The *basic model* of nuclear theory: from atomic nuclei to infinite matter

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The *basic model* of nuclear theory

Major goal: Describe nuclear systems (such as atomic nuclei and infinite matter) from a microscopic point of view. In such model the nucleus' constituents— the nucleons (N), i.e., protons (p) and neutrons (n) interact with each other in terms of many-body (primarily, two and three-body) effective interactions, and with external electroweak probes via effective currents describing the coupling of these probes to individual nucleons and many-body clusters of them

Inputs for the *basic model*:

Hamiltonian: many-body effective interactions between the nucleons (N)

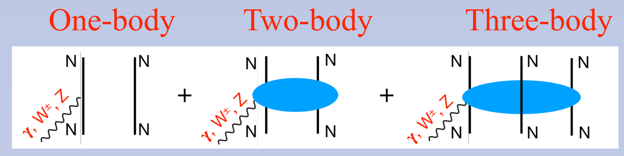
$$H=\sum_{i=1}^{A}\frac{\mathbf{p}_i^2}{2m_i}+\sum_{i<j=1}^{A}v_{ij}+\sum_{i<j<k=1}^{A}V_{ijk}+\ldots$$

Kinetic energy — Two-body — Three-body

Currents: many-body effective electroweak operators

$$j^{\rm EW}=\sum_{i=1}^{A}j_i+\sum_{i<j=1}^{A}j_{ij}+\sum_{i<j<k=1}^{A}j_{ijk}+\ldots$$

One-body — Two-body — Three-body



Theoretical approaches

- Phenomenological: two-body Argonne V18 (AV18) + three-body Illinois-7 (IL7)
- Chiral effective field theory (χEFT): two- and three-body local chiral interactions
  - local chiral two-body interactions contains parameters called low-energy constants (LECs) that are fixed by fitting NN scattering data
  - the fits to data of some of these local interactions have been performed by using POUNDERS, a SciDAC-supported derivative-free optimization solver available in PETSc libraries

Quantum Monte Carlo methods

Physical problem: Calculate the structure and reactions of light-nuclei including spectra, form factors, transitions, low-energy scattering and response as well as equation of state (EoS) of infinite matter. Compare the theoretical results with the experimental data

Numerical method: Use Quantum Monte Carlo (QMC) methods to solve the many-body Schrödinger equation for two- and three-body interactions

$$H\,\Psi(\mathbf{R};s_1,..,s_A;t_1,..,t_A)=E\,\Psi(\mathbf{R};s_1,..,s_A;t_1,..,t_A)$$

3A coordinates in r-space — Nucleon spin — Nucleon isospin (p or n)

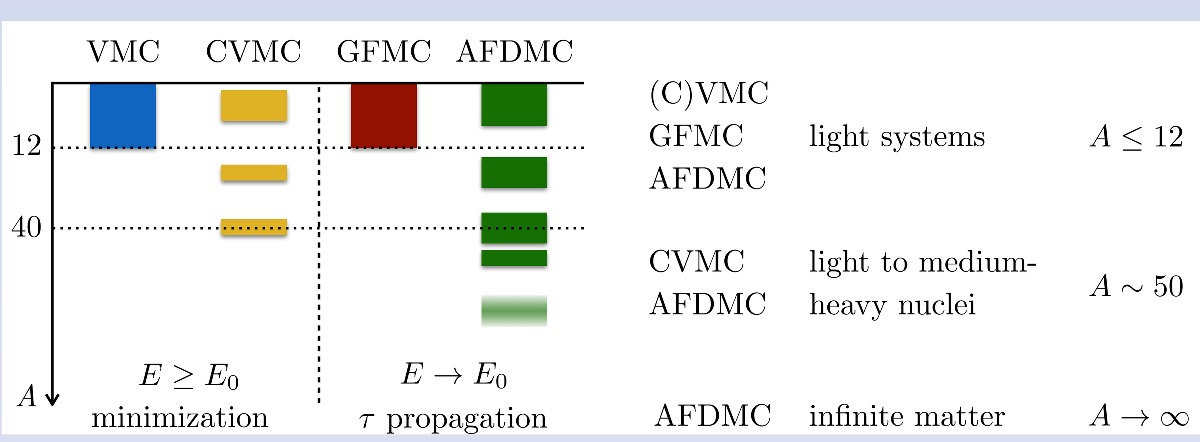


Figure by Diego Lonardoni LANL

- (Cluster)Variational Monte Carlo, (C)VMC
- Green's functions Monte Carlo, GFMC
- Auxiliary Field Diffusion Monte Carlo, AFDMC

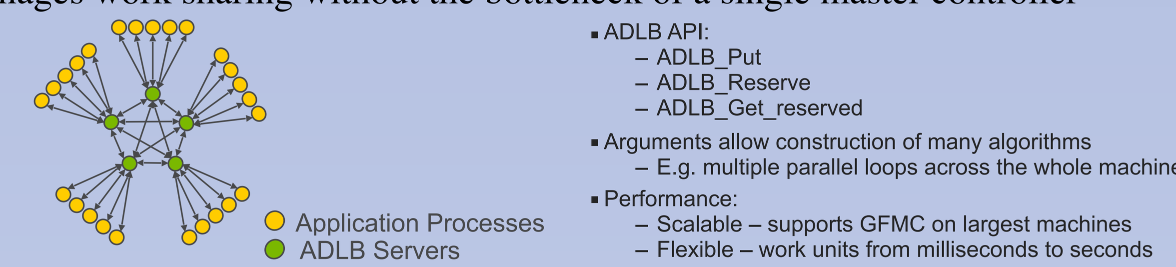
PROS: • QMC does not require a basis expansion or fixed grids and works with bare interactions

CONS: • Keeping track of every nucleon's spin and isospin states: in GFMC these states are summed explicitly, while in AFDMC they are sampled. GFMC is more appropriate for light-nuclei, AFDMC for heavy nuclei and matter

Computer Science impact via SciDAC on GFMC:

GFMC is a hybrid code using both MPI and OpenMP parallelism

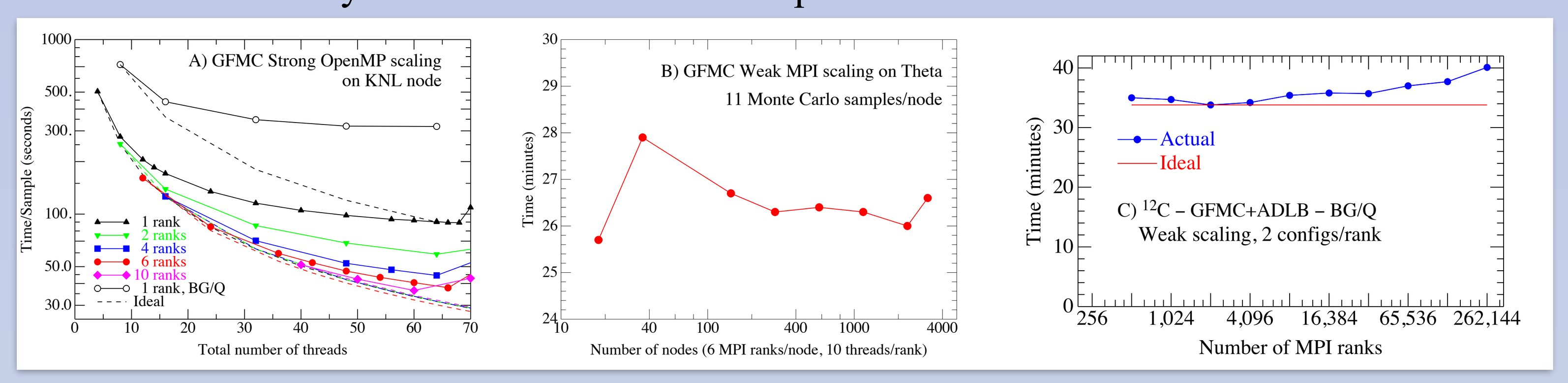
- The Asynchronous Dynamic Load Balancing (ADLB):
  - library that implements a flexible and scalable scheduling and load-balancing system for work units of varying types, sizes, and priorities
  - manages work sharing without the bottleneck of a single master controller



- Distributed Memory (DMEM):
  - carries out memory load balancing by storing large arrays on any node with enough memory and subsequently fetching them when needed
  - manages memory on all clients. Runs as separate thread, sharing memory with application processes, so local operations are fast: great improved performance of ADLB in GFMC

DMEM API:
– DMEM_Put
– DMEM_Get
– DMEM_Free
– DMEM_Copy
– DMEM_Update

ADLB and DMEM rely on MPI for interaddress space communication



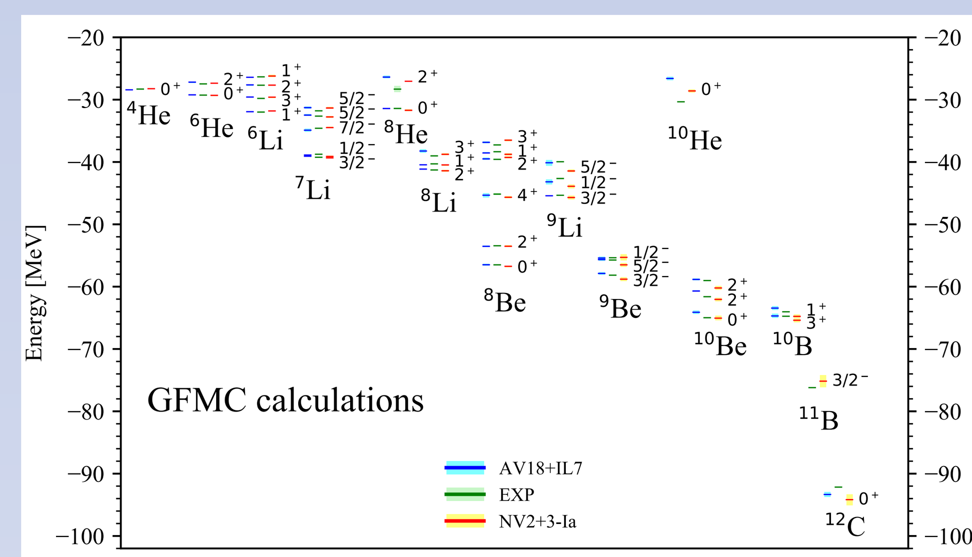
Spectra of light-nuclei A≤12

Objectives:

- Study the spectra of light-nuclei: theory confronts experiment
- Validate theoretical framework used to derive nuclear interactions

Accomplishments:

- GFMC calculations of the spectra of nuclei up to A=12 using Delta-full local chiral interactions (red) compared with the ones obtained using AV18+IL7 (cyan) and experimental data (green)

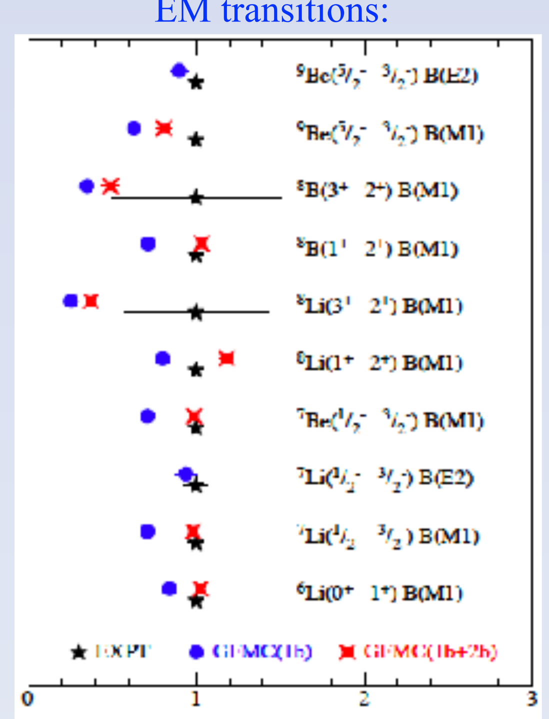


Magnetic moments and electromagnetic decays in light-nuclei

Objectives:

- Understand electromagnetic properties and transition rates of light-nuclei
- Test nuclear interactions and electromagnetic current operators, including complete two-body currents

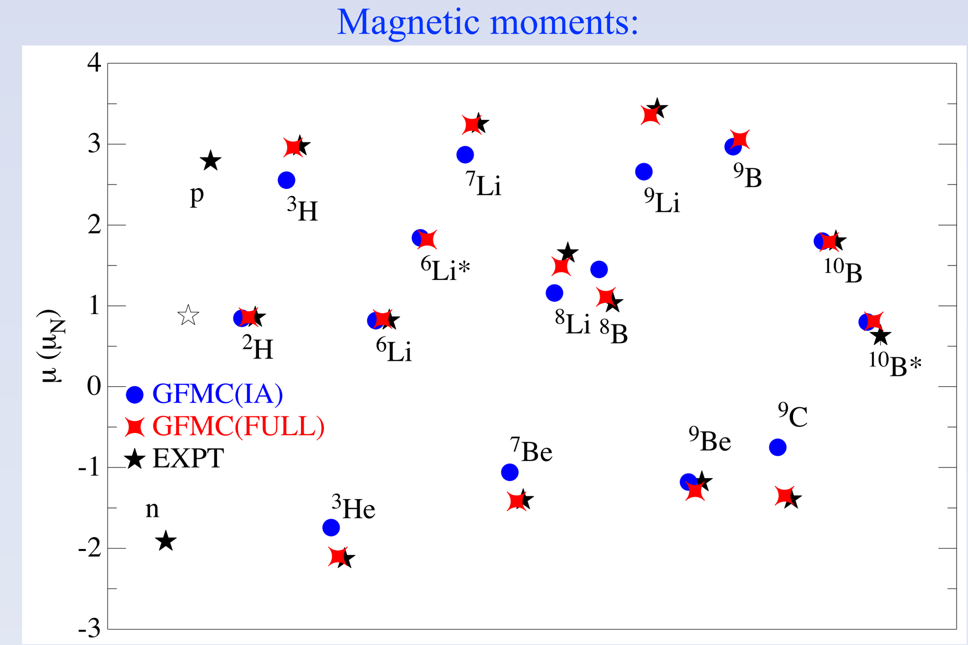
EM transitions:



Accomplishments:

- GFMC calculations of magnetic moments (right panel) and electromagnetic decays (left panel) using AV18+IL7 at lowest-order theory of one-body currents (blue) disagrees with experiment (black)
- Including two-body currents based on effective field theory (red) improves all predictions

Magnetic moments:



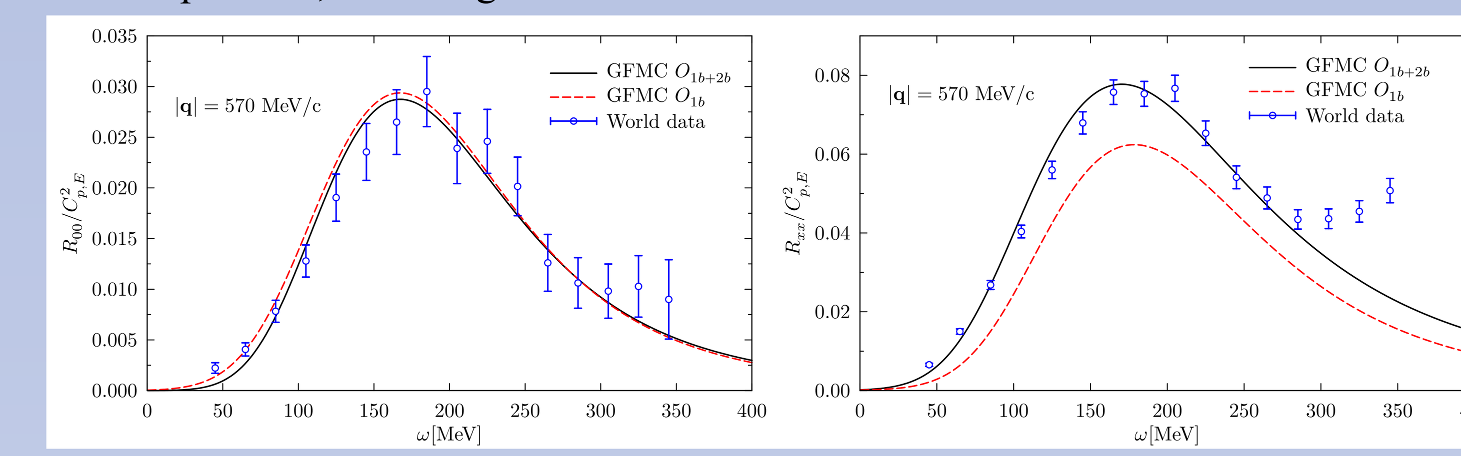
Inelastic lepton-nucleus scattering

Objectives:

- Compute inelastic electron-nucleus scattering for which accurate experimental data are available
- Within the same formalism, study the neutral-current and charge-current response functions that are important inputs for neutrino-nucleus scattering
- Test electroweak current operators, including two-body operators

Accomplishments:

- Development of an algorithm to compute the Euclidean response functions within GFMC
- Using Maximum Entropy technique to obtain the response functions from the Euclidean response

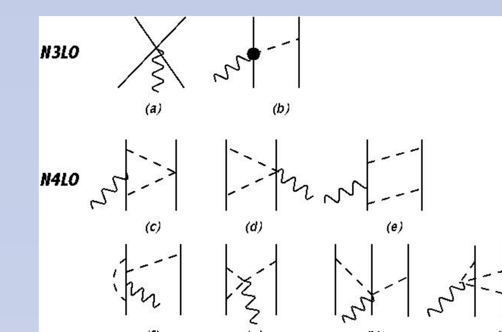


- EM longitudinal (right panel) and transverse (left panel) response function of ^{12}C for q=570 MeV/c with only one-body currents (red) and also two-body currents (black) are compared with experiment data (blue)

Beta-decays and Gamow-Teller matrix elements in light-nuclei

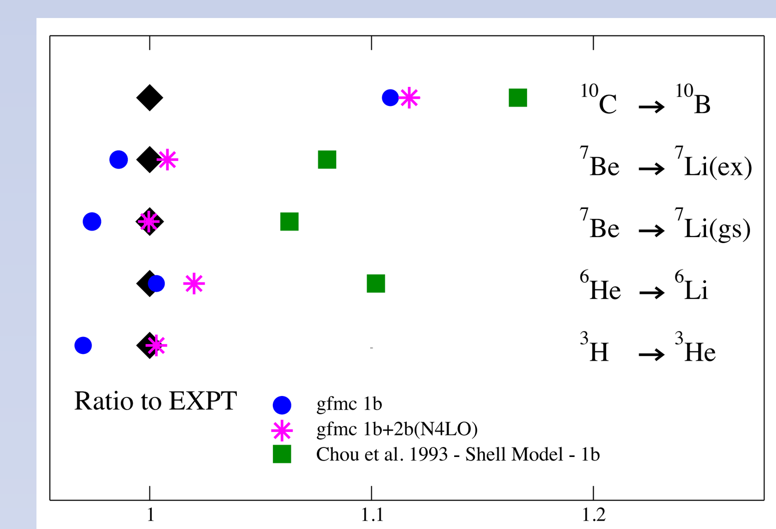
Objectives:

- Understand weak properties and transition rates of light-nuclei
- Test nuclear interactions and weak current operators, including complete two-body currents up to one loop (left panel)
- Address long-standing problem "quenching" of g_A required from shell-calculations: this is relevant for neutrinoless double-beta decay $\sim g_A^4$



Accomplishments:

- GFMC calculations of Gamow-Teller matrix elements (right panel) for light-nuclei at lowest-order theory of one-body currents (blue) using AV18+IL7
- Including two-body currents (magenta), there is an overall improvement of the theoretical predictions compared to the experimental data (black): some issues with ^{10}C



- Comparison with "unquenched" shell model calculations (green) based on the inclusion of one-body current operators: important role of correlation in the wave functions

Larger nuclei and infinite neutron matter

Objectives:

- Validate theoretical framework for nuclear forces and current operators in heavier nuclei, including neutron-rich nuclei important in the r-process, and infinite nuclear matter

Accomplishments:

- Realistic two- and three-body interactions based AV18+IL7 and χEFT have been used in AFDMC to study properties of selected close shell nuclei up to A=16 and EoS pure neutron matter (left panel)
- Realistic two- and three-body interactions based AV18+IL7 have been used in CVMC to validate the computational approach in ^{16}O and then used to study properties of ^{40}Ca (right panel)