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

LOUISIANA STATE UNIVERSITY

Tomáš Dytrych, Jerry P. Draayer, Kristina D. Launey

TEAM — Postdocs & Students — WORK

Daniel Langr (Czech Tech U, Prague) & Alison C. Dreyfuss (Keene State U)
Robert Baker (Austin Peay Statue U), David Kekejian (Armenia), Grigor Sargsyan (Armenia)

NSF PetaApps & DOE EPSCoR Supported Collaboration

Other PIs: James P. Vary (Iowa State) and Umit V. Catalyurek (Ohio State)

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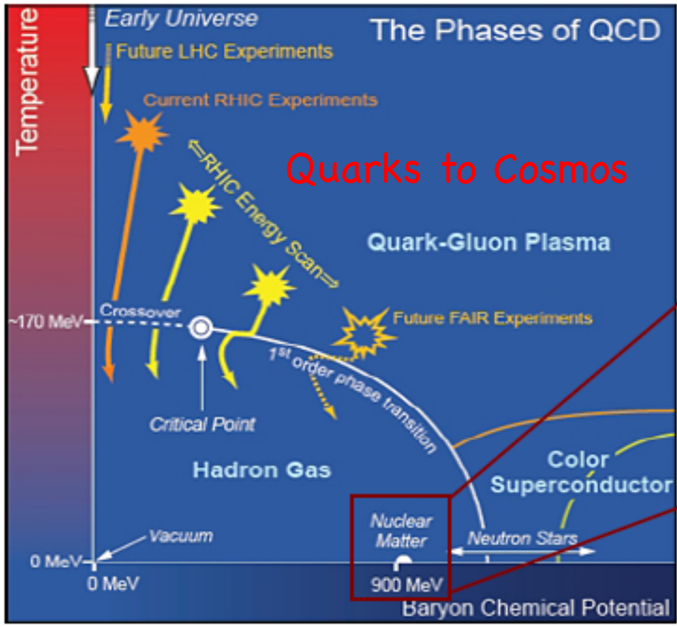
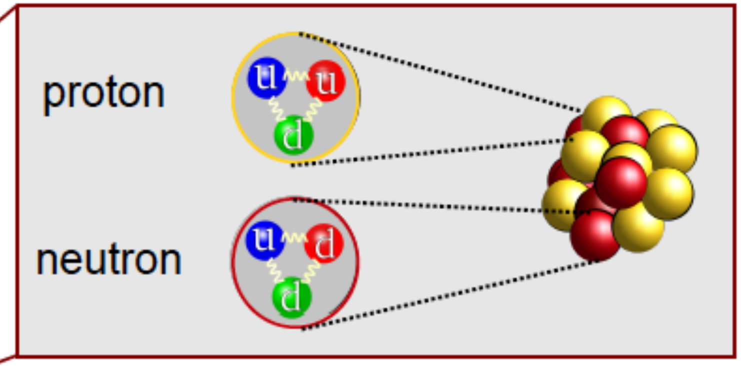
Sunriver Resort, Sunriver, Oregon May 10-13, 2015

# Physics of Atomic Nuclei




## Nuclear interactions

- Residual strong force → highly complex
- two-, three- and four-body forces

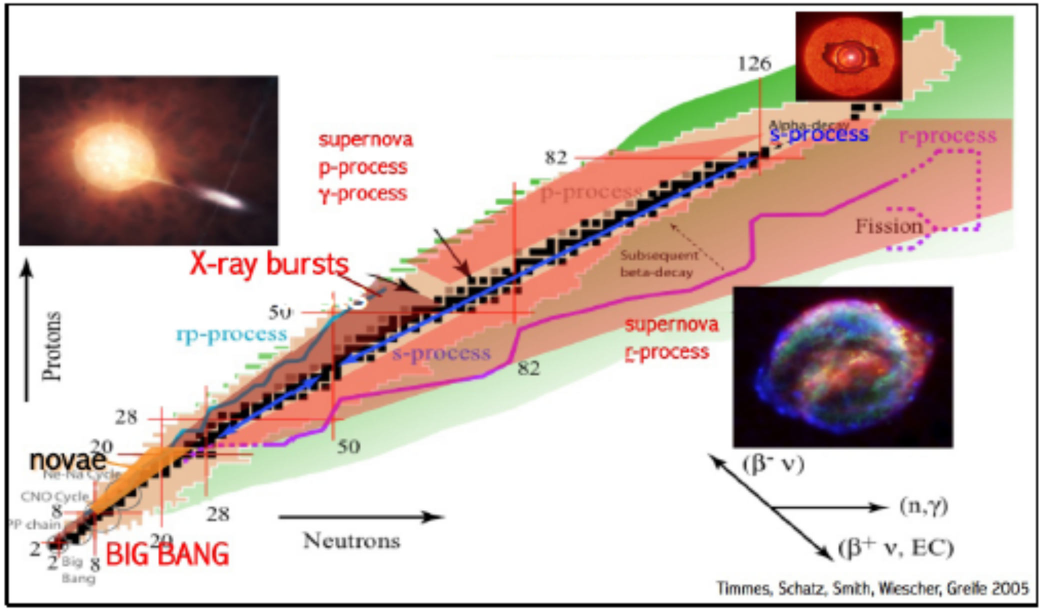
## Discovery potential in nuclear physics

- 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

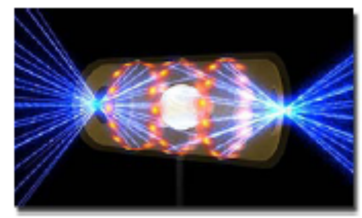
# Applications of Nuclear Structure & Reaction Modeling

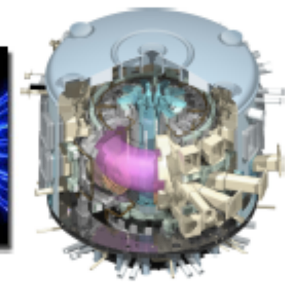
## Astrophysics: thermonuclear processes in the cosmos



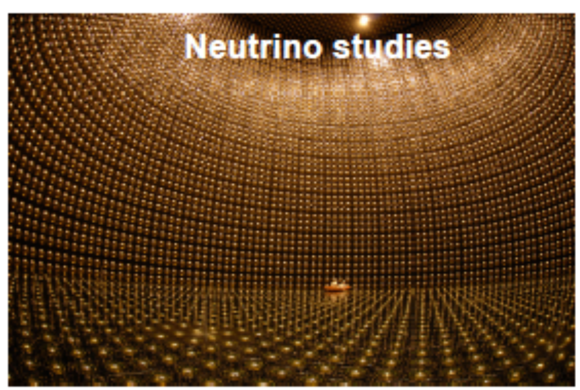

### NIF @ LLNL

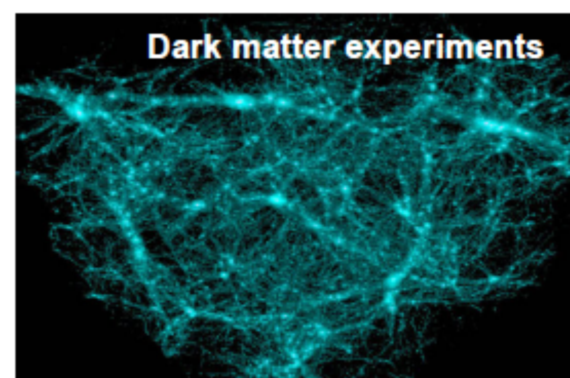
### Nuclear reactions for applied energy studies





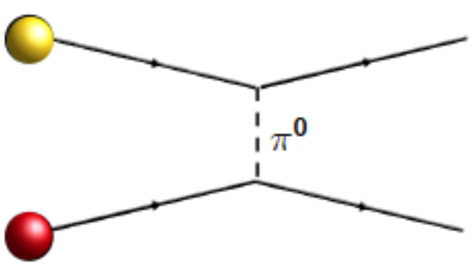
## Neutrino & Cosmology research

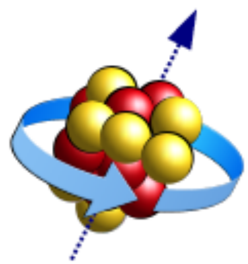
# *Ab initio* Approaches to Nuclear Structure and Reactions

**Strong interaction**



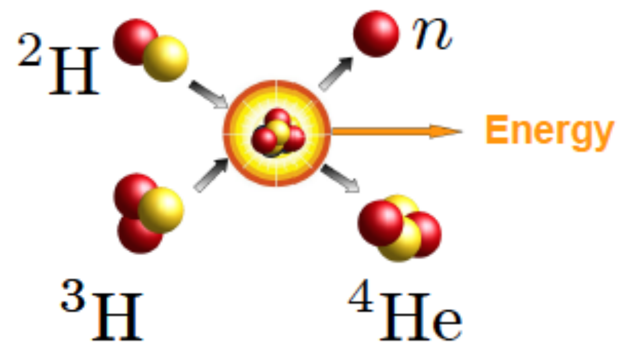

- Realistic nuclear potential models

**Many-body dynamics**



- wave functions nuclear properties

**Nuclear reactions**



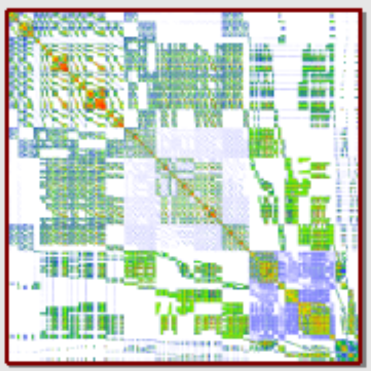

- reaction rates cross sections

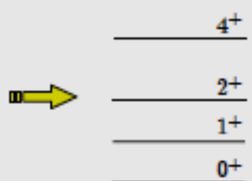
# *Ab Initio* No-Core Shell Model

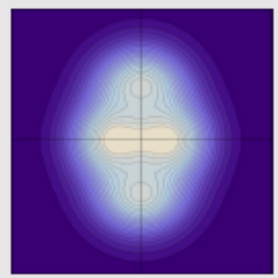
- **Goal:** Solve the non-relativistic quantum problem of A-interacting nucleons

$$\hat{H}|\psi_i\rangle = E_i|\psi_i\rangle \qquad \hat{H} = T + V_{\mathrm{Coul}} + V_{NN} + \dots$$

1. Choose **physically relevant** model space and construct its basis $\{|\phi_1\rangle, \dots, |\phi_d\rangle\}$
2. Compute Hamiltonian matrix $H_{ij} = \langle\phi_i|\hat{H}|\phi_j\rangle$
3. Find lowest-lying eigenvalues and eigenvectors [Lanczos algorithm]



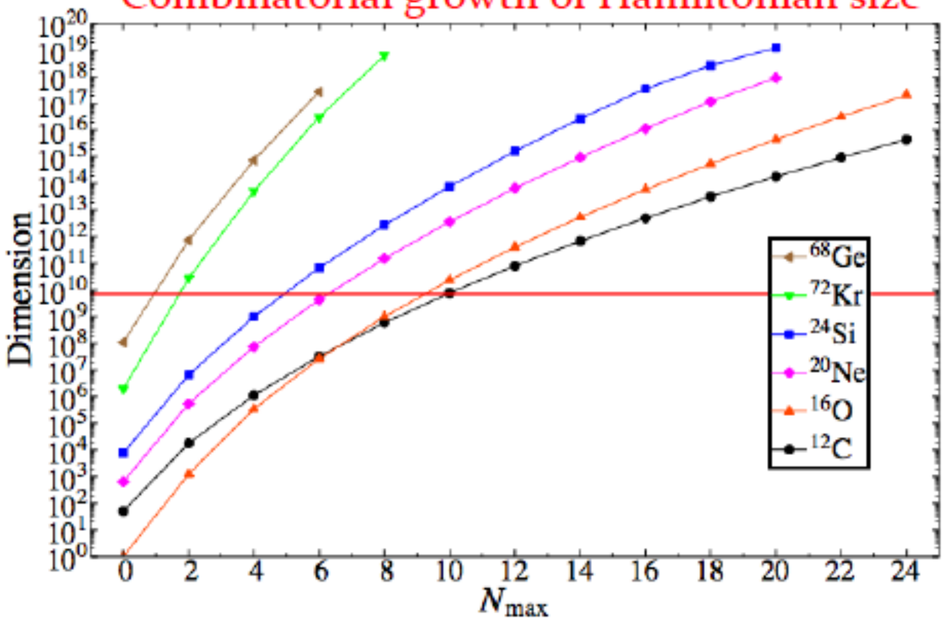


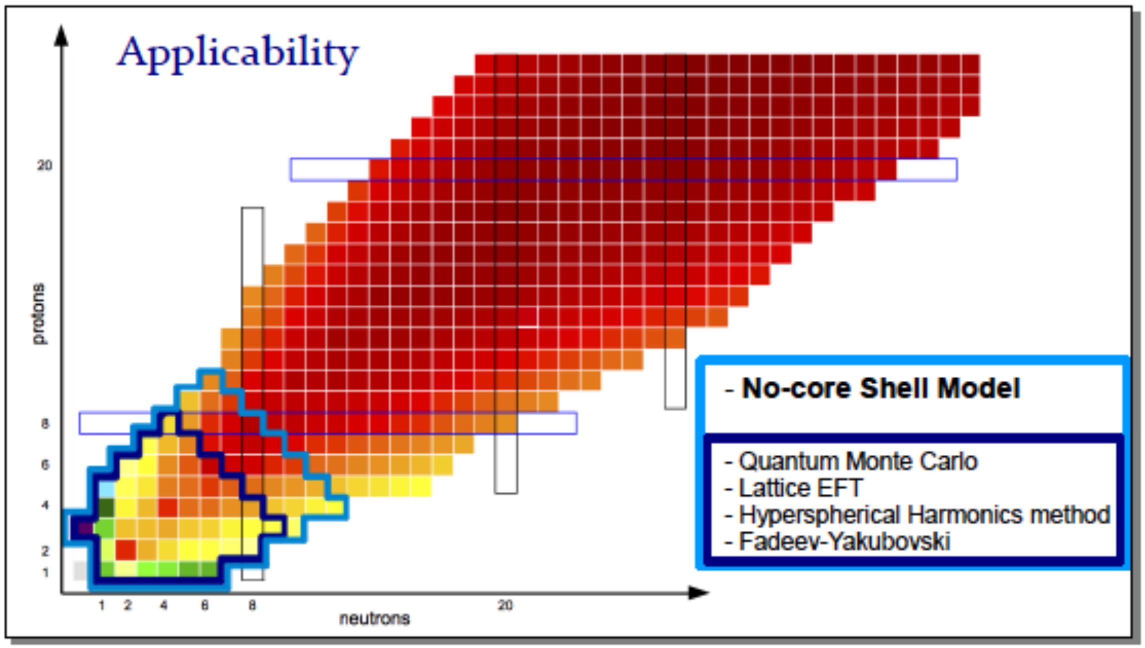



- **Resulting wave functions:**
  - obey Pauli exclusion principle
  - exact separation between intrinsic and center-of-mass motion

# Computational Challenge: Scale Explosion

Combinatorial growth of Hamiltonian size



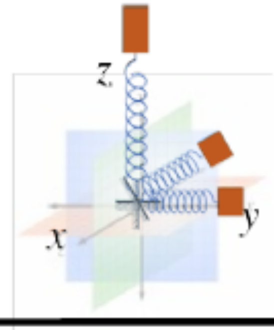
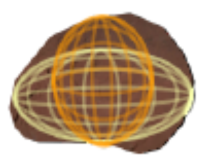
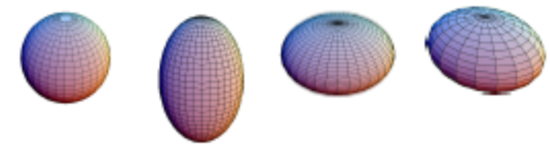




## Computational Scale Explosion

- Applicability limited to light nuclei
- Memory bound

# 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)  | $(\lambda\, \mu)$ |   |
| rotation | SO(3)  | $L$ | |

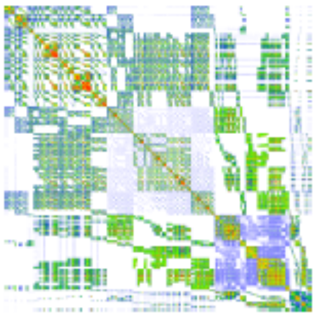
- **Three pillars of Symmetry-Adapted No-Core Shell Model**
  - Computational group theory
  - Nuclear physics
  - High performance computing

# MPI/OpenMP Implementation of Symmetry-Adapted No-Core Shell Model

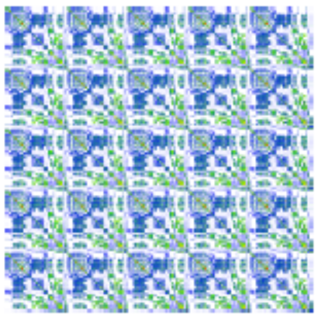
## Computational effort

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

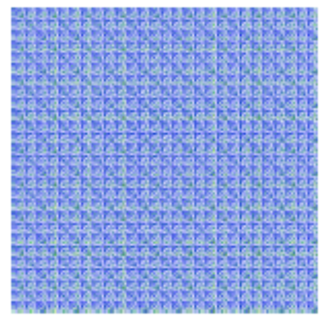
## Load balanced computations



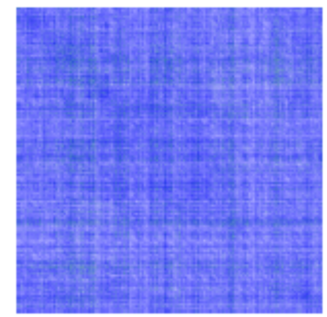
1 process



15 processes

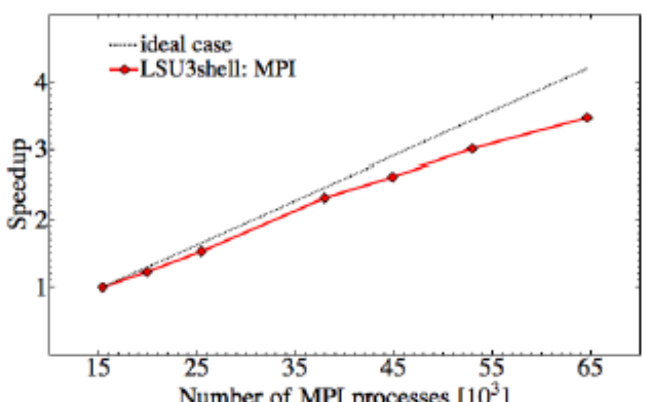


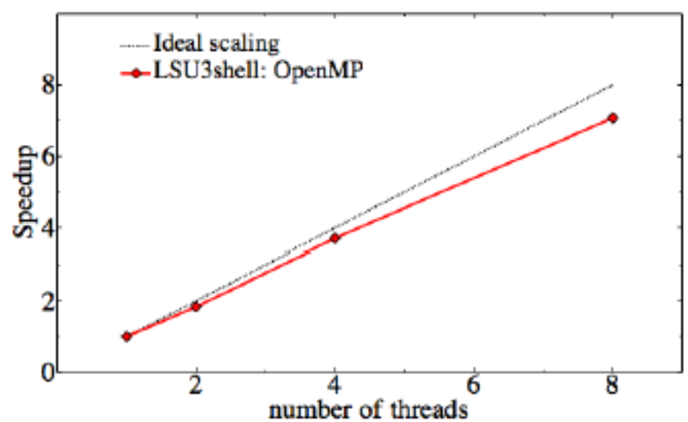
378 processes



37,950 processes

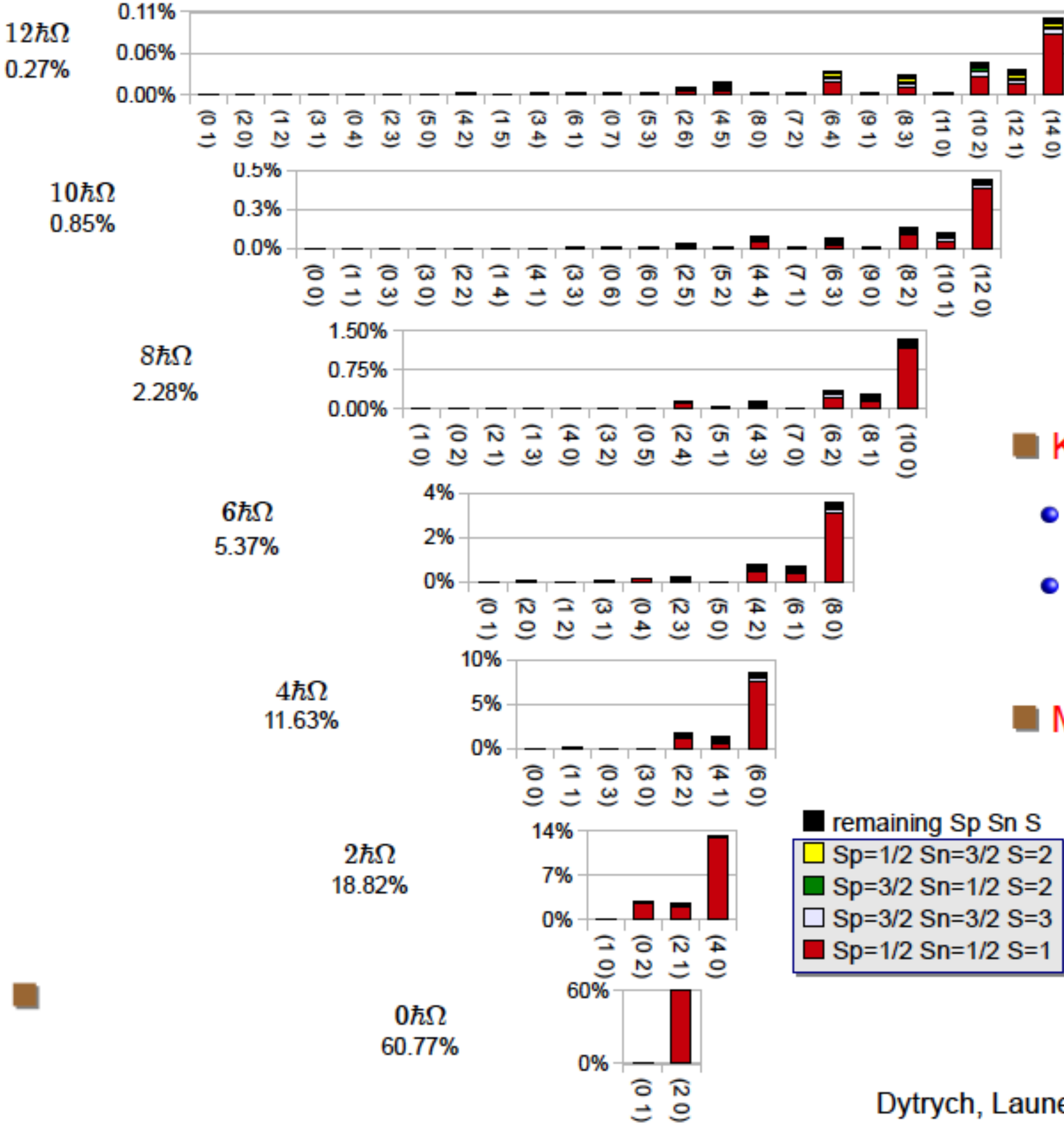
## Excellent scalability



# Discovery: Emergence of Simple Patterns in Complex Nuclei

$^{6}\mathrm{Li} : 1^{+}_{gs}$

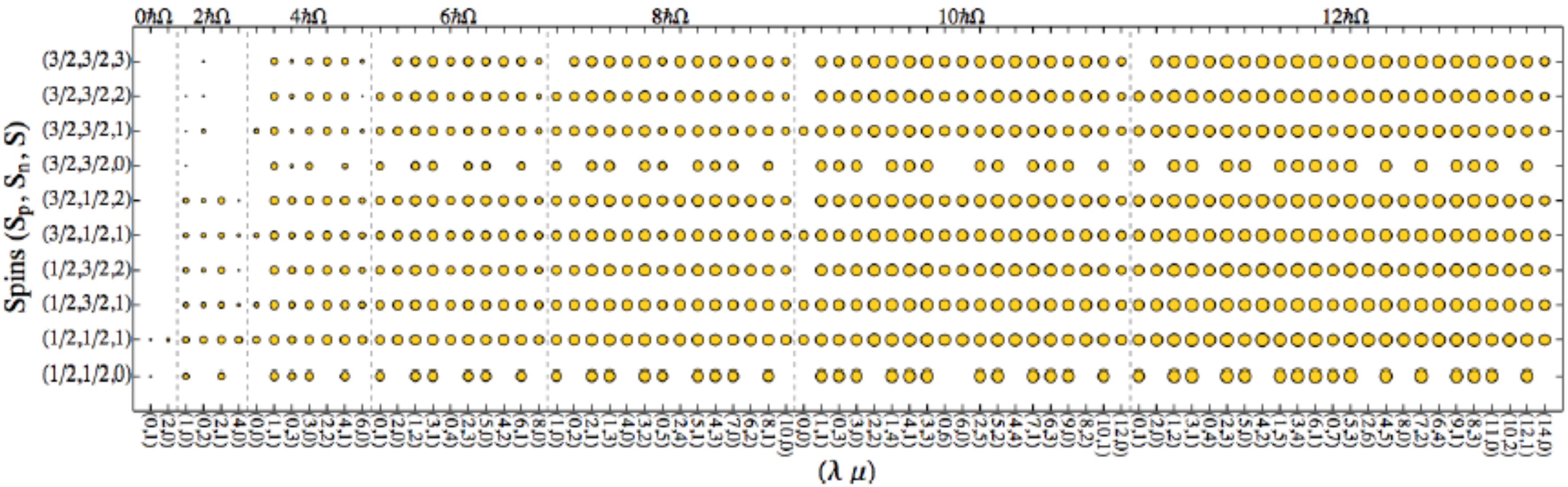



- Key features of nuclear structure
  - Low spin
  - Large deformation
- Model space truncation

Dytrych, Launey, Draayer, et al., PRL 111 (2013) 252501

# Model Space

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




$N\hbar\Omega$ space: direct sum of subspaces [○] of states carrying the same $(\lambda\ \mu)$ and $S_pS_nS$

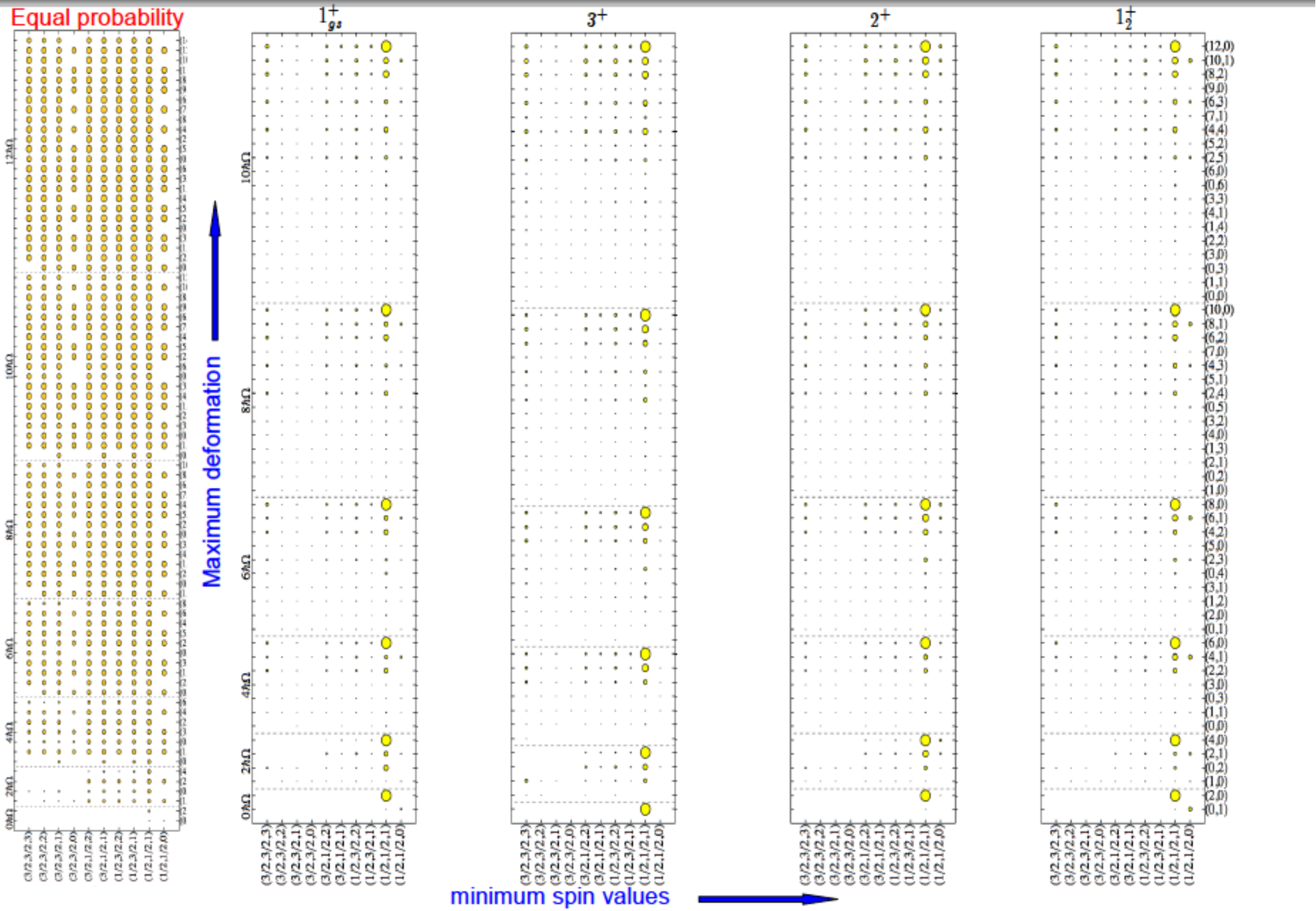
## Symmetry-Adapted Truncation Scheme

(1) maximal number of total HO quanta Nmax

(2) intrinsic spins $S_p\,S_n\,S$

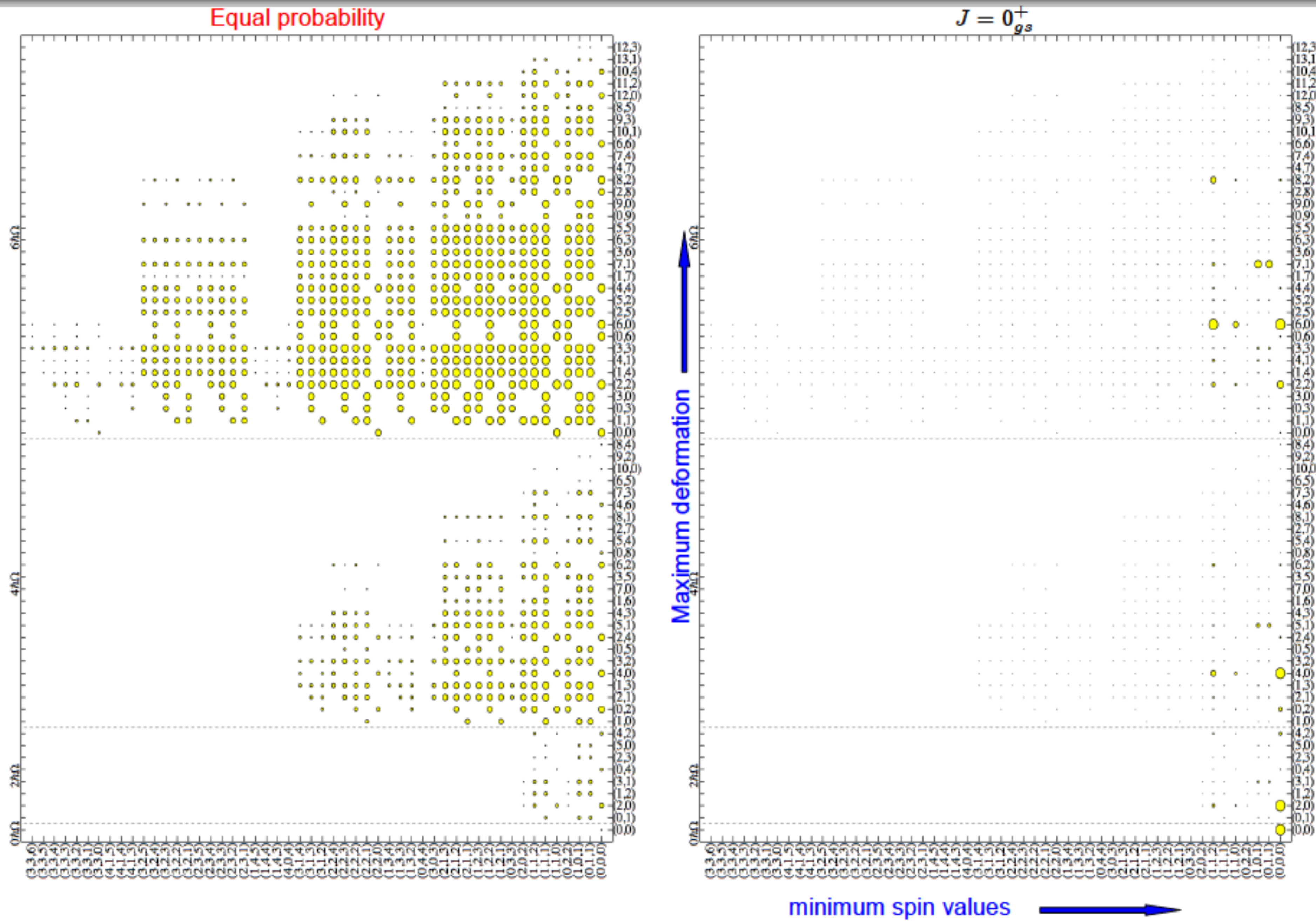
(3) deformations $(\lambda\ \mu)$

# $^{6}Li$ - coherent structure of T=0 states



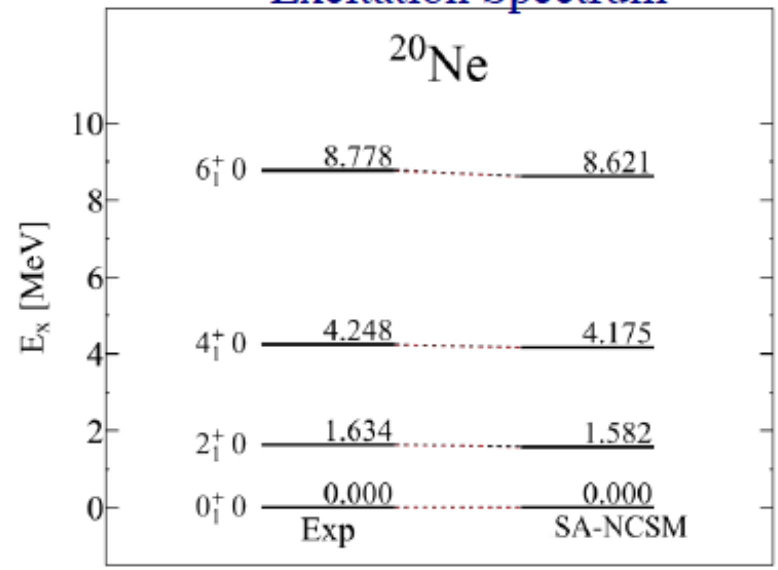
# $^{16}O$

Equal probability — $J = 0^+_{gs}$

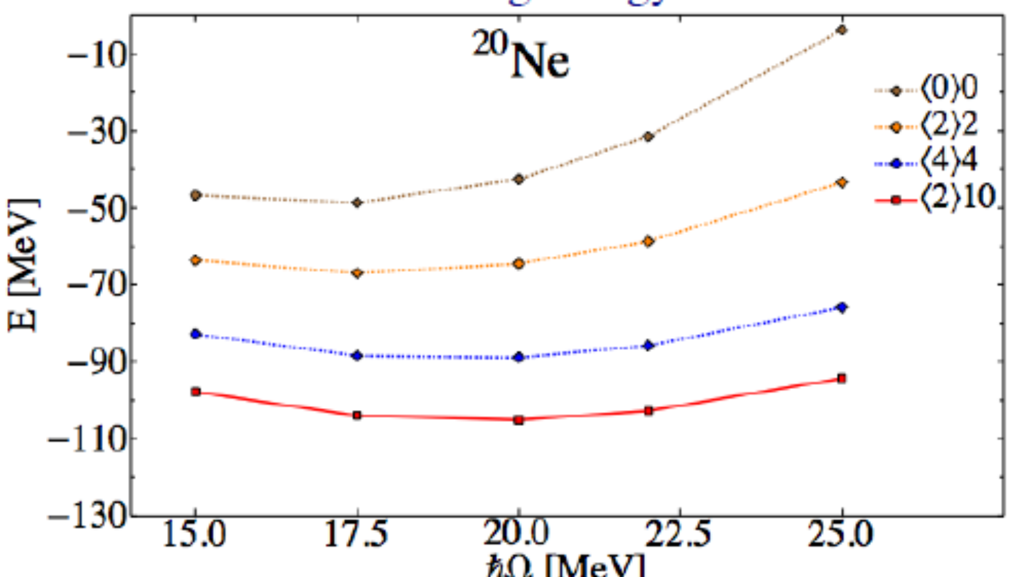


# SA-NCSM on BlueWaters: reaching towards medium mass nuclei

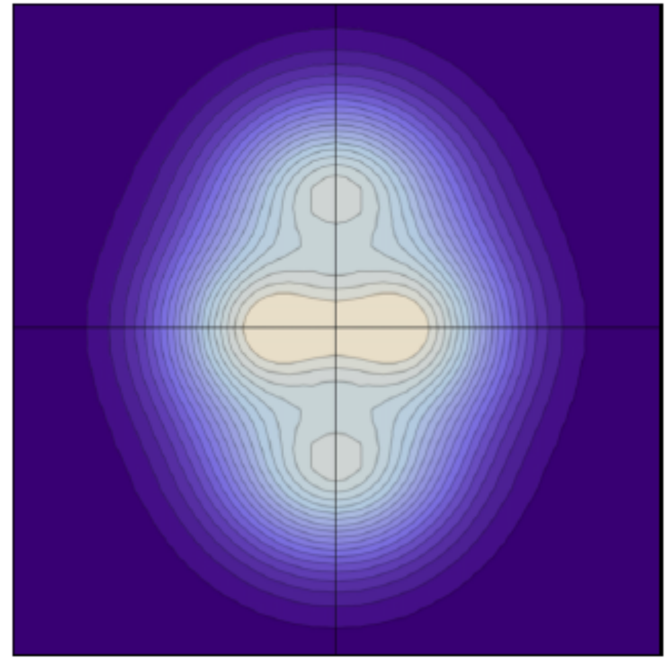
## Excitation Spectrum




## Binding energy



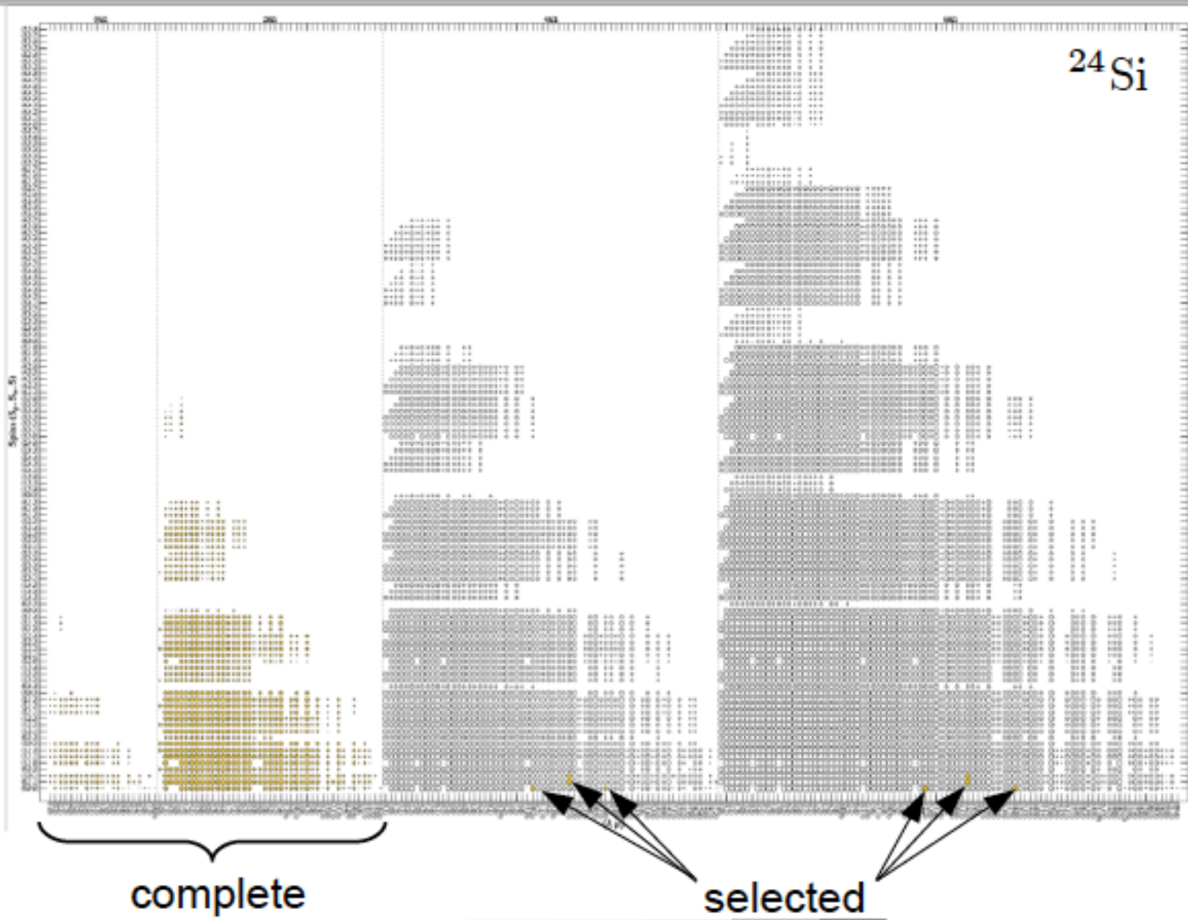

## Nucleon Density



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

Symmetry-adapted space: $1 \times 10^{7}$

# SA-NCSM on BlueWaters: reaching towards medium mass nuclei

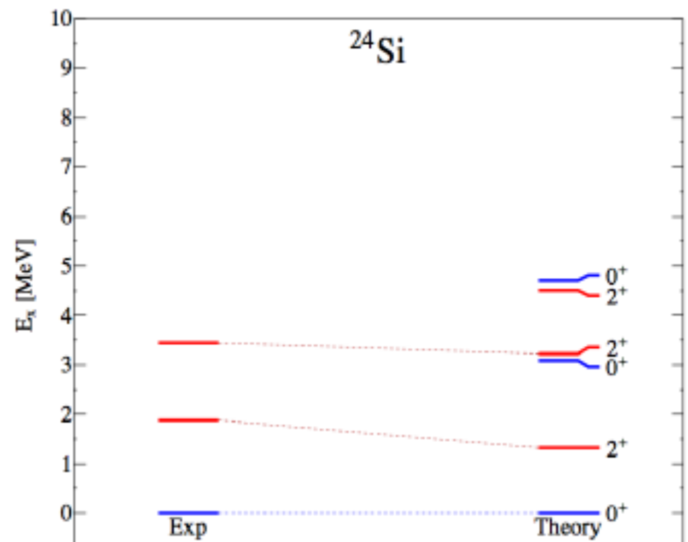



dimension: $3 \times 10^6$

Complete space dimension: $7 \times 10^{10}$

Novae and X-ray bursts

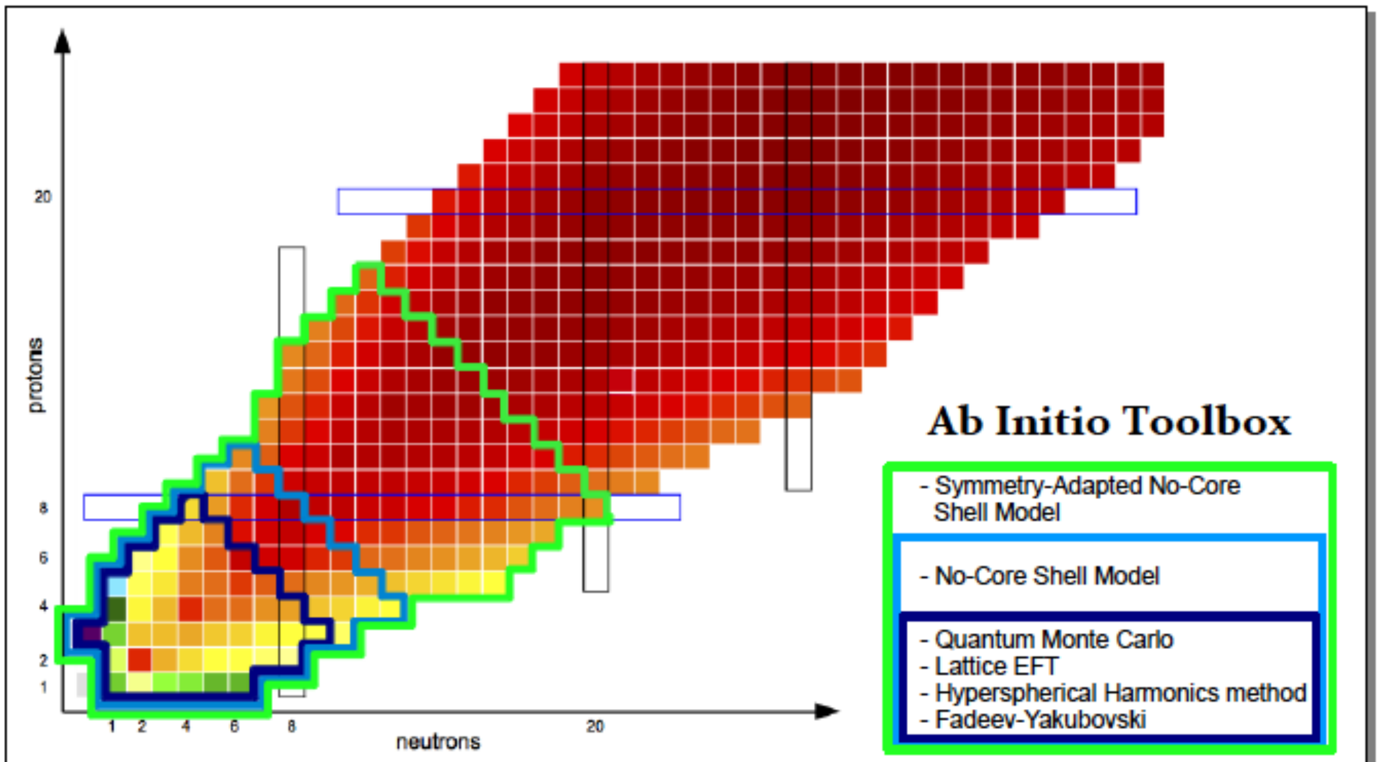
$^{23}\mathrm{Al}(p, \gamma)^{24}\mathrm{Si}$



# Summary

## 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

**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.**