Path Integral Studies of Structure and Dynamics in Nuclear Physics

NUCLEI collaboration (computingnuclei.org)

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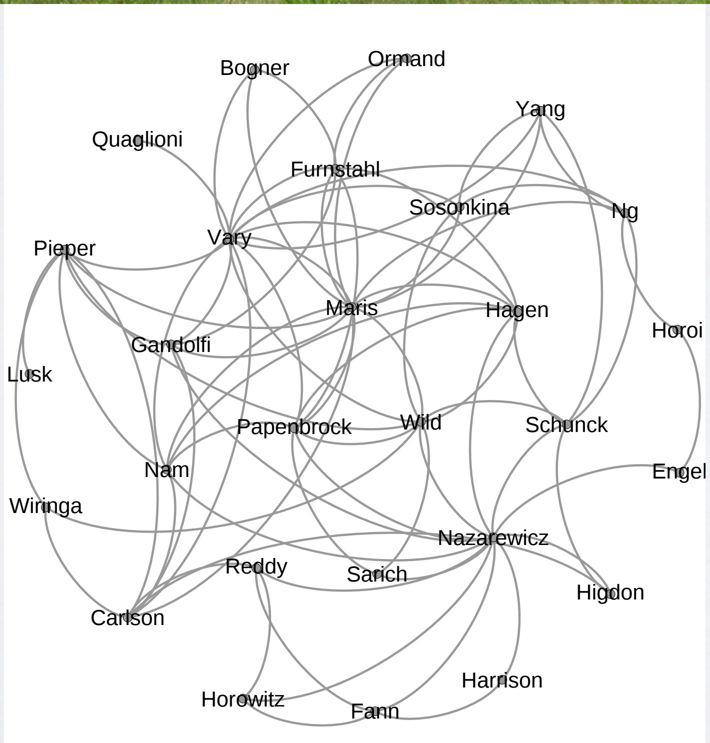
Nuclear Computational Low-Energy Initiative


NUCLEI 2013 Collaboration Meeting Indiana Univ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Ormand
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Maris
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Horoi
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Lusk
Papenbrock
Wild
Schunck
Engel
Nam
Wiringa
Nazarewicz
Reddy
Sarich
Higdon
Carlson
Harrison
Horowitz
Fann

NUCLEI Awards / Recognition 2013

Gaute Hagen: DOE early career award

"State of the art microscopic calculations of weak processes in nuclei"

Hai Ah Nam: showcased in DOE Women@Energy feature

Stefano Gandolfi: IUPAP Young Scientist Prize

Alessandro Lovato: PhD thesis award

"ab-initio calculations of nuclear matter properties"

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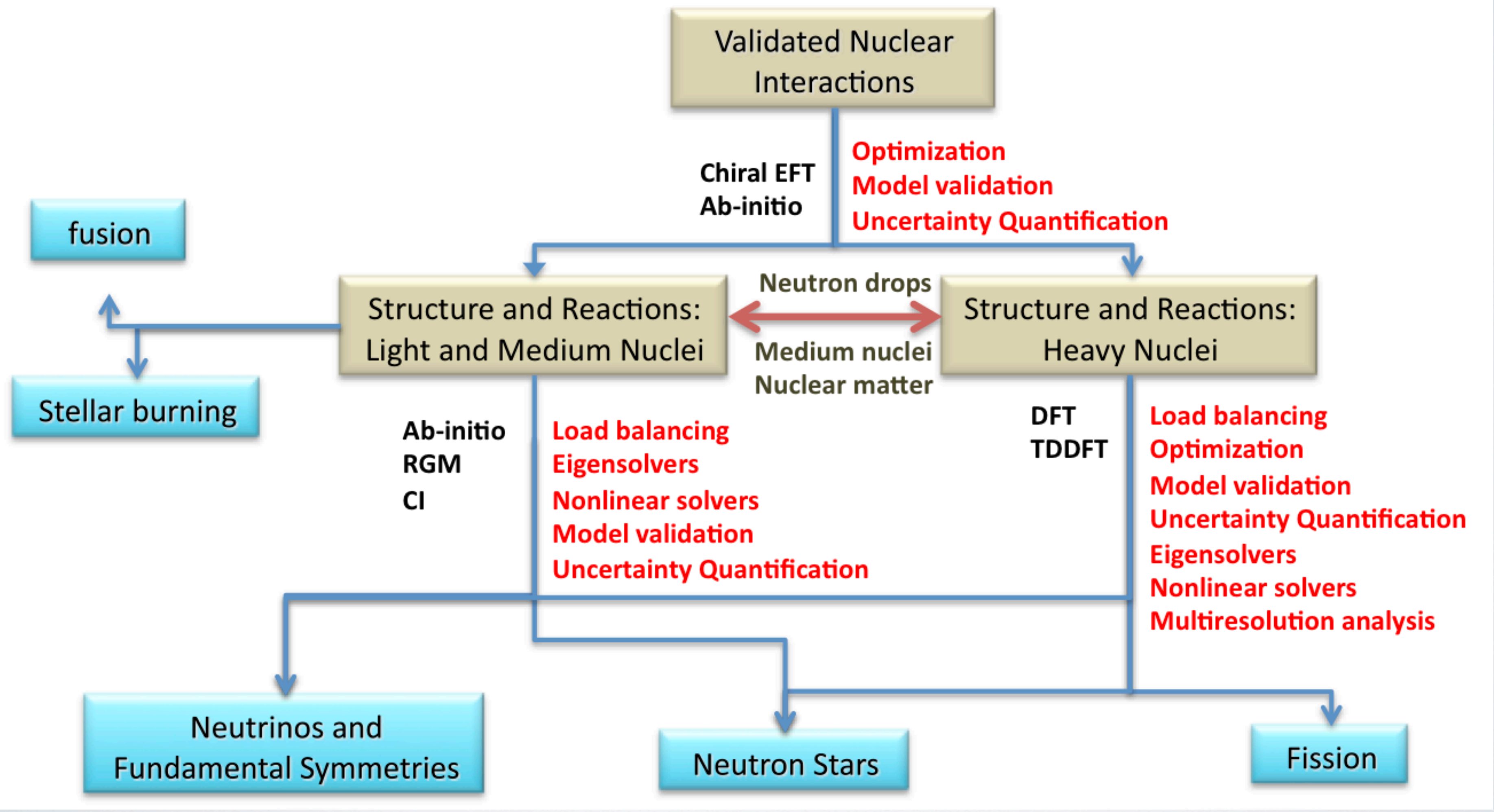

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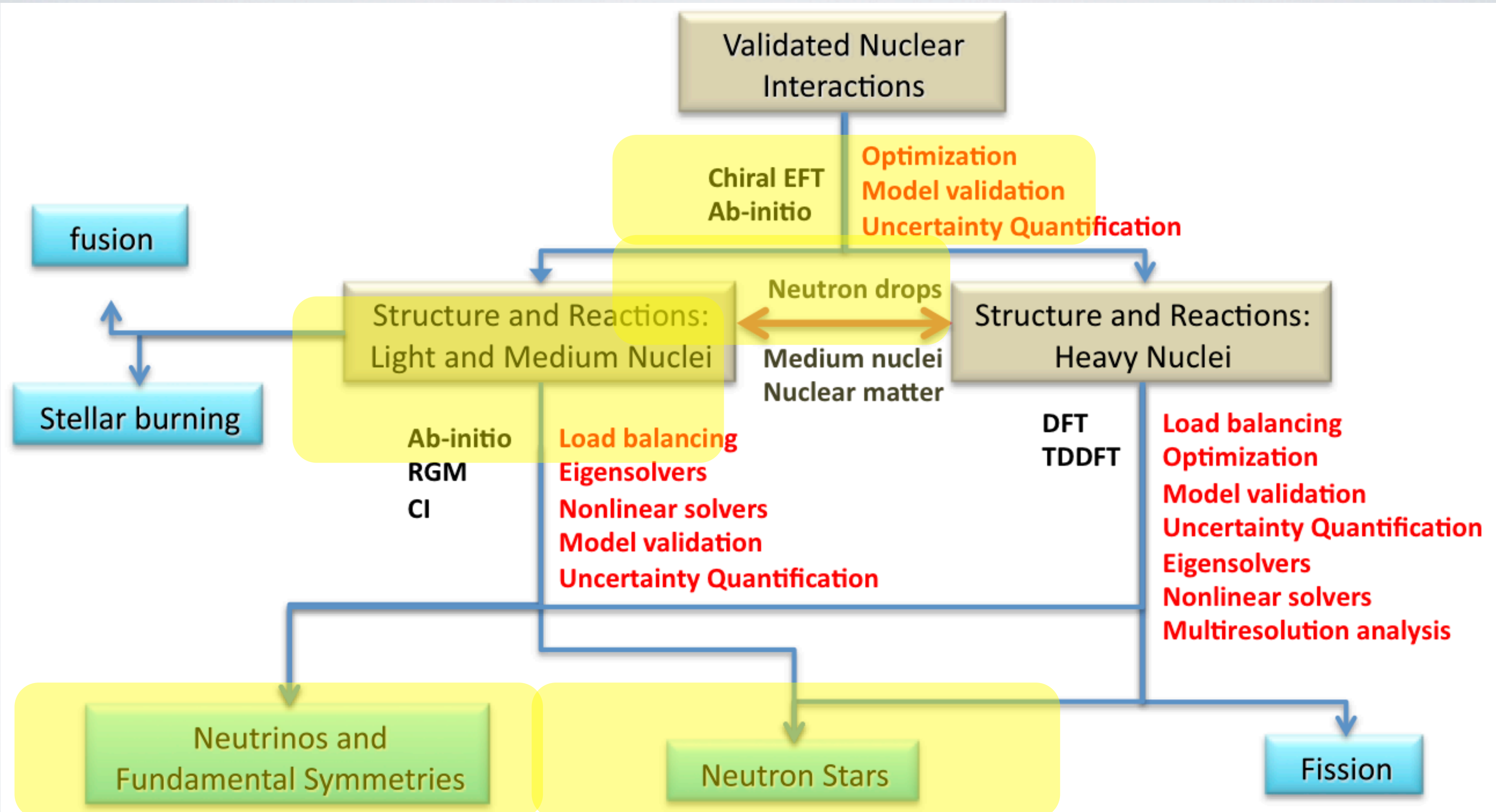


Path Integral Studies of Structure and Dynamics in Nuclear Physics

- Basic Structure of the calculations
- QMC at very large scales
- Ground and low-lying states
- Form Factors and EW transitions
- Inclusive Scattering and Response
- Summary and Outlook

Basic Idea: project specific low-lying states from initial guess (or source)

$$\Psi_0 \ = \exp\left[-H\tau\right]\ \Psi_T$$

Use Feynman path integrals to compute propagator

$$\exp\left[-H\tau\right] = \prod \exp[-H\delta\tau]$$

where the high-T (short-time) propagator can be calculated explicitly.

Applications: condensed matter (Helium, electronic systems, ...
nuclear physics (light nuclei, neutron matter,...)
atomic physics (cold atoms,...)

Algorithm:

Branching random walk in 3A (36 for ^{12}C) dimensions
Asynchronous Dynamic Load Balancing (ADLB)

Each step moves 12 particles and updates

$2^A \times \binom{A}{Z}$ complex amplitudes (2 GB for ^{12}C gs)

significant linear algebra for each step

tuned by physicists and math/CS staff at ANL

Similar branching random walk with linear algebra
used in condensed matter physics (lattice calculations)

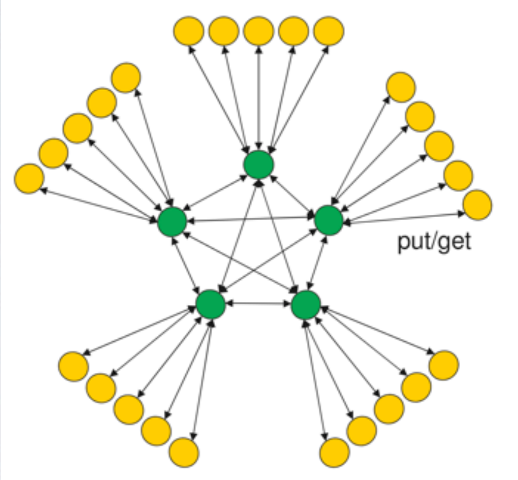
See current INT program on QMC for non-relativistic systems:
http://int.phys.washington.edu/PROGRAMS/current.html

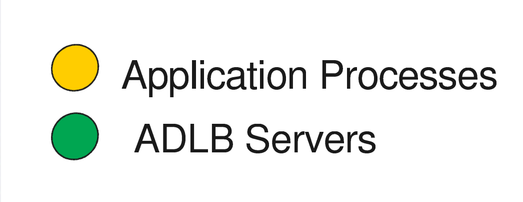
Advancing from Blue Gene P to Blue Gene Q

- ADLB under UNEDF resulted in code working well on BG/P:
  - 2 Gbytes and 4 cores (each one thread) per node
  - $^{12}C(0^+)$ needs 2 Gbytes so OpenMP used for the 4 cores (threads)
  - ADLB gives excellent scaling to 32,768 nodes
- BG/Q offers new possibilities and challenges
  - 16 Gbytes, 16 cores (each 4 threads) per node
  - 48×1024 nodes
  - $^{12}C(0^+)$: 8 ranks/node (8 threads each) or 4, 2, or 1 (64 threads)
  - Other ^{12}C states need much more memory/rank (T=1: 14 Gbytes)

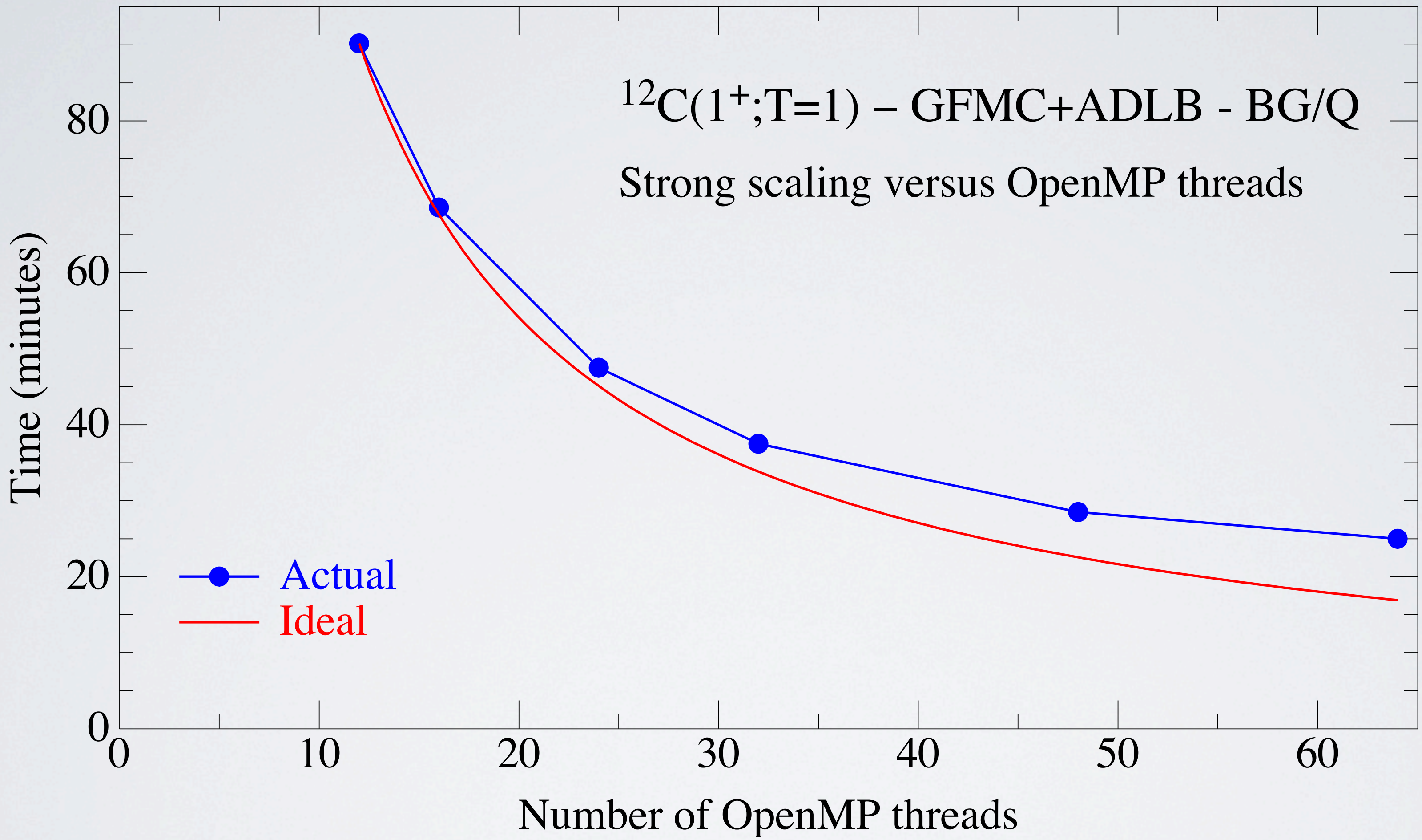
ADLB (Asynchronous Dynamic Load Balancing)

- Large-scale load-balancing is provided to GFMC by the Asynchronous Dynamic Load Balancing (ADLB) library.
- ADLB is a library that implements a scalable version of the venerable master/slave parallel programming model for load balancing.
- There is no master process; rather, a subset of application processes in constant communication with one another is used to manage a shared pool of work units.
- Application processes create and *put* work units into this pool and *get* and process work units from this pool.
- Sophisticated (i.e. complicated) process-load balancing, memory-usage load balancing, and message-traffic load balancing algorithms are used to achieve scalability without burdening the application programmer.
- ADLB uses MPI and is also compatible with other MPI usage by the application.
- ADLB is particularly applicable when work units do little communication with one another and are of widely varying size and computational complexity.
- ADLB is also used as the execution engine for the parallel scripting language Swift.
- ADLB is available for downloading http://www.cs.mtsu.edu/~rbutler/adlb . It includes documentation and example codes.





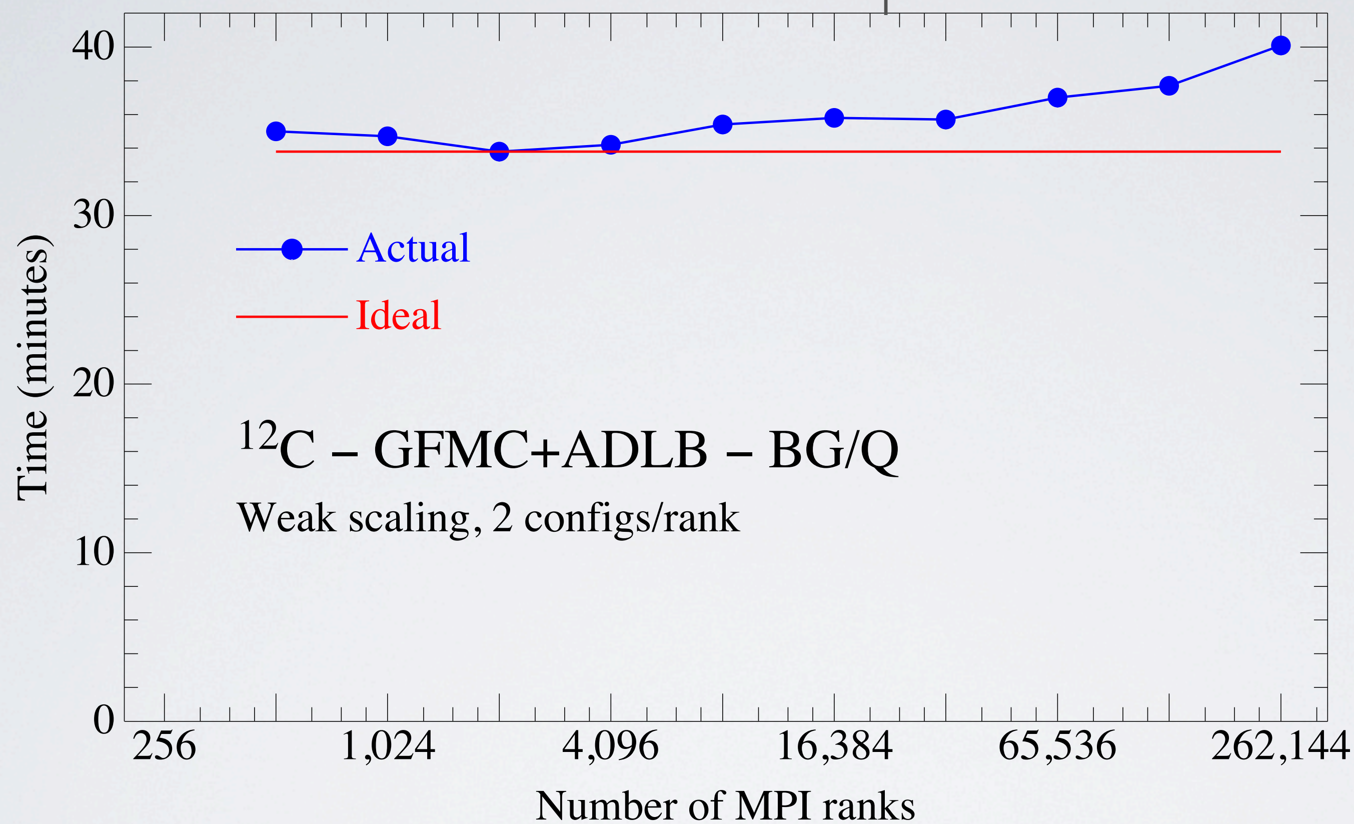
OpenMP Strong Scaling: BG/Q (MIRA)



Combination of ADLB/MPI and OpenMP working very well

ADLB/ GFMC weak scaling

Experiments find best hybrid configurations 4 MPI ranks per node and 16 threads per rank

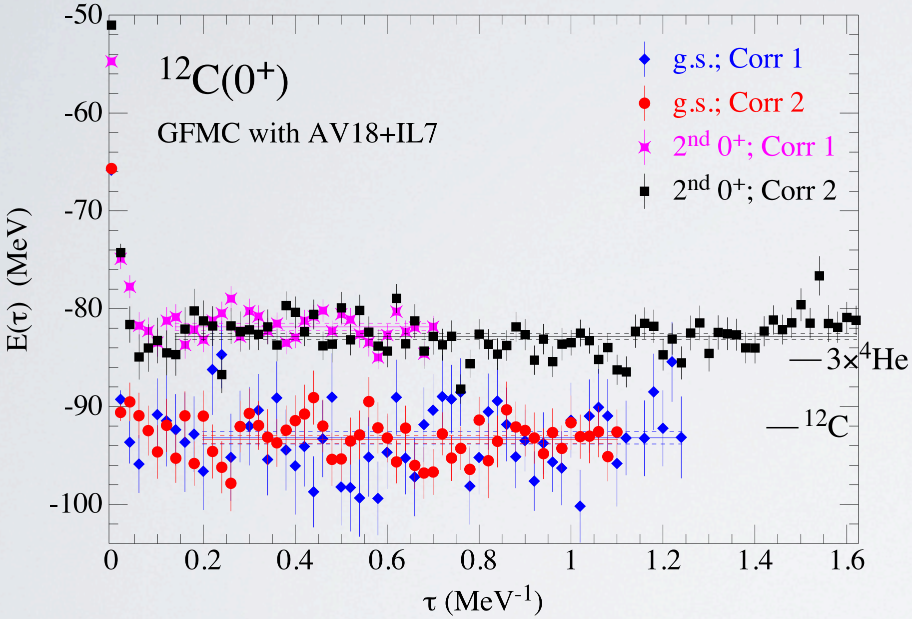


6 (now 8) threads per core >2 M threads total!

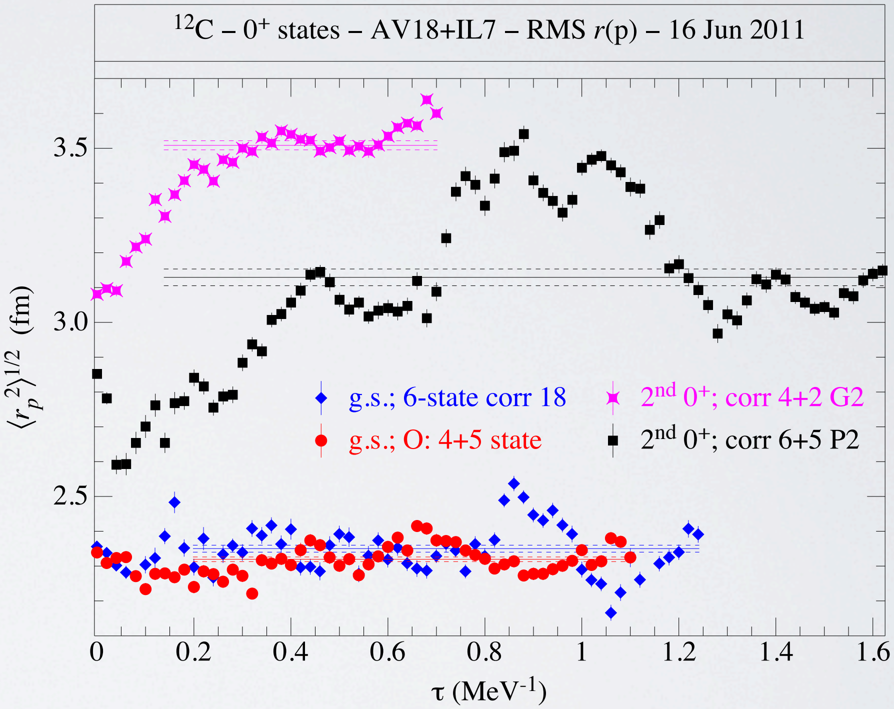
Future developments: use of new MPI-3 features for shared memory and remote memory access

Ground and Hoyle State

Energy



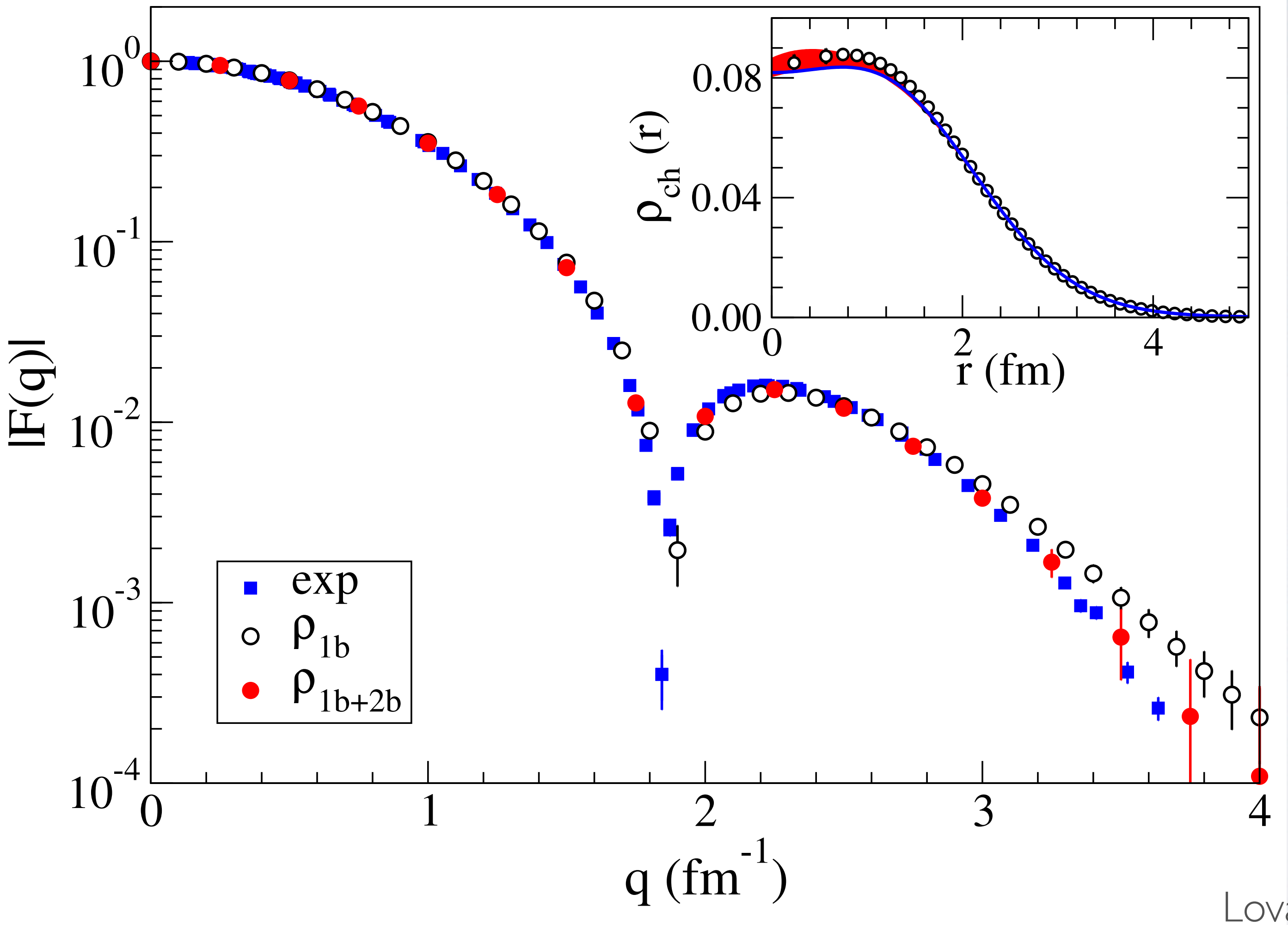
RMS radius



0+ excited state near triple-alpha threshhold postulated by Fred Hoyle to explain nuclear abundances

Pieper, Wiringa, Carlson, Lusk,

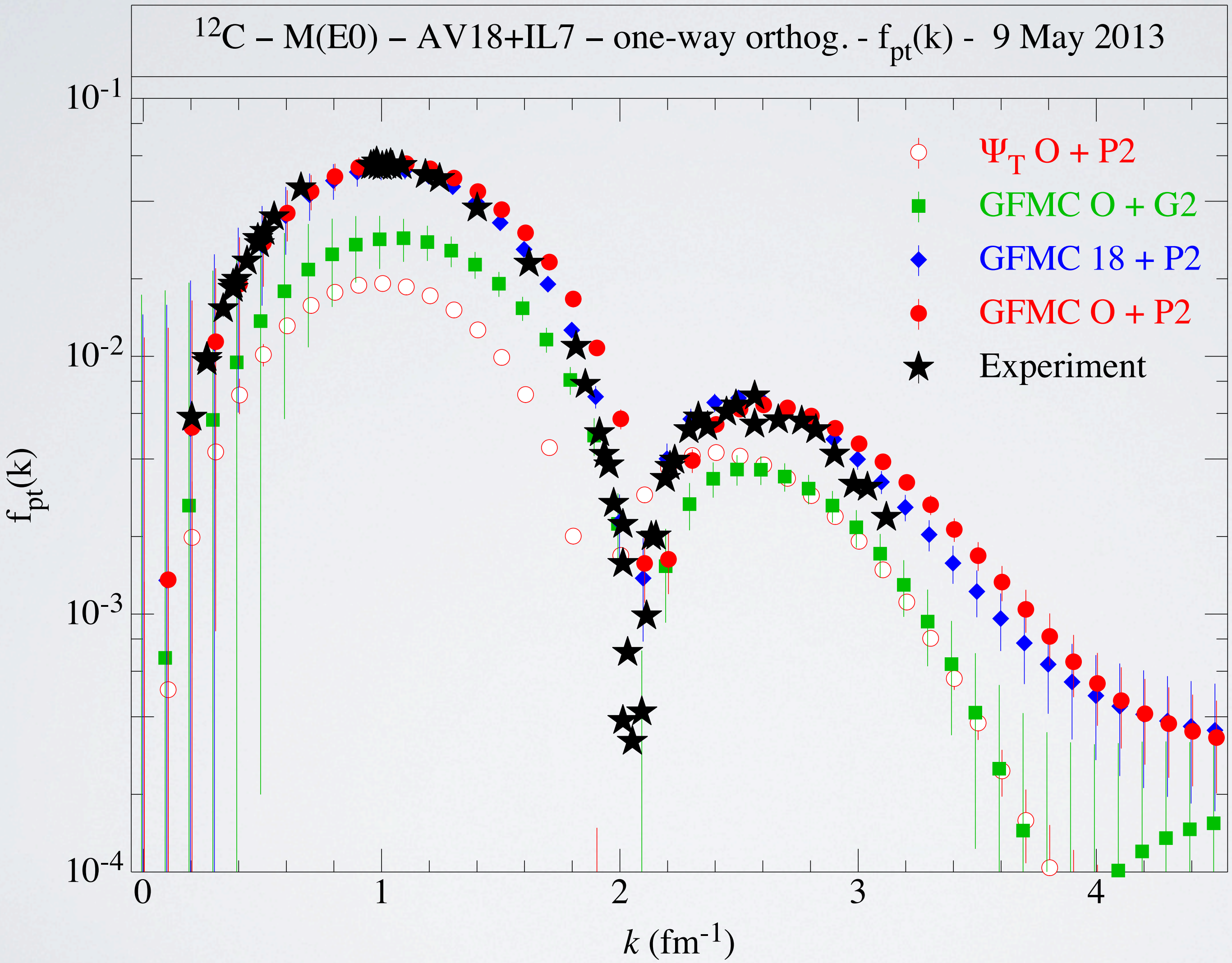
^{12}C Electromagnetic Form Factor



Small role for two-nucleon currents
Excellent agreement with data

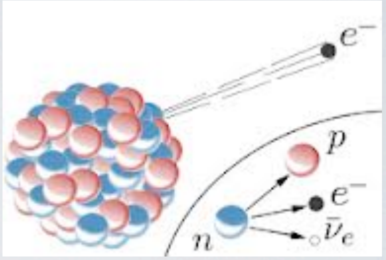
Lovato, Gandolfi, Butler, Carlson, Lusk, Pieper, Schiavilla
arXiv:1305.6959

Ground State - Hoyle State Transition form factor



Fundamental Symmetries

Superallowed Beta Decay in A=10



$^{10}C \rightarrow {}^{10}B$ FERMI BETA DECAY

CIB terms	δ_C VMC	δ_C GFMC
AV18 + IL7; Cluster Ψ_T:		
Coulomb	.00122(5)	.00157(43)
All E&M	.00133(5)	.00216(24)
Coulomb + Strong	.00142(6)	.00273(23)
Full CIB	.00274(4)	.00412(24)
AV18 + IL7; S.M. Ψ_T:		
Full CIB	.00168(4)	.00329(16)
AV8', no V_{ijk}; S.M. Ψ_T:		
Full CIB	.00172(6)	.00282(23)
Following have only Coulomb		
Towner & Hardy a)	.0017	
W. Satula, *et al.* b)	.0065(14)	
"Expt." b)	.0037(15)	

a) Phys. Rev. C. **77**, 025501 (2008); b) Phys. Rev. C 86, 054316 (2012)

Used to test CVC and examine unitarity of the CKM matrix

Pieper and Wiringa

Electromagnetic Response in ^{12}C

The electromagnetic inclusive cross section of the process

$$e +^{12} \mathrm{C} \to e' + X$$

where the target final state is undetected, can be written in the Born approximation as

$$\frac{d^2\sigma}{d\Omega_{e'} dE_{e'}} = -\frac{\alpha^2}{q^4} \frac{E_{e'}}{E_e} L_{\mu\nu} W^{\mu\nu} \ ,$$

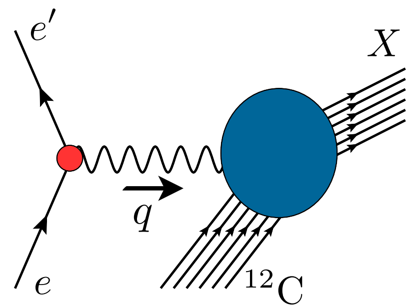
Leptonic tensor

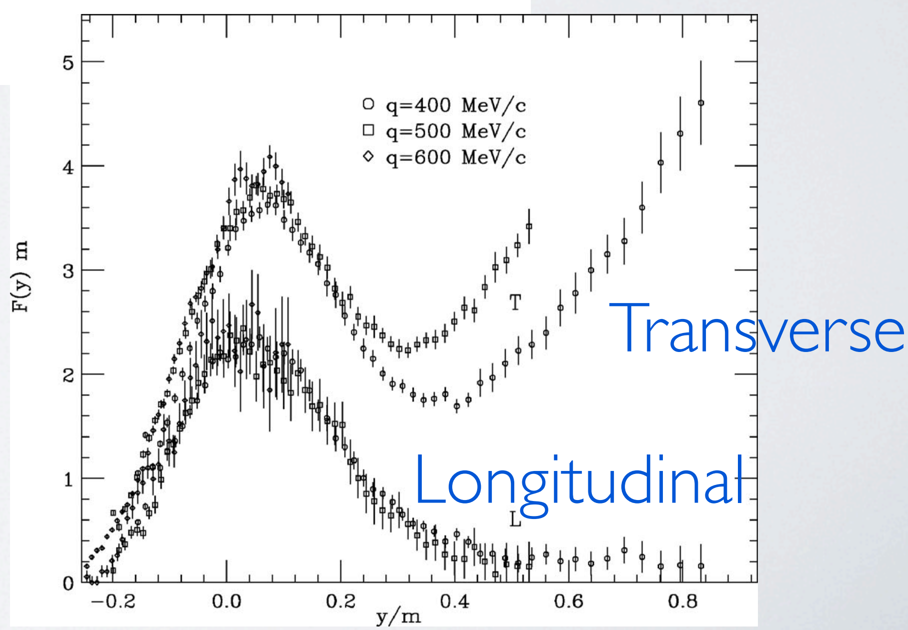
$$L_{\mu\nu} = 2[k_\mu k'_\nu + k_\nu k'_\mu - g_{\mu\nu}(kk')]$$

Hadronic tensor

$$W^{\mu\nu} = \sum_X \langle\Psi_0|J^\mu|\Psi_X\rangle\langle\Psi_X|J^\nu|\Psi_0\rangle\delta^{(4)}(p_0 + q - p_X)$$

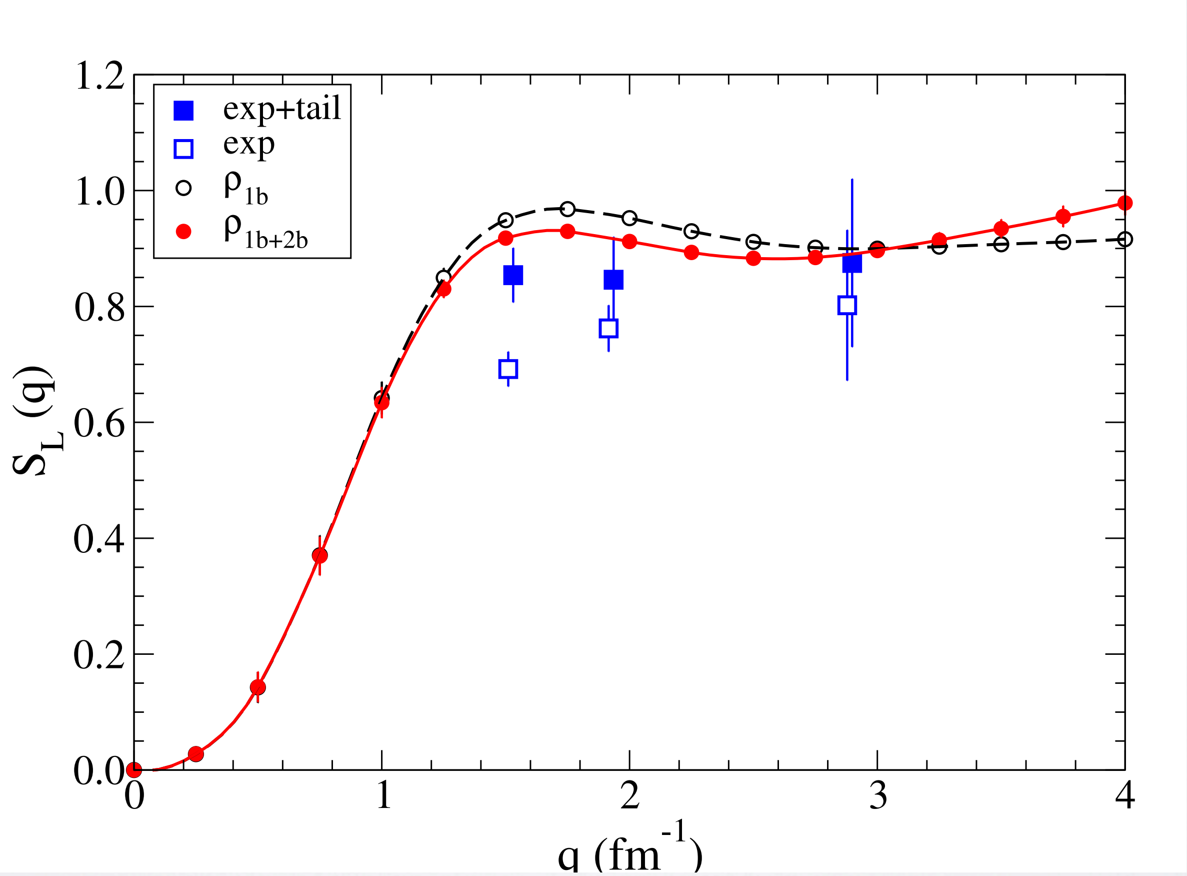
It contains all the information on target structure.





Longitudinal Sum Rule

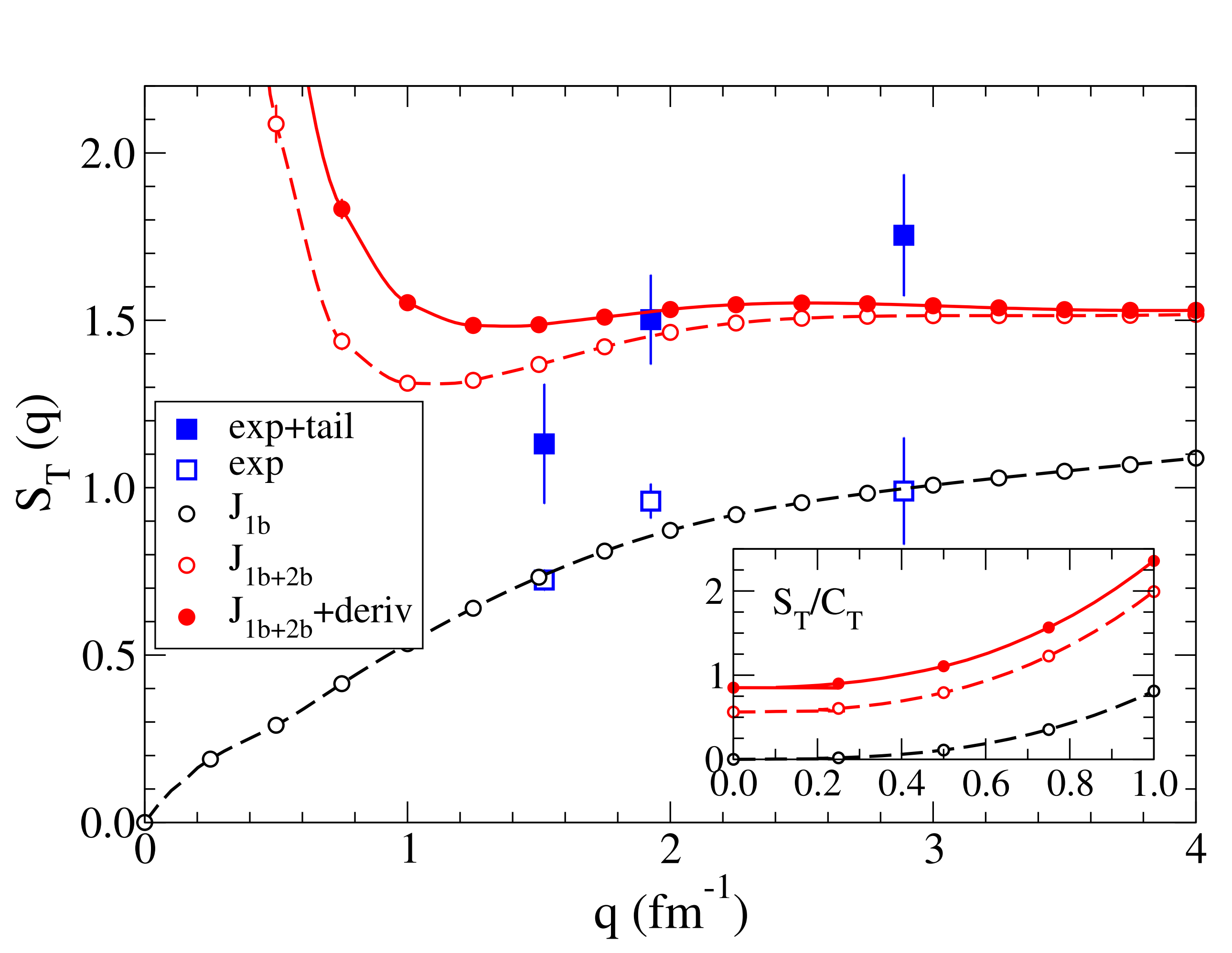
$$S_L(q) \;=\; \langle 0|\; \rho^\dagger(q)\; \rho(q)\; |0\rangle$$



new Jlab experiment soon, also neutrino experiments

again small role for two-nucleon currents

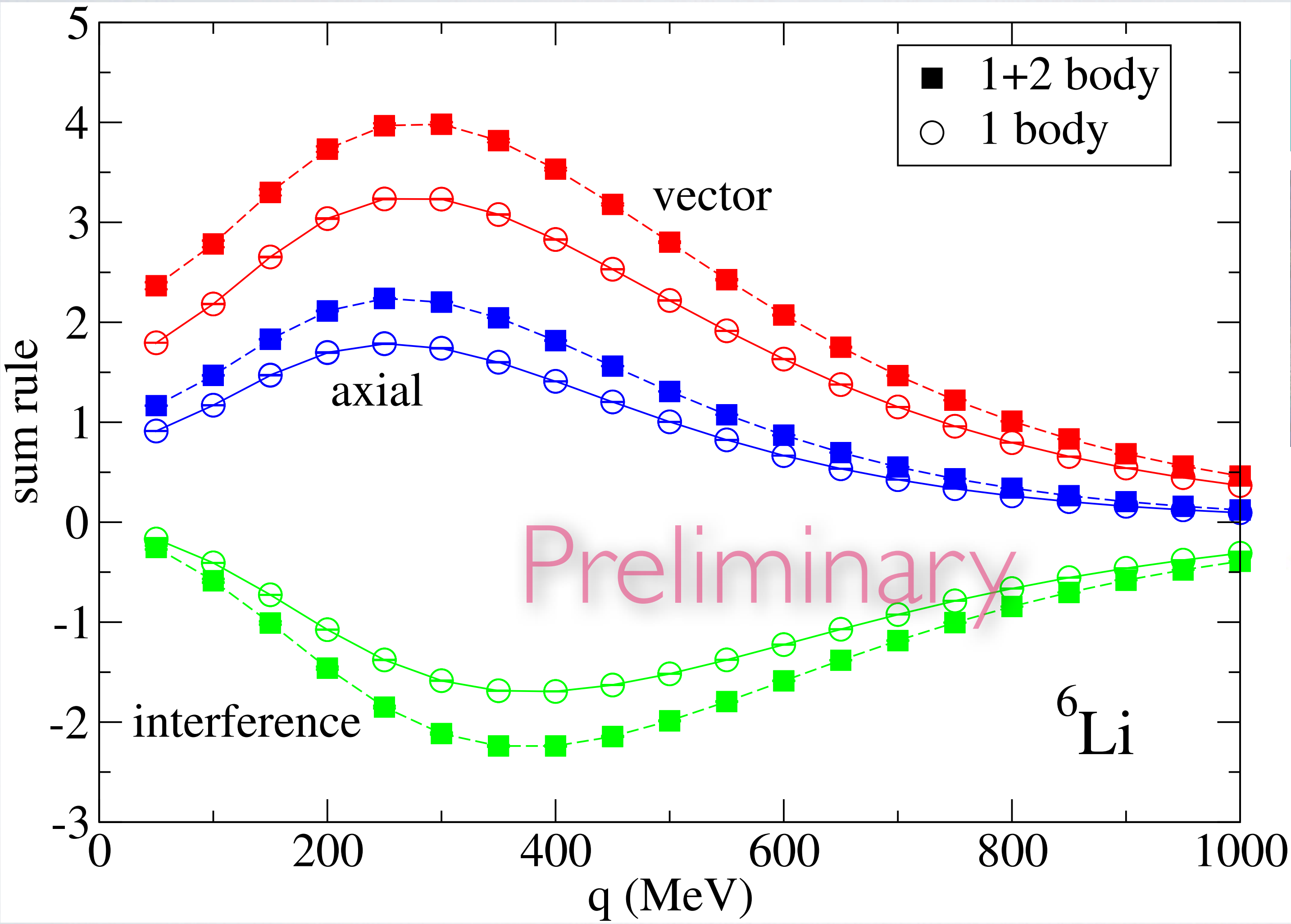
Transverse Sum Rule

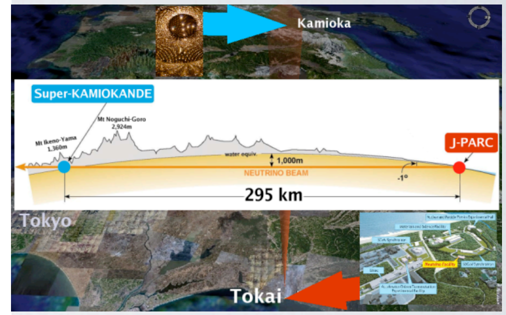


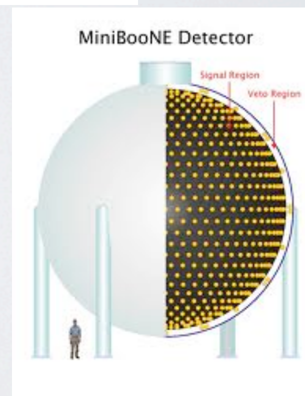
Lovato, Gandolfi, Butler, Carlson, Lusk, Pieper, Schiavilla arXiv:1305.6959

Two-nucleon currents contribute ~ 50% enhancement
Jlab experiments, neutrino experiments

Neutrino/Anti-neutrino Scattering
5 response functions
Neutral current sum rules for Li







Beyond Sum Rules:

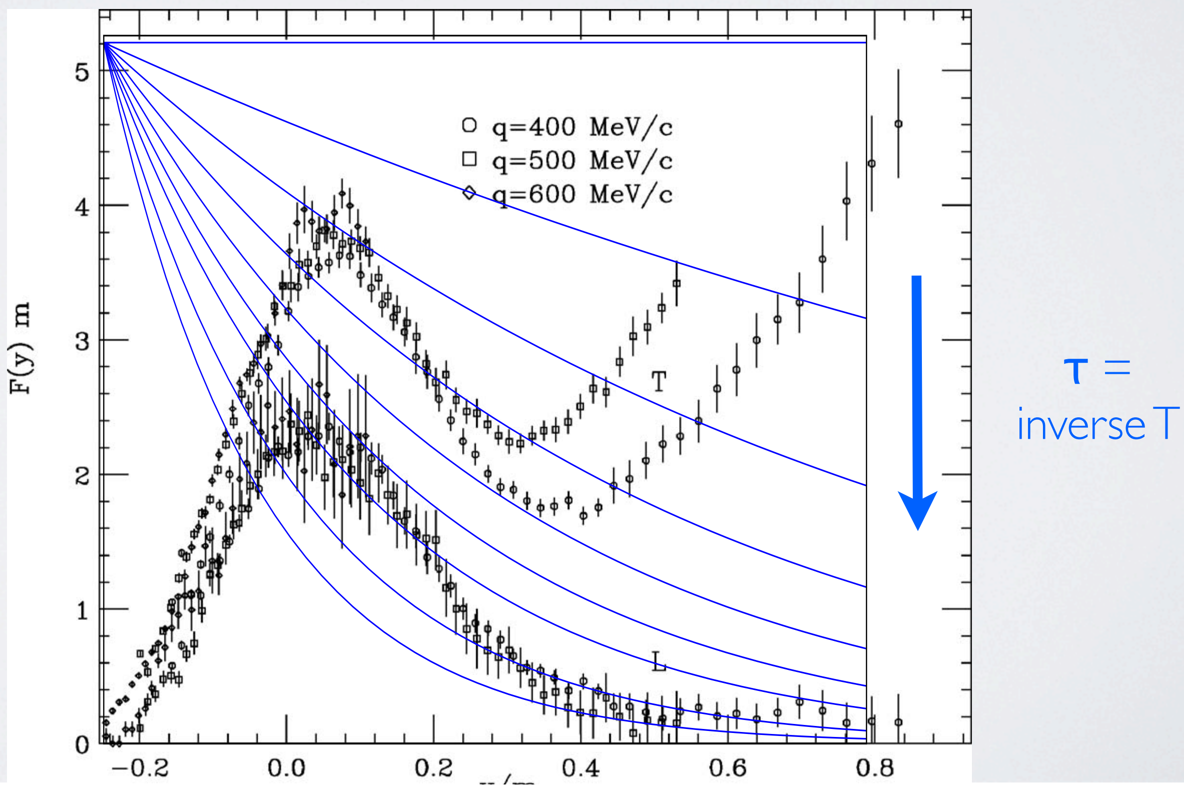
Real-time response

$$R(q,\omega) \ = \ \langle 0|\ \mathbf{j}^\dagger(q)\ |f\rangle\langle f|\ \mathbf{j}(q)\ |0\rangle\ \delta(w-(E_f-E_0))$$

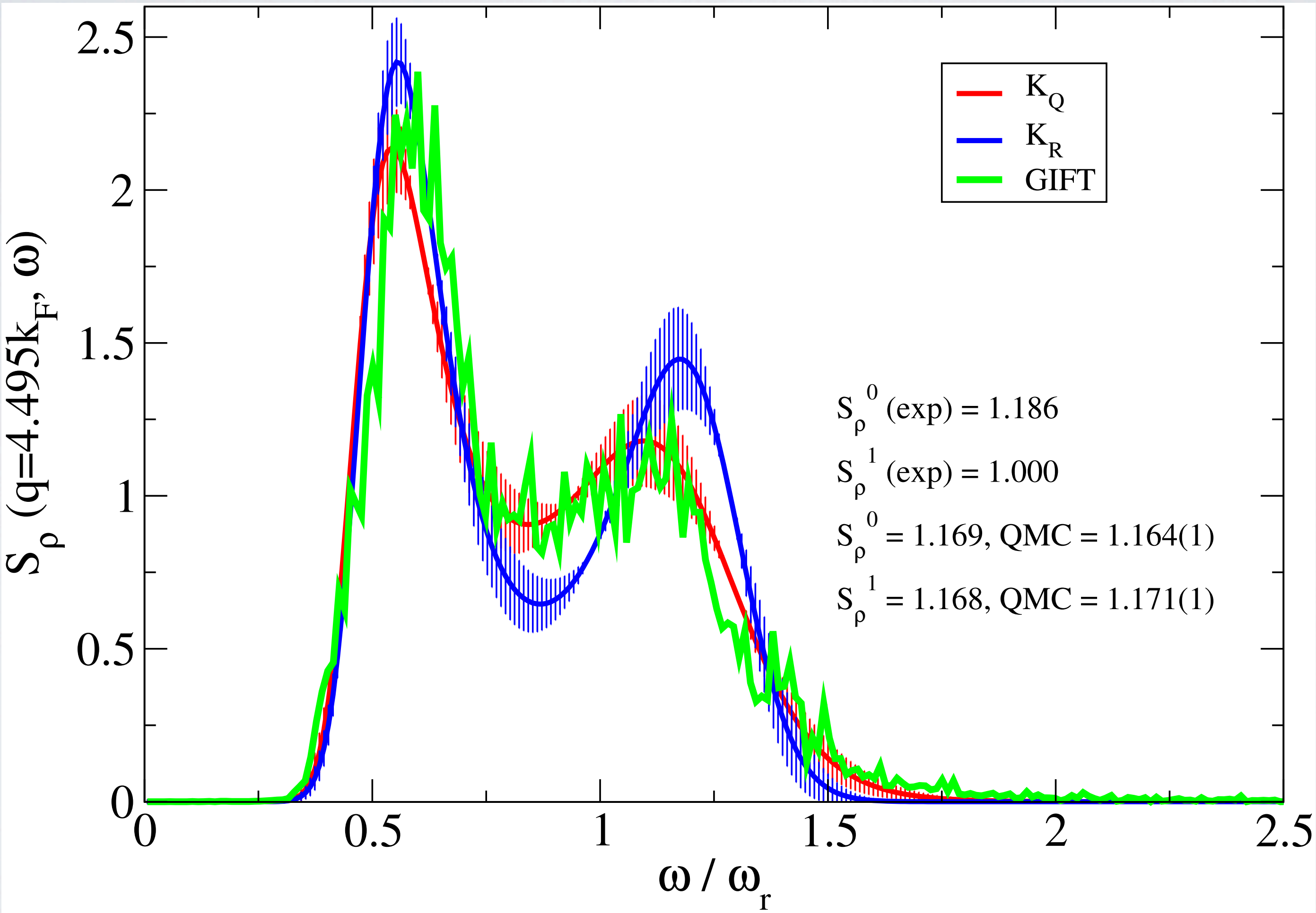
$$R(q,\omega) \ = \ \langle 0|\ \mathbf{j}^\dagger(q) \quad \exp[i\omega t]\ \mathbf{j}(q)\ |0\rangle$$

Imaginary-time correlator (Euclidean Response)

$$R(q,\tau) \ = \ \langle 0|\ \mathbf{j}^\dagger(q) \quad \exp[-H\tau]\ \mathbf{j}(q)\ |0\rangle$$



Challenge:
Extract as much information as possible from imaginary-time matrix elements

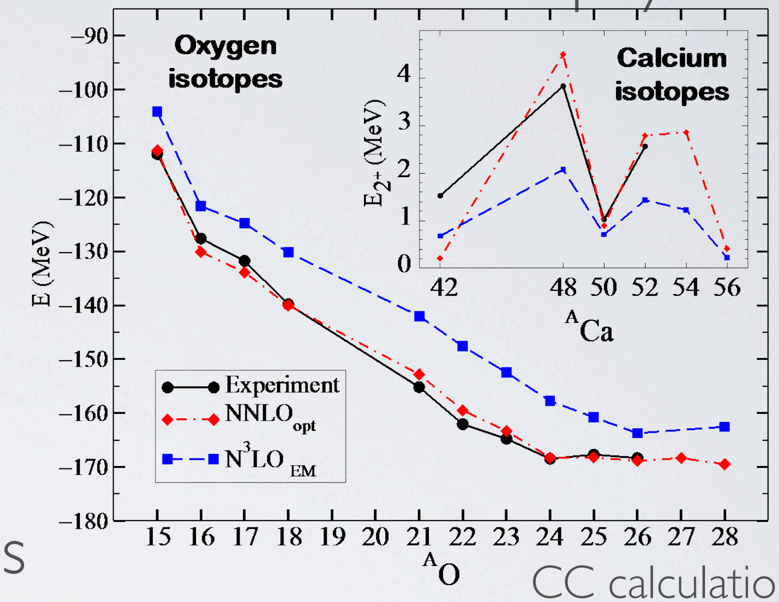


example from cold atom physics - unitary Fermi gas

Include analytic constraints, work with Higdon and others

Conclusions

Great progress in Quantum Monte Carlo in nuclear physics :
lattice approaches,
neutron matter/drops,
EM transitions and response



CC calculations of neutron-rich nuclei (Hagen, Papenbrock)

Many collaborations across methods (CI, CC, ...) and physics areas (nuclei, cold atoms, condensed matter).

Working closely with math/CS and SciDAC institutes:
SUPER, QUEST, FASTMATH

please see two NUCLEI posters:

Alessandro Lovato - QMC math/CS and physics

Hai Ah Nam - diverse projects in NUCLEI and ties to SciDAC institutes