$

NUCLEAR PHYSICS APPLICATIONS

We applied NQS to solve the nuclear many-body problem and for nuclei and dilute neutron matter





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

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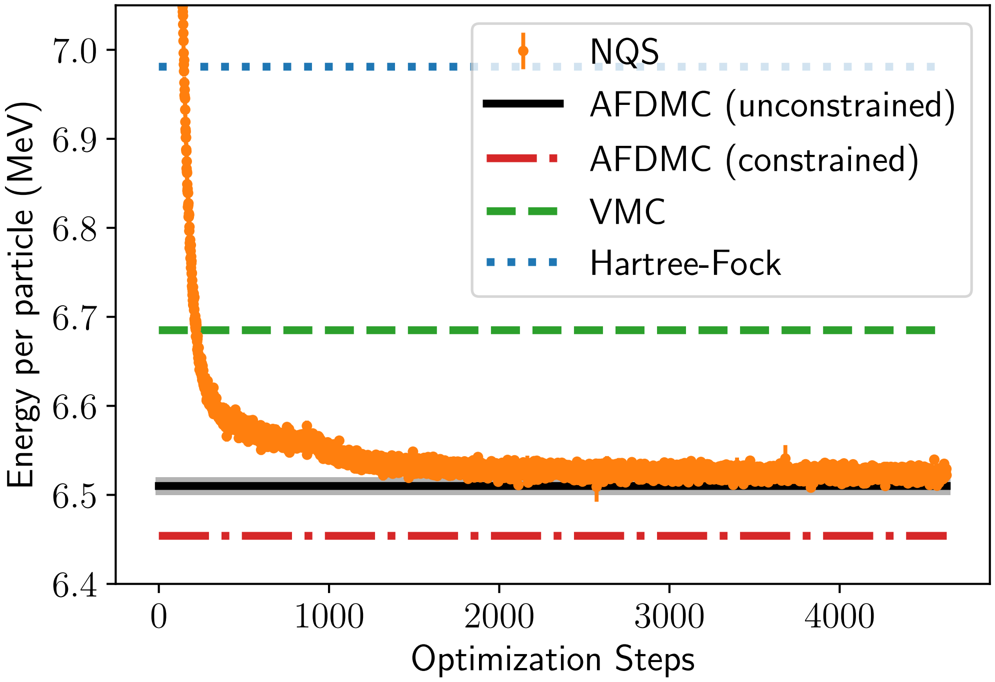


B. Fore, J. Kim, AL, arXiv:2212.04436 [nucl-th]

PATH FORWARD

We are already solving nuclei with ~40 nucleons using ~ 100 GPUs with almost ideal scaling

Heavy nuclei and infinite nuclear matter within reach with leadership-class machines

Can tackle high-momentum nuclear forces (short-range correlations)

No issues with open shell or exotic systems; just need to specify A, Z, and the Hamiltonian

REAL-TIME DYNAMICS

Real-time dynamics relies on the time-dependent variational principle

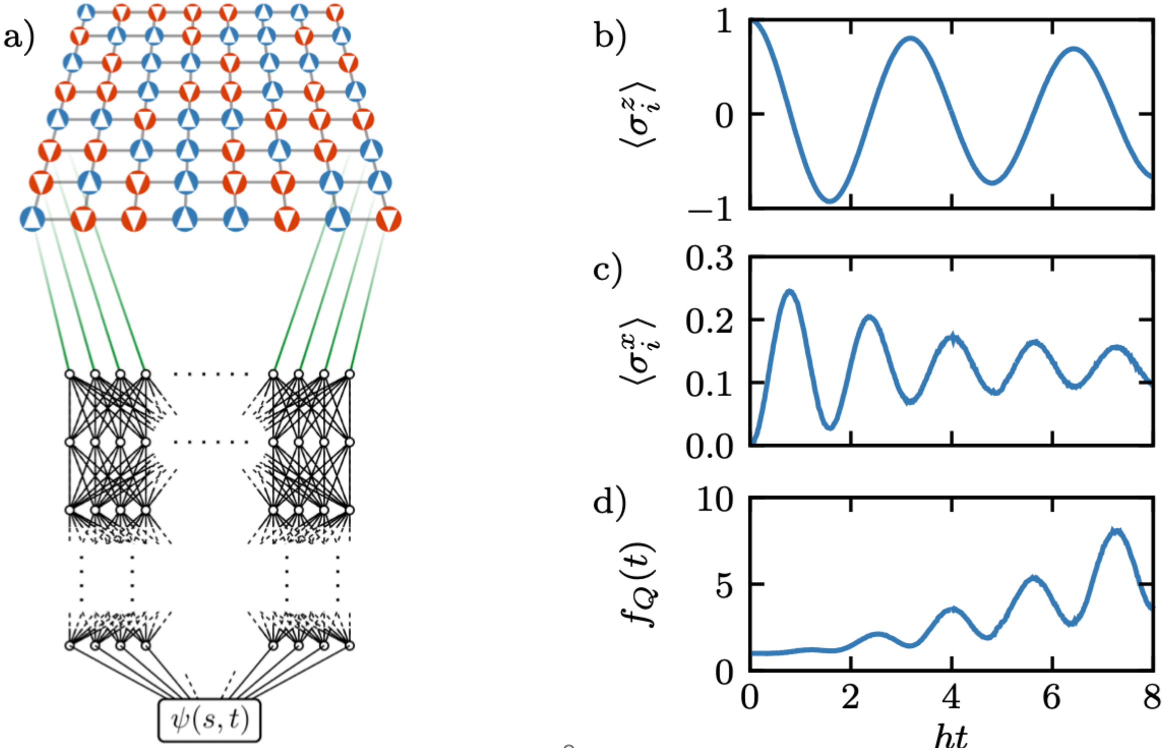
$$\mathcal{D}\left(|\Psi(\mathbf{p}_{t+\delta t})\rangle, e^{-iHt}|\Psi(\mathbf{p}_t)\right)^2 = \arccos\left(\sqrt{\frac{\langle\Psi(\mathbf{p}_{t+\delta t})|e^{-iHt}|\Psi(\mathbf{p}_t)\rangle\langle\Psi(\mathbf{p}_t)|e^{iHt}|\Psi(\mathbf{p}_{t+\delta t})\rangle}{\langle\Psi(\mathbf{p}_{t+\delta t})|\Psi(\mathbf{p}_{t+\delta t})\rangle\langle\Psi(\mathbf{p}_t)|\Psi(\mathbf{p}_{\tau+\delta t})\rangle}}\right)^2$$

Requiring stationary of this distance yields the t-VMC equations → $S_t \frac{d\mathbf{p}}{dt} = \mathbf{g}_t$

- Applications to fusion, fission: generalizes time-dependent Hartree-Fock including correlations
- Lepton-nucleus scattering: JLAB, Dune, and T2K

REAL-TIME DYNAMICS

Neural quantum states have proven suitable ansatz to simulate the dynamics in 2d spin systems



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Requiring stationary of this distance yields the t-VMC equations → $$S_t \frac{d\mathbf{p}}{dt} = \mathbf{g}_t$$

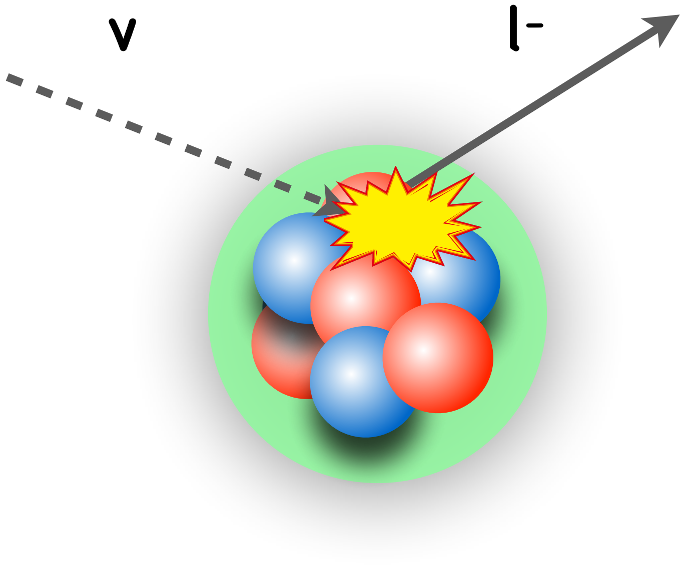
The TDVP equation defines a Hamiltonian dynamics on the variational manifold, which conserves energy.

$$\frac{d}{dt}\frac{\langle\Psi(\mathbf{p}_t)|H|\Psi(\mathbf{p}_t)\rangle}{\langle\Psi(\mathbf{p}_t)|\Psi(\mathbf{p}_t)\rangle} = 0$$

NEUTRINO-NUCLEUS SCATTERING

Goal: evaluate the real-time correlation function

$$R(\mathbf{q},t) = \langle\Psi_0|J^\dagger(\mathbf{q})e^{-iHt}J(\mathbf{q})|\Psi_0\rangle$$



1) Learn the ground state of the system

$$|\Psi_V\rangle \simeq |\Psi_0\rangle$$

2) Learn the state obtained applying the current to the ground state

$$|\Psi_V(\mathbf{p}_{t=0})\rangle \simeq J(\mathbf{q})|\Psi_0\rangle$$

3) Evolve the neural quantum state in real time with t-VMC

$$|\Psi_V(\mathbf{p}_t)\rangle \simeq e^{-iHt}J(\mathbf{q})|\Psi_0\rangle$$

4) Evaluate the overlap with the initial state

$$R(\mathbf{q},t) \simeq \langle\Psi_V(\mathbf{p}_{t=0})|\Psi(\mathbf{p}_t)\rangle$$