Ab-initio Summary

Year-5 Deliverables (from Year-4 annual report summary)

Further calculate homogeneous neutron matter and neutron drops in external fields using GFMC and AFDMC to create pseudo-data for constraining energy density functionals. Calculate the Hoyle state with GFMC.

Continue improvements to ADLB resulting in community usable code.

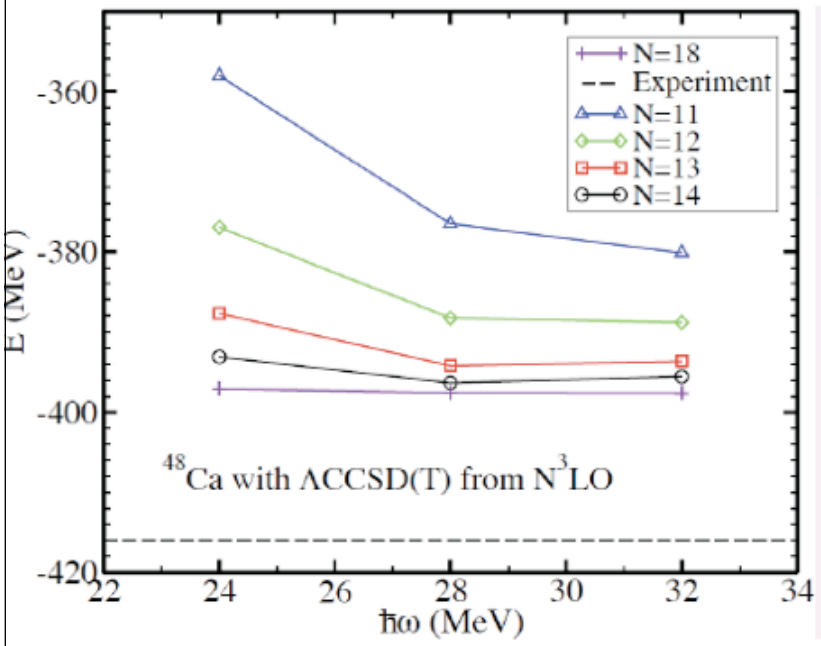
The LCCI project will deliver final UNEDF versions of LCCI codes, scripts, and test cases and the prototype DBMS will be completed and released.

Study role of NNN forces in medium mass nuclei with CC.

Complete CUDA hybrid Monte Carlo (HMC) codes and apply them to the first large-scale HMC calculations of the unitary Fermi gas.

Selected highlights: Coupled Cluster

Saturation of N³LO (NN only) in medium mass nuclei



	CCSD		Λ-CCSD(T)	
Nucleus	E/A	$\Delta E/A$	E/A	$\Delta E/A$
^{16}O	-6.72	1.25	-7.56	0.41
^{40}Ca	-7.72	0.84	-8.63	-0.08
^{48}Ca	-7.40	1.27	-8.26	0.40

Benchmarks in light nuclei:

Coupled-cluster meets few-body benchmarks for ^{4}He. Recent IT-NCSM and UMOA calculations of ^{16}O agree with CCM.

R. Roth *et al*, arXiv:1105.3173 (2011)

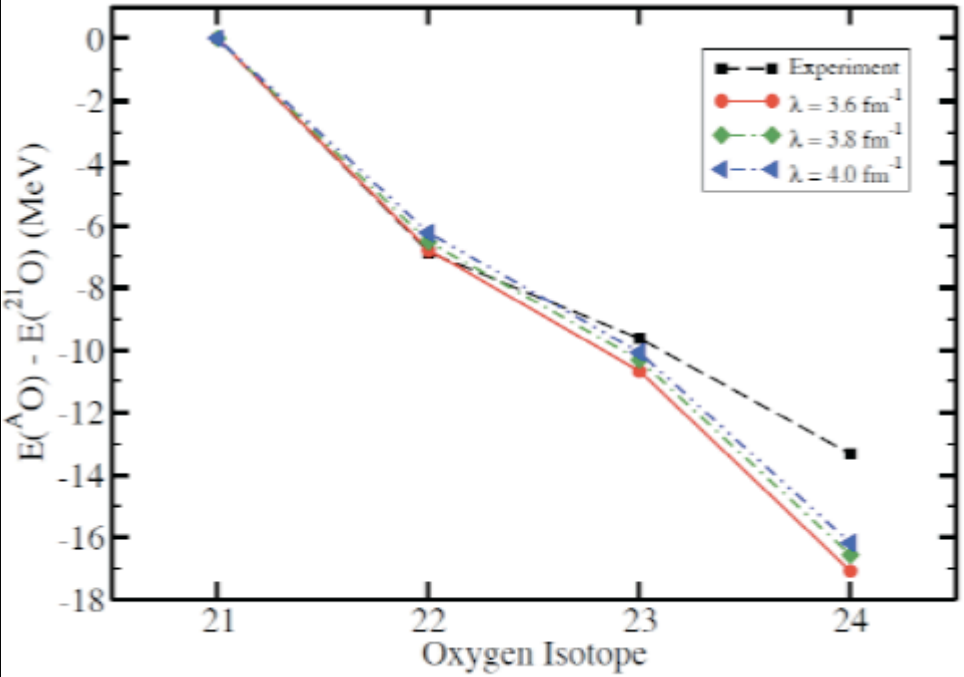
Fujii *et al*, PRL 103, 182501(2009)

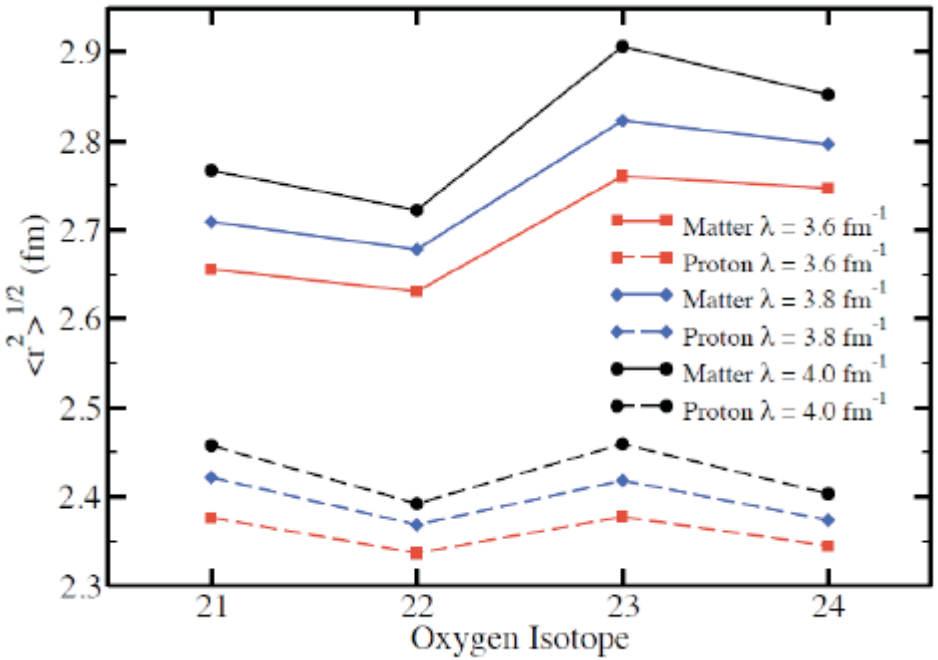
	CCM	(IT-)NCSM	UMOA
	E/A	E/A	E/A
^{4}He	-6.39(5)	-6.35	
^{16}O	-7.56(8)	-7.48(4)	7.47

G. Hagen, T. Papenbrock, D. J. Dean, M. Hjorth-Jensen, Phys. Rev. C 82, 034330 (2010).

Selected highlights: Coupled Cluster

Matter and charge radii in the ^{21,22,23,24}O isotopes





Also: going beyond closed shells
nuclear/neutron matter

Load balancing up to a few thousand processors,
starting with OpenMP

LCCI project

LCCI codes/scripts deposited initially on Oct. 2-4, 2009

Codes/Scripts	Contact	email	Updated	Final update
BIGSTICK	Calvin Johnson	cjohnson@sciences.sdsu.edu	June 2011	Nov 2011
MFDn	Pieter Maris	pmaris@iastate.edu	June 2011	Nov 2011
NuShellX	Mihai Horoi	horoi@phy.cmich.edu	March 2011	Nov 2011
trdens	Petr Navratil	navratil@triumf.ca	April 2010	Nov 2011
ncsmv2eff	Petr Navratil	navratil@triumf.ca	March 2010	Nov 2011
LCCI-wrapper	Maris/Johnson	pmaris@iastate.edu	July 2011	Nov 2011

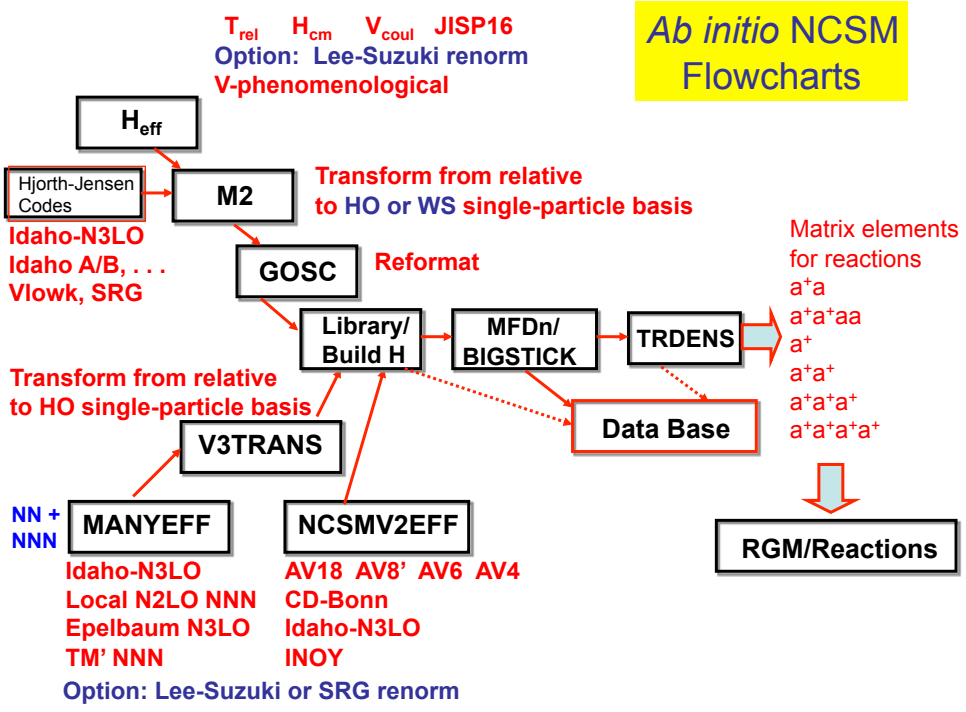
Source codes for each resides in its own subdirectory in NERSC project space:

/project/projectdirs/unedf/lcci

with a README file, one or more scripts, and test cases.

In addition, this introduction and an introduction to the DBMS reside there and are updated as major developments warrant.

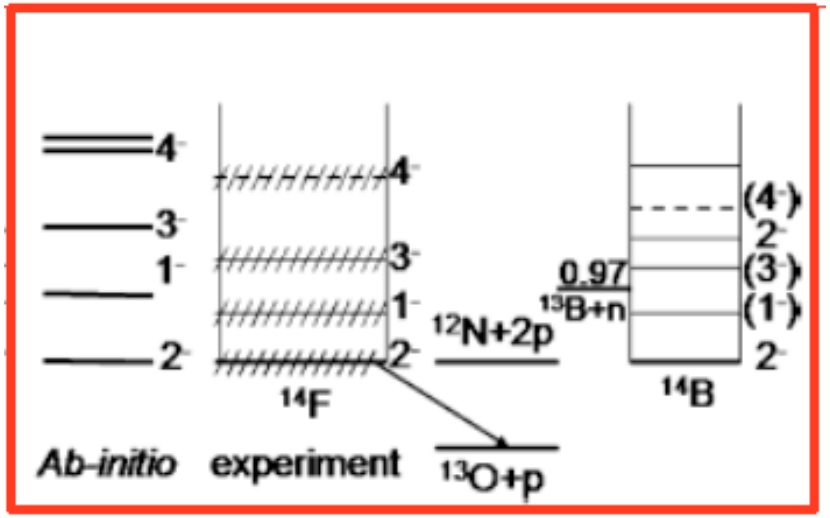
Ab initio NCSM Flowcharts



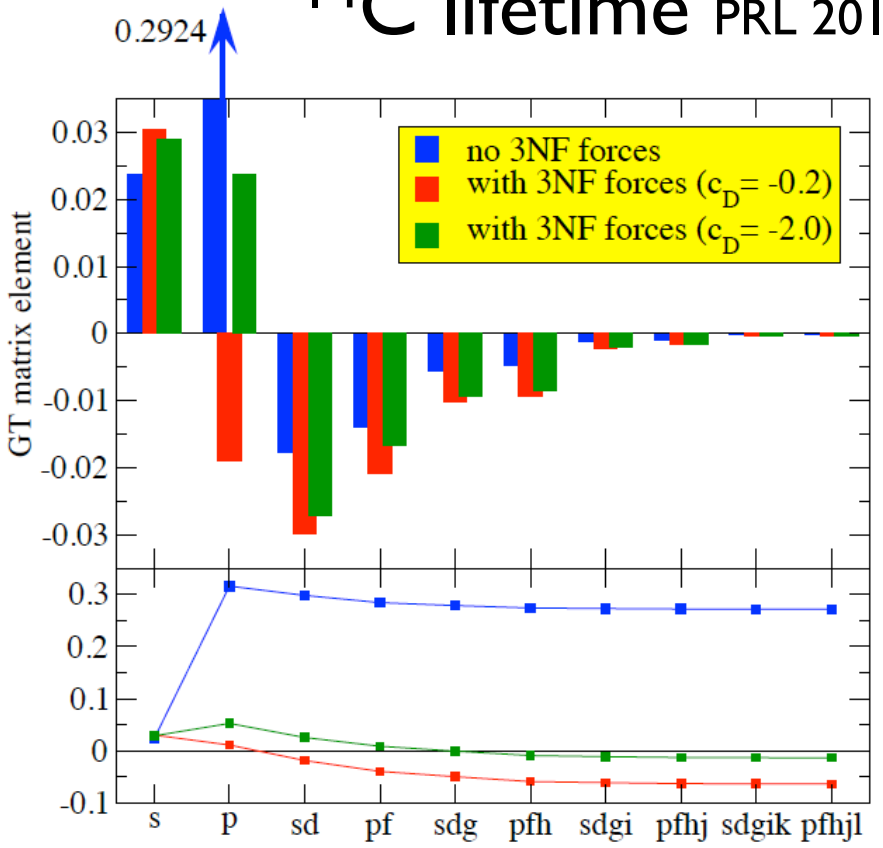
Selected highlights: NCSM

^{14}F

NCFC predictions (JISP16) in close agreement with experiment

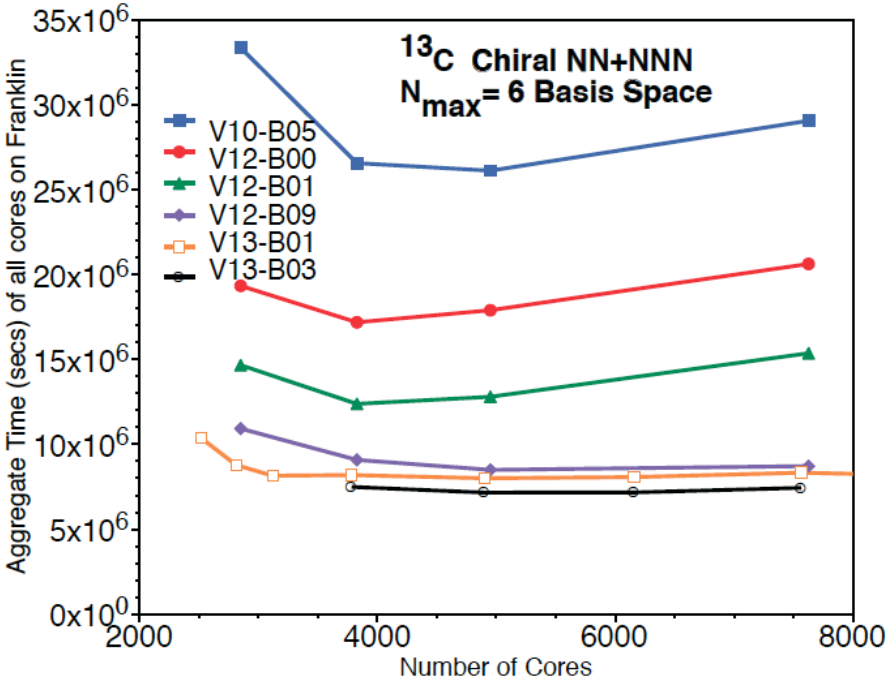


^{14}C lifetime PRL 2011

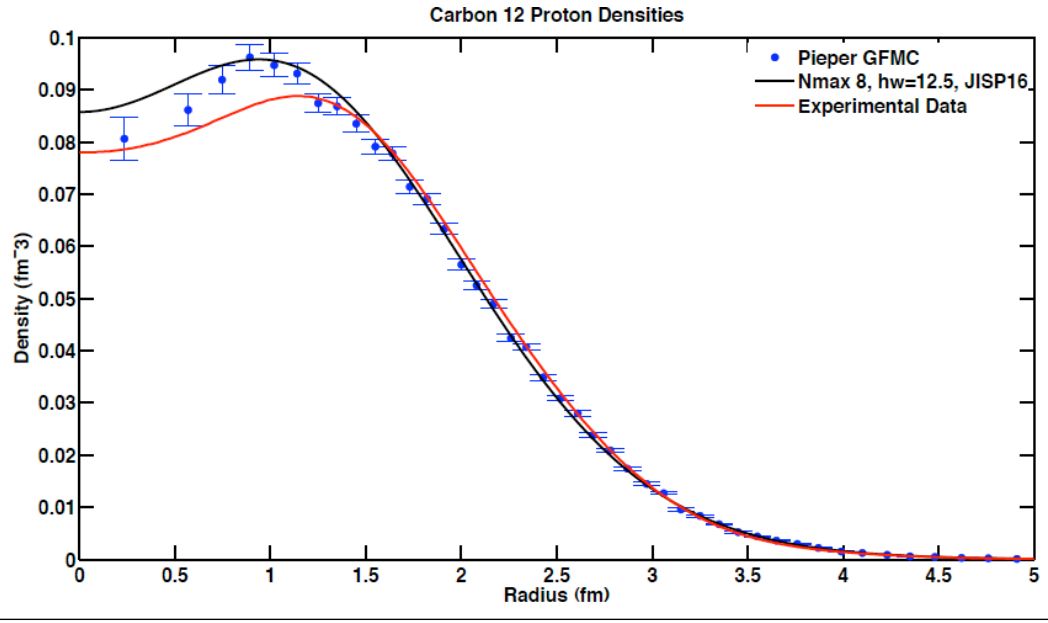


NCSM highlights (cont'd)

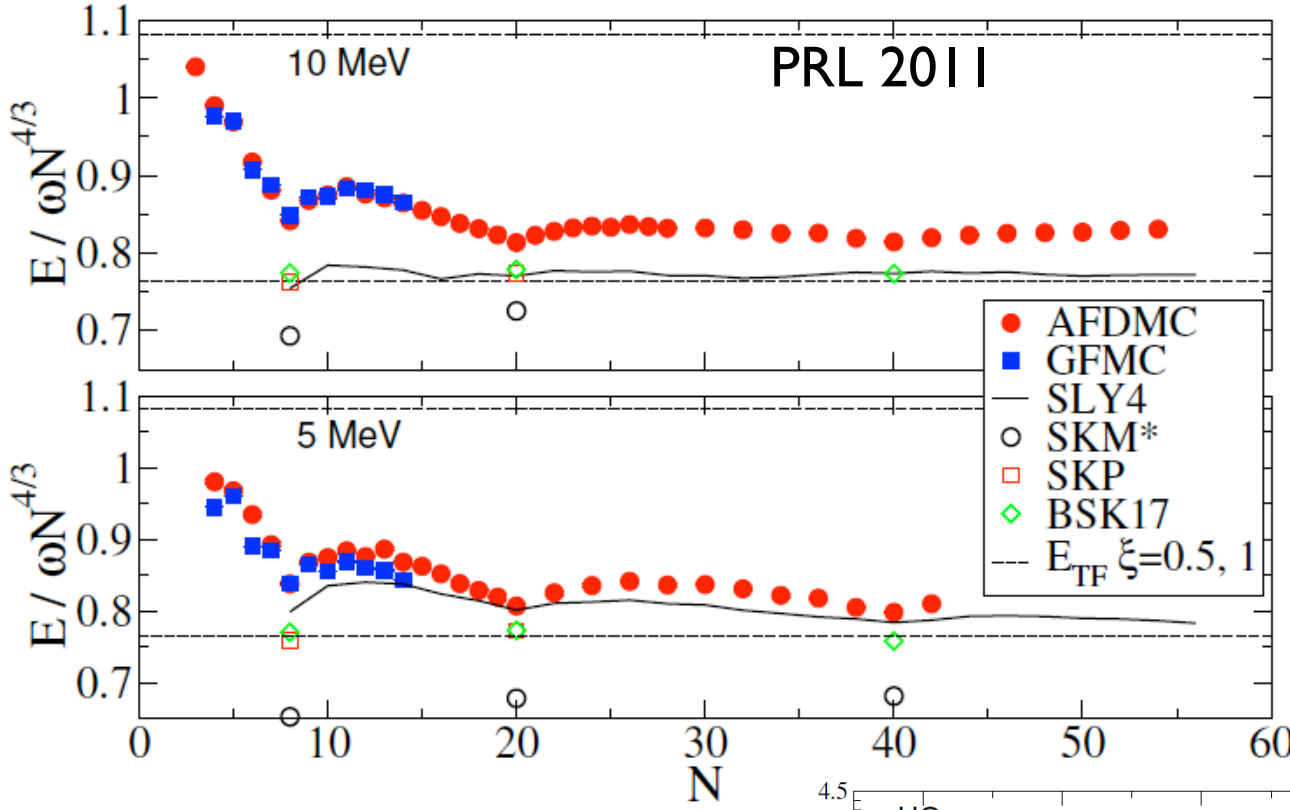
Computational Performance (Franklin at NERSC)

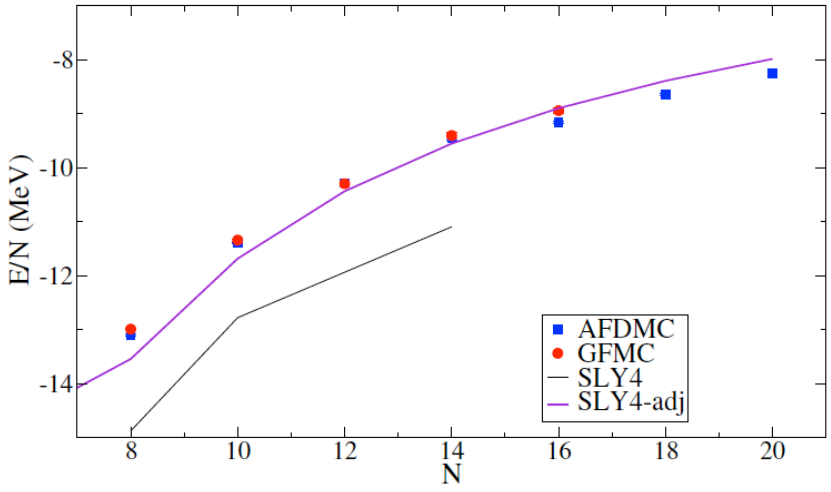


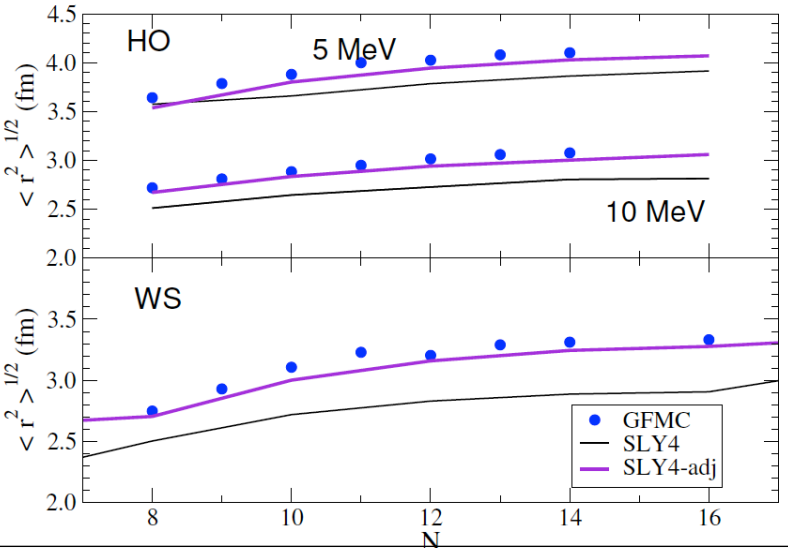
12C proton densities



Selected highlights: AFDMC/GFMC
Neutron Drops

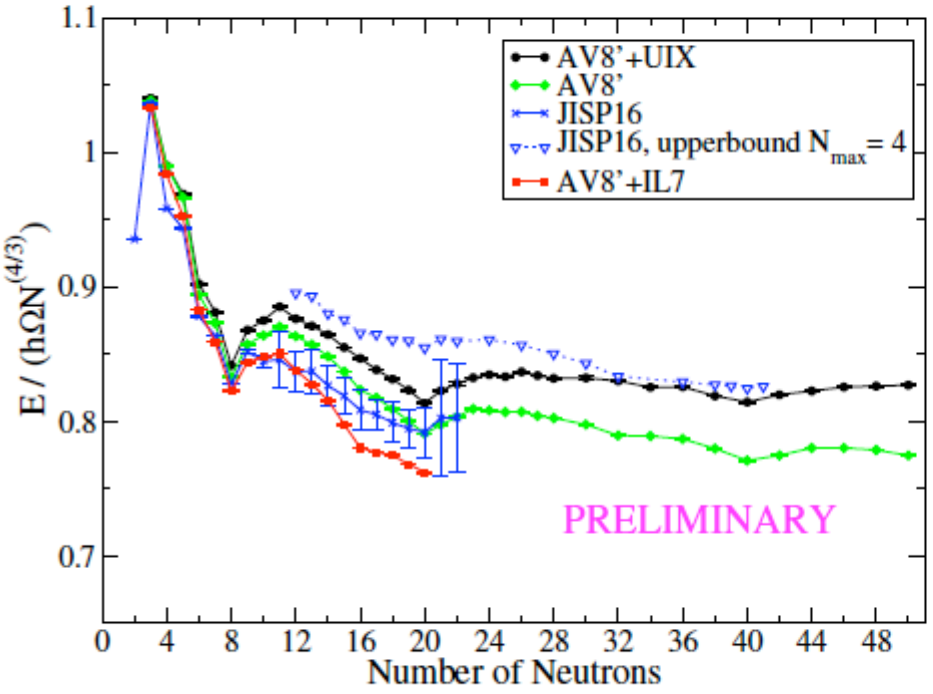




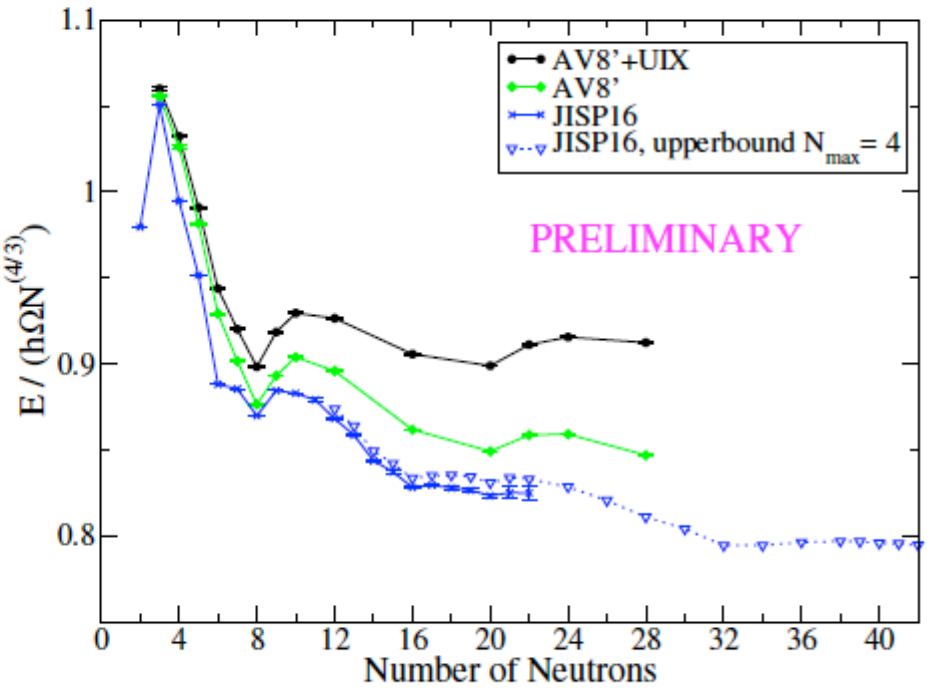


QMC + NCSM (+ DF + DME...)
many more wells, interactions, comparisons

$\hbar\omega = 10$ MeV

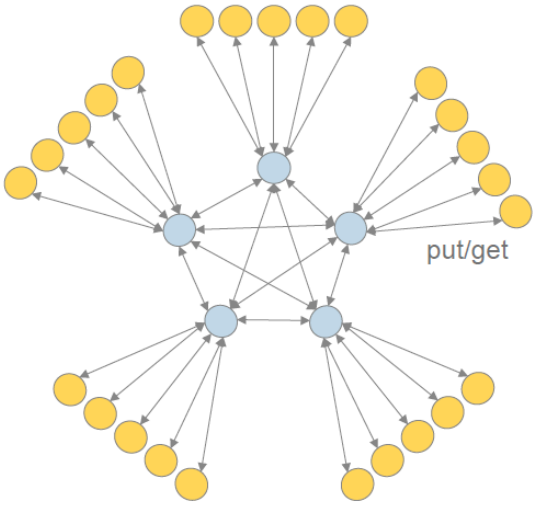


$\hbar\omega = 20$ MeV



Single, Double Energy Differences, Spin-orbit splittings, ...

How It Works (Current production version)



Application Processes

ADLB Servers

ADLB

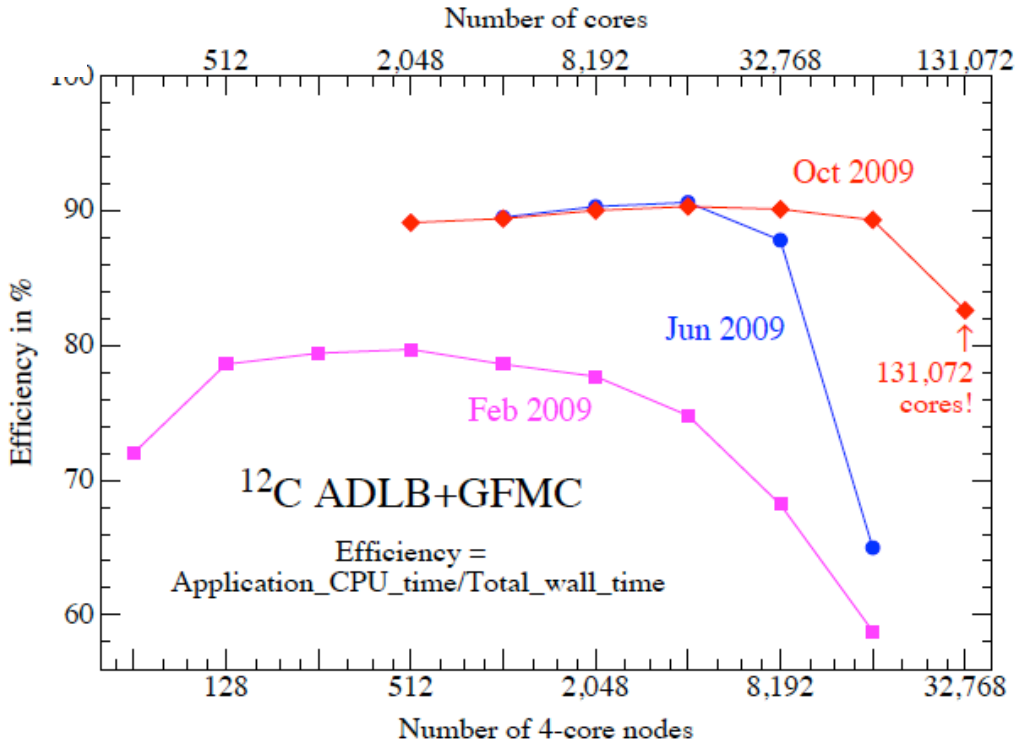
Web site is http://www.cs.mtsu.edu/~rbutler/adlb

To download adlb:

- svn co http://svn.cs.mtsu.edu/svn/adlbm/trunk adlbm

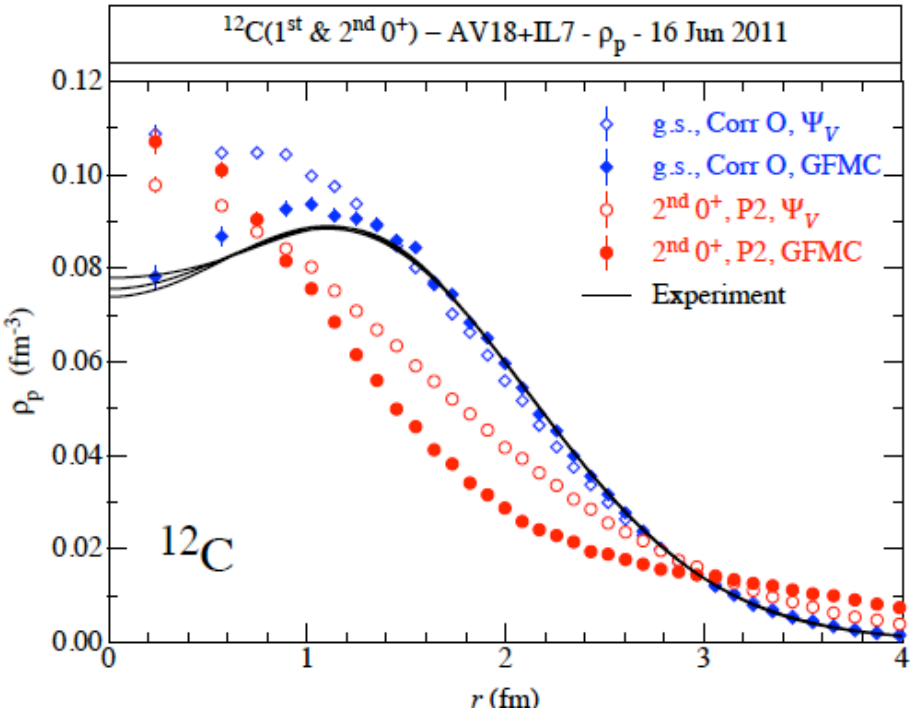
on Blue Gene

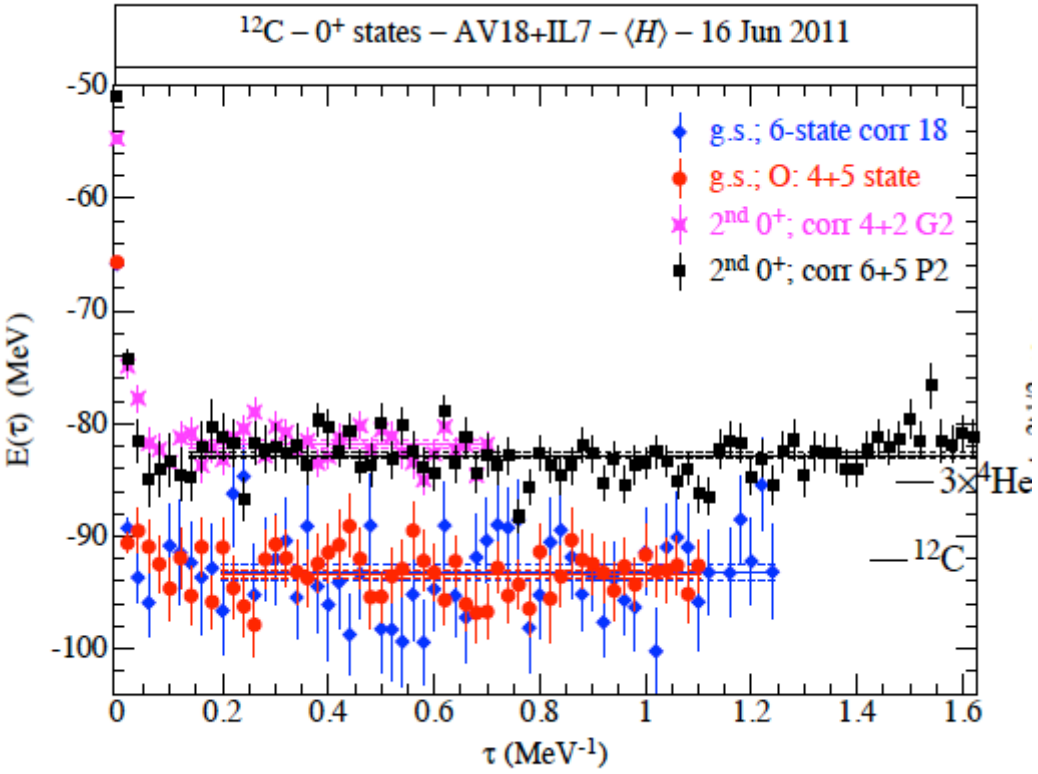
New approaches
(one-sided communication)
New applications:
parameter sweep
"batcher"
Swift substrate



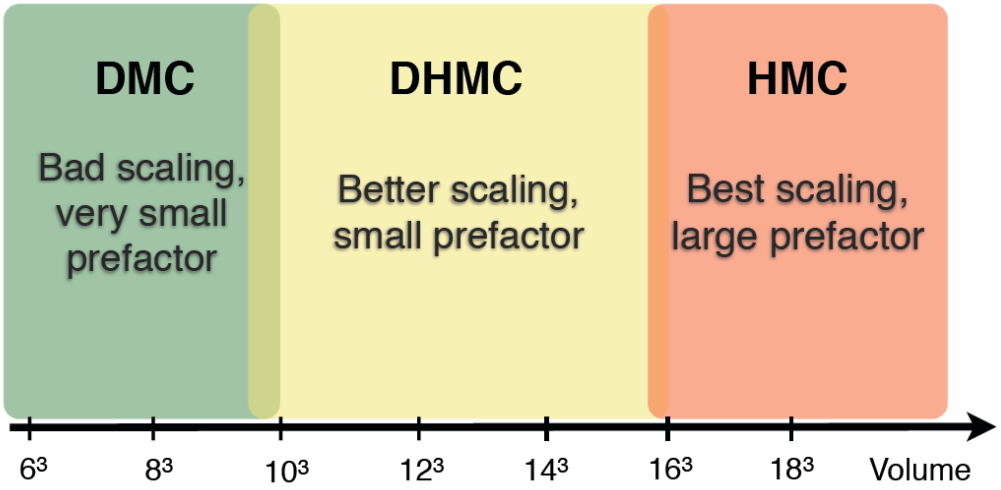
Selected highlights: GFMC

- scaling
- Hoyle State
- ANC
- towards Fermi β-decay
- ...

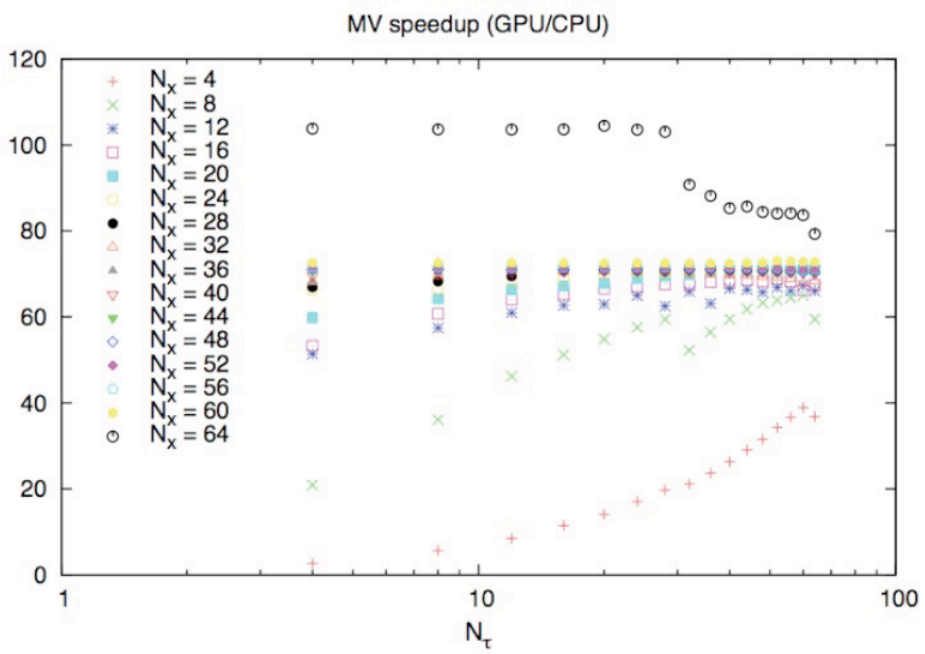




Towards advanced algorithms/architectures

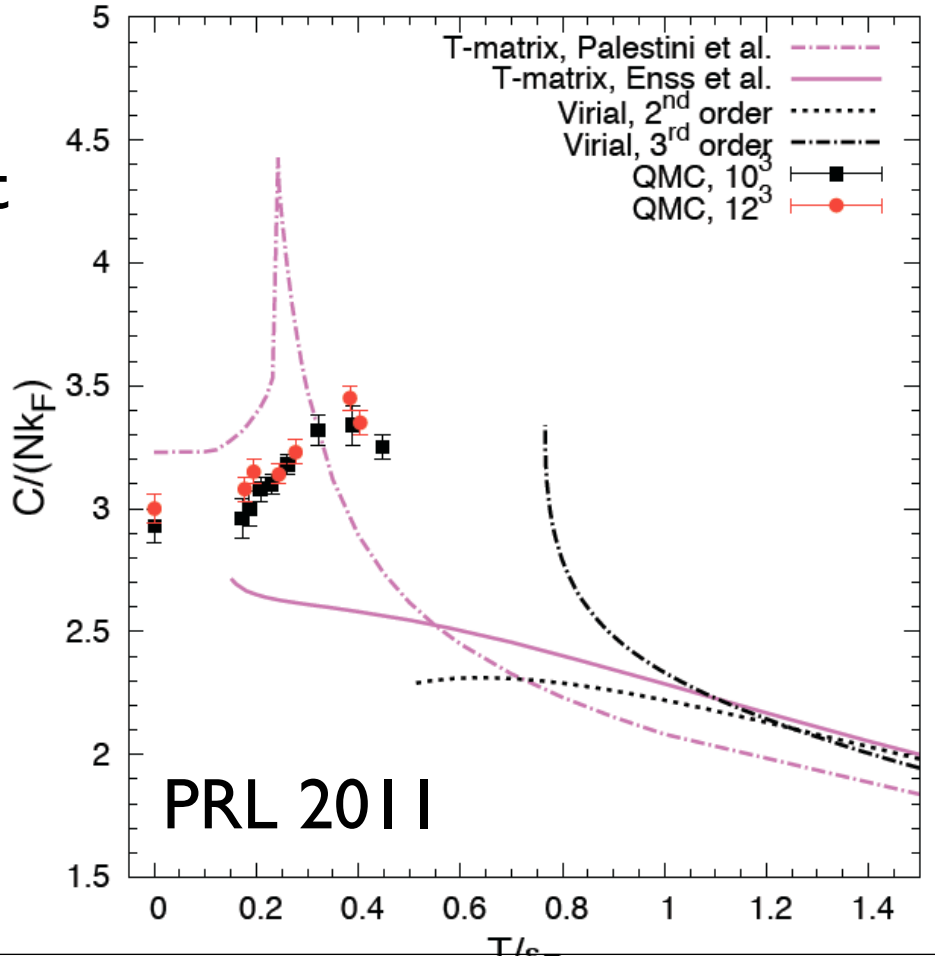


GPU status



Text

Contact in Unitary Fermi Gas (short-distance behavior)



Summary

Excellent progress towards deliverables

Many new collaborations still developing