NUCLEI 2014 – Year 2 status report
June 18, 2014

People
Awards
Papers and Talks
Computing and INCITE
Highlights
Requests
Announcements

NUCLEI Year 2

Graduate Students

- Murat Bakirci, Ames and ODU
- Bridget Bertoni, UW / INT
- Noah Birge, UT (20%)
- Sushant More, OSU
- Titus Morris, MSU (50%)
- Erik Olsen, UT (30%)
- Kemper Talley, UT (50%)
- Dossay Oryspayev, Ames and ODU (100%)
- Nathan Parzuchowski, MSU (40%)
- Hugh Potter, ISU (50%)
- Ermal Rrapaj, UW / INT (100%)
- Shiplu Sarker, CMU
- Andre Schneider, IU
- Thomas Shafer, UNC
- Fei Yuan, MSU (15%)
- Chunli Zhang, UT (100%)

Postdocs

- Andreas Ekstrom, MSU
- Heiko Hergert, OSU (FRIB Fellow at MSU from 8/2014)
- Sebastian Koenig, OSU (50%)
- Nobuo Hinohara, UNC (80%), UT (20%)
- Jeremy Holt, UW
- Guillaume Hupin, LLNL
- Gustav Jansen, UT/ORNL (10%)
- Michael Kruse, LLNL
- Diego Lonardoni, ANL (100%)
- Joel Lynn, LANL (100%)
- Allesandro Lovato, ANL
- Justin Lietz, MSU (15%)
- Jordan McDonnell, LLNL (100%)
- Mika Mustonen, UNC (100%)
- George Papadimitriou, ISU (100%)
- Sergey Postnikov, IU (50%)
- Jhilam Sadhukhan, UT
- Irinia Sagert, IU (50%)
- Andre Schneider, IU (50% through 8/14)
- Roman Senkov, CMU (100%)
- Yue Shi, UT (50%)
- Angelo Signoracci, UT/ORNL (100%)
- Andrew Steiner, UW / INT
- Vaibhav Sundriyal, Ames (100%)
- Kyle Wendt, UT/ORNL (100%)

Congratulations

Heiko Hergert : FRIB

Nobuo Hinohara: Tsukuba

Alessandro Lovato: ANL

Andrew Steiner: UT/ORNL

Permanent Faculty/Lab positions in UNEDF/NUCLEI

- Bogner (MSU)
- Forbes (WSU)
- Gezerlis (Guelph)
- Holt (TRIUMF)
- Maris (ISU)
- Platter (UT/ORNL)
- Steiner (UT/ORNL)
- Wild (ANL)
- Drut (UNC)
- Gandolfi (LANL)
- Hinohara (Tsukuba)
- Lovato (ANL)
- Pei (Peking U)
- Schunck (LLNL)
- Stetcu (LANL)

Awards (UNEDF/NUCLEI)

- Joaquin Drut (OSU), who was awarded the Hermann Kümmel Early Achievement Award in Many-Body Physics in 2009
- Steve Pieper and Robert Wiringa (ANL), who received the Tom W. Bonner Prize in Nuclear Physics in 2010
- Sofia Quaglioni (LLNL), who received a prestigious DOE Early Career award in 2011.
- Witold Nazarewicz (UTK/ORNL), who received the Tom W. Bonner Prize in Nuclear Physics in 2012
- George Fann, a UNEDF member, is a co-leader of the MADNESS software development team that received a R&D 100 Award in 2011
- Stefano Gandolfi (LANL) won the IUPAP Prize in Nuclear Physics in 2013
- Alessandro Lovato (ANL) won the Adelchi Fabrocini Thesis Award in Nuclear and Many-Body Physics in 2013
- Gaute Hagen (ORNL) received a prestigious DOE Early Career award in 2013

Statistics

Papers

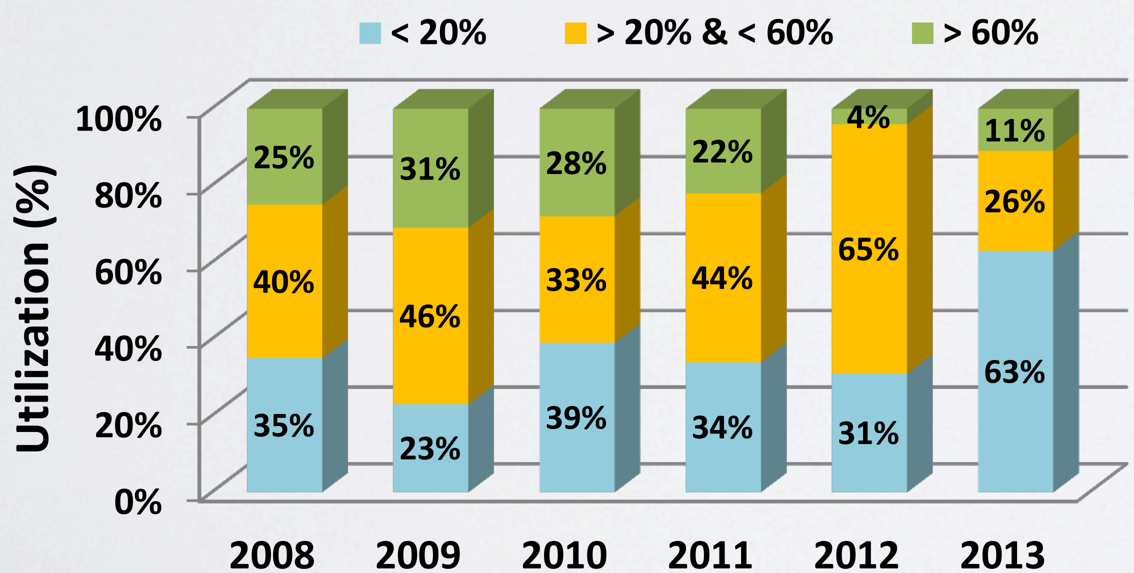
Year 1 (12 months) : 69
Year 2 (9 months) : 60 + 7 + xxx since 4/30

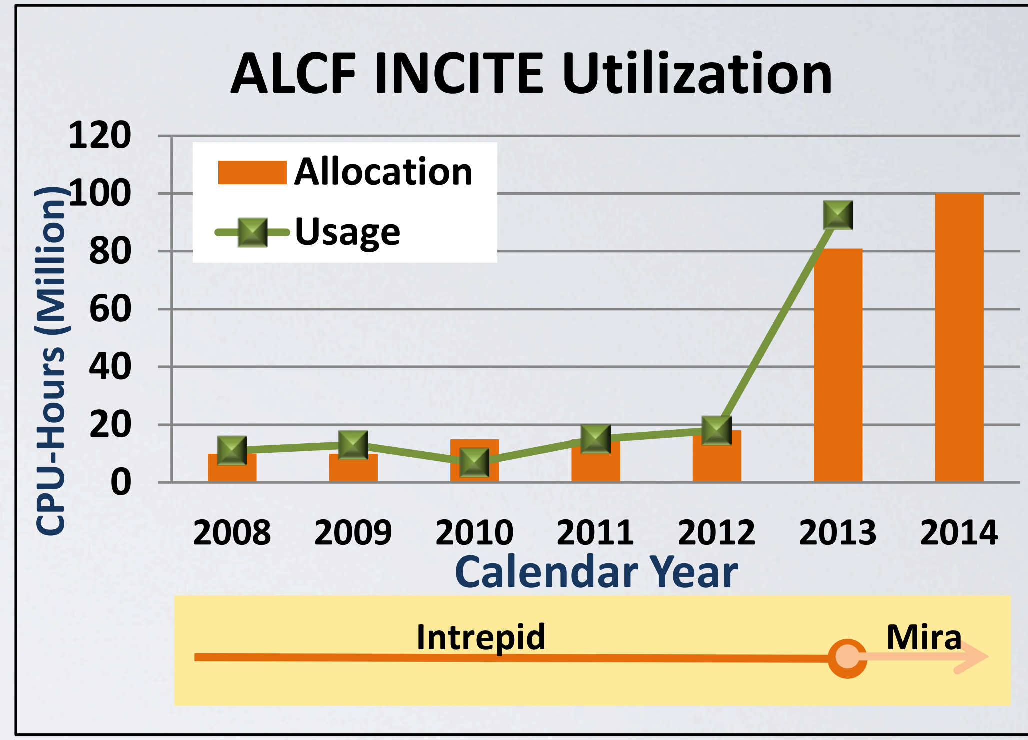
Invited Talks (conferences):

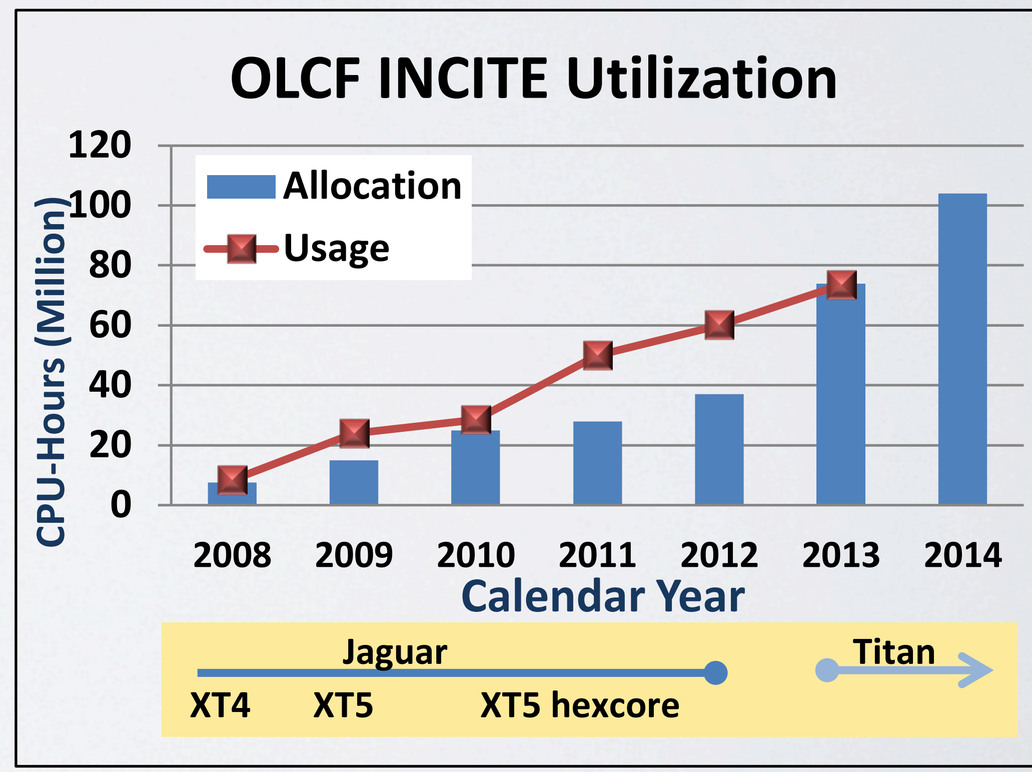
Year 1 (12 months) : 84
Year 2 (9 months) : 52 + 18 since 4/30
+ 30 other

NUCLEI/UNEDF Leadership-class computing

- SciDAC collaborations between applied mathematicians, computer scientists, and nuclear physicists lead to efficient utilization of leadership-class computing resources for nuclear physics problems
- Significant accomplishments in NUCLEI/UNEDF, achieved through leadership-class computing
  - *Ab-initio* calculations of C-12
  - Understanding the long lifetime of C-14
  - *Ab-initio* calculations of Ca-54
  - Improved energy-density functionals
  - Quantifying the limits of nuclear existence
- Over 35% of computing resources consistently used at leadership-class scale (utilization @ OLCF)







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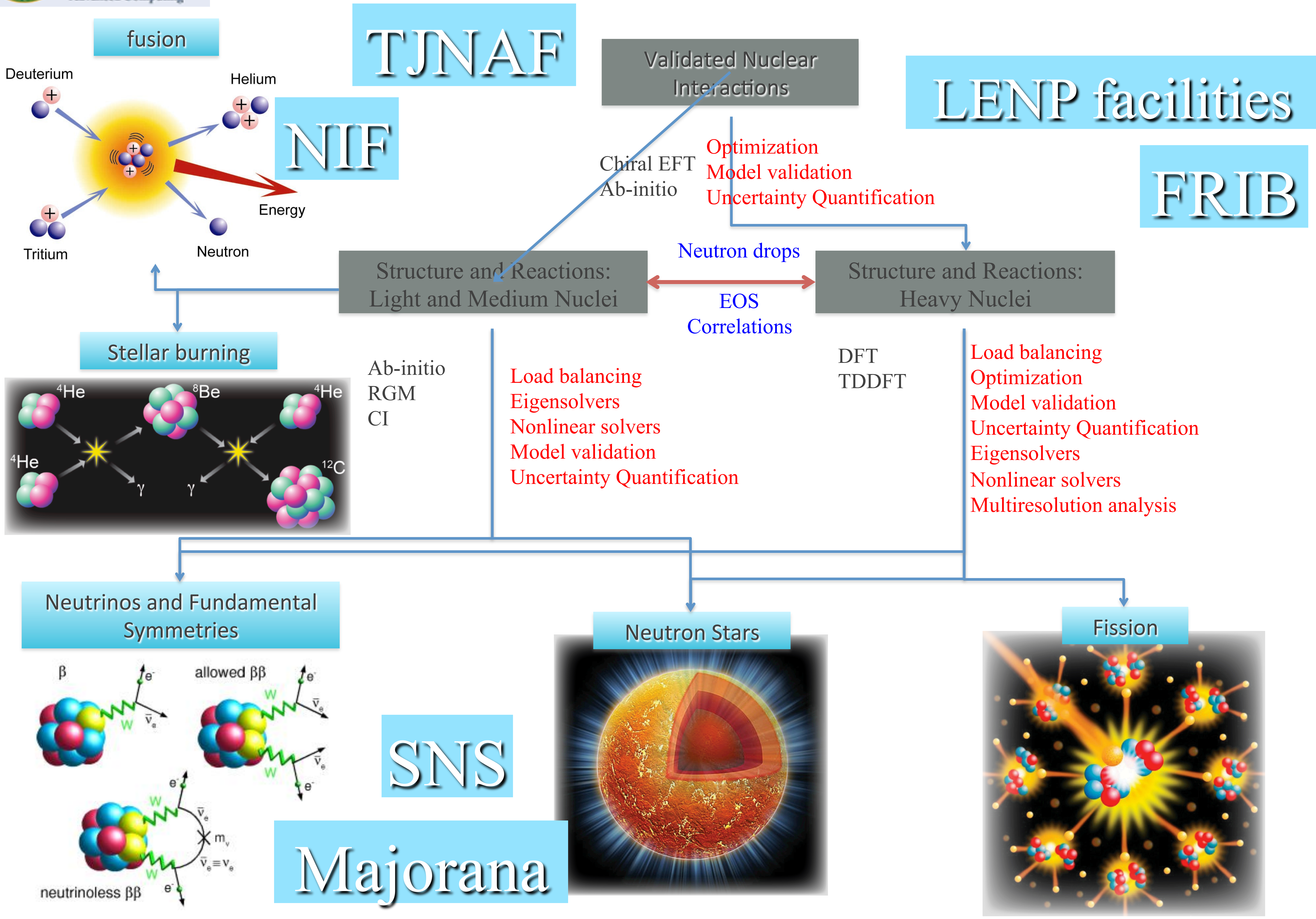
NUCLEI Nuclear Computational Low-Energy Initiative

Contacts: H. Nam, namha@ornl.gov/J. Vary, jvary@iastate.edu

NUclear Computational Low-Energy Initiative



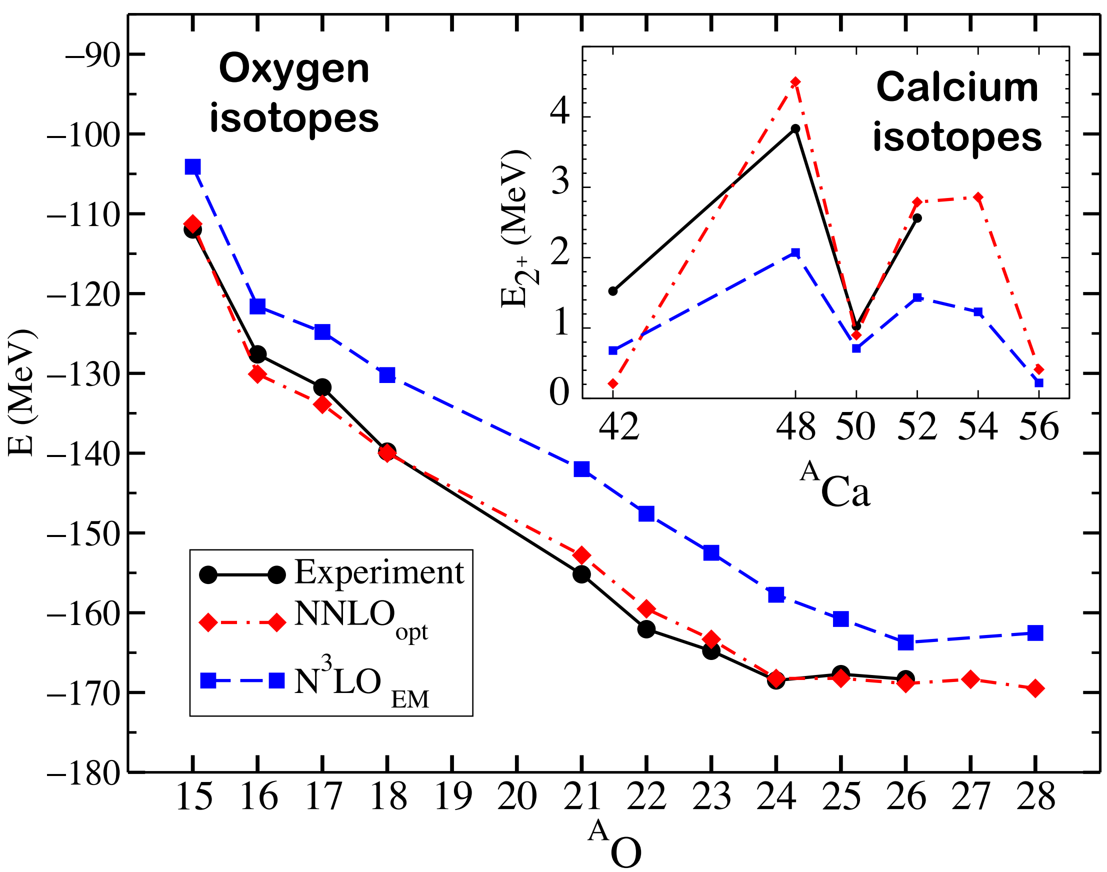
Streamlining the nuclear force

Objectives

- Apply state-of-the-art optimization methods for wide range of calibration problems in nuclear physics for scalable codes spanning ab initio to density functional theory approaches
- Optimization of nuclear interaction from chiral effective field theory at next-to-next-to leading order using the optimization tool POUNDERS in the phase-shift analysis
- Provide uncertainty quantification for nuclear structure modeling

Impact

- Nucleon-nucleon and three-nucleon interactions are key input in *ab initio* nuclear structure computations
- A decade of work has focused on hand-tuned potentials at next-to-next-to-next-to-leading order
- Computationally expensive three-nucleon forces are believed to play a pivotal role in description of nuclei and nuclear matter



Accomplishments

- The derivative-free, nonlinear least squares solver POUNDERS in TAO was used to systematically optimize potentials based solely on two-nucleon forces
- The optimization of the low-energy constants of the new interaction $NNLO_{op}$ yields a χ^2/datum of about one for laboratory scattering energies below 125 MeV. The new interaction yields very good agreement with binding energies and radii for A=3,4 nuclei.
- Less pain and more gain: $NNLO_{opt}$ captures key aspects of nuclear structure without resorting to three-nucleon forces.

Caption: The ground-state energies of oxygen isotopes obtained in coupled cluster method with the $NNLO_{opt}$ interaction obtained in this work and the previous interaction N^3LO_{EM} compared with experiment. The inset shows the first 2^+ state in selected calcium isotopes.

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Reference: A. Ekström et al., Phys. Rev. Lett 110, 192502 (2013) **Contact**: G. Hagen, hageng@ornl.gov, S. Wild, wild@mcs.anl.gov

Scalable Eigensolver for Many-Fermion Dynamics - nuclear (MFDn)

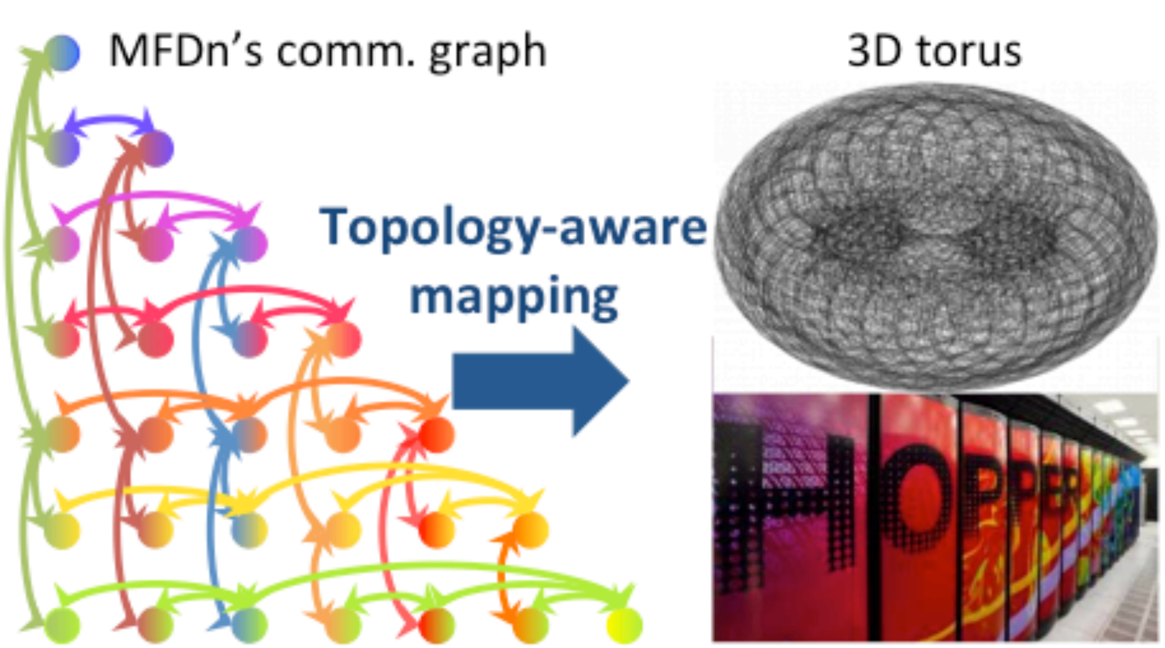
ASCR/NP – Applied Math/Computer Science Highlight

Objective

- Efficient and scalable iterative solvers for extreme-scale eigenvalue problems arising in nuclear physics (MFDn code)

Impact

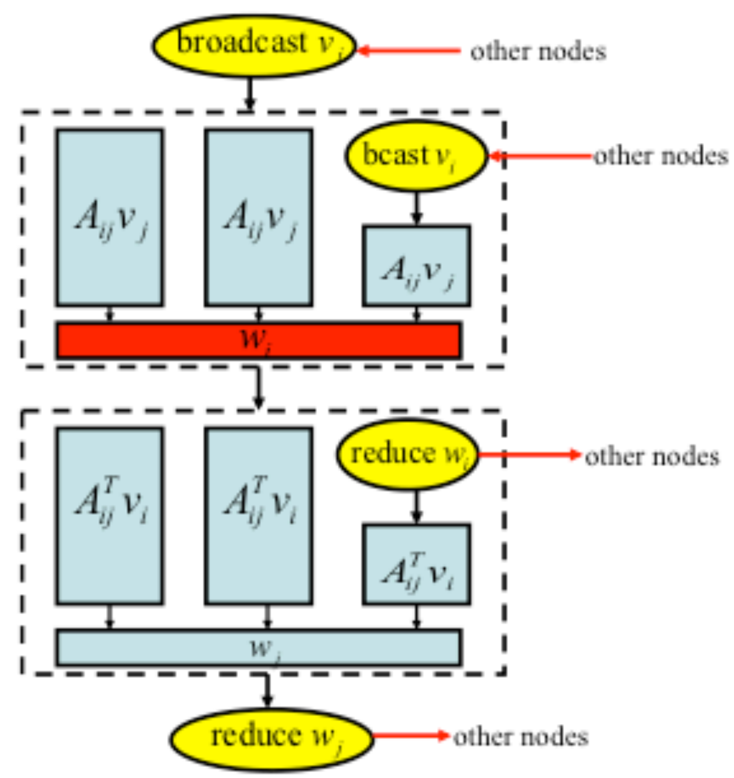
- Drastically reduced communication overheads
- Significant speed-ups over earlier version of MFDn (up to 6x on 18,000 cores)
- Almost perfect strong scaling on up to 260,000 cores on Jaguar



Topology-aware mapping of processes to the physical processors becomes more important as the gap between computational power and bandwidth widens. Communication groups are optimized through a column-major ordering of processes on the triangular grid [1].

Communication Hiding

Flow-chart for multi-threaded SpMV computations during the eigensolve phase of MFDn. Expensive communications are overlapped with computations. Explicit communications are carried out over topology-optimized groups [2].



Contacts: E. Ng, egng@lbl.gov; J. Vary, jvary@iastate.edu

[1] H.M. Aktulga,C. Yang,P. Maris,J.P. Vary,E.G. Ng, “Topology-Aware Mappings for Large-Scale Eigenvalue Problems”, Euro-Par 2012 Conference

[2] H.M. Aktulga,C. Yang,E.G. Ng,P. Maris,J.P. Vary, "Improving the Scalability of a Symmetric Iterative Eigensolver for Multi-core Platforms”, CCP&E, in review

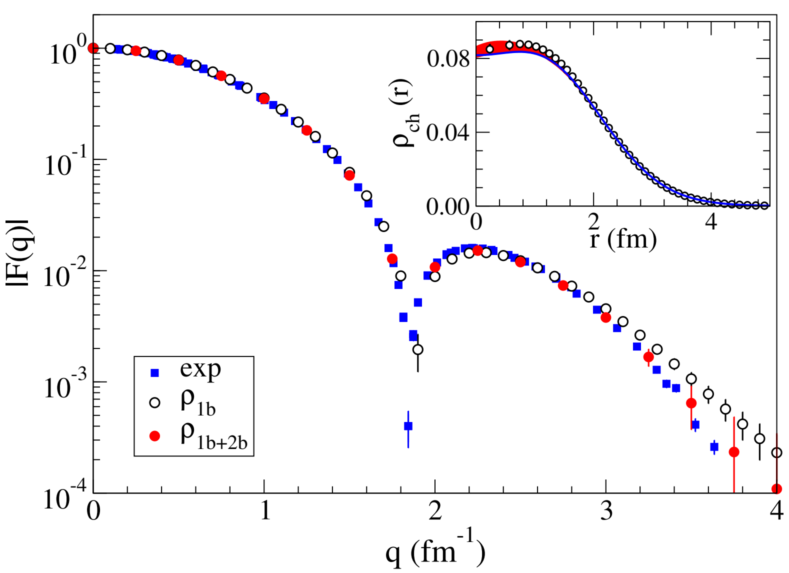
Electromagnetic Form Factor and Sum Rules in ^{12}C

Objectives

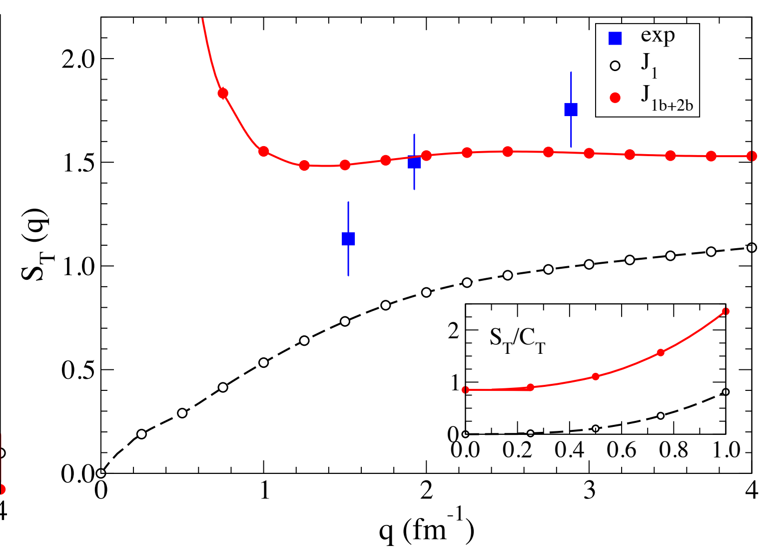
- Compute electroweak response in 12-Carbon. This is a fundamental ingredient in describing the neutrino – ^{12}C scattering.
- As a first step compute the sum rules for the electromagnetic response of ^{12}C including two-body meson exchange currents.

Impact

- This calculation can be used to predict the results of a recent experiment at Jlab, which are not yet released!
- It sets the stage for neutrino scattering calculations relevant to neutrino-nucleus scattering detector calibration (MiniBooNE) and supernovae explosions.



Longitudinal form factor: Two body terms in the density operator bring theoretical prediction closer to experimental data in the high-momentum transfer tail (q).



Transverse sum rule:

- *Two-body contribution is large for all momentum transfers.*
- *Satisfactory agreement with the experimental values.*

Accomplishments

We ported GFMC, our Green's Function Monte Carlo code, together with the ADLB load-balancing library, to the 10-petaflop Mira computer at Argonne and demonstrated scaling to more than 250,000 MPI ranks with over 2 million threads.

We conducted experiments to determine the best configuration of MPI processes per node and OpenMP threads per process for the sum rule calculations (4 ranks/node, 16 threads/rank).

We computed the longitudinal form factor and the sum rules for the electromagnetic response of ^{12}C including two-body meson exchange currents. This is the first step towards our overall objective.

The two-body currents are important for agreement with existing data; the Jlab results soon to be available should provide a more stringent test.

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Reference: http://arxiv.org/abs/1305.6959
Contact: A. Lovato, lovato@anl.gov

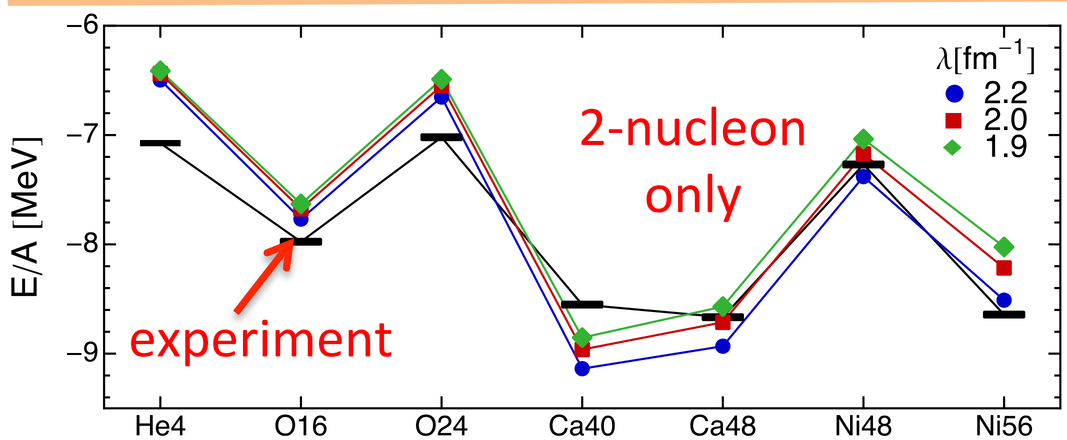
A powerful new ab-initio many-body method for nuclei: The In-Medium Similarity Renormalization Group (IM-SRG)

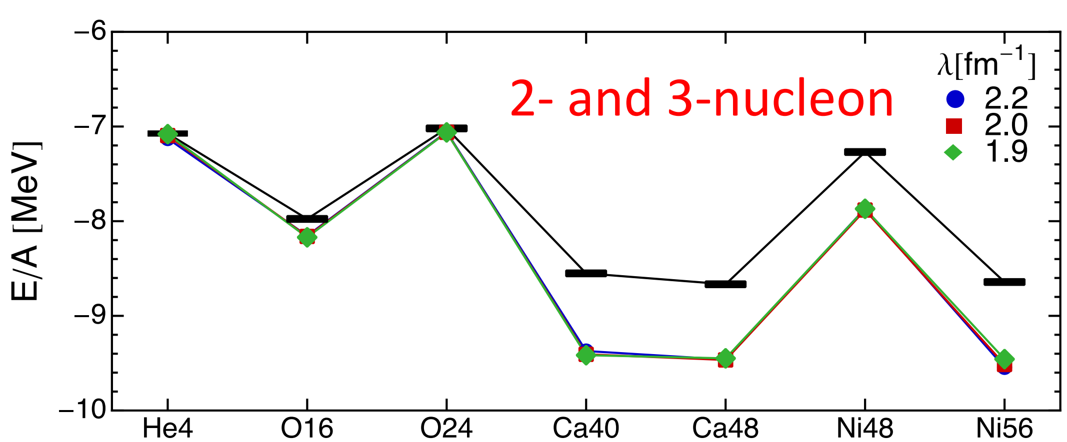
Objectives

- Develop the IM-SRG as an efficient, comprehensive ab initio framework
- Quantify statistical and systematic uncertainties of theoretical predictions
- Study and benchmark chiral 2- and 3-nucleon interaction effects in medium-mass nuclei

Impact

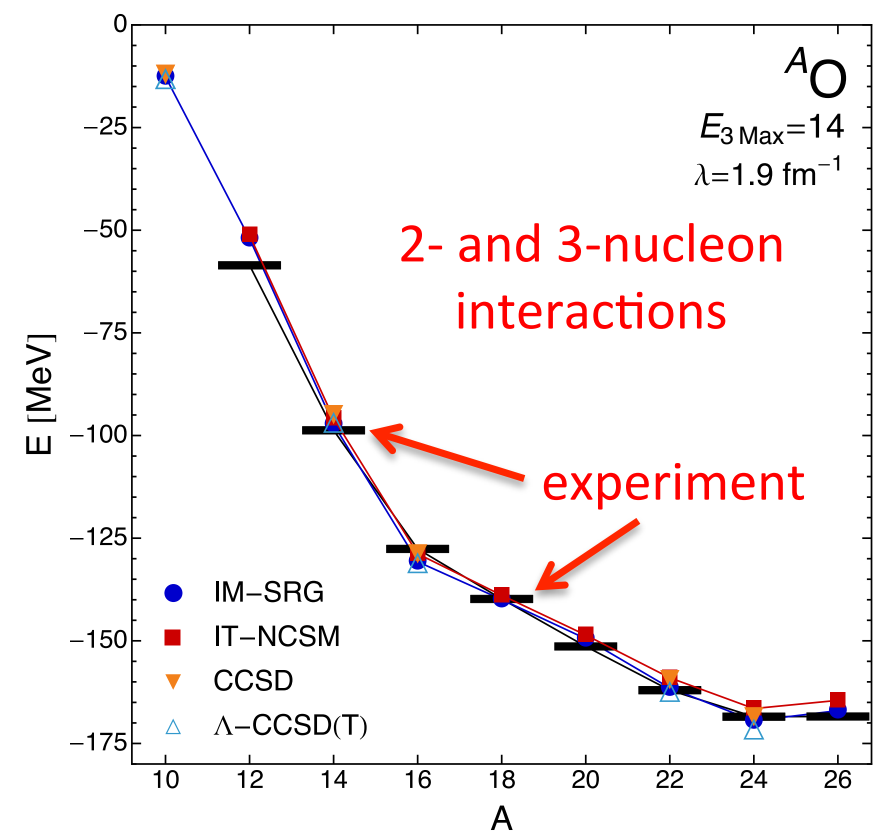
- Ab initio analysis and prediction of properties for isotopic and isotonic chains, including exotics, with quantifiable theoretical uncertainties
- Microscopic origin of Gamow-Teller quenching, effective charges, and other features
- Ab initio structure input for reaction theory and nuclear astrophysics





Accomplishments

- Complete study of closed-shell nuclei with 2- and 3-nucleon interactions
- Ab initio description of oxygen ground-state energies
- Showed 3-nucleon forces needed for correct systematics



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Reference: H. Hergert, S. Bogner et al., Phys. Rev. C 87, 034307 (2013)

Contact: H. Hergert, hergert.3@osu.edu

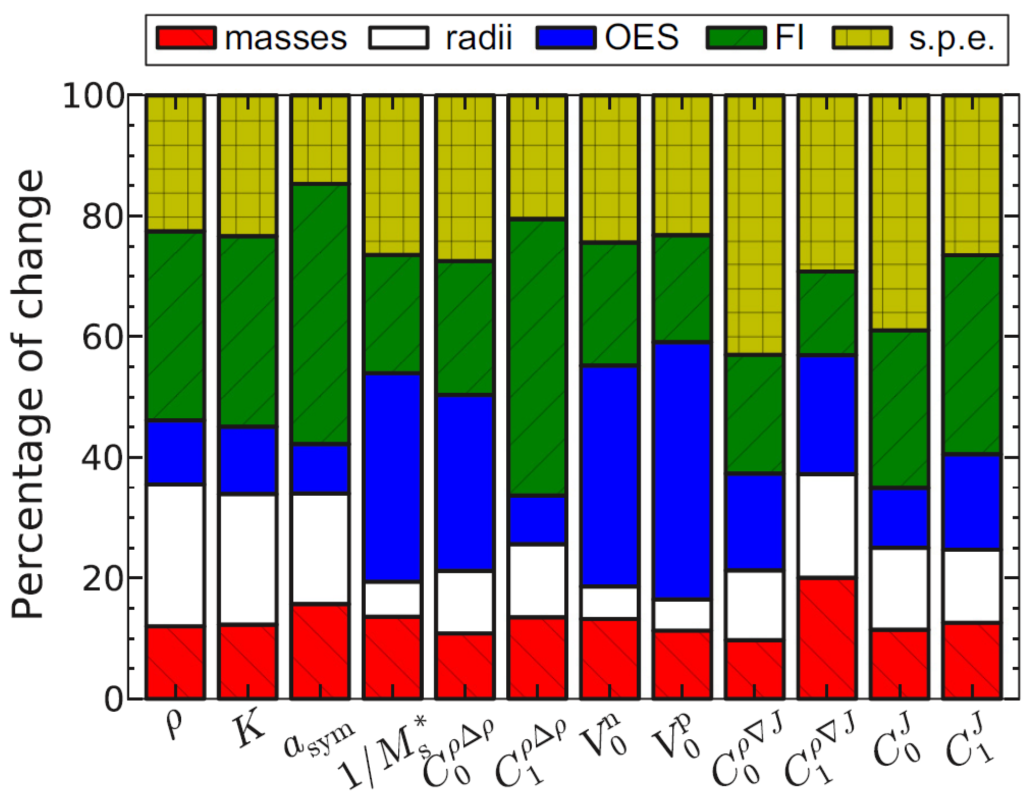
UNEDF2: the Endpoint of Skyrme DFT

Objectives

- Develop predictive nuclear density functional theory to compute properties of light to heavy nuclei to understand global properties of nuclei, nuclear fission, and the formation of elements in the universe.
- Use the advanced optimization framework POUNDERS and carefully selected nuclear data to produce the well-calibrated Skyrme-type nuclear energy density functional UNEDF2 that represents an effective nuclear interaction.

Impact

- Enable rigorous, data-driven, predictive modeling of nuclear structure, which will reduce uncertainties stemming from nuclear science inputs in:
  - basic science research such as tests of fundamental symmetries and nuclear astrophysics
  - stockpile science and reactor physics
- Provide benchmark and template for future developments of nuclear structure models



Sensitivity of the UNEDF2 parameters of the Skyrme energy density to different data types: atomic masses (red), charge radii (white), odd-even mass differences (blue), fission isomer excitation energies (green), and single-particle energies (yellow). The 4 fission isomer excitation energies and 9 single-particle energies represent only about 10% of the experimental data used but have a major impact on the final parameters.

Accomplishments

1. We have developed a general framework to solve the self-consistent equations of nuclear density functional theory.
2. We have shown that:
   - to constrain nuclear density functional, and provide uncertainty quantification, different types of data are required;
   - traditional Skyrme functionals are intrinsically limited.
3. We have used the POUNDERS optimization framework and fast solver HFBTHO, developed and published under UNEDF/NUCLEI SciDAC projects.

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Reference: M. Kortelainen *et al.*, Phys. Rev. C **89**, 054314 (2014).

Contact: N. Schunck, schunck1@llnl.gov

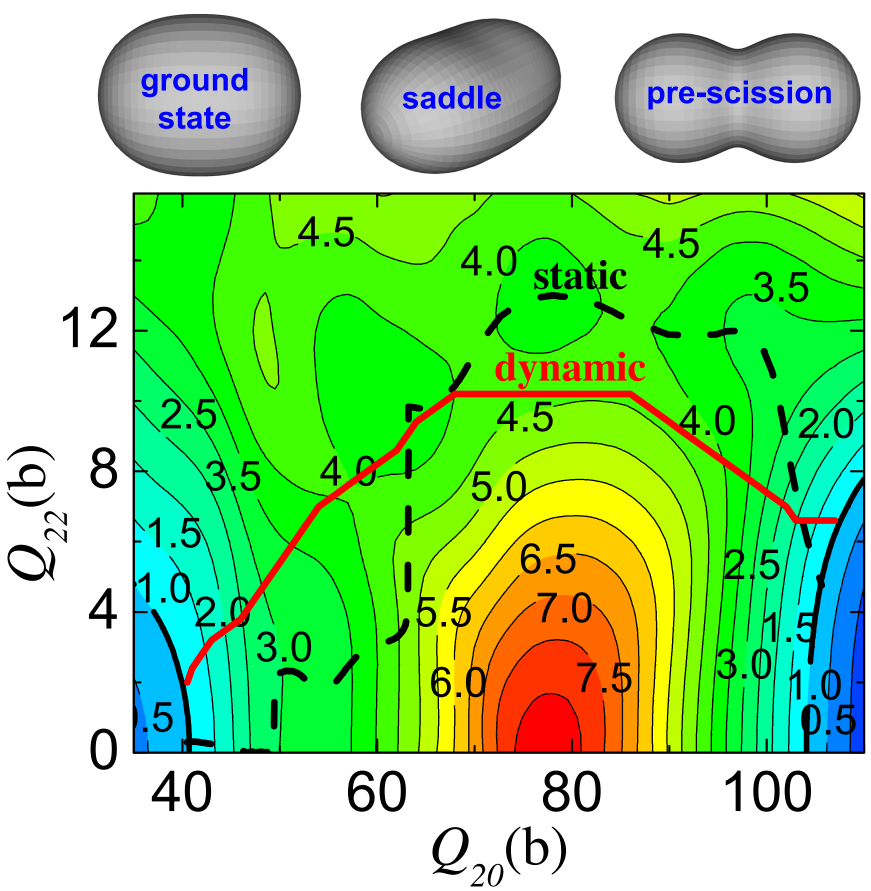
Spontaneous fission lifetimes from the minimization of collective action

Objectives

- Describe spontaneous fission, a magnificent example of quantal collective motion during which the nucleus evolves in a multidimensional space representing shapes with different geometries, going through regions that are forbidden by classical mechanics.
- Use nuclear Density Functional Theory and high performance computing to investigate the dynamical evolution of the heavy nucleus fermium-264 from its ground state to its symmetric split into two tin-132 nuclei.

Impact

- Enable rigorous data-driven predictive modeling in complex physical systems, supported by:
  - inference and calibration from experimental data and observations
  - model selection and learning of model structure
- Provide benchmark for future model developments
- Developments have been initiated in the context of dynamical effects due to the competition between triaxial and reflection asymmetric degrees of freedom, and pairing.



Dynamic and static paths for spontaneous fission of 264Fm in the 2D plane of elongation (Q_{20}) and triaxiality (Q_{22}) obtained by minimizing the collective action integral between the ground state and the outer turning point. The fission pathway connects the slightly deformed ground-state of ^{264}Fm with the ^{132}Sn+^{132}Sn pre-scission configuration through a family of elongated triaxial shapes, thus bypassing the axial saddle (inner fission barrier).

Accomplishments

1. Spontaneous fission has been studied microscopically for the first time within a dynamic approach based on the minimization of the fission action in a two-dimensional collective space of elongation and triaxiality. Strong dynamical effects have been predicted due to the interplay between level crossing dynamics and nuclear superfluidity.
2. Used the research team's symmetry-free HFB solver HFBODD, optimized for performance under UNEDF/NUCLEI SciDAC projects
3. This paper has been chosen by the Editors of Physical Review C for the "Kaleidoscope"

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Reference: Jhilam Sadhukhan et al, Phys. Rev. C 88, 064314 (2013).

Contact: W. Nazarewicz, witek@utk.edu

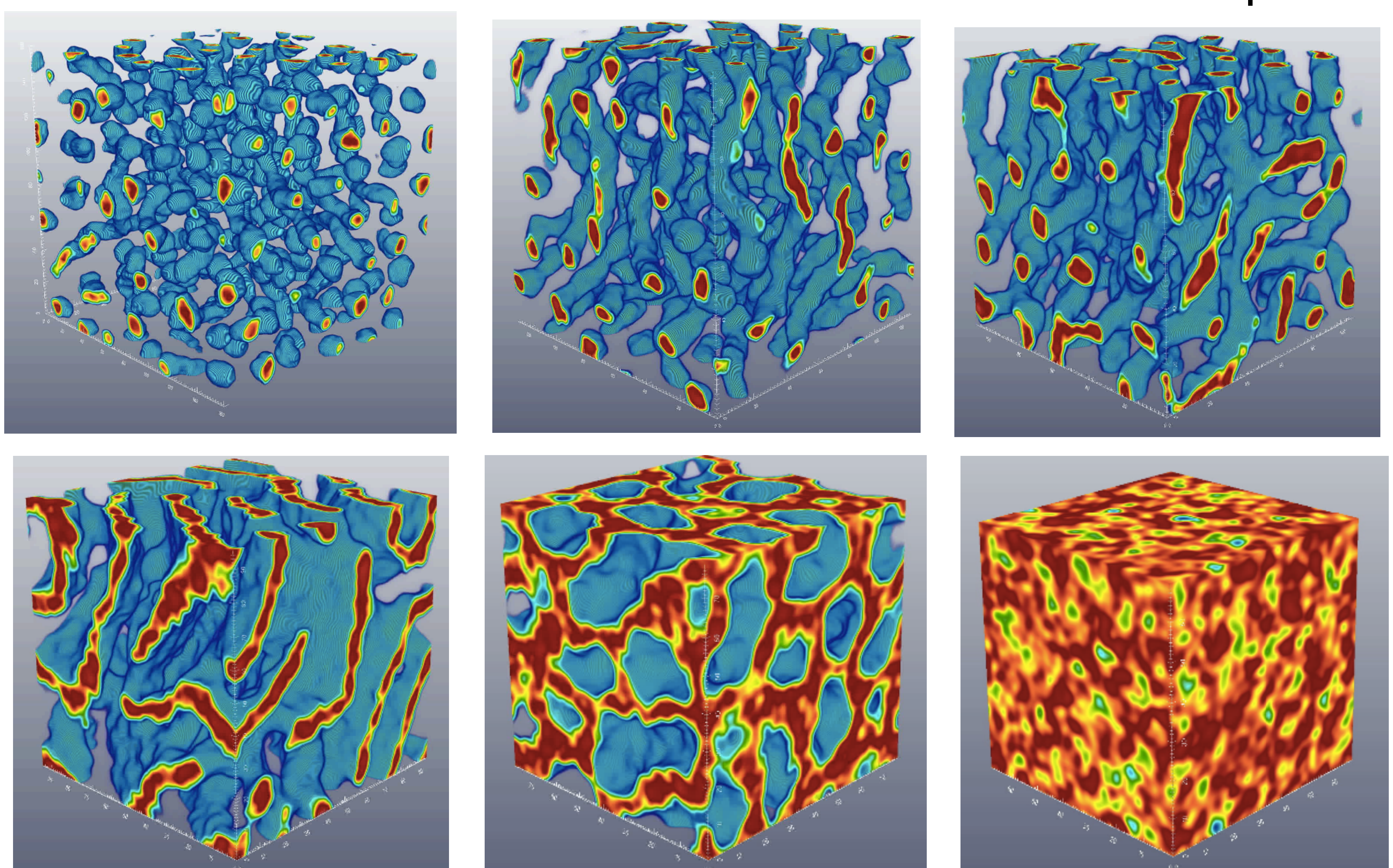
Large scale MD simulations of nuclear pasta formation: Nuclear reactions that make a neutron star

Objectives:

- Determine how core of massive star, during supernova, transforms from 10^{55} separate nuclei into a single large nucleus --- a newly formed neutron star.
- Study large-scale shape oscillations associated with formation of exotic nuclear pasta phases.

Impact:

- Determine time scales for large-scale nuclear shape changes.
- Guidance for multifragmentation and other heavy-ion reactions.
- Determine many transport properties important in astrophysics.



Accomplishments:

- Performed MD simulations with ≦ 300,000 nucleons.
- Directly determined time scales for different nuclear pasta shape changes.

Reference: A. Schneider et al., to be published.

Contact: C. Horowitz
horowit@indiana.edu

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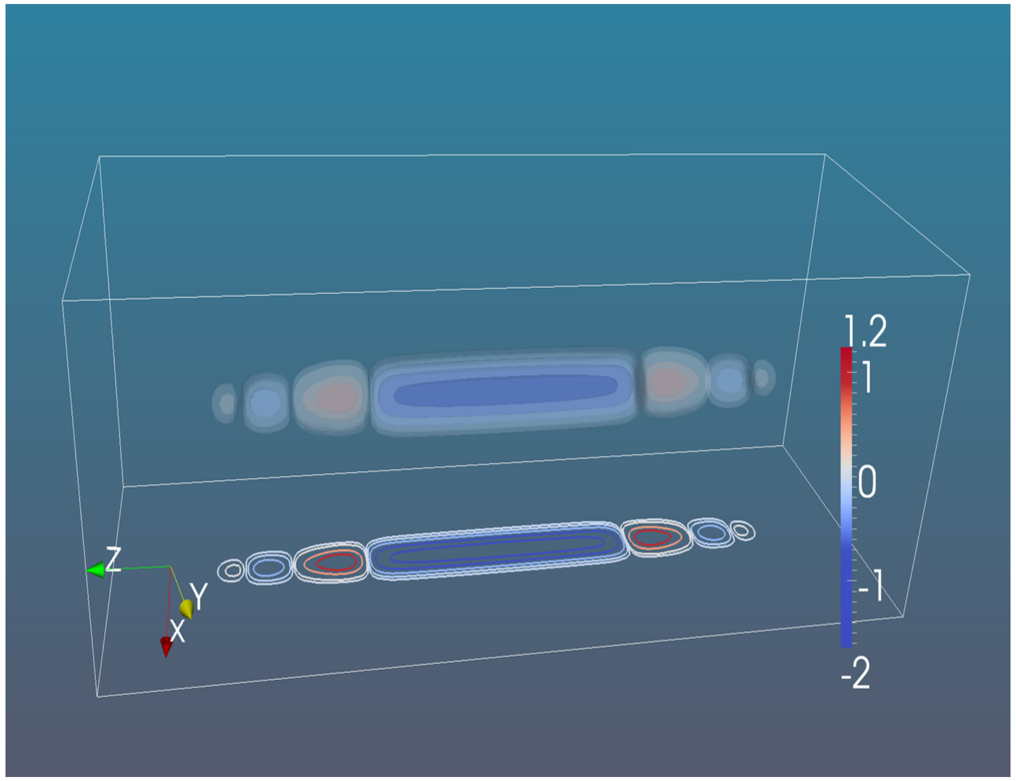
MADNESS-HFB: High Accuracy and Scalable Nuclear DFT Solver for Complex Geometries

Objectives

- Apply state-of-the-art scalable and adaptive computational tools to describe many-body nuclear and atomic problems involving complex geometries within the superfluid density functional theory
- High-order adaptive spectral approximations are used with an Object-Oriented solver environment to reduce simulation uncertainties and numerical errors

Impact

- Enable rigorous computational predictive modeling in complex physical systems in large and asymmetric domains
- Model verification of experimental results



The local 3-D pairing density for a HFB cold-fermion simulation computed by MADNESS-HFB is shown. The transversal oscillations of the pairing field are indicative of the Larkin-Ovchinnikov phase. The simulation used a box of width 320 fermis.

Accomplishments 2012

1. Solved the Hartree-Fock-Bogoliubov equations describing ultracold superfluid Fermi systems
2. Benchmarked in 3-D with 2-D spline based 2-D axial spline solver HFB-AX.
3. MADNESS-HFB is faster and scales better using more processors HFB-AX.

Reference: Pei, Fann, Nazarewicz, et. al., J. Phys. Conf. Series **402** (2012) 012035

Contact: George Fann, fanngi@ornl.gov

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Requests

Many more highlights presented at this meeting!

Please turn these into highlights for the NUCLEI web site:

Excellent Science (physics/math/CS)
Eye-catching graphic
Ties together physics and math/CS

Requests

What are the most important projects you currently cannot attack?

What resources (people, computing) would be required to achieve these goals?

Critical to justify additional funding for Nuclear Physics Long Range Plan

Make sure your ideas are presented to the community.

Announcements:

Dinner tonight: 7 PM
Blue Corn downtown location (Water Street)
Individual bills
Please be patient for paying bills
Blue Corn is also a brewery

Advances and Perspectives in Computational Nuclear Physics

Oct. 5-7 at Hilton/Waikola Village (same as DNP)

Cold/Hot QCD,
Physics of Nuclei,
Nuclear Astrophysics

Joint US/Japan Meeting
Prelim website:
http://indico2.riken.jp/indico/conferenceDisplay.py?confId=1534