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CALCULATION OF NUCLEAR GROUND STATES USING ARTIFICIAL NEURAL NETWORKS.

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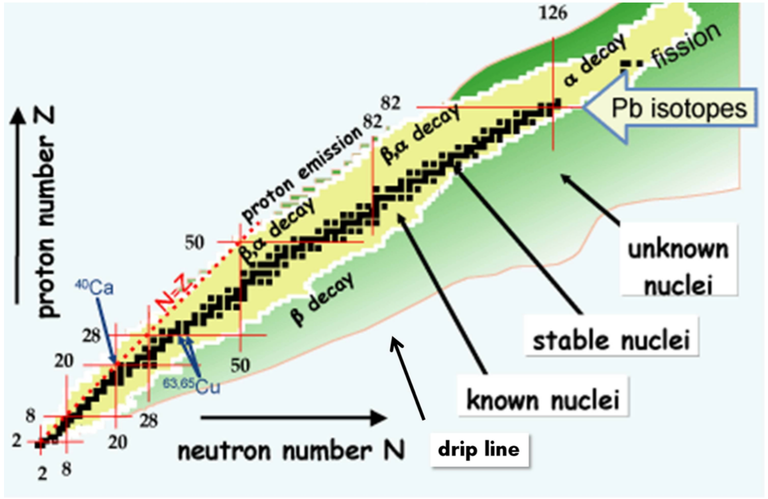
INTRODUCTION

Why nuclear physics?

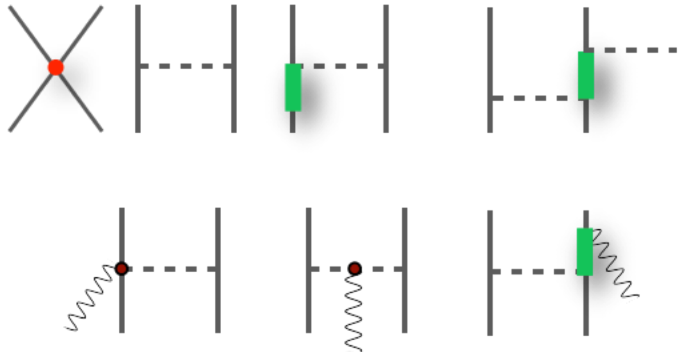
Atomic Nuclei are many-body systems governed by the strong interaction, which exhibit emergent properties such as: shell structure, pairing and superfluidity, deformation, and self-emerging clusters.



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.

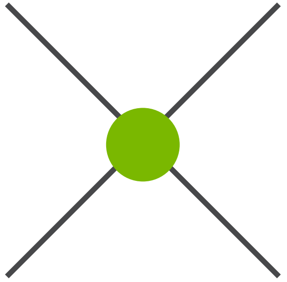


$$H = \sum_i \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

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

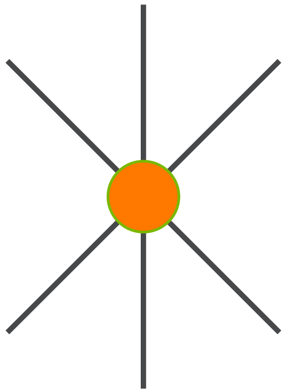
PION-LESS NUCLEAR HAMILTONIAN

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 ^{3}H

THE NUCLEAR MANY-BODY PROBLEM

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

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

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

- 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 trial wavefunction, 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 $3xN_{\text{particles}}$.

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

- 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.

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):

$$P(R) = \frac{|\psi(R)|^2}{\int dR|\psi_T(R)|^2}$$

$$\langle E_T \rangle = \frac{1}{N}\sum_n E_L(R_n)$$

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

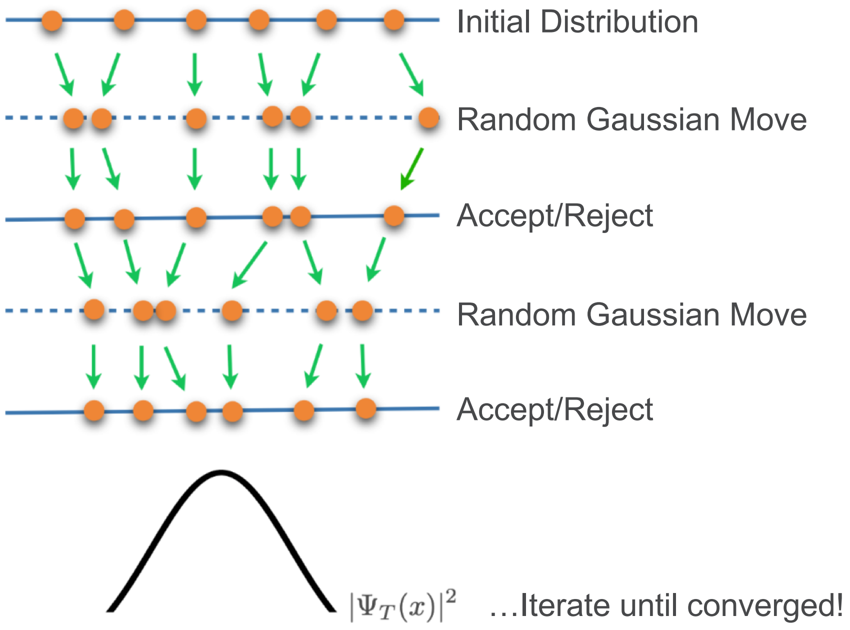
$$\langle E_T^2 \rangle = \frac{1}{N}\sum_n E_L^2(R_n)$$

$$E_L(R) \equiv \frac{H\psi_T(R)}{\psi_T(R)}$$

M(RT)^2 SAMPLING

- Now that we have a tool for computing integrals in high dimensionality, 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 sample as a "walker."

*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

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.

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):

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

- 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.

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

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

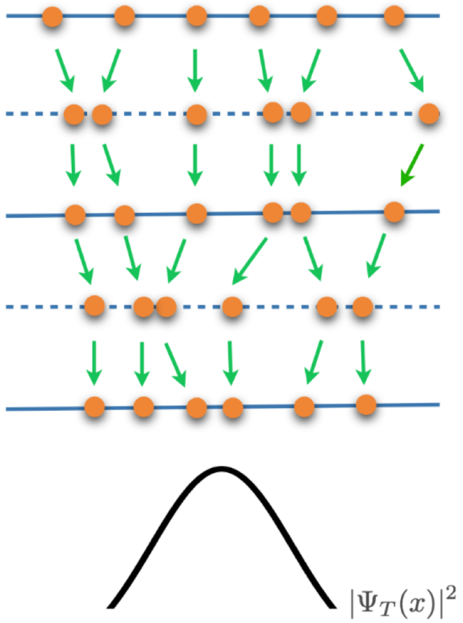
- Effectively, this flattens the space of optimization and is a 2nd order approach

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

- 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

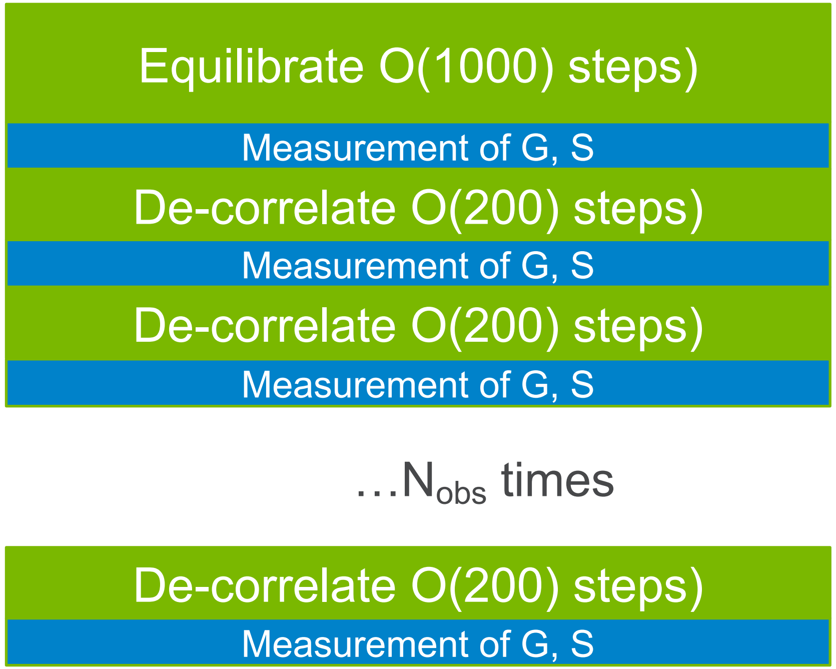
- Accumulate the **observables** for N_{obs} iterations;

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

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

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

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



Equilibrate O(1000) steps)
Measurement of G, S
De-correlate O(200) steps)
Measurement of G, S
De-correlate O(200) steps)
Measurement of G, S
…N_{obs} times
De-correlate O(200) steps)
Measurement of G, S

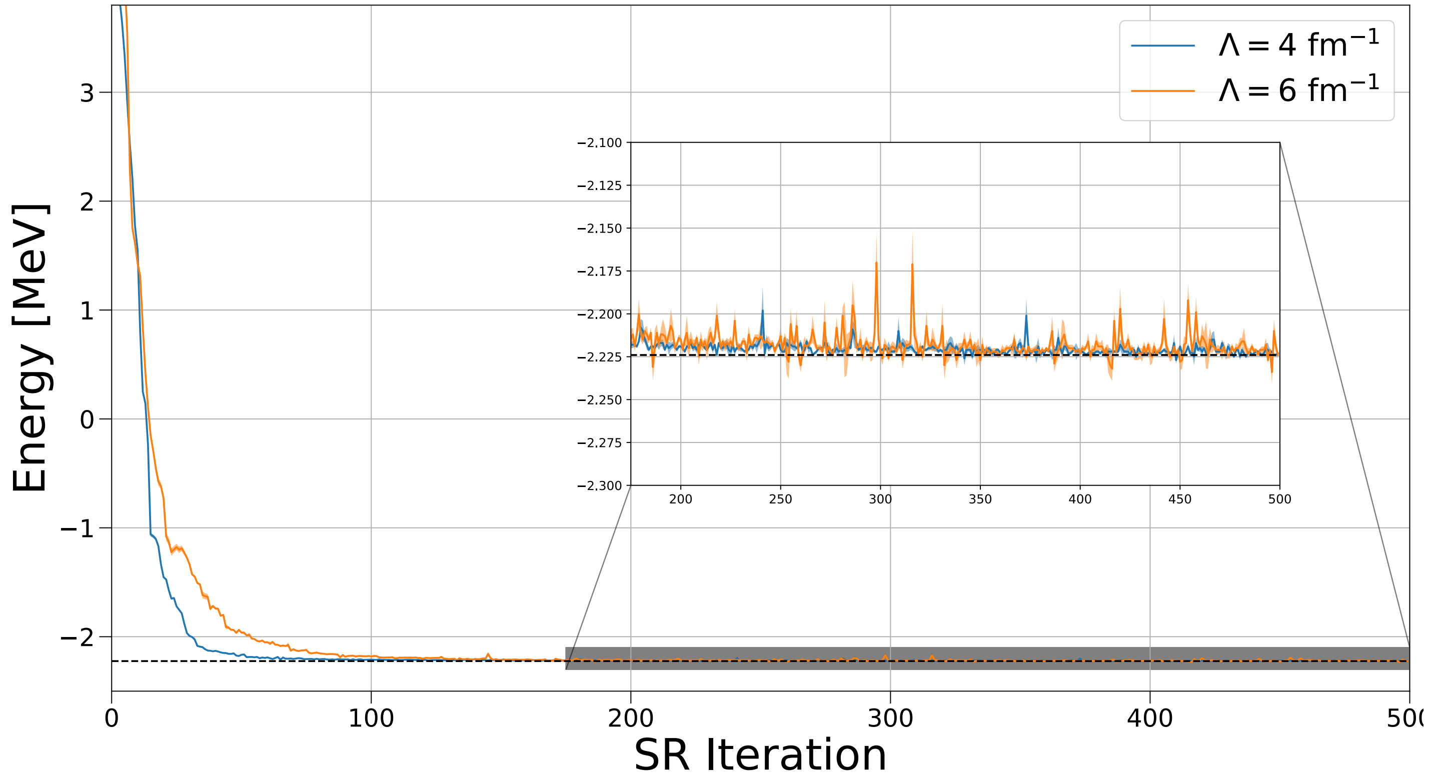
COMPUTATIONAL EFFICIENCY

- 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 a second derivative with respect to input variables, AND a jacobian.
  - 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

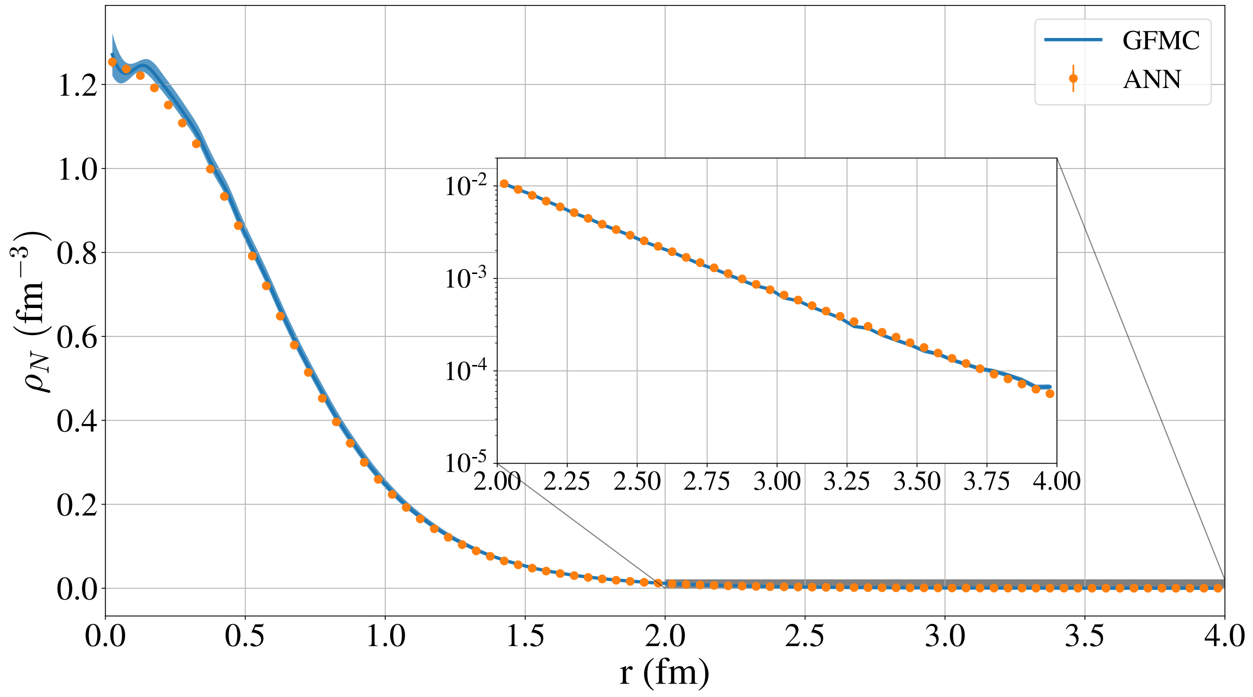


NUCLEI UP TO A=6

Nucleus	Potential	ANN		HH		Exp.	
		E (MeV)	r_{ch} (fm)	E (MeV)	r_{ch} (fm)	E (MeV)	r_{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



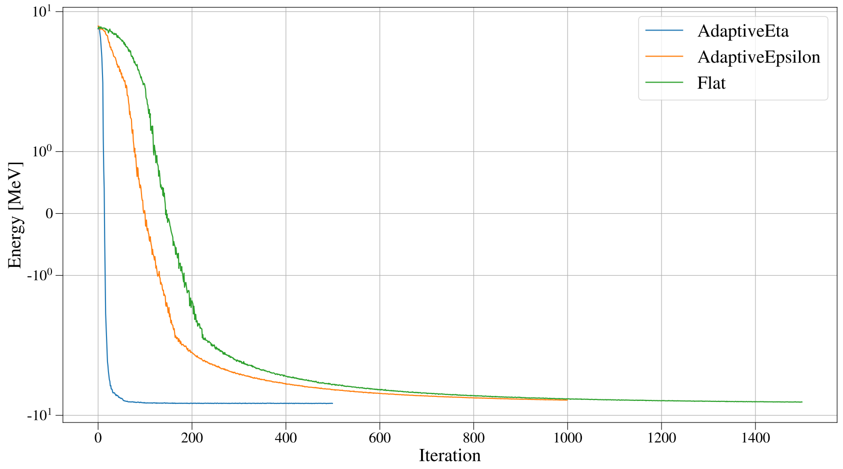
The point-nucleon density of ^{4}He compared to the classical, Green's field Monte Carlo Technique – accurate over 4 orders of magnitude.

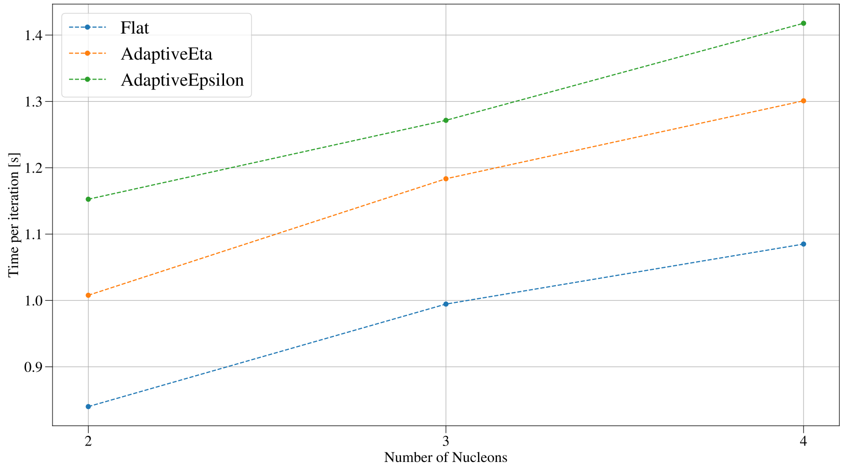
Figure 2 from https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.127.022502

OPTIMIZATION TRICKS

- The iterative update of parameters requires several hyperparameters, particularly the learning rate and the regularization parameter for the inversion of the Stochastic Reconfiguration matrix.
- Instead of picking hyperparameters, we can experiment:
  - Set values for the parameters, ensure the changes in the wavefunction are small.
  - update the wavefunction, recompute the energy
    - Because updates are constrained to be **small,** the previous walk can be reused by rescaling the probability (psi_new^2 / psi_old^2)
  - Choose the step with the best "next" energy

OPTIMIZATION TRICKS

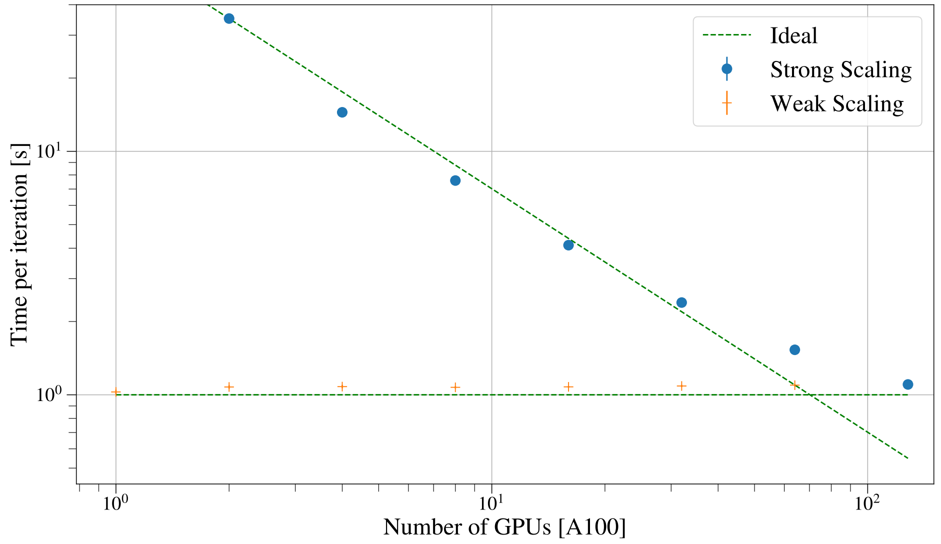




The “AdaptiveEta” (learning rate) quickly out-performs the standard algorithm with minimal additional computational cost (10% slower).

SCALABLE MACHINE LEARNING

- The algorithm, as designed, is easily scalable to multiple compute systems:
  - We compute the observables a total number of N_{obs} times
  - This can be trivially distributed across M GPUs, as long as N_{obs} / M is an integer.
- Nearly perfect weak scaling up to hundreds of A100 GPUs.



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.
- Our software is open source and available on github with minimial software requirements (tensorflow) and no input requirements:
  – https://github.com/Nuclear-Physics-with-Machine-Learning
  – This also includes a tutorial session on these numerical techniques presented at the 2021 AI-in-Nuclear-Physics winter School
    - (Including hands-on exercises in Tensorflow, if you want to try this out – we solve the hydrogen atom with machine learning)

THANK YOU!