Summary of the Computational Nuclear Physics Meeting

July 14-15, 2014
SURA, Washington DC

~40 participants discussing the status and future of Computational Nuclear Physics

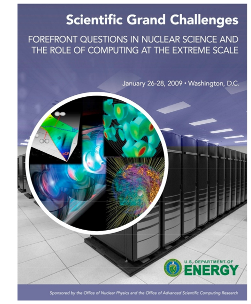
Cold and Hot QCD
Nuclear Structure and Reactions
Nuclear Astrophysics

Background
Highlights since 2007 / Future Program
Findings/Recommendations of the Town Meeting

Background

Computational Nuclear Physics 2014

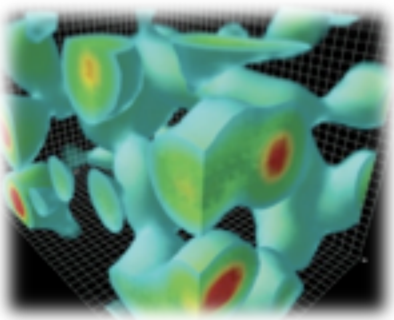
2009 NP HPC
Status and Projected Needs



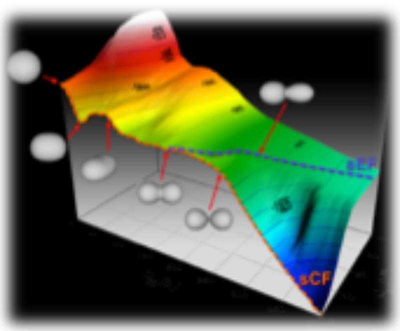
Meeting in Washington DC
Jan 26 , 27, 28 (2009)

Fred Bertrand (Facilitator)

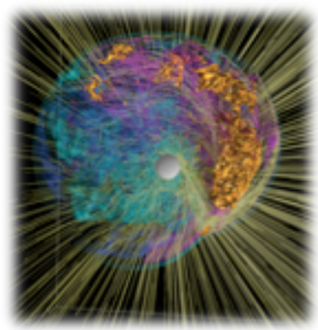
Glenn Young (Chair) , David Dean (co-Chair) , Martin Savage (co-Chair)



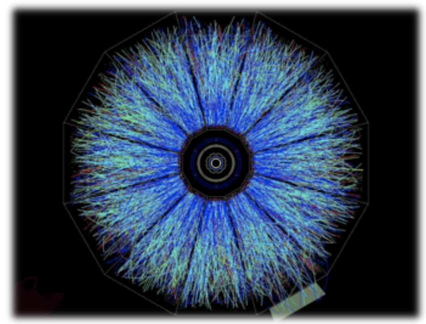
Tom Luu (LLNL)
David Richards (TJNAF)



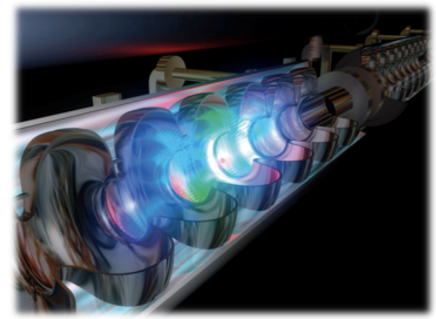
Steven Pieper (ANL)
James Vary (Iowa)



George Fuller (UCSD)
Tony Mezzacappa (ORNL)



Steffen Bass (Duke U.)
Frithjof Karsch (BNL)



Robert Ryne (LBNL)

- 109 Attendees
- Physics, Computer Science, Mathematics and Applied Mathematics
- 27 Universities (US and foreign), 7 Labs, 6 Corporations (US and foreign), 2 Federal Agencies
- PNNL administered/document production (Moe Khaleel, Hope Mathews (technical writer))

Additional Meeting on NNSA Science including Nuclear

2012 Meeting on Computational Nuclear Physics

TOWN MEETING RECOMMENDATIONS

RECOMMENDATION 1

The nuclear physics community should work with DOE and NSF to increase funding for the NP SciDAC programs and other cyber-related initiatives, and to foster partnerships with ASCR, NNSA, OCI, and other agencies to strengthen the impact of these programs. In addition to enabling new physics, these partnerships also open new avenues in the areas of computer science and applied mathematics.

RECOMMENDATION 2

Collaboration amongst the fields of computational nuclear physics, experimental nuclear physics and analytic theory is critical. In particular, new experimental initiatives should be integrated with large-scale theoretical computations to maximize the combined science output.

RECOMMENDATION 3

Concrete steps should be taken to educate and train the next generation of computational nuclear physicists, and to increase the cross-fertilization between the various efforts, exploiting synergies in physics, computer science and applied mathematics. The options include, but are not limited to: computational nuclear physics meetings, workshops, and schools; enhanced connections between SciDAC projects; and student exchanges.

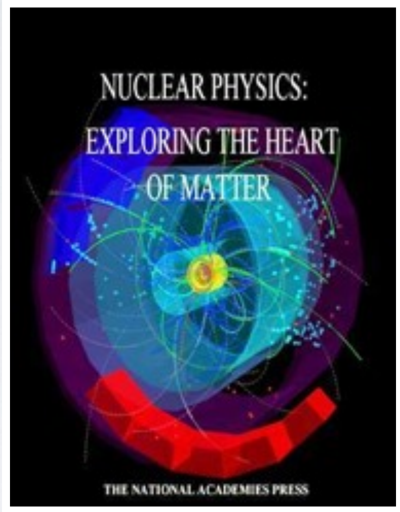
Strengthen SciDAC and Related Initiatives

Computing Integrated with New Experimental Initiatives

Education, Training w/ Applied Math and Computer Science

Background

National Academy Report, Tribble Report….



NAS report "Exploring the Heart of Matter":

High performance computing provides answers to questions that neither experiment nor analytic theory can address; hence, it becomes a third leg supporting the field of nuclear physics.

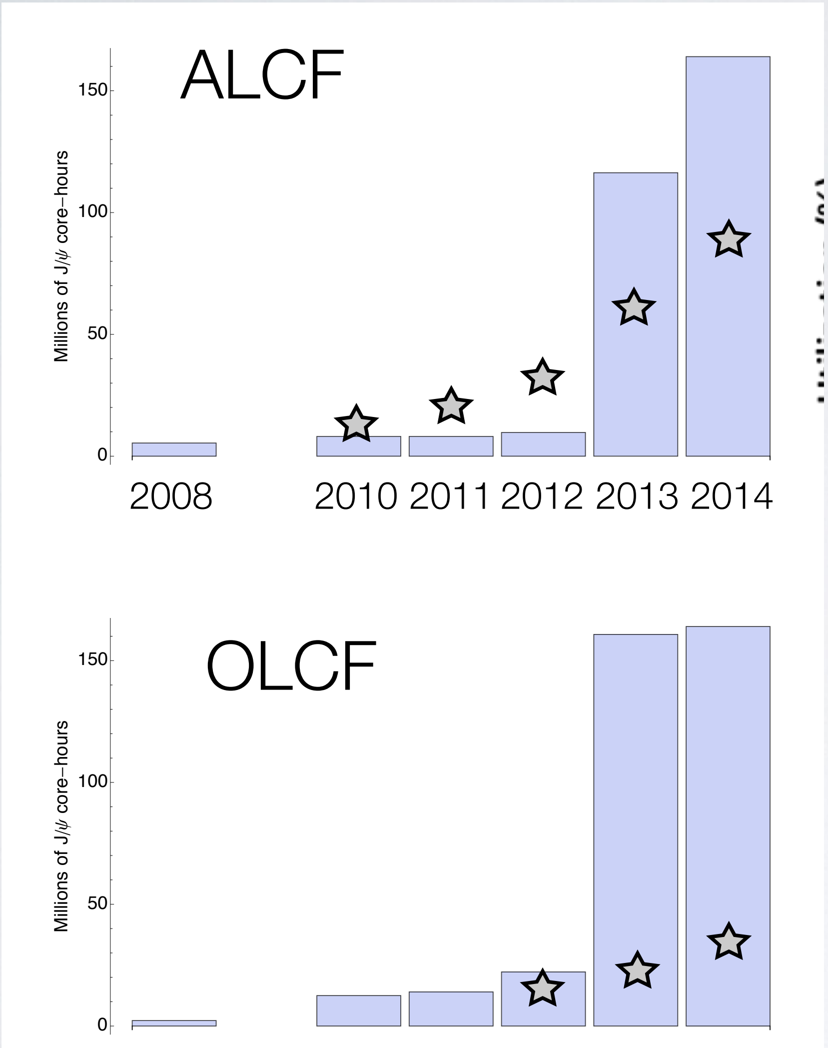
Recommendation:

A plan should be developed within the theoretical community and enabled by the appropriate sponsors that permits forefront computing resources to be exploited by nuclear science researchers, and establishes the infrastructure and collaborations needed to take advantage of exascale capabilities as they become available.

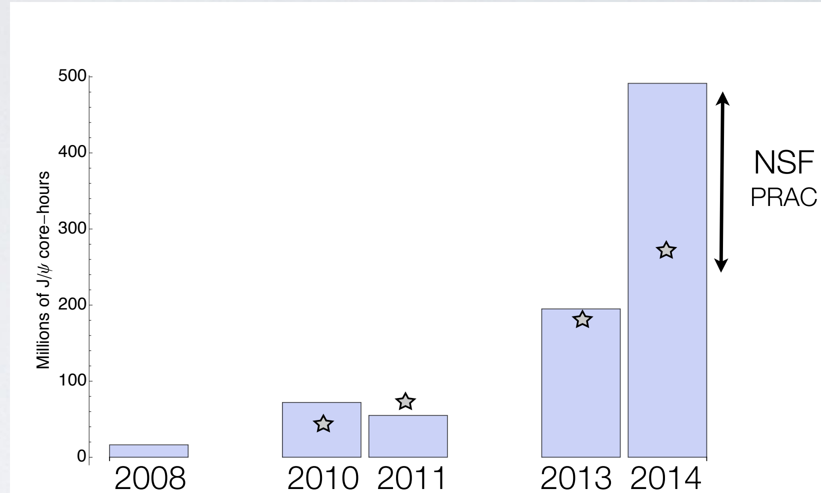
Tribble Report:

"People remain the key factor. In particular, early-career scientists working at the interface between nuclear theory, computer science, and applied mathematics are critical to make future impact, especially in the era of extreme computing that demands the novel coding paradigms and algorithmic developments required by novel architectures."

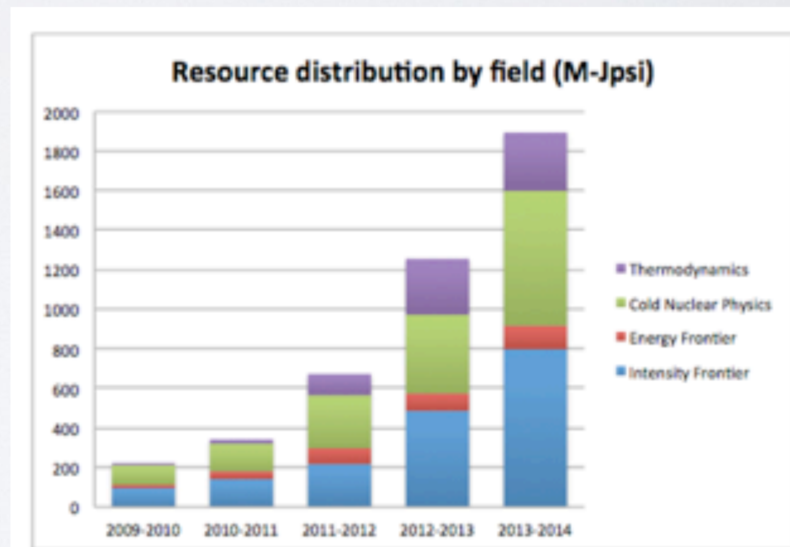
Available Resources Growing Very Rapidly



NUCLEI



Nuclear Astrophysics



Lattice QCD

Architectures Changing Rapidly

Next NERSC Procurement
will be a Xeon Phi system

Training of Young Scientists is Crucial

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%)

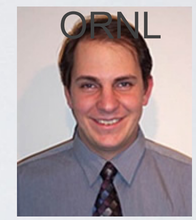
2014 new positions

Heiko Hergert : FRIB

Nobuo Hinohara:

Alessandro Lovato: ANL

Andrew Steiner: UT ORNL

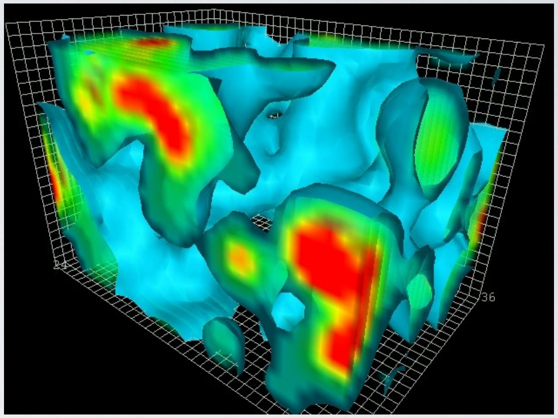


DOE early career awards:
Hagen
Quaglioni

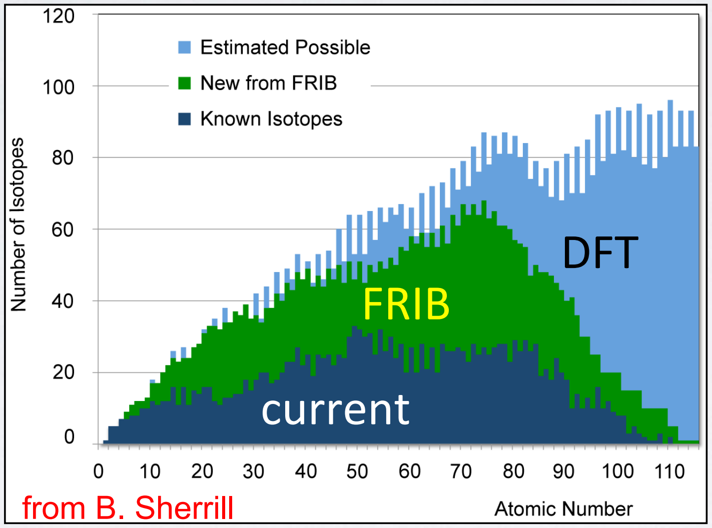
similar support/awards in Nuclear Astrophysics and QCD

Outstanding Science Opportunities

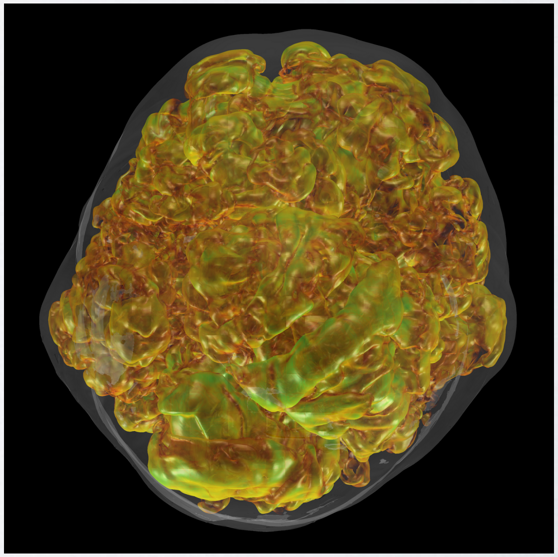
Lattice QCD



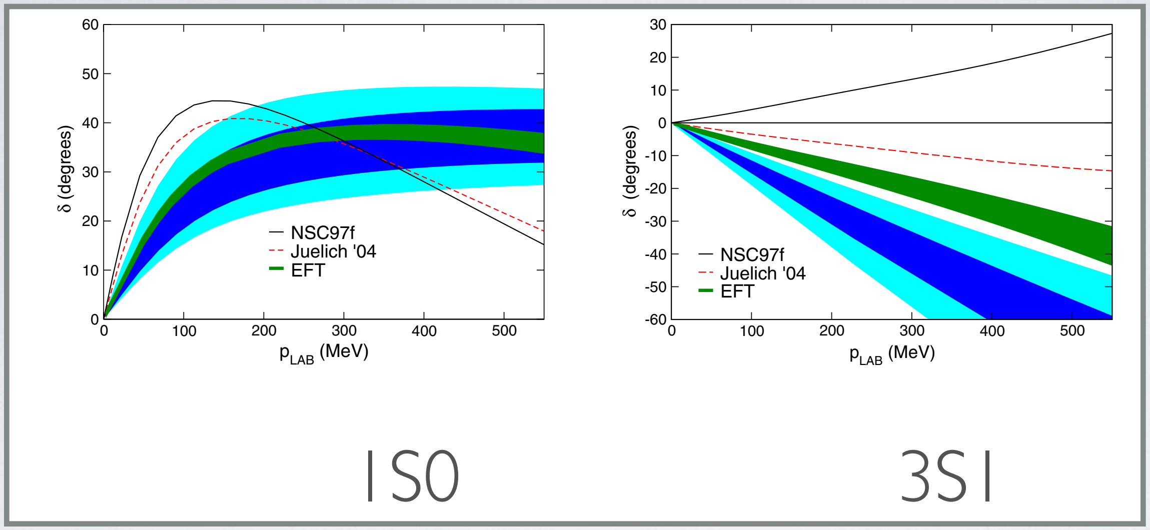
Physics of Nuclei



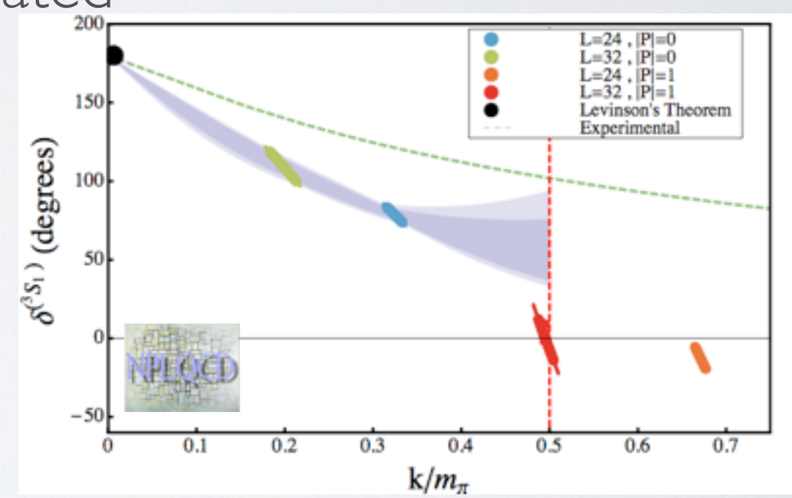
Nuclear Astrophysics



Lattice QCD and Nuclear Physics



Sigma- neutron interactions extrapolated
to physical pion mass

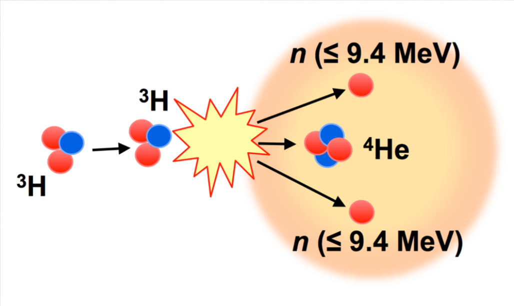


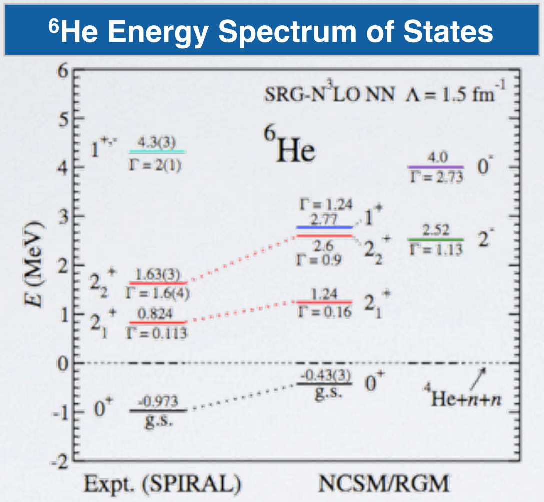
Baryon-Baryon Interactions
Light Nuclear Structure
Properties of dense matter - neutron stars, etc.

Light Nuclei and Reactions

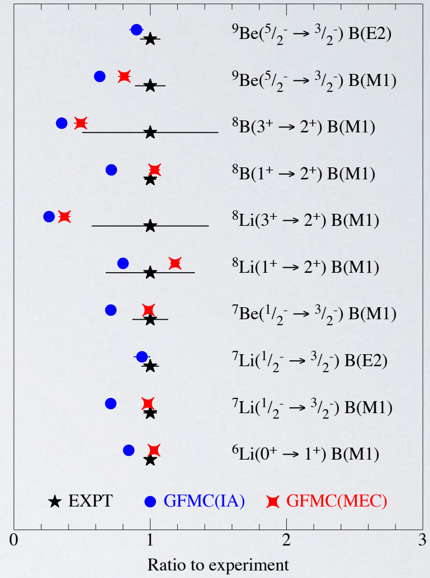
Scattering including 3-body final states

The 3-body continuum energy spectrum of ^{6}He (= ^{4}He+n+n) is needed for the description of the ^{3}H+^{3}H → ^{4}He+n+n fusion

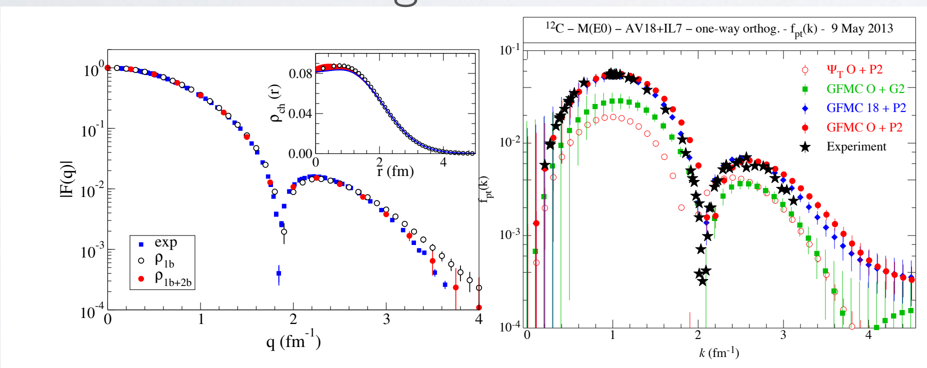


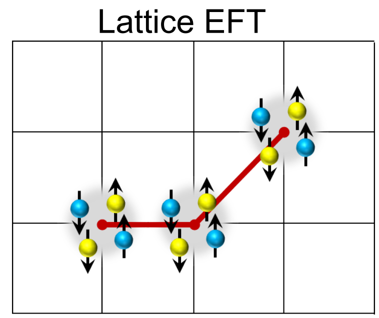


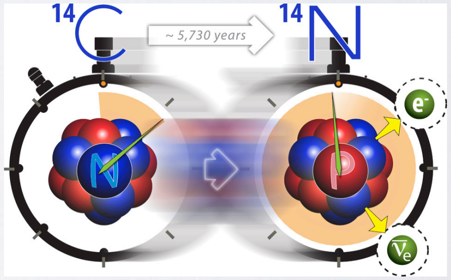
EM transitions and 2 nucleon currents



12C ground state and transition FF



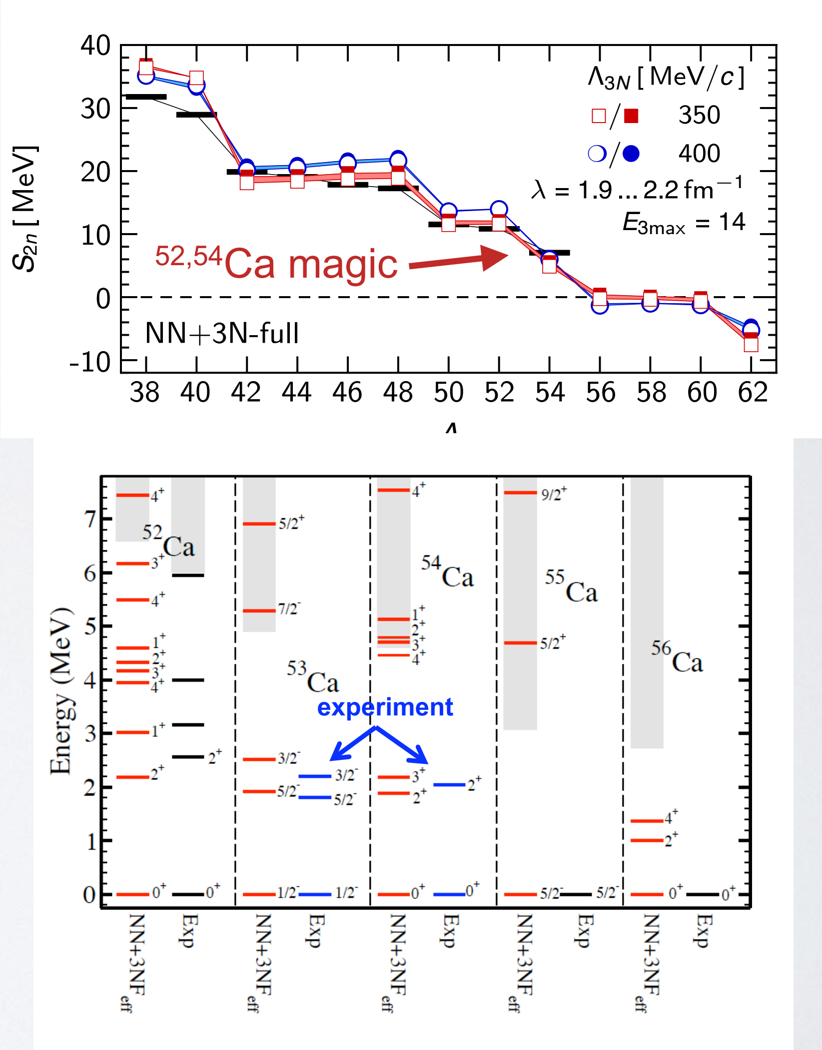




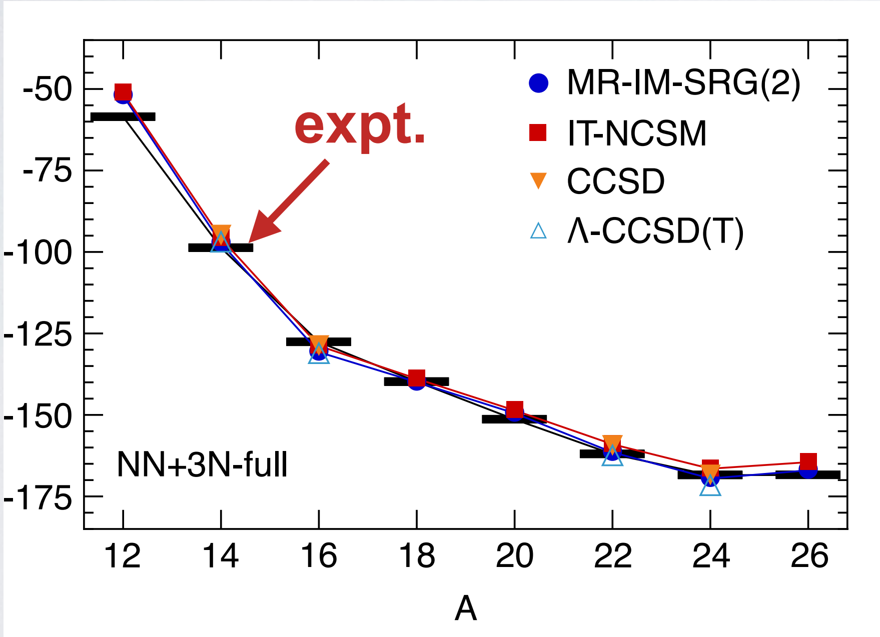
Ties to fundamental symmetries, neutrino physics and astrophysics

Neutron Rich Nuclei

Calcium Isotopes

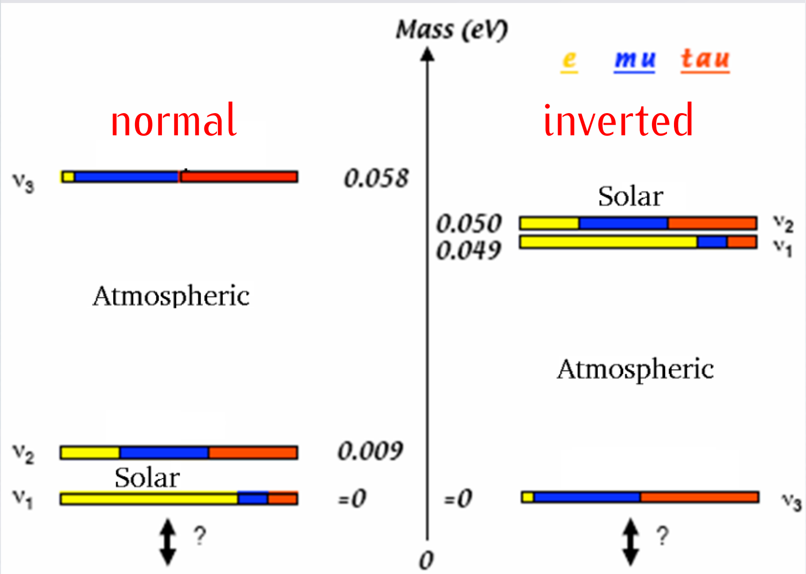


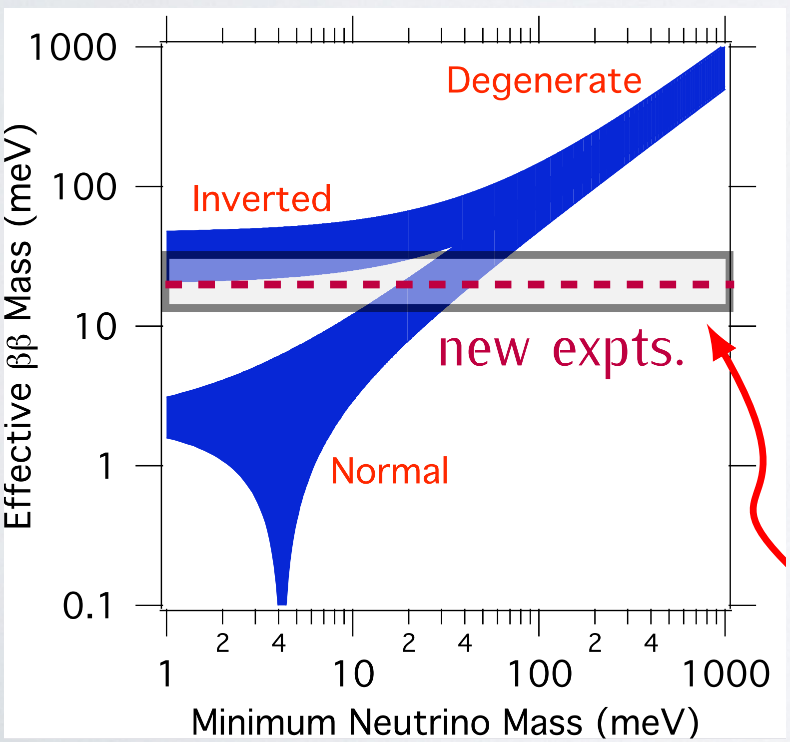
Oxygen Isotopes



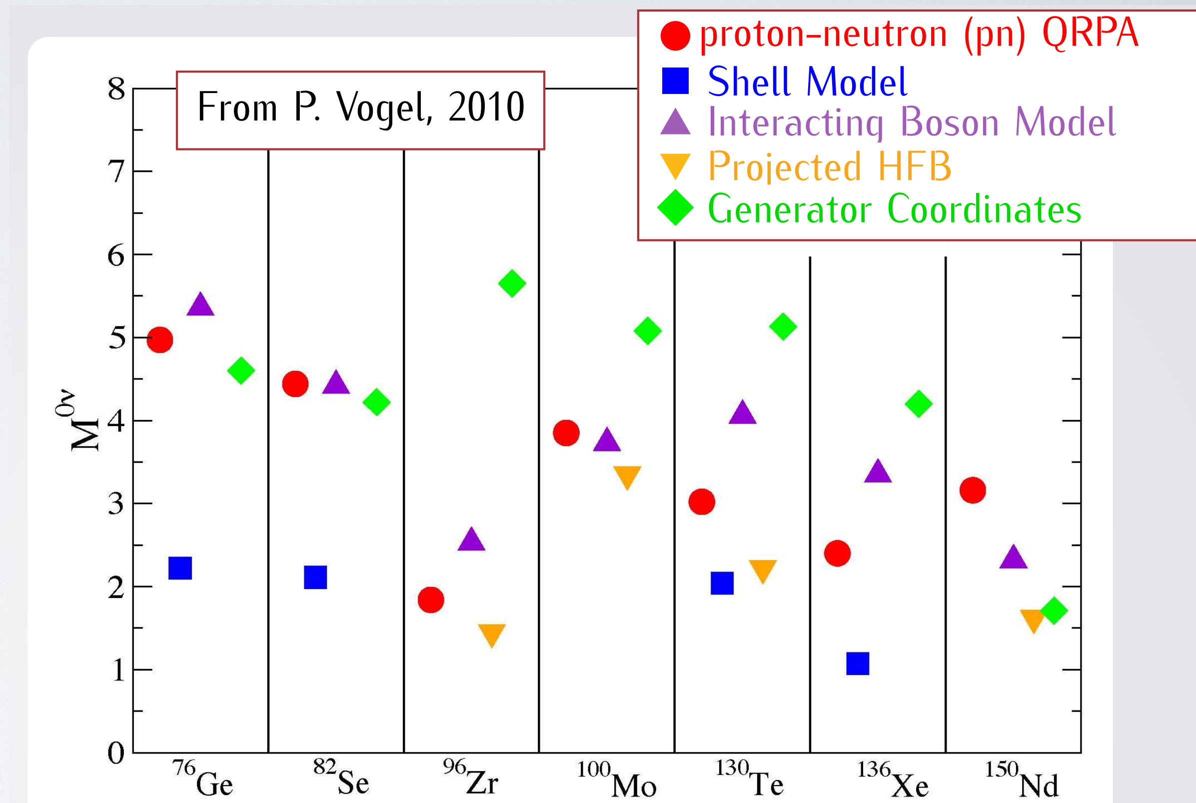
Direct Connection to FRIB, calculations of weak rates, matter

Neutrinoless Double Beta Decay



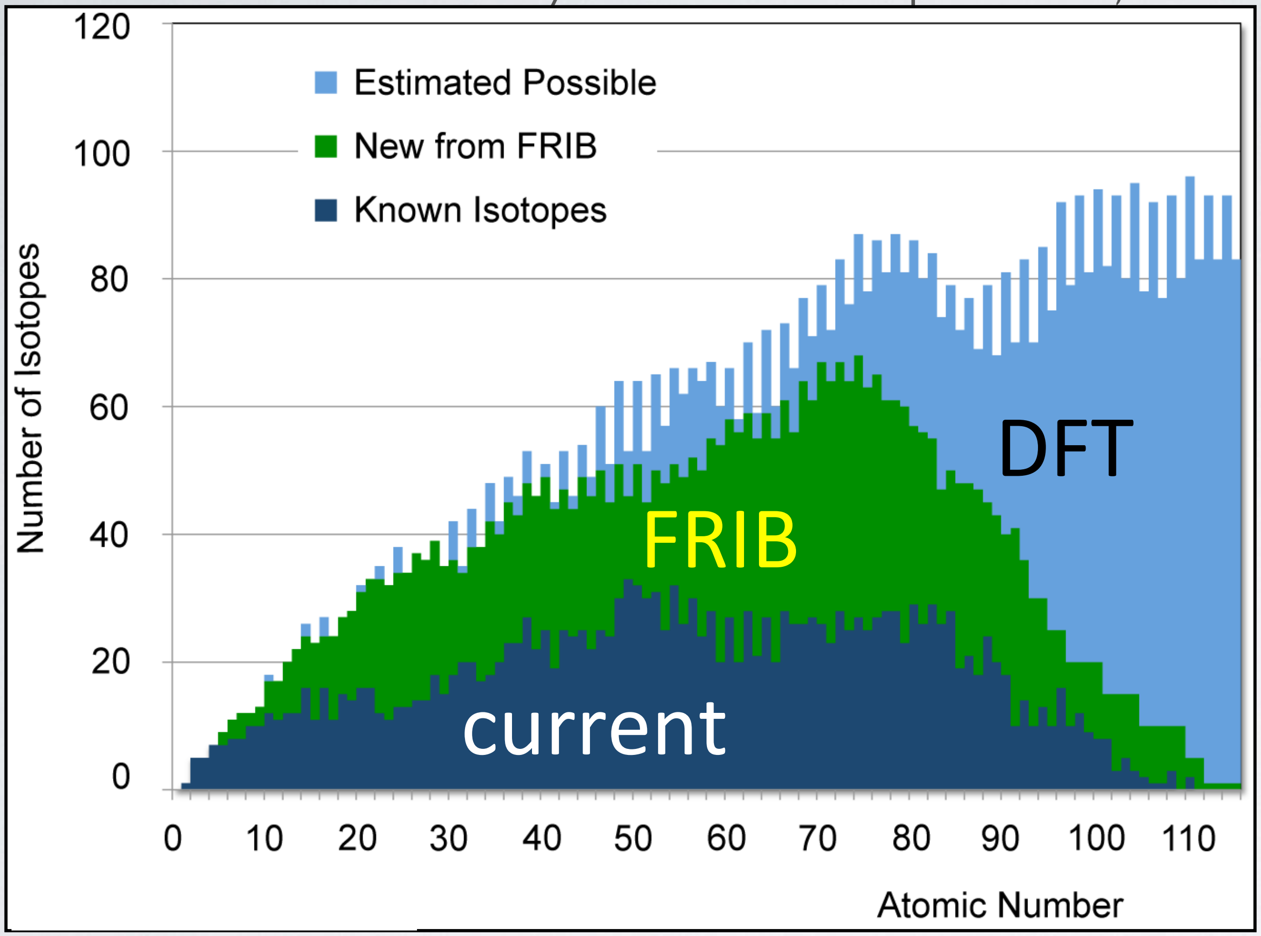


Uncertainties

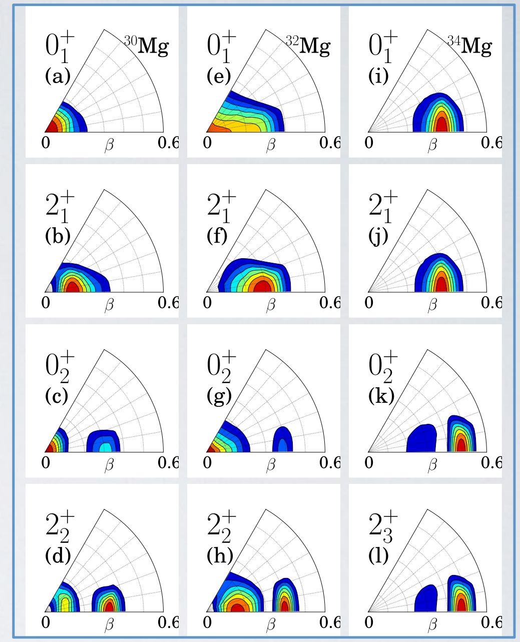


nuclear uncertainties

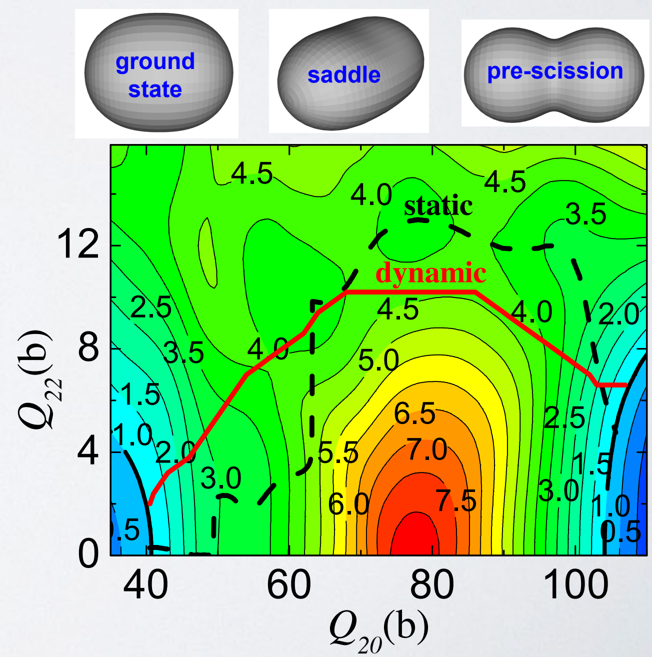
Heavy Nuclei: Drip Lines, Fission



Shape coexistence



Spontaneous fission



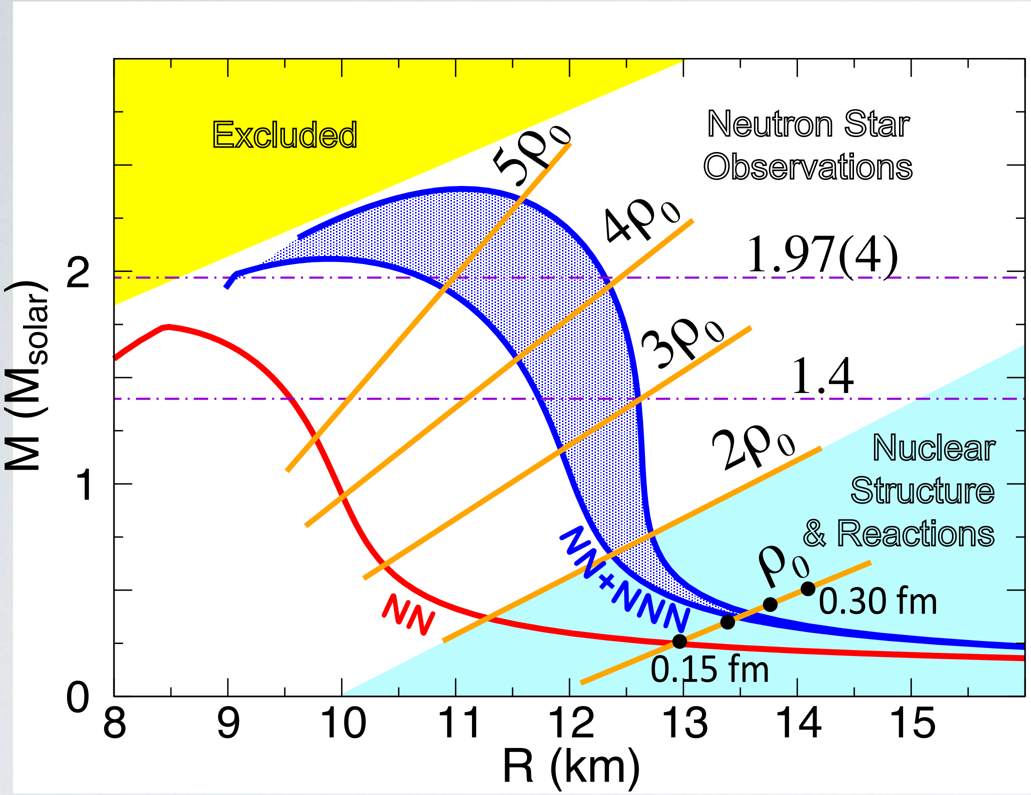
Critical Challenges:

Nuclei far from stability

r-process and Nucleosynthesis

Nuclear Fission

Neutron Stars and Supernovae: Microphysics



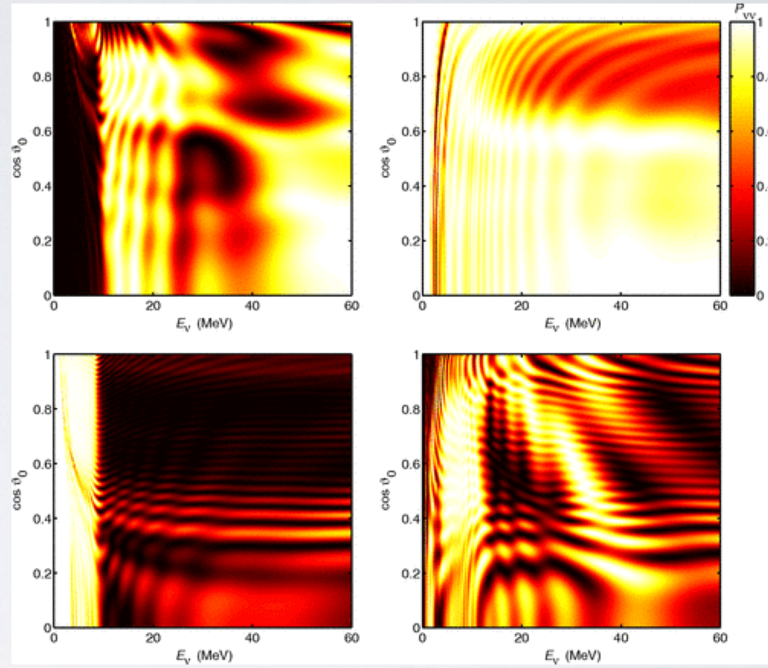
Mass/Radius relationship

Gravitational waves and EOS

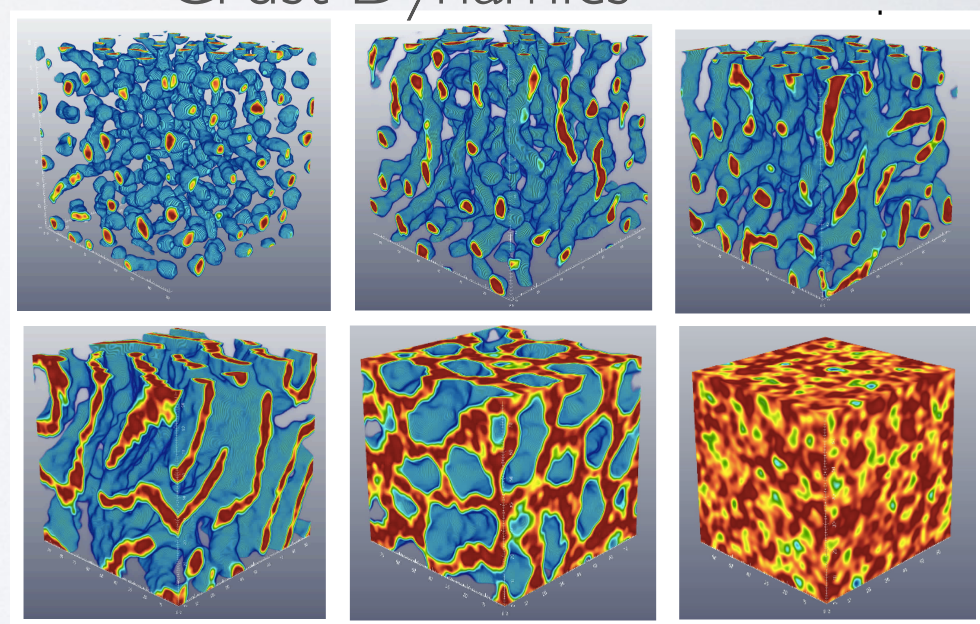
Neutron Star Cooling

Supernovae neutrinos

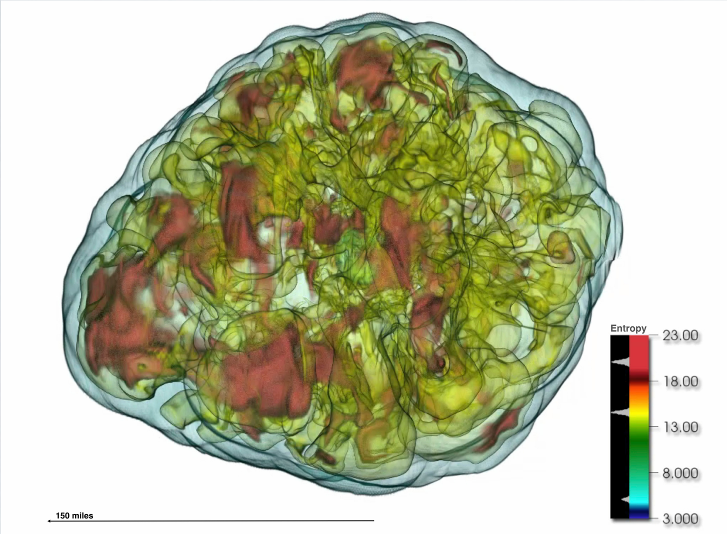
Supernovae Coherent Neutrino Evolution



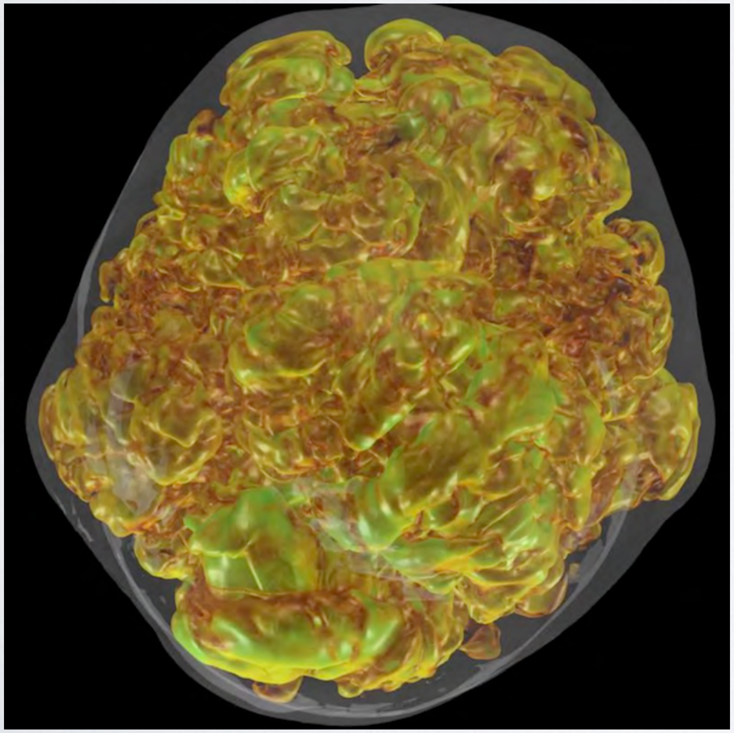
Crust Dynamics



Type II (core-collapse) Supernovae



Entropy in 3D simulation, 15 solar masses



3D codes with
spectral neutrino transport
now becoming available

Unique laboratories for:

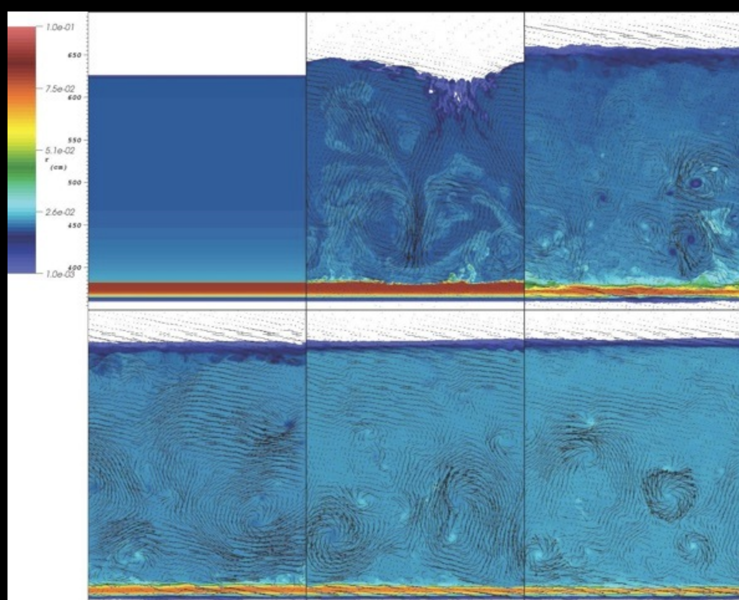
- High density nuclear EOS
- r-process nucleosynthesis
- neutrino-nuclear physics
- neutrino flavor mixing
- gravitational waves

public codes available

Turbulent Fusion Flames in Type Ia Supernovae

- Laboratory for nuclear fusion in the presence of turbulence and instabilities
- SN Ia are the origin of iron and many other heavy elements
- Electron capture, electron screening and heavy ion reactions affect outcome

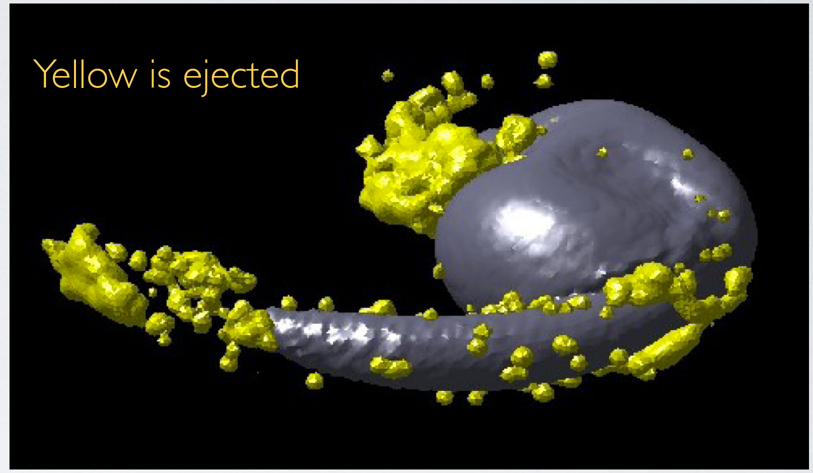
X-ray Bursts on Neutron Stars



Unique laboratories for:

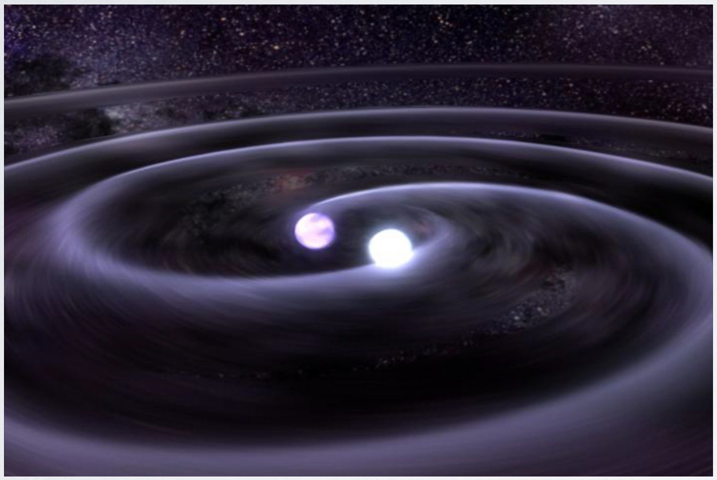
- Nuclear reactions involving nuclei near the proton-drip line (rp-process)
- Science goal of FRIB
- Light curve well studied – depends on properties of very unstable nuclei
- Multi-D effects important, but could constrain neutron star radii – hence EOS

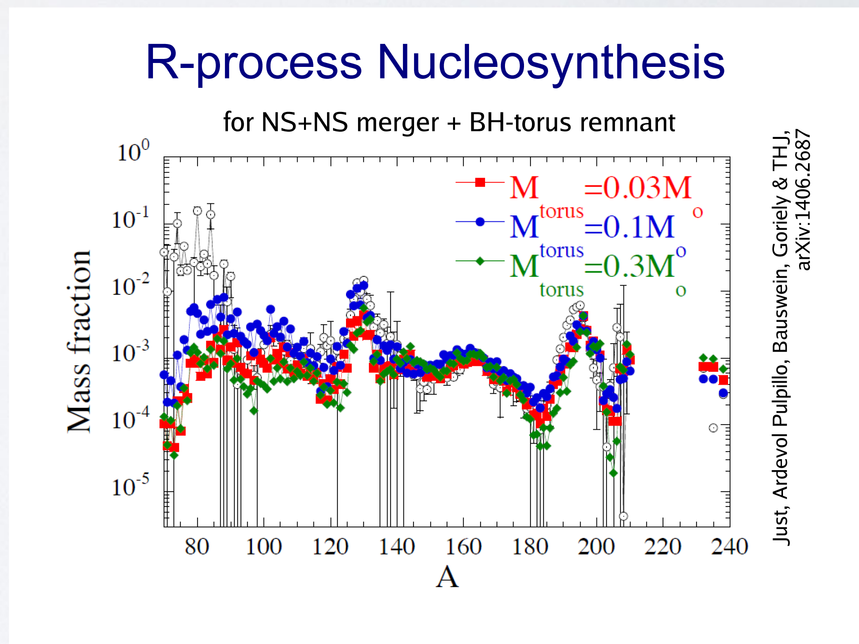
Neutron Star Mergers



requires full GR
microphysics in different regimes

using gravitational waves
to study neutron star structure





nucleosynthesis from NS merger

Key questions:

- R-process site(s)
- Gravitational Waves
- Neutron Star Mass Radius

Recommendation

Realizing the scientific potential of current and future experiments demands large scale computations in nuclear theory that exploit the US leadership in high-performance computing. Capitalizing on the pre-exascale systems of 2017 and beyond requires significant new investments in people, advanced software, and complementary capacity computing directed toward nuclear theory.

Request

• To this end, we ask the Long-Range Plan to endorse the creation of an NSAC subcommitee to plan a diverse program of new investments in computational nuclear theory. We expect this program to include:

– new investments in SciDAC and complementary efforts needed to maximize the impact of the experimental program;

– development of a multi-disciplinary workforce in computational nuclear theory as called for in the Tribble Report;

– deployment of the necessary capacity computing to fully exploit the nations leadership-class computers;

with support ramping up over five years towards a level of around $10M per annum.