Nuclear Structure and Reactions

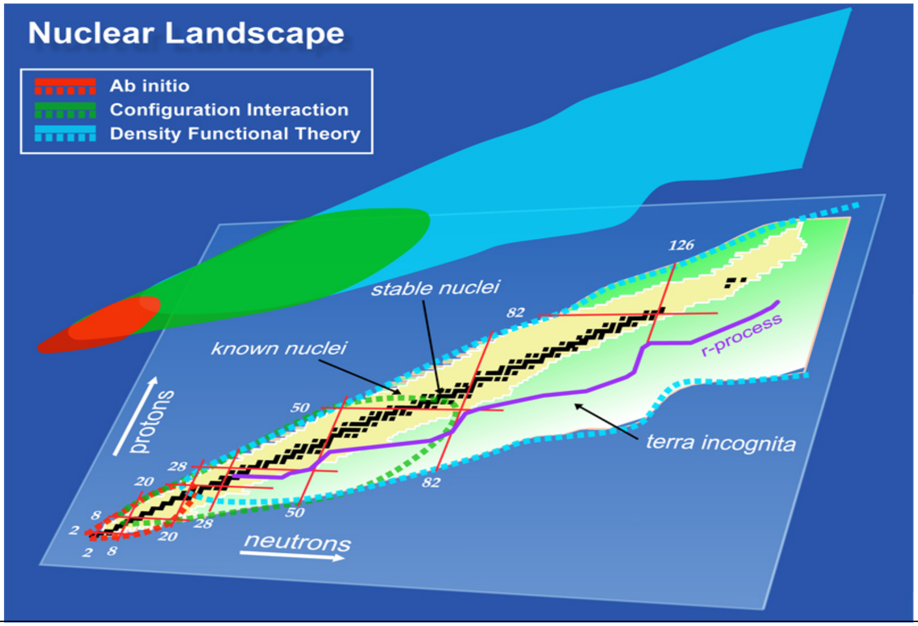
Different codes are used for different applications:

Light nuclei - ab initio calculations:

solve the Schroedinger eq. w/ microscopic interactions
Monte Carlo (GFMC, AFDMC,...) [J. Carlson]
Diagonalization (Shell Model, NCSM,...) [Esmond Ng]

Larger Nuclei: Density Functionals

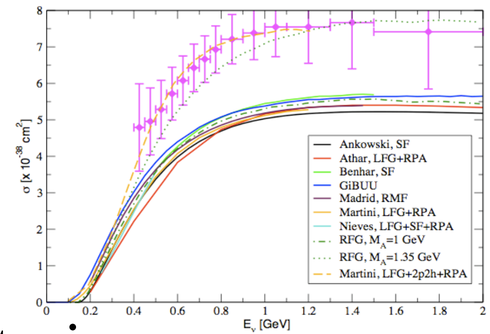
Mean-Field Theories/RPA/QRPA for Ground- and excited states and low-energy reactions [Jon Engel]



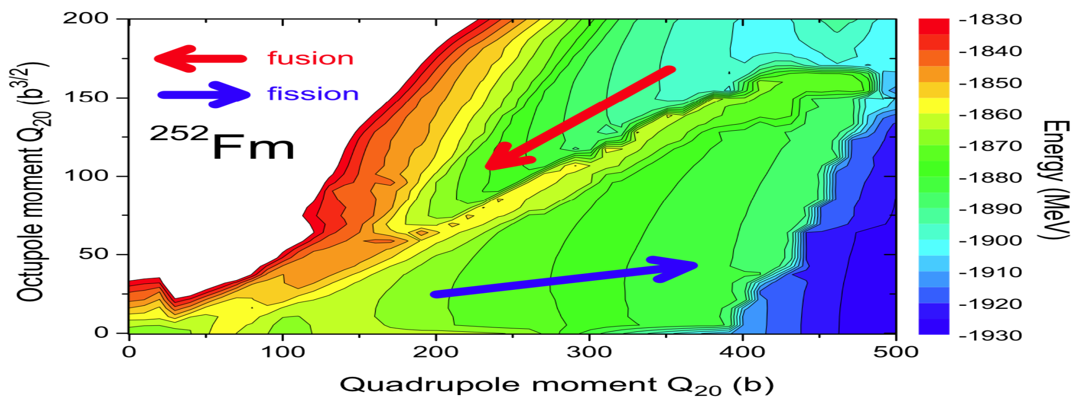
Science Goals:

Nuclear Structure: Energy Levels, EW form factors, β decay...

Reactions: Low-Energy Capture Reactions
Tests of fundamental symmetries



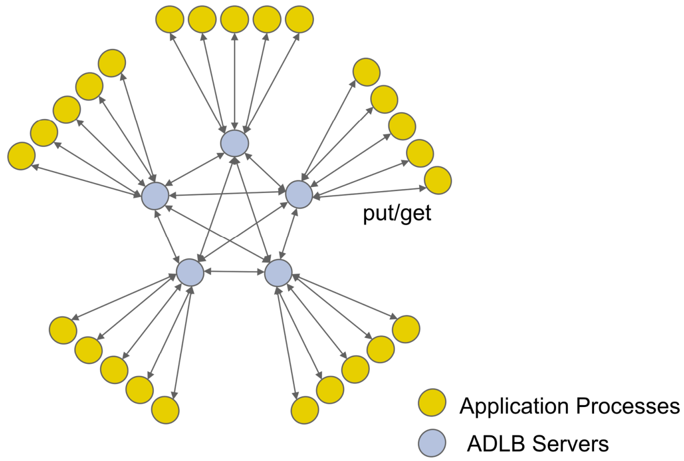
Response: Electron and neutrino/anti-neutrino scattering
from nuclei



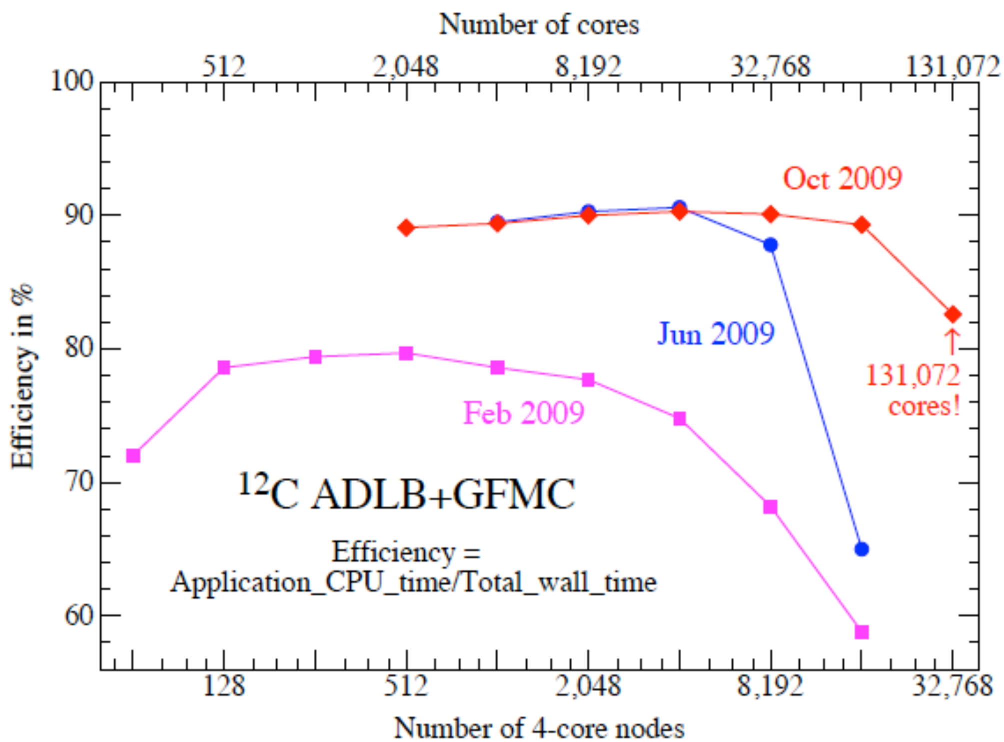
Large Nuclei: Fission, ββ decay, ...

Related Applications: Cold Atoms structure and dynamics
exotic phases, response functions, ...

Quantum Monte Carlo: Branching Random walks for T=0

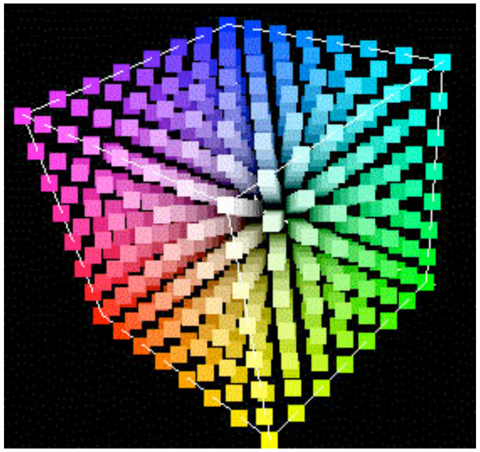


- ADLB (Asynchronous Dynamic Load Balancing) library implements simple Manager/Worker programming model for application.
- Sophisticated use of advanced MPI features "behind the scenes"



- Good scalability up to 130,000 CPUs of BG/P
- New version is typical of DOE moving to Exascale
  - multi-language (Fortran & C)
  - multi-hybrid (MPI, OpenMP, and pthreads
  - advanced MPI-1 and MPI-2
  - shows need for MPI-3

Quantum Monte Carlo: Linear Algebra components



GFMC

2^N complex spin amplitudes
A!/(N!Z!) isospin variables

states as many amplitudes
dominated by (sparse)
matrix-vector multiply

AFMC

orbitals on each site
eg L^3 lattice
FFT on L^3 lattice on each step

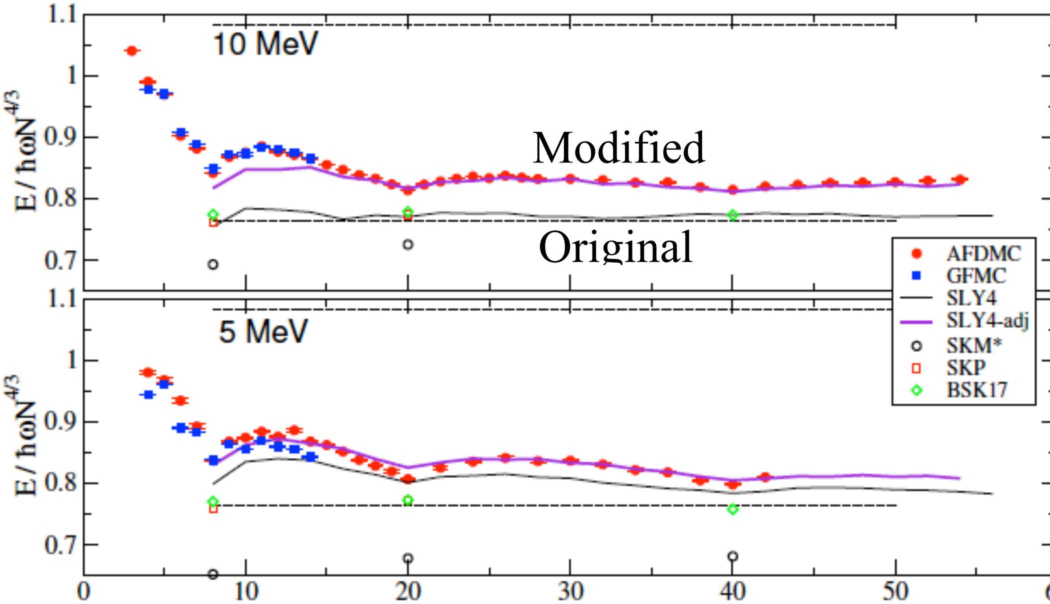
present L~ 20-30

10K configurations
1-5K steps/ configuration

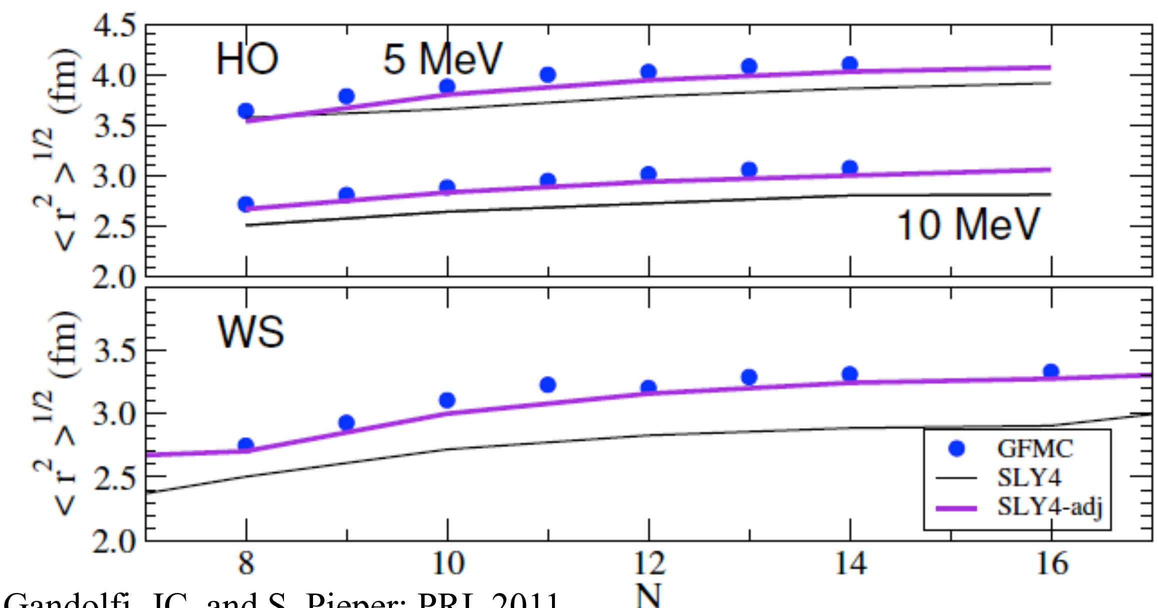
Recent Highlight: Density Functionals in Extreme Isospin Limit

Artificial Nuclei
with Neutrons only

Energies



Radii



Gandolfi, JC, and S. Pieper; PRL 2011

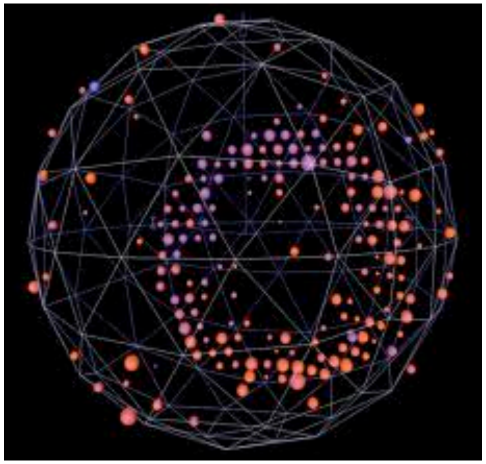
Future: Quantum Monte Carlo

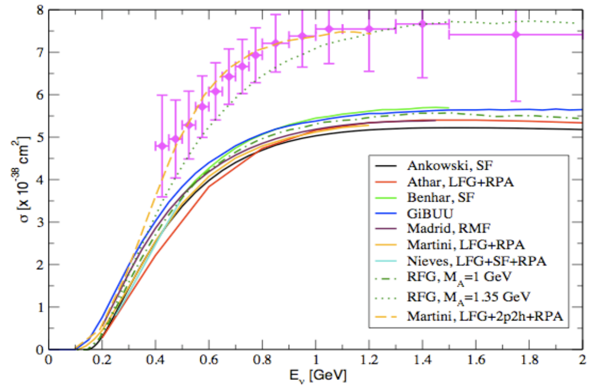
Neutrino and Anti-Neutrino Inclusive Scattering from C, O (10x larger than ground state calculations)

Hoyle State and triple-alpha capture

...

Neutrino response from Oxygen is an exascale problem





HPC in Nuclear Structure Calculation: Shell Model

- The goal is to obtain, based on first principles, a detailed microscopic understanding of how neutrons and protons are bound together in the nucleus, how the nuclear nodes of excitation are formed, and eventually how nuclear reactions take place.

- The challenge is to solve the nuclear Schrodinger equation.

- Large-Scale Sparse Eigenvector/Eigenvalue calculation

- After discretization, the resulting problem is the diagonalization of the nuclear Hamiltonian to get the eigenstates.
  - Large-scale sparse eigenvalue calculation
  - Need only a small number of eigenstates

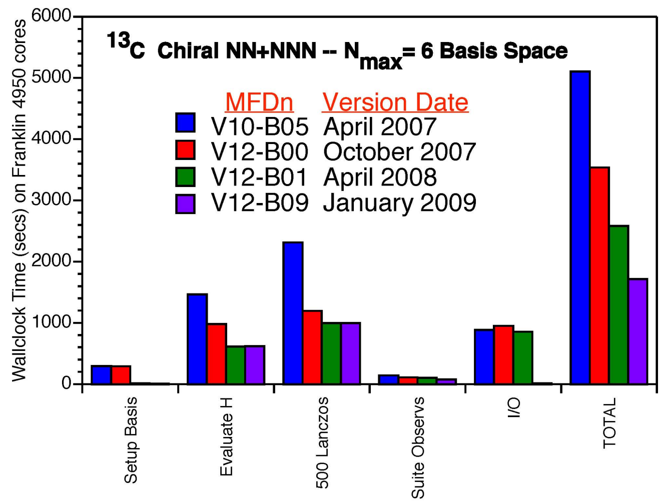
HPC in Nuclear Structure: Shell Model

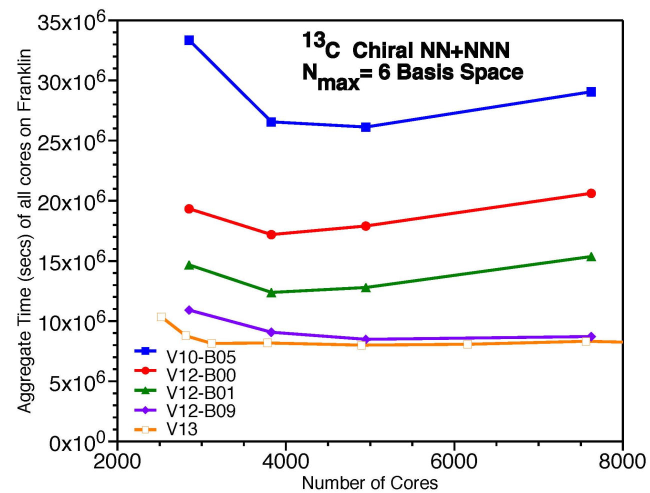
- The Hamiltonian matrix is very sparse.
  - Use the Lanczos algorithm to compute the eigenvalues.
  - Involve pimarily matrix-vector multiplies.
  - But there are also reorthogonalization steps.
- Dimension of the Hamiltonian matrix depends on N_{max}, a parameter that limits the total number of oscillator quanta allowed in the many body states.
- Sparsity depends on what potentials are included.
  - 2-body potentials or 3-body potentials are read from files.
  - I/O performance.

Current HPC Requirements

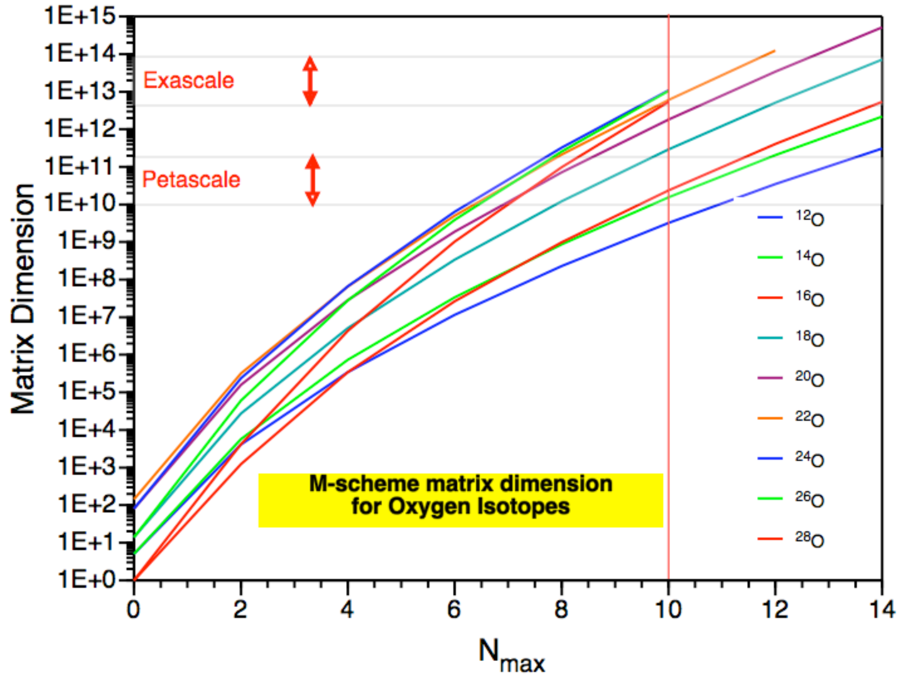
- MFDn is the primary code. It is based on MPI.
  - Highly optimized.
  - OpenMP directives have been incorporated recently.

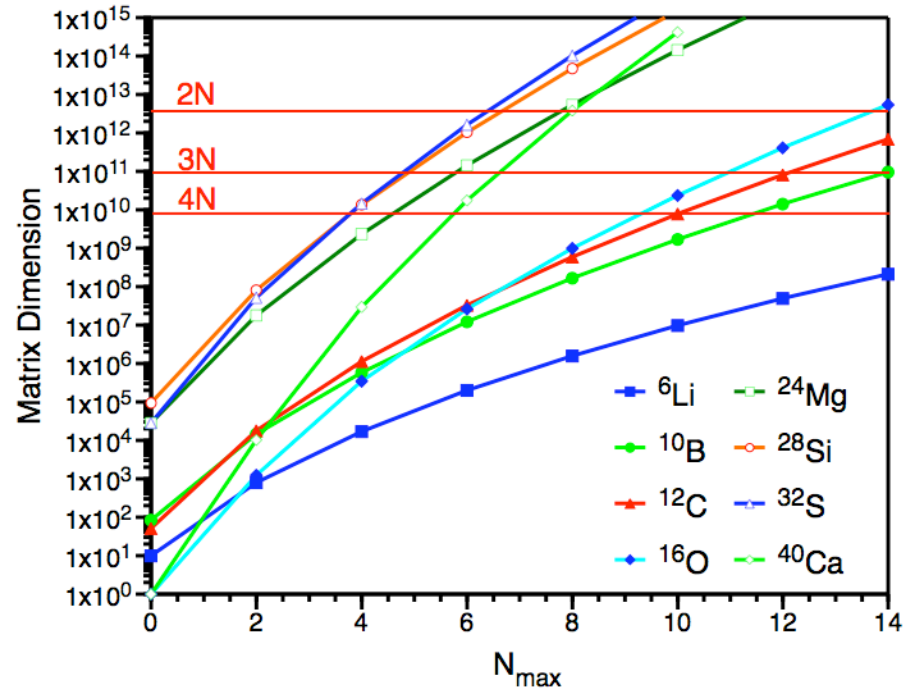
- HPC usage can be huge.
  - Even for small nuclei, matrix dimensions can be millions or even billons.
  - Can use ALL memory available.
  - Have used substantial number of core counts.



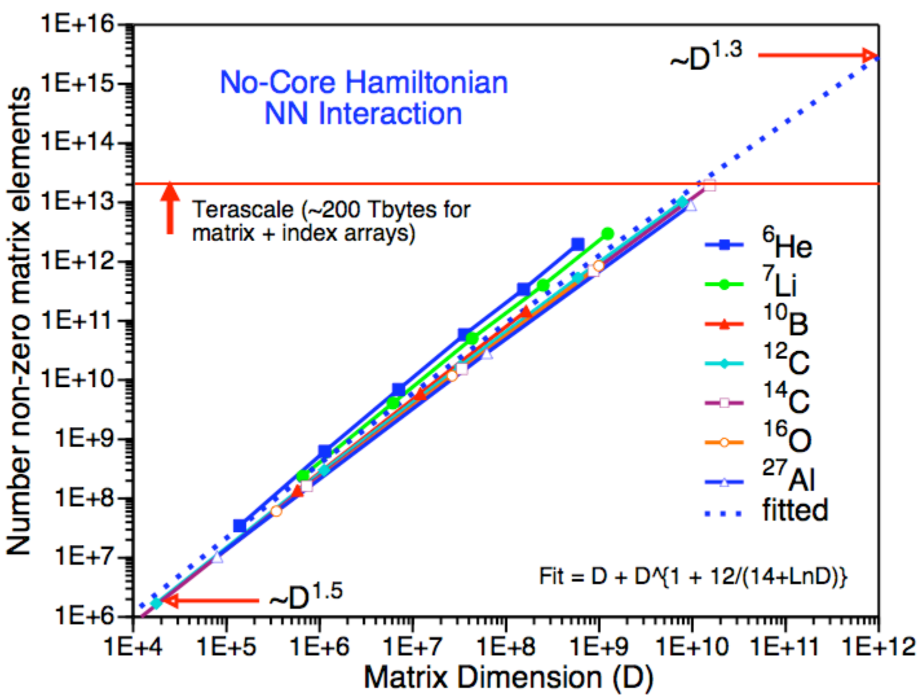


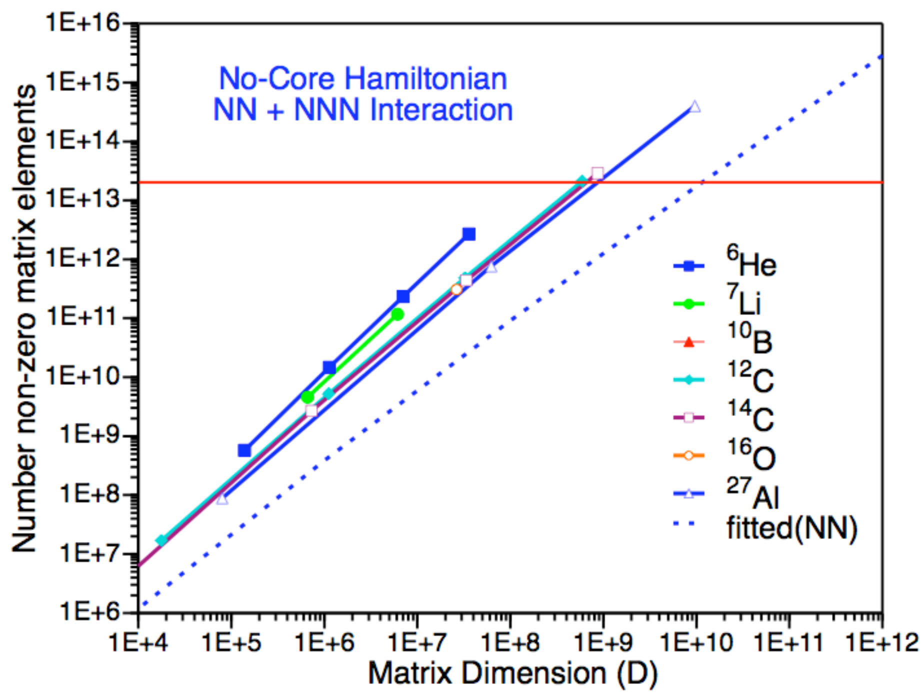
Challenges in nuclear structure calculations





Challenges in nuclear structure calculations





HPC Usage and Methods for the Next 3-5 Years

- Memory requirement is expected to grow as larger nuclei are to be studied.
- May have to explore “compute-on-the-fly” strategy when we run out of memory.
  - I/O issues.

- R&D direction
  - codes are currently MPI based, but we are beginning to look at mixed programming model
  - algorithmic changes are expected to accommodate multi-/many-cores architectures
  - more load balancing work may be needed

HPC Usage and Methods for the Next 3-5 Years

- Fast turnaround very desirable for testing and evaluation purposes

- Tools for performance profiling, tuning, and optimization are essential on future architectures

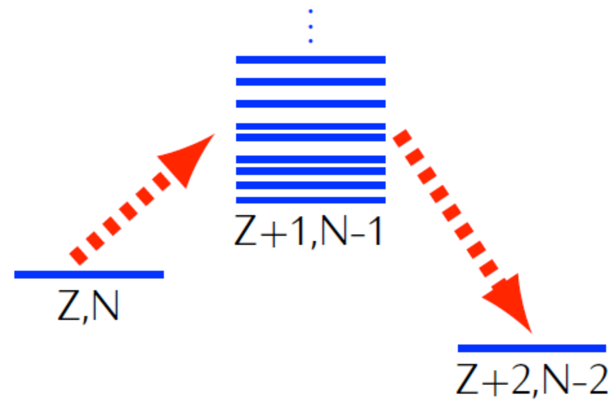
- Strategy for heterogeneous architectures (including those with accelerators):
  - HELP ☹

New Science with New Resources

- More memory, larger core count in the system (and larger allocation) will allow larger nuclei to be studied and higher fidelity simulations to be performed (e.g., larger N_{max}).

Large Nuclei - DFT and QRPA : Double-β decay

To extract neutrino mass (or mass limit) from new experiments, need good calculation of nuclear matrix elemen decay. Current uncertainty a factor of 2 or 3.



Near future: Fully self-consistent DFT-based QRPA calculation, using best density functionals and including deformation. QRPA generates linear response of mean-field ground states to beta-decay operators (and thus transition matrix elements to virtual intermediate states).

Farther future: Replace single mean-field by superposition of many, each with different deformation. Analog of QRPA is linear response of this complicated superposition.

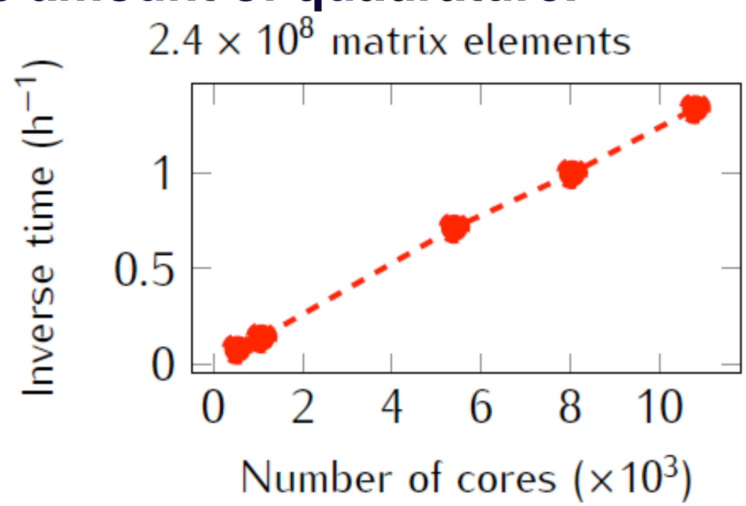
Computational Approach and Scaling

"Matrix" QRPA, requires calculation of two-body matrix elements
=> lots of 2-d (axial symmetry) quadrature . For near future:

- **~ 40 matrices with dimension ~ 10^4 (different multipoles based on initial and final ground states)**
- **Each matrix element consists of many 2-d integrals; single core computes 30,000 matrix elements/hr.**
- **Construction and diagonalization of Hamiltonian matrix from result requires communication but not much time.**
- **Transition matrix element: comparable amount of quadrature.**

Scaling

At present each core assigned a subset of the matrix elements, so that scaling is very good.



Farther Future: double beta decay

A generalized QRPA based on superposition of many triaxial mean field allows inclusion of all difficult physics known to affect ββ decay: deformation, pairing, neutron-proton correlations . . .

Superposing **N** mean fields requires **$O(N) – O(N^2)$** times more quadrature (overlap integrals between states with different deformation), and more communication to construct Hamiltonian matrix.

Quadrature is “embarrassingly parallel” and should benefit from GPUs or other accelerators.

Hope to have full implementation within a few years

Present Usage Overall (Approximate)

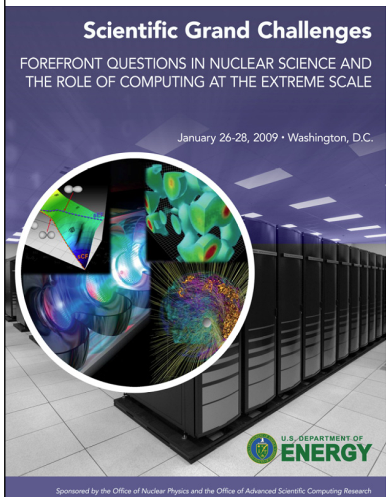
Through NERSC, INCITE, and other awards usage per project is approximately (core-hours):

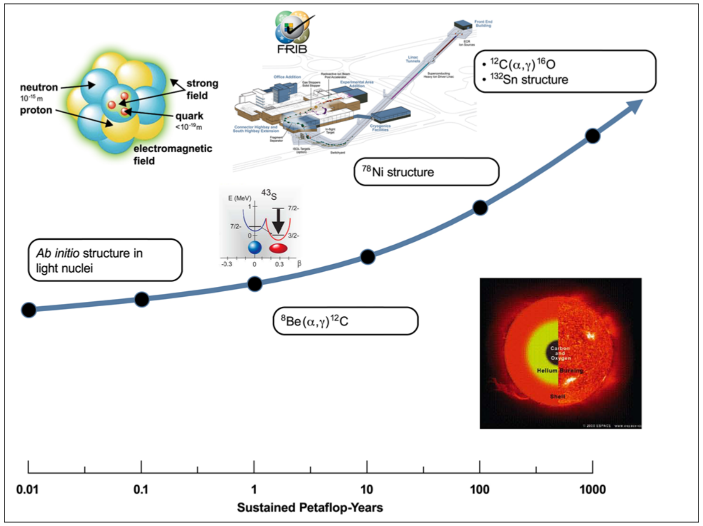
MFDn (shell model) :	20 M
Quantum Monte Carlo:	20 M
DFT/RPA and QRPA and SLDA:	25 M

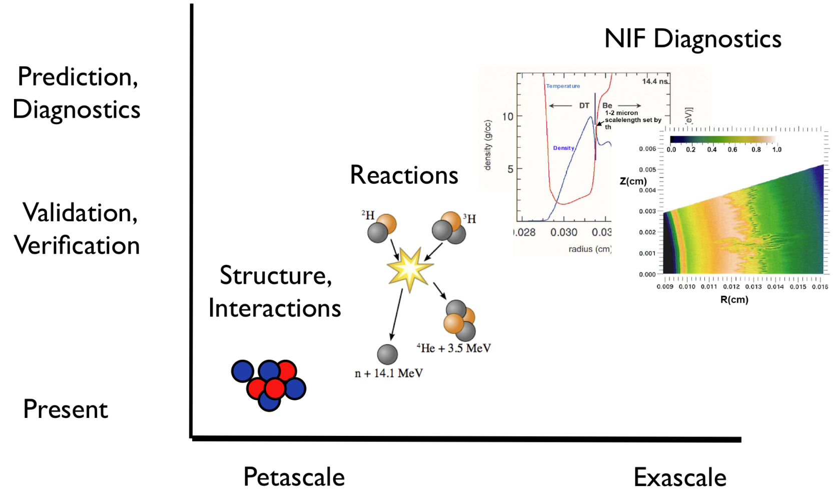
Total approximately 65M

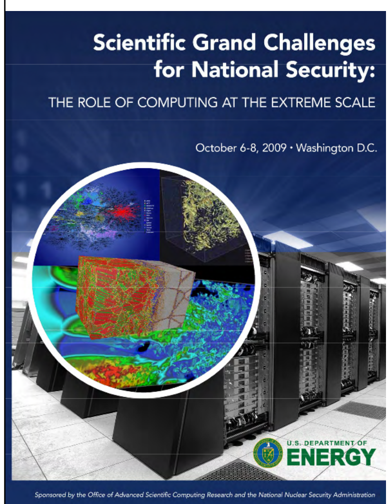
Usage is spread across many machines and architectures:
NERSC, Jaguar, Intrepid, LANL, ...

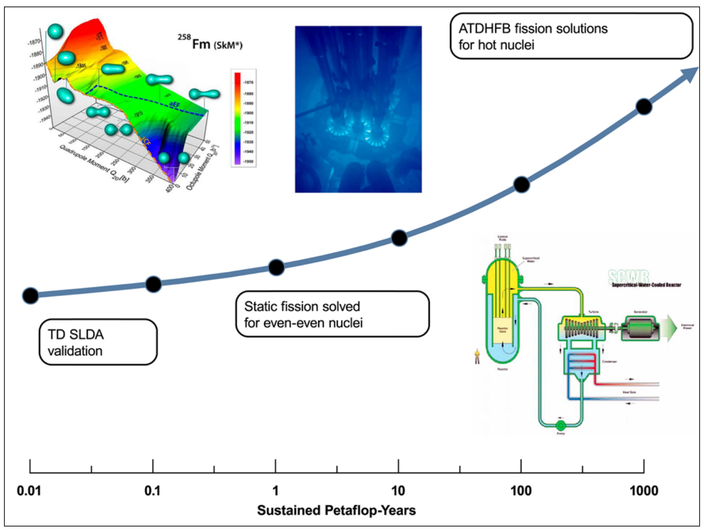
Future











Moving from
Structure to Dynamics

Need SciDAC-3
and continued collaborations
with Math/CS

Requirements next 3 years

Overall factor of 5 in core-hours

NERSC critical for development
factor of 10 required as new ideas / new people
become involved

Many people rely on NERSC for development
or testing of new ideas.