MANYBODY

National PI: Francesco Pederiva (TIFPA)

Nodes:

- Bologna
- Lecce
- Pavia ← ~50 Kcore/hr
- Roma 1 ← ~100 Kcore/hr
- Torino
- Trento-TIFPA ← ~6 Mcore/hr (~2 from INFN)

Other accessible resources: LLNL and NERSC through collaboration agreements.

Many-Body theory: projection Monte Carlo

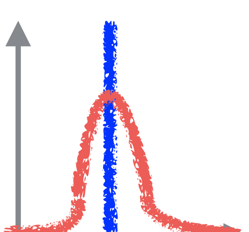
We compute ground state energies of nuclei by means of projection Monte Carlo methods. The ground state of a many-body system is computed by applying an “imaginary time propagator” to an arbitrary state that has to be non-orthogonal to the ground state (power method):

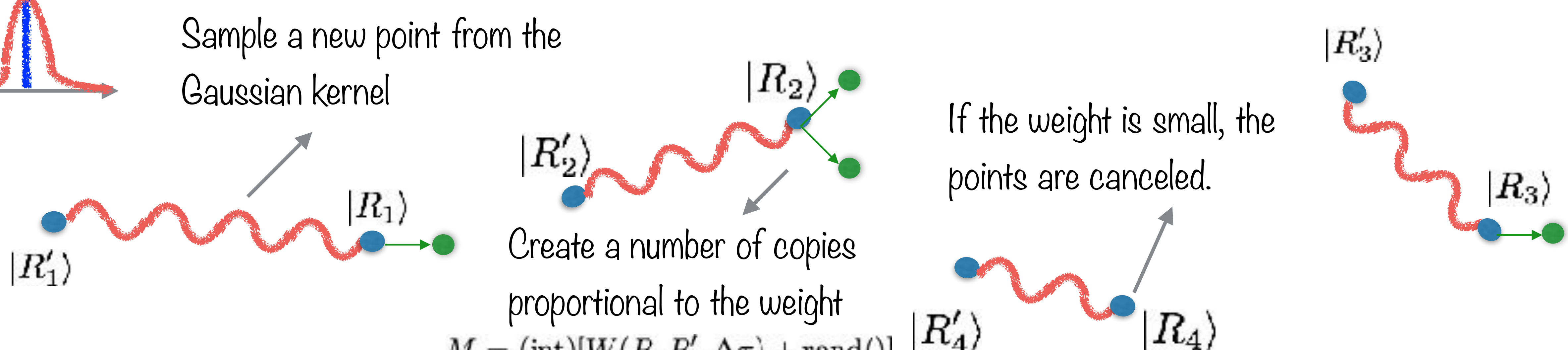
$$\langle R|\Psi(\tau)\rangle = \langle R|e^{-(\hat{H}-E_0)\tau}|R'\rangle\langle R'|\Psi(0)\rangle$$

In the limit of “short” τ (let us call it “$\boldsymbol{\Delta\tau}$”), the propagator can be broken up as follows (Trotter-Suzuki formula):

$$\langle R|e^{-(\hat{H}-E_0)\Delta\tau}|R'\rangle \sim \underbrace{e^{-\frac{(R-R')^2}{2\frac{\hbar}{m}\Delta\tau}}}_{\text{Kinetic term}} \; \underbrace{e^{-\left(\frac{V(R)+V(R')}{2}-E_0\right)\Delta\tau}}_{\text{Potential term (“weight”)}}$$

$W(R,R',\Delta\tau)$





$M = (\mathrm{int})[W(R,R',\Delta\tau) + \mathrm{rand}()]$

Projection MC many-nucleon systems

Multicomponent wave functions are needed!
How large is the system space? For a system of A nucleons, Z protons, the number of states is $2^A \binom{A}{Z}$

	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

Number of states in many nucleon wave functions for a few selected nuclei

- Very accurate results, possibility of using accurate wave functions for the evaluation of general estimators (e.g. response functions
- Due to the high computational cost, application limited so far to $A \leq 12$: **COMPUTATIONAL CHALLENGE!**

AFDMC

The operator dependence in the exponent has become linear.

In the Monte Carlo spirit, the integral can be performed by sampling values of x from the Gaussian $e^{-\frac{x^2}{2}}$. For a given *x* the action of the propagator will become:

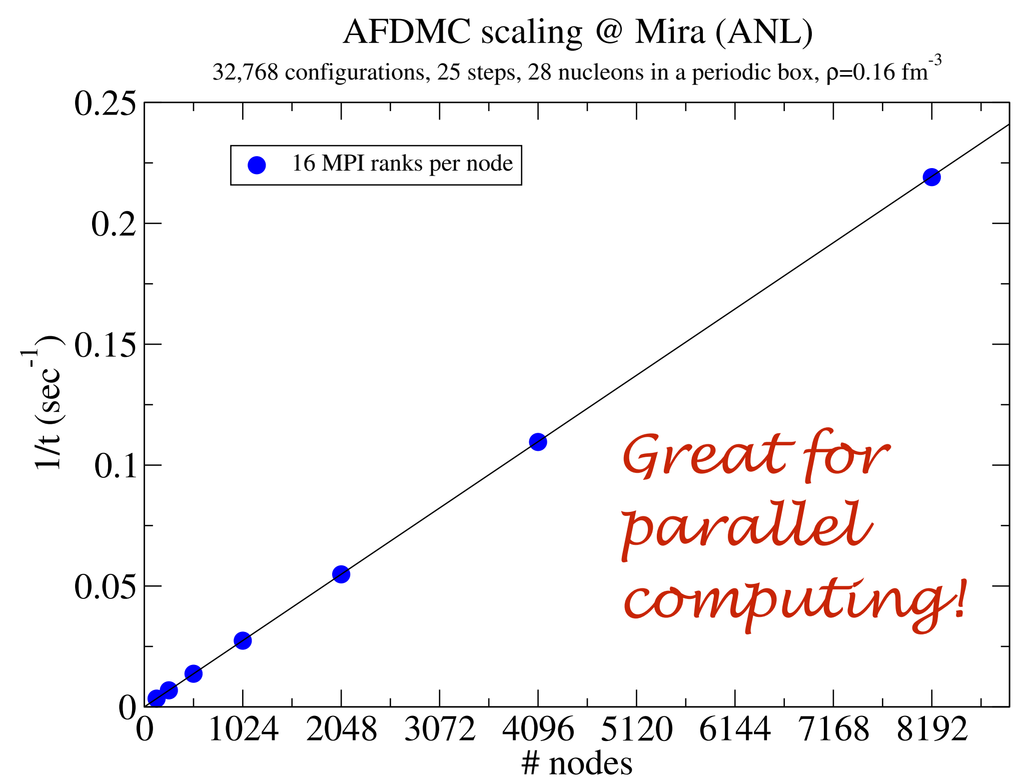
$$e^{-x\sqrt{\lambda\Delta\tau}\hat{O}_n}|S\rangle = \prod_{k=1}^{3A} e^{-x\sqrt{\lambda\Delta\tau}\phi_n^k\sigma_k}|S\rangle$$

In a space of spinors, each factor corresponds to a rotation induced by the action of the Pauli matrices

The sum over the states
has been replaced by sampling rotations!

AFDMC

The crucial advantage of AFDMC is that the scaling of the required computer resources is no longer exponential: **the cost scales as *A*^{3}** (the scaling required by the computation of the determinants in the antisymmetric wave functions) → **LARGER SYSTEMS ACCESSIBLE!**



Progress

- The HS transformation can be used ONLY FOR THE PROPAGATOR Accurate wave functions require an operatorial dependence! “Cluster expansion” introduced and working!(Gandolfi, Lovato, Schmidt)
- Some problems in treating nuclear spin-orbit have been addressed.
- Three-body forces are now implemented in a quasi-perturbative way, but results are very promising.

Fock space calculations

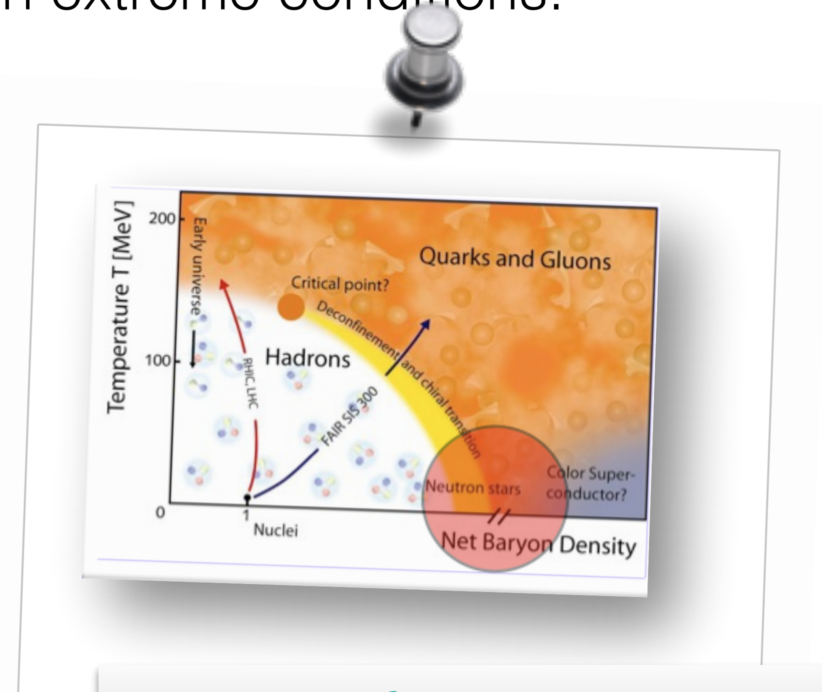
The stochastic power method can also be used in Fock space. In this case the propagator acts on the occupation number of a basis set used to span the Hilbert space of the solution of a given Hamiltonian. In particular, given two basis states $|\mathbf{m}\rangle$ and $|\mathbf{n}\rangle$ the quantity:

$$\langle \mathbf{m}|\mathcal{P}_{\Delta\tau}|\mathbf{n}\rangle = \langle \mathbf{m}|1 - (\hat{H} - E_0)\Delta\tau|\mathbf{n}\rangle$$

is interpreted as the probability of the system of switching the occupation of the state $|\mathbf{n}\rangle$ into the occupation of the state $|\mathbf{m}\rangle$. This propagation has in principle the same properties of the coordinates space version.

Equation of state of dense matter

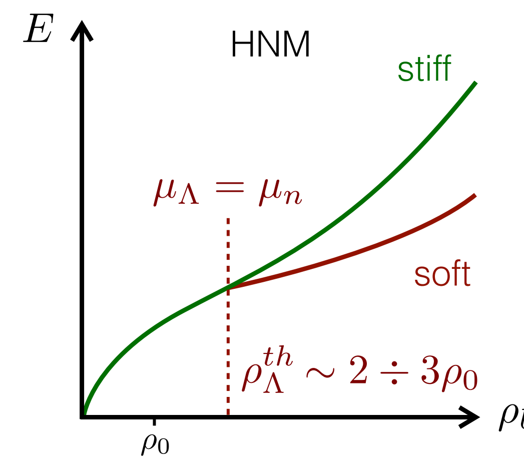
The *fine tuning* of the hyperon-nucleon interaction is essential to understand the behaviour of matter in extreme conditions.

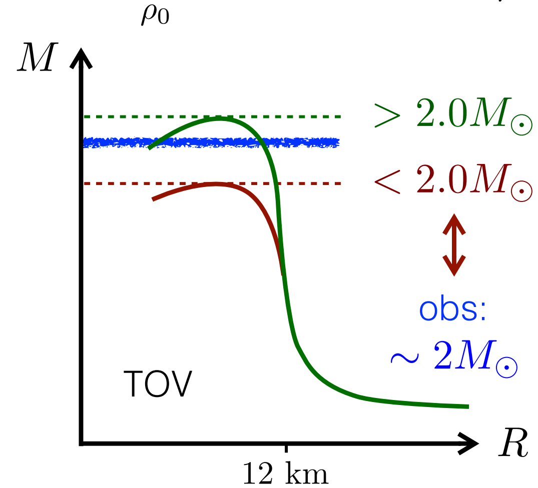


Far away from any possible perturbative treatment..

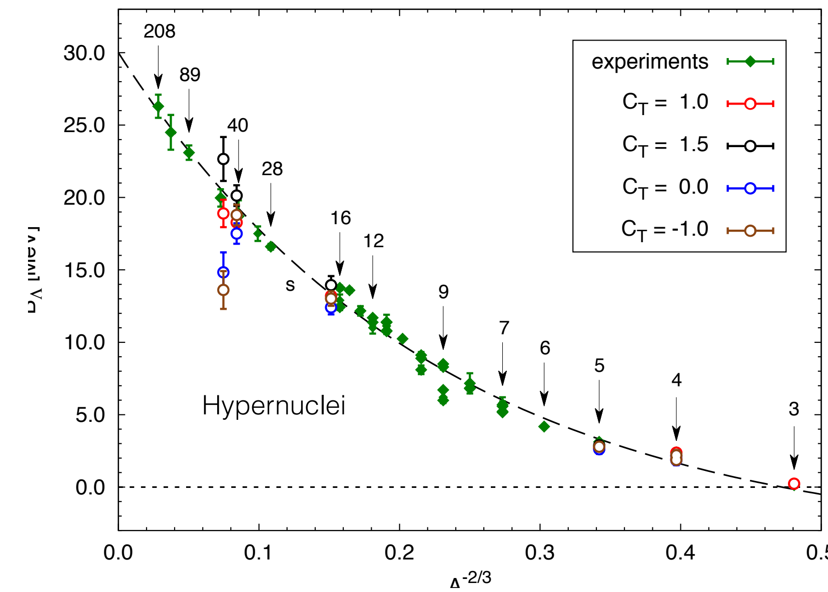
Example: Neutron stars

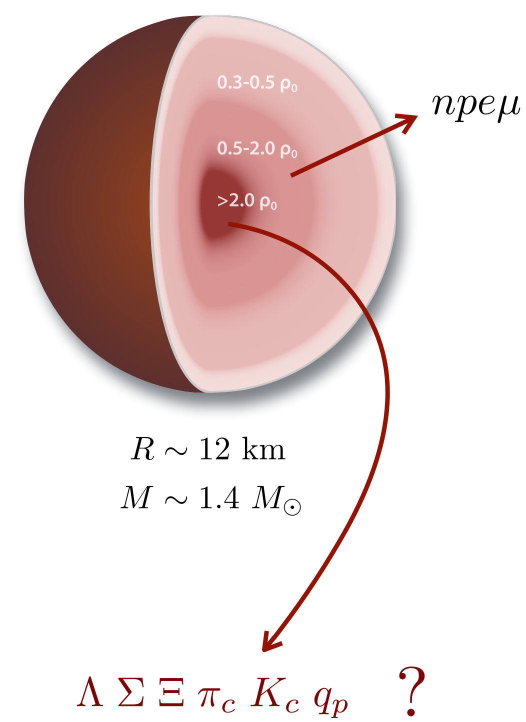
Equation of state



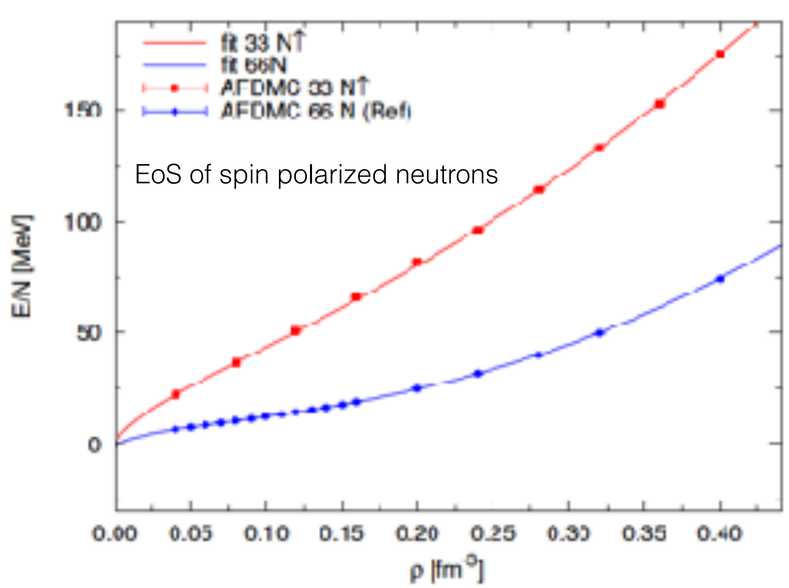


Neutron star structure





Internal composition still largely unknown



Effective π-less theories

L.Contessi, A. Lovato, FP, J. Kirscher, U. van Kolck, N.Barnea, D. Gazit

Plan: build a π-less effective Hamiltonian in coordinate space on few-body system and check the results for nuclei with larger masses.

Test: a nuclear physics with m_π=800MeV - LQCD calculations available for A=3,4

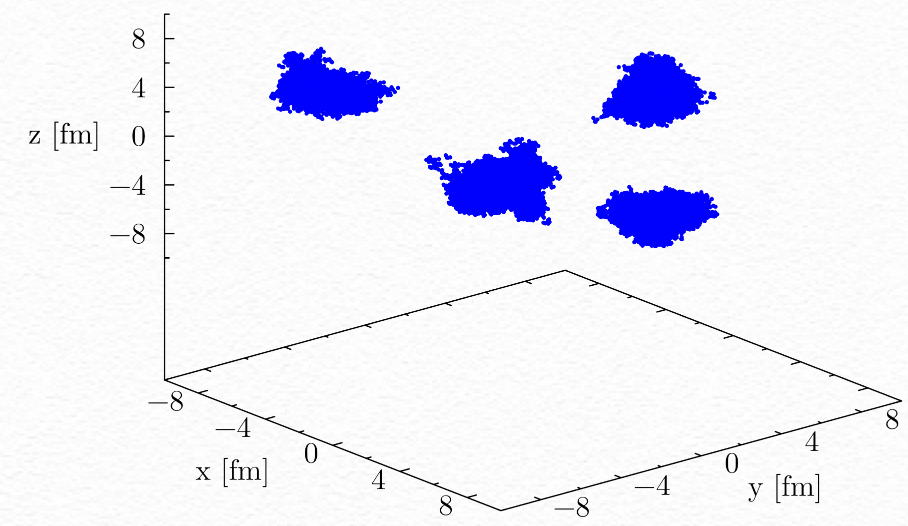
$$V_{LO} = C_1^{LO} + C_2^{LO}\sigma_1 \cdot \sigma_2$$

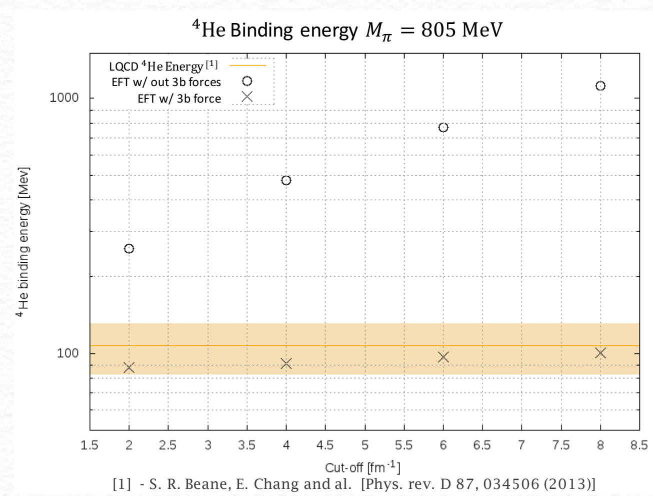
$$V_{LO}^{3b} = D_1 \tau_1 \cdot \tau_2$$

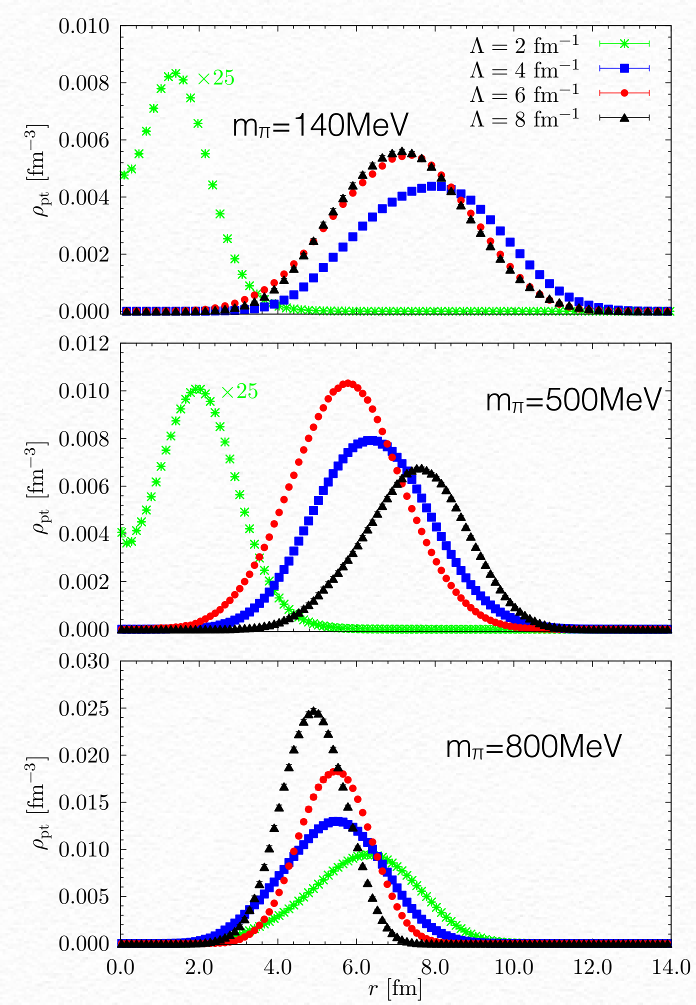
Regularization in r space

$$V_{LO}(r) = (C_1^{LO} + C_2^{LO}\sigma_1 \cdot \sigma_2) I_0(\Lambda, r)$$

$$I_k(\Lambda, r) = \Lambda^k e^{-\Lambda^2 r^2/4}$$







Future needs

- The scaling on the KNL partition of Marconi at CINECA is decent, but not perfect.

33 neutrons 0.04 fm^-3
VMC 25 equilibrium blocks, 25 average blocks, 10 steps/block

walkers	cpu	nodes	cpu-time [h]	job-time [min]
68	68	1	2.934	2.591
136	68	1	5.160	4.560
340	68	1	11.650	10.268
136	136	2	6.215	2.748
272	136	2	10.814	4.767

Calculation of the EoS on about 10 points for a single model requires ~ 1M hours

- Calculations for ^{40}Ca with pi-less EFT interactions (LO only) would presently require ~ 4Mhours (a factor 40 with respect to ^{16}O). Repeating ^{16}O calculations with operatorial-dependent correlations would require 2.5Mchrs (a factor 256 with respect to present calculations). A similar estimate holds for calculations of ${}_{\Lambda}^{39}$K/^{39}K required in preparation of the approved hypernuclear program at JLab.
- Considering the already available resources (therefore excluding possible resources coming from grants) a reasonable request of resources from INFN would be 7Mchrs for 2018, 10Mchrs for 2019 and 13Mchrs for 2020, for a total of 30Mchrs over the 3 years. This would in principle accommodate also similar (scaled) needs of the other groups.