Computing the nucleus of the atom from first principles

San Diego State University
March 13, 2009

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Iowa State University

In conjunction with

Leadership-Class Configuration Interaction (LCCI)
Code/Environment Development Workshop
March 12-14, 2009

Major questions we aim to answer

"Connecting Quarks with the Cosmos: 11 Science Questions for the New Century", NAS/NRC Committee on Physics of the Universe, 2003 Report

1. How were the heavy elements from iron to uranium made?
2. Do neutrinos have mass?

....

How - adopt available *ab initio* theory to assure predictive power with results based on QCD and controlled uncertainties

Present stage - method validation in light nuclei, novel physics
Next decade - describe heavy nuclei and reactions, novel physics

....

Really big dream - computational nuclear physics achieves a precision competitive with experimental uncertainties

=> Coordination/balance between experiment and computation

UNEDF SciDAC Collaboration

Universal Nuclear Energy Density Functional

QCD
Theory of strong interactions

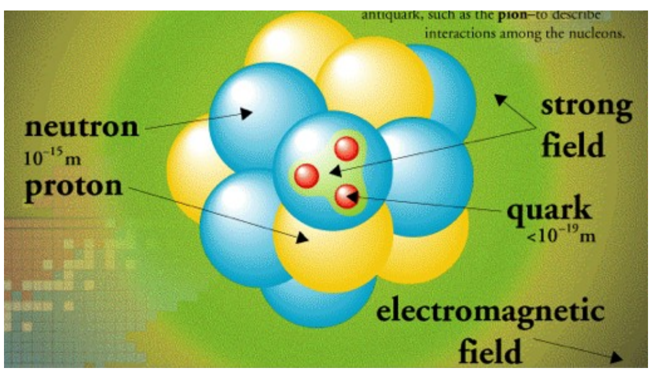
χEFT
Chiral Effective Field Theory

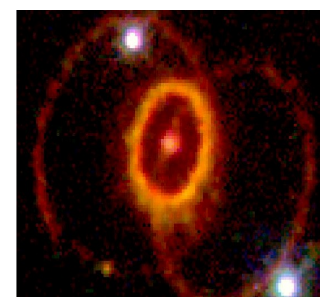
Inter-Nucleon
NN, NNN Interactions
AV18, EFT, V_{low-k}

Theory of Light Nuclei
Spectroscopy and selected reactions
Verification: NCSM=GFMC=CC
Validation: nuclei with A<16

Big Bang
Nucleosynthesis
& Stellar Reactions

Density Functional Theory
improved functionals
remove computationally-imposed constraints
properties for all nuclei with A>16





Dynamic Extensions of DFT
LACM by GCM,TDDFT,QRPA
Level densites

r,s processes
& Supernovae

Low-energy Reactions
Hauser-Feshbach
Feshbach-Kerman-Koonin
Fission
mass and energy distributions

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The 3-Fold Challenge = Computationally Hard

- Multiple scales - keV to GeV (collective modes, EOS, SRC’s)
- Strong interaction - SRC’s, renormalization, NN+NNN
- Self-bound quantum N-body systems - preserve all underlying symmetries

DOE Major Facilities with related experimental programs

Facility for Rare Isotope Beams (FRIB)
Thomas Jefferson Lab (TJ Lab)
Neutrino detector facilities (several)

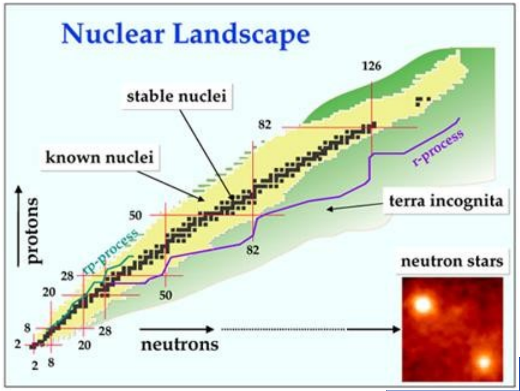
Nuclear Physics interfaces with other fields - input/benefits

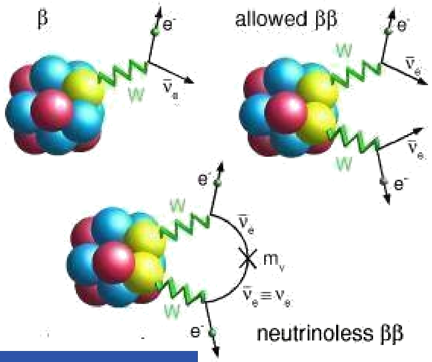
Math/Comp Sci
Particle physics
Astrophysics/Cosmology
Many-body physics

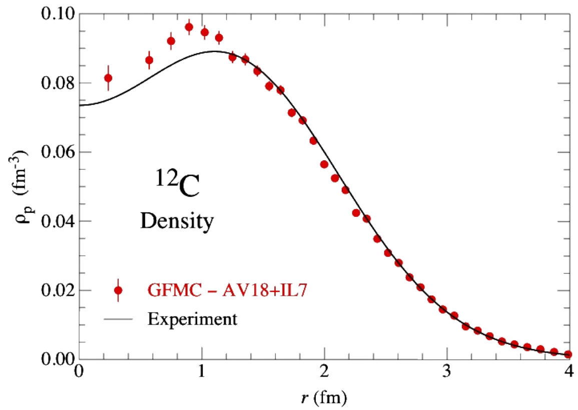
DOE Workshop on Forefront Questions in Nuclear Science
and the Role of High Performance Computing,
Gaithersburg, MD, January 26-28, 2009
Nuclear Structure and Nuclear Reactions

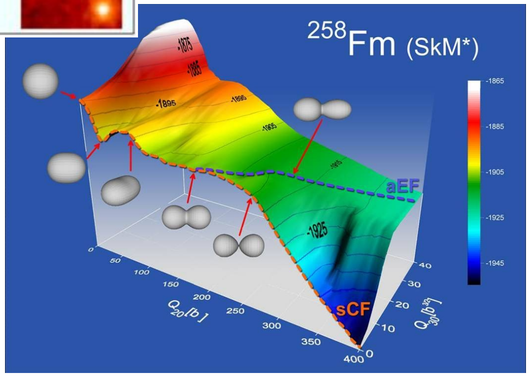
List of Priority Research Directions

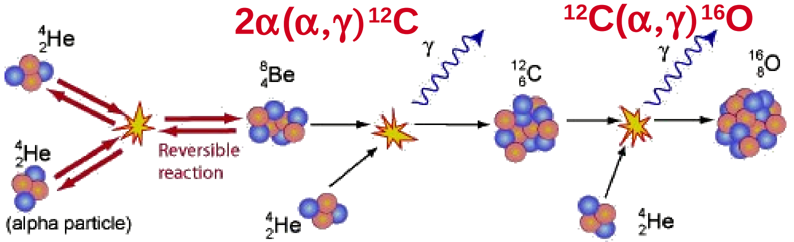
- **Physics of extreme neutron-rich nuclei and matter**
- **Microscopic description of nuclear fission**
- **Nuclei as neutrino physics laboratories**
- **Reactions that made us - triple α process and $^{12}C(\alpha,\gamma)^{16}O$**











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Nuclear Structure and Nuclear Reactions

Nuclei as Neutrino Physics Laboratories

Scientific and computational challenges

- **Develop effective interactions and weak currents based upon fundamental theory and experiments.**
- **Diagonalize matrices of dimension 10^{12-13}**

Summary of research direction

- **Develop extreme scale nuclear structure codes; estimate uncertainties with competing methods.**
- **Create techniques for ν-reactions relevant to oscillation experiments.**

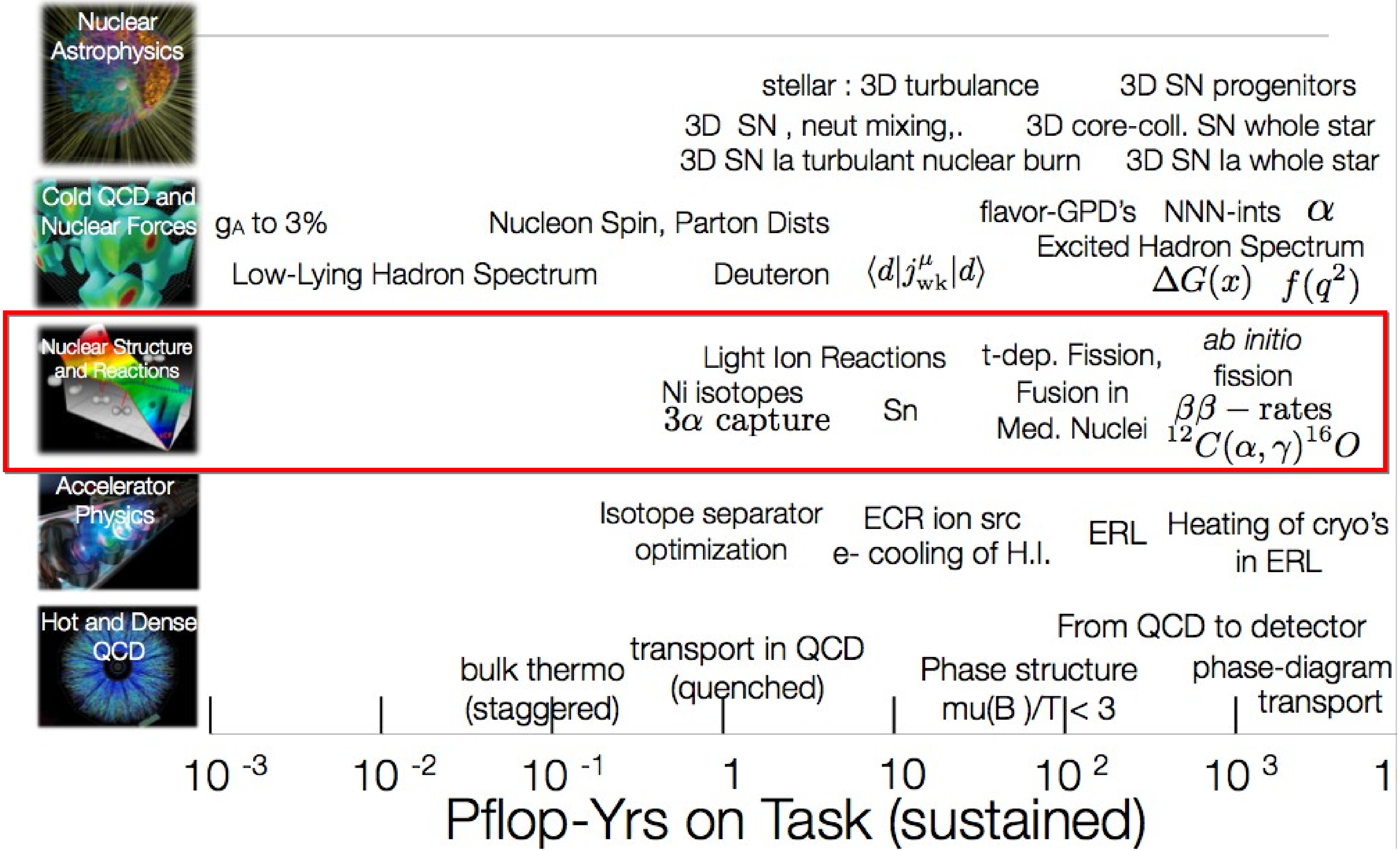
Expected Scientific and Computational Outcomes

- **Dependence of $0\nu\ \beta\beta$-decay nuclear lifetimes on neutrino mass with theoretical uncertainty to 30-50%.**
- **ν-nucleus cross sections to 20%.**
- **Fault-tolerant, load-balanced highly scalable sparse eigensolver; load balancing for Monte Carlo simulations.**

Potential impact on Nuclear Science

- **Interpret experiments to explain the nature of the neutrinos and their masses.**
- **Calculate rates of nuclear reactions that drive stars and stellar explosions.**

Nuclear Physics Requires Exa-scale Computation



The Nuclear Many-Body Problem

The many-body Schroedinger equation for bound states consists of $2\binom{A}{Z}$ coupled second-order differential equations in 3A coordinates using strong (NN & NNN) and electromagnetic interactions.

Ab initio approaches projected for exascale machines

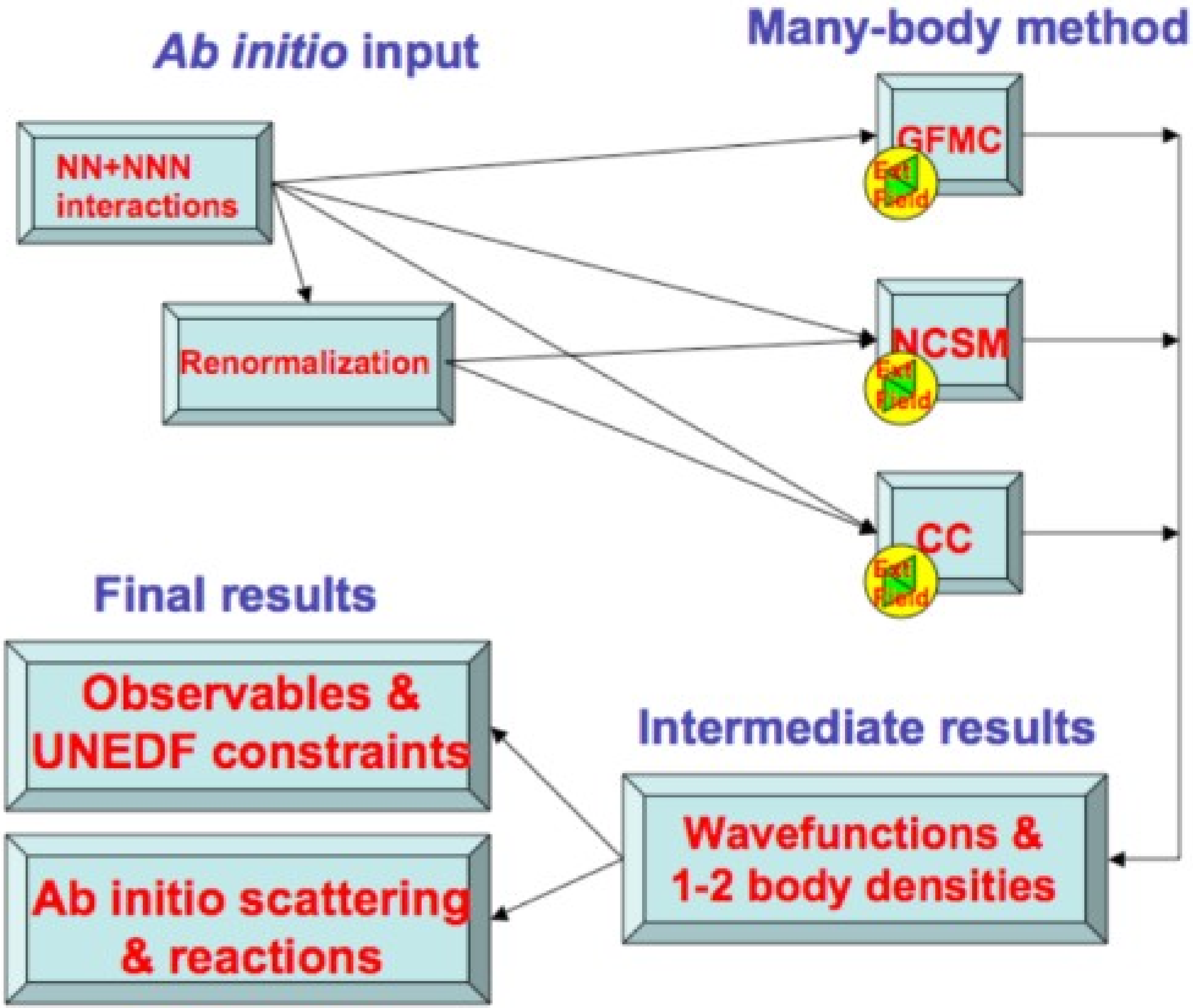
Stochastic approach in coordinate space
Greens Function Monte Carlo (**GFMC**)

Hamiltonian matrix in basis function space
No Core Shell Model (**NCSM**)

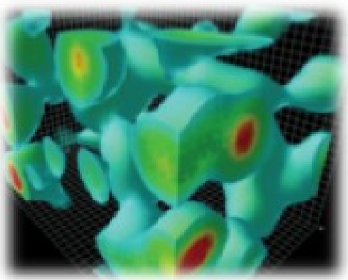
Cluster hierarchy in basis function space
Coupled Cluster (**CC**)

Comments
All work to preserve and exploit symmetries
Extensions of each to scattering/reactions are well-underway
They have different advantages and limitations

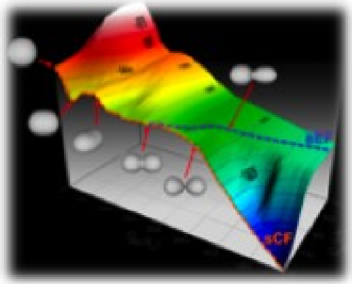
Example of a multi-code environment



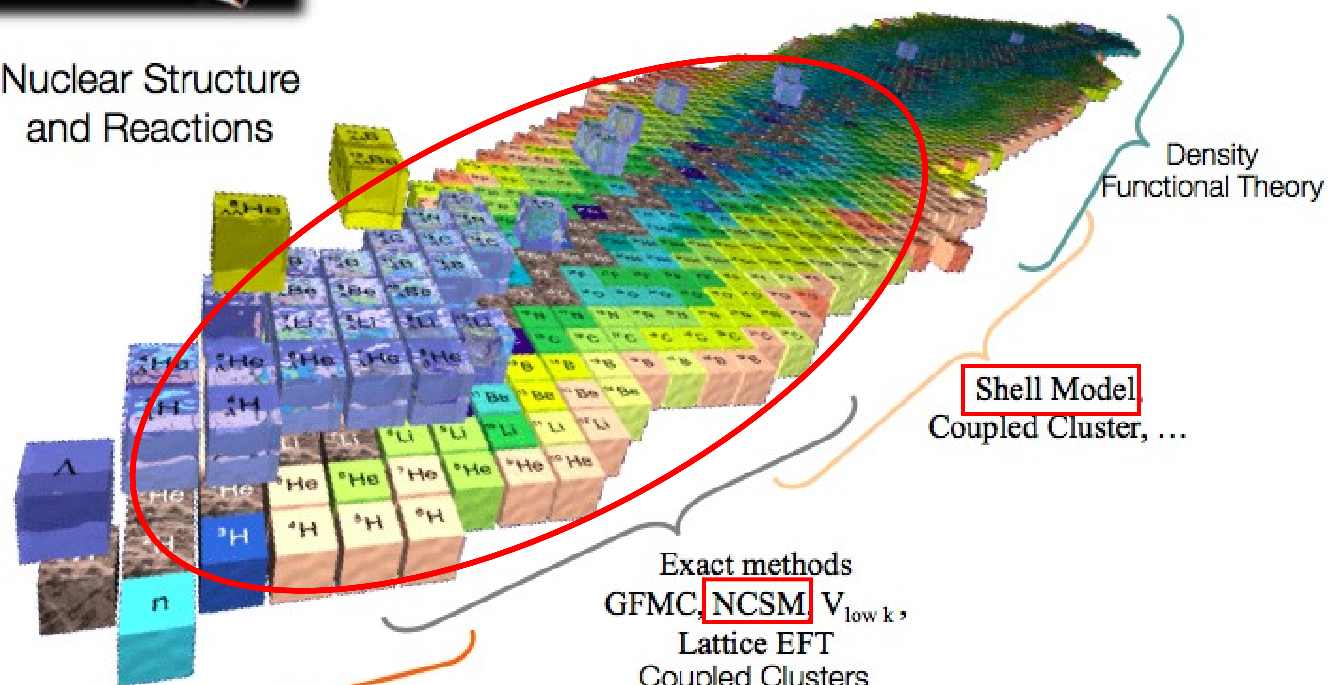
Exa-scale computing will unify Nuclear Physics



Cold QCD and
Nuclear Forces



Nuclear Structure
and Reactions



+ Reactions

ab initio No-Core Shell Model (NCSM) Problem Statement

Solve eigenvalue problem in large enough basis to converge

$$H = T_{rel} + V_{NN} + V_{3N} + \cdots$$

$$H\left|\Psi_i\right\rangle = E_i\left|\Psi_i\right\rangle$$

$$\left|\Psi_i\right\rangle = \sum_{n=0}^{\infty} A_n^i \left|\Phi_n\right\rangle$$

$$\text{Diagonalize } \{\left\langle\Phi_m\right|H\left|\Phi_n\right\rangle\}$$

Employ eigenvectors to calculate experimental observables

$$\text{Transition Rate } (i \rightarrow k) \propto \left|\left\langle\Psi_k\right|\hat{O}\left|\Psi_i\right\rangle\right|^2$$

Issues limiting the physics

- Strong interaction complexity (e.g. NN vs NN + NNN)
- Size & character of basis space needed for convergence
- Eigensolver algorithm improvements
- Memory available to store matrix and vectors

What are the basic elements to solving the problem?

- Adopt a realistic NN (and 3N) interaction & renormalize as needed - retain induced many-body interactions
- Adopt the 3-D Harmonic Oscillator (HO) for the single-nucleon basis states, α, β,…
- Evaluate the nuclear Hamiltonian, H, in basis space of HO (Slater) determinants (manages the bookkeepping of anti-symmetrization)

$$\left|\Phi_n\right\rangle = [a_a^+ \qquad a_V^+]_n \left|0\right\rangle$$

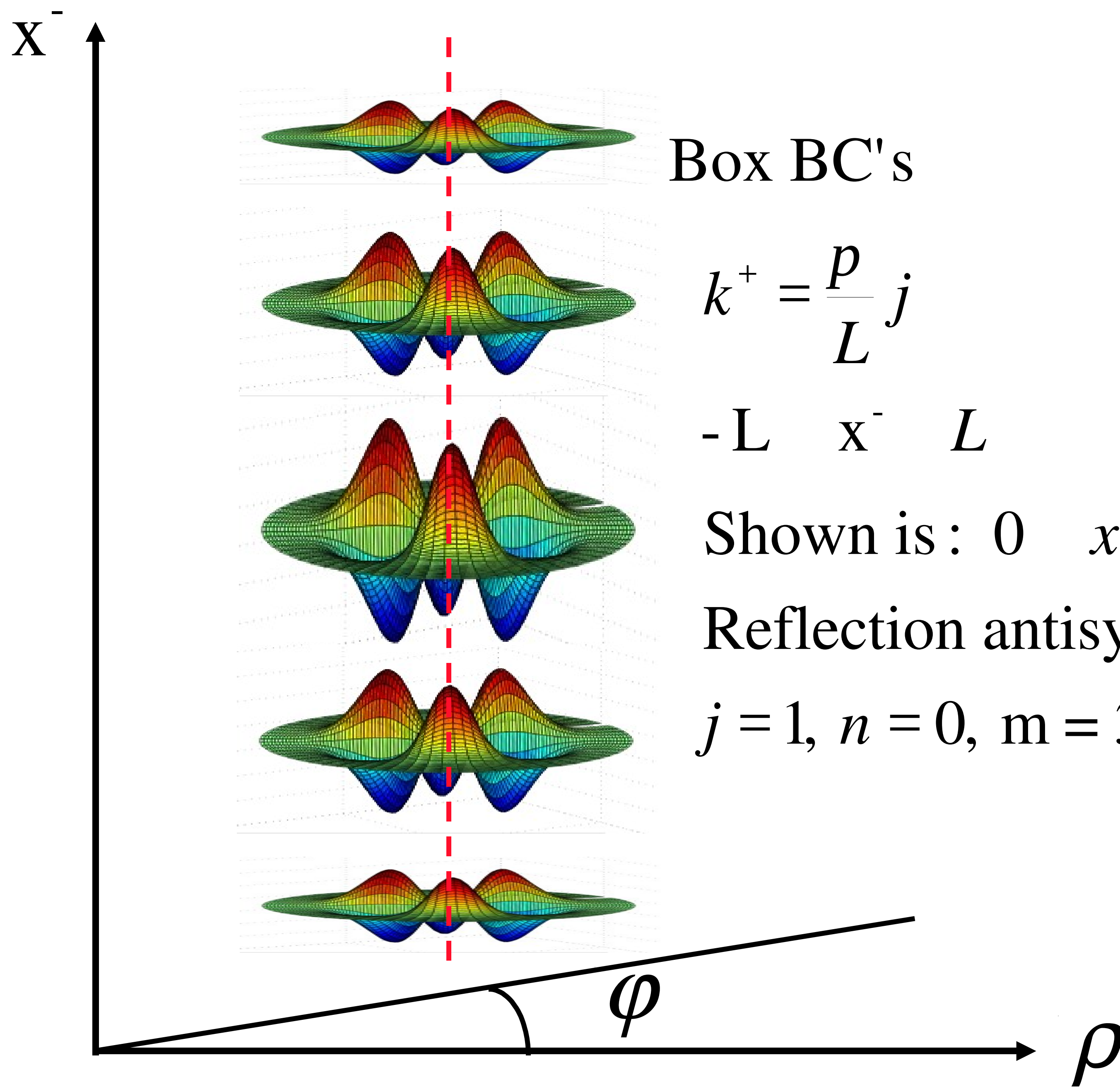
- Diagonalize resulting sparse many-body H in this “m-scheme” where

$$n = 1,2,\ldots,10^{10} \text{ or more!}$$

- Evaluate observables and compare with experiment

Comments:

- Straightforward but computationally demanding => new algorithms/computers
- Requires convergence assessments and extrapolation tools
- Achievable for nuclei up to A=16 (40) today with leadership-class computers



Box BC's

$k^+ = \frac{p}{L} j$

$- \mathrm{L} \quad \mathrm{x}^- \quad L$

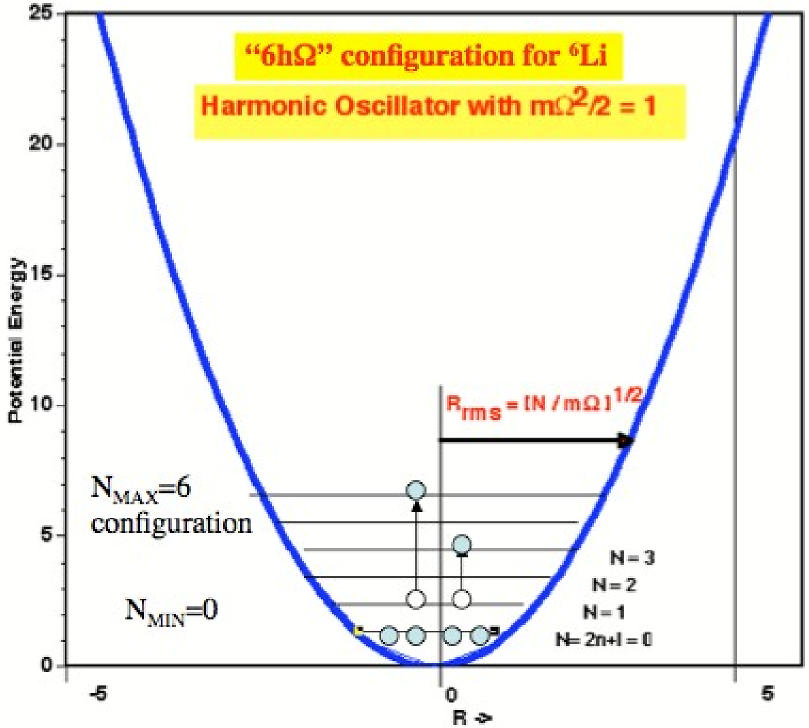
Shown is : $0 \quad x^- \quad L$

Reflection antisym.

$j = 1,\ n = 0,\ \mathrm{m} = 3$

Single-particle basis

- Harmonic oscillator single-particle basis states (Shell Model)



- General single-particle basis
  - Wood–Saxon basis implemented, further generalizations under development

Lanczos Diagonalization

$$H|\Psi_\alpha\rangle = E_\alpha|\Psi_\alpha\rangle$$

$$|\chi_1\rangle = \tau\rho\iota\alpha\lambda\#1 \quad = \quad \text{“pivot vector”}$$

$$\alpha_1 = \langle\chi_1|H|\chi_1\rangle$$

$$\beta_1 = 0$$

Recursive determination of additional terms:

$$b_{n+1}|\chi_{v+1}\rangle = H|\chi_v\rangle - \alpha_v|\chi_v\rangle - \beta_v|\chi_{v-1}\rangle$$

implies

$$H \qquad \begin{matrix} \alpha_1 & \beta_2 & 0 & 0 & .. \\ \beta_2 & \alpha_2 & \beta_3 & 0 & .. \\ 0 & \beta_3 & \alpha_3 & \beta_4 & .. \\ 0 & 0 & \beta_4 & \alpha_4 & .. \\ .. & .. & .. & .. & .. \end{matrix}$$

Lanczos diagonalization develops a dynamical basis in which the full H is tri-diagonal.

In practice, one diagonalizes this (truncated) tri-diagonal H after each iteration and compares the lowest eigenvalues until a desired precision is reached.

Even for very large many-Fermion problems, e.g. $D = 10^9$, 30-50 iterations can give a ground state energy accurate to one part in a million using 32-bit accuracy.

Efficient Algorithm for Lanczos Diagonalization

$$|\eta_{n+1}\rangle = H|c_n\rangle - b_n|c_{n-1}\rangle$$

$$a_n = \langle h_{n+1}|c_n\rangle$$

$$|h'_{n+1}\rangle = |h_{n+1}\rangle - a_n|c_n\rangle$$

$$b_{n+1} = [\langle h'_{n+1}|h'_{n+1}\rangle]^{1/2}$$

$$|c_{n+1}\rangle = \frac{|h'_{n+1}\rangle}{b_{n+1}}$$

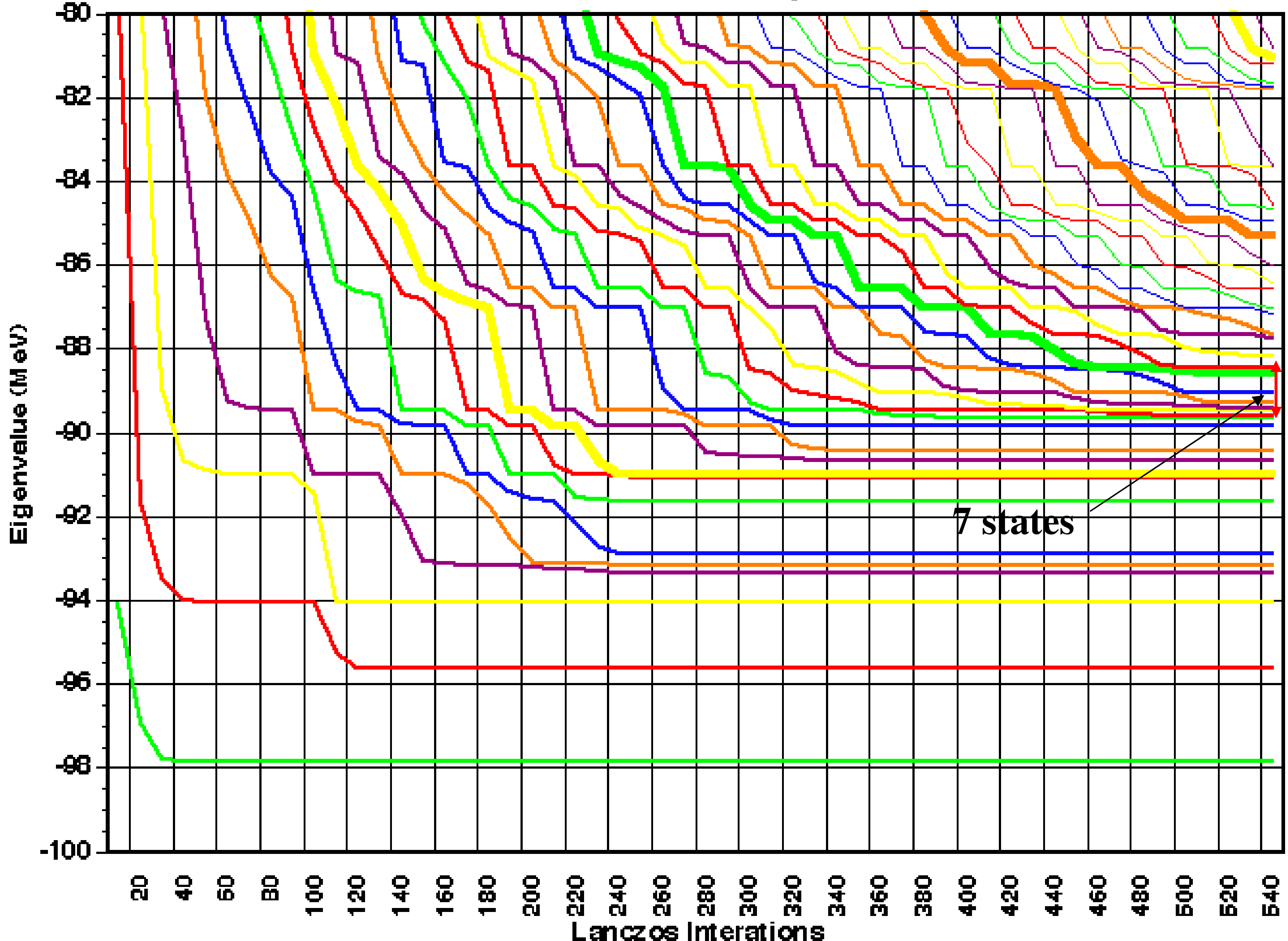
Only two vectors must be stored as we can use same storage for:

$$|\chi_{n-1}\rangle, |h_{n+1}\rangle, |h'_{n+1}\rangle, and\, |c_{n+1}\rangle$$

Possible difficulties

- Loss of orthogonality leading to spurious and duplicate eigenvalues => reorthogonalize
- slower convergence of degenerate or near-degenerate states
- sensitivity of convergence rate to initial pivot vector

16-O with CD-Bonn(2K) in 6hw space, hw = 15 MeV
Excited State Spectrum



Many Fermion Dynamics (MFD) – nuclear physics

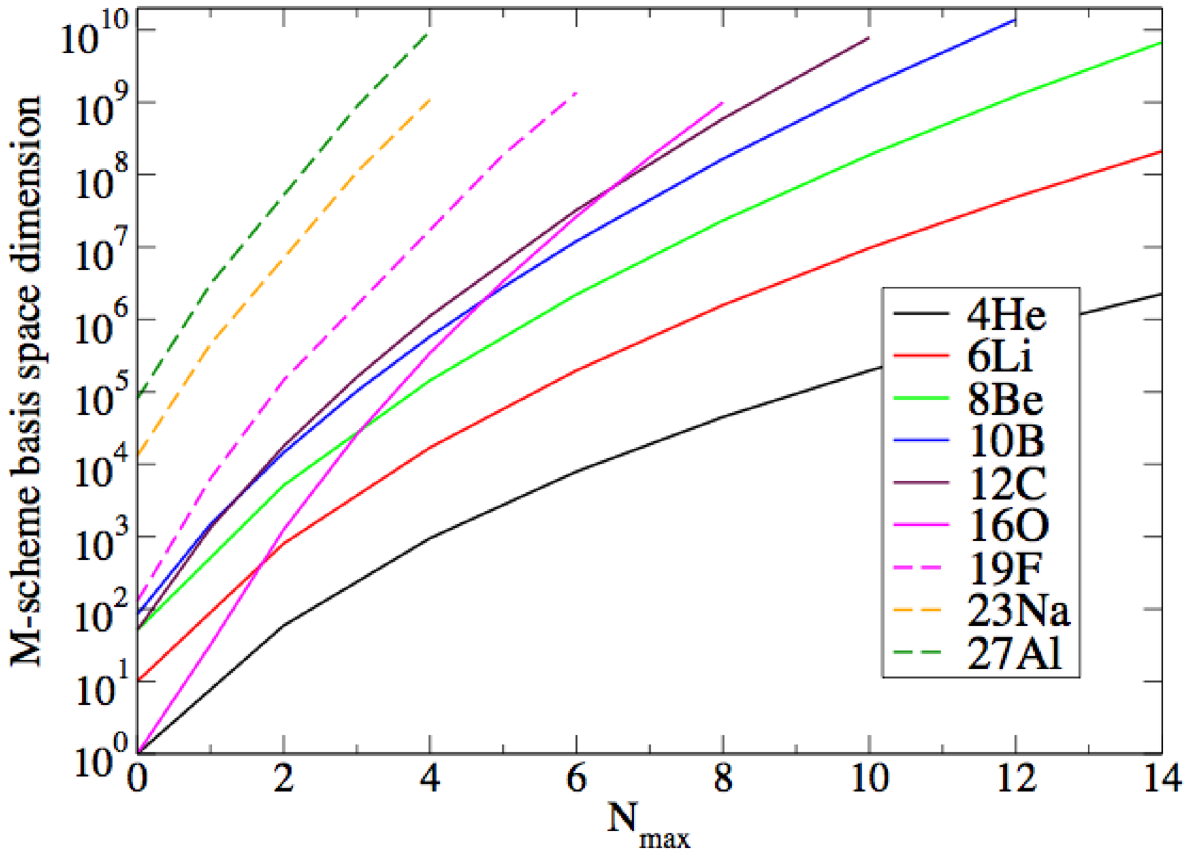
Numerical approach for bound states of nucleons
using basis-space expansion methods

- Given
  - a V_{NN} and V_{NNN} (and V_{NNNN}) interaction
  - number of protons and neutrons: Z, N

  calculates
  - bound state spectrum and corresponding wave functions
  - one-body density matrices (in development)
  - selected observables:
    rms radii, magnetic moments, quadrupole moments,
    transition rates between ground state/excited states
- Other applications
  - Hadron physics:
    relativistic field theory, number of particles not conserved
  - Atomic physics: trapped bosons and/or fermions

Basis space – memory considerations

Basis space dimensions for stable nuclei $N \approx Z$



Need to distribute single vector over multiple processors

Basis space – memory considerations

Memory requirements for many-body basis
Current implementation

- integer2 array mbstates(num_nucleons, num_states)
  where mbstates(i, j) indicates
  the single-particle state of nucleon i of many-body state j
- total memory for array mbstates(num_nucleons, num_states)

nucleus	$N_{\mathrm{max}} = 4$	$N_{\mathrm{max}} = 6$	$N_{\mathrm{max}} = 8$	$N_{\mathrm{max}} = 10$
^{6}Li	204 kB	2.4 MB	19 MB	116 MB
^{12}C	27 MB	0.78 GB	14 GB	0.19 TB
^{16}O	11 MB	0.85 GB	32 GB	0.77 TB
^{19}F	840 MB	52 GB		
^{23}Na	50 GB			

Need to distribute many-body basis over multiple processors

Storage and solution of sparse matrix

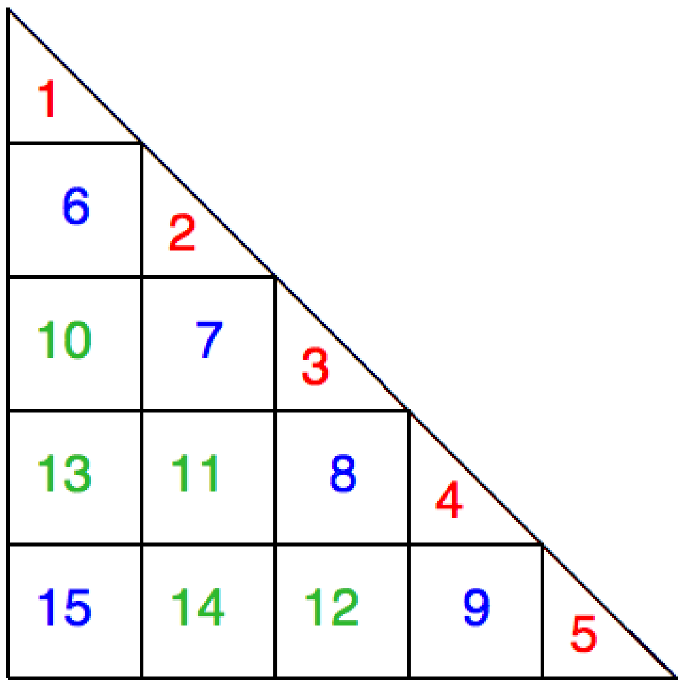
Current implementation:

- Store matrix in Compressed Column format
  - Integer4 array column_ptrs(num_local_states)
  - Integer4 array matrix_ptrs(num_local_nonzeros)
  - Real4 array matrix_elements(num_local_nonzeros)
- Calculate eigenvalues using Lanczos procedure
  - use of current implementation of PARPACK not efficient due to 2-dimensional distrubution of matrix
  - modification of PARPACK under development
- Numerical precision issue
  - perform matvec in single precision but need to perform orthogonalization and normalization in double precision
  - more general: acccumulation of inner products of vectors need to be done in double precision
  - standard BLAS routines not always suitable

Distribution of matrix and vectors

- Store lower half of symmetric matrix, distributed over $n = d \cdot (d+1)/2$ processors with d "diagonal" proc's
- Store Lanczos vectors on one of $(d+1)/2$ groups of d proc's

lower triangle matrix



storage Lanczos vectors

1	6	10
2	7	11
3	8	12
4	9	13
5	15	14

Dimensions and sparsity of matrices – summary

Estimates of aggregate memory needed for storage
of sparse symmetric Hamiltonian matrix

(does not include memory for column pointers nor for vectors)

nucleus	N_{max}	dimension	2-body	3-body	4-body
^{12}C	8	$6.0 \cdot 10^8$	4 TB	180 TB	4 PB
^{12}C	10	$7.8 \cdot 10^9$	80 TB	5 PB	140 PB
^{16}O	8	$9.9 \cdot 10^8$	5 TB	300 TB	5 PB
^{16}O	10	$2.4 \cdot 10^{10}$	230 TB	12 PB	350 PB
^{8}He	12	$4.3 \cdot 10^8$	7 TB	300 TB	7 PB
^{11}Li	10	$9.3 \cdot 10^8$	11 TB	390 TB	10 PB
^{14}Be	8	$2.8 \cdot 10^9$	32 TB	1100 TB	28 PB
^{20}C	8	$2.0\ \ 10^{11}$	2 PB	150 PB	6 EB
^{28}O	6	$1.0 \cdot 10^9$	6 TB	220 TB	4 PB
^{28}O	8	$1 \cdot 10^{11}$	1 PB	56 PB	2 EB

<u>Need</u>
Is 4N impt?

<u>Need</u>
increased memory

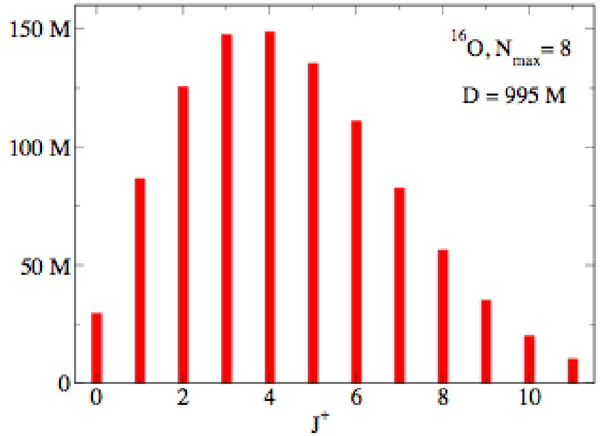
<u>Need</u>
Improved I/O

200 TB
petascale limit

200 PB
exascale limit

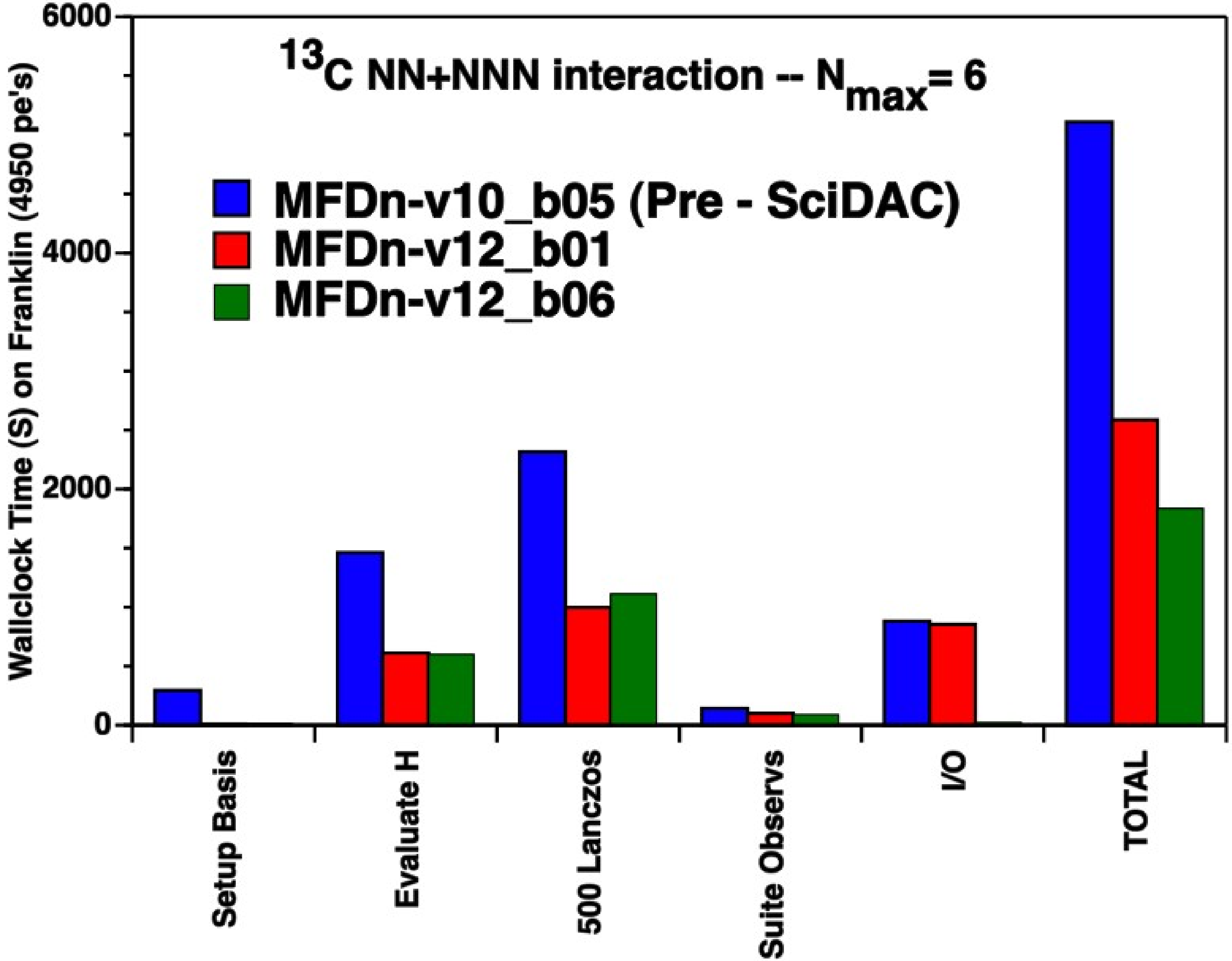
Under development

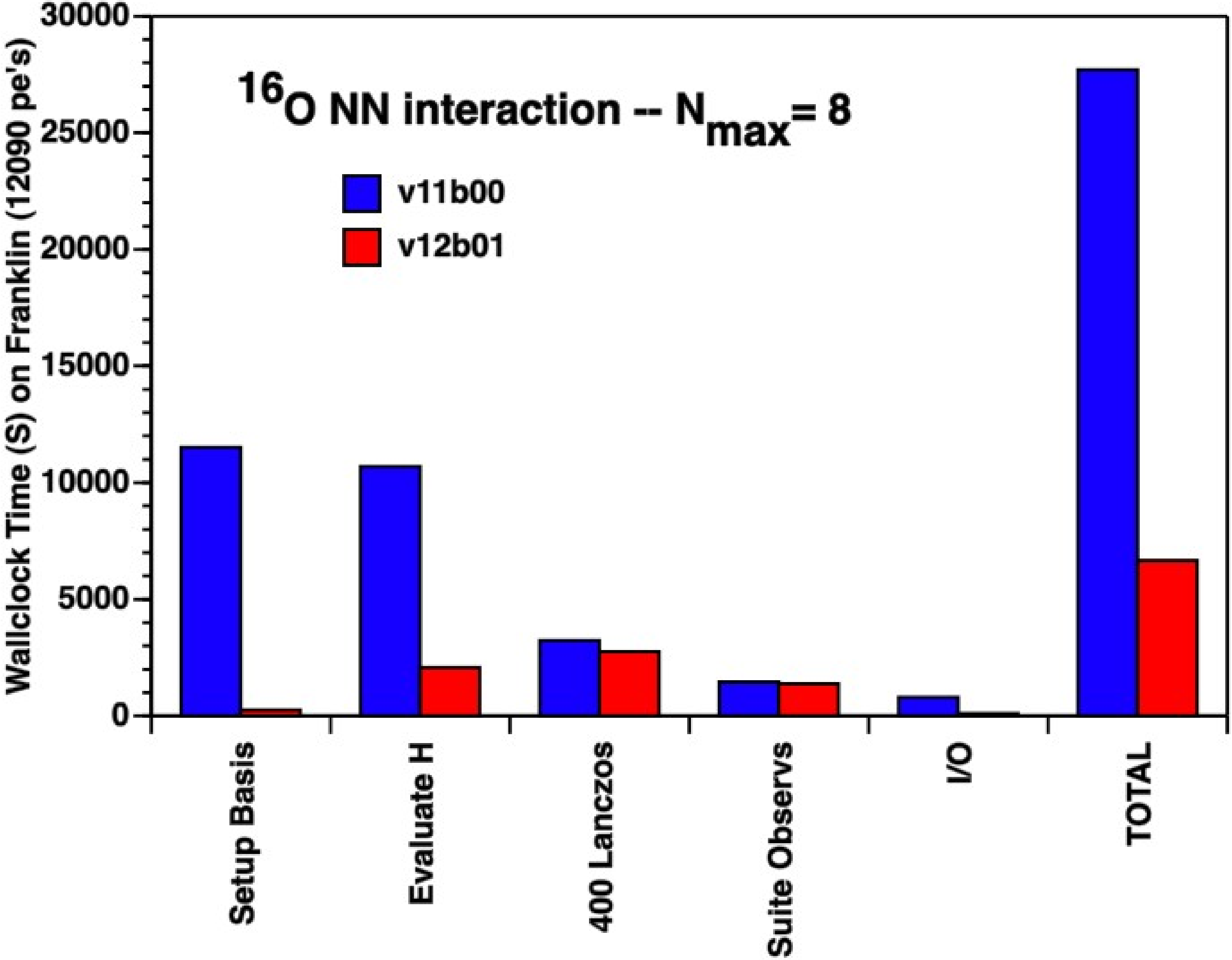
- Generalized single-particle basis
  - basis functions with realistic asymptotic behavior should improve convergence of observables such as $\langle r^2 \rangle$ and Q
- Expand and generalize external fields
  - necessary for connection with DME/DFT
- Output of one-body density matrices
- Extend 3-body forces to larger model spaces
- Hybrid MPI and OpenMP
- Coupled J-basis
  - significant reduction in # of basis states
  - matrices less sparse



- Scattering applications
  - RGM (Navratil), other methods (Shirokov, Elster?)

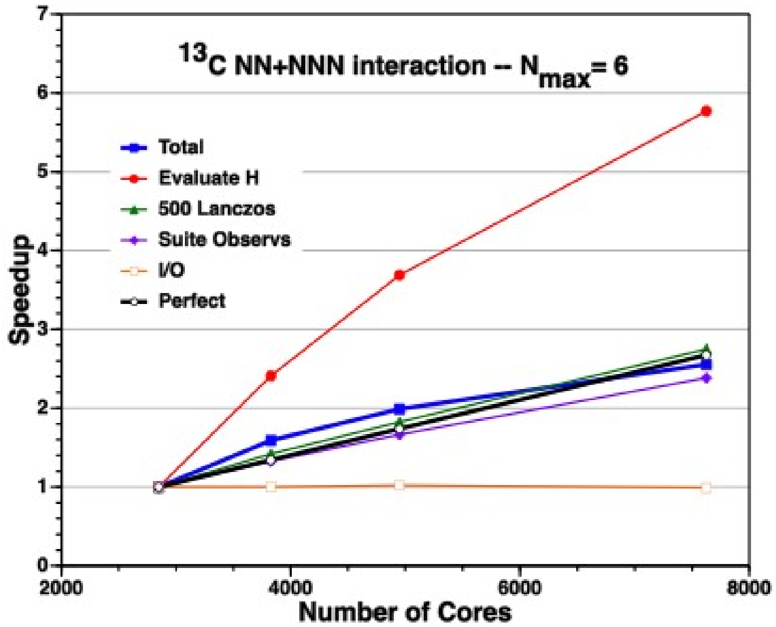
Overall Performance of MFDn

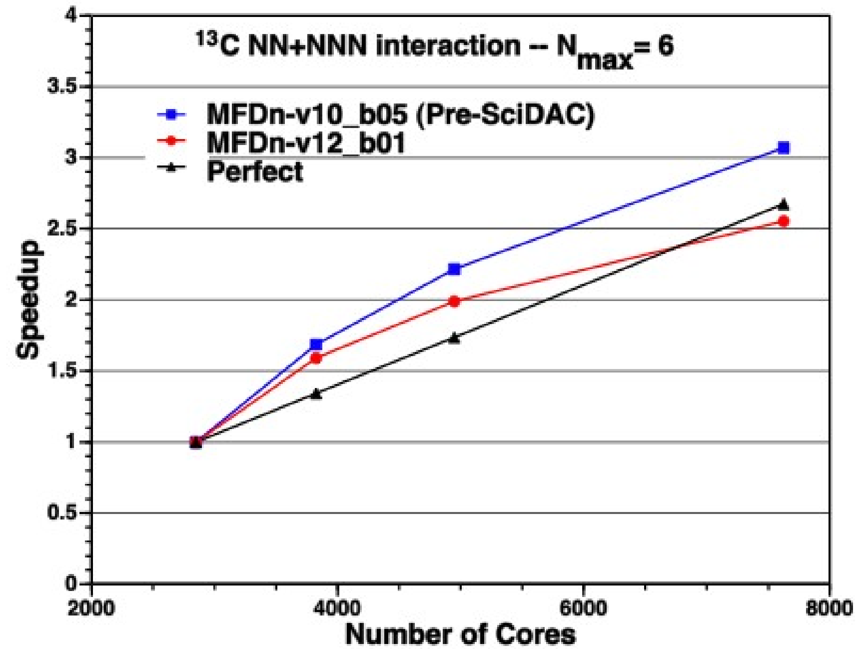




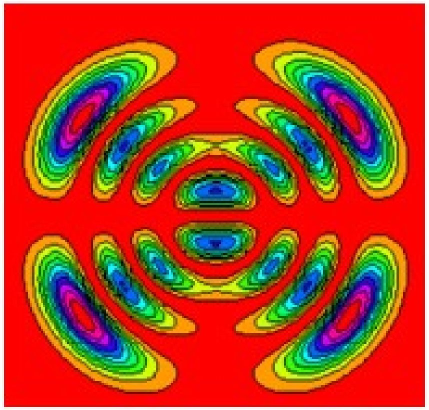
^{16}O NN interaction -- N_{max}= 8
v11b00
v12b01
Wallclock Time (S) on Franklin (12090 pe's)
30000
25000
20000
15000
10000
5000
0
Setup Basis
Evaluate H
400 Lanczos
Suite Observs
I/O
TOTAL

Scalability of MFDn





Frontier Nuclear Science Enabled By SciDAC Partnership



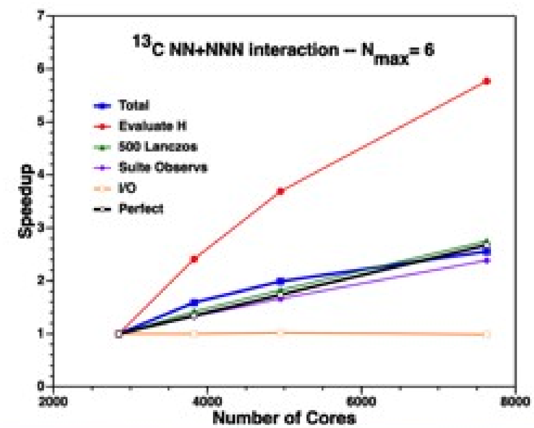
sample harmonic oscillator basis function

14F, an exotic nucleus with an extreme proton to neutron ratio, not previously discovered, is predicted through advanced simulations using MFDn, a parallel code for configuration interaction modeling in a harmonic oscillator basis (see fig. on left). The properties of this “beyond proton drip line” nucleus present significant constraints on theories of strong interactions and may be measured at the planned DOE facility for rare isotope beams.

Collaboration among Physics, Applied Mathematics, and Computer Science enabled the simulations through critical improvements in MFDn by a factor of 4-6 on the Cray XT-4.

Improvements in MFDn include new data structures, new parallel blocking and combinatorial algorithms, and enhanced inner loop and I/O performance.

Computing the 10 lowest eigenstates using the improved MFDn for ^{14}F requires 3 hours on 30,628 Cray XT-4 nodes at ORNL. This would have taken at least 18 hours using previous versions of MFDn.



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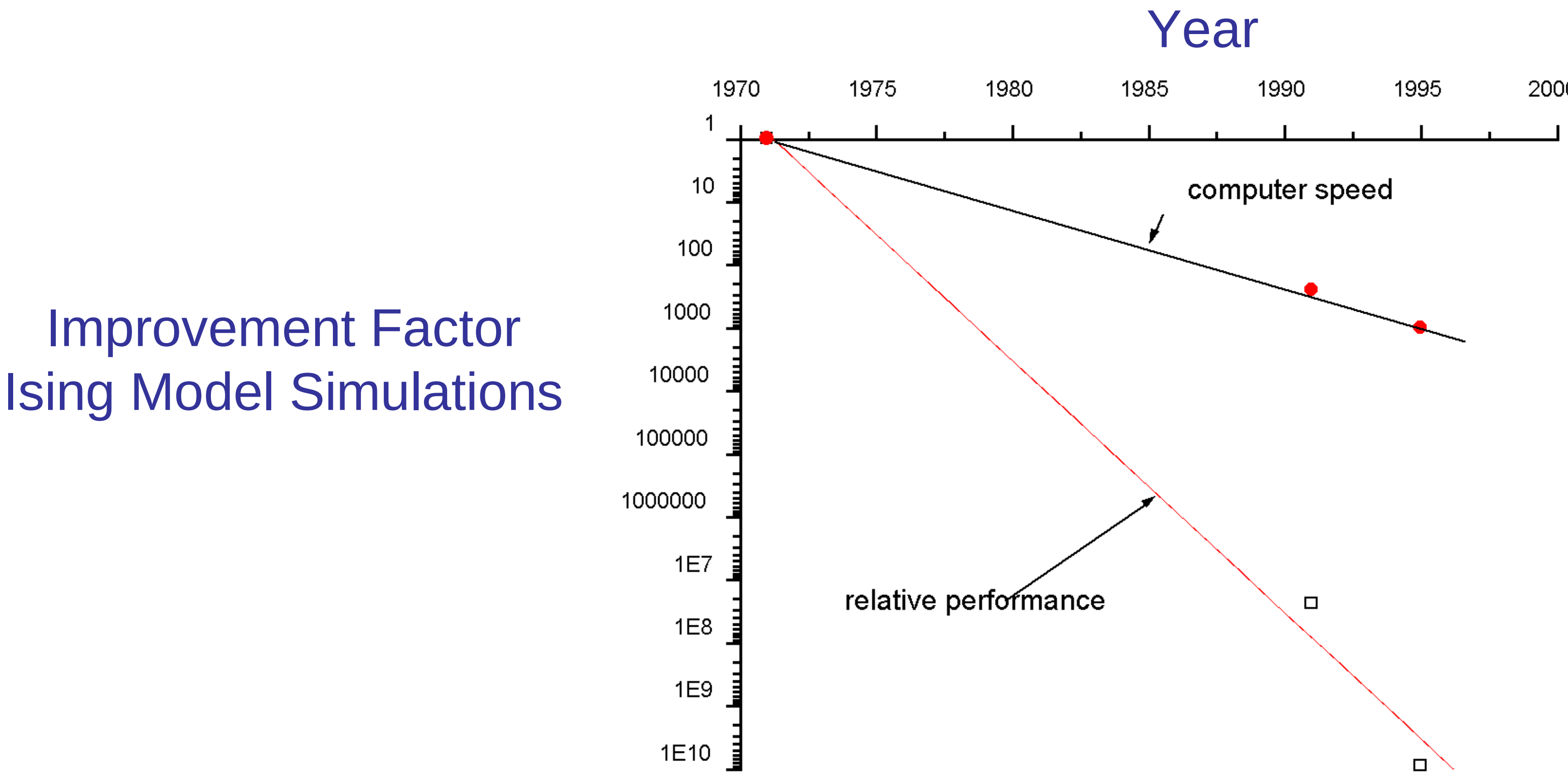
Human Resources

- To fully utilize Exa-scale at 2017 we need to grow expertise in the NP community
  - faster than Moores Law
  - not business as usual

- The standard interdisciplinary hiring problems exist
  - challenge at Labs and Universities
  - new training models , start today for 2017?

- Broad collaborations
  - Graduate students and postdocs hired into collaboration
    - naive scaling from RHIC and UNEDF programs = SIGNIFICANT enhancement in person-power (+10+10 per project ?)
  - Organization in the Nuclear Physics community

Gains from investments in research well-matched with Moore's gains in computer speed



Thanks to David P. Landau

Conclusions and Outlook

Theory + Leadership Class Computers

||

Discovery potential

Federal support increasing dramatically

||

Career opportunities

Thank you

For your attention

To colleagues and collaborators