Next-Generation Ab Initio Symmetry-Adapted No-Core Shell Model and Its Impact on Nucleosynthesis

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Other PIs: James P. Vary (Iowa State) and Umit V. Catalyurek (Ohio State)
**Physics of Atomic Nuclei**

**The Phases of QCD**
- Early Universe
- Future LHC Experiments
- Current RHIC Experiments
- Quark-Gluon Plasma
- Quark-Gluon Energy Surface
- Hadron Gas
- Nuclear Matter
- Neutron Stars
- Neutron Stripes
- Nuclear Superconductor
- Color Superconductor
- First order phase transition
- Critical Point
- Vacuum
- Baryon Chemical Potential
- Crossover

**Quarks to Cosmos**

**Nuclear interactions**
- Residual strong force → highly complex
- Two-, three- and four-body forces

**Discovery potential in nuclear physics**
- Universal internucleon interaction derived from QCD
- Properties and reactions of nuclei at the edge of their existence
- Accurate tests of fundamentals laws of nature
- Emergence of simple features from highly complex interactions

Estimated 98% of Mass/Energy in the Universe
Astrophysics: thermonuclear processes in the cosmos

NIF @ LLNL
Nuclear reactions for applied energy studies

Neutrino & Cosmology research
Ab initio Approaches to Nuclear Structure and Reactions

**Strong interaction**
- Realistic nuclear potential models
- Wave functions

**Many-body dynamics**
- Nuclear properties

**Nuclear reactions**
- Reaction rates cross sections
- Energy
Ab Initio No-Core Shell Model

**Goal:** Solve the non-relativistic quantum problem of $A$-interacting nucleons

\[ \hat{H} |\psi_i\rangle = E_i |\psi_i\rangle \quad \hat{H} = T + V_{\text{Coul}} + V_{NN} + \ldots \]

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]

**Resulting wave functions:**

- obey Pauli exclusion principle
- exact separation between intrinsic and center-of-mass motion
Combinatorial growth of Hamiltonian size

Computational Challenge: Scale Explosion

- Applicability limited to light nuclei
- Memory bound

- No-core Shell Model
- Quantum Monte Carlo
- Lattice EFT
- Hyperspherical Harmonics method
- Fadeev-Yakubovski
Symmetry-Adapted No-Core Shell Model

- Many-nucleon basis natural for description of many-body dynamics of nuclei

  Number of HO excitations: \( N \)

  Total proton, total neutron and total intrinsic spins: \( S_p S_n S \)

  Deformation: \( SU(3) \)

  Rotation: \( SO(3) \)

  \( \lambda \mu \) states:
  - \((0,0)\)
  - \((\lambda,0)\)
  - \((0,\mu)\)
  - \((\lambda,\mu)\)

Three pillars of Symmetry-Adapted No-Core Shell Model:
- Computational group theory
- Nuclear physics
- High performance computing
### Computational effort

- 95% - computing matrix elements
  - Embarassingly parallel problem
- 3% - solving eigenvalue problem

### Load balanced computations

1 process | 15 processes | 378 processes | 37,950 processes

### Excellent scalability

![Graph showing speedup vs. number of MPI processes](image1.png)

![Graph showing speedup vs. number of threads](image2.png)
Discovery: Emergence of Simple Patterns in Complex Nuclei

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

Key features of nuclear structure:
- Low spin
- Large deformation

Model space truncation

Dytrych, Launey, Draayer, et al., PRL 111 (2013) 252501
$^6\text{Li}: \ N_{\text{max}} = 12$

<table>
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<th>Spins $(S_p, S_n, S)$</th>
<th>(0\hbar\Omega)</th>
<th>(2\hbar\Omega)</th>
<th>(4\hbar\Omega)</th>
<th>(6\hbar\Omega)</th>
<th>(8\hbar\Omega)</th>
<th>(10\hbar\Omega)</th>
<th>(12\hbar\Omega)</th>
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*N\hbar\Omega* space: direct sum of subspaces [●] of states carrying the same \((\lambda\ \mu)\) and \(S_p S_n S\)

- **Symmetry-Adapted Truncation Scheme**

  1. maximal number of total HO quanta \(N_{\text{max}}\)
  2. intrinsic spins \(S_p S_n S\)
  3. deformations \((\lambda\ \mu)\)
$^6$Li - coherent structure of $T=0$ states
SA-NCSM on BlueWaters: reaching towards medium mass nuclei

**Excitation Spectrum**

$^{20}\text{Ne}$

- $6^+ 0$: 8.778, 8.621
- $4^+ 0$: 4.248, 4.175
- $2^+ 0$: 1.634, 1.582
- $0^+ 0$: 0.000, 0.000

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<th>$E_x$ [MeV]</th>
<th>Exp</th>
<th>SA-NCSM</th>
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**Nucleon Density**

Complete space: $4 \times 10^{12}$

Symmetry-adapted space: $1 \times 10^7$
SA-NCSM on BlueWaters: reaching towards medium mass nuclei

Novae and X-ray bursts

$^{23}\text{Al}(p, \gamma)^{24}\text{Si}$
Symmetry-Adapted No-Core Shell Model on Blue Waters

- Collective modes emerge from first principles
- Physically relevant model spaces for ab initio modeling of nuclear structure
- First applications of ab initio theory to open shell medium mass nuclei
Outcomes: Kjellrun Olson’s “List”

- **Key Challenges**: description of the science/engineering problem being addressed – Nature of Matter; nuclei account for 99.9% of the mass in universe

- **Why it Matters**: description of the potential impact of solving this research problem – Ultimate source of energy in universe – Quarks to Cosmos concept

- **Why Blue Waters**: explanation of why you need the unique scale and attributes of Blue Waters to address these challenges – good balance of node count, cpu power, and memory plus CPU utilization available for development work

- **Accomplishments**: explanation of results you obtained – Many papers in top journals, plus pushing beyond the reach of other competitive theories

- **Blue Waters team contributions**: explanation of how the Blue Waters team contributed to your research – Excellent support and guidance as needed

- **Broader Impact**: description of the broader impact that resulted from your work on Blue Waters – Training next generation STEAM workforce

- **Shared Data**: description of the data shared with others as well as the method of sharing – Everything is publically available, even codes

- **Products**: description of the products (e.g. software) that were created as a part of or as a result of your Blue Waters project – Next generation NCSM: SA-NCSM

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**To Date**: 1,127,929 node hours from start 04/02/2013 forward. Of our current March 10, 2015 allocation of 600,000 node hour, we have used 47,284. PRAC proposal in the works.