A Diffusion Monte Carlo implementation of EFT

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MOTIVATIONS

- ✓ Quantum Monte Carlo based techniques have been providing an efficient way of computing ground-state and low-lying excitations of nuclei and nuclear matter (quasi-) exactly.
- ✓ In order to perform QMC calculations one needs a potential with no momentum dependence. Argonne/Urbana – Illinois interactions are commonly used. But no use of interesting developments ($V_{low\text{-}k}$ or EFT-derived potentials) can be made.
- ✓ Main question is then: can we make use in any way of EFT at all within a QMC scheme? Are we just stuck with AV18?

OUTLINE

- “Standard” Quantum Monte Carlo methods (VMC, GFMC): results, limitations and problems.
- Auxiliary Field Diffusion Monte Carlo (AFDMC).
- AFDMC and pion-full Effective Field Theory.
- Conclusion and future prospects

"Standard" Monte Carlo methods : VMC & GFMC

Variational Monte Carlo (VMC)

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{A}\nabla_i^2 + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

Expectation values can be efficiently computed with stochastic methods:

$$E_T = \frac{\langle\psi_T|H|\psi_T\rangle}{\langle\psi_T|\psi_T\rangle} \geq E_0$$

Use wave function with Jastrow correlations, up to 3 body

$$|\psi_T\rangle = \left[S\prod_{ij}\left(v_c(r_{ij}) + v_\sigma(r_{ij})\vec{\sigma}_i\cdot\vec{\sigma}_j + ...\right)\right]|\phi\rangle$$

[Wiringa, PRC 43, 1585, (1991)]

[Wiringa, NPA, 543, (1992)]

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"Standard" Monte Carlo methods : VMC & GFMC

Green's Function Monte Carlo

Project the ground state

$$\psi(R,t) = e^{-(H-E_T)t}\psi(R,0)$$

$$\psi(R,t) = \int dR' \, G(R,R',t)\psi(R',0)$$

Use Jastrow correlations as in VMC

Spin-isospin states grow as $\approx \frac{A!}{Z!(A-Z)!}2^A$

⇨ exponential scaling with A

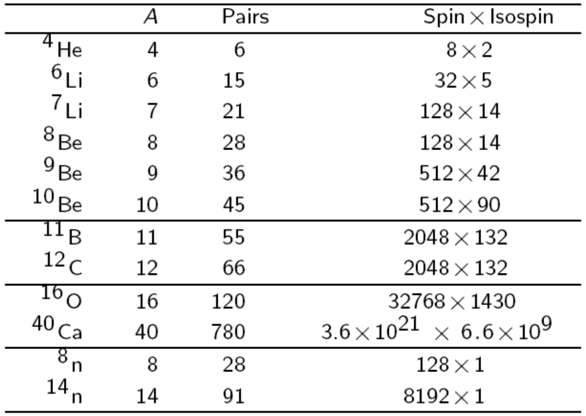
GFMC limit is (now) A=12

Local potential required like Argonne+Urbana/Illinois

[Carlson, PRC 36(5),2026, (1987)]

[Pudliner, Pandharipande, Carlson, Pieper,Wiringa, PRC 56(4), 1720 , (1997)]

[Pieper, NPA, 751, (2005)]



	A	Pairs	Spin $\times$ Isospin
^{4}He	4	6	8×2
^{6}Li	6	15	32×5
^{7}Li	7	21	128×14
^{8}Be	8	28	128×14
^{9}Be	9	36	512×42
^{10}Be	10	45	512×90
^{11}B	11	55	2048×132
^{12}C	12	66	2048×132
^{16}O	16	120	32768×1430
^{40}Ca	40	780	$3.6 \times 10^{21} \times 6.6 \times 10^9$
^{8}n	8	28	128×1
^{14}n	14	91	8192×1

Auxiliary Field Diffusion Monte Carlo (AFDMC)

Hubbard Stratonovich transform

$$e^{\frac{1}{2}\Delta t O^2} = \frac{1}{\sqrt{2\pi}} \int dx e^{-\frac{x^2}{2} + x\sqrt{\Delta t} O}$$

2 body operators ⇒ $\int$ Auxiliary Field x + 1 body operator

AFDMC = DMC + HS-transform

$$\psi(R, t) = e^{-(H - E_T)t} \psi(R, 0)$$

Sign-problem "treated" with Fixed-Phase approximation

[Schmidt & Fantoni, PLB 446, 99 (1999)]

[Fantoni,Sarsa ,Schmidt,Prog.Part.Nuc.Phys. 44 2000)]

[Gandolfi et al, PRL 99,022507, (2007)]

Auxiliary Field Diffusion Monte Carlo (AFDMC)

Capabilities and problems

PLUS

- Only single particle spin-isospin space dimension required

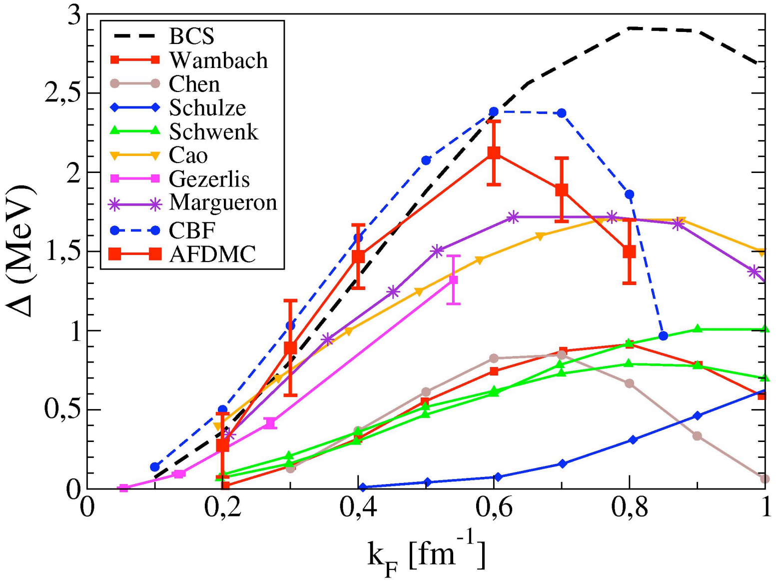
(4A and not $\frac{A!}{Z!(A-Z)!}2^A$)

- Polynomial scaling (larger systems, up to ~ 150 nucleons)

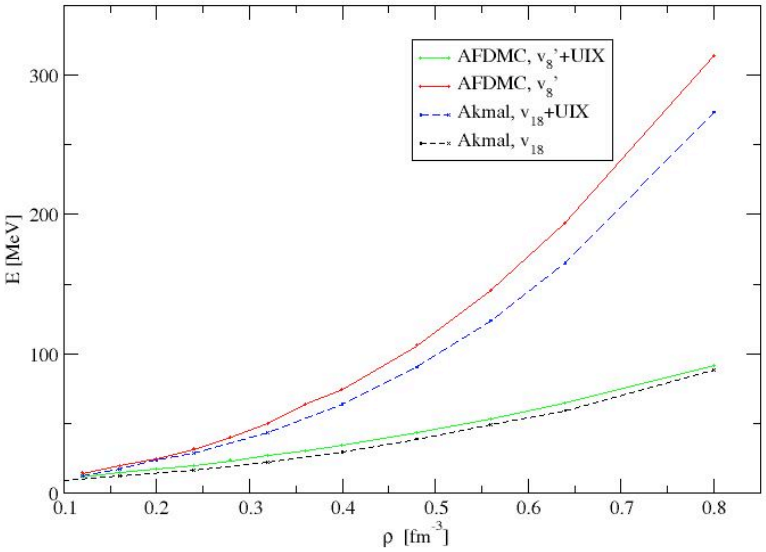
MINUS

- So far inclusion of 3-body operatorial terms and nonlocal terms except spin-orbit ones is problematic when protons and neutrons are used (ok for pure neutron matter).

Auxiliary Field Diffusion Monte Carlo (AFDMC)



Gap computed in low density neutron matter



Eos of neutron matter compared with Akmal-Pandharipande results

Method	^{4}He	^{8}He	^{16}O	^{40}Ca
FP-AFDMC	-27.13(10)	-23.6(5)	-90.8(1)	-272(2)
GFMC	-26.93(1)	-23.6(1)	-	-

(AV6' potential)

[Wiringa & Pieper PRL 89, 18 (2002) ; Gandolfi et al. PRL 99, 022507 (2007)]

AFDMC with Effective Field Theory (EFT)

The idea!

- Auxiliary fields of HS transform ⟺ pion fields
- 3-body potential term are generated (also) by 2nucleon-pion EFT terms

- Fundamental EFT Hamiltonian used instead of phenomenological potentials
- Include explicitly pion fields regularized on a lattice, assume a fixed nucleon number
- Original 3-nucleon forces could be treated with AFDMC as 2nucleon-pion terms
- Hamiltonian can be improved systematically by adding higher terms of the EFT chiral expansion, and eventually other degrees of freedom (e.g. Δ baryon)

Leading order Lagrangian

$$
\begin{aligned}
\mathscr{L}_0 = &-\frac{1}{2}\left[(\vec{\nabla}\pi_i)^2 - (\partial_0\pi_i)^2 + m_\pi^2\pi_i^2\right] \\
&+ N^\dagger\left[i\partial_0 - \frac{1}{2f_\pi}\epsilon_{ijk}\tau_i\pi_j\partial_0\pi_k - M_0 + \boxed{\frac{\nabla^2}{2M_0}}\right]N \\
&- \frac{g_A}{2f_\pi}N^\dagger\tau_i\sigma_j\nabla_j\pi_i N \\
&- \frac{1}{2}C\left(N^\dagger N\right)\left(N^\dagger N\right) \\
&- \frac{1}{2}C_I\left(N^\dagger\tau_i N\right)\left(N^\dagger\tau_i N\right)
\end{aligned}
$$

Higher order, but we keep it to maintain the DMC scheme

[Ordonez, Ray, Kolck, PRC 53(5), 2086, (1995)]

Regularized Hamiltonian at leading order

$$H = H_\pi + H_{\pi N} + H_N$$

$$H_\pi = \frac{1}{2}a^3 \sum_{\vec{l}} \Pi^2_{\pi_i}(\vec{l}) + \frac{1}{2}a^3 \sum_{\vec{l},\vec{n}} \pi_i(\vec{l})\ K_{\vec{l}\vec{n}}\ \pi_i(\vec{n})$$

$$H_{\pi N} = \frac{g_a}{2f_\pi} \sum_{m=1}^{A} \tau_i \sigma_j \frac{\pi_i(\lfloor a^{-1}\vec{x}_m \rfloor + \hat{j}) - \pi_i(\lfloor a^{-1}\vec{x}_m \rfloor - \hat{j})}{2a}$$

$$H_N = AM_0 - \sum_{m=1}^{A} \frac{\nabla^2_m}{2M_0} + \frac{1}{2}\sum_{m=1}^{A} \sum_{\substack{n=1 \\ n\neq m}}^{A} \delta_a(\vec{x}_m - \vec{x}_n)(C + C_I \vec{\tau}_m \cdot \vec{\tau}_n)$$

$$K_{\vec{l}\vec{n}} = \left(m^2_\pi + \frac{1}{a^2}\frac{3}{2}\right)\delta_{\vec{l}\vec{n}} - \frac{1}{2a^2} \sum_{\vec{\mu}=\hat{x},\hat{y},\hat{z}} \delta_{\vec{l},\vec{n}+2\vec{\mu}}$$

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AFDMC with Effective Field Theory (EFT)

EFT Hamiltonian & trial wave function

- **Leading order Hamiltonian:**

$$H = \underbrace{\partial_\pi^2 + V_c(\pi\pi)}_{\text{Pure pions terms}} + \overset{\text{1-nucleon operator}}{\sigma_N\tau_N}\,\overset{\text{HS auxiliary fields}}{\nabla\pi} + \underbrace{V_c(NN) + V_\tau(NN)}_{\text{Regularization counterterms}}$$

Hilbert space:

$$\mathscr{H} = \mathscr{F}_\pi \otimes \mathscr{F}_N$$

$$\mathscr{F}_\pi = \bigotimes_{i=0}^{\infty} S\mathscr{H}_\pi^i$$

$$\mathscr{F}_N = \bigotimes_{i=1}^{A} A\mathscr{H}_N^i$$

- **Trial wave function:**

Single nucleon spin-isospin wavefunction

$$|\Psi_T\rangle = J_c\Psi_0(\pi)Det\left[O(N\pi)|\chi(N)\rangle\right]$$

NN central Jastrow

Pion vacuum wavefunction

Nπ correlation

Vacuum energy

It is possible to exactly solve the discretized Hamiltonian in absence of nucleons.

The pion vacuum wavefunction is

$$\Psi_0 = \exp\left(-\frac{1}{2}\sum_{i,j,\alpha} \pi_i^\alpha \; E_{ij} \; \pi_j^\alpha\right)$$

where the kernel E_{ij} is given by:

$$E_{\vec{i}\vec{j}} = \frac{1}{n_l^3}\sum_k \sqrt{\vec{p}^2 + m_\pi^2}\, e^{i\frac{2\pi}{n_l}\vec{k}\cdot(\vec{i}-\vec{j})} \qquad \textbf{with} \qquad \vec{k} = \frac{a n_l}{2\pi}\vec{p}$$

The corresponding eigenvalue E_0 is: $\frac{1}{2}\sum_{\vec{k}}\sqrt{m_\pi^2 + \frac{1}{a^2}\sum_{\vec{\mu}=\hat{x},\hat{y},\hat{z}} \sin^2\left(\frac{2\pi}{n_l}\vec{k}\cdot\vec{\mu}\right)}$

Trial Wavefunction(al)

Trial wave function

$$\Psi_0 \cdot \prod_n \left[\exp\left(-\frac{1}{2}\sum_{i,j,\alpha} Q_i^\alpha(n)\, E_{ij}\, Q_j^\alpha(n)\right) \cdot \exp\left(-\sum_{i,j,\alpha} Q_i^\alpha(n)\, E_{ij}\, \pi_j^\alpha\right)\right] \Big| \chi \Big\rangle$$

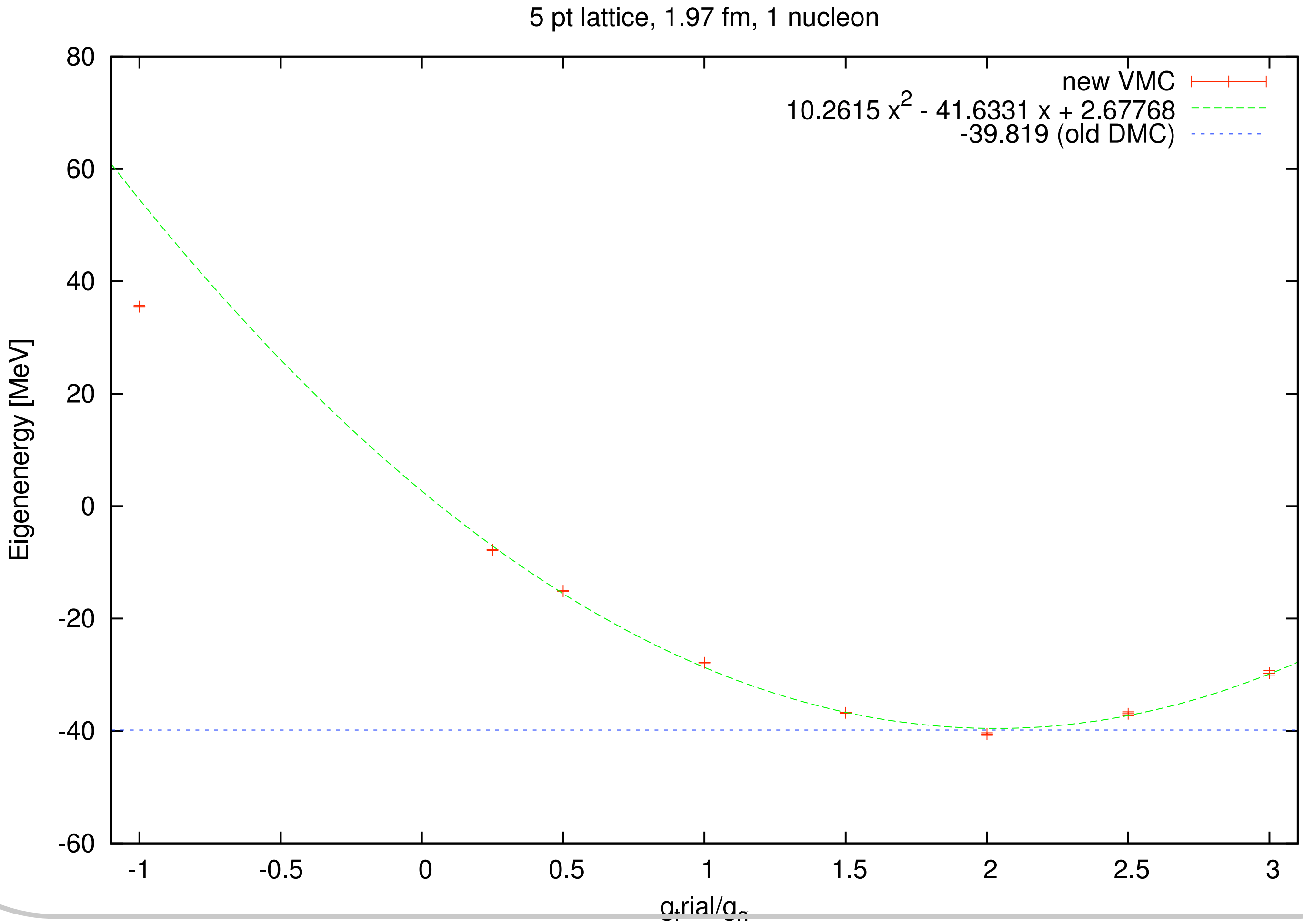
with $$Q_i^\alpha(n) = -\frac{g}{2}\tau^\alpha \sum_\beta \sigma^\beta \partial_\beta \Delta(i - x_n)$$

Variational parameter!

2-nucleon correlator

$$O_{nn} = \mathcal{S} \prod_{i<j} f_c(r_{ij}) \left(1 + f_\tau(r_{ij}) \vec{\tau}_i \cdot \vec{\tau}_j\right)$$

Nucleon Eigenenergy



AFDMC with Effective Field Theory (EFT)

Problems (partially solved)

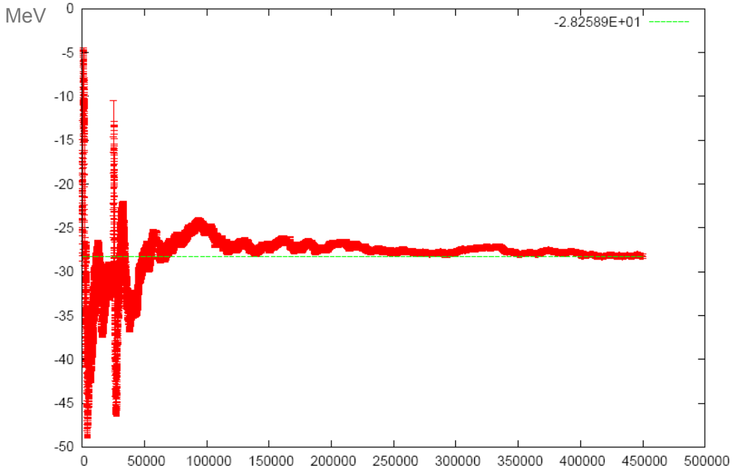
- Pion vacuum energy ~ 20 GeV
- Nucleon eigenenergy ~ 40 MeV

We need an accurate wavefunction including nucleon-nucleon, pion-pion, and pion-nucleon correlations in order to make the variance of the energy as small as possible

Because the Hamiltonian is regularizaion-dependent, we also need to fit the coefficient over some data. At present the good candidates are the binding energy of ^{4}He and Tritium (np, nn, and pp present some unexpected (?) problem)

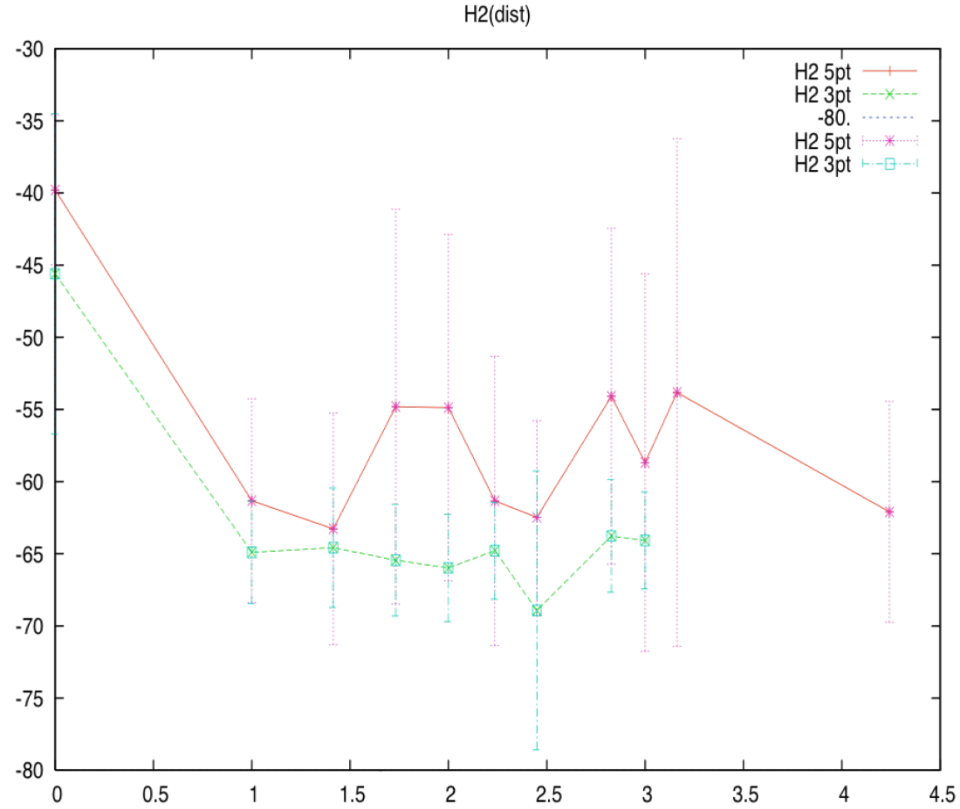
Preliminary results

- Nucleon bare mass computed
- Algorithm scales linearly with nucleon number ⇨ medium size nuclei (^{16}O,^{40}Ca) study is feasible [^{4}He example run of only 48 cpu hours]



- Inclusion of higher Hamiltonian terms does not change the scalability

np ENERGY AS FUNCTION OF DISTANCE

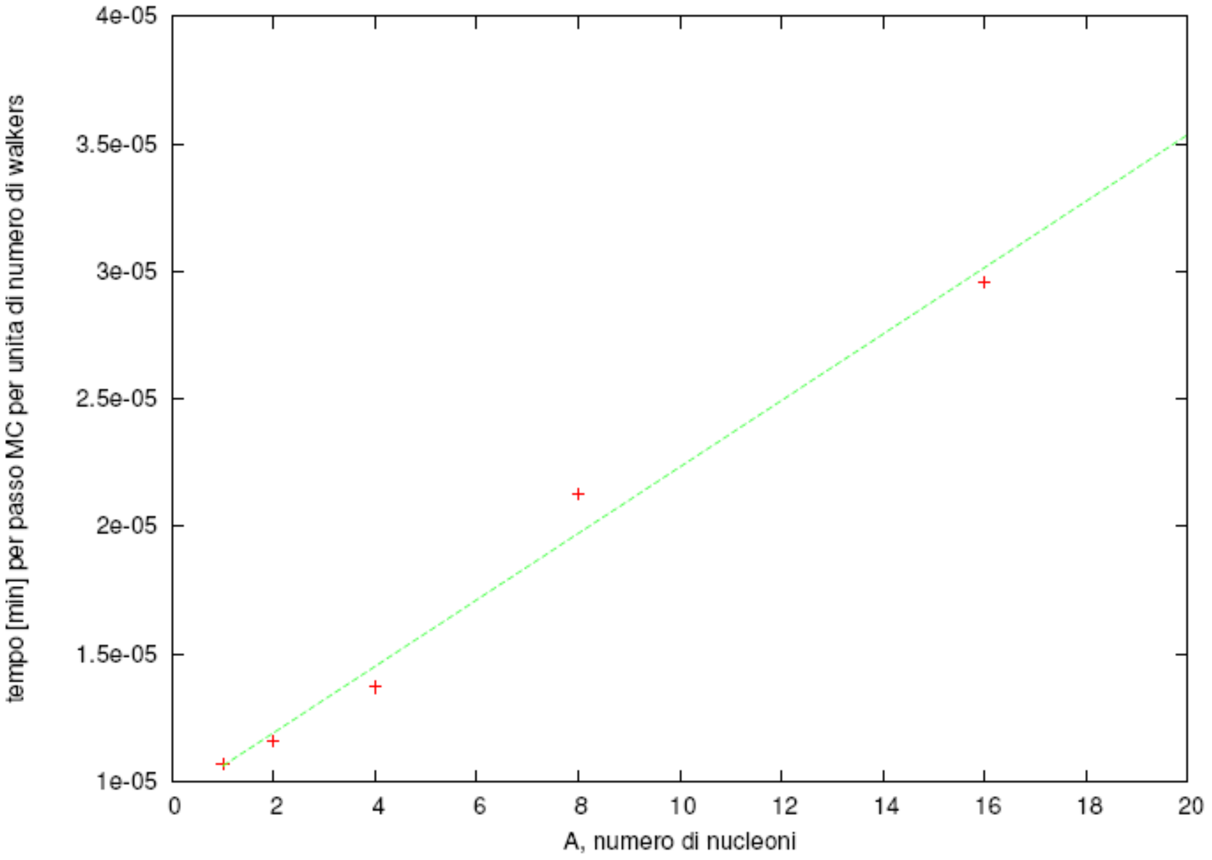


·Plain GFMC
(sum over states)

Approximate np correlation (linearized in the operators $\sigma\tau$ part)

Nucleon kinetic term dropped, nucleons on the lattice sites at different distances

Scalability with nucleon number



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CONCLUSIONS & WISH LIST

- AFDMC algorithm gives the possibility to study large systems with the accuracy typical of few body methods, and with a relatively limited request of computational resources.
- AFDMC method has to be improved by including non local and three body terms in the propagator.

- The combination of EFT with AFDMC is very promising:
  - implicit inclusion of 3-nucleons terms
  - use of a fundamental and systematic improvable Hamiltonian
- Convergence of Chiral expansion within EFT must be checked
- Study differences between phenomenological potentials and Effective Field Theory.

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