Annual UNEDF Meeting 2011

DFT Extensions (DFTE): Year 5 deliverables and future plans

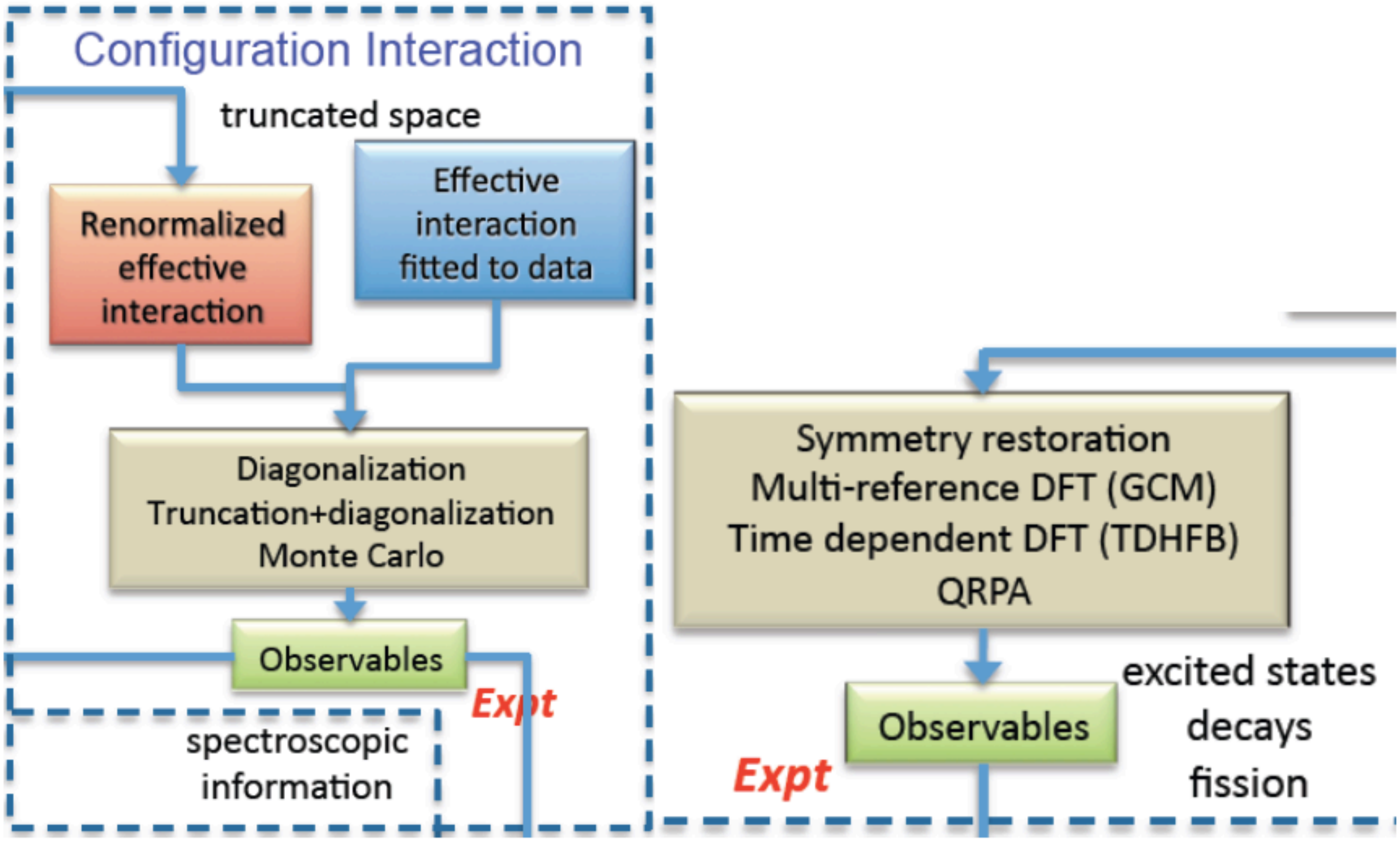


Figure 29: UNEDF's DFT EXTENSIONS Effort

DFTE: Year 5 Deliverables

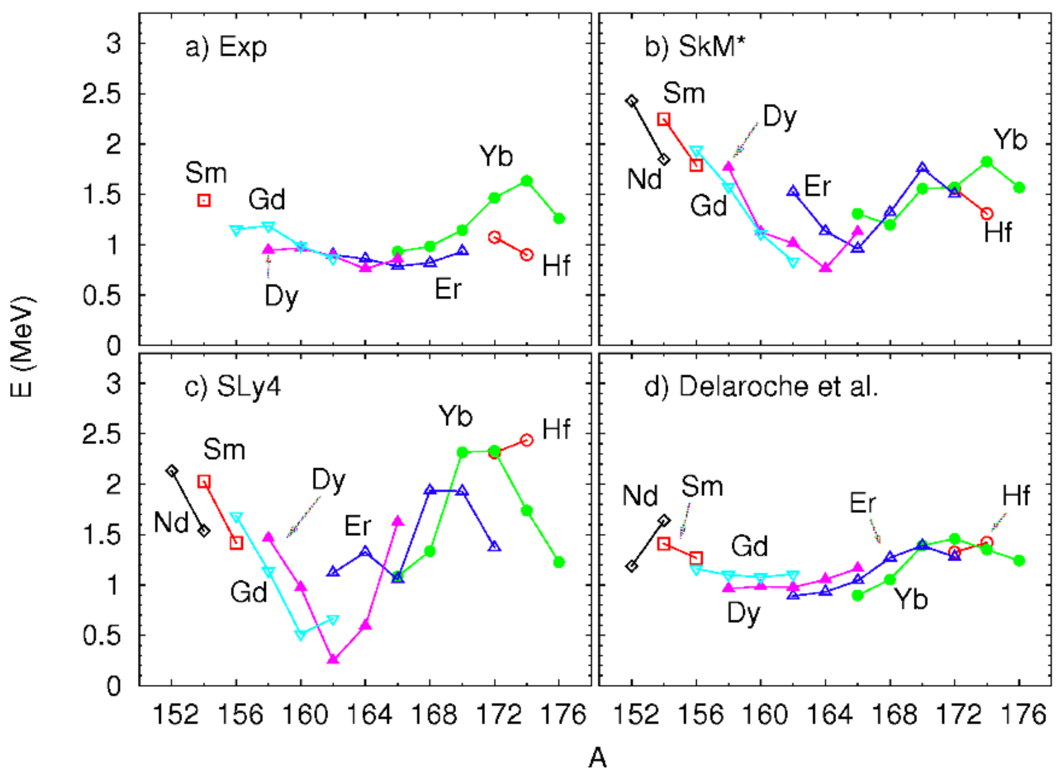
- **Engel, Terasaki, University of North Carolina at Chapel Hill:**
  - ➢ Complete calculation of β decay.
    - In progress
  - ➢ Develop DFT-consistent code beyond RPA.
    - In progress
- **Bulgac, Stetcu, Magierski (UW), Roche (PNNL):**
  - ➢ Improve the performance of the TD-SLDA code.
    - ✓ Accomplished; more tests in progress
  - ➢ Test the small amplitude regime for light nuclei.
    - ✓ Some cases worked out; more to be done
- **Horoi, Senkov, Central Michigan Unversity:**
  - ➢ Develop and test the J-Moments NLD code that removes the center-of-mass spurious contributions.
    - ✓ Accomplished; improving scalability in progress (may use ADLB ?)
  - ➢ Calculate more reaction rates in the rp-process path.
    - ✓ Some cases worked out; more examples to be done

DFTE: Year 5 Deliverables

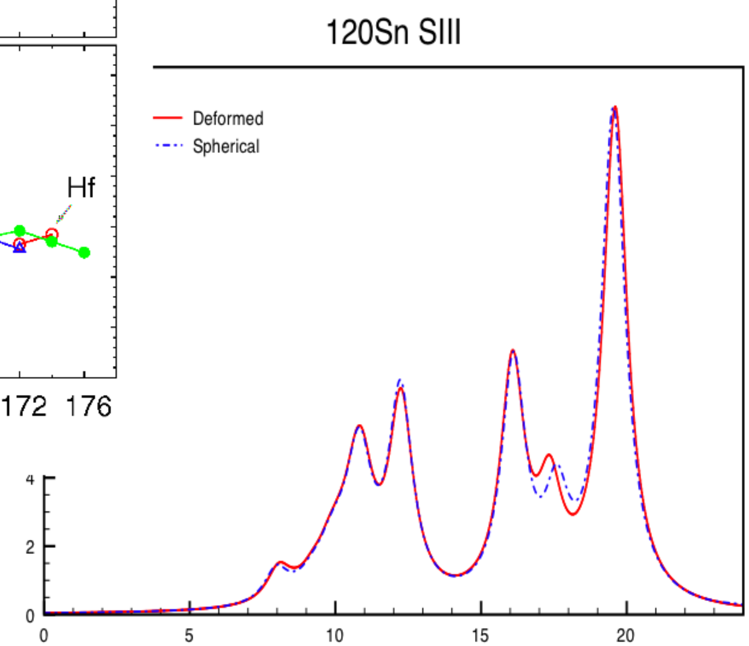
- **Brown, McDonald, Michigan State University:**
  - Understand the scalability barriers in NuShellX to enable the most effective use of GPUs and leadership-class (LC) machines.
    - ✓ Hybrid MPI/OpenMP code ready; testing in progress on LC machines
- **Johnson, Krastev, San Diego State University, Ormand (LLNL):**
  - Improve the scalability of REDSTICK CI code up to 50,000 cores.
    - Main barrier was reorthogonalization; now putting Lanczos ; vectors in memory to minimize I/O
  - Use REDSTICK to investigate isosping breaking in pf shell.
    - Delayed due to problem with I/O hardware on Sierra

Deformed QRPA

γ vibrations in rare earths



GT strength

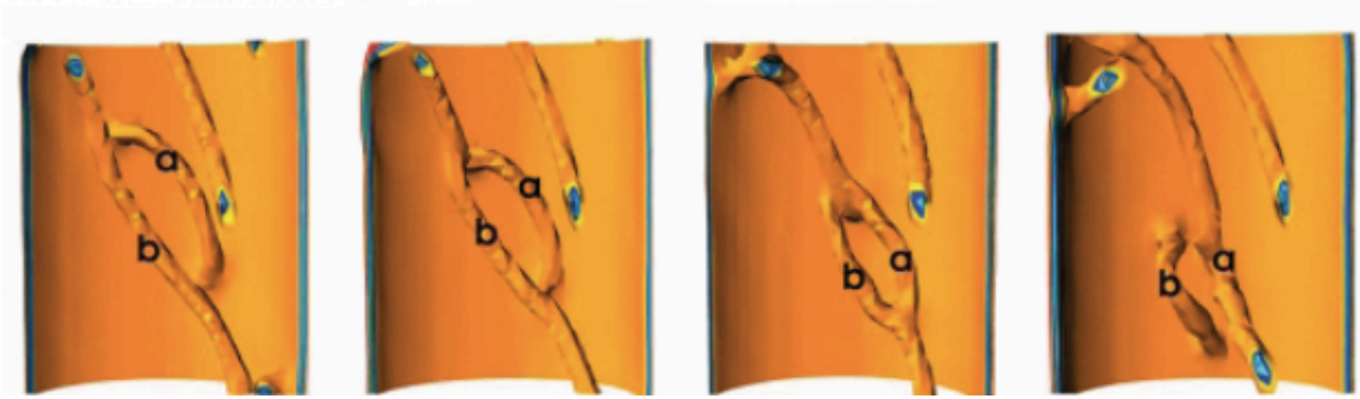


Deformed charge-changing code ready

Stirring superfluids

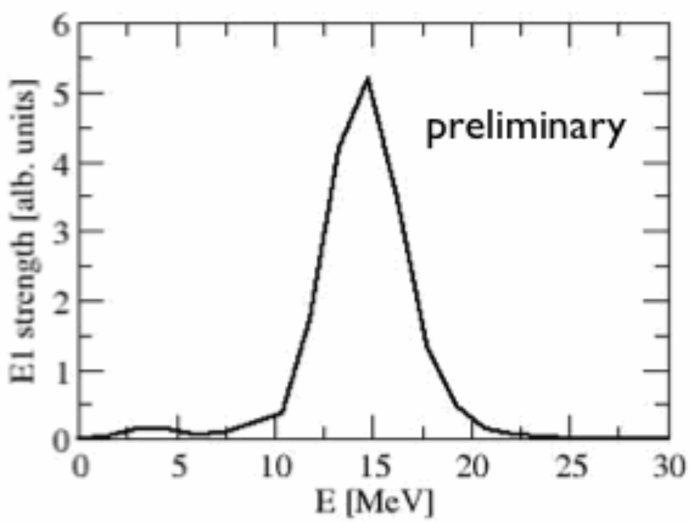
By Physics Today on June 13, 2011 10:52 AM | No TrackBacks

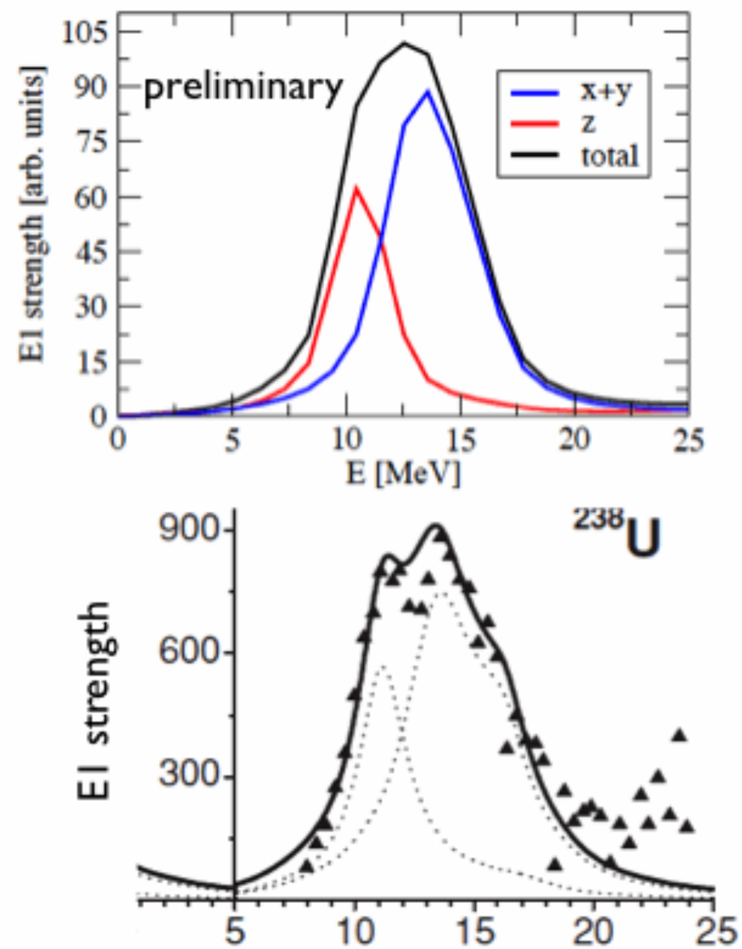
If you chill fermions enough, they can pair up to form bosons and settle into a single collective ground state, a Bose–Einstein condensate. In the case of helium-3 atoms, the resulting BEC is a superfluid that flows without dissipation—provided the flow is not so energetic that it breaks the pairs apart or destroys the ground state's coherence. Until now, theorists could characterize placid flows in fermionic superfluids, but not the vigorous turbulence that results from shaking or stirring. Aurel Bulgac of the University of Washington in Seattle and his colleagues have adapted density functional theory—a computational approach originally devised to calculate molecular energy levels—and applied its time-dependent extension to model turbulent fermionic superfluids. Although the underlying quantum mechanical equations are straightforward, solving them required the use of one of the world's most powerful supercomputers, Jaguar at Oak Ridge National Laboratory in Tennessee. In their simulations, Bulgac and his colleagues agitated a fermionic superfluid by shooting spherical projectiles through it or by stirring it with a laser beam. Turbulent superfluids are known to harbor tubes of quantized vorticity. As the figure below shows, the simulation could track how two vortex tubes (marked a and b) joined to form a ring, which then opens in a manner reminiscent of the unzipping of a DNA molecule during transcription. Bulgac's model could help astronomers understand another agitated superfluid: the interior of a rapidly spinning neutron star. (A. Bulgac et al., *Science* **332**, 1288, 2011.)—Charles Day



Time Dependent Approach: Applications to nuclei

Dipole response ^{136}Xe and ^{238}U





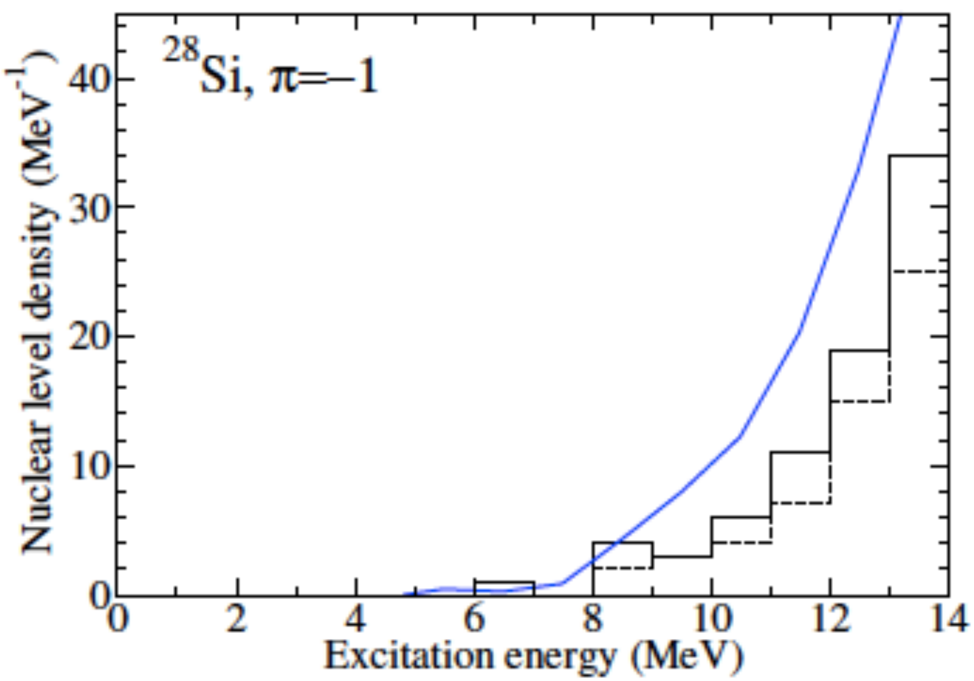
Scalable JMOMENTS PN Code for Nuclear Level Density (NLD): Removal of CoM Spurious Contributions

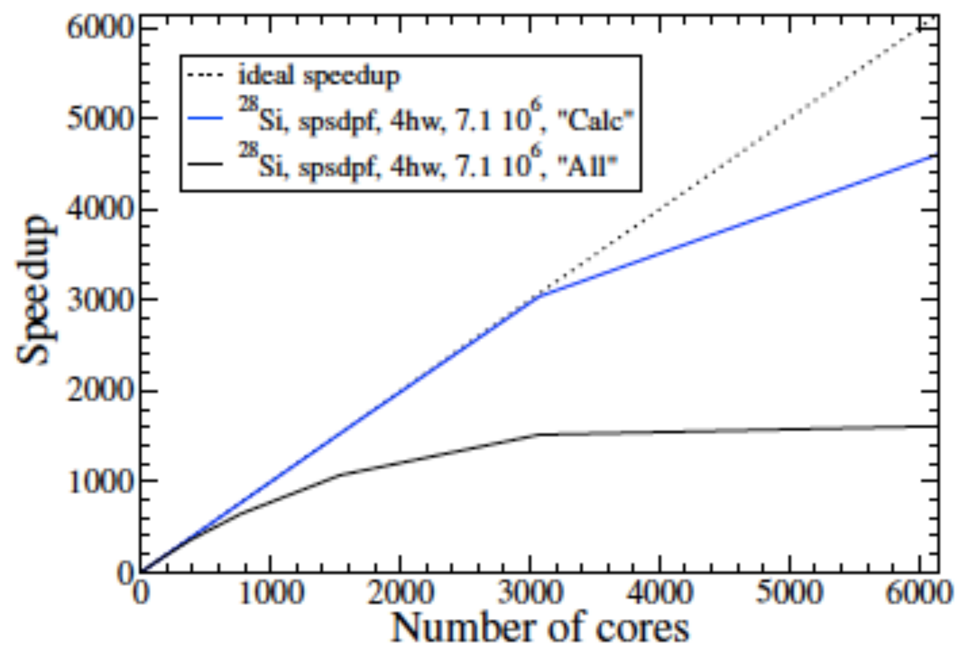
Domain decomposition: many-body configurations

Algorithm: Dynamical Load Balancing

Machine: Hopper/NERSC

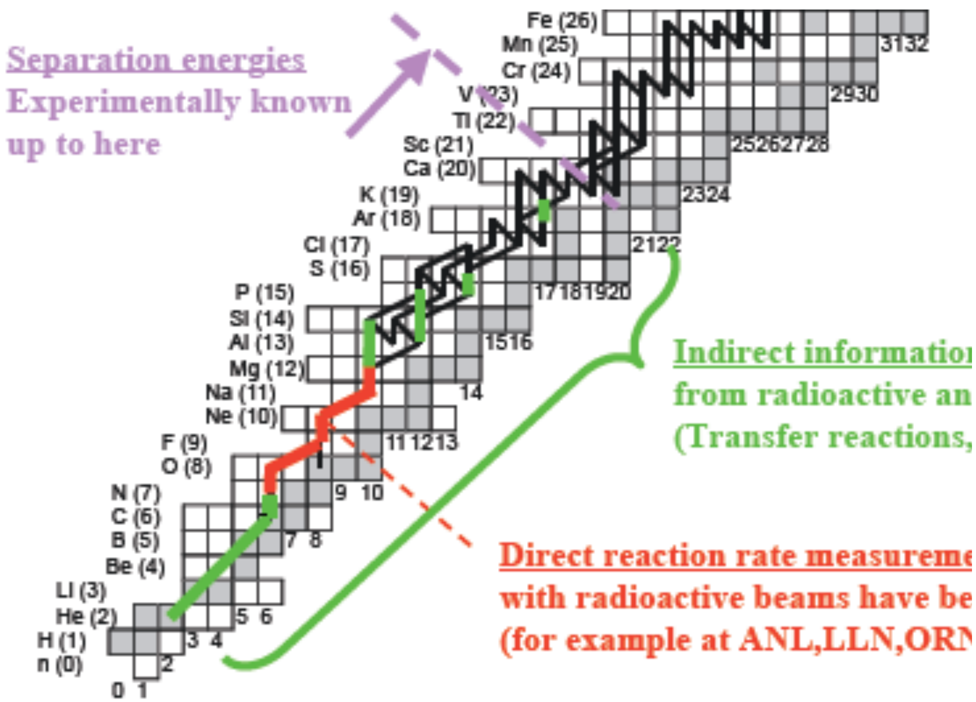
4 Major shells, Nmax=1

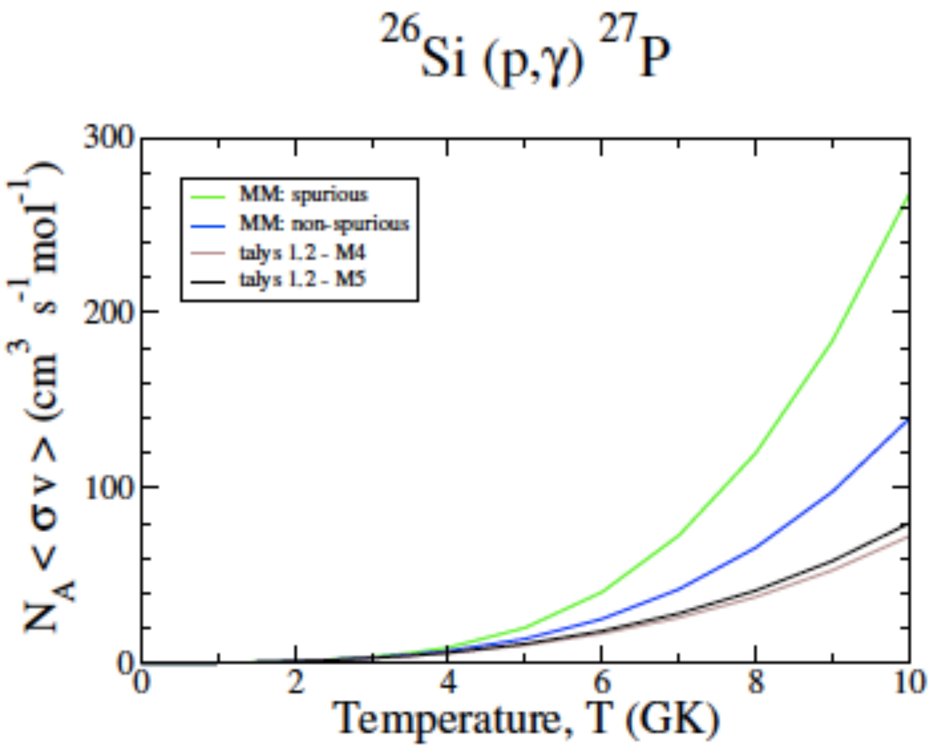




Strong scaling

Calculations of rp-process reaction rates using Moments Method NLDs





Year 5 Deliverables: Publications

1. "Real-Time Dynamics of Quantized Vortices in a Unitary Fermi Superfluid," A. Bulgac, Y.-L. Luo, P. Magierski, K.J. Roche, and Y. Yu, Science **332**, 1288 (2011), arXiv:1011.5999.

2. "Coupled-Channels Calculations of Nonelastic Cross Sections Using a Density-Functional Structure Model", G.P.A. Nobre, F.S. Dietrich, J.E. Escher, I.J. Thompson, M. Dupuis, J. Terasaki, and J. Engel, Phys. Rev. Lett. 105 (2010) 202502.

3. "Configuration Interactions Constrained by Energy Density Functionals", B. A. Brown, A. Signoracci and M. Hjorth-Jensen, Phys. Lett. B 695, 507 (2011).

4. "High-Performance Algorithm for Calculating Non-Spurious Spin- and Parity-Dependent Nuclear Level Densities" , R. Senkov, M. Horoi, and V. Zelevinsky, accepted for publication in Phys. Lett. B, arXiv:1102.0940.

5. "Improved Accuracy Moments Method for Spin-Dependent Shell Model Nuclear Level Densities", M. Scott and M. Horoi, EPL **91**, 52001 (2010).

6. "Self-Consistent Skyrme QRPA for Use in Axially-Symmetric Nuclei of Arbitrary Mass", J. Terasaki and J. Engel, Phys. Rev. C 82 (2010) 034326.

7. "Testing Skyrme Energy-Density Functionals with the QRPA in Low-Lying States of Rare-Earth Nuclei", J. Terasaki and J. Engel, arXiv:1105.3817v1 [nucl-th], to appear in Phys. Rev. C.

8. "Three and four harmonically trapped particles in an effective field theory framework", J. Rotureau, I. Stetcu, B.R. Barrett, and U. van Kolck, Phys. Rev. A **82**, 032711 (2010).

9. A. Bulgac and M.M. Forbes, Time-Dependent Superfluid Local Density Approximation, chapter in ``Quantum Gases: Finite Temperature and Non-Equilibrium Dynamics(Cold Atoms Series)," Nick Proukakis, Simon Gardiner, Matthew Davis, Marzena Szymanska and Nicolai Nygaard (eds.), Imperial College Press: London, in press.

10. A. Bulgac, M.M. Forbes, and P. Magierski, The Unitary Fermi Gas: From Monte Carlo to Density Functionals, arXiv:1008.3933, chapter in ``BCS-BEC Crossover and the Unitary Fermi Gas" (Lecture Notes in Physics), edited by W. Zwerger (Springer, 2011), in press.

11. "A High-Performance Algorithm to Calculate Spin- and Parity-Dependent Nuclear Level Densities", arXiv:1004.5027, R. Senkov and M. Horoi, Phys. Rev. C **82**, 024304 (2010).

12. "Can one identify the intrinsic structure of the yrast states in ^{48}Cr after the backhanding?", Z-C. Gao, M. Horoi, and Y. S. Chen, Y. J. Chen, and Tuya, Phys. Rev. C **83**, 057303 (2011).

13. "An Update of B(E2) Evaluation for $0_{1}^{+} \rightarrow 2_{1}^{+}$ Transitions in Even-Even Nuclei near N$\sim$Z$\sim$28", B. Pritychenko, J. Choquette, M. Horoi, B. Karamy, B. Singh, accepted for publication in At. Data. Nucl. Data. Tabels, arXiv:1102.3365 (BNL-94720-2011-JA).

14. "The Role of Shell Model Nuclear Level Densities for Nuclear Astrophysics", M. Horoi and R. Senkov, Proceedings of the International Symposium on Nuclear Astrophysics "Nuclei in Cosmos - XI", Heidelberg, Germany, July 19-23, 2010, **PoS(NIC-X)222**, (2010), http://pos.sissa.it/ .

15. "Nuclear Shell Model Analyses and Predictions of Double-Beta Decay Observables", M. Horoi, Proceedings of the Carpathian Summer School of Physics "Exotic Nuclei & Nuclear/Particle Astrophysics II. From Nuclei to Stars', Sinaia, Romania, June 20 - July 3, 2010, AIP Proceedings **1304**, 106 (2010)

16. "Renormalized Interactions with a Realistic Single-Particle Basis", A. Signoracci, B. A. Brown and M. Hjorth-Jensen, Phys. Rev. C 83, 024315 (2011).

17. "The onset of the pseudogap phase in ultracold Fermi gases," P. Magierski, G. Wlazlowski, and A. Bulgac, arXiv:1103.4328.

18. "The onset of the pseudogap phase in ultracold Fermi gases," P. Magierski, G. Wlazlowski, and A. Bulgac, arXiv:1103.4382, submitted to PRL.

Year 5 Deliverables: Talks

1. J. Engel, Charge-Changing Processes and Nuclear Response, Meeting of the Topical Collaboration on Hot and Dense Matter, Los Alamos, NM, June 6, 2011.

2. J. Terasaki, Test of Skyrme Energy Functionals with QRPA in Low-Lying States of Rare-Earth Nuclei, 5th LACM EFES JUSTIPEN Workshop, Oak Ridge, TN, March 15, 2011.

3. A. Bulgac, Lectures, Summer School on Nuclear Collective Dynamics V, F.Gursey Institute for Theoretical Physics, Istambul Turkey, July 4-10, 4. 2010.

5. A. Bulgac, Invited talk, Quantum solids, liquids, and gases, July 19 - August 27, 2010, Stockholm, Sweden.

6. A. Bulgac, Invited talk, Frontiers of condensed matter physics, Stockholm, Sweden, January 3-8, 2011.

7. A. Bulgac, Lectures, 14th Taiwan Nuclear Physics School, January 17-22, 2011, Taiwan.

8. A. Bulgac, Seminar, UW, January 27th, 2011.

9. A. Bulgac, Seminar, INT program Fermions from Cold Atoms to Neutron Stars: Benchmarking the Many-Body Problem, April 18th, 2011
10. A. Bulgac, Invited talk, INT Ultra-Cold Atoms Symposium, May, 16-20, 2011.

11. A. Bulgac, Seminar, INT program Extreme Computing and its Implications for the Nuclear Physics/Applied Mathematics/Computer Science Interface, June 8th, 2011.

12. A. Bulgac, Invited talk, Workshop on the Nuclear Physics/ Applied Math/Computer Science Interface Applied Math/CS, June 27 - July 1, 2011.

13. A. Bulgac, Invited talk, Finite-temperature Non-Equilibrium Superfluid Systems, September 18-21, 2011, Heidelberg, Germany.

14. I. Stetcu, K. J. Roche, Time-dependent Approach to Nuclear Systems, East Lansing, Michigan, June 20-24, 2011.

15. K. J. Roche, Data Intensive Analysis: Computing Case Study from Low-Energy Nuclear Theory (Prepared for Drs. Atsuto Suzuki, Masanori Yamauchi), PNNL-SA-80383, Richland, Washington, June 3, 2011.

16. I. Stetcu, Nuclear dynamics in real time, invited talk at the International Workshop on Nuclear Physics, Stellenbosch, South Africa, May 2011.

17. I. Stetcu, Harmonic EFT, the beginning: from nuclei to trapped atoms, talk at the ECT* workshop on "Effective theories and the nuclear many-body problem," Trento, Italy, March 2011.

18. I. Stetcu, The road from trapped cold atoms to nuclear physics, talk at the ECT* workshop on "The limits of existence of light nuclei," Trento, Italy, Oct. 2010.

19. I. Stetcu, Nuclear structure and dynamics in a time-dependent SLDA framework, seminars at MSU, Warsaw Inst. Tech., NIPNE-HH Bucharest, Sept.-Nov. 2010.

20. M. Horoi, "Challenges for a reliable shell-model description of the neutrinoless double beta decay matrix elements", MEDEX'11 Workshop, Prague, June 13-16, 2011.

21. M. Horoi, "Updates on Nushellx", LCCI collaboration meeting, BLNL, March 17-19, 2011.

22. M. Horoi, "Effective Forces Responsible for Enhanced Proton-Neutron Correlations in N $\approx$ Z Nuclei", ECT* workshop "Effective Theories and the Nuclear Many-Body Problem", Trento, Italy, March 7-11, 2011.

23. M. Horoi, "Nuclear Structure Theory Relevant to the Facility for Rare Isotope Beams", colloquium at Western Michigan University, Kalamazoo, MI, January 24, 2011.

24. M. Horoi, "Proton-neutron pairing correlations in nuclei: a shell model perspective", invited talk at the International Workshop *Probing Proton-Neutron Pair Correlations* held at Nishina Center, RIKEN Wako-shi campus, Japan, November 19-20, 2010.

25. M. Horoi, "Structure Theory for the Facility of Rare Isotope Beams", invited talk at the Annual Meeting of Division of Nuclear Physics of the American Physical Society, Santa Fe, New Mexico, November 4, 2010.

26. M. Horoi, "Nuclear Shell Model Analyses and Predictions of Double-Beta Decay Observables", invited talk at the Carpathian Summer School of Physics 'Exotic Nuclei \& Nuclear/Particle Astrophysics II. From Nuclei to Stars', Cyclotron Institute at Texas A&M, International Center for Theoretical Physics Trieste, Horia Hulubei National Institute of Physics and Nuclear Engineering, Romania, Sinaia, Romania (June 30, 2010).

27. R. Senkov and M. Horoi, "High Performance Algorithm for Non-Spurious Spin- and Parity-Dependent Nuclear Level Density", Annual Meeting of Division of Nuclear Physics of the American Physical Society, Santa Fe, New Mexico, November 4, 2010.

28. S. Stoica, A. Neacsu, and M. Horoi, "Shell model calculations of double-beta decay lifetimes of ^{76}Ge and ^{82}Se", Annual Meeting of Division of Nuclear Physics of the American Physical Society, Santa Fe, New Mexico, November 4, 2010.

29. B.A. Brown, Renormalized interactions for CI constrained by EDF methods and NuShellX@MSU, Carpathian Summer School of Physics 2010, Exotic Nuclei and Nuclear/Particle Astrophysics (III), From Nuclei to Stars, June 20 – July 3, 2010, Sinaia, Romania.

30. B.A. Brown, Configuration Interactions Constrained by Energy-Density Functionals, University of Aizu- JUSTIPEN - EFES Symposium on "Cutting-Edge Physics of Unstable Nuclei", University of Aizu, Aizuwakamatsu, Fukushima, Japan, November 10-13, 2010.

31. C.W. Johnson, "Add, multiply, divide, and conquer," UCSD Quantum Chemistry Seminar, Oct. 2010

32. C.W. Johnson, "Factorization algorithms for configuration-interaction," Perspectives on the no-core shell model, TRIUMF, Feb 2011.

33. C.W. Johnson, "Cold atomic gases and effective interactions," Benchmarking the many-body problem, Institute for Nuclear Theory/University of Washington, March 2011

UNC: Year 5 Deliverables

Accomplishments:

- Completed study of 2^+ states in rare earths
- Developed charge-changing deformed QRPA and began application to beta decay and double beta decay
- Collaborated with ORNL group to develop sum-rule approach to including giant resonances in optimization of functionals.

Remaining:

- Complete calculations of r-process beta decay, double-beta decay.
- Begin to develop beyond-QRPA approach

UW: Year 5 Deliverables

Accomplishments:

- Improved numerical accuracy and optimized further the SLDA/TDSLA codes- Significant portions of codes have been recoded from Fortran90 to C
- Performed a series of GDR calculations in several open shell nuclei (to be submitted)
- First implementation of neutron scattering off open-shell nuclei
- Performed extensive studies of vortex dynamics in unitary Fermi gas, established a number of new qualitative phenomena (published)
- Revealed the existence of shock waves and dark solitons in collisions of cold Fermi clouds (to be submitted)
- Performed the first series of exploratory stochastic real-time solutions of Schroedinger equation for interacting fermions (to be submitted)

UW: Year 5 Deliverables

What remains to be done in year 5

- Continue the study of real-time path integral for interacting fermions
- Study excitation of single and multiple GDR excited with relativistic heavy-ions
- Rewriting SLDA/TDSLDA codes in C
- Several papers to be submitted:

a) I. Stetcu, A. Bulgac, P. Magierski, K.J. Roche, Excitation of GDR in open-shell nuclei

b) A. Bulgac, Y.-L. Luo, K.J. Roche, Excitation of dark solitons and shock waves in collision of cold fermi gases

c) A. Bulgac, Y.-L. Luo, K.J. Roche, Y. Yu , Real-time path integral for interacting many fermion systems

CMU: Year 5 Deliverables

Deliverables for year 5

- new algorithm of removal of the contribution of center-of-mass spurious states was successfully developed and tested
- the code is parallelized and was tested using up to 6,000 processors
- calculations of NLD in large model spaces were performed
- calculations of reaction rates in the rp-process path were made

What's next?

- improve the scaling
- develop interface, scripts
- write documentation, examples. publish the code
- more applications: NLD, reaction rates, schematic interactions

MSU: Year 5 Deliverables

NuShellX Summary

- We met our Year 5 goals of:
  - analyzing scalability constraints on the code,
  - evaluating options for reaching the petascale level,
  - and producing a working MPI/OMP hybrid code.
- The hybrid code has been shown to scale to a much larger number of cores than the original OpenMP-only code.
- We have a number of goals for further improvements to the code. These will be discussed during the presentation.

NSCL

SciDAC Scientific Discovery through Advanced Computing

Rest of Year 5: optimize the hybrid MPI/OpenMP code

SDSU: Year 5 Deliverables

UNEDF Deliverables for BIGSTICK:

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

Current version (6.5) at NERSC; expect final version by end of year; plans to publish in CPC or similar venue.

•Improve the scalability of BIGSTICK CI code up to 50,000 cores.

Main barrier was reorthogonalization; now putting Lanczos vectors in memory to minimize I/O

• Use BIGSTICK code to investigate isospin breaking in pf shell

Delayed due to problem with I/O hardware on Sierra

LCCI Meeting March 17-19, 2011

Issues discussed:

Progress on code & script developments
Update schedules (slide 5)
Modifications to Year 5 goals, deliverables (slide 25)
What to propose for SciDAC-3

Some specific questions discussed:

LCCI thrust areas to propose for SciDAC3:
- double beta decay (slides 16, 18)
- ab-initio nuclear reactions (slides 16, 19)
- structure of medium mass nuclei: 78Ni, 132Sn (slides 16, 19)

If/how to fold the upstream codes into wrapper -> SciDAC3
Will additional researchers deposit .info files to DBMS -> Yes
Desired features for DBMS/Workflow and their priorities -> Ongoing
What happens to UNEDF web site & m308 at end of UNEDF?
-> UNEDF Council to address
Making the LCCI repository public, e.g. via UNEDF web site,
or via FRIB or via NNDC -> possibly all 3

Questions:

- Different codes optimized for different problems

- Do we need all these codes

DFTE Plans for SciDAC-3

Physics Drivers:

Ab-initio calculations of reactions:

- Fusion: e.g. $^{8}Be\ (\alpha,\gamma)\ ^{12}C$
- TN reaction
- Reactions relevant to NIF
- nucleon-nucleus and reactions generally

Weak interactions in nuclei:

- Solar neutrino reactions
- Accelerator neutrinos (~1 GeV)
- $\beta\beta$ decay

Physics of Extreme Neutron-Rich Nuclei and Matter

- Ab-initio and Density Functional
- Coupled Cluster for neutron-rich nuclei

Microscopic Description of Fission

- Density Functionals
- Fission Barriers
- SLDA/TDSLDA

UW: Plans for SciDAC-3

a) **Extend the application of SLDA and TDSLDA to study nuclear LACM, induced fission, nuclear reactions, and various collective modes in nuclei and related systems**

b) **Study the feasibility of stochastic TDSLDA and perform the first simulations of many-fermion systems including fluctuations of the meanfield**

c) **Implement lattice QMC with EFT interactions for N=Z nuclei, neutron and symmetric nuclear matter on leadership class supercomputers**

d) **Study the dynamics of vortices in neutron star crust**

Microscopic Description of Fission

- Density Functionals
- Fission Barriers
- SLDA/TDSLDA

DFTE Plans for SciDAC-3

Physics Drivers:

Ab-initio calculations of reactions:

- Fusion: e.g. $^{8}Be\ (\alpha,\gamma)\ ^{12}C$
- TN reaction
- Reactions relevant to NIF
- nucleon-nucleus and reactions generally

Weak interactions in nuclei:

- Solar neutrino reactions
- Accelerator neutrinos (~1 GeV)
- $\beta\beta$ decay

Physics of Extreme Neutron-Rich Nuclei and Matter

- Ab-initio and Density Functional
- Coupled Cluster for neutron-rich nuclei

Microscopic Description of Fission

- Density Functionals
- Fission Barriers
- SLDA/TDSLDA

LCCI Meeting March 17-19, 2011

Issues discussed:

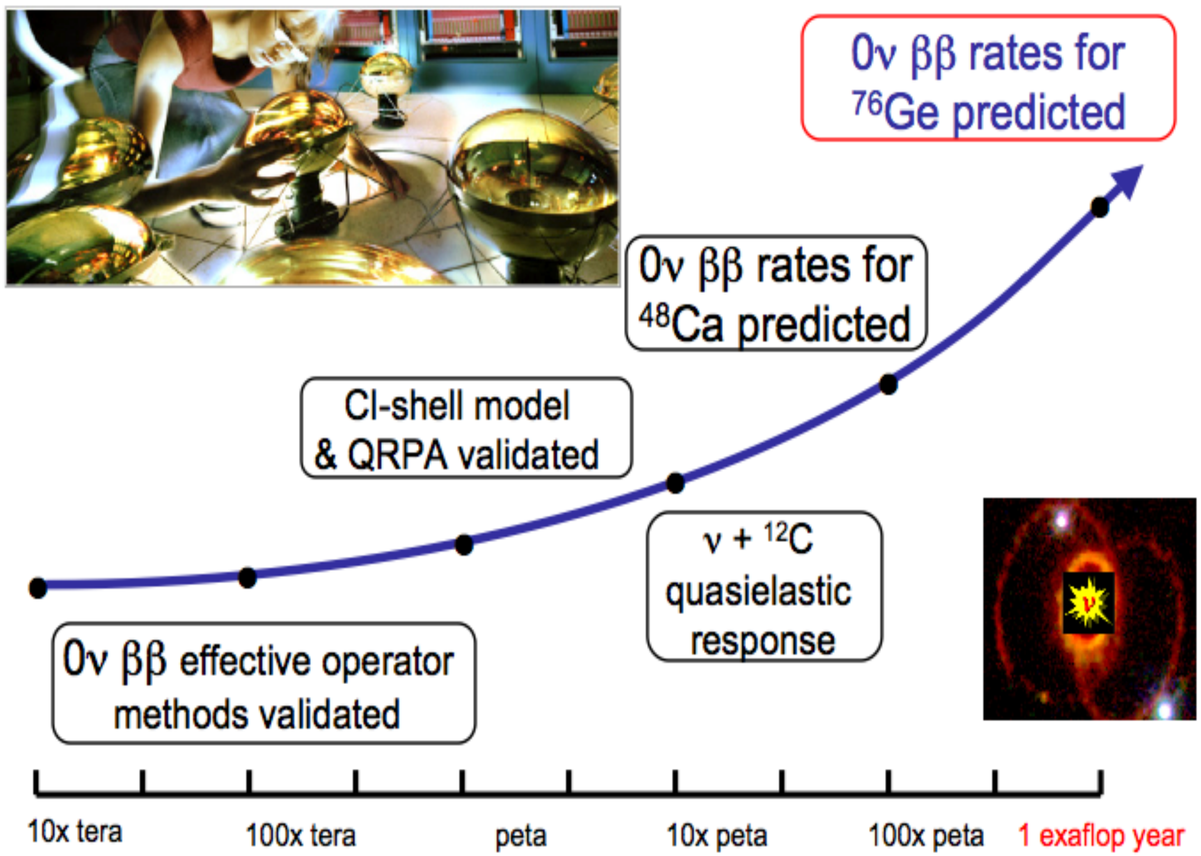
Progress on code & script developments
Update schedules (slide 5)
Modifications to Year 5 goals, deliverables (slide 25)
What to propose for SciDAC-3

Some specific questions discussed:

LCCI thrust areas to propose for SciDAC3:
- double beta decay (slides 16, 18)
- ab-initio nuclear reactions (slides 16, 19)
- structure of medium mass nuclei: 78Ni, 132Sn (slides 16, 19)

If/how to fold the upstream codes into wrapper -> SciDAC3
Will additional researchers deposit .info files to DBMS -> Yes
Desired features for DBMS/Workflow and their priorities -> Ongoing
What happens to UNEDF web site & m308 at end of UNEDF?
 -> UNEDF Council to address
Making the LCCI repository public, e.g. via UNEDF web site,
 or via FRIB or via NNDC -> possibly all 3

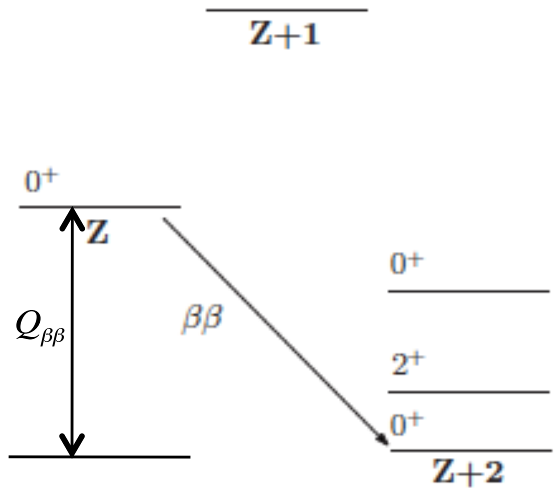
LCCI Highlights for ASCR



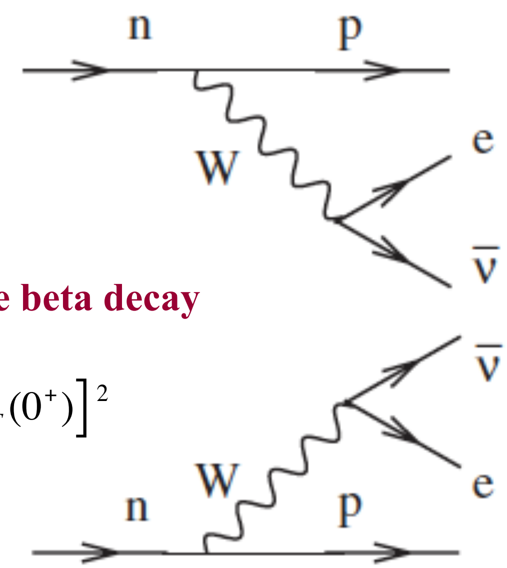
Office of Science Financial Assistance Funding Opportunity Announcement DE-PS02-09ER09-24 *Topical Collaborations in Nuclear Theory*

- a. Effective field theory descriptions of nuclear forces
- b. Properties of nuclei far from stability
- c. Microscopic studies of nuclear input parameters for astrophysics
- d. Calculations of electroweak corrections to precision data
- e. Microscopic nuclear reaction theory
- f. Analysis of the spectrum of excited baryons and mesons
- g. Studies of the phases of strongly-interacting matter
- h. Phenomenology of hard probes of hot, dense matter
- i. Phenomenology of thermal probes of hot matter
- j. Simulations of core collapse supernovae
- k. Lattice simulations of hadron properties
- l. Lattice simulations of thermal quantum chromodynamics
- m. *Ab initio* many-body calculations
- n. Phenomenology of neutrino oscillations
- o. Dynamics of fission
- p. Calculations of double beta decay nuclear matrix elements
- q. Extensions of the Standard Model

Double Beta Decay Problem

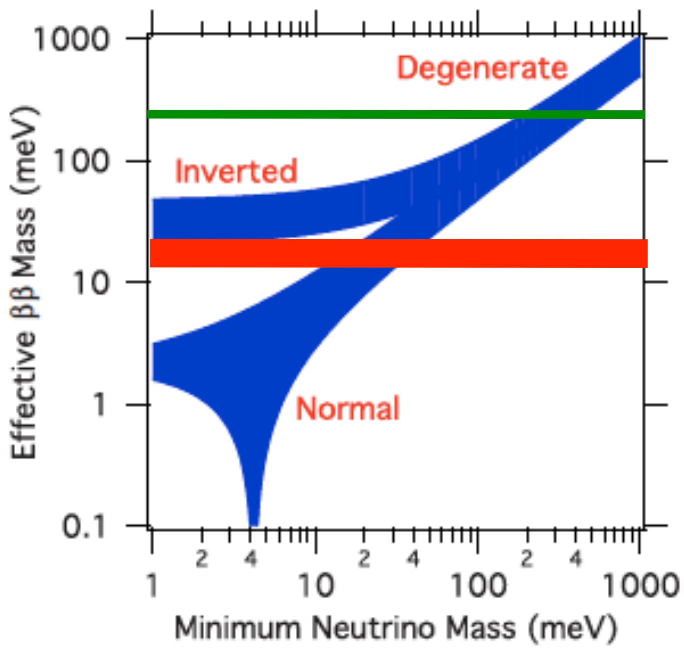


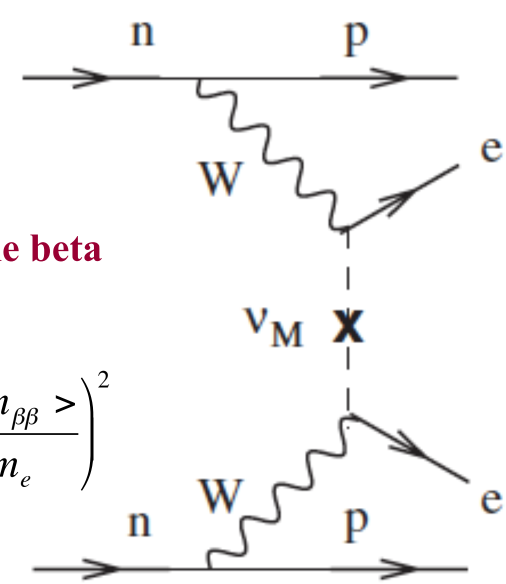
Adapted from Avignone, Elliot, Engel, Rev. Mod. Phys. 80, 481 (2008) -> RMP08



2-neutrino double beta decay

$$T_{1/2}^{-1}(2\nu) = G_{2\nu}(Q_{\beta\beta})\left[M_{GT}^{2\nu}(0^+)\right]^2$$





neutrinoless double beta decay

$$T_{1/2}^{-1}(0\nu) = G_{0\nu}(Q_{\beta\beta})\left[M^{0\nu}(0^+)\right]^2\left(\frac{< m_{\beta\beta} >}{m_e}\right)^2$$

$$\langle m_{\beta\beta}\rangle = \left|\sum_k m_k U_{ek}^2\right|$$

Neutrinoless DBD matrix element

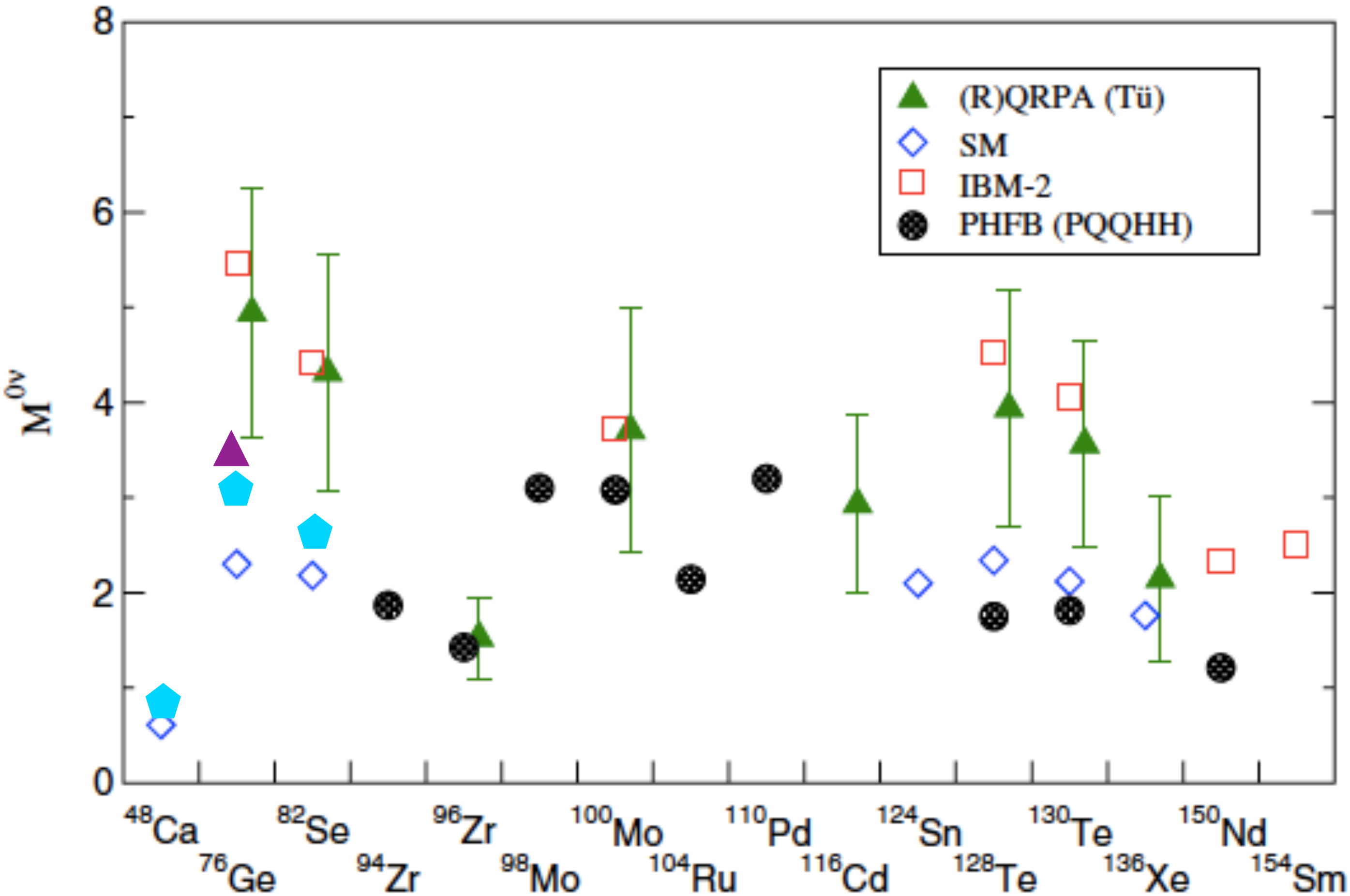
$$T_{1/2}^{-1}(0\nu) = G_{0\nu}(Q_{\beta\beta})\left[M^{0\nu}(0^+)\right]^2\left(\frac{<m_{\beta\beta}>}{m_e}\right)^2$$

$$\langle m_{\beta\beta}\rangle = \left|\sum_k m_k U_{ek}^2\right|$$

A. Escuderos et al, J. Phys. G, 37, 125108 (Nov 2010)

▲ **Menendez et al arXiv:0906.0179 (rg.prolate int)**

⬟ **CMU results**



$$Prediction\ for\ {}^{76}Ge: \langle M^{0\nu}\rangle = 3 \xrightarrow{T_{1/2}(0\nu)\geq 10^{26}y} \langle m_{\beta\beta}\rangle \leq 0.220\, eV$$

Experimental Status of DBD

Japan

Homestake

Experiment	Isotope	Mass	Technique	Present status
CANDLES	^{48}Ca	few tons	CaF_2 scint. crystals	Prototype
CARVEL	^{48}Ca	1 ton	$CaWO_4$ scint. crystals	Development
COBRA	^{116}Cd	418 kg	CZT semicond. det.	Prototype
CUORICINO	^{130}Te	40.7 kg	TeO_2 bolometers	Running
CUORE	^{130}Te	741 kg	TeO_2 bolometers	Proposal
DCBA	^{150}Ne	20 kg	^{enr}Nd foils and tracking	Development
EXO-200	^{136}Xe	200 kg	Liq. ^{enr}Xe TPC/scint.	Construction
EXO	^{136}Xe	1–10 ton	Liq. ^{enr}Xe TPC/scint.	Proposal
GEM	^{76}Ge	1 ton	^{enr}Ge det. in liq. nitrogen	Inactive
GENIUS	^{76}Ge	1 ton	^{enr}Ge det. in liq. nitrogen	Inactive
GERDA	^{76}Ge	≈35 kg	^{enr}Ge semicond. det.	Construction
GSO	^{160}Gd	2 ton	Gd_2SiO_5:Ce crys. scint. in liq. scint.	Development
MAJORANA	^{76}Ge	120 kg	^{enr}Ge semicond. det.	Proposal
MOON	^{100}Mo	1 ton	^{enr}Mo foils/scint.	Proposal
SNO++	^{150}Nd	10 ton	Nd loaded liq. scint.	Proposal

KamLAND2-Zen at MEDEX'11

400 kg ^{136}Xe experiment with sensitivity down to 50 meV for effective neutrino mass is about to start

UNC: Plans for SciDAC-3

Comprehensive EDF calculation of double-beta decay. Three phases:

1. Development of triaxial HFB with full mixing of neutrons and protons, including the important phenomena of isoscalar pairing. Development of appropriate pairing functional
2. Full QRPA on top of this HFB state.
3. GCM-like mixing of resulting QRPA vacua. With fast QRPA, this will be less computationally intensive than I had originally thought, but will still be a major enterprise.

Also would like to collaborate with coupled-cluster and in-medium SRG groups to develop shell-model effective interaction and effective double-beta operator.

Weak interactions in nuclei:

Solar neutrino reactions

Accelerator neutrinos (~1 GeV)

ββ decay

CMU: Plans for SciDAC-3

1. Investigate the role of missing spin-orbit partners to the CI $2\nu\beta\beta$ matrix elements or A>56
2. Investigate the role quenching and short range correlations to the $0\nu\beta\beta$ matrix elements; use light nuclei (p-sd) in increasingly larger model spaces.
3. Calculate the $0\nu\beta\beta$ matrix elements with error ranges less than 20%.
4. Understand the differences between the CI and QRPA matrix elements

Weak interactions in nuclei:

Solar neutrino reactions

Accelerator neutrinos (~1 GeV)

$\beta\beta$ decay

MSU: Plans for SciDAC-3

1. Investigate the $2\nu\beta\beta$ in A>56
2. Gamow-Teller strengths and validation of $2\nu\beta\beta$
3. Investigate the $0\nu\beta\beta$ in A>56

Past years: About 15 papers where Nushellx is used for collaboration with experimental groups, many on GT strength

Weak interactions in nuclei:

Solar neutrino reactions

Accelerator neutrinos (~1 GeV)

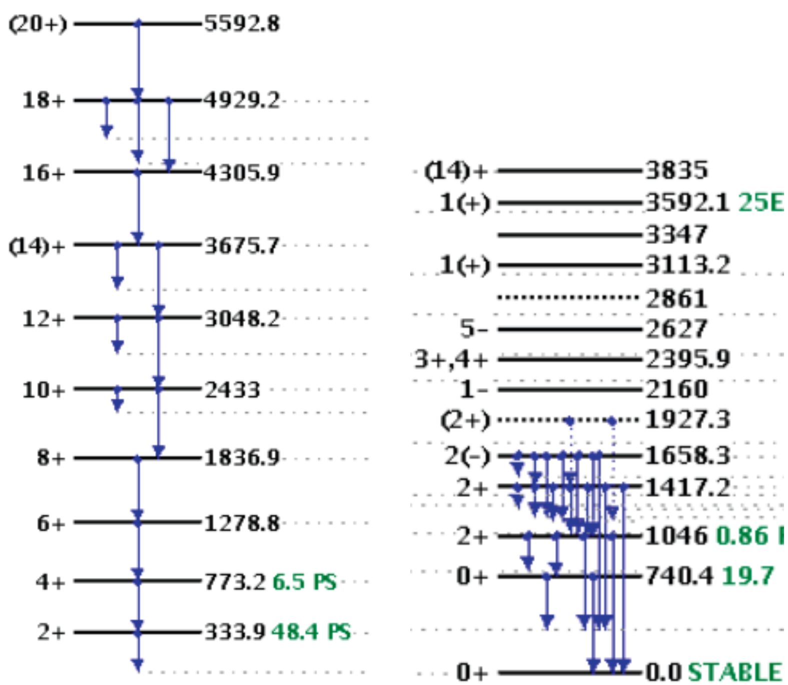
$\beta\beta$ decay

Two 0νββ decay cases

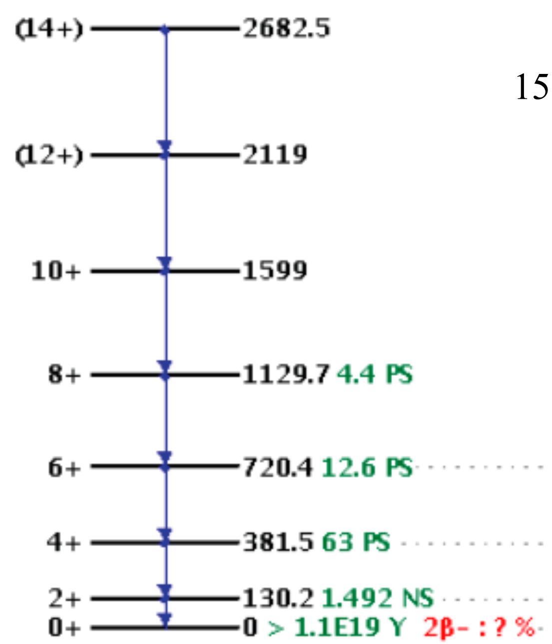
- ^{76}Ge -> ^{76}Se
- fp-g9/2 valence space
- p,n: 0f7/2 0f5/2 1p3/2 1p1/2 0g9/2
- ^{76}Ge: **dim 1,296,156,991,047**
- ^{76}Se: **dim 18,333,463,355,503**

- ^{150}Nd -> ^{150}Sm
- p: 0g7/2 1d5/2 1d3/2 2s1/2 0h11/2
- n: 1f7/2 1f5/2 0h9/2 2p3/2 2p1/2 0i13/2
- ^{150}Nd: **dim 222,314,413,121,622**
- ^{150}Sm: **dim 32,199,157,066,956**

^{150}Sm



^{150}Nd



SDSU: Plans for SciDAC-3

(End of SciDAC-2: 3-body forces on 100,000 cores)

•Run with 3-body up to 1,000,000 cores on Sequoia, Nmax =10/12 for ^{12,14}C

•Add in 4-body forces; investigate alpha-clustering with effective 4-body forces (via SRG or Lee-Suzuki)

•Currently interfaces with Navratil's TRDENS to generate densities, spectroscopic factors, etc, needed for RGM reaction calculations; will improve this: develop fast post-processing with factorization

•Investigate general unitary-transform effective interactions, adding constraint to observables