Innovative *ab initio* symmetry-adapted no-core shell model for advancing fundamental physics and astrophysics

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Nuclear Physics

Nuclear interactions:
- residual strong force
- composite particles, two-, three-, and four-body forces

Potential benefits:
- discover properties of nuclei at the edge of existence
- test fundamental understanding of nature
Application areas

Astrophysics and nucleosynthesis
- X-ray bursts
- r-process

Neutrinos and beyond the standard model physics
Ab initio approach

Interaction

<table>
<thead>
<tr>
<th>LO $\sigma(\bar{r})^2$</th>
<th>$XH$</th>
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<tbody>
<tr>
<td>NLO $\sigma(\bar{r})^2$</td>
<td>$XXH$</td>
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<tr>
<td>NLO $\sigma(\bar{r})^3$</td>
<td>$XAX$</td>
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Model

Observables

realistic nuclear potentials

wave functions and binding energies

reaction rates, cross sections, and densities

$^2H$, $^3H$, $^4He$
Solve non-relativistic Schrödinger equation:

\[ \hat{H} |\psi_i\rangle = E_i |\psi_i\rangle \]

where \[ \hat{H} = \hat{T} + \hat{V}_{NN} + \cdots + \hat{V}_{Coul} \]

1. Choose **physically relevant** model space and construct its basis \{ |\phi_1\rangle, \ldots, |\phi_d\rangle \}

2. Compute Hamiltonian matrix \[ H_{ij} = \langle \phi_i |\hat{H}|\phi_j\rangle \]

3. Find lowest-lying eigenvalues and eigenvectors [Lanczos algorithm]
Challenges

Combinatorial growth of Hamiltonian matrix

Limited to light nuclei
Construct many-body basis from physically-intuitive quantities:

- number of HO excitations: $N$
- total proton, total neutron and total intrinsic spins: $S_p S_n S$
- deformation: SU(3) and (λ μ)
- rotation: SO(3) and $L$
Computational effort:
- calculate matrix elements (95%)
- solving eigenvalue problem (3%)

Load balancing:

Scalability:
Model space example

$^6\text{Li} : N_{\text{max}} = 12$

$N\hbar\Omega$ space: direct sum of subspaces $[\bullet]$ of states carrying the same $(\lambda \mu)$ and $S_p S_n S$

Dimension: $3.9 \cdot 10^6$
Emerging Patterns

Key features:
- high deformation
- low spin

\[ ^6\text{Li} : 1^+ \text{gs} \]

Consistent Patterns
Toward medium-mass nuclei

Excitation Spectrum

Binding energy

Nucleon Density

complete space dimension: $4 \cdot 10^{12}$
symmetry-adapted space dimension: $1 \cdot 10^7$
Goal: Improve computation of density matrices with GPUs/MICs

Task details:
- Calculating density matrices requires vector-matrix-vector multiplication.
- Key observation: (large, sparse) matrix is made up of a small set of (small, dense) submatrices

New approach:
- compute only these submatrices, then do vector-submatrix-vector multiplication on-the-fly
- outsource this multiplication to GPU or MIC
Serial implementation: **4 orders of magnitude** faster than legacy code!

OpenMP implementation: **done**

GPU implementation: under development with associated deployment on Blue Waters

Looking forward to continued productive engagement of NSF PAID program to harvest and deliver key advances now and into the future.
Summary

• Collective modes arise naturally from first principles
• Physically-relevant basis provides a useful truncation scheme
• Applications of ab initio theory to medium mass nuclei currently underway
• Accelerated delivery of associated discovery science is expected to be enabled by exciting interdisciplinary computational advances on Blue Waters and future NSF Tier 1 systems.

Ab Initio Toolbox

- Symmetry-Adapted No-Core Shell Model
- No-Core Shell Model
- Quantum Monte Carlo
- Lattice EFT
- Hyperspherical Harmonics method
- Fadeev-Yakubovski
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LSU3shell code is publically available at [http://sourceforge.net/projects/lsu3shell](http://sourceforge.net/projects/lsu3shell).