

Ab initio calculations of nuclear thermodynamics

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Collaborate with: (Nuclear Lattice EFT Collaboration)

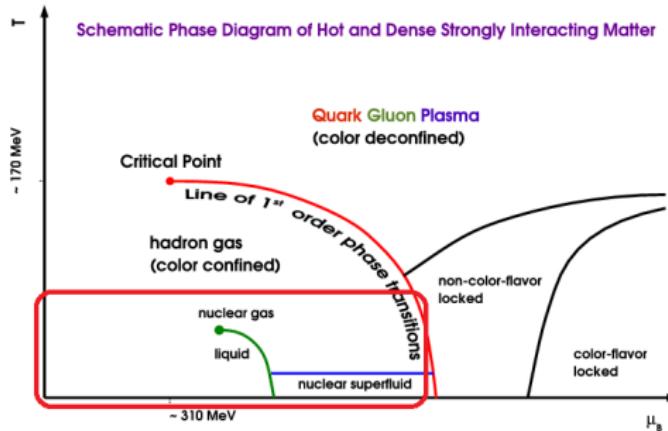
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Nuclear thermodynamics

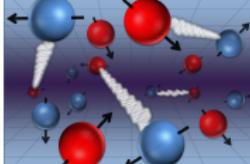
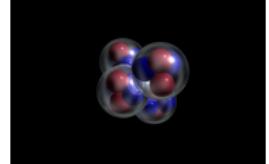
- At low temperature and density, nuclear matter can have different phases.
- Indirect evidences of liquid-gas phase transition are found in heavy-ion collision at intermediate energy (Temperature ~ 10 MeV).

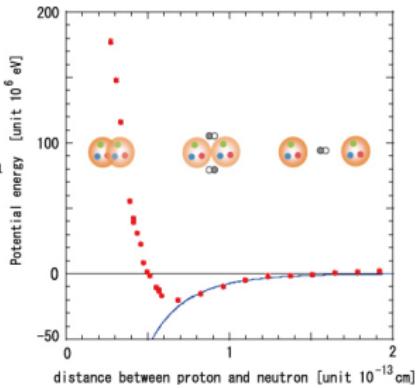
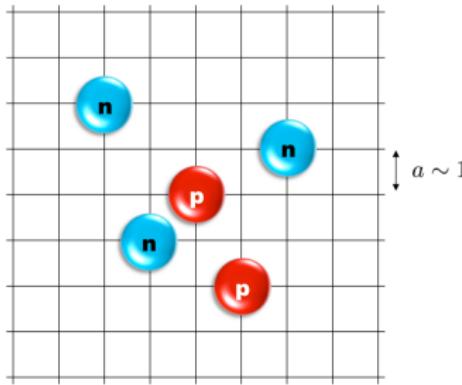


Goal of Lattice Chiral Effective Field Theory: Understand the low-energy nuclear physics based on the knowledge of the bare $N - N$ interaction (Hopefully from lattice QCD!).

Fig. taken from T. Csorgo, arXiv:0911.5015

Lattice chiral effective field theory

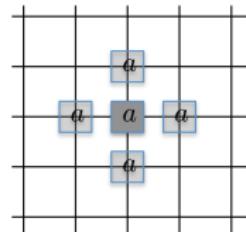
			
Quarks, Gluons	Nucleons, Pions	Alpha-clusters	Surface shape
Lattice QCD	Lattice χ EFT	Few-body models	Collective models



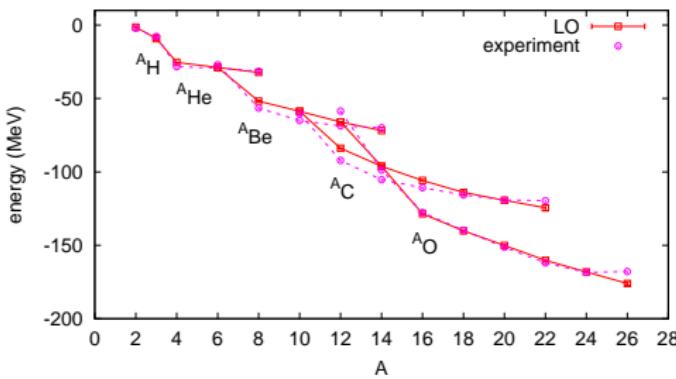
New leading order interaction

- A new non-locally smeared interaction for LEFT was proposed. [Elhatisari, Epelbaum, Krebs, Lahde, Lee, Li, BNL, Meissner, Rupak, PRL 119, 222505 \(2017\)](#)
- Reproduce both the N - N phase shift and the light nuclei binding energies with only 3 adjustable parameters.

$$a_{\text{NL}}(n) = a(n) + s_{\text{NL}} \sum_{\langle n' n \rangle} a(n')$$
$$a_{\text{NL}}^\dagger(n) = a^\dagger(n) + s_{\text{NL}} \sum_{\langle n' n \rangle} a^\dagger(n')$$



a



Euclidean time projection

- Get interacting g. s. from imaginary time projection:

$$|\Psi_{g.s.}\rangle \propto \lim_{\tau \rightarrow \infty} \exp(-\tau H) |\Psi_A\rangle$$

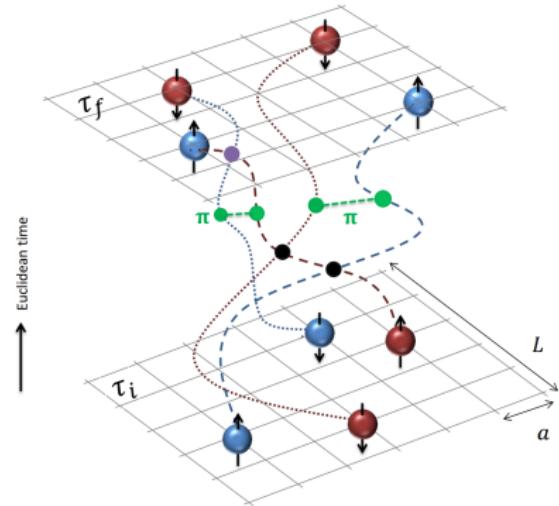
with $|\Psi_A\rangle$ representing A free nucleons.

- Expectation value of any operator \mathcal{O} :

$$\langle \mathcal{O} \rangle = \lim_{\tau \rightarrow \infty} \frac{\langle \Psi_A | \exp(-\tau H/2) \mathcal{O} \exp(-\tau H/2) | \Psi_A \rangle}{\langle \Psi_A | \exp(-\tau H) | \Psi_A \rangle}$$

- τ is discretized into time slices:

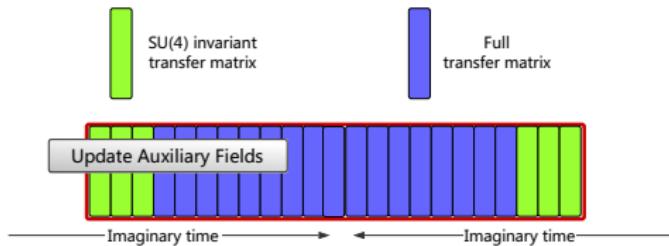
$$\exp(-\tau H) \simeq \left[: \exp\left(-\frac{\tau}{L_t} H\right) : \right]^{L_t}$$



All possible configurations in $\tau \in [\tau_i, \tau_f]$ are sampled.

Complex structures like nucleon clustering emerges naturally.

Hybrid Monte Carlo method



Samples are generated by updating the Auxiliary Fields using Hybrid Monte Carlo algorithm.

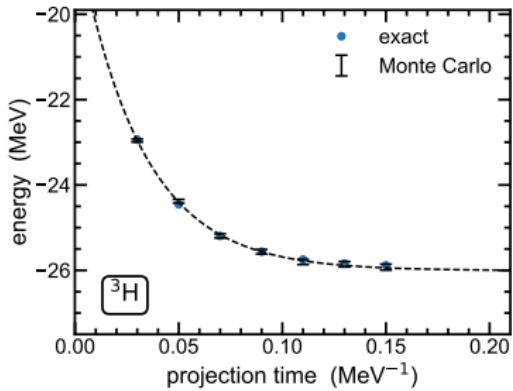
The total energies at large t follow

$$E_{\mathbf{A}}(t) = E_{\mathbf{A}}(\infty) + c \exp[-\Delta E t].$$

For inserted operator \mathcal{O} ,

$$\mathcal{O}_{\mathbf{A}}(\tau) = \mathcal{O}_{\mathbf{A}}(\infty) + c_4 \exp[-\Delta E \tau/2],$$

where ΔE is the excitation energy of the first excited state.



Pinhole algorithm: track the individual nucleon

In Lattice EFT it is hard to measure observables in the center of mass frame.

Solution: track the the status of individual nucleons using pinhole algorithm.

- Let $n = (r, s, i)$ denotes the position, spin and isospin, the density operator

$$\rho(n) = a^\dagger(n)a(n)$$

measure the number of nucleons occupying quantum state n .

- The A -body density operator

$$\rho_A(n_1, \dots, n_A) =: \rho(n_1) \cdots \rho(n_A) :$$

measure the probability of A -nucleons occupying quantum state n_1, n_2, \dots, n_A .

- The ground state probability density distribution can be written as

$$|\Phi(n_1, \dots, n_A)|^2 = \langle \rho_A \rangle = \lim_{\tau \rightarrow \infty} \frac{\langle \Psi_A | \exp(-\tau H/2) : \rho(n_1) \cdots \rho(n_A) : \exp(-\tau H/2) | \Psi_A \rangle}{\langle \Psi_A | \exp(-\tau H) | \Psi_A \rangle}$$

Elhatisari, Epelbaum, Krebs, Lahde, Lee, Li, BNL, Meissner, Rupak, PRL 119, 222505 (2017)

Pinhole algorithm: Sampling

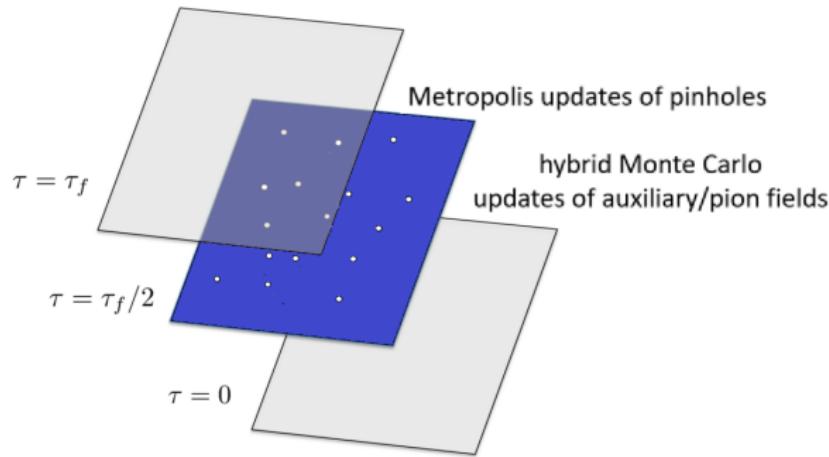
The expectation value of operator $O = O(n_1, \dots, n_A)$ can be expressed as

$$\langle O \rangle = \lim_{\tau \rightarrow \infty} \frac{\sum_{n_1, \dots, n_A} \int \mathcal{D}s \mathcal{D}\pi \langle \Psi_A | e^{-\frac{\tau}{2} H(s, \pi)} \rho_A(n_1, \dots, n_A) e^{-\frac{\tau}{2} H(s, \pi)} | \Psi_A \rangle O(n_1, \dots, n_A)}{\sum_{n_1, \dots, n_A} \int \mathcal{D}s \mathcal{D}\pi \langle \Psi_A | e^{-\frac{\tau}{2} H(s, \pi)} \rho_A(n_1, \dots, n_A) e^{-\frac{\tau}{2} H(s, \pi)} | \Psi_A \rangle},$$

We generate an ensemble with probability distribution

$$P(s, \pi, n_1, \dots, n_A) = \left| \langle \Psi_A | e^{-\frac{\tau}{2} H(s, \pi)} \rho_A(n_1, \dots, n_A) e^{-\frac{\tau}{2} H(s, \pi)} | \Psi_A \rangle \right|$$

with Hybrid Monte Carlo and Metropolis algorithms.

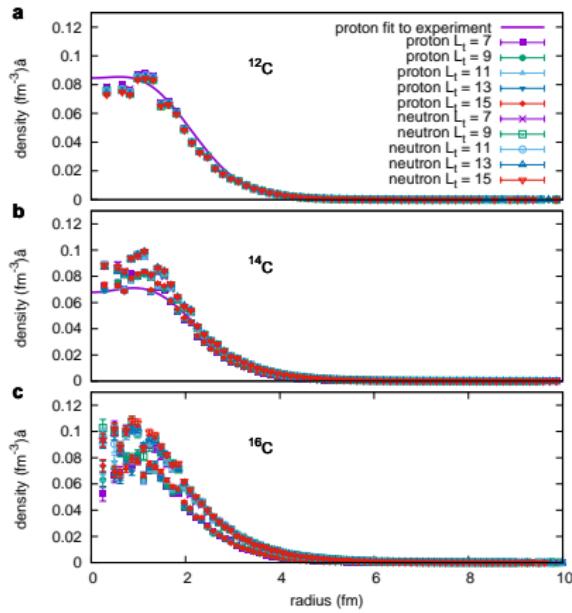


Pinhole algorithm: Intrinsic density distributions

Intrinsic densities can be measured directly in the pinhole mode:

$$\rho_{\text{c.m.}}(r) = \sum_{n_1, \dots, n_A} |\Phi(n_1, \dots, n_A)|^2 \sum_{i=1}^A \delta(r - |r_i - R_{\text{c.m.}}|)$$

Elhatisari, Epelbaum, Krebs, Lahde, Lee, Li, BNL, Meissner, Rupak, PRL 119, 222505 (2017)



Pinhole trace algorithm: Partition function

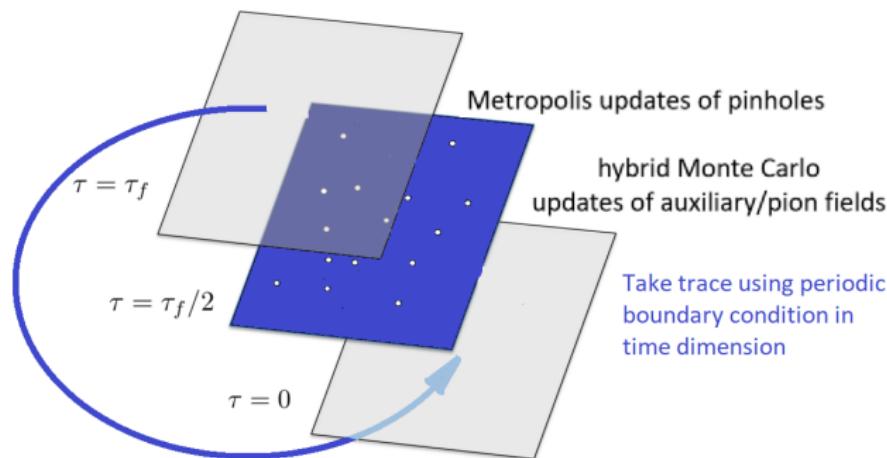
The pinhole states span the whole A -body Hilbert space.

The canonical partition function can be expressed using pinholes ($\beta = 1/k_B T$):

$$Z_A = \text{Tr}_A [\exp(-\beta H)] = \sum_{n_1, \dots, n_A} \int \mathcal{D}s \mathcal{D}\pi \langle n_1, \dots, n_A | \exp[-\beta H(s, \pi)] | n_1, \dots, n_A \rangle$$

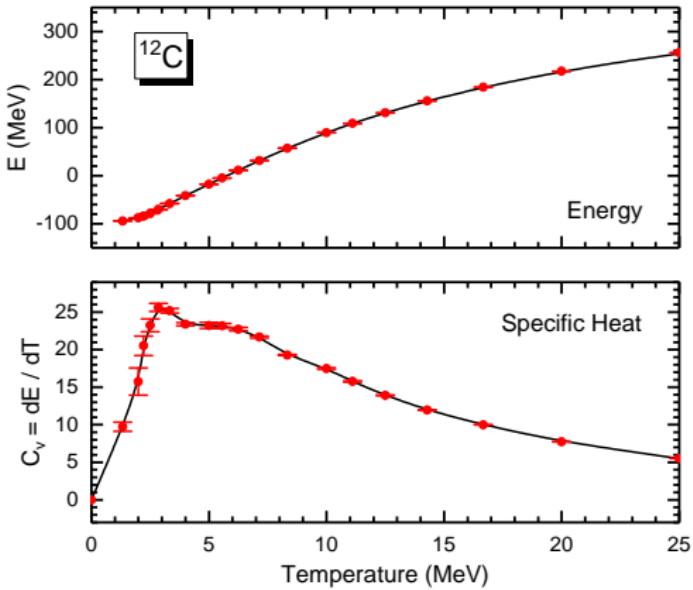
The expectation value of operator $O = O(n_1, \dots, n_A)$ can be expressed as

$$\langle O \rangle = \lim_{\tau \rightarrow \infty} \frac{\sum_{n_1, \dots, n_A} \int \mathcal{D}s \mathcal{D}\pi \langle n_1, \dots, n_A | \exp[-\beta H(s, \pi)] | n_1, \dots, n_A \rangle O(n_1, \dots, n_A)}{\sum_{n_1, \dots, n_A} \int \mathcal{D}s \mathcal{D}\pi \langle n_1, \dots, n_A | \exp[-\beta H(s, \pi)] | n_1, \dots, n_A \rangle}$$



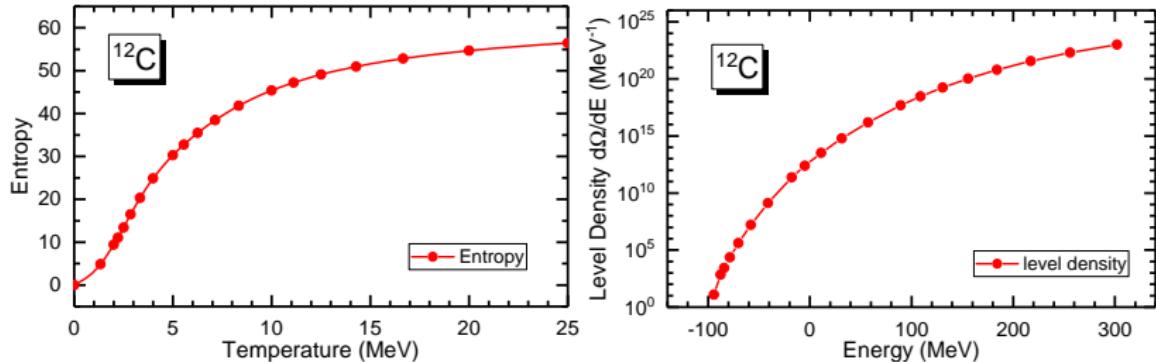
Application of Pinhole Algorithm: Hot nucleus in a box

- 6 neutrons and 6 protons enclosed in a $L = 12$ fm box with periodic boundaries.
- specific heat peaks at $T = 3.3$ MeV, $E_{e.x.} = 36.2$ MeV.
- liquid to alpha-particle-gas transition smeared due to finite size effect.



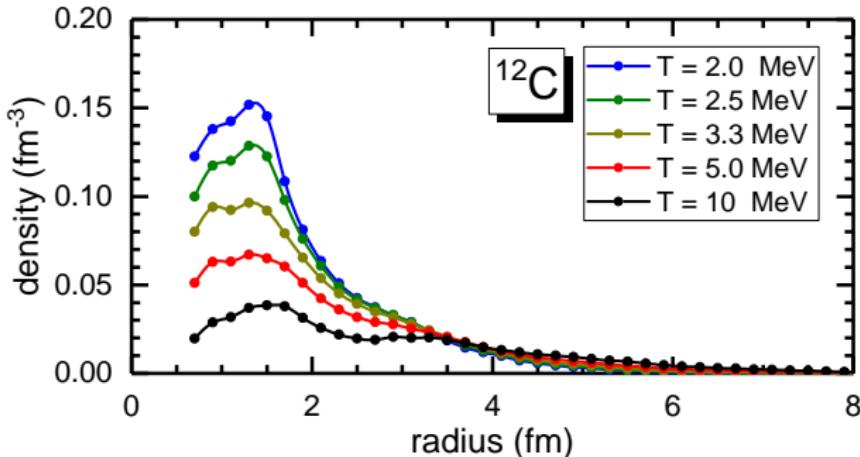
Hot nucleus in a box

- Entropy $S(T_0) = \int_0^{T_0} \frac{1}{T} dU$.
- Level Density $\rho(E) = \frac{e^S}{\sqrt{2\pi C_V} T}$



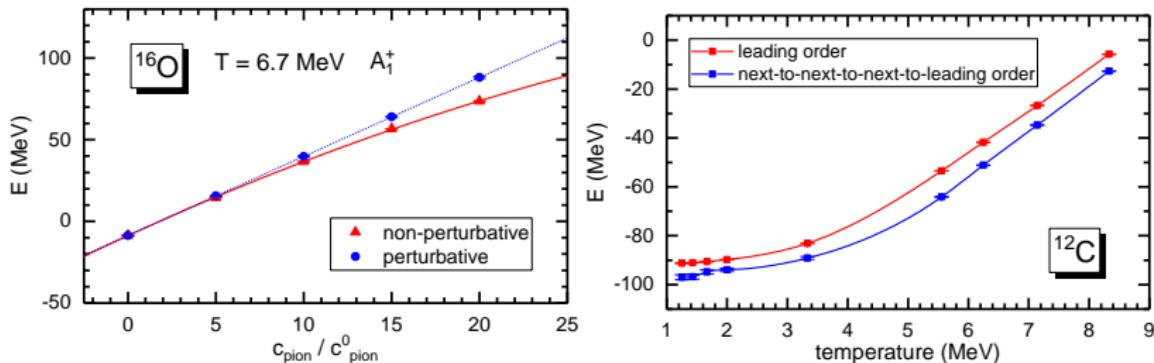
Hot nucleus in a box

- Intrinsic density profile collapse as temperature increase.
- α clusters evaporate from the liquid drop.
- Radius increase gradually, evidencing a smeared phase transition.



Pinhole perturbation theory

- $N - N$ interaction fitted to $N - N$ phase-shift up to $N^3\text{LO}$.
- Leading order included *non-perturbatively*, higher order *perturbatively*.
- Higher order plus Coulomb ~ 10 MeV, total binding ~ 100 MeV.
 \implies Perturbation theory works well.

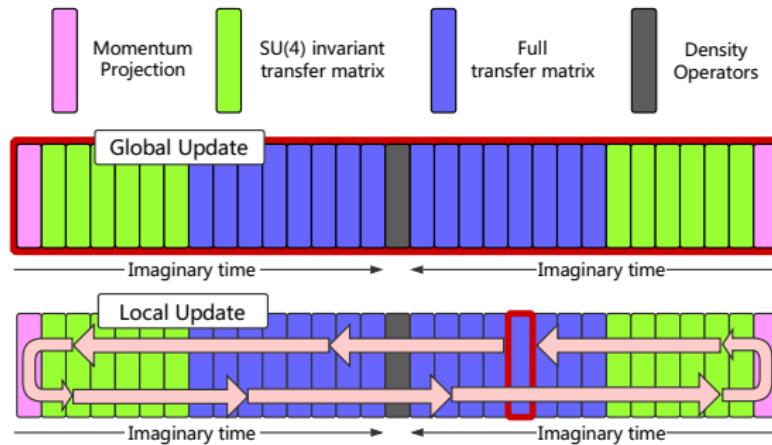


\implies Hot nucleus simulation starting from full chiral $N - N$ interaction!

Speed-up: shuttle algorithm

The Hybrid Monte Carlo algorithm used in LEFT can be simplified by updating the time slices locally instead of globally.

Most of the CPU hours spent on propagating the wave functions can be saved.

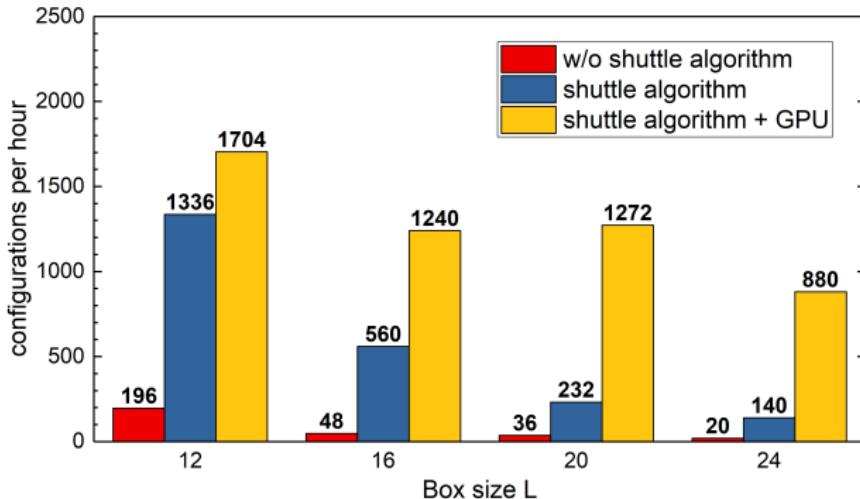


Speed-up: shuttle algorithm + GPU

The Lattice EFT algorithms are very compatible with the GPU acceleration.

Large scale parallelization, almost no communication.

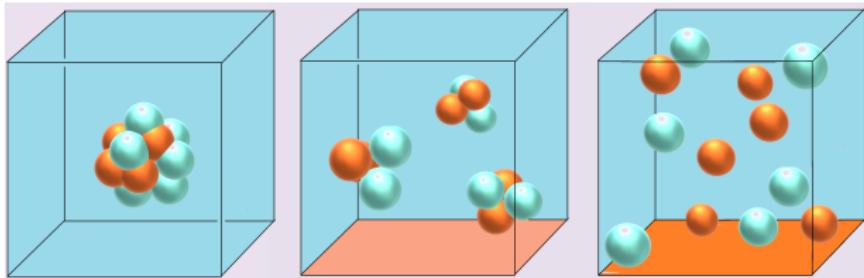
The program is recently rewritten using CUDA (Nvidia GPU language).



For $L \geq 10$, the new algorithm and GPU transplantation together give speed-up factors up to 40. BNL, Elhatisari, Li, Lee, in preparation

Summary and perspective

- The *Lattice Chiral Effective Field Theory* simulates the nuclear thermodynamics with a newly developed *pinhole algorithm*.
- Starting from a $N - N$ chiral nuclear force fitted to the empirical $N - N$ phase shifts, we calculate various thermodynamic properties of 12 nucleons in a box. Evidence of a liquid to alpha-gas phase transition is found.
- With the help of new algorithms and GPU-acceleration, we expect to simulate the hot nuclear matter with much higher densities in the future.



Thank you for attention!