Present and Future Computing Requirements for Ab Initio Calculations of Nuclear Reactions and Light Exotic Nuclei

Large Scale Computing and Storage Requirements for Nuclear Physics (NP): Target 2017

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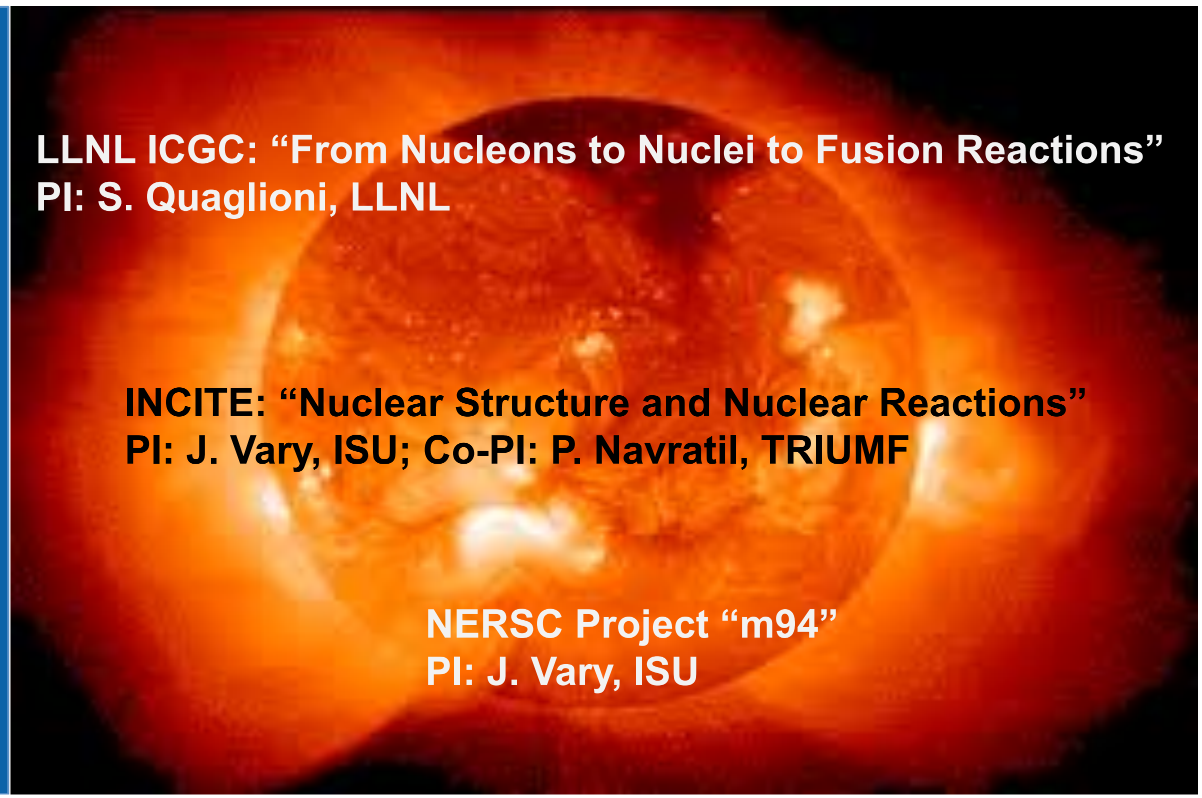
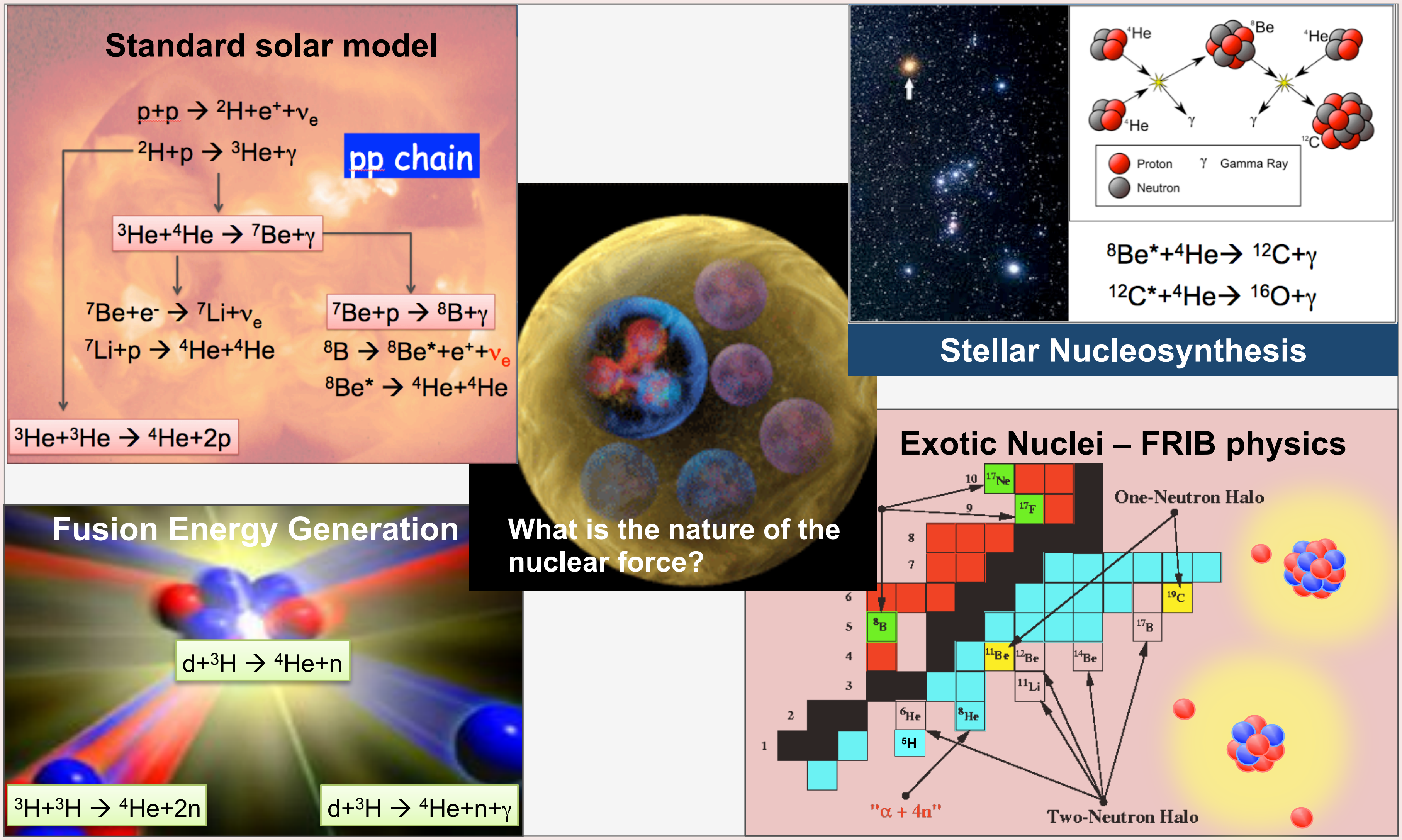


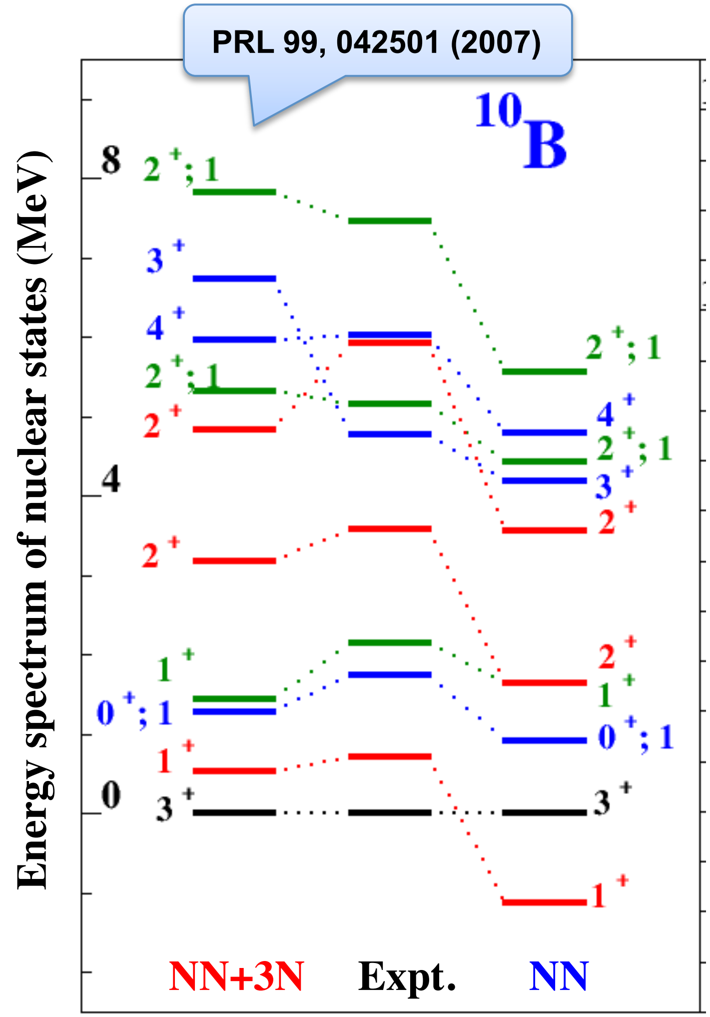
Our goal is to develop a fundamental theory for the description of thermonuclear reactions and exotic nuclei



Large-scale computations have already allowed us to describe static properties of nuclei from first principles

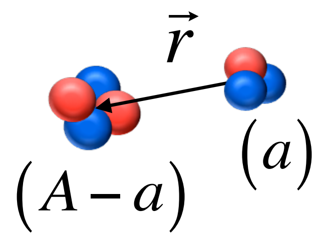
- *Ab initio* no-core shell model (NCSM) approach
  - Bound states
  - Two- and three-nucleon (NN+3N) forces based upon Quantum Chromodynamics

Helped to point out the fundamental importance of 3N forces in structure calculations.



We extended this approach by adding the dynamics between nuclei with the resonating-group method (RGM)

- Reconstruct the interaction potential between a projectile and a target starting from:
  - *Ab initio* NCSM wf. of the clusters
  - Nucleon-nucleon (NN) interactions

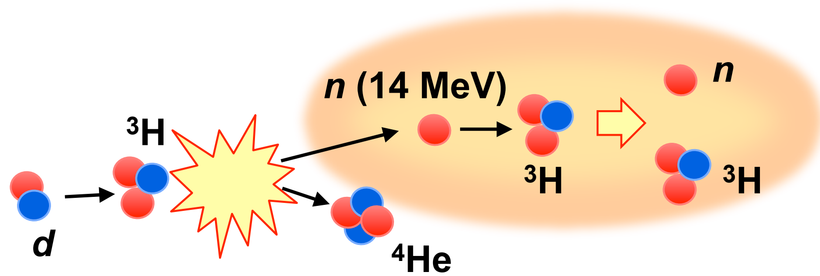


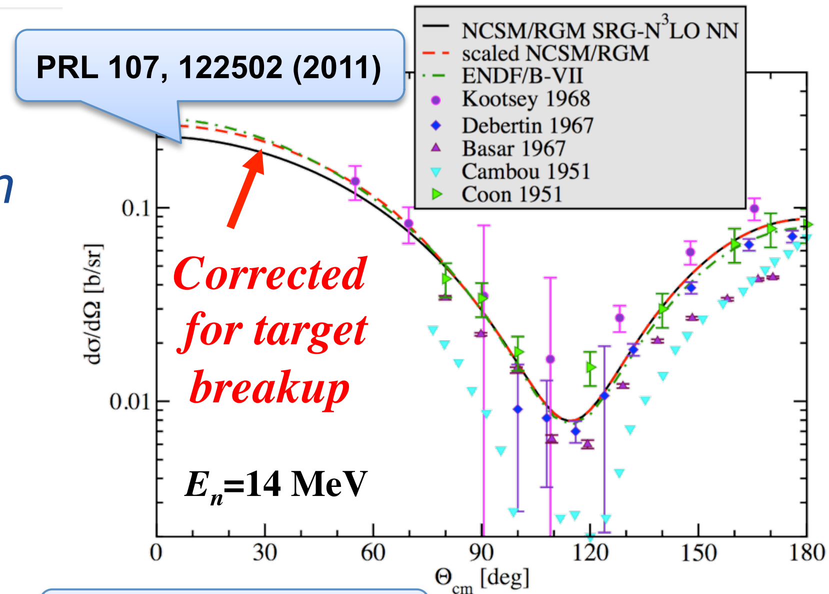
- Solve for projectile-target relative motion
- Investments from: DOE/SC/NP, SciDAC-2 (UNEDEF)

Pioneered ab initio calculations of light-nuclei fusion reactions starting from NN interactions

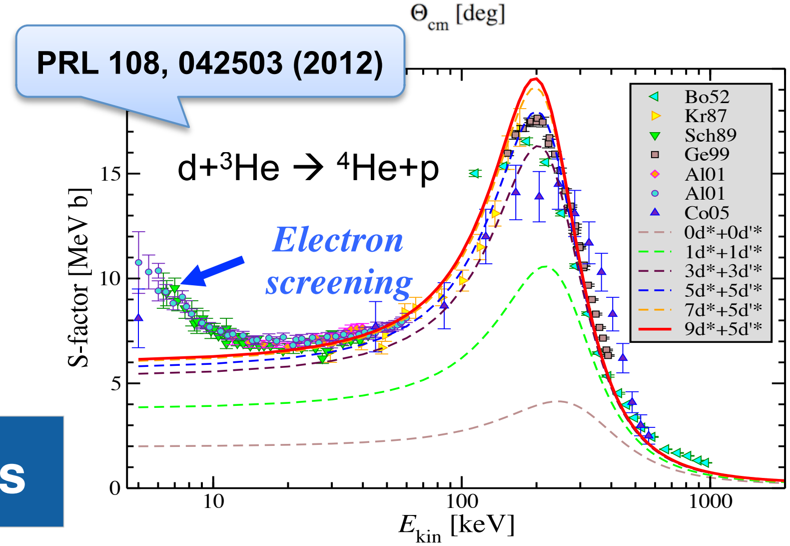
Started with nucleon-nucleus collisions & gradually built up capability to describe fusion reactions with NN force

- *Evaluated n+^{3}H→n+^{3}H cross section for fusion diagnostics with required 5% accuracy*





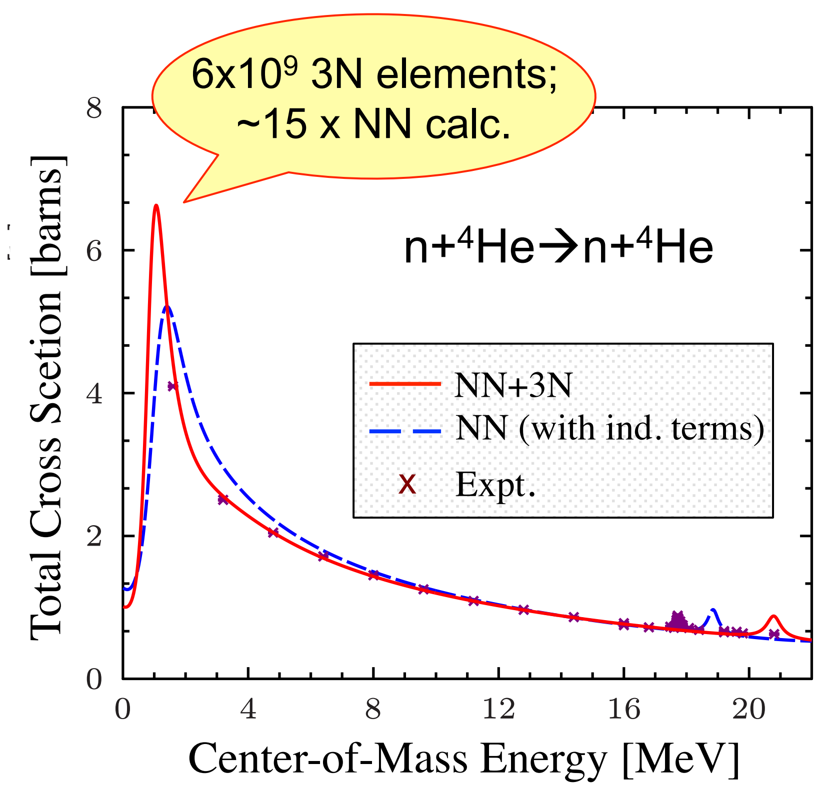
- *Deuterium-^{3}H & deuterium-^{3}He fusion important for Big Bang nucleosynthesis, fusion research, atomic physics*



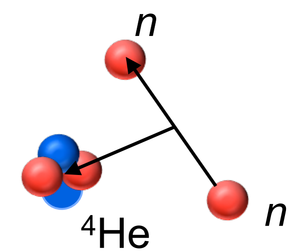
To do: 3N force; 3-body dynamics

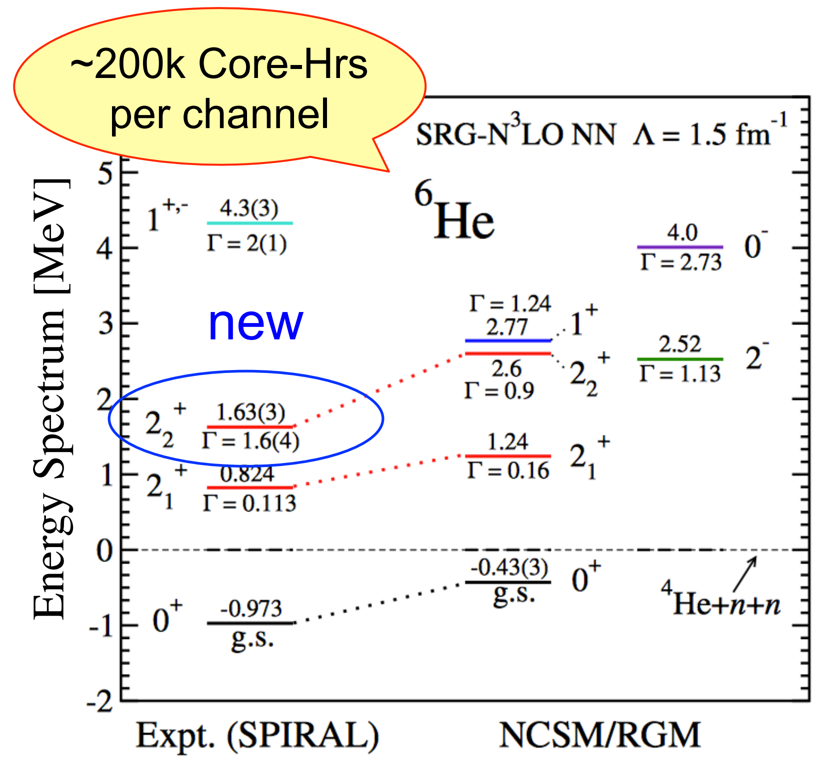
Now including 3N force in reactions and describing continuum of three clusters (DOE/SC/NP Early Career)

- *3N force needed for high-fidelity simulations*



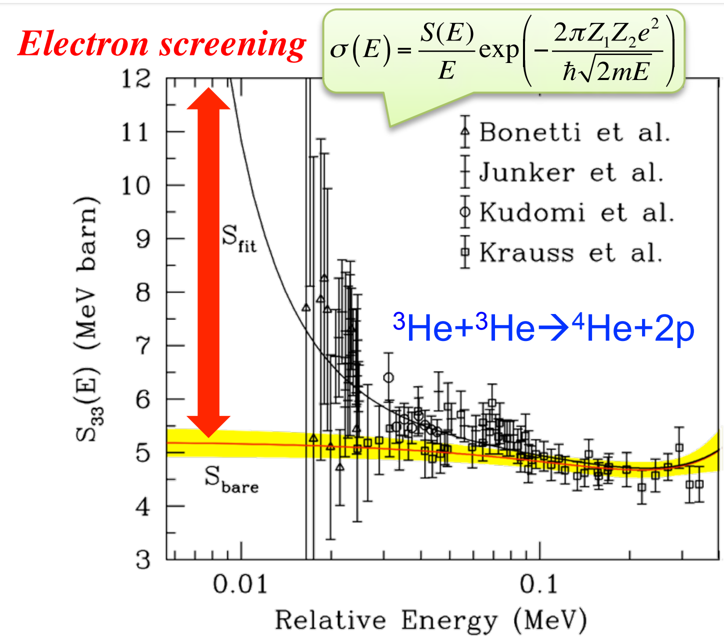
- *We want to describe systems with 3-body decay channels*



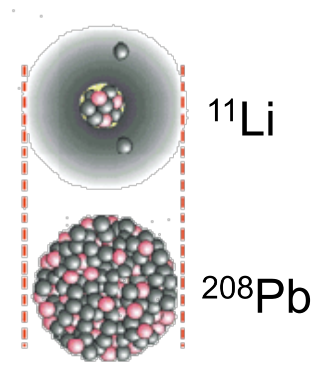


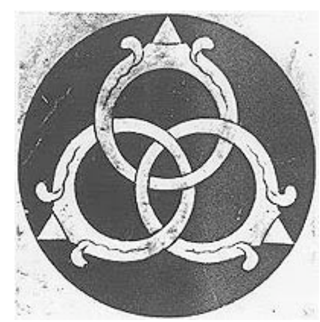
From now through 2017: deliver high-fidelity simulations complete of both 3N-force & 3-cluster dynamic effects

- **In 2017**: $^3H + ^3H \rightarrow ^4He + n + n$ (fusion research) and $^3He + ^3He \rightarrow ^4He + p + p$ (solar astrophysics)
  - As an intermediate step calculation with only NN interaction



- **In 2017:** Spectroscopy of Borromean exotic nucleus ^{11}Li as $^9Li + n + n$ (FRIB physics)
  - At first $^6He (= ^4He + n + n)$ and $^5H (= ^3H + n + n)$ with NN+3N force

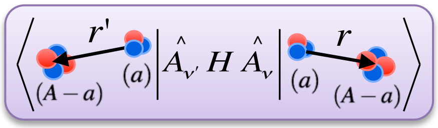


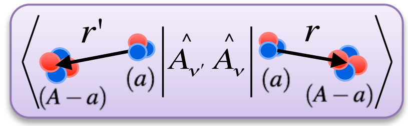


Our problem, our solution

- Problem: $$\sum_{\nu} \int d\vec{r} \, \left[H_{\nu'\nu}(\vec{r}', \vec{r}) - E \; N_{\nu'\nu}(\vec{r}', \vec{r}) \right] g_{\nu}(\vec{r}) = 0$$

Hamiltonian couplings





Overlap couplings

1) Input: NN, 3N interactions; projectile, target wave functions

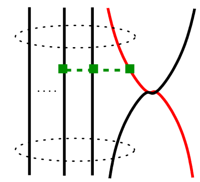
2) Compute: Hamiltonian and Overlap couplings
   - Non trivial specialized algebra, depends on projectile mass
   - Sparse matrices; dim = f(# oscillator shells,# projectile nucleons)
   - Sparsity not easily predictable, depends on interaction in input

3) Solve: 2-, 3-body coupled-channel equations
   - At each energy step: dense linear algebra

4) Output: Scattering matrix, wave functions, phase shifts

Our biggest computational challenges come from couplings depending on many-body densities

N+(A-1) with 3N interaction



$$\propto {}_{SD}\left\langle \psi^{(A-1)}_{\alpha_1'} \middle| a^+_h a^+_i a^+_j a_m a_l a_k \middle| \psi^{(A-1)}_{\alpha_1} \right\rangle_{SD}$$

- Storing in memory many-body density matrices not feasible

A. Compute and store (coupled) reduced matrix elements

- Efficient when doable
- Only very light systems

$$\sum_\beta {}_{SD}\left\langle \psi^{(A-1)}_{\alpha_1'} \middle\| \left(a^+_h (a^+_i a^+_j)^{\kappa'\tau'}\right)^{\mathrm{K'T'}} \middle\| \psi^{(A-4)}_{\beta} \right\rangle_{SD}$$
$$\times\, {}_{SD}\left\langle \psi^{(A-4)}_{\beta} \middle\| \left((a_m a_l)^{\kappa\tau} a_k\right)^{\mathrm{KT}} \middle\| \psi^{(A-1)}_{\alpha_1} \right\rangle_{SD}$$

B. On the fly calculation of (uncoupled) density matrices

- Well suited for parallel computing
- Can address heavier systems

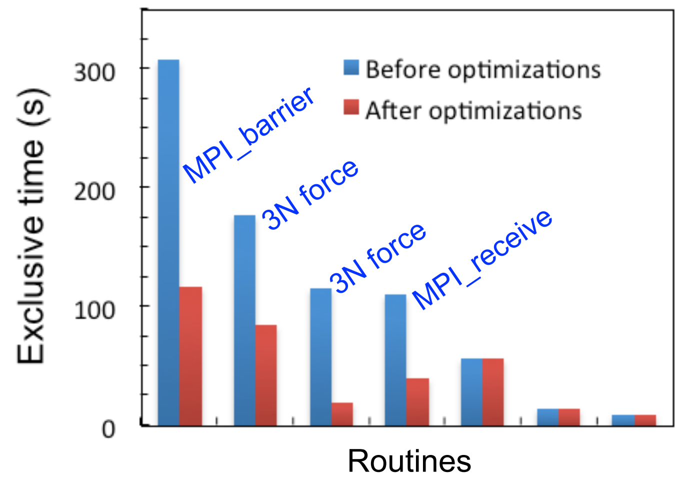
$$\left| \psi^{(A-1)}_{\alpha_1} \right\rangle_{SD} = \sum_i \left| SD \right\rangle_i$$

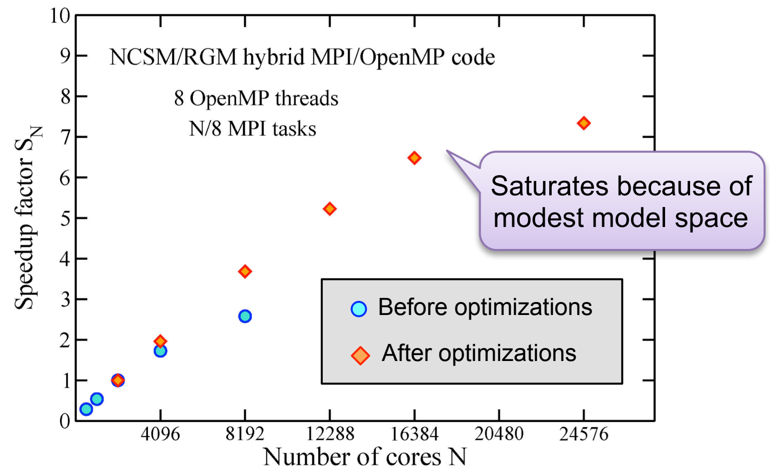
In 2017 we expect to transition more and more towards strategy B.

The primary code is NCSM_RGM, based on strategy A.

- Hybrid MPI/OpenMP
  - up to 98,304 cores on TITAN
- Algorithms include
  - Mostly specialized, in house
  - Matrix multiplications, inversions, diagonalizations
- Recent optimizations include
  - MPI I/O for large input data
  - Hybrid “all slaves” algorithms
  - MKL threaded libraries for dense algebra components

Excellent scaling should continue in larger model spaces (to study)





Current HPC Usage (2012-2013)

- LLNL Institutional Computing Grand Challenge (SIERRA)
  - 1,944 nodes, 12 cores/node
  - 261 teraflop/s, 24 GB/node
  - ➢ 10M Core-Hrs, ~70 runs/year
  - ➢ Typically 1,000 MPI tasks and 12 OpenMP threads/task for 12 Hrs

- INCITE allocation, PI: J. Vary, co-PI: P. Navratil (TITAN)
  - ➢ 23M Core-Hrs, ~50 runs/year
  - ➢ Up to 6,144 nodes for 8 Hrs: 12,288 MPI tasks, 8 OpenMP threads/task (98,304 cores)

- NERSC project “m94”, PI: J. Vary (Edison, early users)
  - ➢ 12M Core-Hrs
  - ➢ Typically 200-600 nodes, i.e. 3 to 10% of machine
  - ➢ Could use 20% now

Current HPC Usage (2012-2013)

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- INCITE allocation, PI: J. Vary, co-PI: P. Navratil (TITAN)
- NERSC project “m94”, PI: J. Vary (Edison, early users)

- Memory Usage:
  - All memory on the node
  - Need at least 2GB/core
  - Use all global memory
- Data Usage:
  - Input < 100 GB
  - Output < 0.5 TB
  - Use mostly /scrach

HPC Requirements for 2017

- Estimate: 15 x (usage for 3-cluster simulations)
- Selected, more challenging science goals
- Concurrent storage of 3N matrix elements & 3-cluster configurations
- Approach under development
- Unprecedented large scale
- Store more scattering data for later use

- ➢ Minimum 25M Core-Hrs
- ➢ Fewer, larger runs (20-50% of Edison), same typical run time
- ➢ Will need all memory on node, i.e., # MPI tasks = # nodes
  - Use threads with OpenMP
- ➢ Expect algorithmic changes
- ➢ May need more load balancing
- ➢ Larger data requirement

Summary

- With HPC we are addressing previously unsolvable problems:
  - ☑ NNN force in light-nucleus reactions
  - ☑ *Ab initio* description of three clusters in the continuum

- **More memory**, larger core count, larger allocations will allow higher-fidelity simulations of complex reactions & exotic nuclei
  - Solar astrophysics, fusion research, FRIB physics

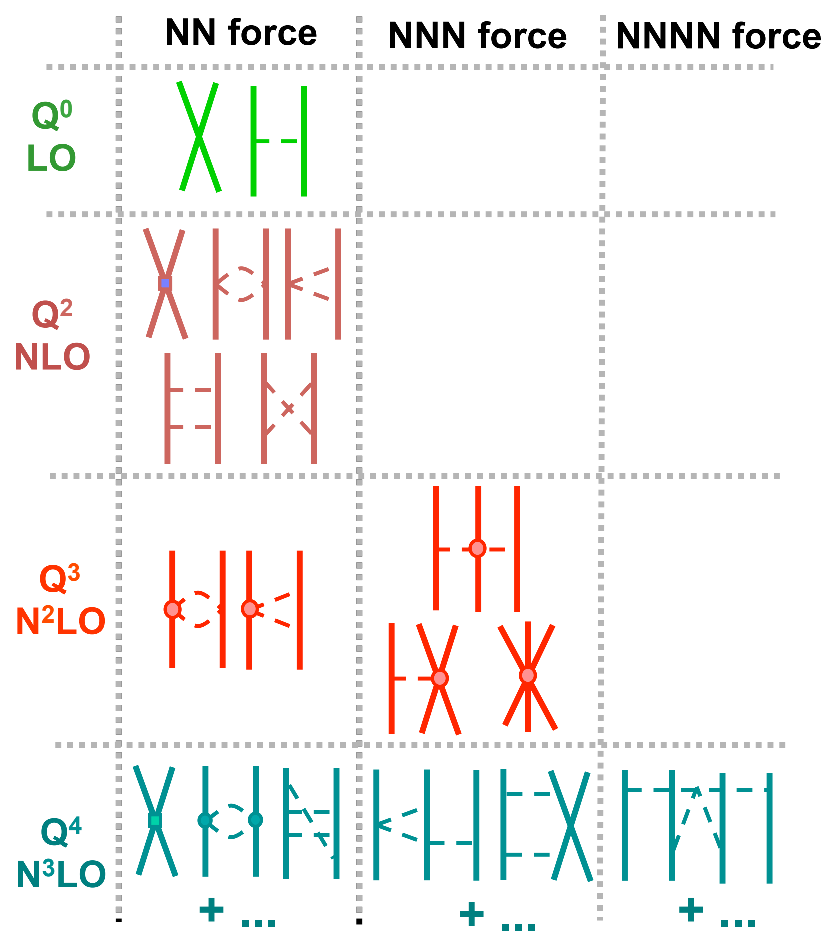
- To achieve these goals and make optimal use of new HPC architectures we will need the help of NERSC experts!
  - Not yet using GPUs (MPI/OpenMP more adapt to our problem);
  - Not porting/optimizing for MIC (Or are we?);

- Need more SciDAC type of support; dedicated positions to foster new generation of computational+nuclear scientists that can help us keep up with new technologies and reach the exascale

Extras

Accurate nuclear interactions (and currents)

- Nuclear forces are governed by quantum chromodynamics (QCD)
  - QCD non perturbative at low energies
- Chiral effective filed theory (χEFT)
  - retains all symmetries of QCD
  - explicit degrees of freedom: π, N
- Perturbative expansion in positive powers of $(Q/\Lambda_\chi) \ll 1$ ($\Lambda_\chi \sim$ 1 Gev)
  - nuclear interactions
  - nuclear currents
- Chiral symmetry dictates operator structure
- Low-energy constants (LECs) absorb short-range physics
  - some day all from lattice QCD
  - now constrained by experiment



Worked out by Van Kolck, Keiser, Meissner, Epelbaum, Machleidt, ...

Major Publications

PRL **110**, 022505 (2013) PHYSICAL REVIEW LETTERS week ending 11 JANUARY 2013

Ab Initio Description of the Exotic Unbound ^{7}He Nucleus

Simone Baroni,[1,2,*] Petr Navrátil,[2,3,†] and Sofia Quaglioni[3,‡]

PHYSICAL REVIEW C **87**, 034326 (2013)

Unified _ab initio_ approach to bound and unbound states: No-core shell model with continuum and its application to ^{7}He

Simone Baroni,[1,2,*] Petr Navrátil,[2,3,†] and Sofia Quaglioni[3,‡]

PHYSICAL REVIEW C **88**, 034320 (2013)

Three-cluster dynamics within an _ab initio_ framework

Sofia Quaglioni,[1,*] Carolina Romero-Redondo,[2,†] and Petr Navrátil[2,‡]

PHYSICAL REVIEW C **88**, 054622 (2013)

Ab initio many-body calculations of nucleon-^{4}He scattering with three-nucleon forces

Guillaume Hupin,[1,*] Joachim Langhammer,[2,†] Petr Navrátil,[3,‡] Sofia Quaglioni,[1,§] Angelo Calci,[2,‖] and Robert Roth[2,¶]