Computing Nuclei: Present Status, Future Prospects

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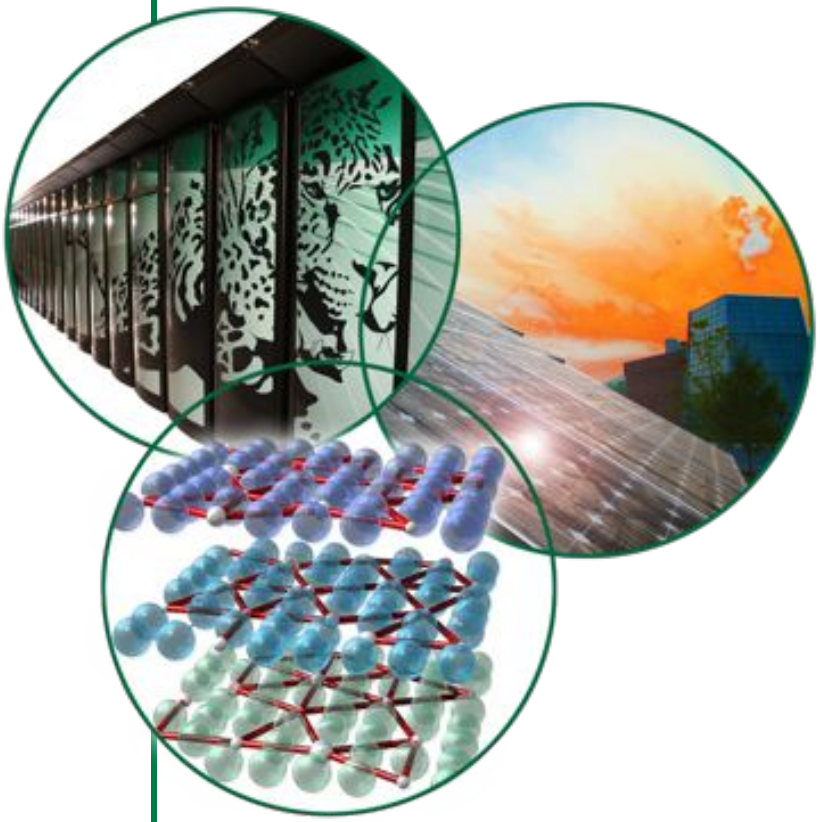
ACSS workshop



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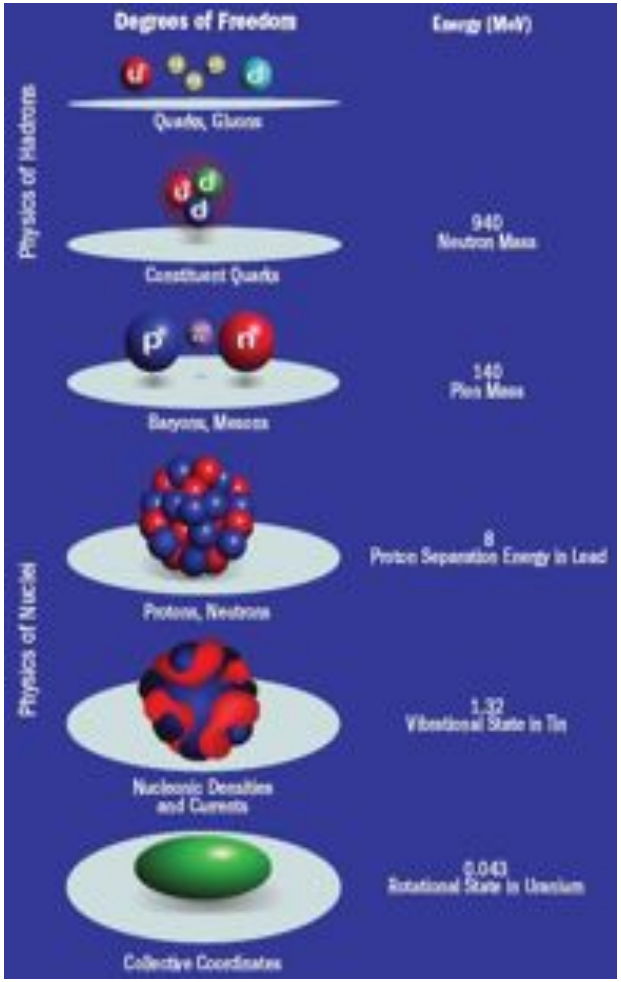
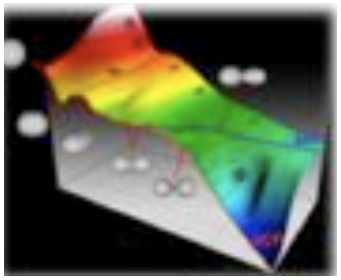
Outline

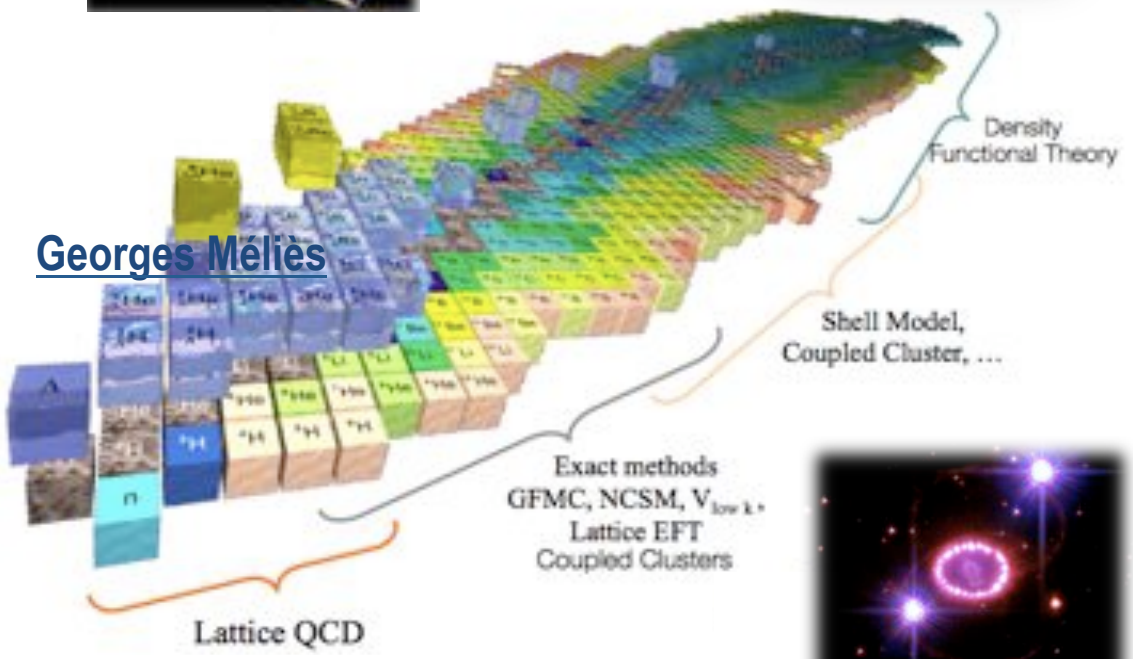
- The Physics
- Where we are:
  - Nuclear Density Functional Theory
  - Nuclear Coupled Cluster theory
- Prospects for the future

The Physics

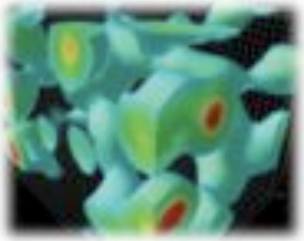
Thematic unification of nuclear physics







Georges Méliès



Some unresolved physics questions

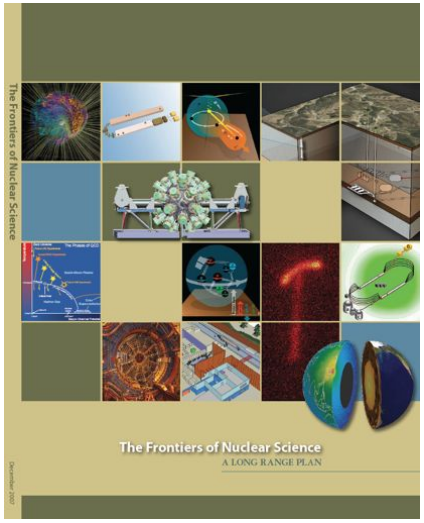
- What is the nature of the nuclear force that binds protons and neutrons into stable nuclei and rare isotopes?
- What is the origin of simple patterns in complex nuclei?
- What is the origin of the elements in the cosmos?
- What is the nature of neutrinos?

Forces

Structure

Origins

Application



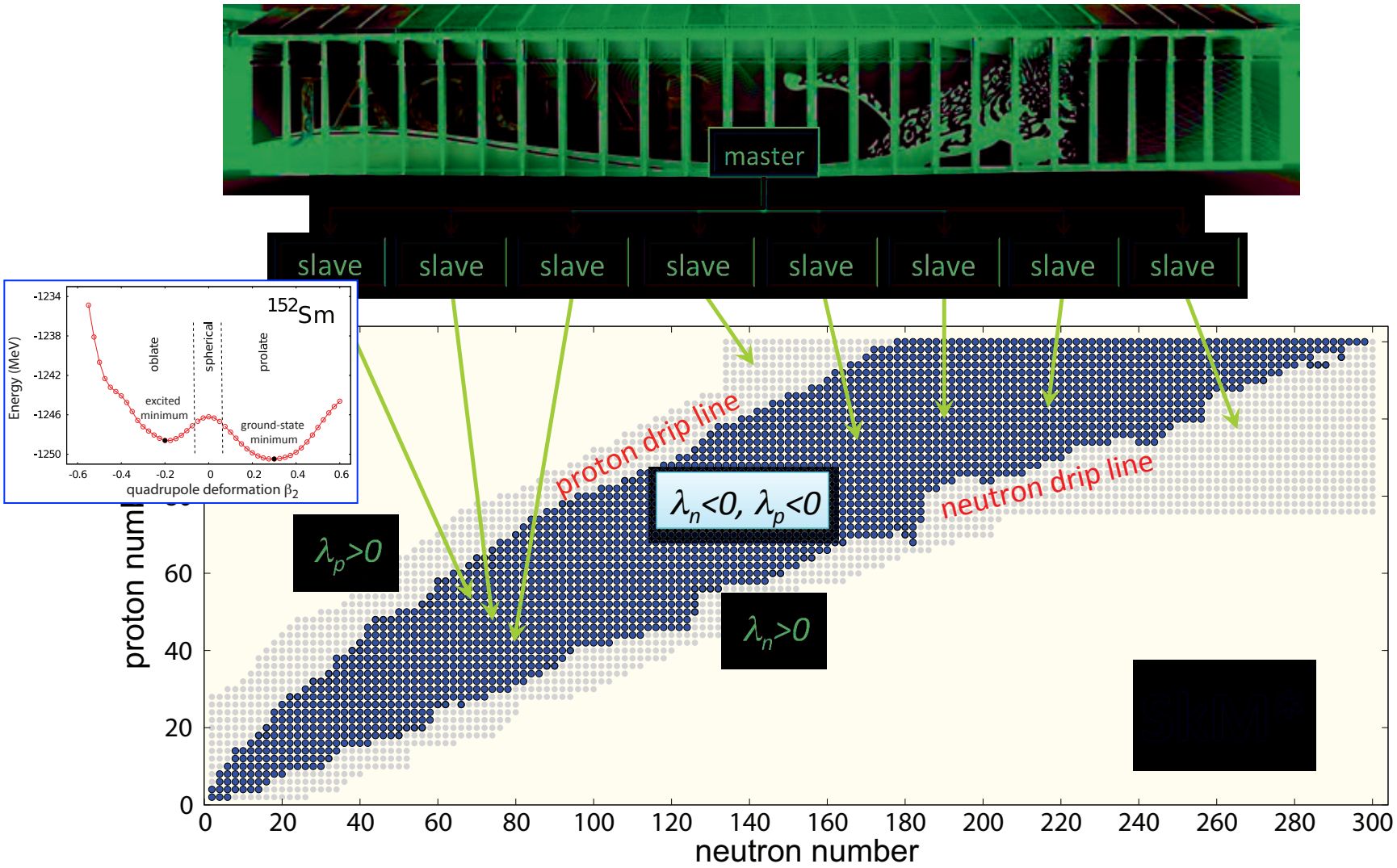
Cannot synthesize all elements created in stellar explosions
Require accurate descriptions for certain applications
→ PREDICTIVE Theory

Where we are: Nuclear Density Functional Theory

Degree of freedom: nuclear densities and quasiparticle densities (think HFB)

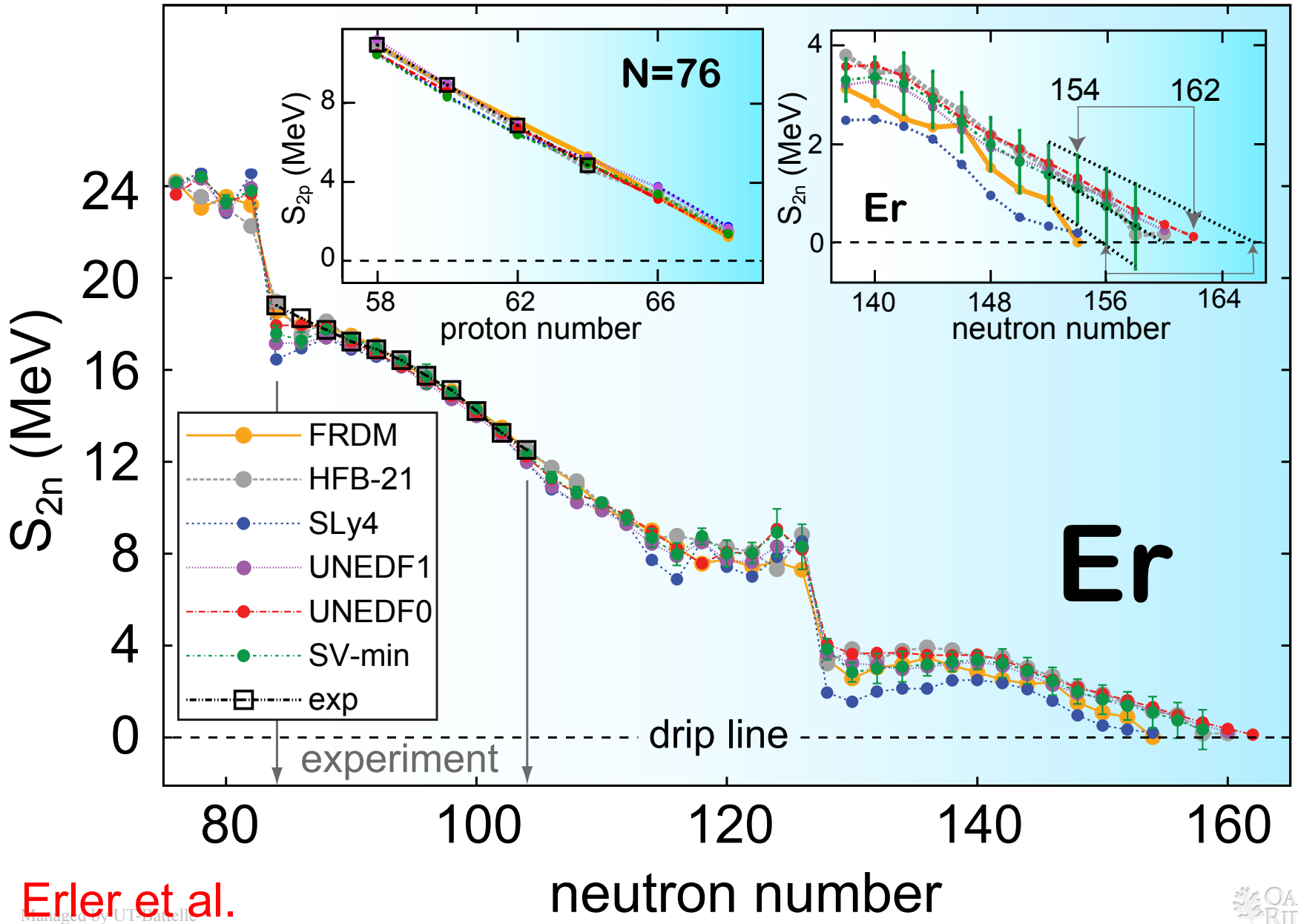
Example: Large Scale Mass Table Calculations

HFB+LN mass table, HFBTHO



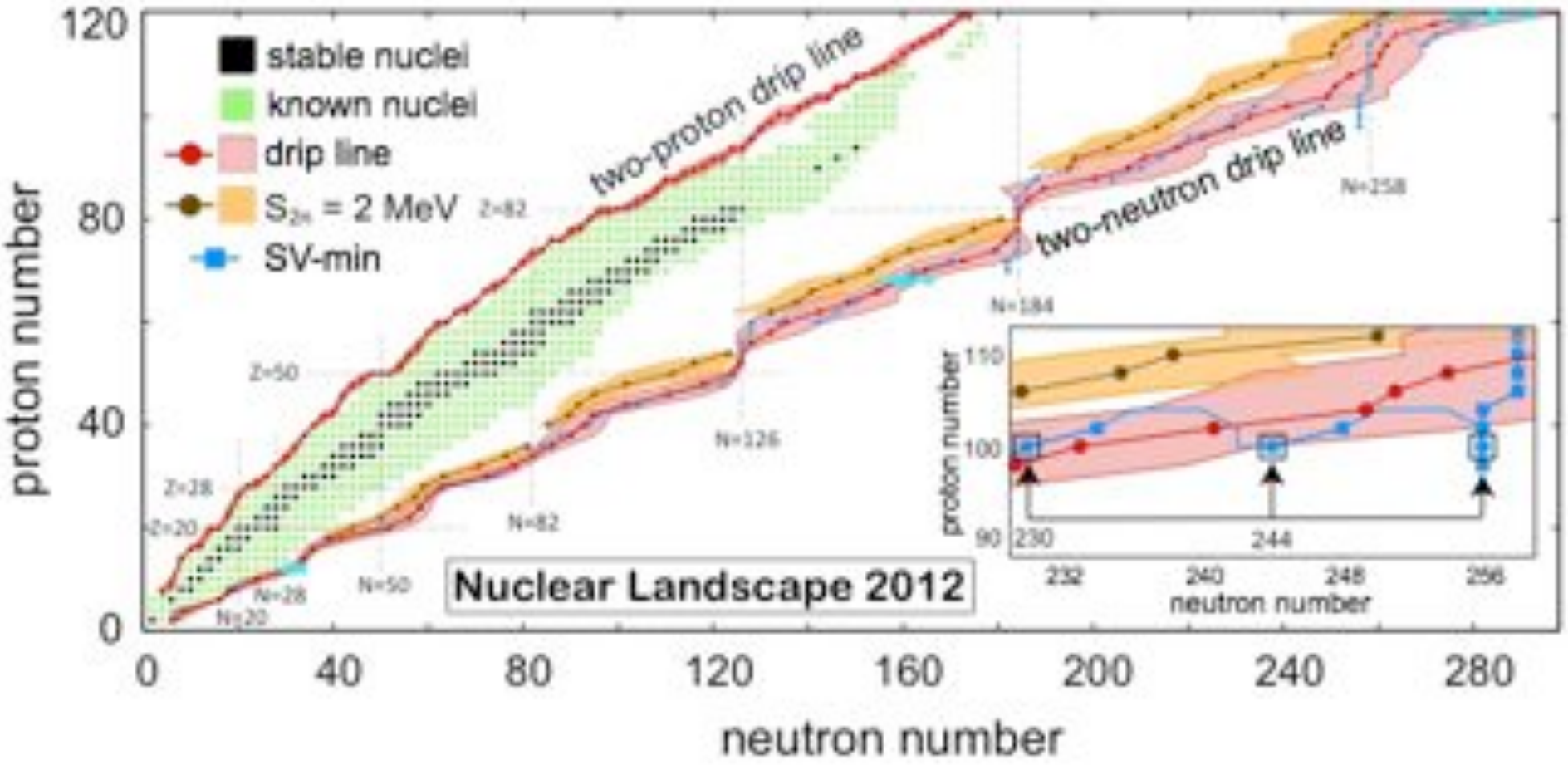
- 5,000 even-even nuclei, 250,000 HFB runs, 9,060 processors – about 2 hours
- Full mass table: 20,000 nuclei, 12M configurations — full JAGUAR

Where is the neutron drip line? UQ in action



Erler et al.

Nuclear DFT Benchmark 2012



How many protons and neutrons can be bound in a nucleus?

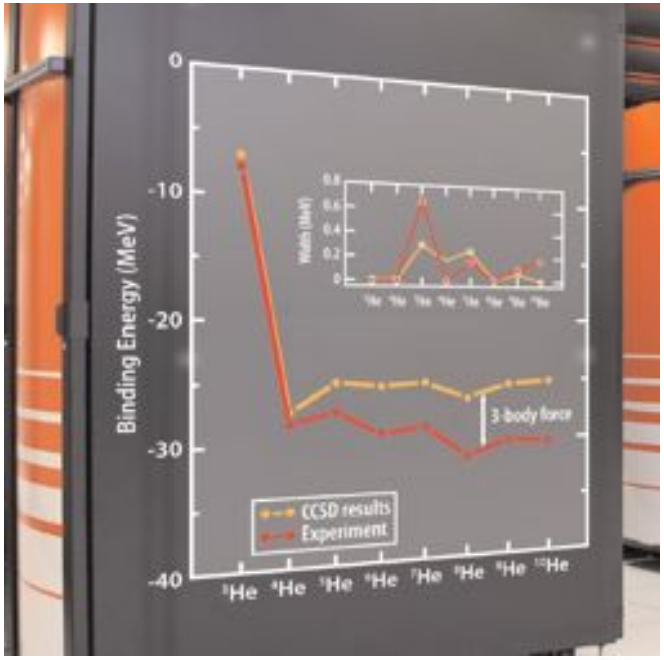
6900±500

Where we are: Nuclear Coupled Cluster Theory

Degrees of freedom: protons and neutrons (nucleons)

Nuclear Coupled Cluster Theory: 2001 – 2010

- First paper, 2004, Dean & Hjorth-Jensen...laid out some things we wanted to do. Followed by exploratory papers with chemists (PRLs, PRC)…
- Major steps forward (2007-2010, all Hagen et al.):
  - 3-body hamiltonians
  - CC in the continuum
  - CC benchmark (2-body) through Ca-40
  - Solution to center of mass problem
- I went to DC…Gaute now leads the effort…

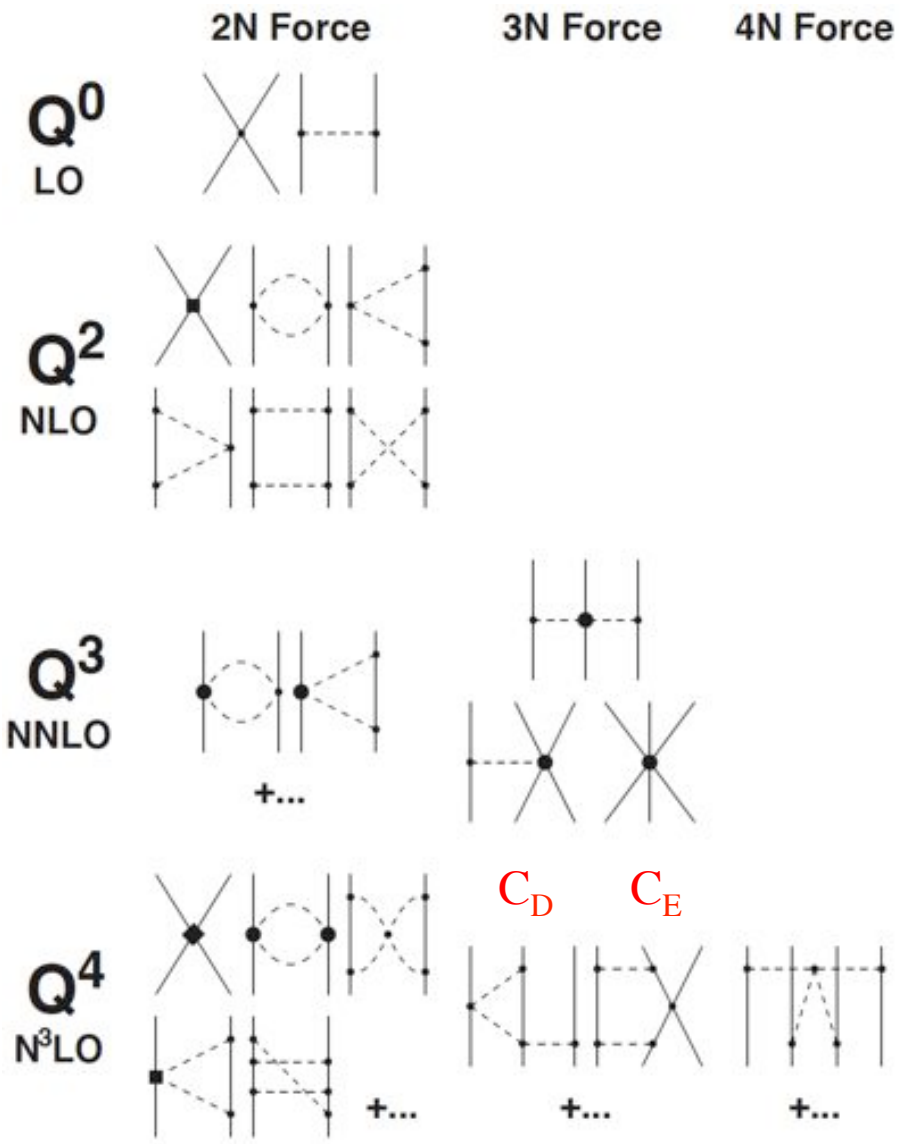


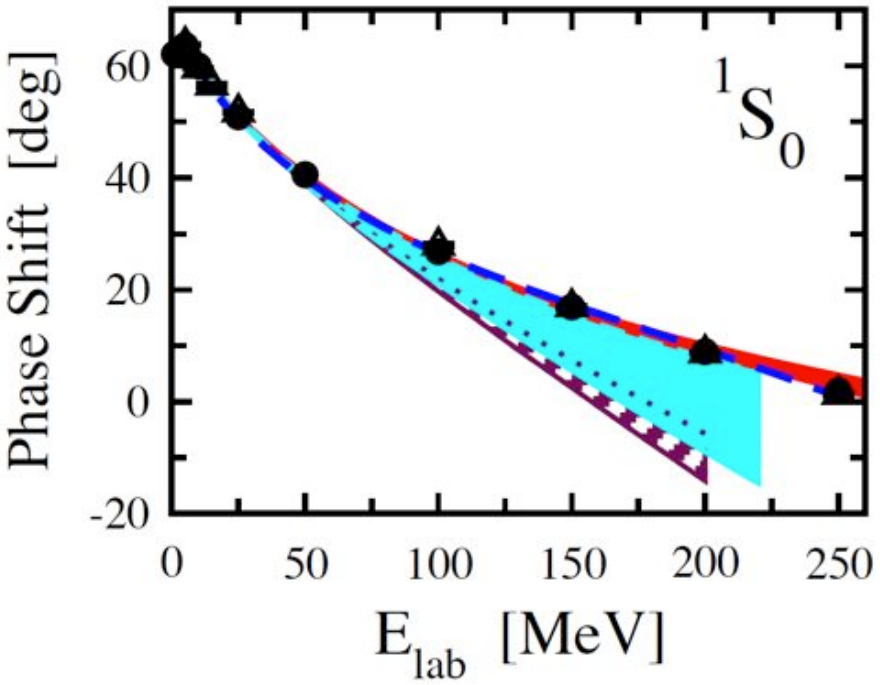
What does it take for CC…

- Excellent scientists and computational science ties
- A “GOOD” Hamiltonian
- A “machine appropriate” algorithm
  - Evolves over time
  - HW design affects algorithms
- Today:
  - 150k cores to look at one nucleus at current model spaces
  - Bundled runs across ~20k cores…oscillator parameter varied
  - CCSD scaling (with symmetry)
  - Λ-CCSD(T) scaling

Nuclear Hamiltonian from chiral effective field theory

[Weinberg; van Kolck; Epelbaum *et al*.; Entem & Machleidt; …]





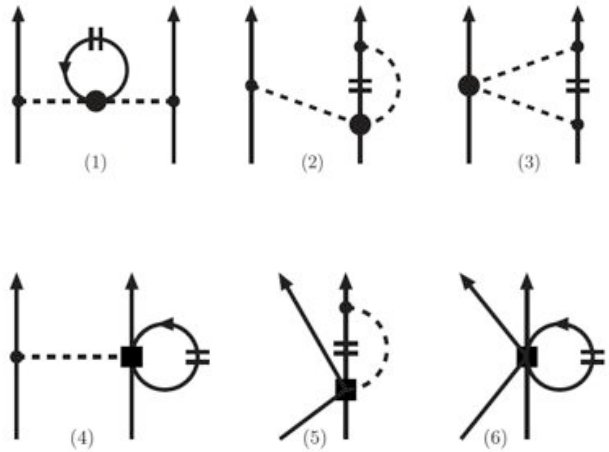
[Epelbaum, Hammer, Meissner RMP 81, 1773 (2009)]

Low energy constants from fit of NN data, A=3,4 nuclei, or light nuclei.

Oxygen isotopes from chiral interactions

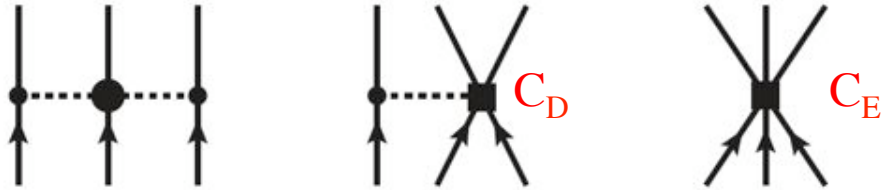
- Integrate over the third leg in infinite nuclear matter
- Derive density dependent corrections to the nucleon-nucleon interaction

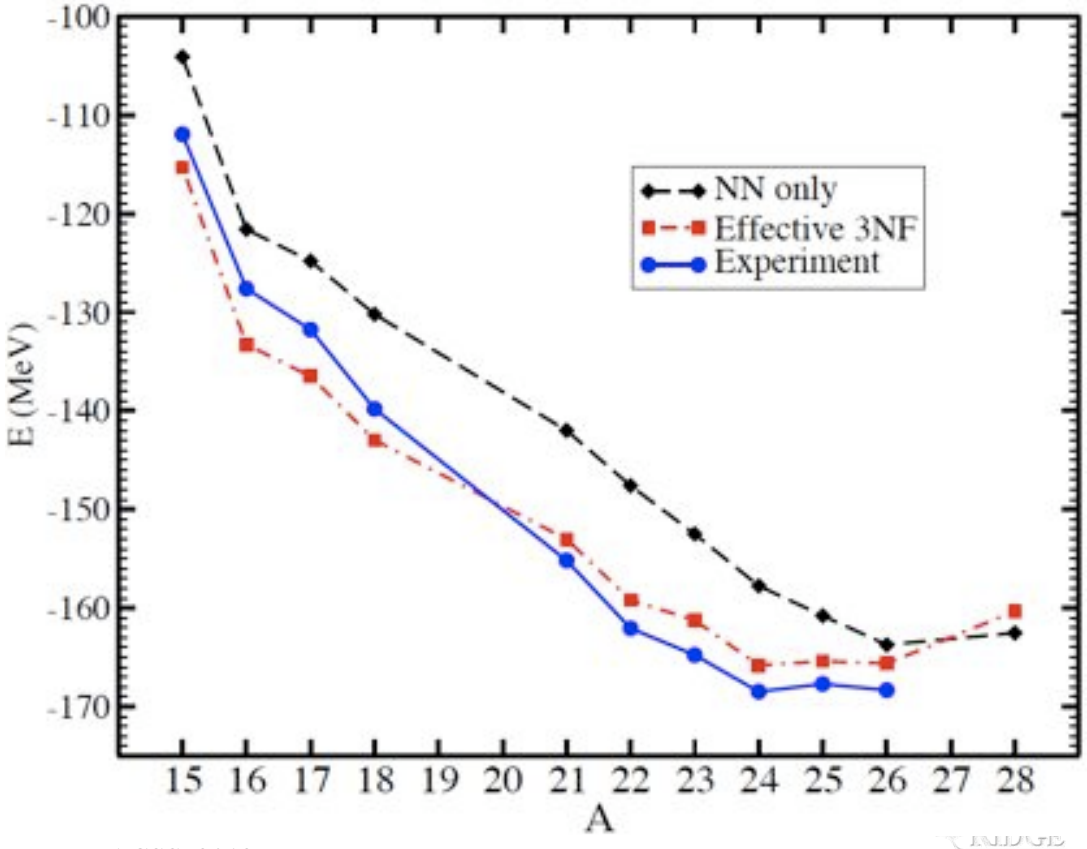
J. Holt . Phys.Rev.C81, 024002, (2010)



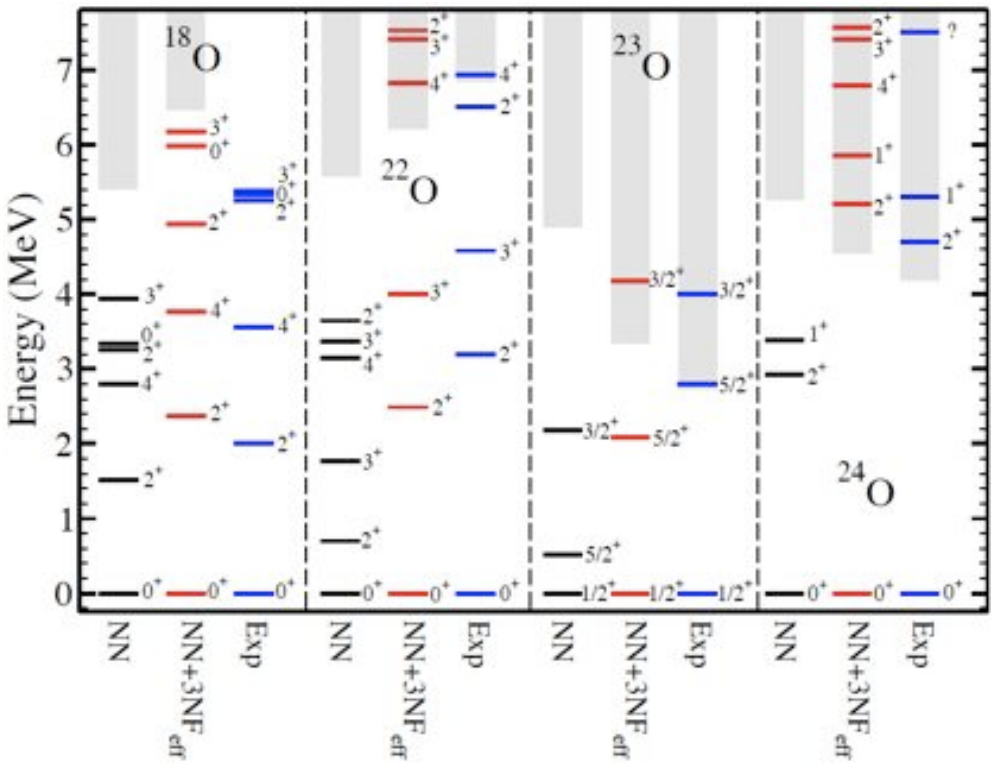
G. Hagen, M. Hjorth-Jensen, G. R. Jansen, R. Machleidt, T. Papenbrock
PRL, in press (2012)

Chiral three-nucleon force at order N2LO
C_D = 0.2, C_E = 0.7 (fitted to to the binding energy of ^{16}O and ^{24}O).





Oxygen isotopes from chiral interactions



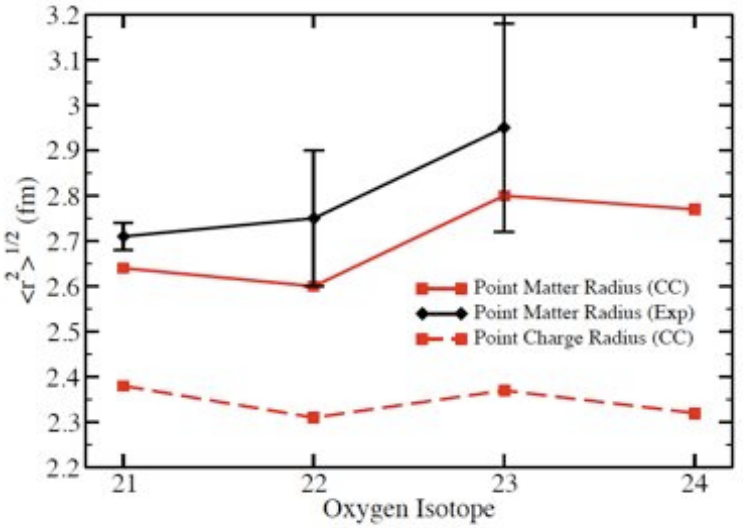
- three-nucleon forces decompress the spectra
- good agreement with experiment

We predict the newly observed resonance at 7.5MeV in ^{24}O to be a super position of several states with spin and parity 4^+,3^+,2^+

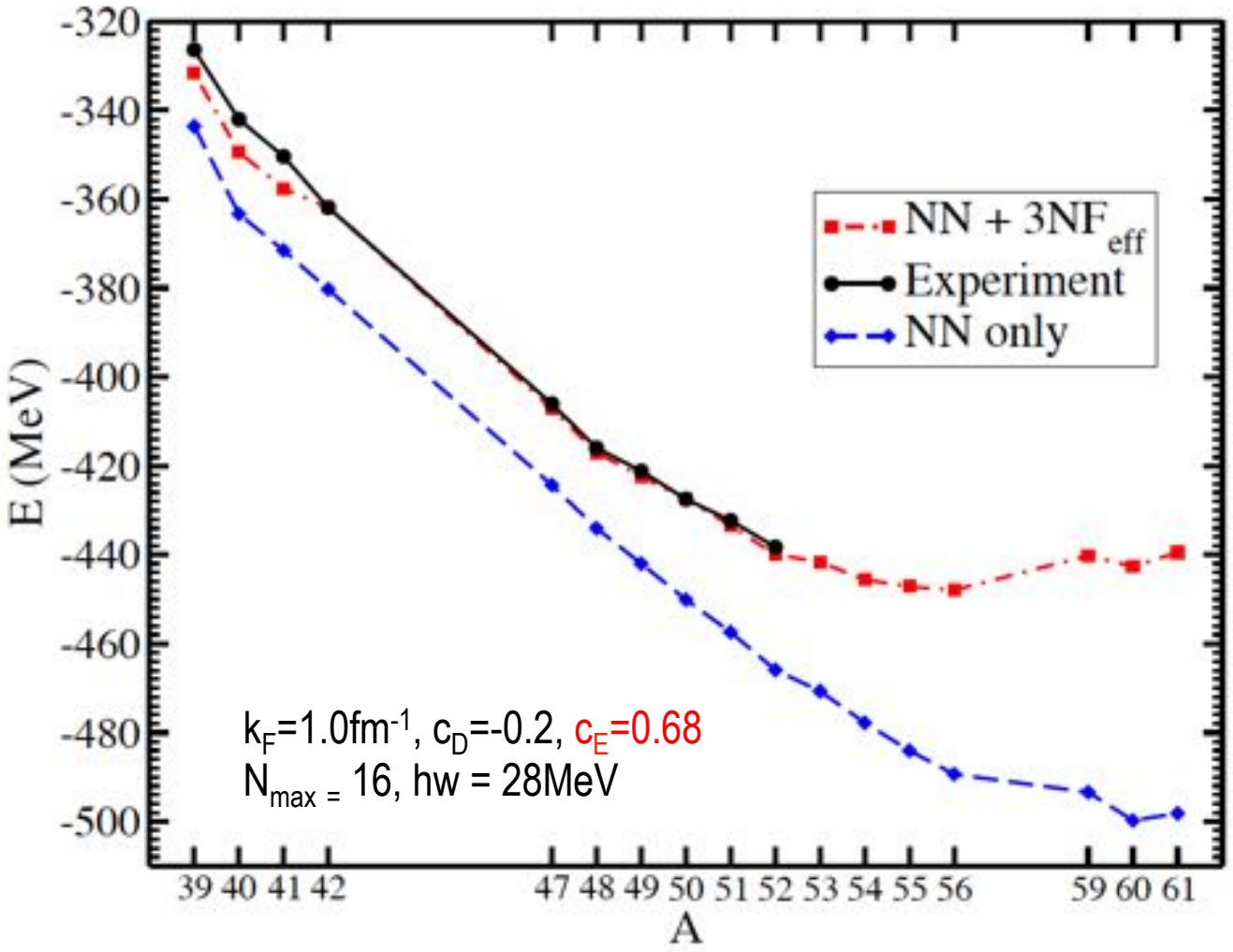
Excited states in ^{24}O computed with EOM-CCSD and Compared to experiment

J^π	2_1^+	1_1^+	4_1^+	3_1^+	2_2^+	1_2^+
E_{CC}	5.2	5.9	6.8	7.4	7.6	8.9
E_{Exp}	4.7(1)	5.33(10)				
Γ_{CC}	0.03	0.05	0.006	0.02	0.04	0.57
Γ_{Exp}	$0.05^{+0.21}_{-0.05}$	$0.03^{+0.12}_{-0.03}$				

Matter and charge radii for $^{21\text{-}24}$O Computed from intrinsic densities and Compared to experiment.



Calcium isotopes from chiral interactions

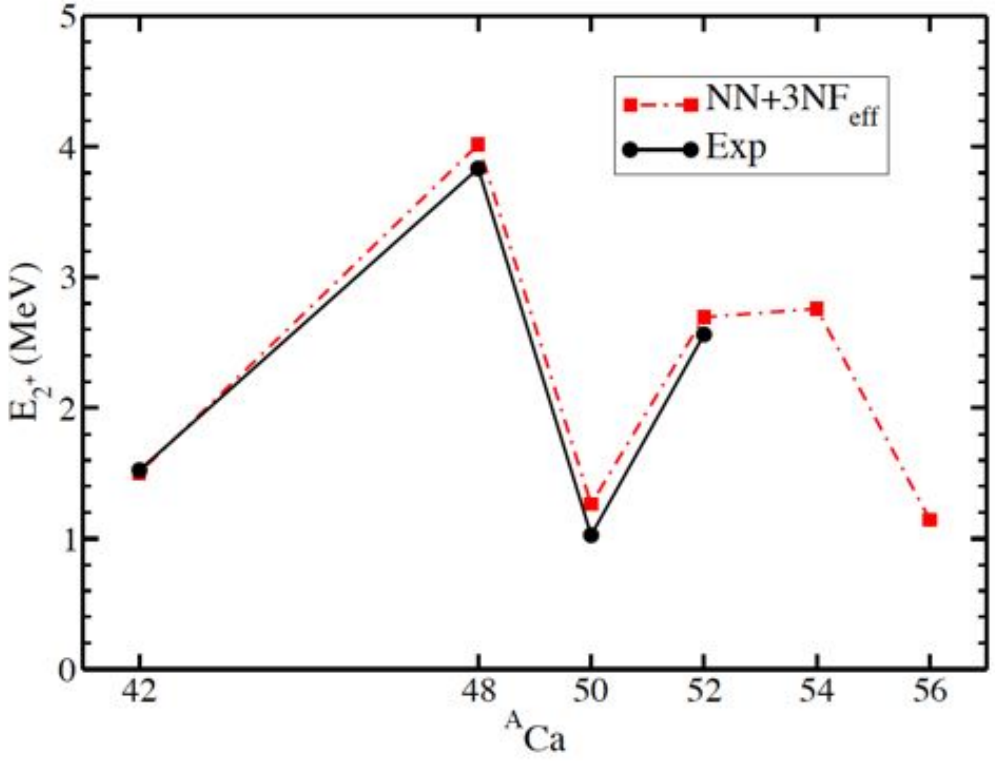


Main Features:

1. Total binding energies agree very well with experimental masses.
2. Masses for $^{40\text{-}52}$Ca are converged in 17 major shells.
3. ^{60}Ca is not bound in 19 major shells.

G. Hagen, M. Hjorth-Jensen, G. R. Jansen, R. Machleidt, T. Papenbrock, in preparation (2012)

2+ systematics in Calcium isotopes from chiral interactions



Main Features:

1. Very nice agreement between theory and experiment.
2. Our calculations for 2^+ and 4^+ in ^{54}Ca do not point to a new magic shell closure.

G. Hagen, M. Hjorth-Jensen, G. R. Jansen, R. Machleidt, T. Papenbrock, in preparation (2012)

	^{48}Ca			^{52}Ca			^{54}Ca		
	2^+	4^+	$4^+/2^+$	2^+	4^+	$4^+/2^+$	2^+	4^+	$4^+/2^+$
CC	4.02	4.67	1.13	2.70	5.349	1.92	2.76	5.83	2.16
Exp	3.83	4.50	1.17	2.56	?	?	?	?	?

“Machine appropriate” algorithms

2001-2003

- M-scheme code “unrestricted symmetry”
- Single and multi-core parallel
- CCSD

2003-2008

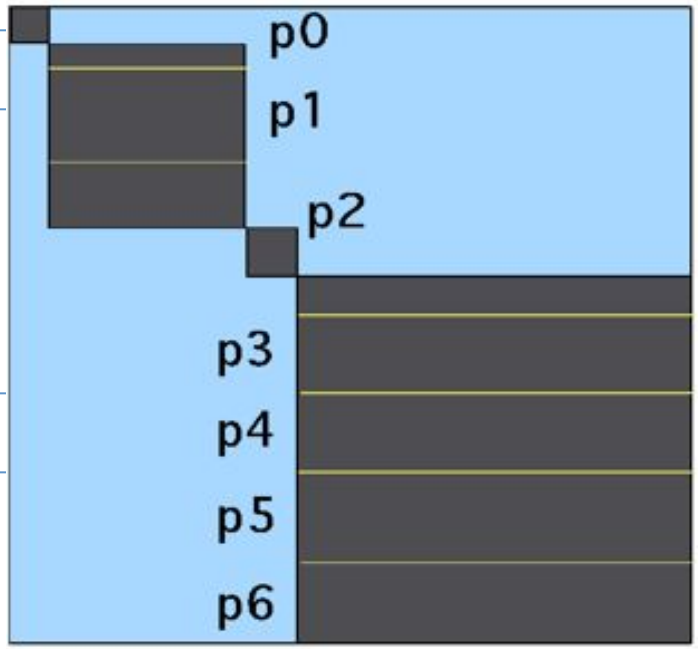
- Multi core
- Continue “M”-scheme code; CCSD, EOM, CCSD(T), A+/-1
- Begin imposing rotational Symmetry (J-coupled)

2008-2011

- Less memory/core → J-coupled becomes workhorse
  - MPI/Open MP development
  - Λ-CCSD(T), densities, spectroscopy
- M-scheme used in time-dependent development

2012

- CPU/GPU will cause another rewrite

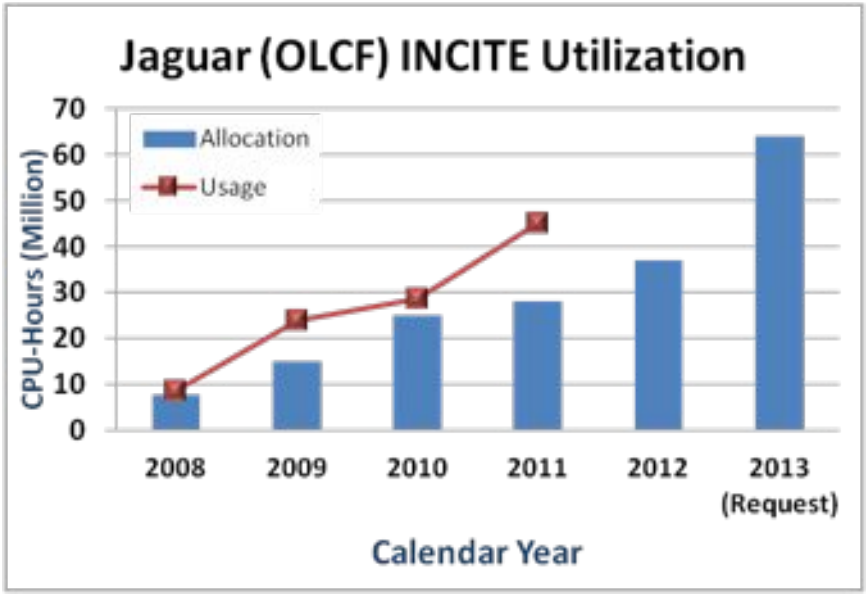


Recent work on triples speedups:
Hagen and Nam, arxiv.org/pdf/1203.3765.pdf

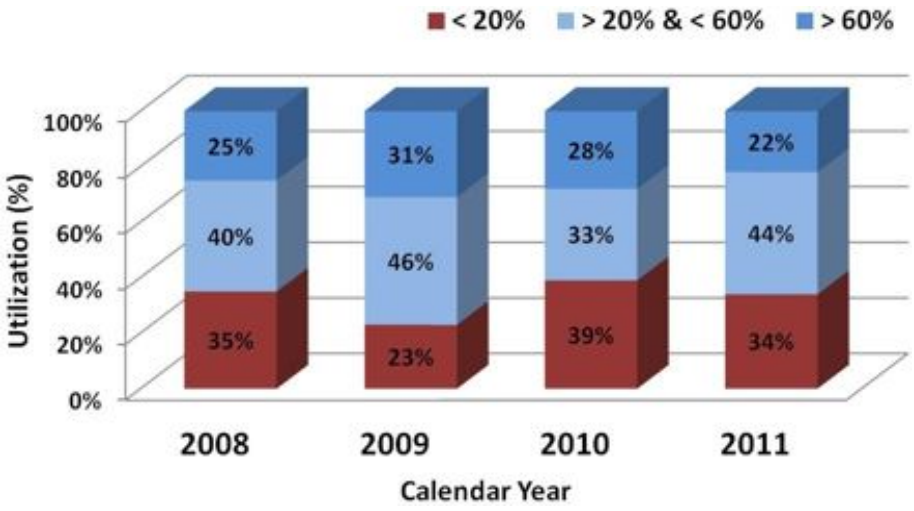
Prospects for the future

Nuclear Structure INCITE on Jaguar; UNEDF SciDAC

- Three basic codes fold into INCITE
  - Shell Model (CI) James Vary
  - Nuclear DFT (Nazarewicz)
  - Coupled Cluster
- UNEDF (SciDAC-II) played a major role in developments; 9 universities, 7 national labs



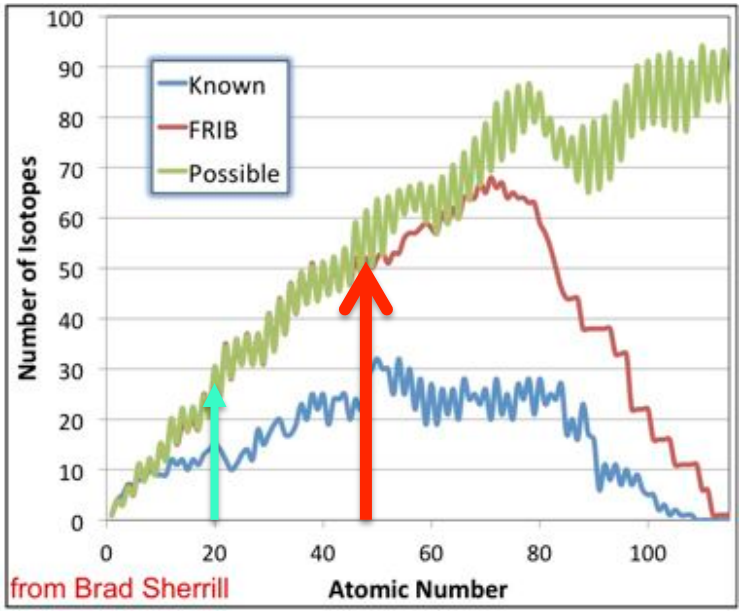
For a popular description of UNEDF, see:
• SciDAC Review Winter 2007
http://www.scidacreview.org/0704/pdf/unedf.pdf
• Nucl. Phys. News 21, No. 2, 24 (2011)

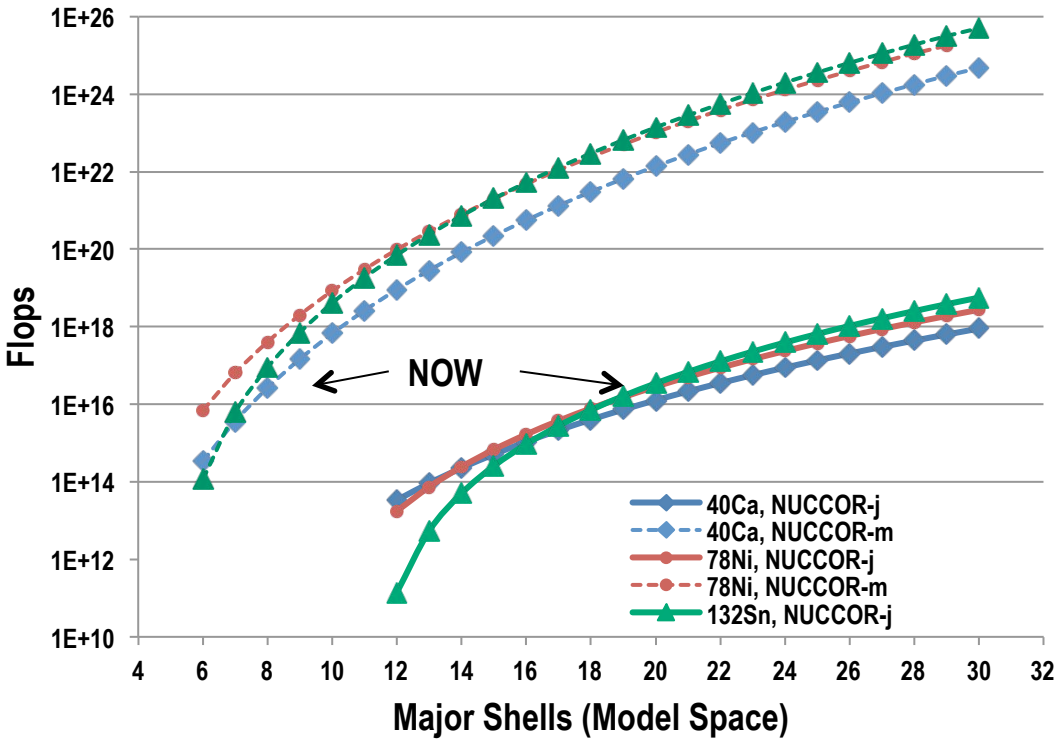


54 Papers in 2011, 6 in 2012: 1 Science, 15 PRL

Coupled-cluster scaling

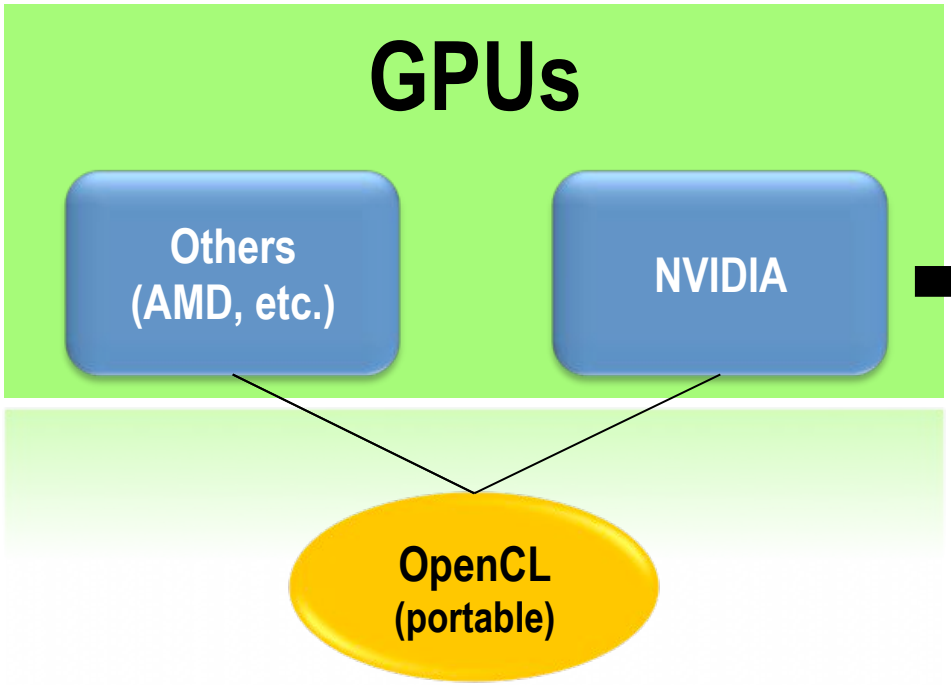
- System of non-linear coupled algebraic equations: solve by iteration; lots of matrix-matrix and matrix-vector multiplies
  - CCSD $O(n^2N^4)$ (n=number of nucleons; N=size of space)
  - Λ-CCSD(T) $O(n^2N^5)$
- Rotational symmetry
  - REDUCED by power of 2/3





Major Shell	8	20	30
J-coupled	72	420	930
M-scheme	480	6160	19720

Acceleration Options on Jaguar XK6



GPU Programming Tools		
CUDA C (NVIDIA)	CUDA Fortran (PGI)	Compiler Directives* • Cray • PGI • CAPS HMPP

*(Cray, PGI, HMPP will adopt the same OpenACC standard. They do not have a common syntax now.)

Accelerated Libraries**			
Libsci_acc (Cray)	MAGMA (ICL/ UT) (GNU)	CULA (EM Photonics)	cuBLAS/ cuSparse (NVIDIA)

** Libraries are based on CUDA

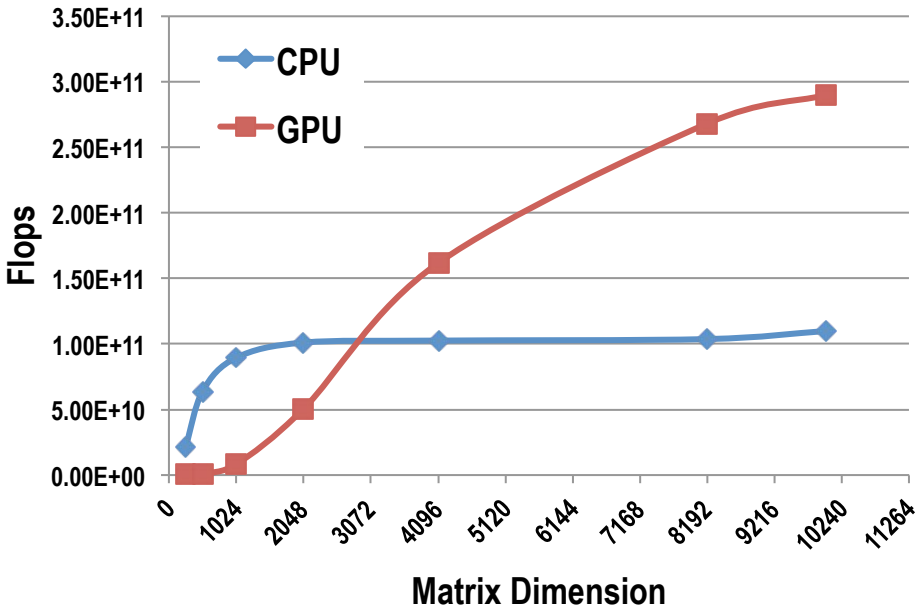
Accelerating CC equations

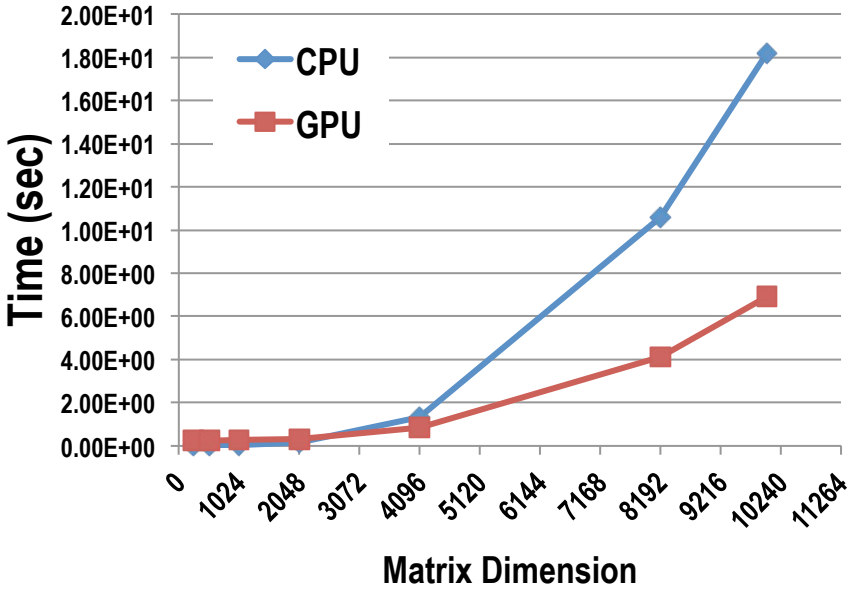
Basic numerical operation:

$$t_{new}(ab, ij) = \sum_{\substack{k,l=1,n \\ c,d=n+1,N}} V(kl, cd) t_{old}(cd, ij) t_{old}(ab, kl)$$

Many such terms exist
Use matrix-matrix multiply algorithm

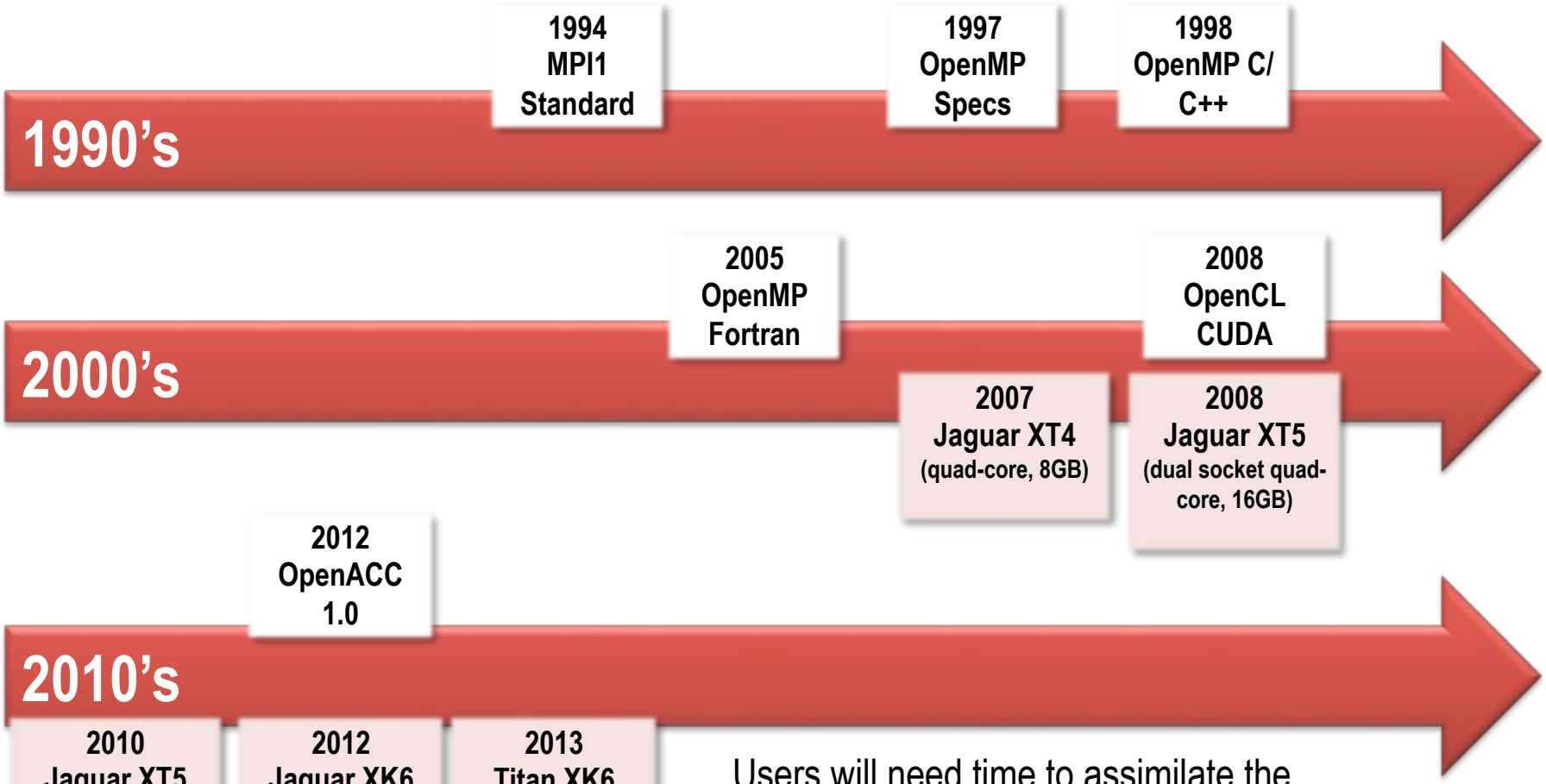
- A first foray into accelerators
  - Libsci_acc (Cray)
  - OpenACC, cce
- Modified DGEMM in t2 eq.
- 1 MPI process + 16 OpenMP threads vs. 1 MPI process + GPU per node
- Time for a single iteration (~30+ iterations for convergence)





Time to mature

OpenMP/MPI are supported on a variety of architectures with C/C++/ Fortran



Users will need time to assimilate the architectural changes into applications and allow tools to become refined.
There is a lot of potential.

Final notes

- Excellent science to do!
- For faster adoption of GPUs across disciplines
  - Improve GPU Programming tools (i.e. directives, libraries)
    - Standardization
    - Increased documentation/examples
    - Portability
  - What is the “MPI” for GPUs (robust/portable)?
- Codes can be restructured as we know the rules
  - i.e. use of allocatable derived types does not work with GPU directives
  - Size of data/work on GPUs is crucial