Advancing first-principle symmetry-guided nuclear modeling for studies of nucleosynthesis and fundamental symmetries in nature

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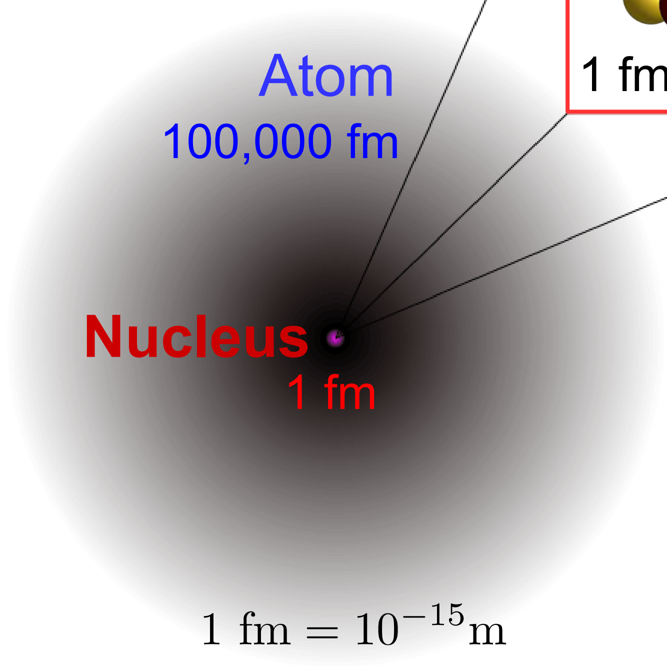
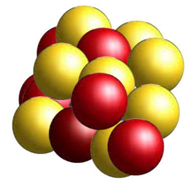
NCSA Blue Waters Symposium for Petascale Science and Beyond, 2019

Nuclear Physics

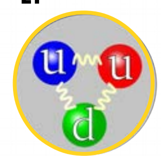


Nucleus

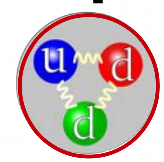


- extremely tiny compared to the size of the atom
- contains nearly all mass of the atom
- made up of protons and neutrons

nucleons [protons and neutrons] made up of quarks



proton



neutron

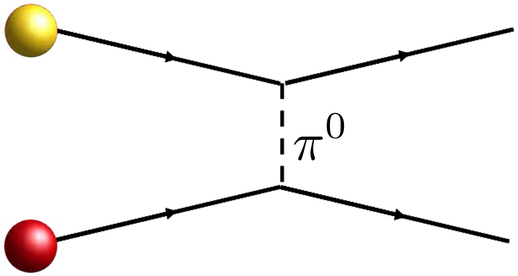
0.8 fm

Nuclear force holds nucleons together

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

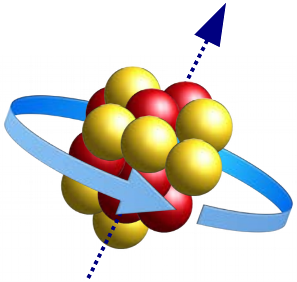
Ab initio Approaches to Nuclear Structure and Reactions

Nuclear interaction



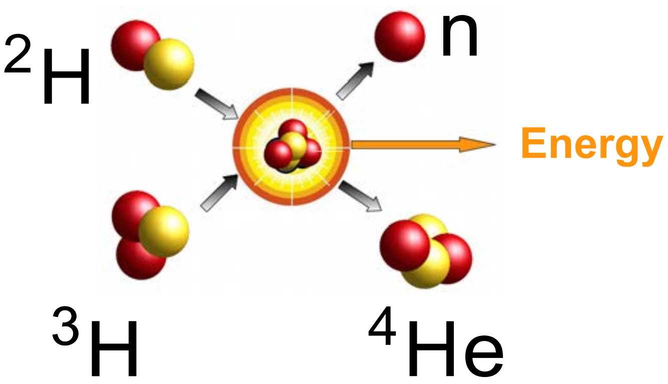
- Realistic nuclear potential models

Many-body dynamics



- wave functions nuclear properties

Nuclear reactions



- reaction rates cross sections

Solving Nuclear Problem

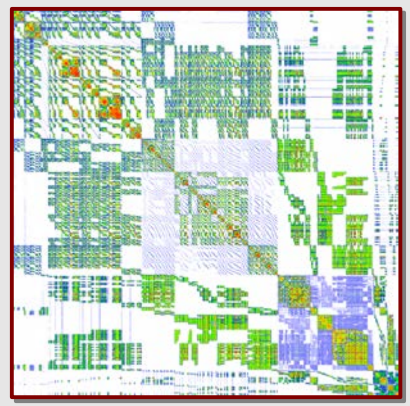
Fundamental task: solve the Schrodinger equation for a system of interacting nucleons

Input: Nuclear Hamiltonian – operator of energy $\hat{H} = \hat{T} + \hat{V}_{\text{Coul}} + \hat{V}_{NN} + \ldots$

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 $\hat{H}|\psi_i\rangle = E_i|\psi_i\rangle$

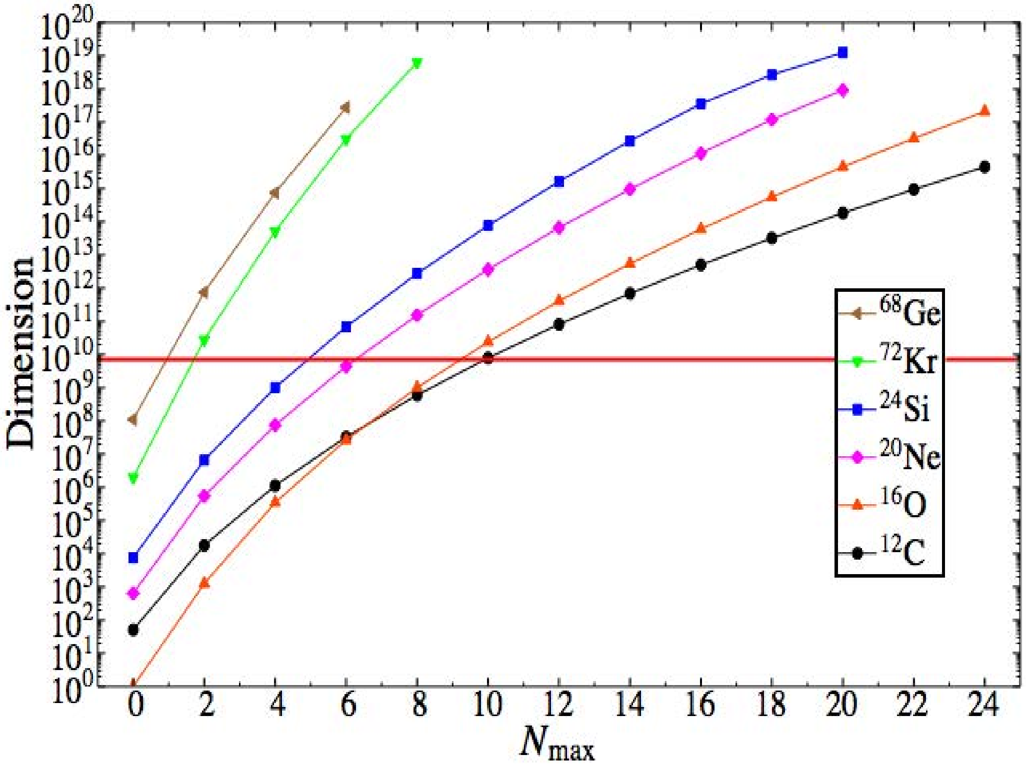
Lanczos algorithm

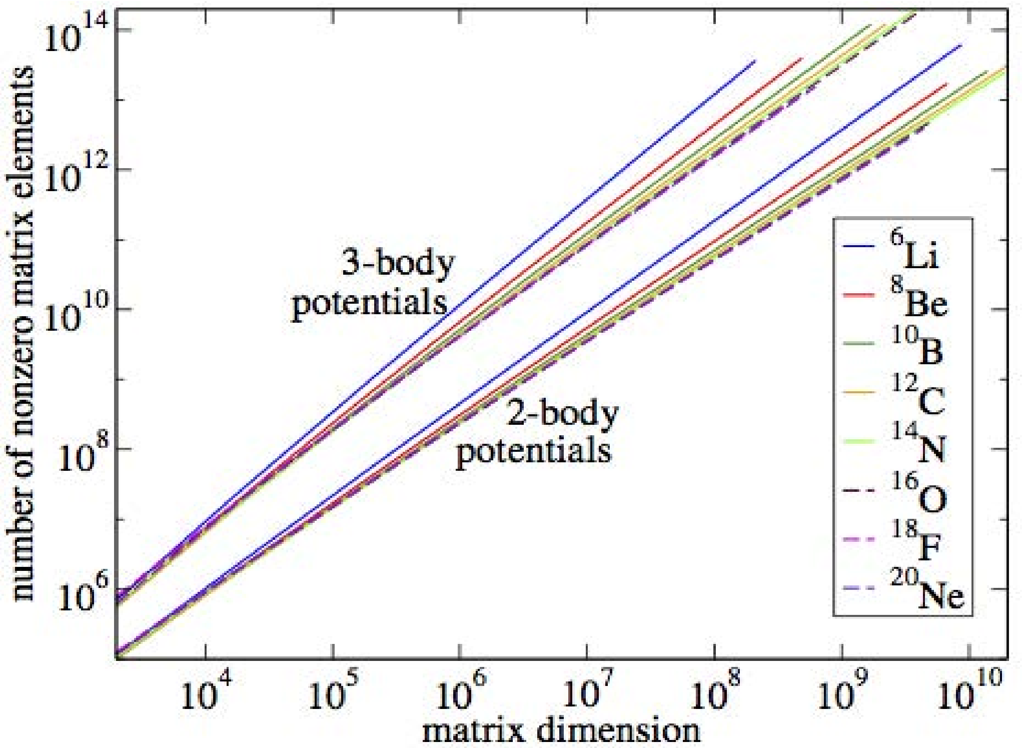
eigenvalues

$$|\psi_i\rangle = \sum_{j=1}^{d} c_j |\phi_j\rangle$$

eigenvectors

Key Challenge: Scale Explosion





[courtesy of Pieter Maris]

Computational Scale Explosion

- Limits application of ab initio studies to lightest nuclei

Why Blue Waters?

- Large aggregate memory and amount of memory per node (64GB)
- High peak memory bandwidth (102.4 GB/s)

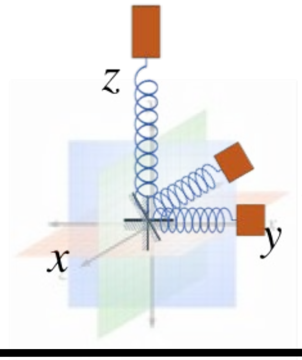
Why symmetry-adapted approach?

- Use partial symmetries of nuclear collective motion to adopt smaller physically relevant model spaces

Symmetry-Adapted No-Core Shell Model

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

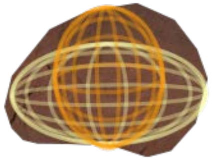
number of harmonic oscillator excitations



N

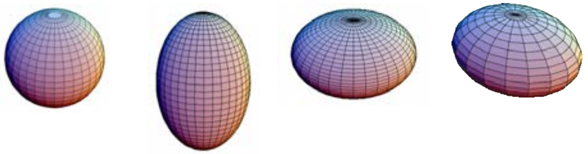
total proton, total neutron and total intrinsic spins S_p S_n S

deformation SU(3)



$(\lambda\,\mu)$

$(0\,0)$ $(\lambda\,0)$ $(0\,\mu)$ $(\lambda\,\mu)$



rotation SO(3)

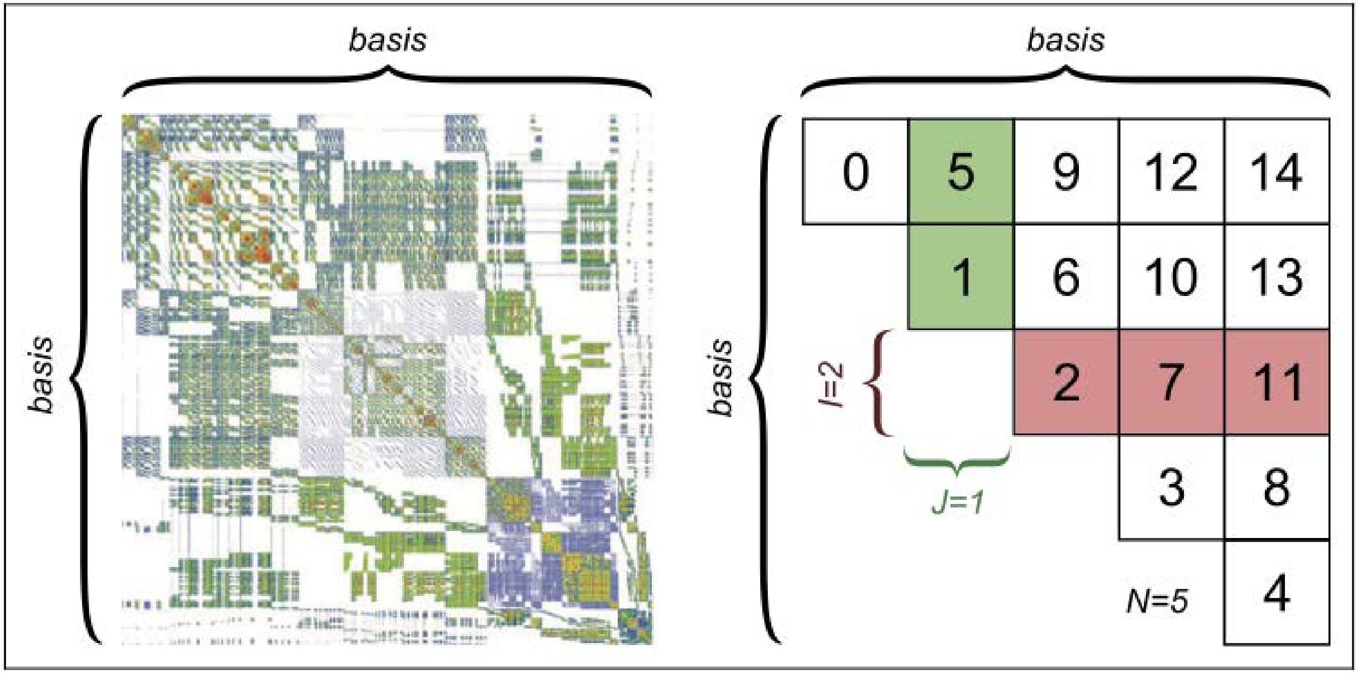
L

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

Implementation

- C++/Fortran code parallelized using hybrid MPI/OpenMP
- Open source: https://sourceforge.net/p/lsu3shell/home/Home/
- Computational effort: 90 % - computing matrix elements 10% - solving eigenvalue problem

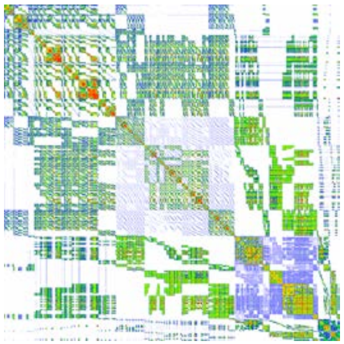
Mapping of Hamiltonian matrix to MPI processes



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

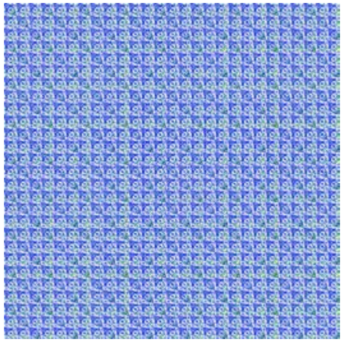
- Round-robin distribution of basis states among MPI processes

  Leads to load balanced computations

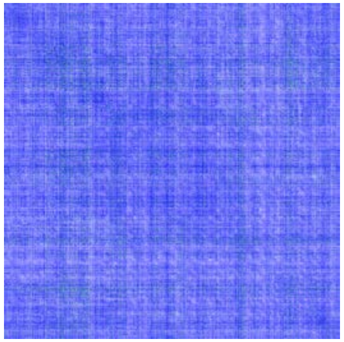


Original density structure of Hamiltonian matrix

15 processes

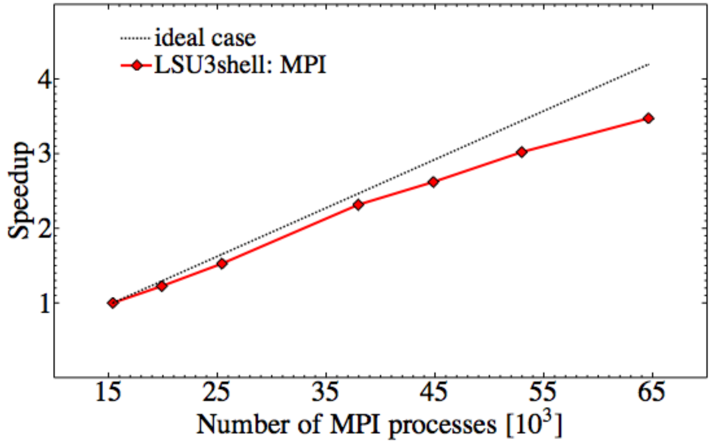


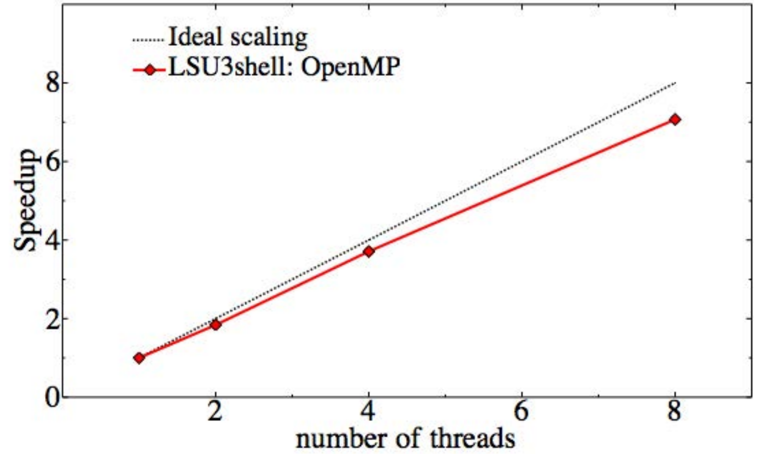
378 processes



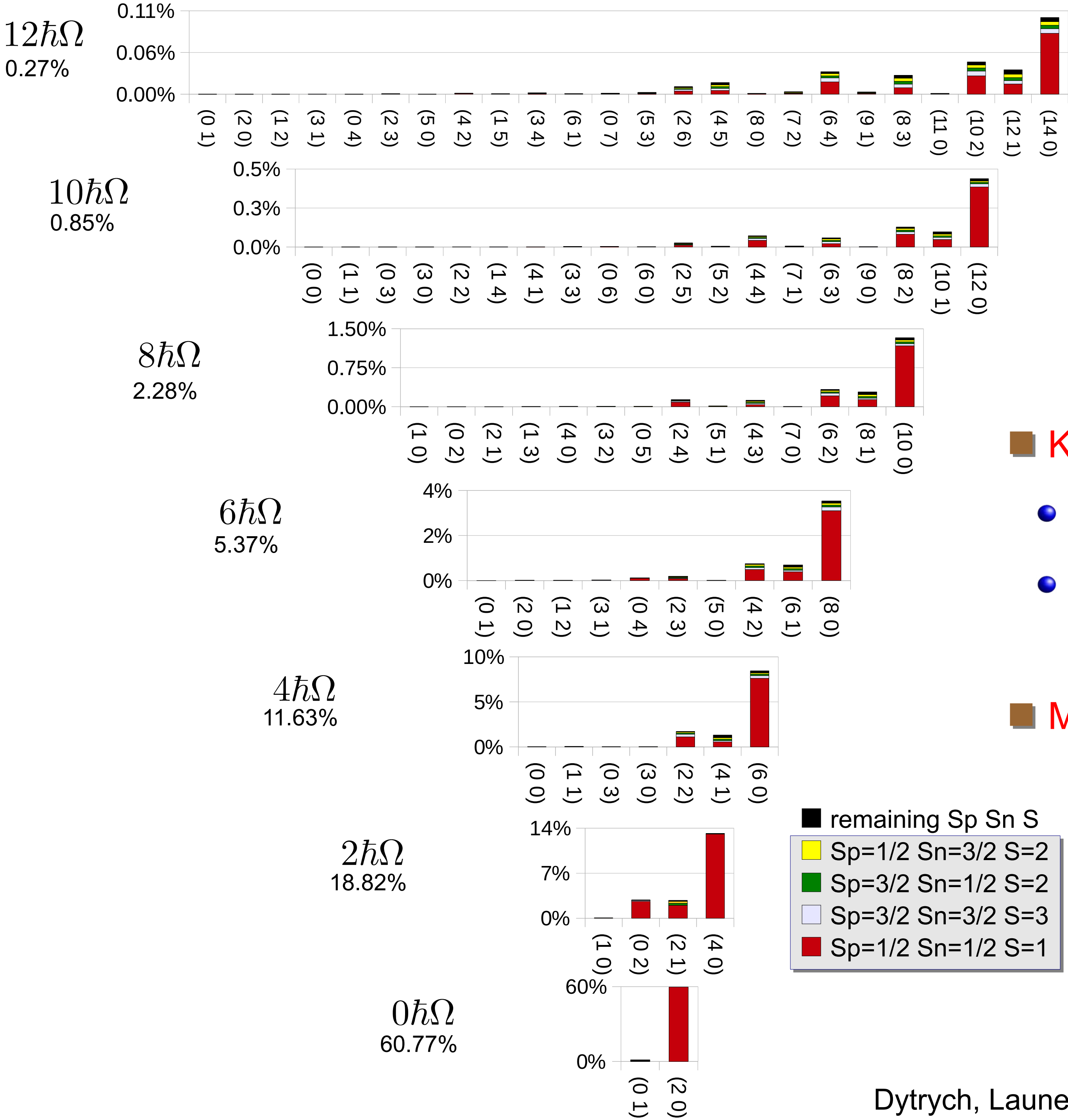
37,950 processes

- Excellent scalability





Discovery: Emergence of Simple Patterns in Complex Nuclei



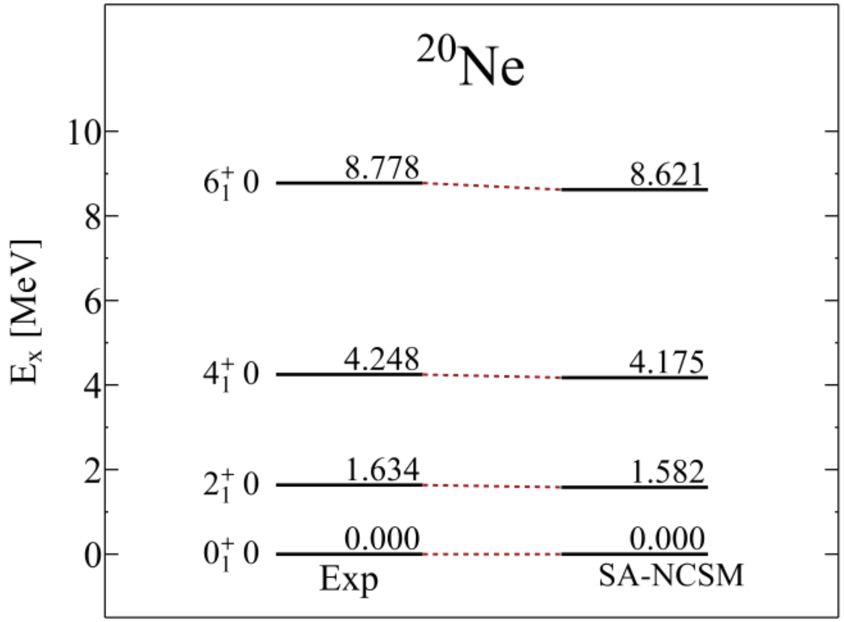
$^6Li : 1^+_{gs}$

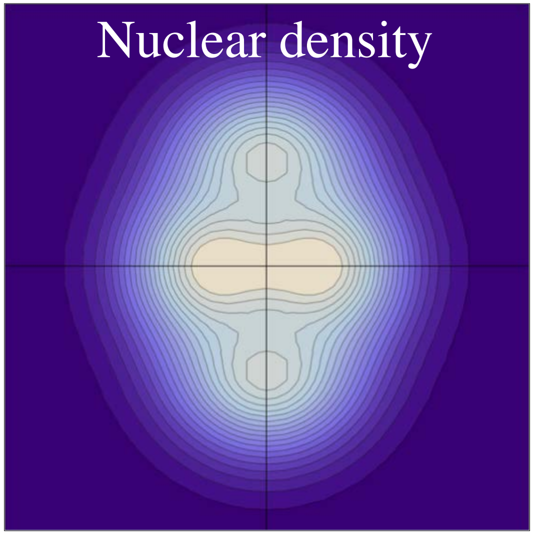
- **Key features of nuclear structure**
  - Low spin
  - Large deformation

- **Model space truncation**

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

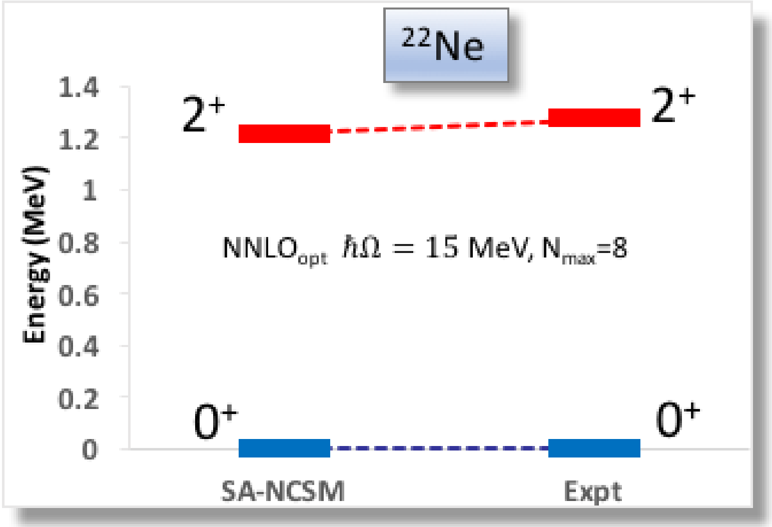
SA-NCSM on BlueWaters: reaching towards medium mass nuclei

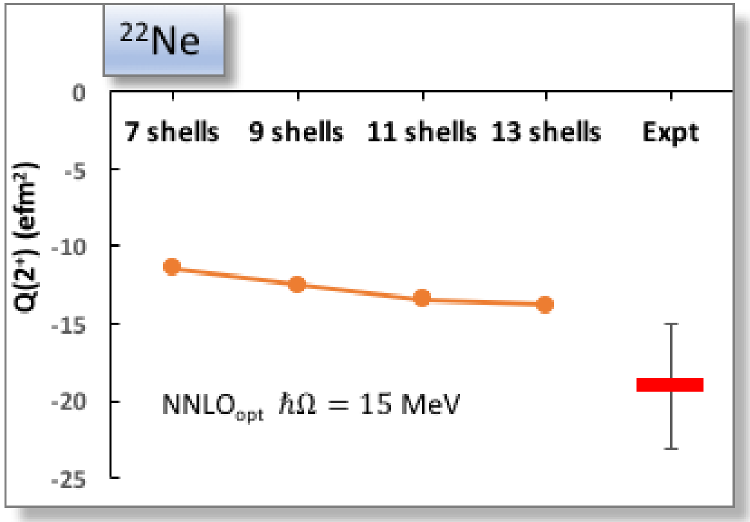




Complete space: 4×10^{12}

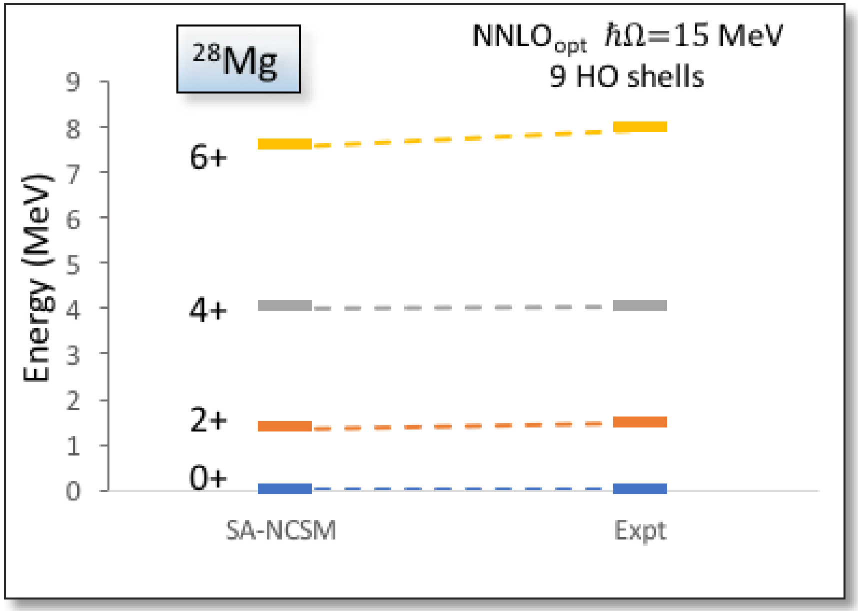
Symmetry-adapted space: 1×10^{7}





Quadrupole moment

SA-NCSM on BlueWaters: reaching towards medium mass nuclei



Complete space: $513, 747, 466, 539$

Symmetry-adapted space: $23, 127, 674$

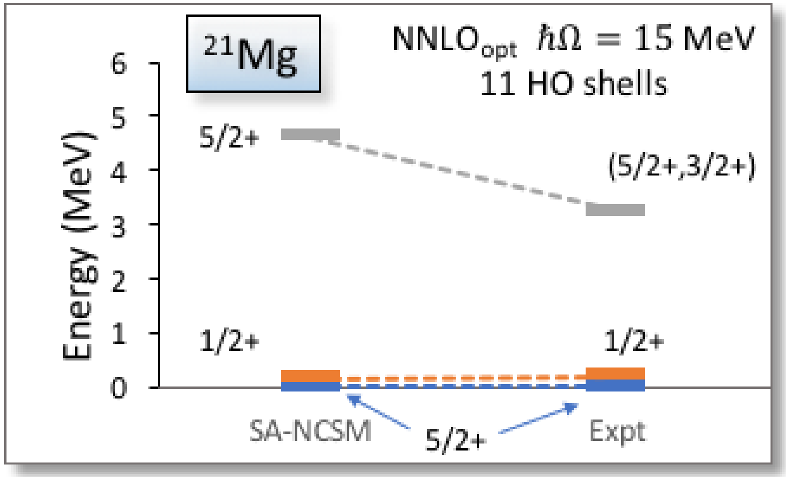
Number of BW nodes: 3335

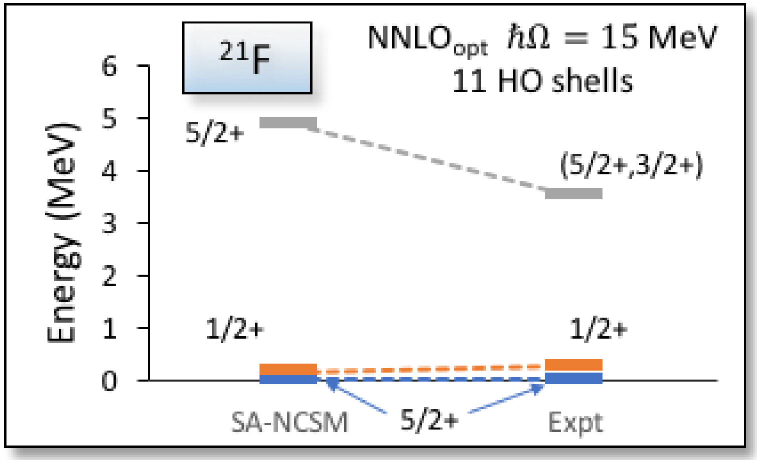
Size of Hamiltonian matrix: 20 TB

Performance on BW system

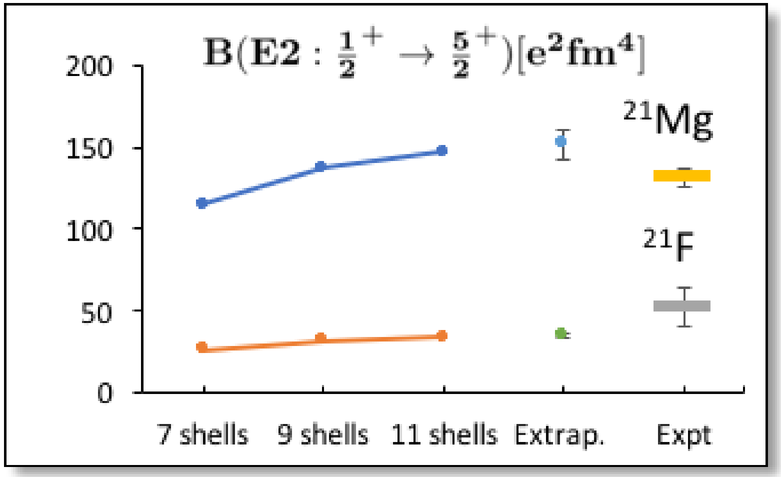
Basis construction:	10 s
Matrix calculation:	1518 s
Solving eigenproblem:	113 s
Total:	1641 s

SA-NCSM on BlueWaters: reaching towards medium mass nuclei

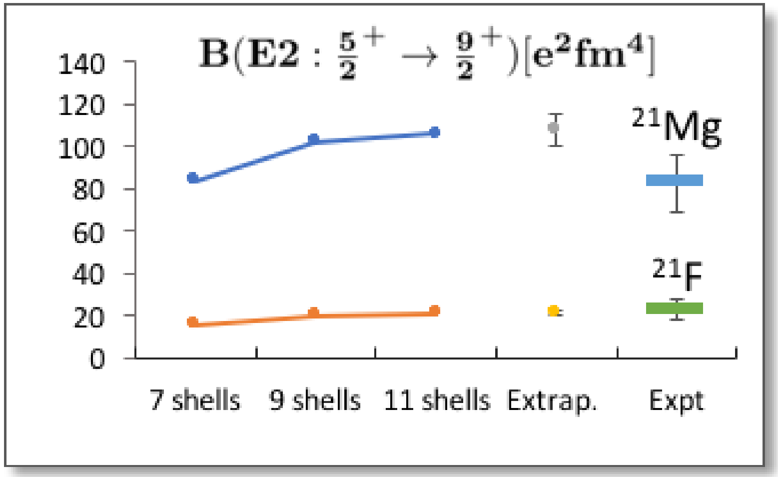




B(E2) transition strengths



B(E2) transition strengths



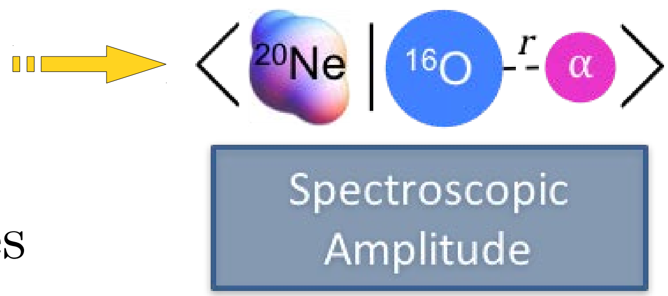
Ruotsalainen et al., PRC 99, 051301 (R) (2019)

Calculation of reaction rates

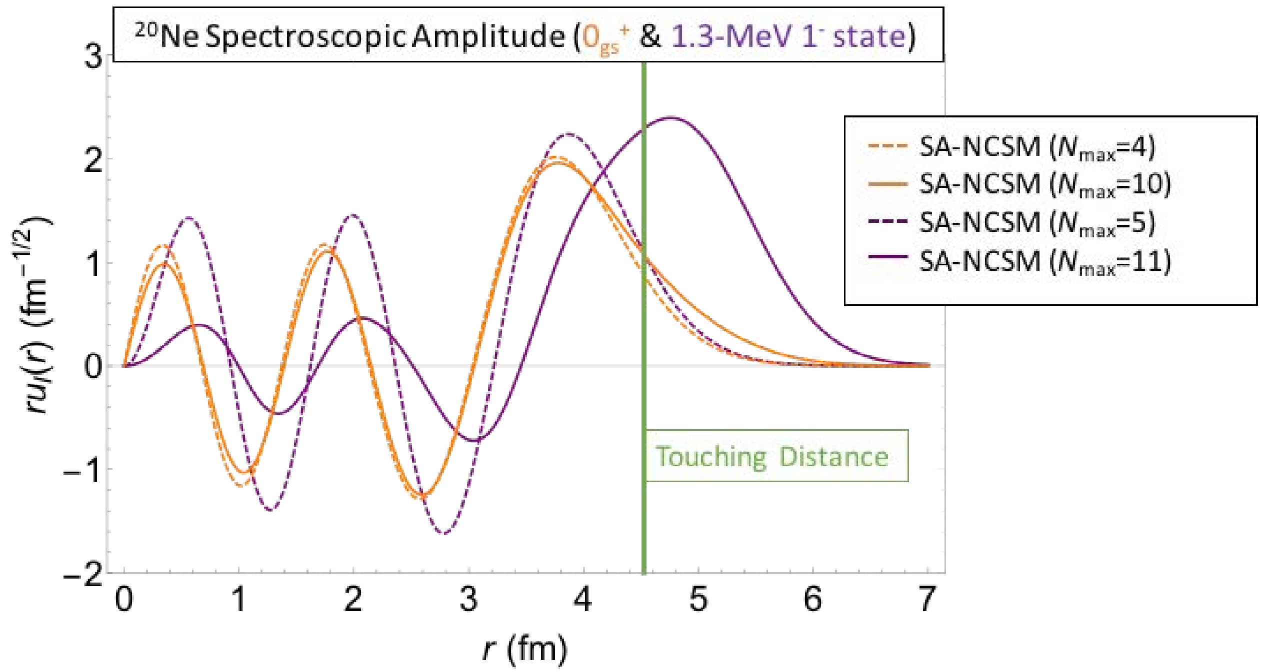
Nuclear reaction: $^{16}\mathrm{O}(\alpha,\gamma)^{20}\mathrm{Ne}$

SA-NCSM

$^{20}\mathrm{Ne} : 0^+_{gs},\ \ 1^-\mathrm{states}$



Probability to find cluster structure



Calculation of reaction rates

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Blue Waters

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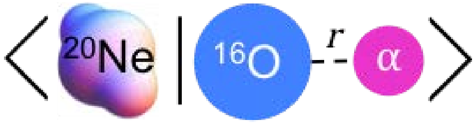
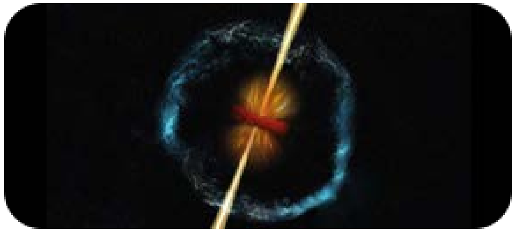


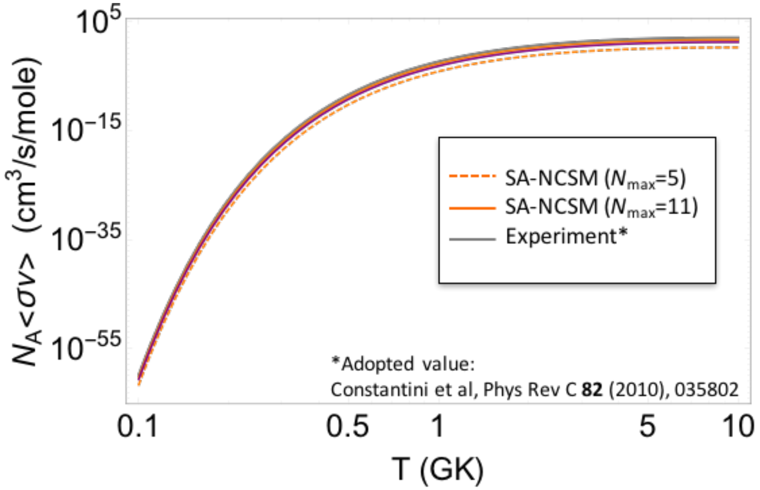
Spectroscopic Amplitude

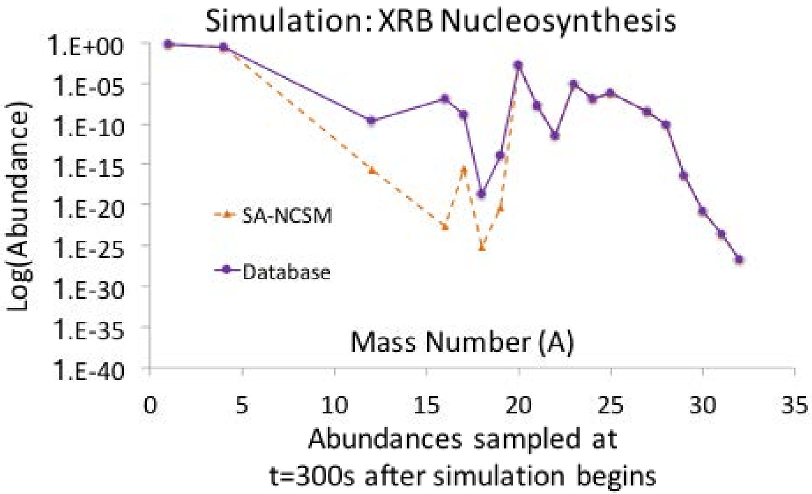
Probability to find cluster structure

Resonance Reaction Rate



astrophysical simulation





Response function

- Nucleus response to external probe (photon, neutrino, etc ..)

- New approach: SA-NCSM + Lorentz Integral Transform Method

SA-NCSM

$|\Psi_0\rangle$

calculate ground state wave function in *ab initio* SA-NCSM

→ $M_{00}, D_{1\mu}, Q_{2\mu}$

choose operator of interest

→ $|v_1\rangle = \dfrac{\hat{O}\,|\Psi_0\rangle}{\sqrt{\langle\Psi_0|\,\hat{O}^\dagger\hat{O}\,|\Psi_0\rangle}}$

construct pivot vector for Lanczos algorithm

↓

tridiagonalize Hamiltonian and construct LIT

SA-NCSM

$$L(E_x,\Gamma) = -\frac{1}{\Gamma}\mathrm{Im}\left[\frac{\langle\Psi_0|\,O^\dagger O\,|\Psi_0\rangle}{z-a_0-\frac{b_1^2}{z-a_1-\frac{b_2^2}{z-a_2-\dots}}}\right]$$

Energy Parameter

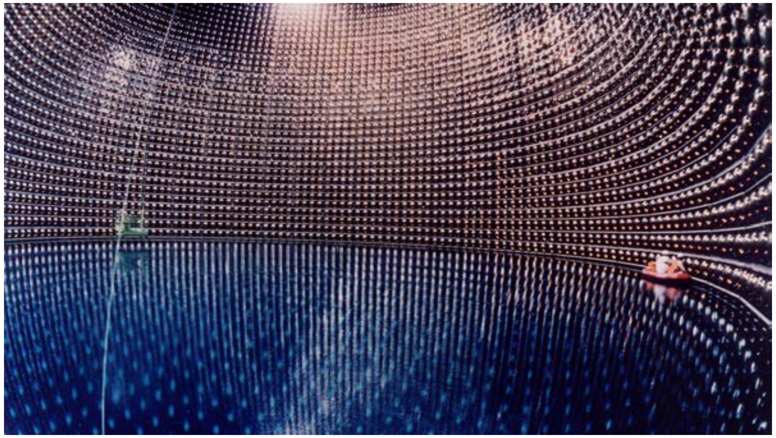
Lanczos coefficients

$$L(E_x,\Gamma) = \frac{\Gamma}{\pi}\int \mathrm{d}\omega\,\frac{R(\omega)}{(\omega - E_x)^2+\Gamma^2}$$

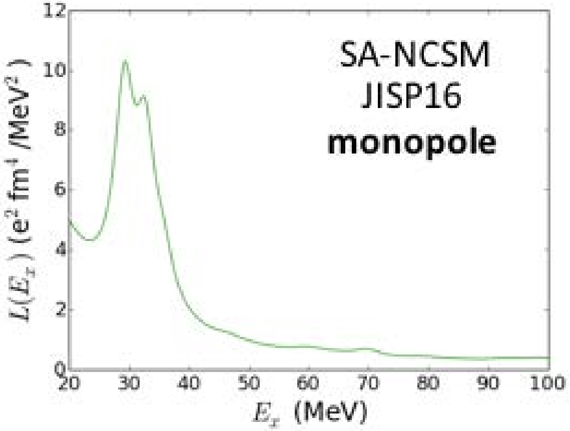
Response functions for neutrino studies

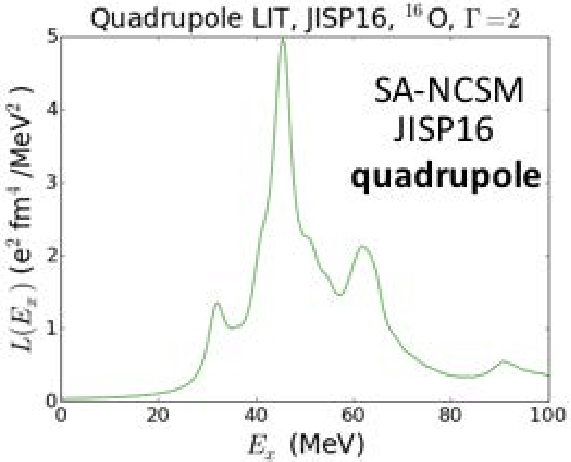
- Response functions – input for neutrino experiments
- Nuclear input - 2nd largest source of uncertainties

^{16}O : component of neutrino detectors



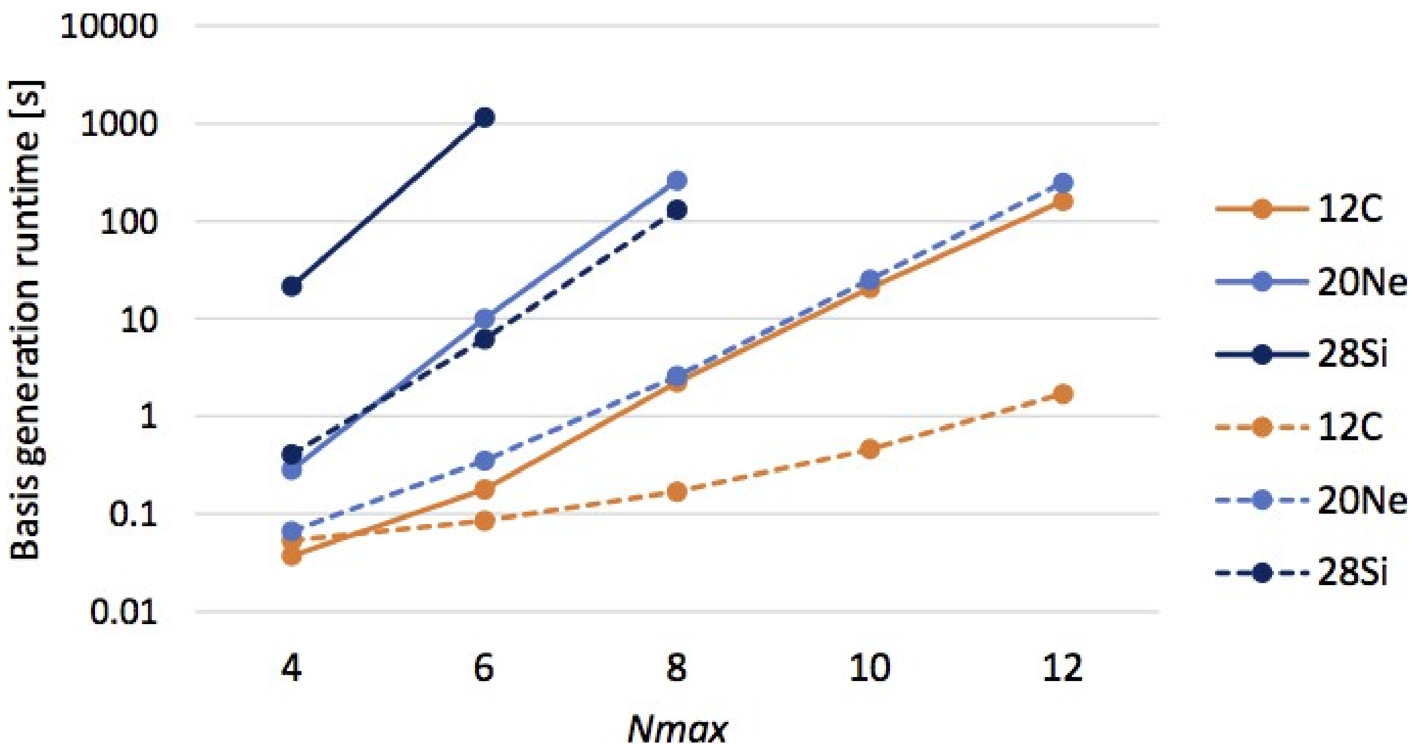
SA-NCSM + LIT: preliminary results





Accelerating basis construction algorithm

- Baseline implementation became bottleneck for heavier nuclei and large Nmax spaces

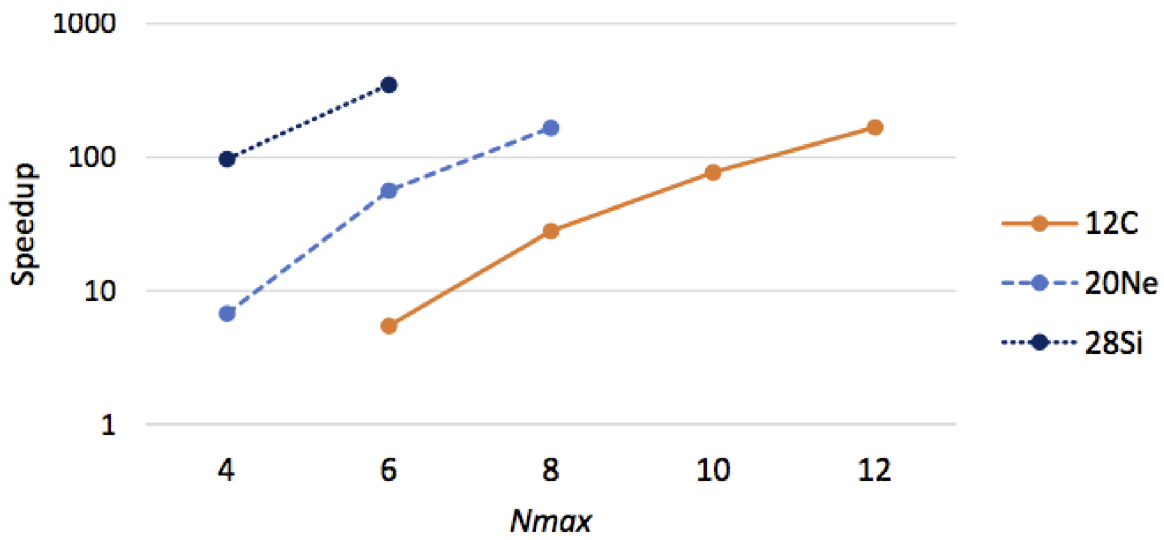


- Workaround: precompute basis segments; store on disk; read during initial step

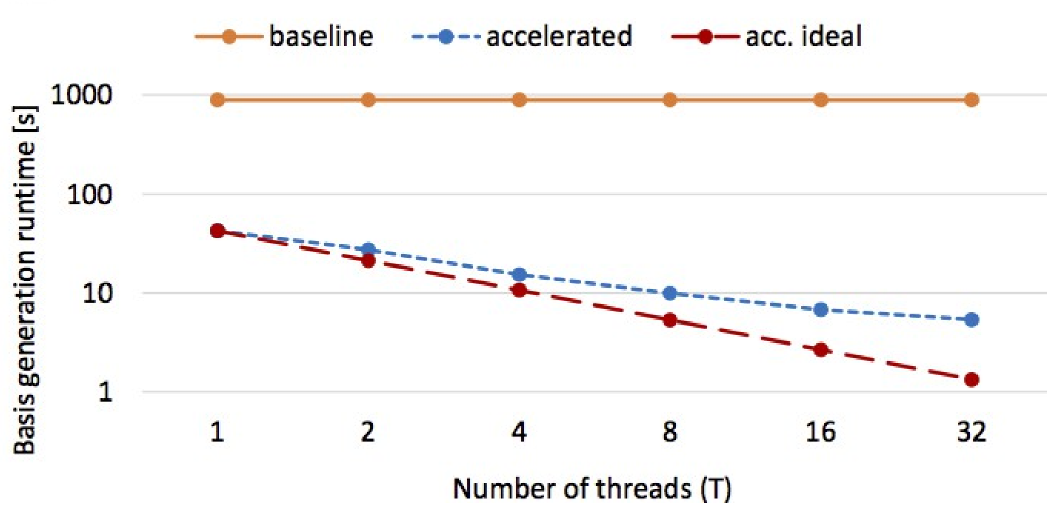
- Unable to utilize threads as the algorithm was inherently sequential

Accelerating basis construction algorithm

- New algorithm: two orders of magnitude speedup



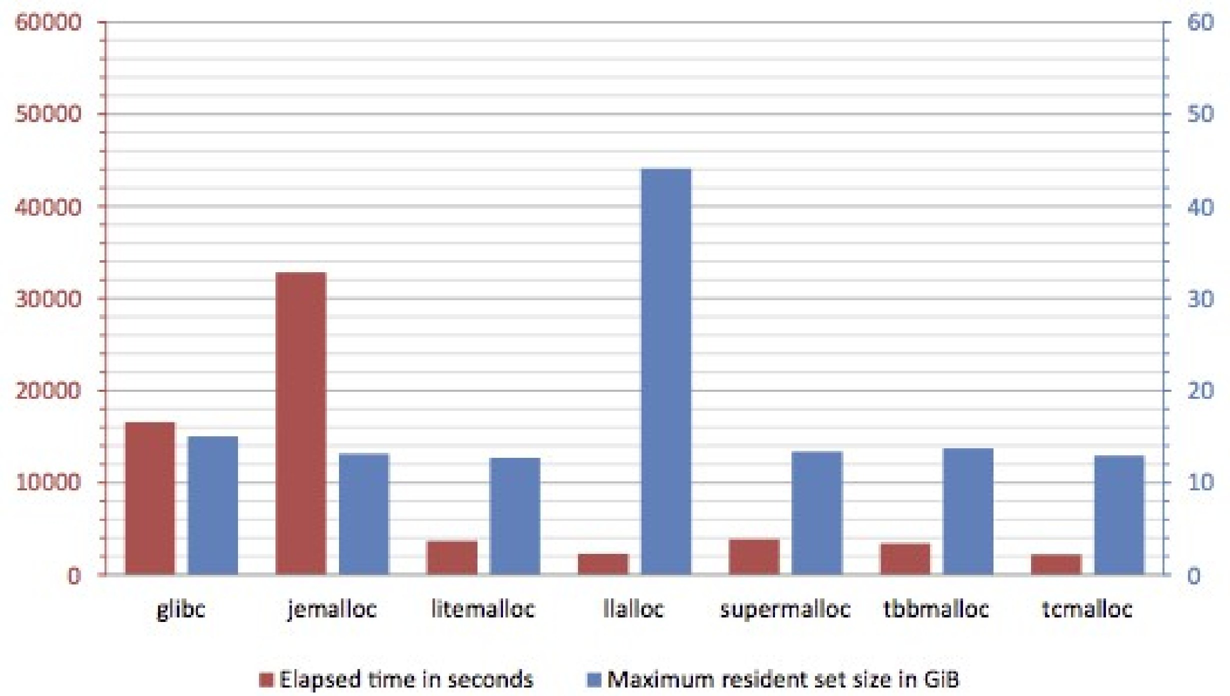
- Good scalability



D. Langr, et al., Int. J. High Perform. Comput. Appl. 33 (2019)

Code optimizations

- **Dynamic memory allocation optimizations**
  - Matrix construction involves lot of concurrent small allocations
  - Dynamic allocation – slow and dependend on malloc implementation.
- **malloc replacement**
  - tcmalloc (Google), jemalloc (Facebook), tbbmalloc (Intel), litemalloc, LLAlloc, SuperMalloc



  - tcmalloc – best performance & memory footprint decrease

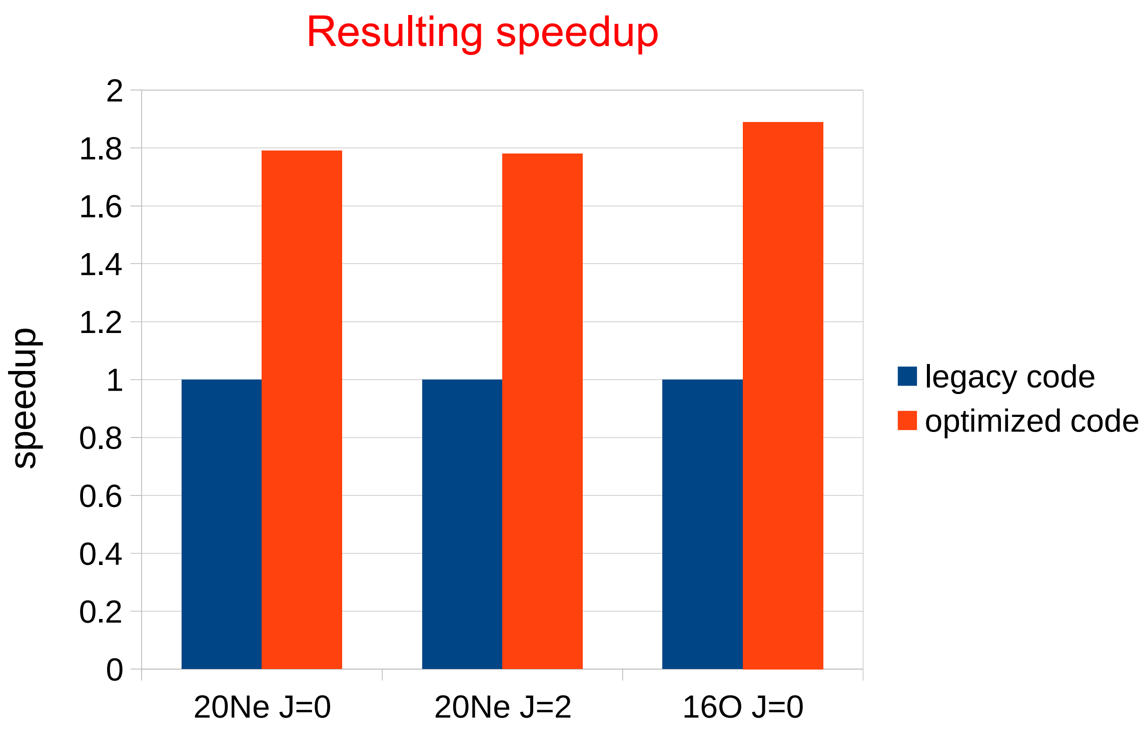
Code optimizations

Memory pooling

- allocating large number of small objects of constant size is inneficient
- Solution: memory pooling
- Boost.Pool – best performance

Small buffer optimizations

- small static buffer for a small number of elements, and dynamic memory over the specified threshold.



For more results see Martin Kocicka's MSc thesis: https://dspace.cvut.cz/handle/10467/80473

Summary

- Key challenges
  - Description of 99.9% mass of the Universe
- Why it matters
  - Ultimate source of energy in the Universe
- Why Blue Waters
  - Aggregate memory and high memory bandwidth
- Accomplishments
  - Many papers in top journals and reaching beyond what competitives theories could accomplish
- Blue Waters team contributions
  - Excellent support and guidance as needed
- Broader impacts
  - Training students in using HPC resources
- Shared Data
  - Codes and results publicly available
- Products
  - https://sourceforge.net/p/lsu3shell/home/Home/