Large Scale Simulations of Nuclear Dynamics

J. Carlson, LANL

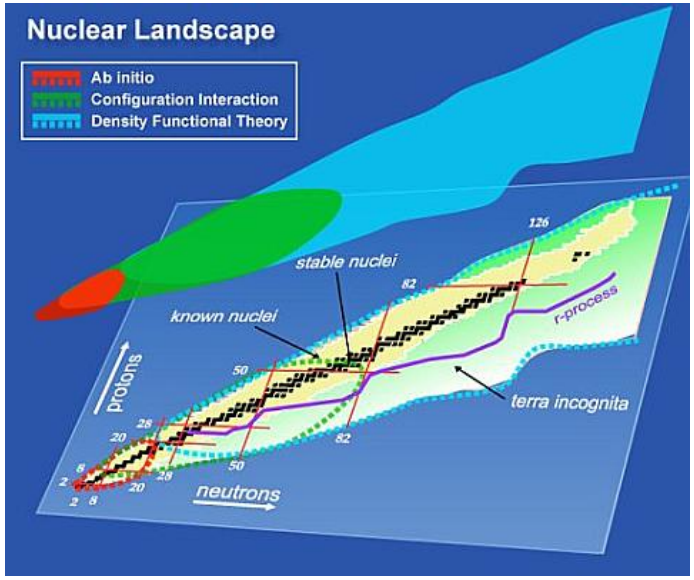
Universal Nuclear Energy Density Functional

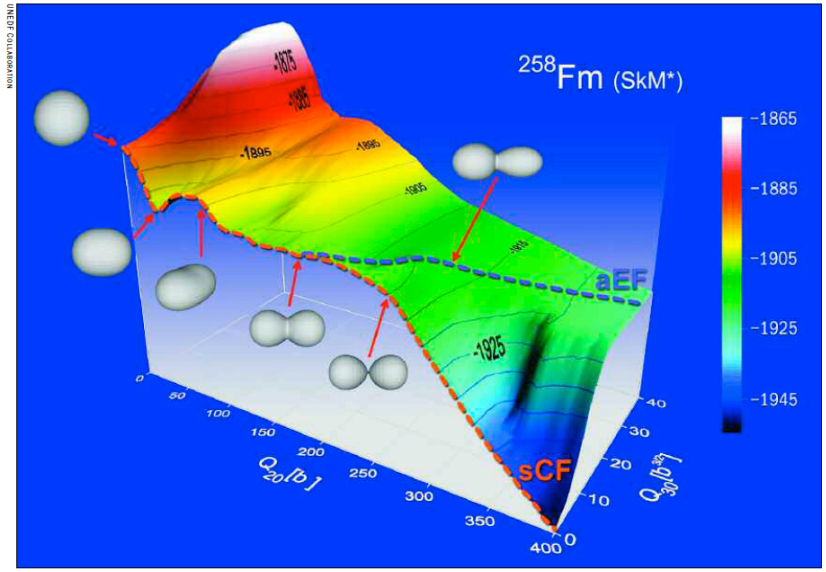
Nuclear Density Functional

Few-Nucleon Reactions: Computational Progress & Initial Physics Results

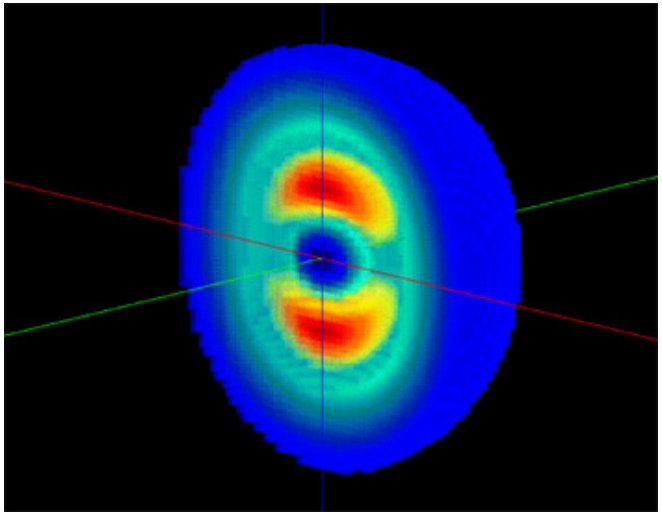
Fission in Heavy Nuclei: Computational Progress & Initial Physics Results

Impact Beyond Nuclear Physics : Real-time Superfluid Vortices

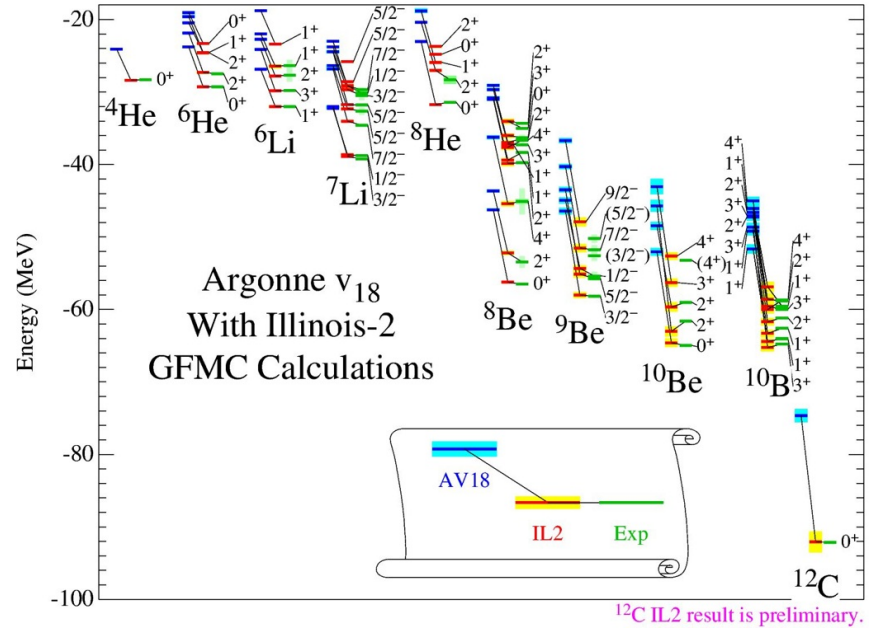




Ab-Initio Calculations (light nuclei and neutron matter)



Deuteron (courtesy JLab)



Pieper, Wiringa, ANL

Strongly-Correlated, Cluster Structures

Large Spin and Isospin Dependence

Wave function has 2^A (A! / N! Z!) components

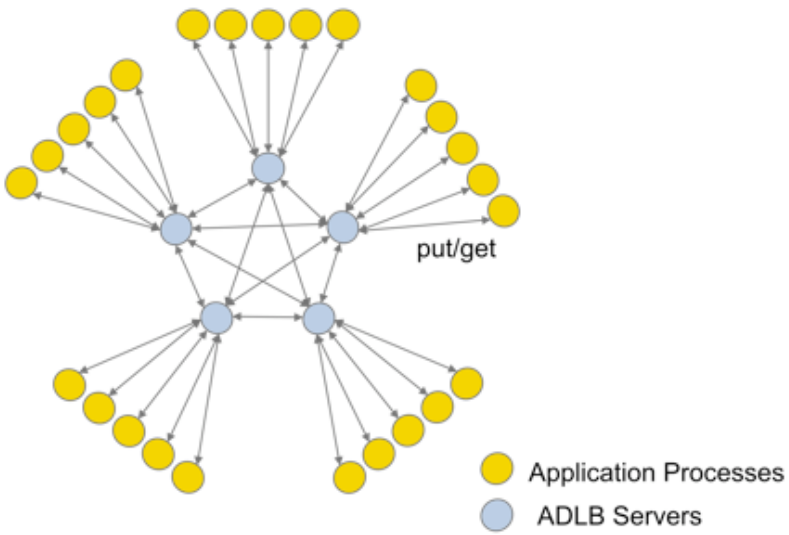
Algorithms: Configuration-Interaction (Shell Model)

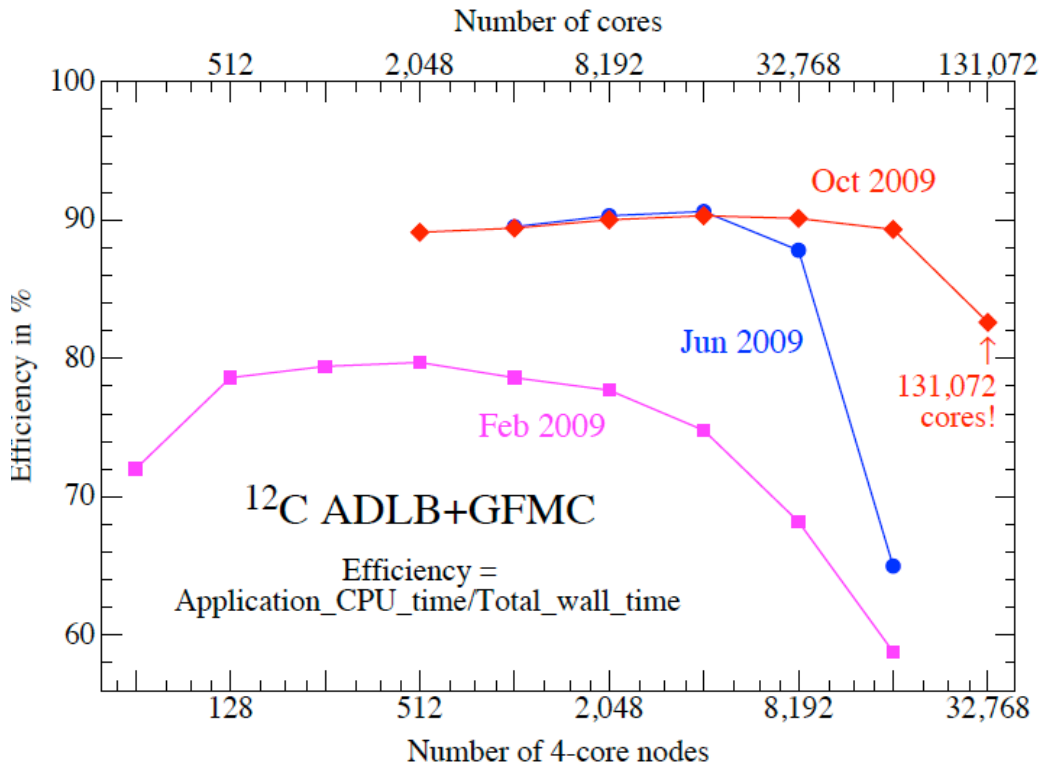
Quantum Monte Carlo

Making GFMC work:

Asynchronous Dynamic Load Balancing

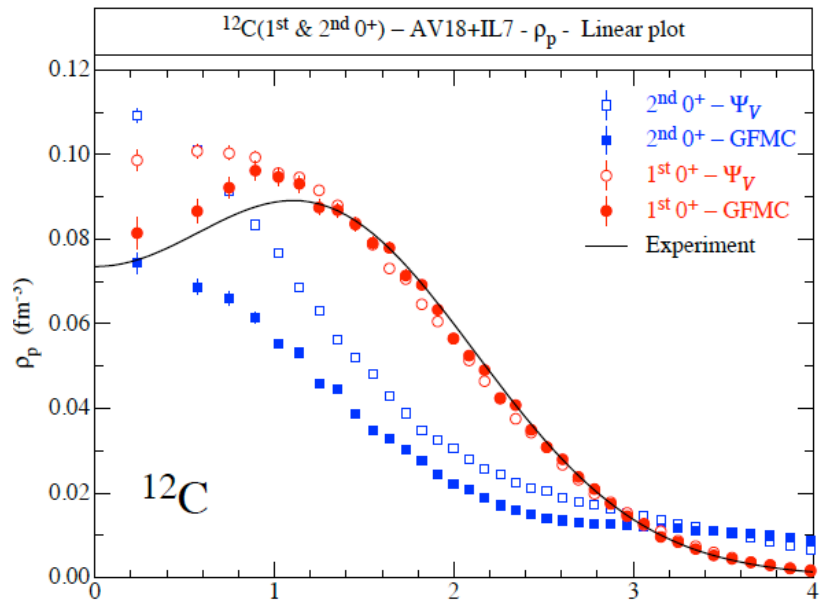
Lusk, Pieper, Butler: SCIDAC Review 2010





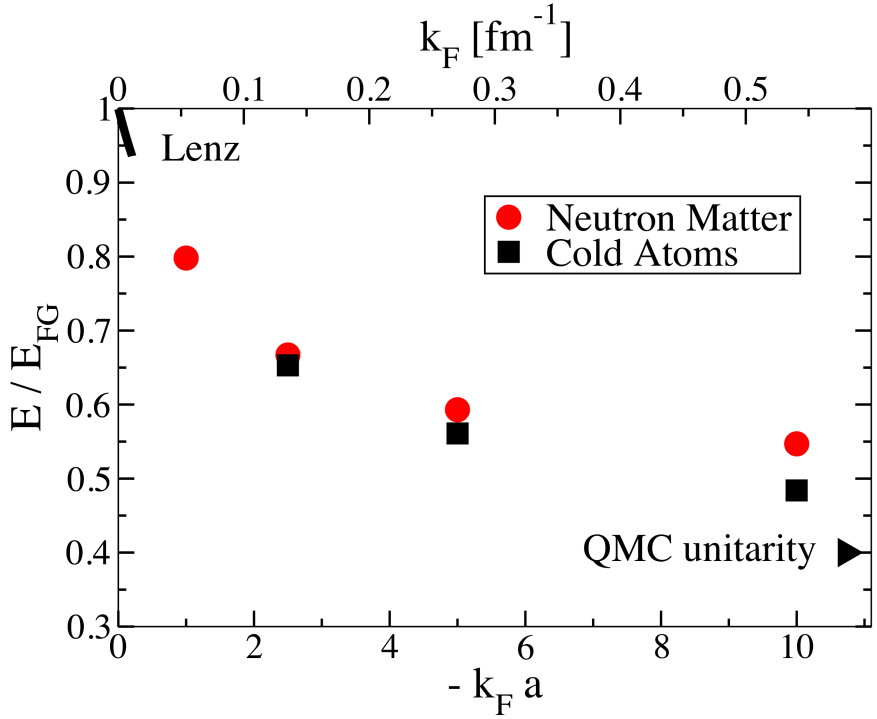
Asynchronous Dynamic Load Balancing
Distributing work elements

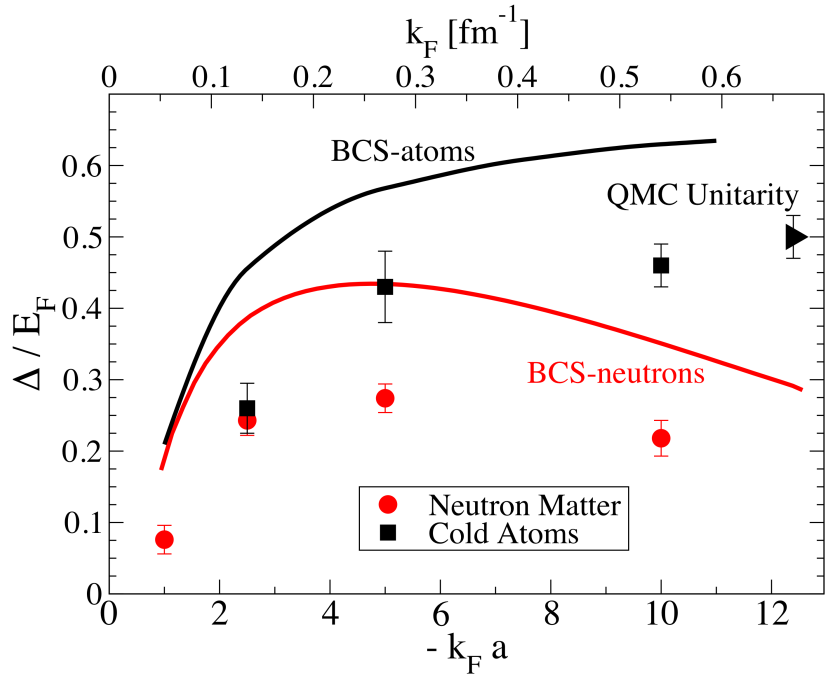
Nuclei



Pieper

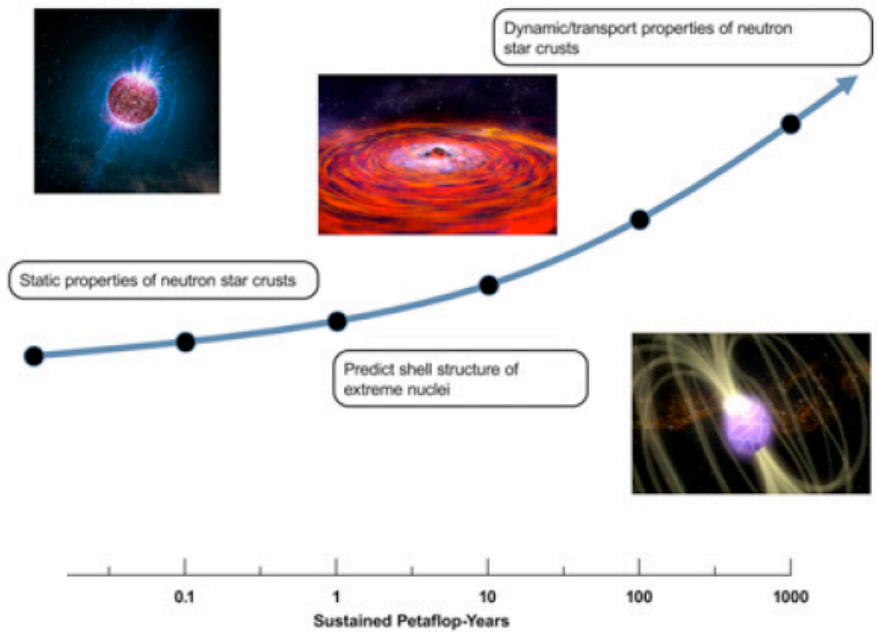
Neutron Matter

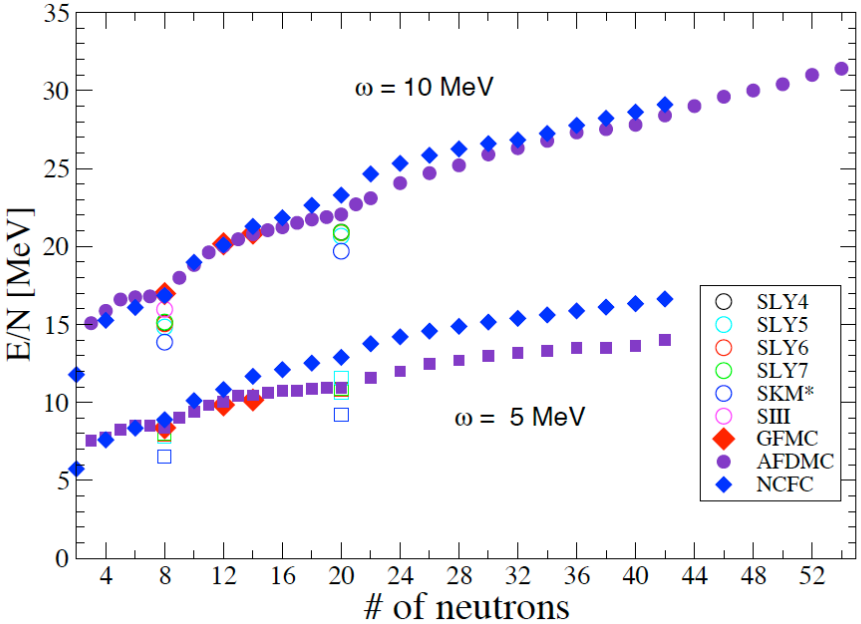




Gezerlis, JC

Neutrons in External Fields

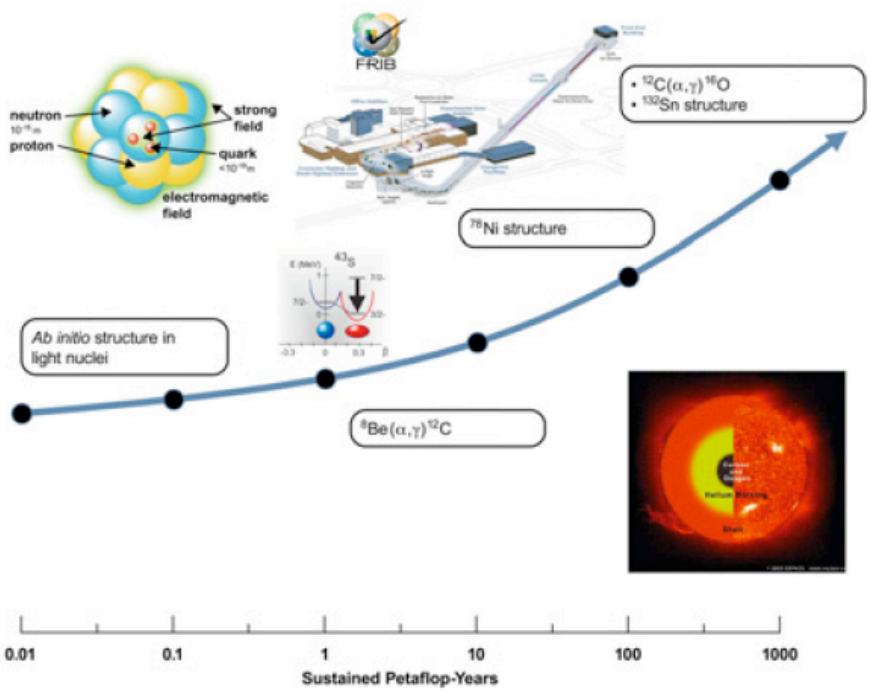




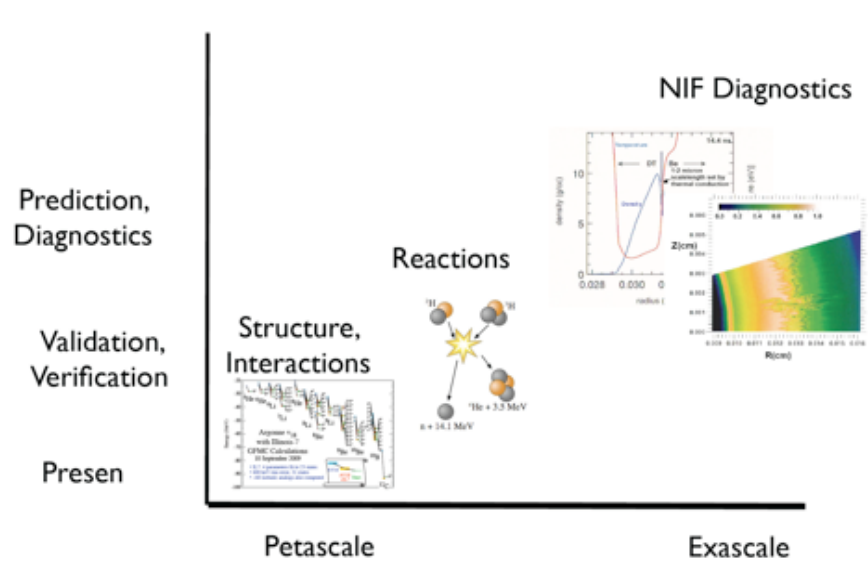
Gandolfi, Pieper, JC 2010

`Pseudo-data':
Used to predict properties of neutron star crust, heavy neutron rich nuclei, …

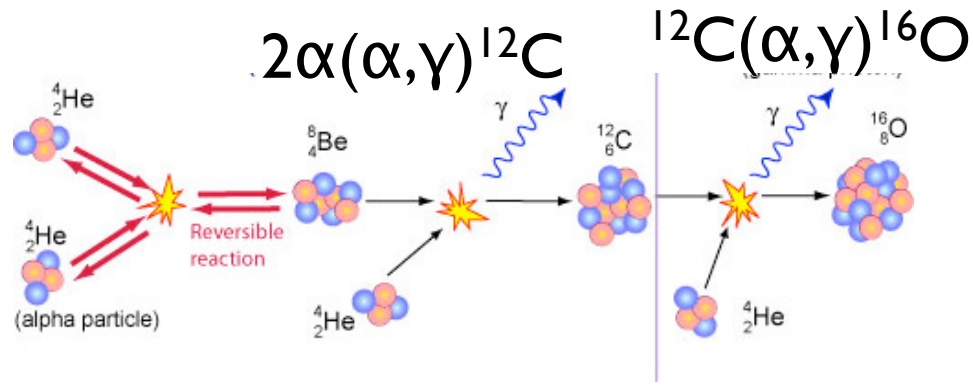
Few-Nucleon Reactions:
Goals in Basic and Applied Physics



NP exascale report



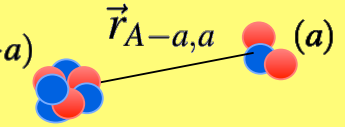
NNSA exascale report



Reactions: No Core Shell Model (CI) / Resonating Group Method

Navratil, Quaglioni

$$\Psi^{(A)} = \sum_{\nu} \int d\vec{r}\, \varphi_\nu(\vec{r})\, \hat{\mathcal{A}}\, \Phi^{(A-a,a)}_{\nu\vec{r}}$$



$$\psi^{(A-a)}_{1\nu}\, \psi^{(a)}_{2\nu}\, \delta(\vec{r} - \vec{r}_{A-a,a})$$

eigenstates of $H_{(A-a)}$ and $H_{(a)}$ in the *ab initio* NCSM basis

- Many-body Schrödinger equation:

$$H\Psi^{(A)} = E\Psi^{(A)}$$

$$T_{\rm rel}(r) + \mathcal{V}_{\rm rel} + \bar{V}_{\rm Coul}(r) + H_{(A-a)} + H_{(a)}$$

realistic nuclear Hamiltonian

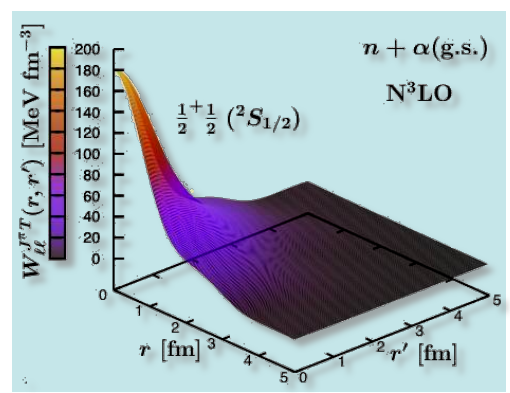
$$\sum_{\nu} \int d\vec{r} \left[\mathcal{H}^{(A-a,a)}_{\mu\nu}(\vec{r}\,',\vec{r}) - E\mathcal{N}^{(A-a,a)}_{\mu\nu}(\vec{r}\,',\vec{r}) \right] \varphi_\nu(\vec{r}) = 0$$

$$\langle \Phi^{(A-a,a)}_{\mu\vec{r}\,'} | \hat{\mathcal{A}} H \hat{\mathcal{A}} | \Phi^{(A-a,a)}_{\nu\vec{r}} \rangle$$

Hamiltonian kernel

$$\langle \Phi^{(A-a,a)}_{\mu\vec{r}\,'} | \hat{\mathcal{A}}^2 | \Phi^{(A-a,a)}_{\nu\vec{r}} \rangle$$

Norm kernel

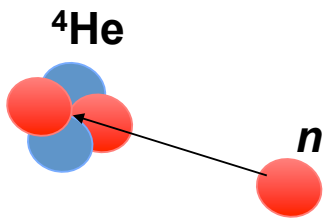


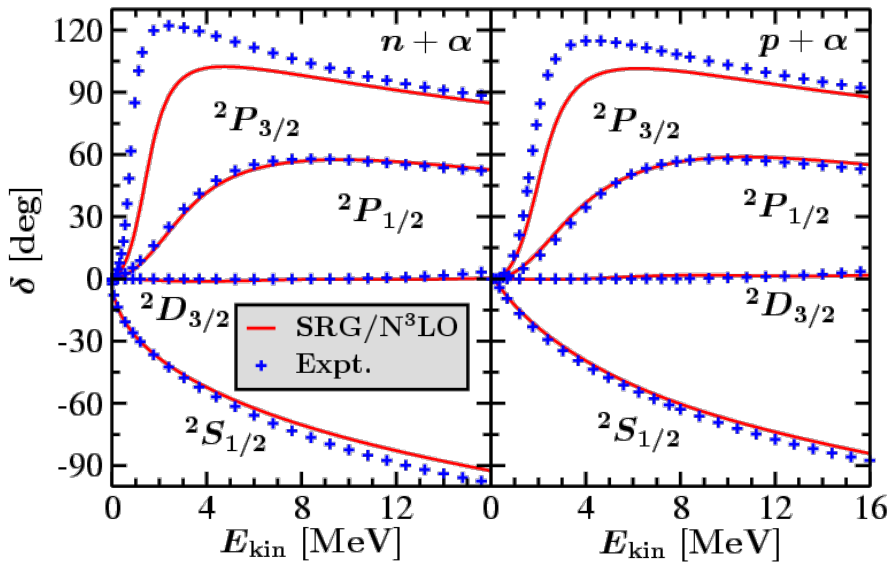
- Non-local integro-differential coupled-channel equations:

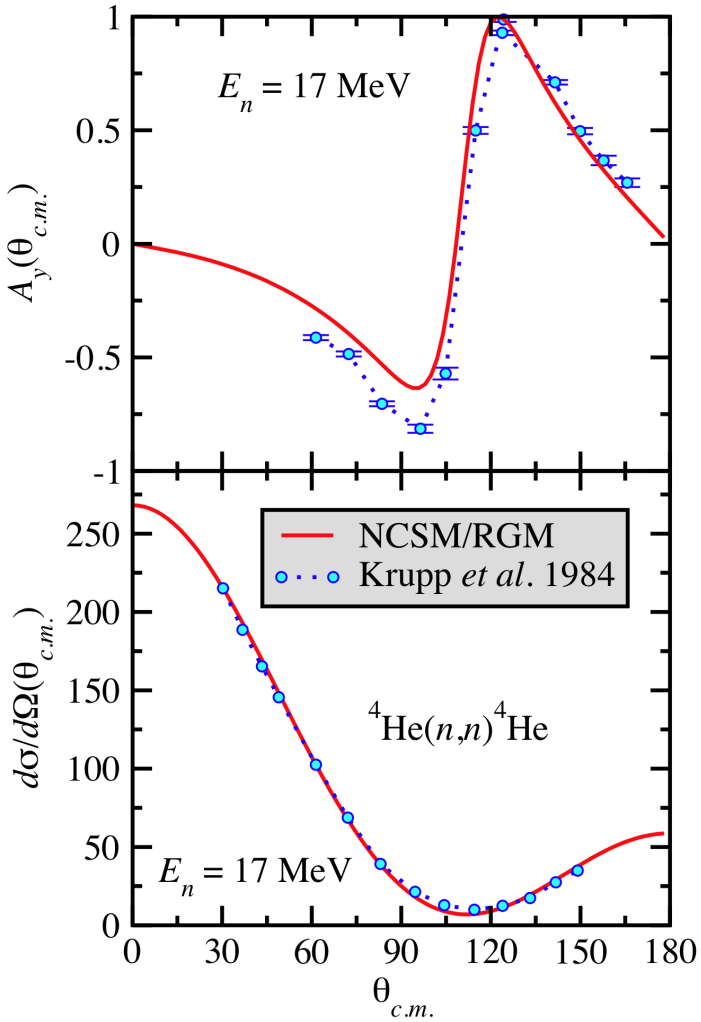
$$[\hat{T}_{\rm rel}(r) + \bar{V}_{\rm C}(r) - (E - E_\nu)]\, u_\nu(r) + \sum_{\nu} \int dr'\, r'\, W_{\nu\nu'}(r,r')\, u_\nu(r') = 0$$

NCSM/RGM: NCSM microscopic wave functions for the clusters involved, and realistic (bare or derived NCSM effective) interactions among nucleons. Proper boundary conditions for scattering and/or bound states

n-^{4}He differential cross-section and analyzing power



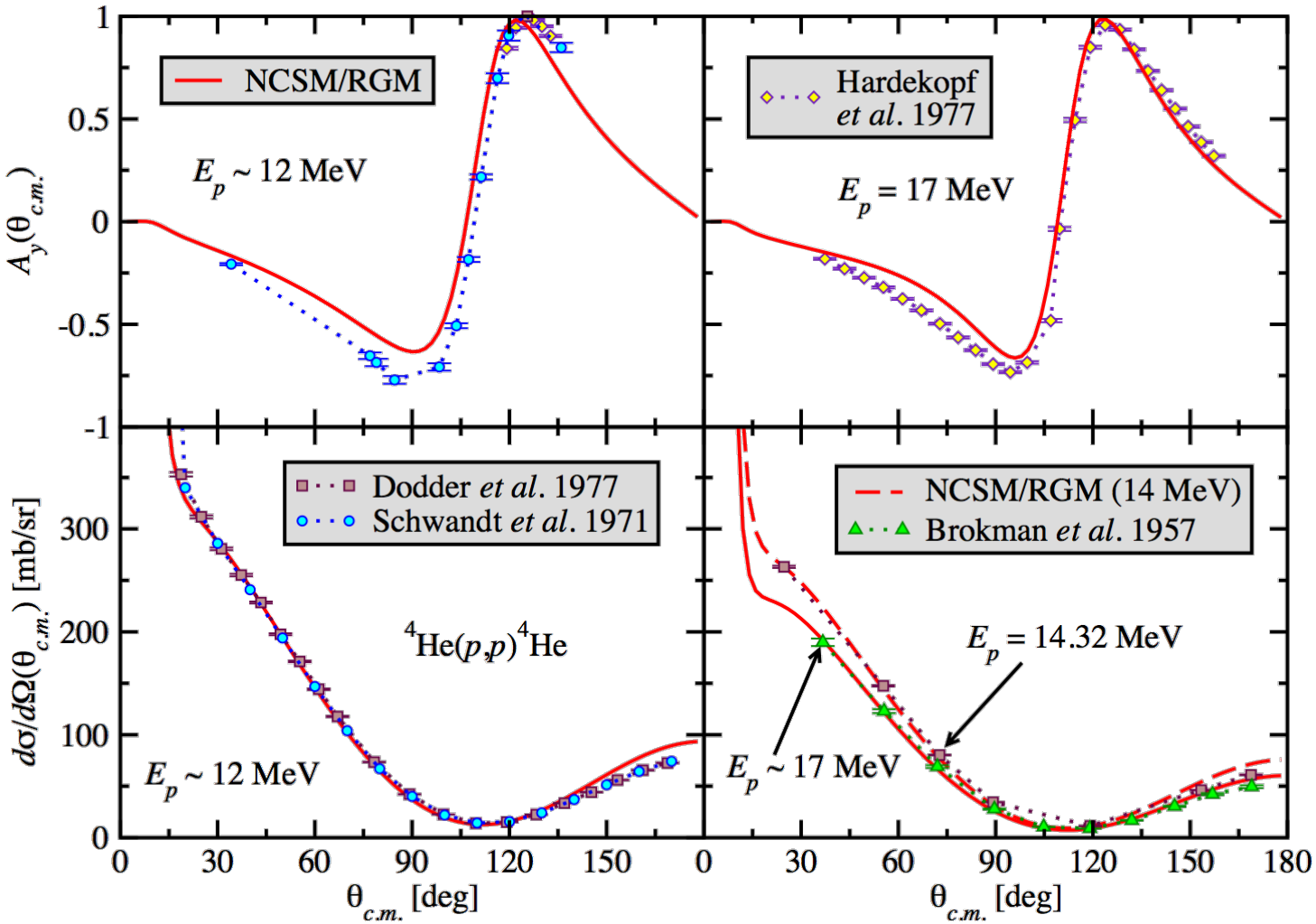




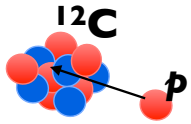
- Differential cross section and analyzing power @17 MeV neutron energy
- Polarized neutron experiment at Karlsruhe

NNN missing: Good agreement only for energies beyond low-lying 3/2$^-$ resonance

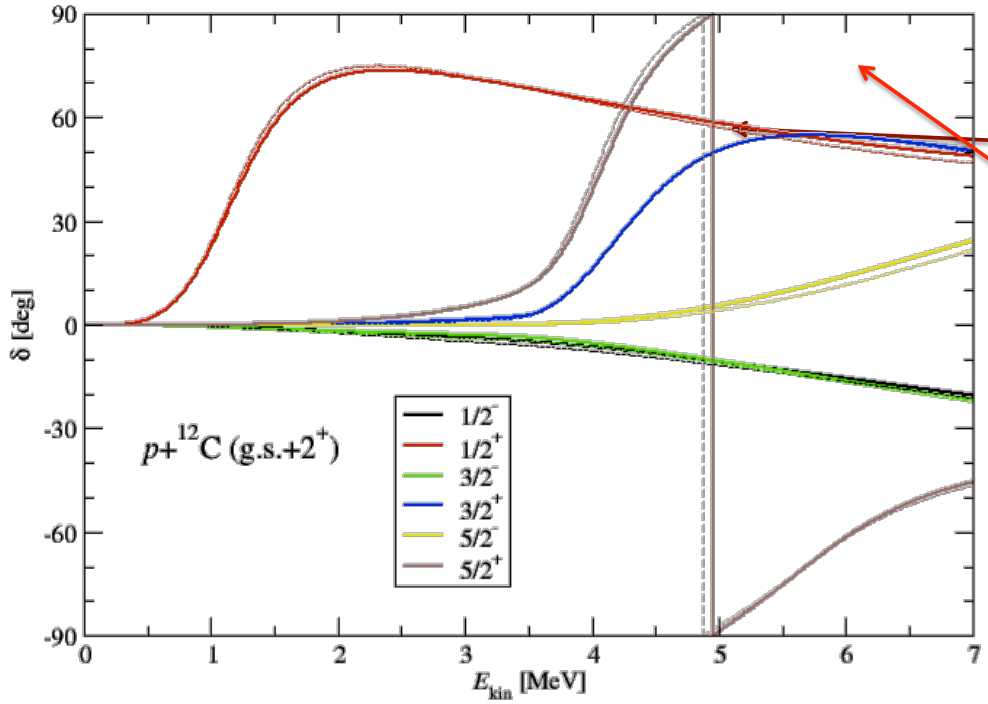
p + ^{4}He cross section and analyzing power

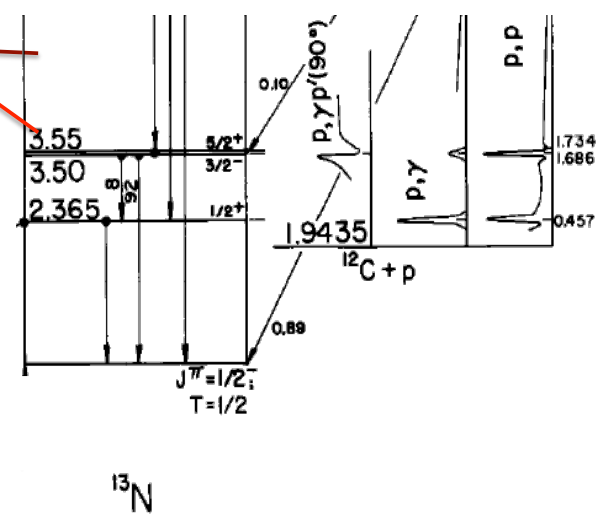


^{13}N ground state and p-^{12}C



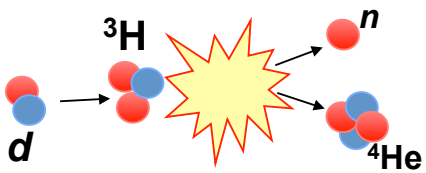
- Experiments with a polarized proton target under way
- N_{max} = 16 NCSM/RGM calculation with n + ^{12}C(g.s.,2^+_1)
- SRG-N^{3}LO NN potential with Λ = 2.02 fm^{-1}
  - ^{13}N $1/2^-$ ground state (bound by 2.9 MeV), other states unbound
  - $1/2^+$ and $5/2^+$ narrow resonance

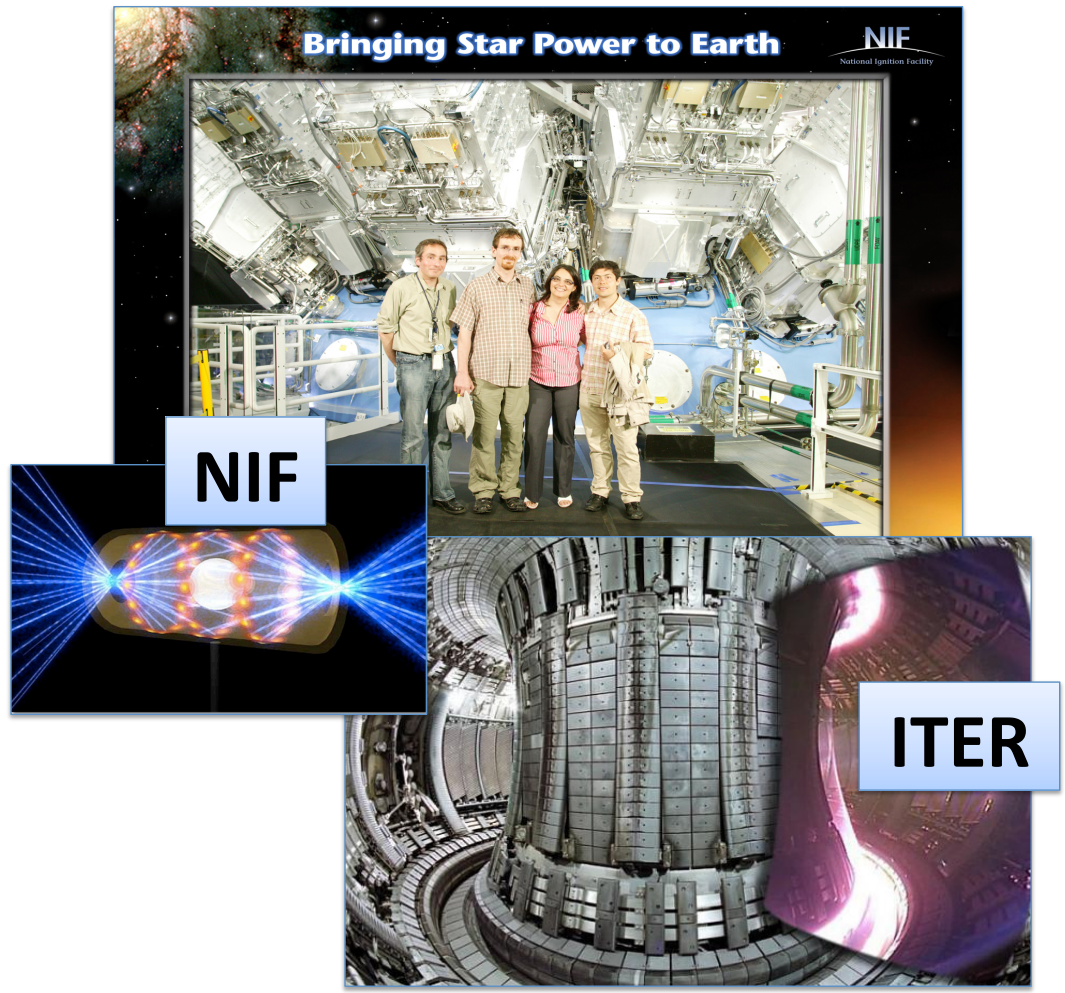




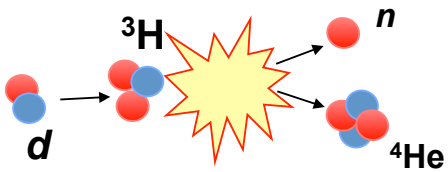
Toward Reactions: d+t

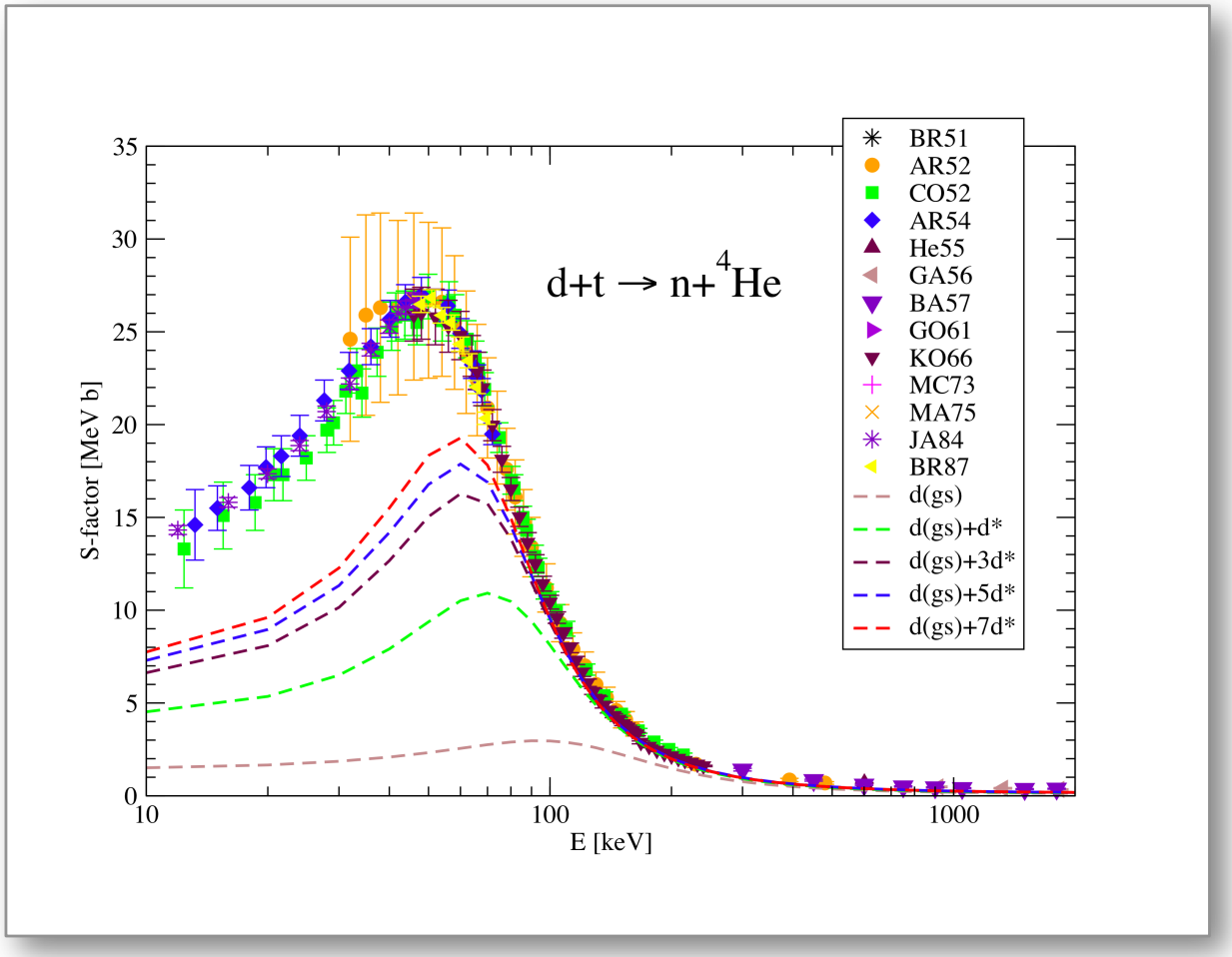
$$\int dr\, r^2 \begin{pmatrix} \left\langle \hat{A}_1 (H-E) \hat{A}_1 \right\rangle & \left\langle \hat{A}_1 (H-E) \hat{A}_2 \right\rangle \\ \left\langle \hat{A}_2 (H-E) \hat{A}_1 \right\rangle & \left\langle \hat{A}_2 (H-E) \hat{A}_2 \right\rangle \end{pmatrix} \begin{pmatrix} \frac{g_1(r)}{r} \\ \frac{g_2(r)}{r} \end{pmatrix} = 0$$





d-t fusion

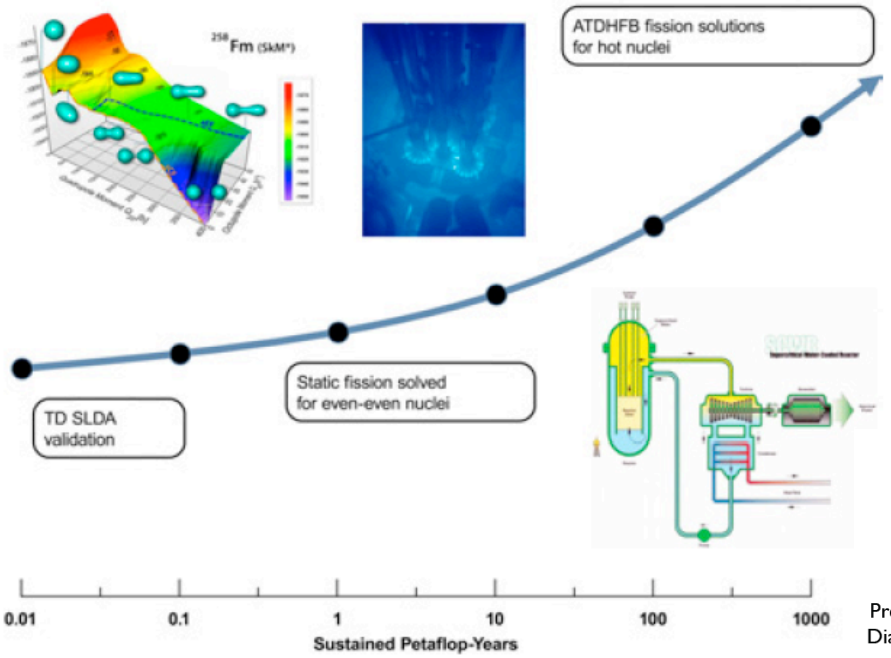


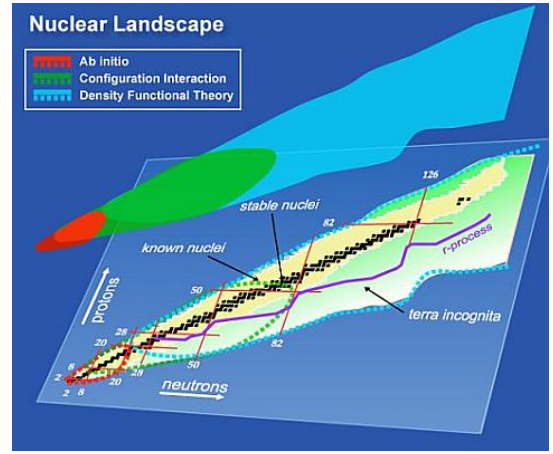


$$S(E) = E\sigma(E)\exp\left(\frac{2\pi\ Z_1 Z_2 e^2}{\hbar\sqrt{2mE}}\right)$$

Navratil, Quaglioni, LLNL

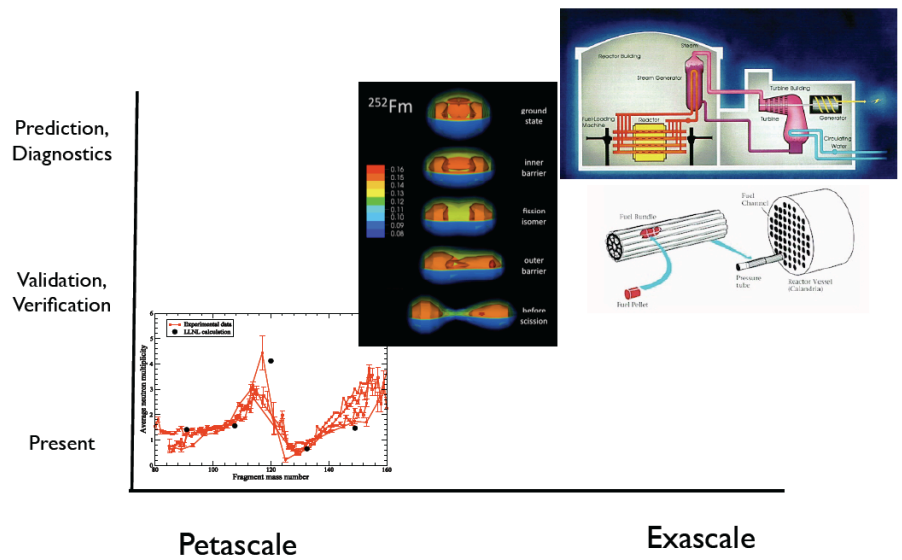
Nuclear Fission



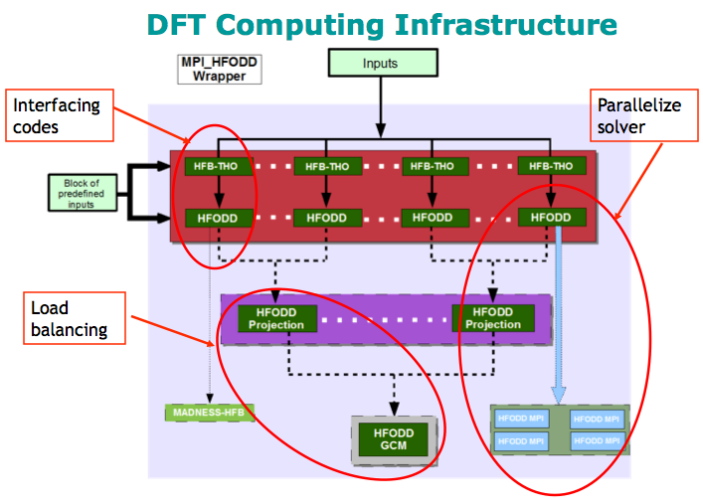


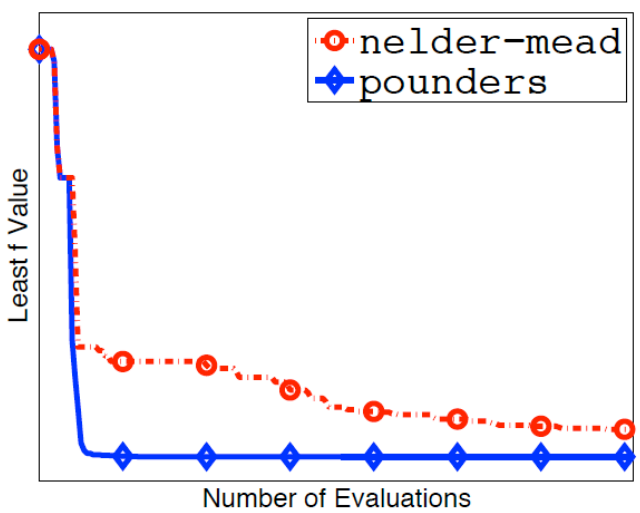
Nuclear Power (fast designs)
Threat Reduction

Nucleosynthesis (fission recycling in SN)



Computational Challenges for DFT





- Self-consistency = **iterative process**:
  - Not naturally prone to parallelization
  - Computational cost :

(number of iterations) × (cost of one iteration)

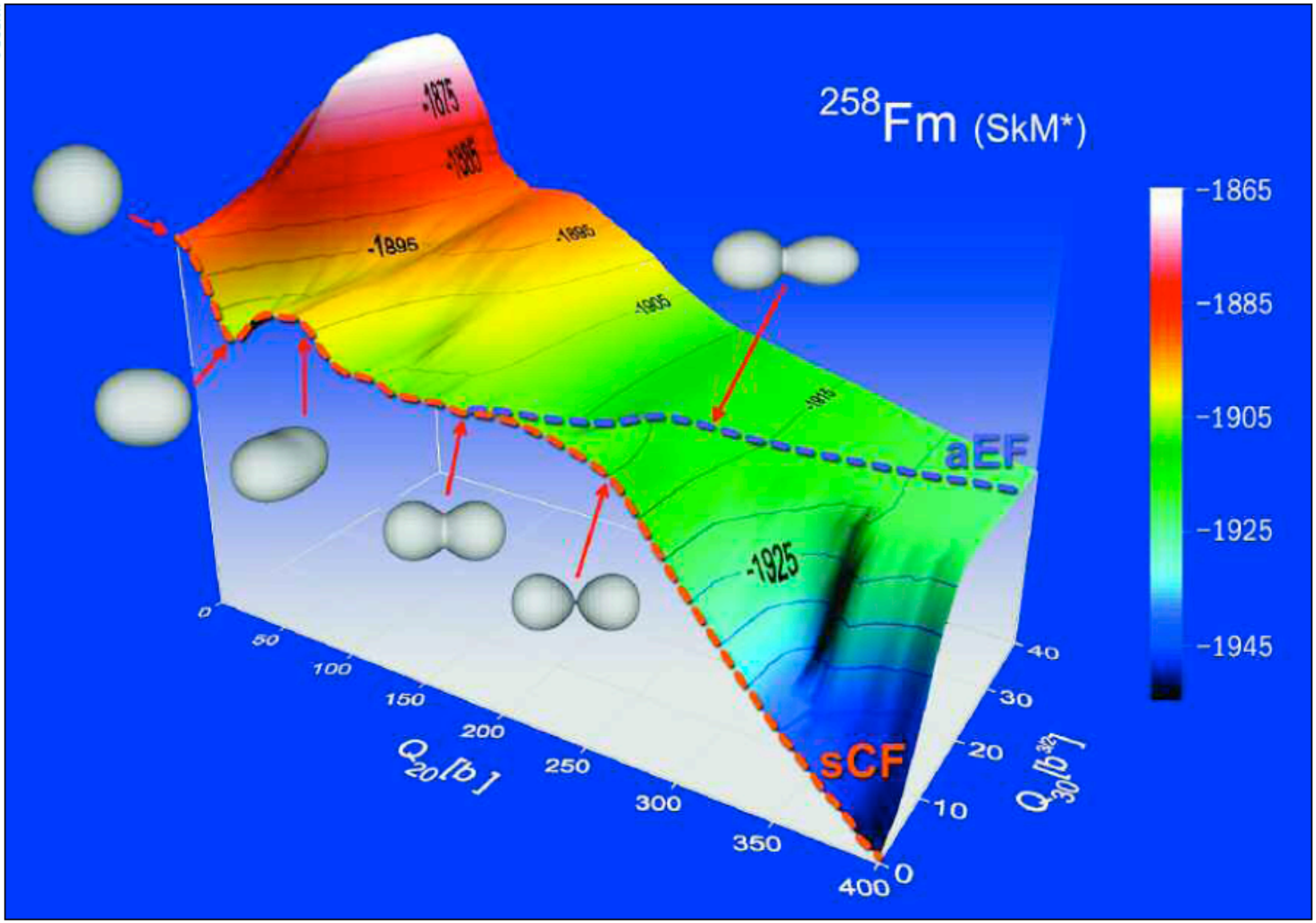
Cost of symmetry breaking: triaxiality, reflection asymmetry, time-reversal invariance

  - **Large dense matrices** (LAPACK) constructed and diagonalized many times – size of the order of (2,000 x 2,000) – (10,000 x 10,000)
  - Many **long loops (threading)**

- Finite-range forces/non-local functionals: exact Coulomb, Yukawa-, Gogny-like
  - Many **nested loops (threading)**
  - Precision issues

Nazarewicz, Schunk, More, …

Fission Energy Surface and Fission Pathways



Dynamics

Time Dependent Superfluid LDA

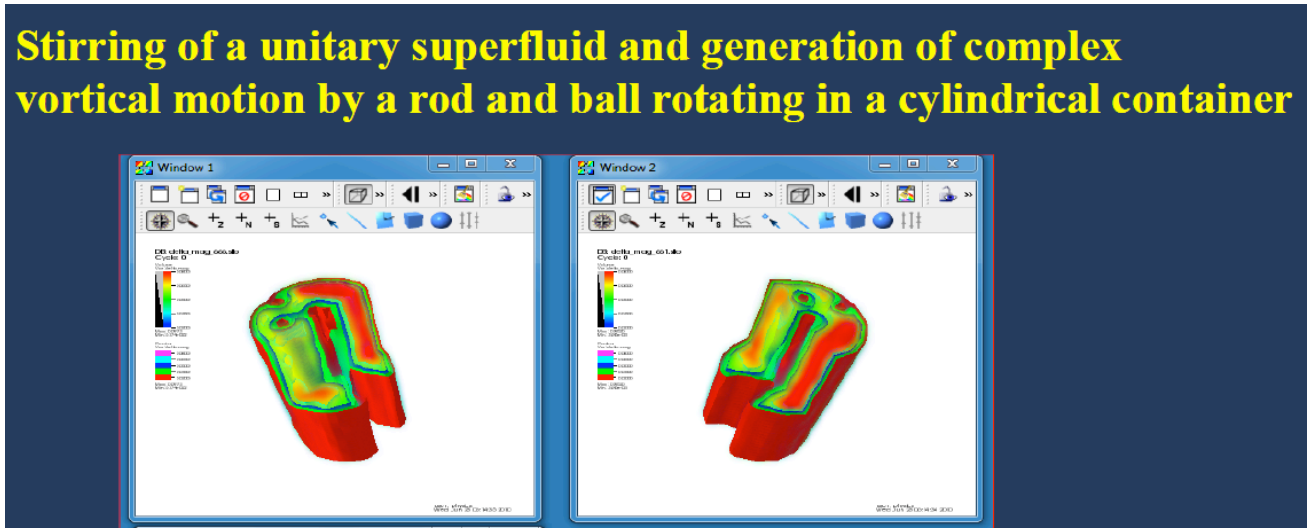
Bulgac, Forbes, Magierski, Luo, Roche, Stetcu, Yu (UW, PPNL,..)

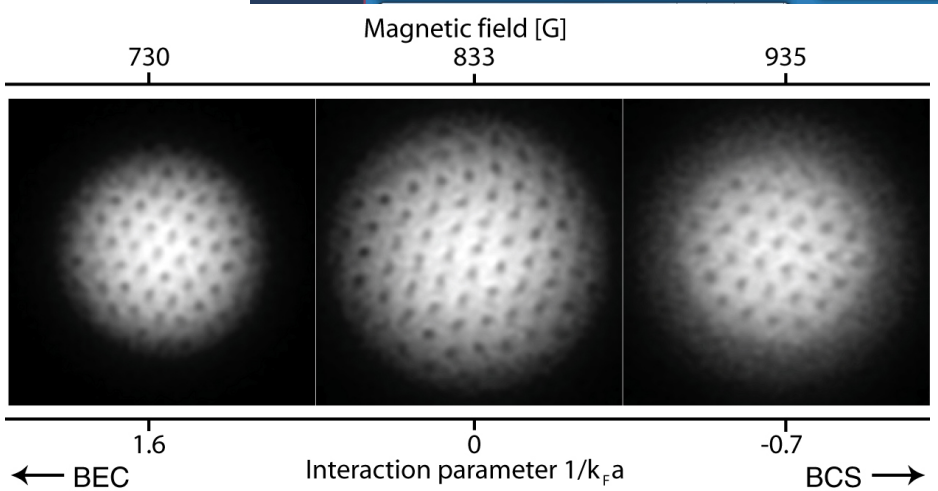
Equations on 3D spatial lattice

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{n\uparrow}(\vec{r},t) \\ u_{n\downarrow}(\vec{r},t) \\ v_{n\uparrow}(\vec{r},t) \\ v_{n\downarrow}(\vec{r},t) \end{pmatrix} = \begin{pmatrix} \hat{h}_{\uparrow\uparrow}(\vec{r},t)-\mu & \hat{h}_{\uparrow\downarrow}(\vec{r},t) & 0 & \Delta(\vec{r},t) \\ \hat{h}_{\downarrow\uparrow}(\vec{r},t) & \hat{h}_{\downarrow\downarrow}(\vec{r},t)-\mu & -\Delta(\vec{r},t) & 0 \\ 0 & -\Delta^*(\vec{r},t) & -\hat{h}^*_{\uparrow\uparrow}(\vec{r},t)+\mu & -\hat{h}^*_{\uparrow\downarrow}(\vec{r},t) \\ \Delta^*(\vec{r},t) & 0 & -\hat{h}^*_{\downarrow\uparrow}(\vec{r},t) & -\hat{h}^*_{\downarrow\downarrow}(\vec{r},t)+\mu \end{pmatrix}\begin{pmatrix} u_{n\uparrow}(\vec{r},t) \\ u_{n\downarrow}(\vec{r},t) \\ v_{n\uparrow}(\vec{r},t) \\ v_{n\downarrow}(\vec{r},t) \end{pmatrix}$$

Applications: Nuclear Physics,
Cold Atom Experiments, ...

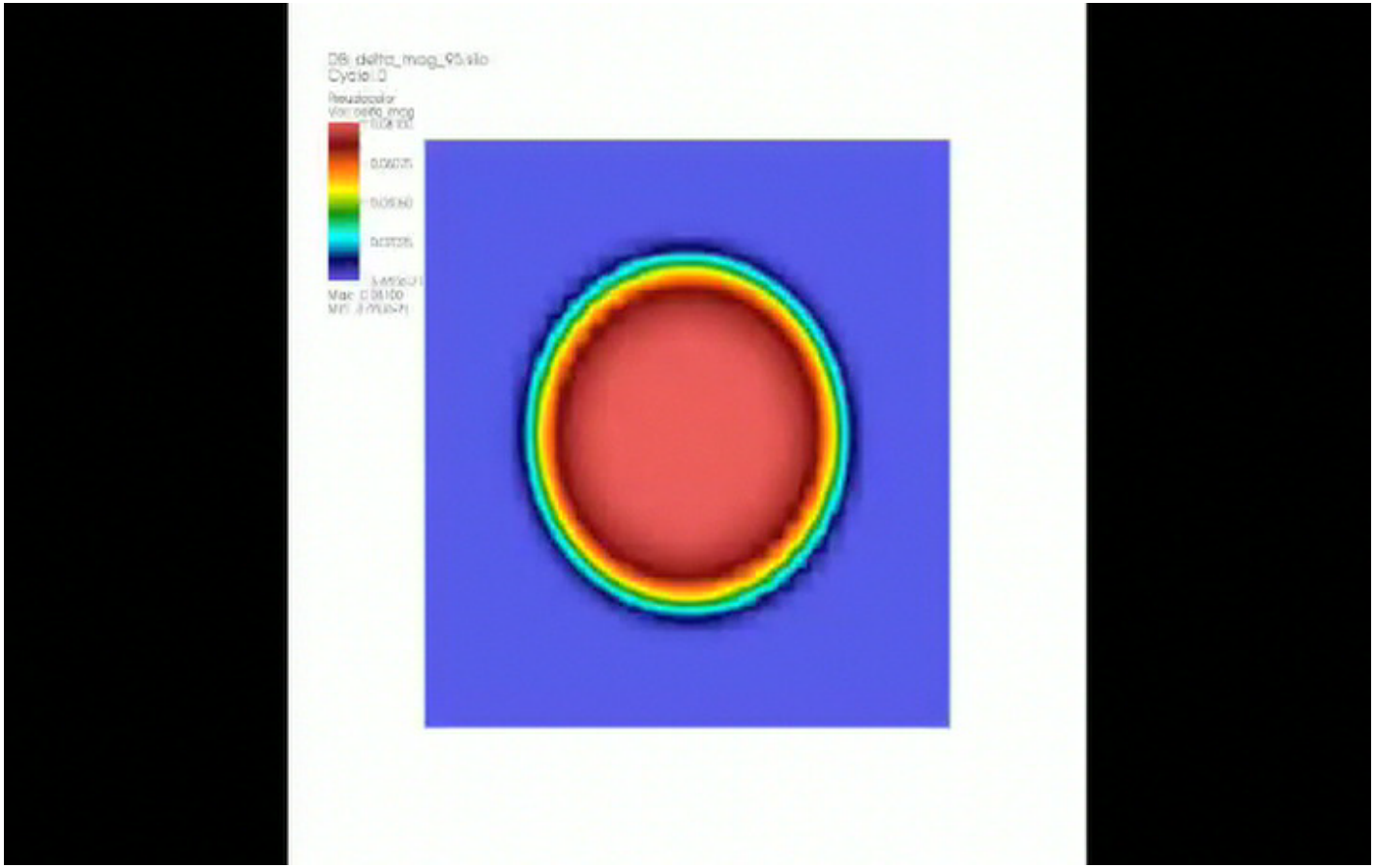
Calculations on Jaguar 32x32x32 spatial lattice
10K-100K time steps
30K-40K quasiparticle orbitals

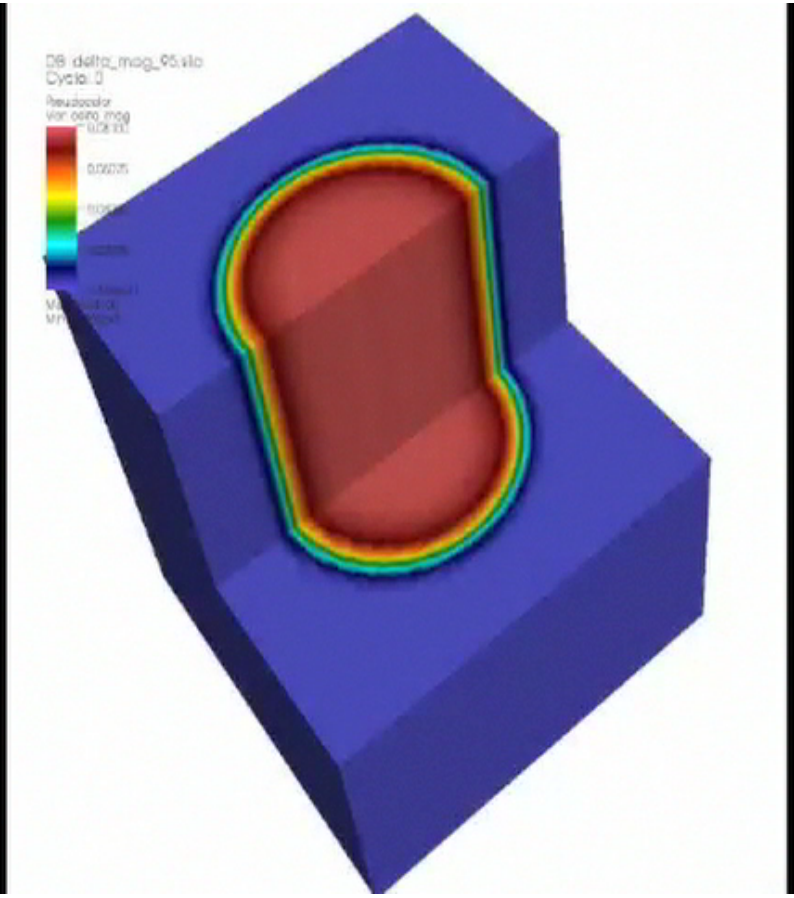




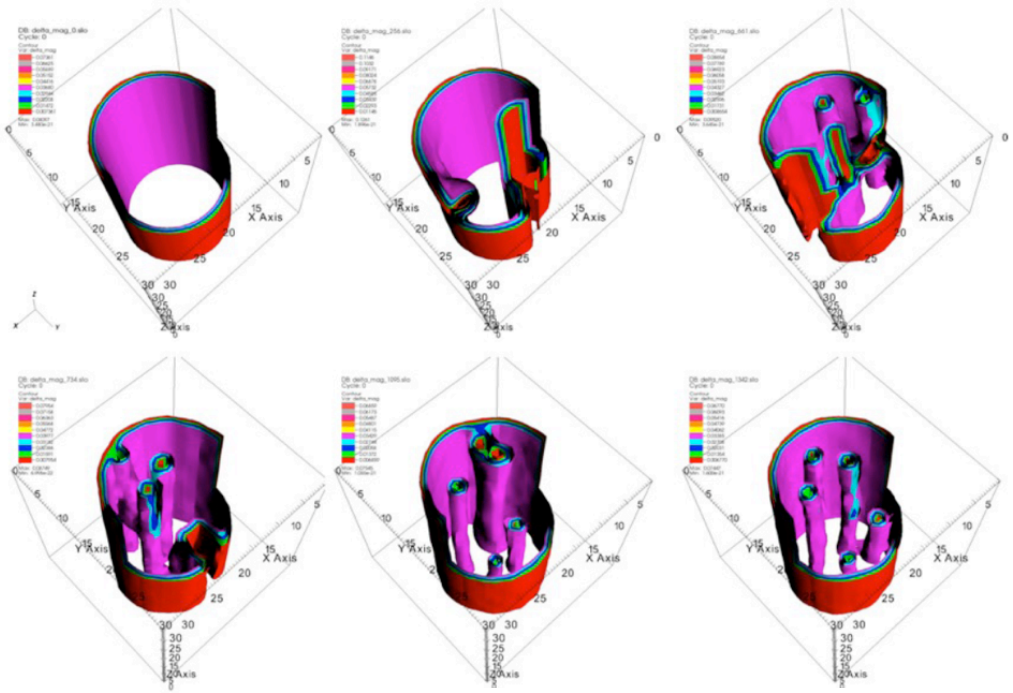
Ketterle, MIT, 2005

Vortex Formation : 2D Symmetry




DB: delta_mag_95.silo
Cycle: 0
Pseudocolor
var: delta_mag

Numerical Studies of Vortex Formation and Dynamics in Superfluid Fermi Systems



62^3 lattice
220K quasi-particle wvfn
97% of Jaguar

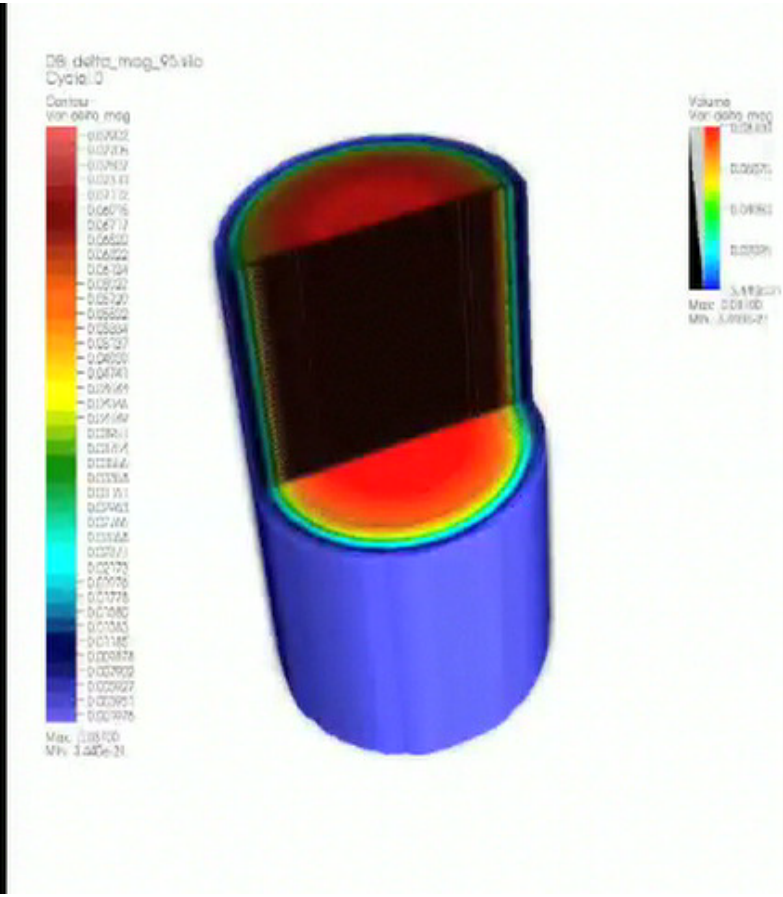
Benchmark(1) on JaguarPF for ASCR's OMB PART Software Effectiveness Metric: UG Problem

5216 particles ; 103,917 wavefunctions ; 50x50x100 lattice ; 2,051 (100K) time steps ; 26 I/O events of analysis data

Solver (Run1)
- 51 parallel , parallel groups
- 144 PEs / group
- simultaneous vs in sequence, perfect strong scaling
- 129 iterations to converge

TD (Run2)
- initialize (read soln) TD code
- 1 time step
- 1 data analysis io event
- checkpoint TD wavefunctions
  - 8TB data written
  - 24 Lustre write groups

TD (Run3)
- restart TD code
- 2050 time steps
- 25 data analysis io events
- clean exit


DB: delta_mag_95.vlo
Cycle: 0
Contour
Var: delta_mag
Volume
Var: delta_mag

Outlook

Present:

Nuclear Structure - Light Nuclei
- Large Neutron-Rich Nuclei
- Nucleonic Matter

Moving toward dynamics
- reactions for basic & applied physics
- fusion and fission
- beyond nuclear physics