AB INITIO NUCLEAR SHELL MODEL CALCULATIONS

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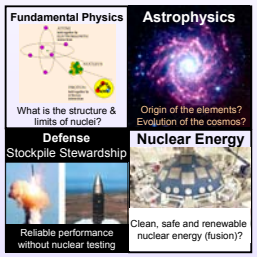
A consistent microscopic theory of the atomic nucleus is necessary to explain a wide range of nuclear phenomena and to predict nuclear behavior that cannot be measured experimentally. Over the past decade, theoretical investigations have fundamentally shifted from phenomenological methods to *ab initio* approaches to understanding nuclei. The availability of high performance computing resources allow for the more reliable, but computationally intensive first principles methods to be tractable.

The No-Core Shell Model (NCSM) is an *ab initio* approach that has been successful in describing light nuclei. Nuclear properties are obtained through diagonalization of the Hamiltonian matrix, which is large (dimension > 10^8) and sparse. The computational effort increases exponentially with nucleon number using a 2-body Hamiltonian, and becomes particularly difficult when including 3-body forces. New algorithms and load balancing techniques are needed to scale this method for larger nuclei (A > 16). We analyze the computational challenges of REDSTICK, a nuclear shell model program, and implement several techniques to scale REDSTICK to investigate high p-shell and low sd-shell nuclei.

INTRODUCTION

A reliable understanding of nuclear reactions is needed for fields as diverse as astrophysics and stewardship of the nation's weapons stockpile. When possible, scientists experimentally measure the reaction rates of interest. Though new accelerator facilities allow us to study a wide range of nuclei with greater sensitivity, there are still a large number of reactions that cannot be reproduced in a laboratory.



A consistent and comprehensive microscopic formulation of nuclear structure, grounded in the fundamental interactions between constituent nucleons, has yet to be achieved. This is desired, to replace existing phenomenological models of nuclear structure and to be used predictively to determine nuclear properties of interest that cannot be measured experimentally.

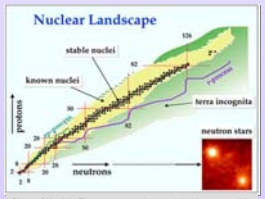


Chart of Nuclei: There are approximately 3,000 known nuclei, many of which have been produced and studied experimentally in labs. Yet, there still remains an estimated 6,000 that have yetto be created.

Due to the complex interactions within nuclei, implementing these models require the use of high-performance computing resources. Shell model codes are constrained by run-time performance and/or memory for large-scale calculations of interests. Codes need to be optimized with unique algorithms to overcome these limitations.

REDSTICK is a general utility interacting nuclear shell model program that performs NCSM calculations. Previous shell model calculations of light nuclei have been limited to two-body interactions due to the computational difficulties of higher body calculations. Results from two-body calculations, though much improved due to higher precision interactions, still remain inconsistent with experiment.

In order to accurately characterize nuclei, a 3-body force is essential in the calculations. Recent advances in theory and computational power allows for the 3-body interactions in the NCSM. There have been systematic studies of the effects of three-body interactions on p-shell nuclei up to ^{13}C in the 4ħΩ and 6 ħΩ model spaces with favorable results.

To continue these investigations using 3-body forces, considerable improvements need to be made to nuclear shell model programs.

NUCLEAR SHELL MODEL

The shell model approach solves the quantum many body problem with a **matrix eigenvalue problem**. It assumes a single particle potential and expands the full many-body solution with a convenient choice of **orthogonal basis**. From which the many-body **Hamiltonian matrix elements** are constructed to solve for the energy spectrum and wavefunctions.

$$H\Psi_i = E_i\Psi_i$$

$$\Psi_i = \sum_i C_{in}\phi_n$$

$$H_{ij} = \langle\phi_j|H|\phi_i\rangle$$

INPUT:

Hamiltonian Operator

$$H = \sum_i \varepsilon_i a_i^+ a_i + \frac{1}{4}\sum_{ijkl} V_{ijkl} a_i^+ a_j^+ a_l a_k$$

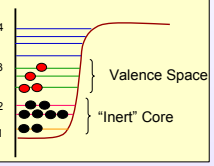
(2-body operator in second quantization formalism, with creation operator a^+ and annihilation operator a)

Effective Interaction – V_{ijkl}

Single Particle Energies - $\mathcal{E}_i$

Model Space:valence space and # of active particles

Ab initio calculations assume all particles are active (No-Core). This is more computationally intense due to the larger model space.



REDSTICK:
Generalized shell model program written by W. E. Ormand and C. W. Johnson

- written in Fortran90 and MPI
- 2 body & 3 body versions available
- calculates Hamiltonian matrix elements on the fly
- Diagonalizes the matrix using the Lanczos method

$$\begin{pmatrix} H_{11} & H_{12} & \cdots & H_{1N} \\ H_{21} & H_{22} & & \\ \vdots & & \ddots & \\ H_{N1} & & \cdots & H_{NN} \end{pmatrix}$$

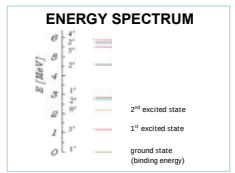
$$Hv_i = \beta_i v_{i-1} + \alpha_i v_i + \beta_{i+1} v_{i+1}$$

(efficiently finds the lowest eigenvalues of a large, sparse matrix)

COMPUTE NUCLEAR PROPERTIES
(i.e. magnetic dipole moment, reaction probabilities, etc.)

Transition Rate $i \to j \propto \langle\Psi_j|\hat{O}|\Psi_i\rangle$

ENERGY SPECTRUM



$$E_i, \Psi_i$$

EIGENVALUES WAVEFUNCTIONS

COMPUTATIONAL CHALLENGES

Storing the Matrix Elements?:
Even on today's fastest and largest supercomputers, there are limits to the possible investigations by shell model codes. The dimensions of the Hamiltonian matrix grow dramatically with number of particles and valence space.

$$Dim \approx \binom{N_{sps}^p}{n^p}\binom{N_{sps}^n}{n^n}$$

(N_{sps}^x = # of single particle states in valence space, *nx* = # of active particles for species *x*)

To scale this problem, storage of the matrix elements must be addressed.

Store on Disk

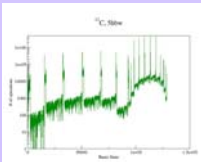
- Requires terabytes (10^{12}) of disk space which is generally not available to one user. Retrieving from disk is ~1000 slower.

Store on RAM

- Limited by the number of nodes available

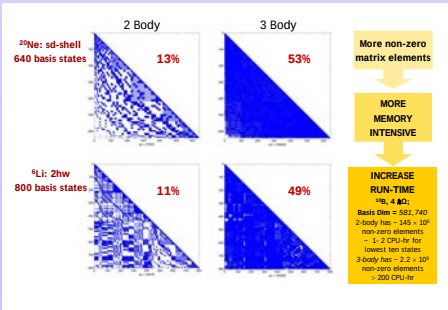
No Storage → On-the-Fly

- Optimal scaling, but requires efficient determination of non-zero matrix elements
- Run-time constraints require optimized programming methods
- Obvious workload distribution is not balanced



The natural work distribution scheme for the problem is to give each processor an equal number of proton basis states. This graph shows that some states require several orders of magnitude more flops. To avoid a workload bottleneck and ensure proper scaling of the application, an advanced workload distribution method is necessary.

2-Body → 3-Body = Less Sparse:



To optimally apply the on-the-fly technique, unique algorithms are necessary to overcome these challenges. My current work involves devising and implementing new approaches to allow for investigations of high *p*-shell and low *sd*-shell nuclei.