ALCF WORKSHOP 2023

Argonne NATIONAL LABORATORY

CALCULATION OF NUCLEAR GROUND STATES USING ARTIFICIAL NEURAL NETWORKS.

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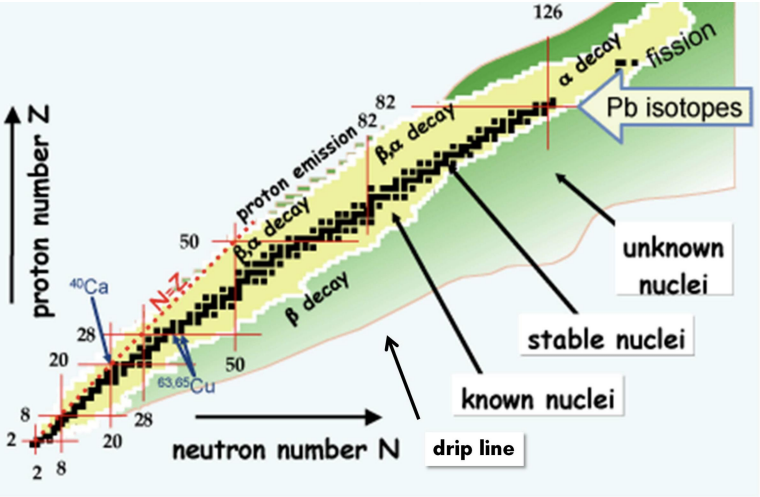
INTRODUCTION

Why nuclear physics?

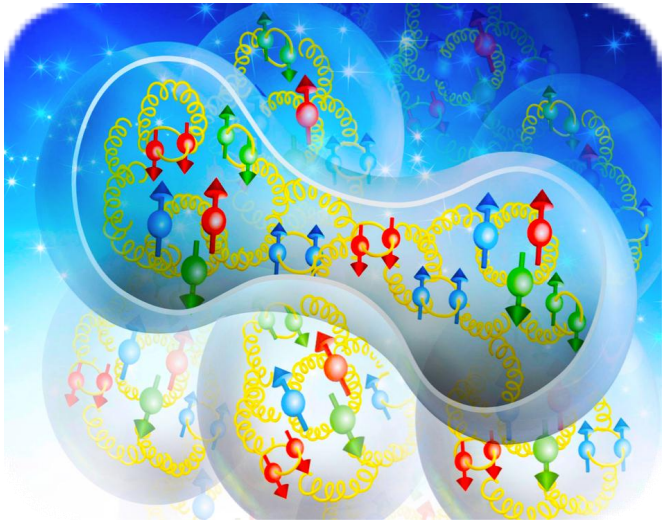
Atomic Nuclei are many-body systems governed by the strong interaction, which exhibit emergent properties such as: shell structure, pairing and superfluidity, deformation, and self-emerging clusters.

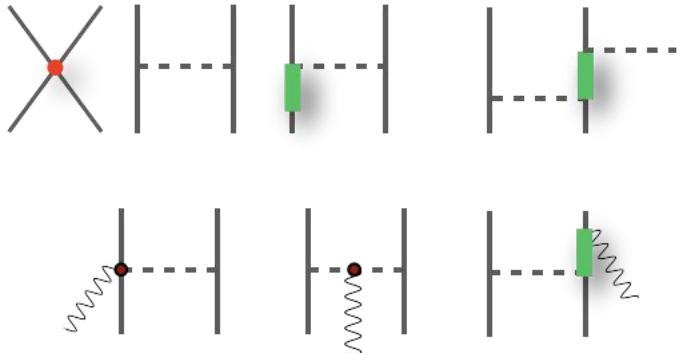


Understanding how the properties of nuclei emerge from QCD is a long-standing goal of nuclear physics.

NUCLEAR MANY BODY PHYSICS

At low energies, the quarks and gluons are **confined** within the hadrons: protons, neutrons and pions.



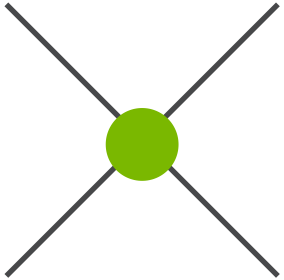


$$H = \sum_i \frac{\vec{p}_i^2}{2m} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

We can approximate QCD through **effective field theories,** allowing us to compute observables

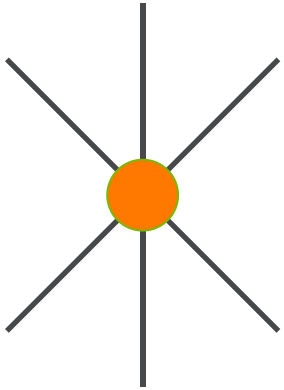
PION-LESS NUCLEAR HAMILTONIAN

An Effective Field Theory with 2- and 3- body interactions



$$v_{12} = C_1 v_\Lambda(r_{12}) + C_2 v_\Lambda(r_{12})\sigma_{12}$$

C_1 and C_2 fit to nucleon-nucleon scattering data



$$v_{123} = D_0 \sum_{cyc} v_\Lambda(r_{12}) v_\Lambda(r_{13})$$

D_0 fixed with the binding energy of ^{16}O

THE NUCLEAR MANY-BODY PROBLEM

§ The non-relativistic many body theory is solving the Schrodinger equation:

$$H\psi_n(R) = E_n\psi_n(R) \qquad R = (\vec{x}_1, s_{1,z}, \tau_{1,z}...)$$

$$H \equiv V(R) - \frac{\hbar^2}{2m}\nabla^2$$

§ The exact solution of this is **exponentially hard.**

§ The methods described in this talk solve this equation approximately, and while we target Nuclear many-body systems it is broadly applicable to many-body quantum systems.

VARIATIONAL MONTE CARLO

§ The Variational Principle of Quantum Mechanics guarantees that for any variational state, the expectation of the energy of that wavefunction is greater than the ground state:

$$\psi_T = \psi_T(R, \vec{\theta}) \qquad E_T = \frac{\langle \psi_T | H | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle} \geq E_0$$

§ Trial wavefunctions are parametrized in some way, and so you may optimize the trial wavefunction to reduce the expectation of the energy.

$$min(E_T) : \theta_j \rightarrow \theta_j - \eta \frac{\partial}{\partial \theta_j} E_T$$

§ Ultimately, the lowest energy found represents the best approximation of the ground state.

COMPUTING EXPECTATION VALUES

§ The trial wavefunction, in just one dimension, is simple to compute numerically. But with many-body problems in 3 dimensions, the number of dimensions in the integral scales as $3xN_{particles}$.

$$E_t = \frac{\int dr \Psi_T^*(r,\vec{\theta}) H \Psi_T(r,\vec{\theta})}{\int dr \Psi_T^*(r,\vec{\theta}) \Psi_T(r,\vec{\theta})} \qquad r \equiv (\vec{r_1}, \vec{r_2}, ...\vec{r_N})$$

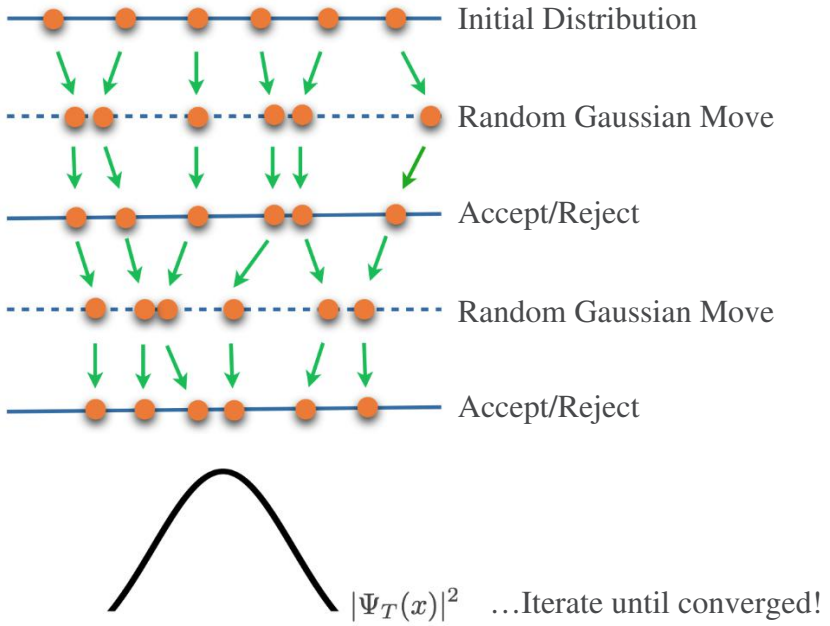
§ Sampling this integral in a dense or even adaptive way is computationally very very hard!

§ The **central limit theorem** provides a way to approximate this multi-dimensional integral.

M(RT)² SAMPLING

- We can compute the energy for any trial wavefunction as long as we sample x_i from the probability distribution $P(x_i)$.
- The M(RT)² algorithm* provides a technique to sample from any arbitrary probability distribution under general conditions.
- Referring to each collection of nucleons as a "walker," compute the observables with N total walkers
- This algorithm performs a walk in both Cartesian coordinates AND spin/isospin.

*named for N. Metropolis, A. Rosenbluth, M. Rosenbluth, A. Teller, E. Teller



https://github.com/Nuclear-Physics-with-Machine-Learning/AI4NP_School/blob/main/Lectures/MLNP_school_I.pdf

ANTI-SYMMETRY

§ A wavefunction of many fermions must be anti-symmetric under the exchange of any two particles. We enforce this directly in the network with the Slater determinant, in combination with a fully-symmetric DeepSets based correlator (U)

$$S = \begin{pmatrix} \langle x_1|\zeta_1\rangle & \langle x_2|\zeta_1\rangle & \dots & \langle x_N|\zeta_1\rangle \\ \langle x_1|\zeta_2\rangle & \langle x_2|\zeta_2\rangle & \dots & \langle x_N|\zeta_2\rangle \\ \vdots & & \ddots & \vdots \\ \langle x_1|\zeta_N\rangle & \langle x_2|\zeta_N\rangle & \dots & \langle x_N|\zeta_N\rangle \end{pmatrix}$$

$$S_{\text{deuteron}} = \begin{pmatrix} \langle x_1|R_1 p\uparrow\rangle & \langle x_2|R_1 p\uparrow\rangle \\ \langle x_1|R_2 n\uparrow\rangle & \langle x_2|R_2 n\uparrow\rangle \end{pmatrix}$$

x_i is a generalized coordinate of spatial position, spin, and isospin.

$$|\zeta_i\rangle = |R_i\rangle\,|s_i\rangle\,|\tau_i\rangle$$

NEURAL NETWORK QUANTUM STATES

§ In general, we need a wavefunction of the form (S is matrix):

$$\psi(\vec{r}_1, ...\vec{r}_N) = e^{U(\vec{r}_1, ...\vec{r}_N)} \det(S)$$

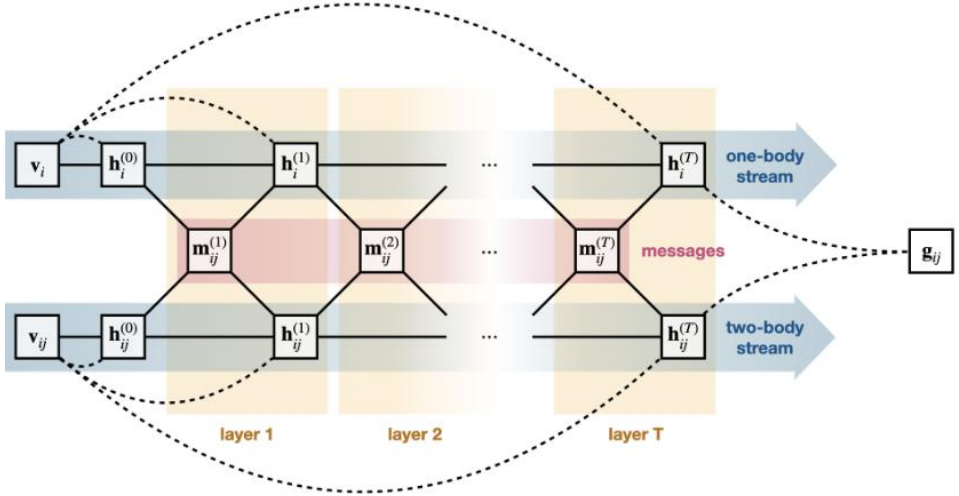
§ In practice, we enforce full symmetry of the correlator under exchange of particles using the **DeepSets** formalism:

$$U(\vec{r}_1, ..., \vec{r}_A) = \rho_U \left(\sum_{\vec{r}_i} \phi_U(\vec{r}_i) \right) \qquad \phi, \rho = ANN$$

§ Each particle's location is mapped to a latent space, and the latent space of all particles is summed to destroy individual interactions, then mapped to a single value.

ENCODING CORRELATIONS

§ We can enhance the encoding of particle-to-particle correlations with Message Passing Graph Neural Networks -maintaining .



We **replace** the inputs to the Slater determinant and correlator with the output of the message passing graph neural network.

This approaches a universal approximator as the variational state.

NEURAL NETWORK PHYSICALITY

§ The neural network implementation must also obey physical constraints: must be twice differentiable, continuous in the first derivative, and for a bound state must go to 0 at infinity.

§ In practice, we enforce this with select activation functions (yes to tanh/sigmoid, no to ReLU!). A correlator function U is also augmented with a confinement term (goes to 0 at infinity):

$$U(\vec{r}_1, ..., \vec{r}_A) = \rho_U \left(\sum_{\vec{r}_i} \phi_U(\vec{r}_i) \right) - \alpha \sum_i \vec{r}_i^2$$

STOCHASTIC RECONFIGURATION

§ The gradients computed above can be improved via “Stochastic Reconfiguration”
  – https://journals.aps.org/prb/abstract/10.1103/PhysRevB.71.241103

$$S_R^{mn} \equiv \langle O^m O^n \rangle - \langle O^m \rangle \langle O^n \rangle \qquad S_{R,\epsilon}^{-1} \equiv (S_R + \mathbb{I}\epsilon)^{-1}$$

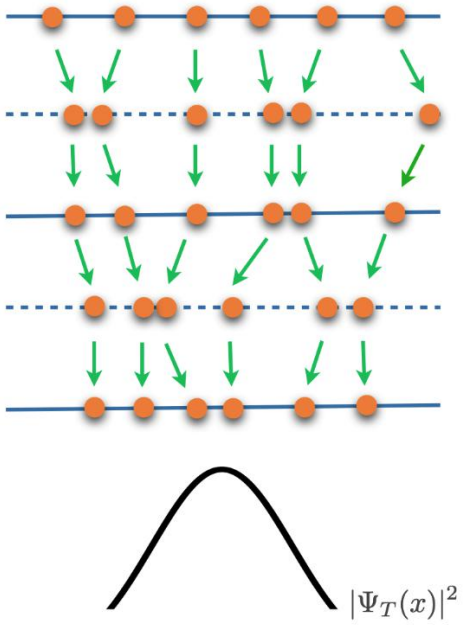
§ Effectively, this flattens the space of optimization and is a 2nd order approach

$$\theta_j \to \theta_j - \eta \sum_j S_{R,\epsilon}^{-1} \frac{\partial}{\partial \theta_j} E_T$$

§ But, this requires the jacobian matrix of the network!

ALGORITHM SUMMARY 1

- For a trial wavefunction, create sets of $N_{walkers}$ to use for a numerical integration.
- Thermalize the walkers for N_{therm} iterations at the start; between each measurement use N_{void} steps to remove correlations in measurements.
- For each set of thermalized, de-correlated walkers, compute the observable properties:
  - E_T, it's variational derivatives, the reconfiguration matrix S_{ij}.



ALGORITHM SUMMARY 2

§ Accumulate the **observables** for N_{obs} iterations;

$$G^i \equiv \frac{\partial \langle E_T \rangle}{\partial \theta_i} = 2\left(\langle O^i H \rangle - \langle E_T \rangle \langle O^i \rangle\right)$$

$$S_R^{mn} \equiv \langle O^m O^n \rangle - \langle O^m \rangle \langle O^n \rangle$$

§ Update the wave function according to the accumulated observables and the update rule:

$$\theta_j \to \theta_j - \eta \sum_j S_{R,\epsilon}^{-1} \frac{\partial}{\partial \theta_j} E_T$$

Thermalize O(5000) steps

Measurement of G, S, Update θ

De-correlate O(500) steps

Measurement of G, S, Update θ

De-correlate O(500) steps

Measurement of G, S, Update θ

…Until Convergence

De-correlate O(500) steps

Measurement of G, S, Update θ

COMPUTATIONAL EFFICIENCY

§ This algorithm can (and has been) implemented in there DL frameworks (TF, Torch, Jax). Jax is the clear winner for computational efficiency.

§ Torch is imperative: the ”walk” algorithm is too slow, and makes terrible use of the GPU.
  – LibTorch is better, but has concurrency issues when computing the Jacobian matrix.
  – Generally torch is great when each GPU op is Big. It falls over when there are many many small ops.

§ Tensorflow is better, but it’s graph compilation stage can be tedious and detrimental to start-up times as the problem size scales up.
  – Has excellent scaling properties, though!

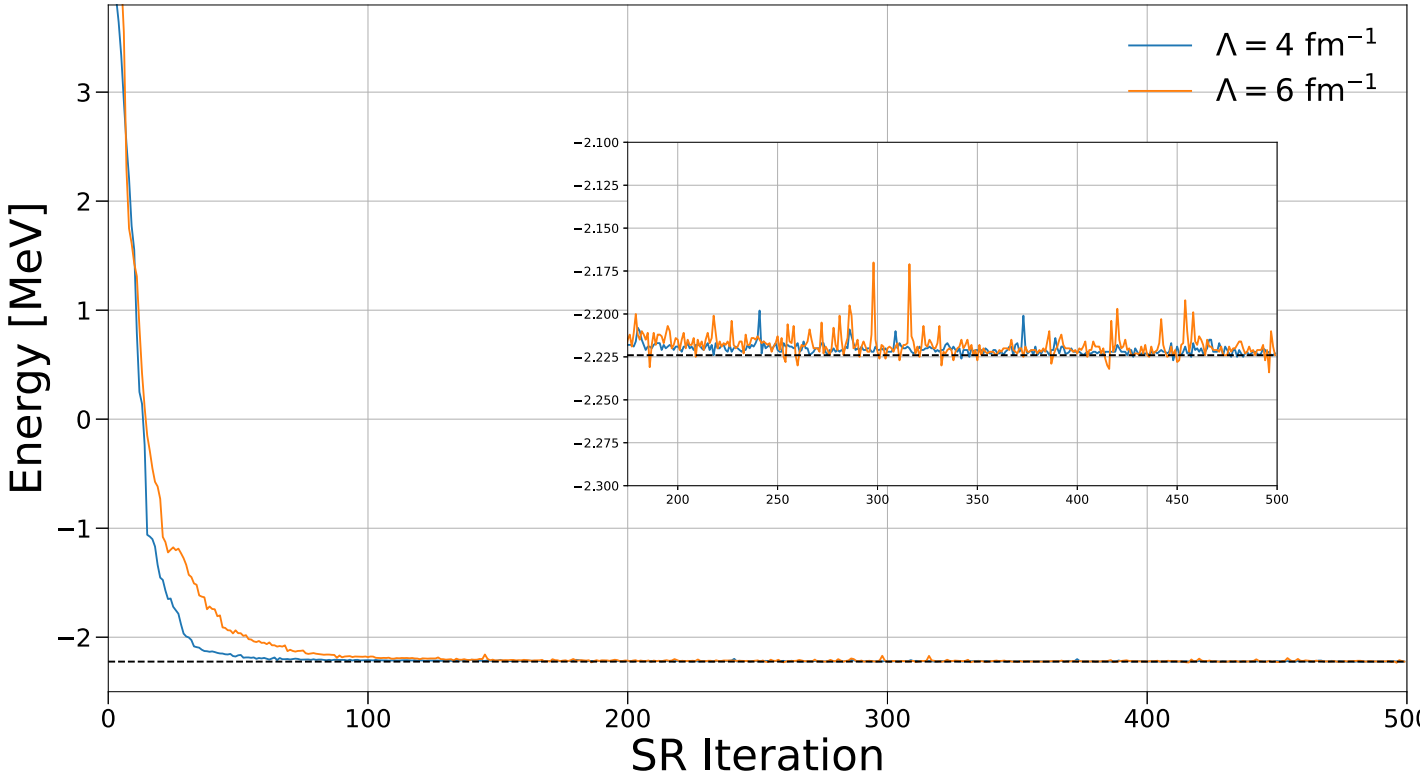
COMPUTATIONAL EFFICIENCY (2)

§ The non-traditional derivatives of this algorithm also are a challenge:
- Need first and second derivative with respect to input variables
- Need a jacobian with respect to model parameters
- No simple vectorization and poor performance with both TF (jacobian) and Torch (both!)

§ Jax offers a solution to all of this:
- Easy to compile the many-small-ops Metropolis algorithm
- Easy to vectorize the gradient of the wavefunction over all parameters (Jacobian)
- Easy to vectorize the 2nd derivatives.

§ In short: if you have a "weird" algorithm using machine learning, Jax is awesome.

SOLVING THE DEUTERON



NUCLEI UP TO A=6

Nucleus	Potential	ANN		HH		Exp.	
		E (MeV)	$r_{\rm ch}$ (fm)	E (MeV)	$r_{\rm ch}$ (fm)	E (MeV)	$r_{\rm ch}$ (fm)
^{2}H	NN	$-2.242(1)$	$2.120(5)$	-2.242	$2.110(2)$	-2.225	2.128
^{3}H	NN	$-9.511(1)$	$1.658(4)$	-9.744	$1.656(4)$	-8.475	$1.755(86)$
	$3N$	$-8.232(1)$	$1.750(3)$	-8.475	$1.747(6)$		
^{3}He	NN	$-8.800(1)$	$1.845(3)$	-9.035	$1.848(6)$	-7.718	$1.964(1)$
	$3N$	$-7.564(1)$	$1.961(3)$	-7.811	$1.969(8)$		
^{4}He	NN	$-36.841(1)$	$1.484(3)$	-37.06	$1.485(4)$	-28.30	1.678
	$3N$	$-27.903(1)$	$1.643(2)$	-28.17	$1.646(4)$		
^{6}He	NN	$-37.25(4)$	$1.895(2)$	$-37.96(8)$	$1.71(1)$	-29.27	$2.05(1)$
	$3N$	$-27.46(2)$	$> 4.89(1)$	$-27.41(8)$	> 2.73		
^{6}Li	NN	$-42.04(1)$	$2.248(3)$	$-42.51(5)$	$2.09(2)$	-31.99	$2.54(3)$
	$3N$	$-30.82(3)$	$3.049(2)$	$-31.00(8)$	> 2.74		

Table 1 from https://link.springer.com/article/10.1007/s00601-021-01706-0

CONVERGENCE OF HELIUM

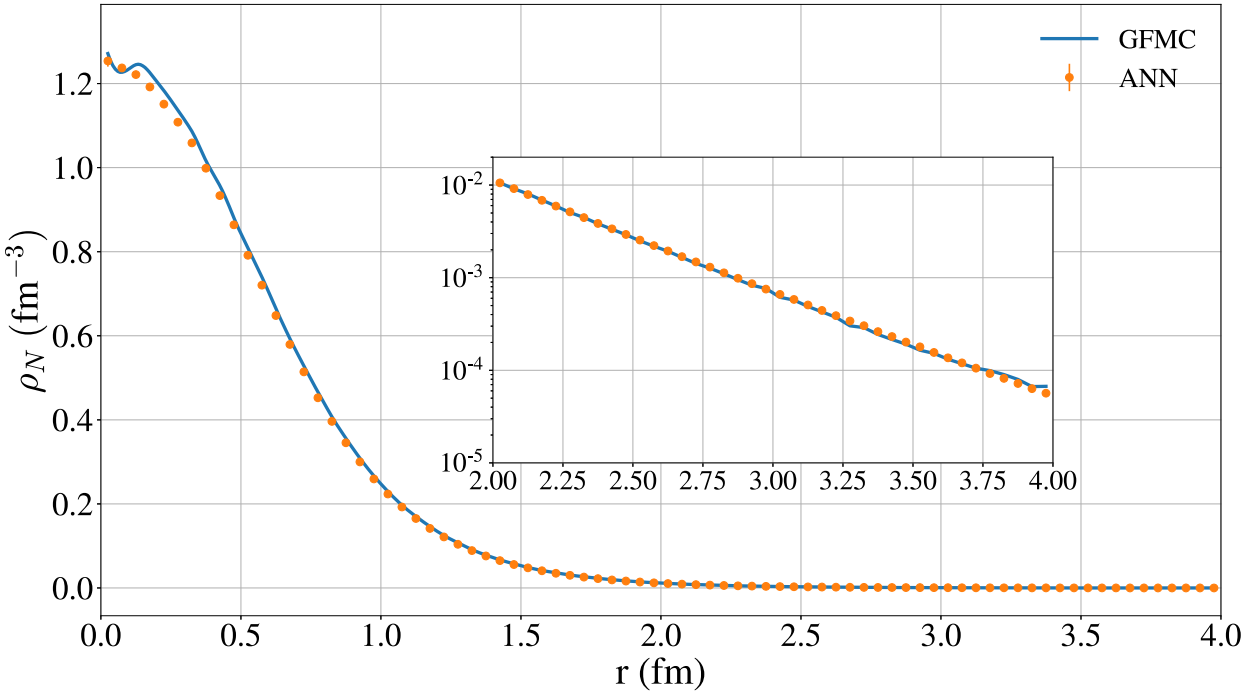
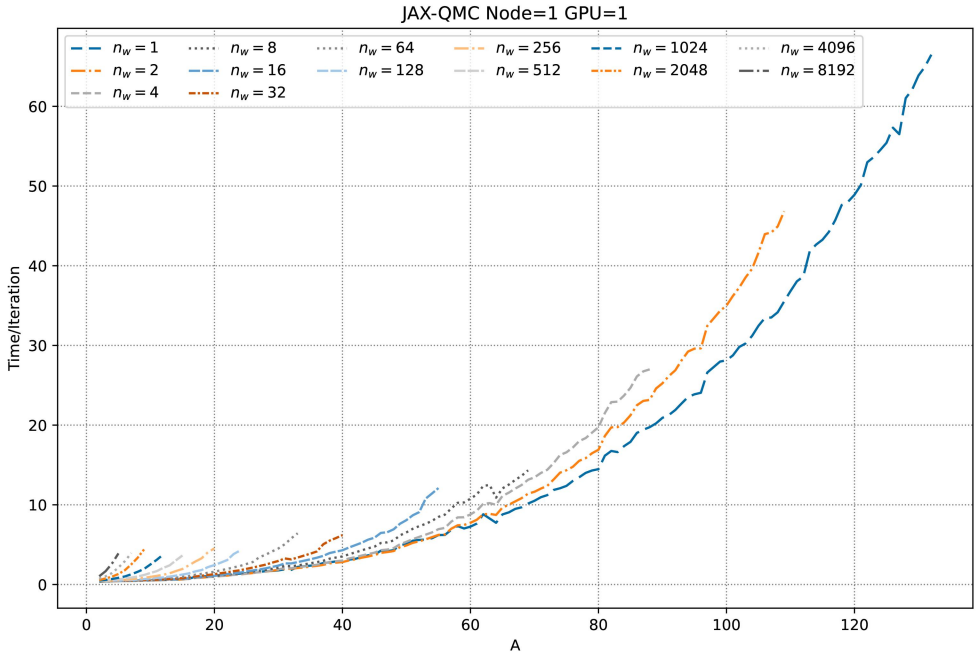


Figure 2 from https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.127.022502

The point-nucleon density of ^{4}He compared to the classical, Green's field Monte Carlo Technique –accurate over 4 orders of magnitude.

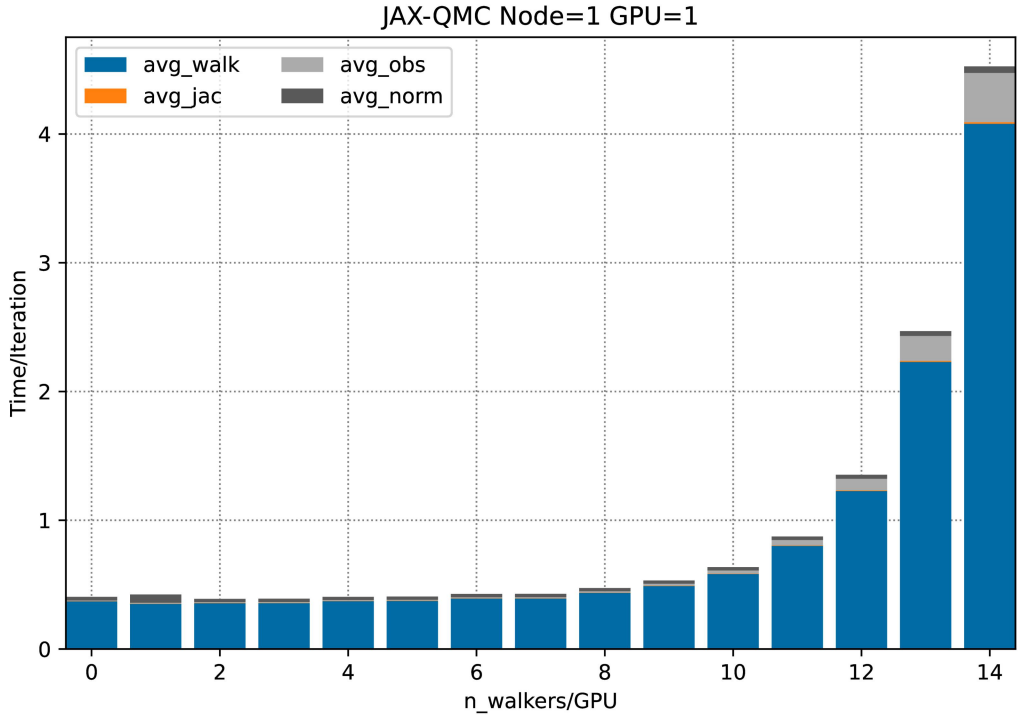
SCALING TO LARGER NUCLEI



As the number of walkers increases, both computational time and memory usage increases.

The only solution to reach larger nuclei is to **parallelize** the algorithm.

SCALING TO LARGER NUCLEI



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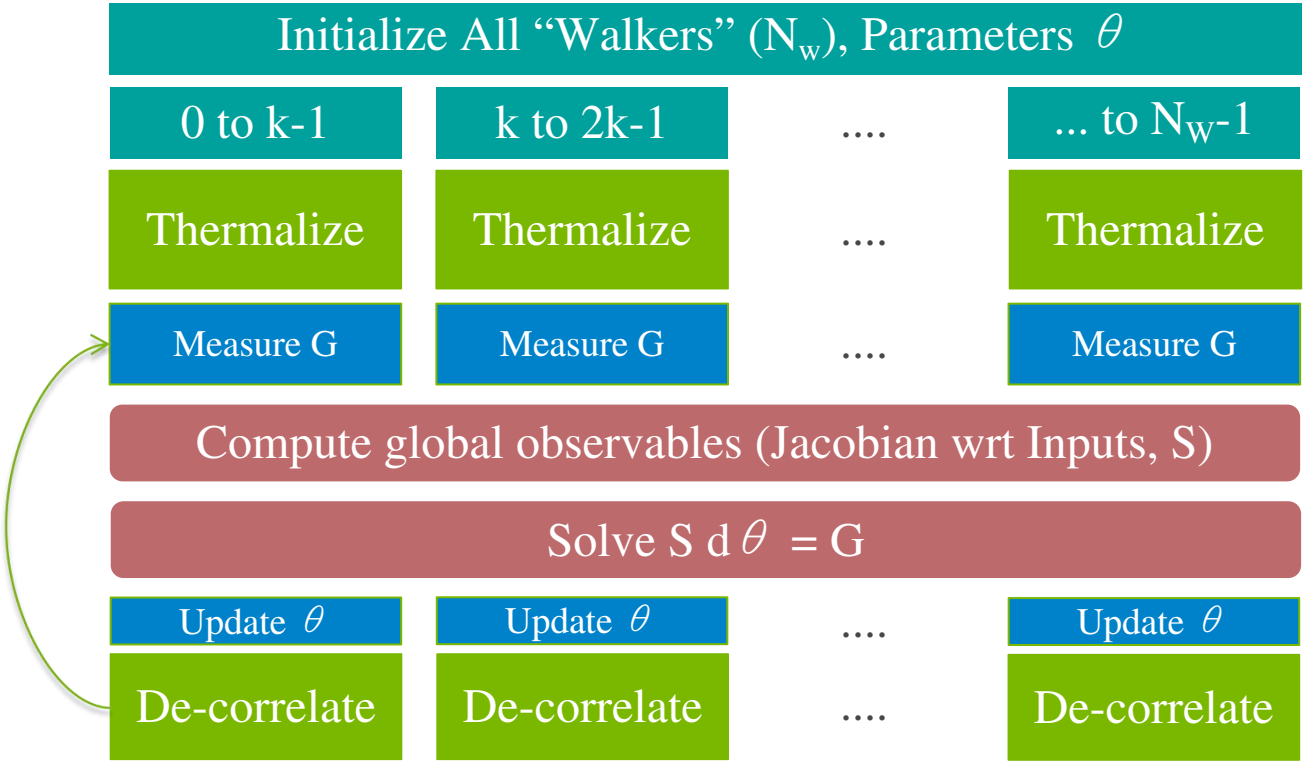
The only solution to reach larger nuclei is to **parallelize** the algorithm.

PARALLELIZATION STRATEGY

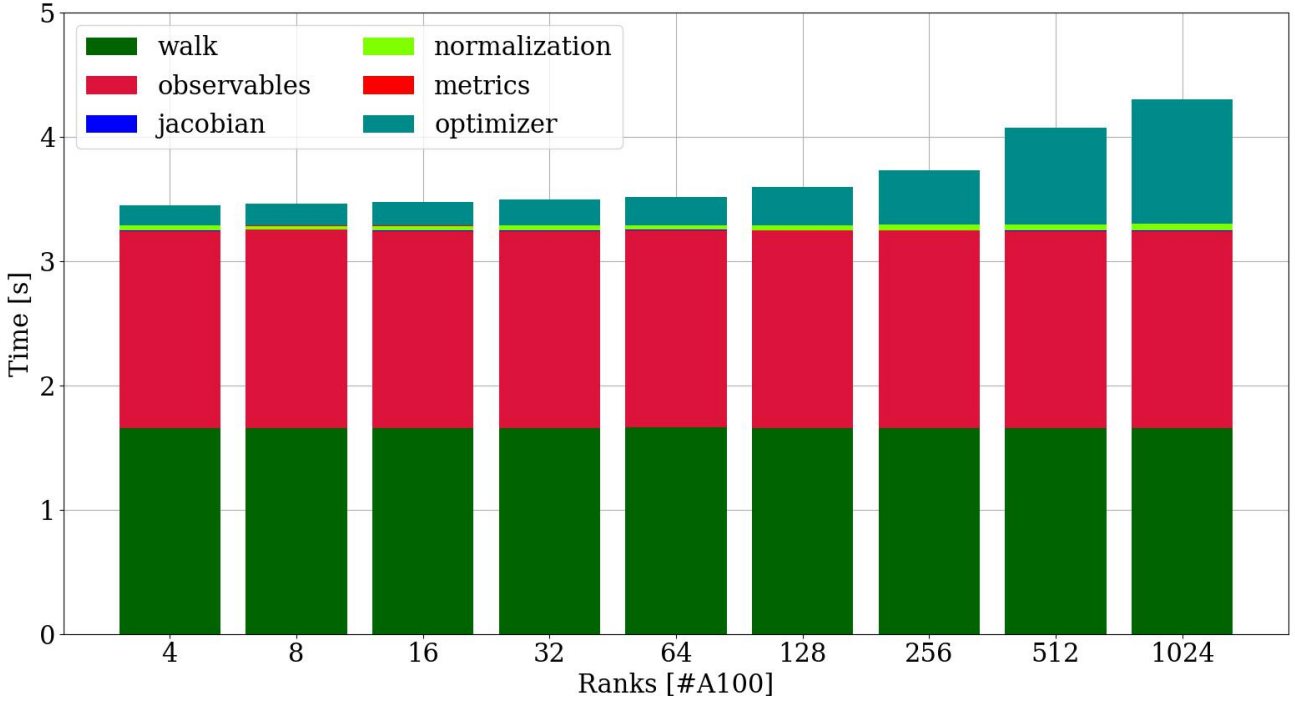


N_R ranks,
$k = N_W/N_R$ walkers per rank

G is the 1st order parameter updates

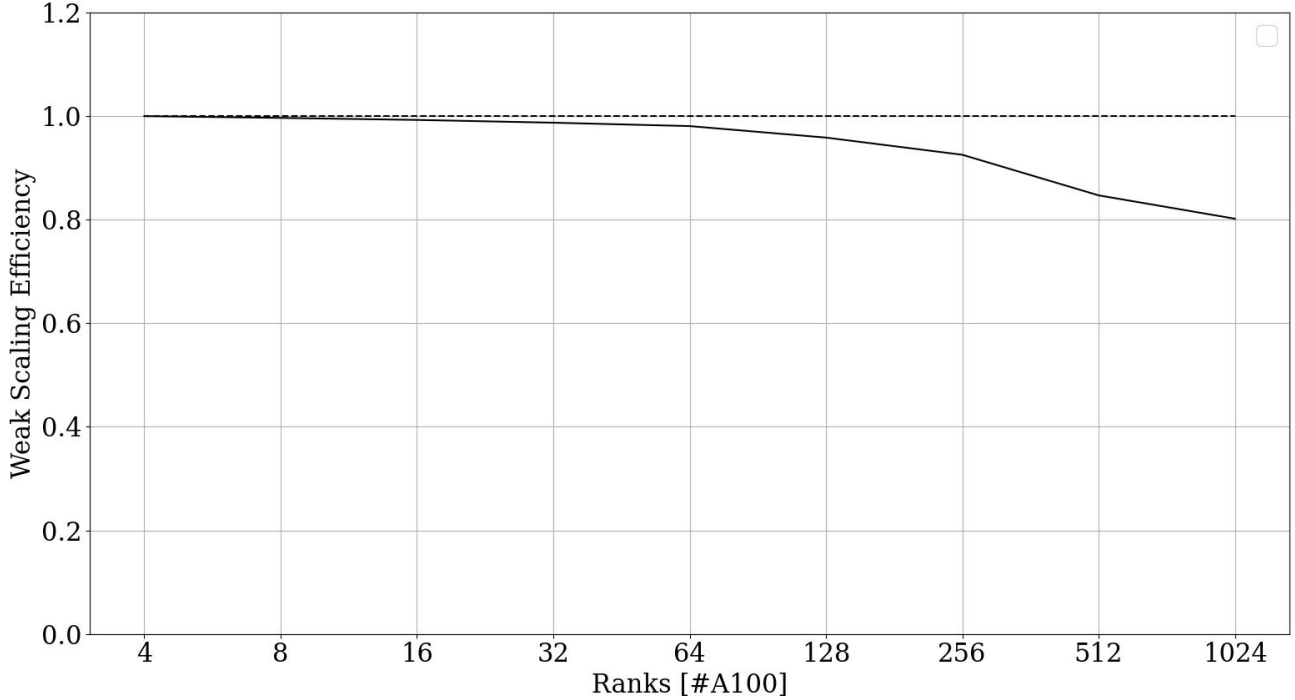
Multiple options for inverting S

SCALING UP ON POLARIS



Scaling efficiency is dominated by the conjugate gradient algorithm to solve for the second-order parameter updates.

SCALING UP ON POLARIS



Scaling efficiency is dominated by the conjugate gradient algorithm to solve for the second-order parameter updates.

ONGOING WORK

§ We continue to develop these techniques with the aim of solving bigger and bigger systems.
  – We intend to solve the Calcium nucleus on Polaris this year.

§ With Aurora, we will be able to solve nuclei near A=100.
  – Biggest challenge will be ensuring the inversion of the matrix S_{ij} does not become a bottleneck at scales beyond 1000 ranks.

§ We are also looking into applying these same techniques to different Hamiltonians, namely molecules.

THANK YOU!

CENTRAL LIMIT ESTIMATES

§ Let P(x) be a probability distribution, and (x_1, … x_N) be drawn from P(x). For the function f(x), you can define a new random variable:

$$S_N = \frac{1}{N}\sum_{i=1}^{N} f(x_i)$$

§ By the central limit theorem:

$$\bar{S}_N = \int dx P(x) f(x) \qquad \sigma_N = \sqrt{\frac{1}{N}\left[\int P(x) f(x)^2 dx - \bar{S}_N\right]}$$

$$I = \int dx f(x) = \int dx P(x) \frac{f(x)}{P(x)}$$

VARIATIONAL MEASUREMENTS

§ The integral to estimate the energy of a trial wavefunction is:

$$E_T = \frac{\langle \psi_T | \, H \, | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle} = \frac{\int dR \, \langle \psi_T | R \rangle \, \langle R | H | \psi_T \rangle}{\int dR \, \langle \psi_T | R \rangle \, \langle R | \psi_T \rangle}$$

§ Define a quantity $E_L(R)$: $$E_L(R) \equiv \frac{H\psi_T(R)}{\psi_T(R)}$$

$$E_T = \frac{\int dR |\psi_T(R)|^2 E_L(R)}{\int dR |\psi_T(R)|^2}$$

TRIAL ENERGY ESTIMATE

§ Numerically approximate the integral by sampling R from the probability distribution P(R):

$$P(R) = \frac{|\psi(R)|^2}{\int dR |\psi_T(R)|^2} \qquad \langle E_T \rangle = \frac{1}{N} \sum_n E_L(R_n)$$

§ And, the integration error can be estimated just as easily:

$$\langle E_T^2 \rangle = \frac{1}{N} \sum_n E_L^2(R_n) \qquad E_L(R) \equiv \frac{H\psi_T(R)}{\psi_T(R)}$$

PRACTICAL CONSIDERATIONS

§ The M(RT)^2 algorithm has some nice properties:
- We can sample nearly any function;
- It is numerically and analytically fairly simple;
- It is easily parallelized up to however many configurations we want

§ Also: The M(RT)^2 algorithm has some unfortunate convergence properties:
- It takes a large number of steps to converge to the target distribution, especially initially.
- Subsequent samples are often frequently correlated with each other, requiring intermediate steps to re-thermalize.
- Discarding sampled configurations initially and with each re-thermalization is quite wasteful.

ENERGY MINIMIZATION

§ Recall the wavefunction, and the values we must compute:

$$\psi_T = \psi_T(R, \vec{\theta}) \qquad E_L(R) \equiv \frac{H\psi_T(R)}{\psi_T(R)}$$

§ So,

$$\frac{\partial \langle E_T \rangle}{\partial \theta_i} = 2\left(\frac{\langle \partial_i \psi_T | H | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle} - E_T \frac{\langle \partial_i \psi_T | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle} \right)$$

§ Define:

$$O^i \psi_T(R, \vec{\theta}) \equiv \frac{\partial}{\partial \theta_i} \psi_T(R, \vec{\theta}) \qquad G^i \equiv \frac{\partial \langle E_T \rangle}{\partial \theta_i} = 2\left(\langle O^i H \rangle - \langle E_T \rangle \langle O^i \rangle \right)$$

CALCULUS INTERLUDE

§ So far, we've encountered a number of derivatives:
  – The Hamiltonian operator requires a second derivative to compute the energy of the trial model, as a function of the inputs.
  – The Gradient Calculation requires derivatives of the trial model as a function of the parameters.

§ We can either figure out these derivates analytically (hard), numerically (slow), or leverage a machine learning framework that has automatic differentiation.
  – Which one?

§ In short: represent our "trial wavefunction" with a machine learning neural network.