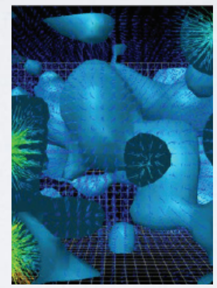
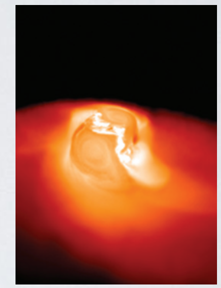
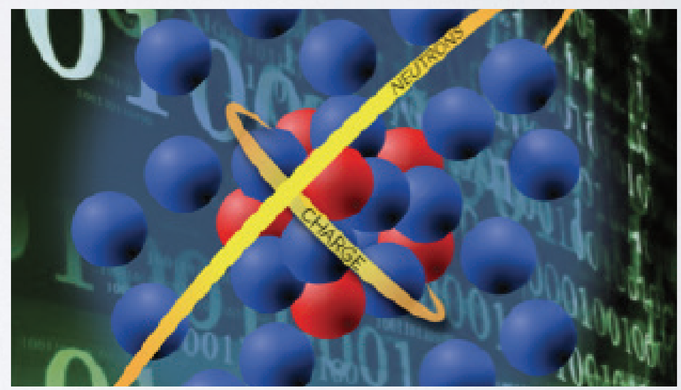
Computational Nuclear Physics in the Exascale Era
- towards the quantum computing era -

computational nuclear physics provides key bridges between different areas of nuclear science:
from the quark-gluon plasma to hadrons to nuclei and stars

Outline:

- Hot QCD
- Cold QCD
- Nuclear Structure and Reactions
- Nuclear Astrophysics
- Experimental Nuclear Physics

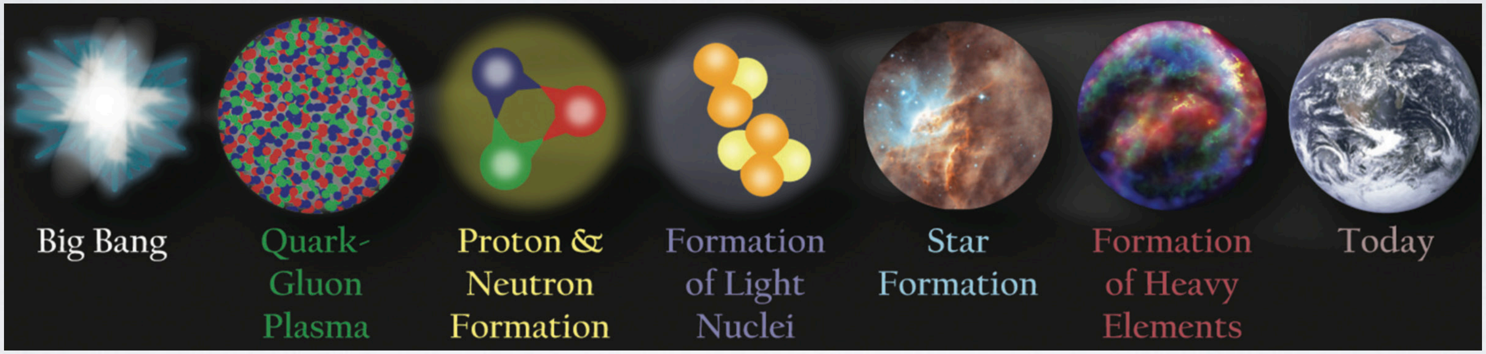


US efforts described in report available at http://exascaleage.org
workshop June 15-17, 2016; M. Savage, JC, and many others

New exascale computing ecosystem offers a unique opportunity:

- Huge increase in computational capability
- Important advances in software and algorithms
- Diverse nuclear science enabled through exascale computing



Grand Challenges

How Did Visible Matter Come into Being and how Does It Evolve?

How Does Subatomic Matter Organize Itself and What Phenomena Emerge?

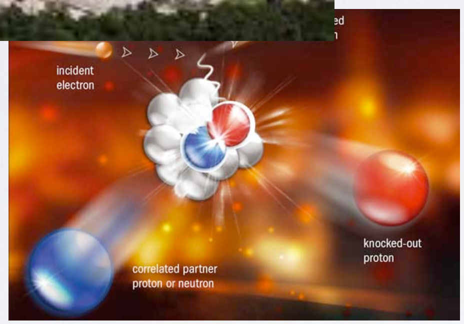
Are the Fundamental Interactions Basic to the Structure of Matter Fully Understood?

How Can the Knowledge and Technological Progress Provided by Nuclear Physics Best Be Used to Benefit Society?

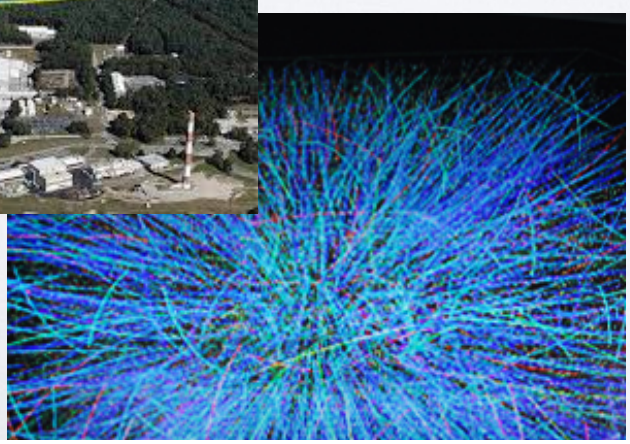
Jefferson Lab

Nuclear Physics Facilities & Experiments

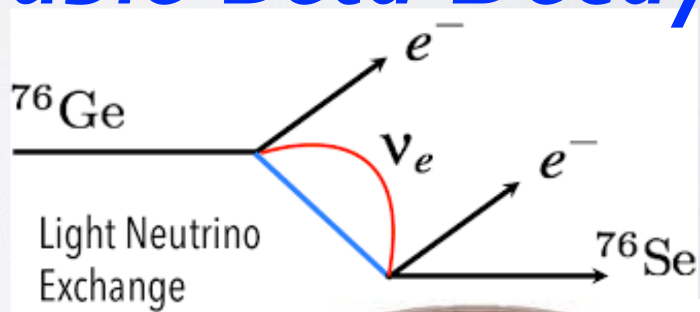
FRIB

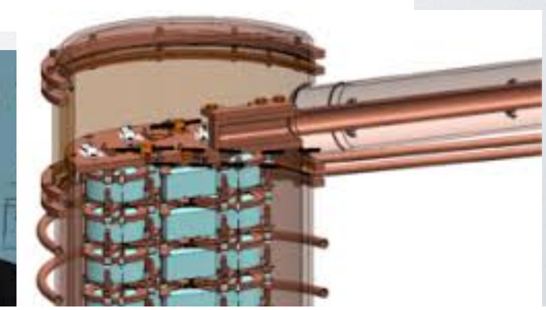


RHIC

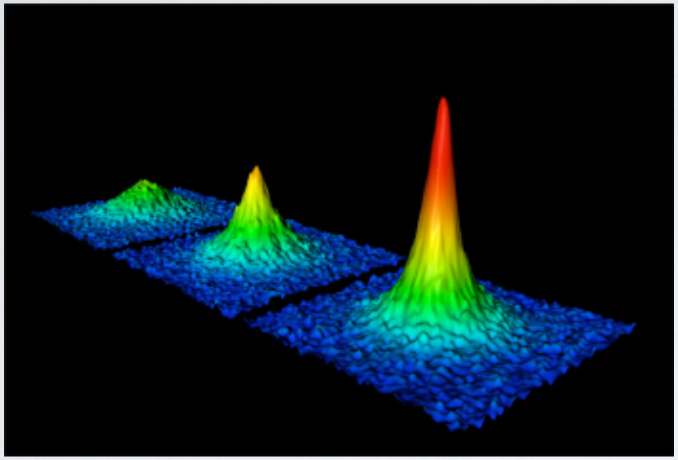


Double Beta Decay

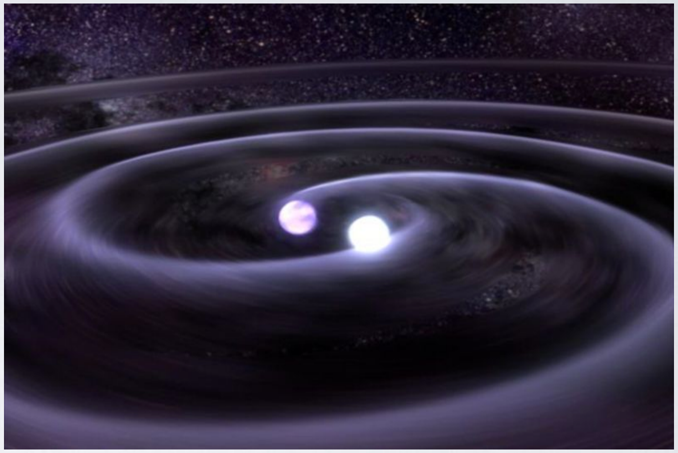




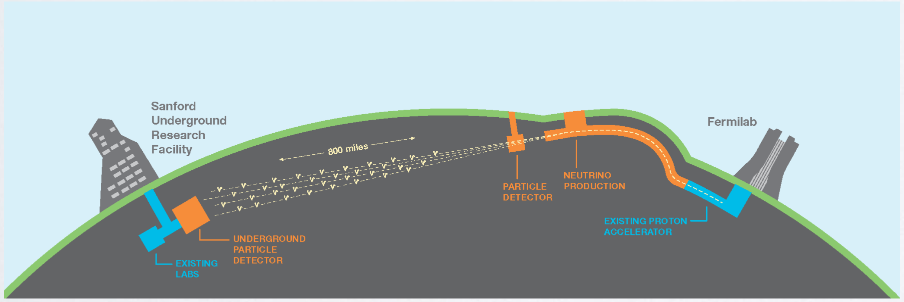
Rich Ties to Many Fields of Physics



Cold Fermionic Atoms



2 solar mass neutron stars and mergers



accelerator neutrino experiments

core-collapse supernovae

Strongly Correlated Quantum Many-Body Physics

Must solve the quantum many-body problem

cautions:

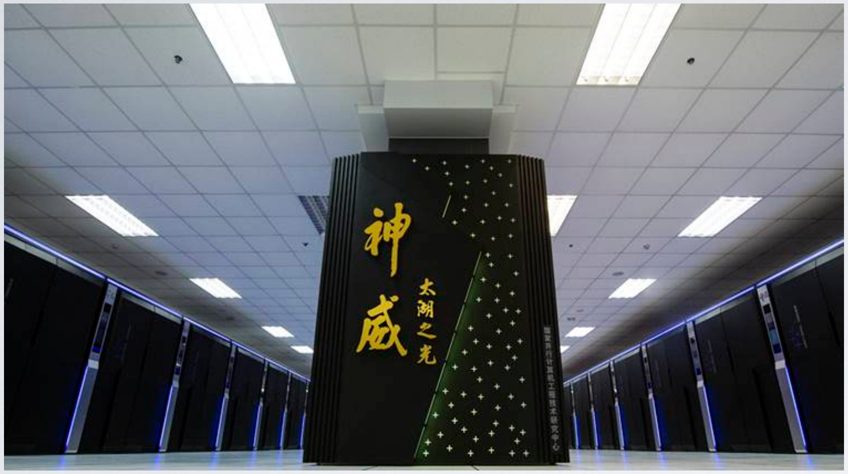
The Schrodinger equation cannot be solved accurately when the number of particles exceeds about 10. No computer existing, or that will ever exist, can break this barrier because it is a catastrophe of dimension ...
Pines and Laughlin (2000)

In general the many electron wave function Ψ ... for a system of N electrons is not a legitimate scientific concept [for large N]
Kohn (Nobel lecture, 1998)

but often we do not need a complete description of the system: thermal properties, samples of path integral, cluster expansions,…

Quantum Monte Carlo, Coupled Cluster, CI, IMSRG, …

World-wide effort



Sunway TaihuLight (China)

K Computer (Japan)

Piz Daint (Switzerland)

Titan (US)

Rapidly Evolving Field (top 500)

2017

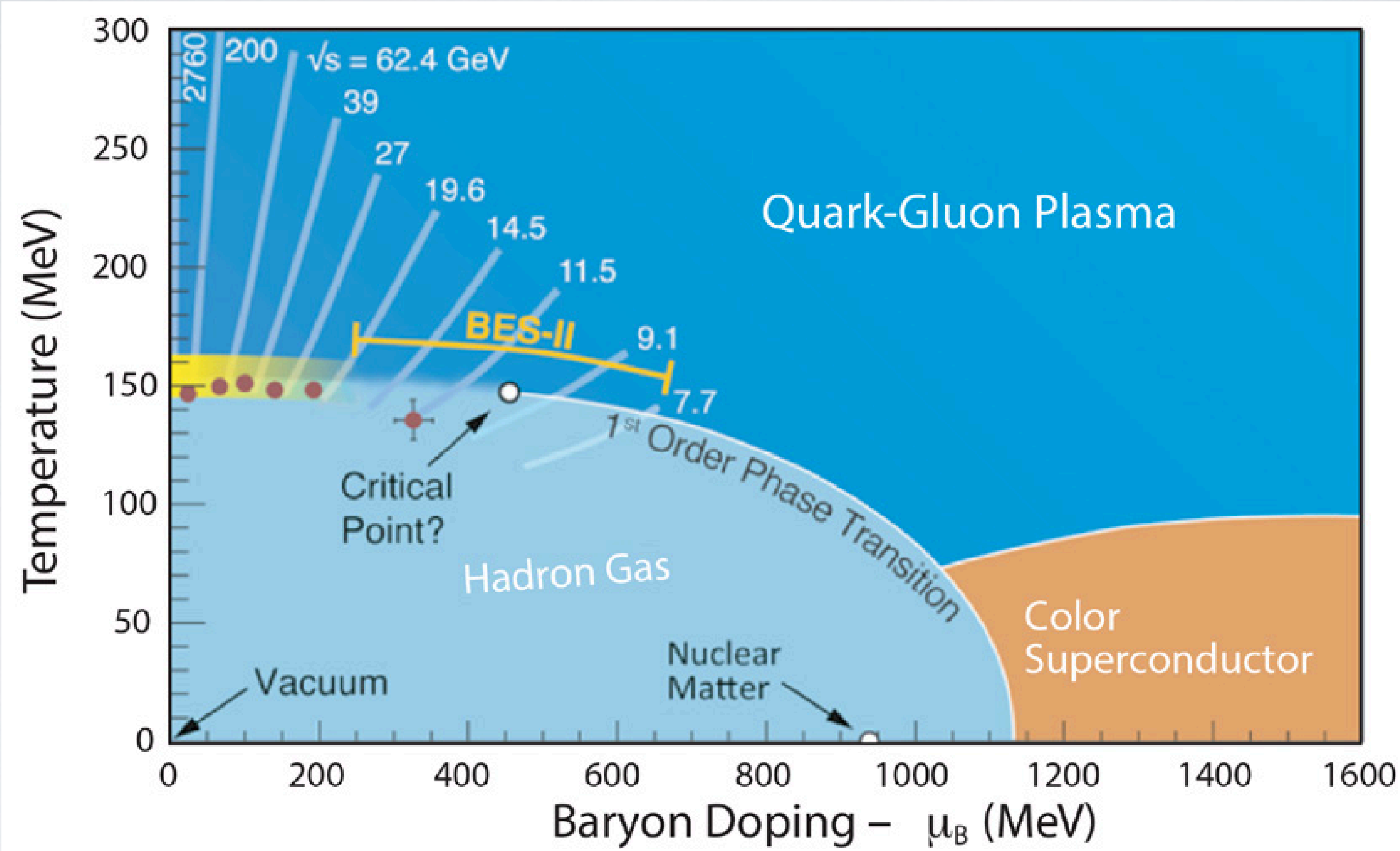
Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway (/system/178764), NRCPC National Supercomputing Center in Wuxi (/site/50623) China	10,649,600	93,014.6	125,435.9	15,371
2	**Tianhe-2 (MilkyWay-2)** - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P (/system/177999), NUDT National Super Computer Center in Guangzhou (/site/50365) China	3,120,000	33,862.7	54,902.4	17,808
3	**Piz Daint** - Cray XC50, Xeon E5-2690v3 12C 2.6GHz, Aries interconnect , NVIDIA Tesla P100 (/system/177824), Cray Inc. Swiss National Supercomputing Centre (CSCS) (/site/50422) Switzerland	361,760	19,590.0	25,326.3	2,272
4	**Gyoukou** - ZettaScaler-2.2 HPC system, Xeon D-1571 16C 1.3GHz, Infiniband EDR, PEZY-SC2 700Mhz (/system/179102), ExaScaler Japan Agency for Marine-Earth Science and Technology (/site/49318) Japan	19,860,000	19,135.8	28,192.0	1,350
5	**Titan** - Cray XK7, Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x (/system/177975), Cray Inc. DOE/SC/Oak Ridge National Laboratory (/site/48553)	560,640	17,590.0	27,112.5	8,209

2012

Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom (/system/177556), IBM DOE/NNSA/LLNL (/site/49763) United States	1,572,864	16,324.8	20,132.7	7,890
2	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect (/system/177232), Fujitsu RIKEN Advanced Institute for Computational Science (AICS) (/site/50313) Japan	705,024	10,510.0	11,280.4	12,660
3	**Mira** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom (/system/177718), IBM DOE/SC/Argonne National Laboratory (/site/47347) United States	786,432	8,162.4	10,066.3	3,945
4	**SuperMUC** - iDataPlex DX360M4, Xeon E5-2680 8C 2.70GHz, Infiniband FDR (/system/177719), IBM/Lenovo Leibniz Rechenzentrum (/site/48248) Germany	147,456	2,897.0	3,185.1	3,423

6x speed, 7x cores, 2x power (10-12x from 10 years ago)

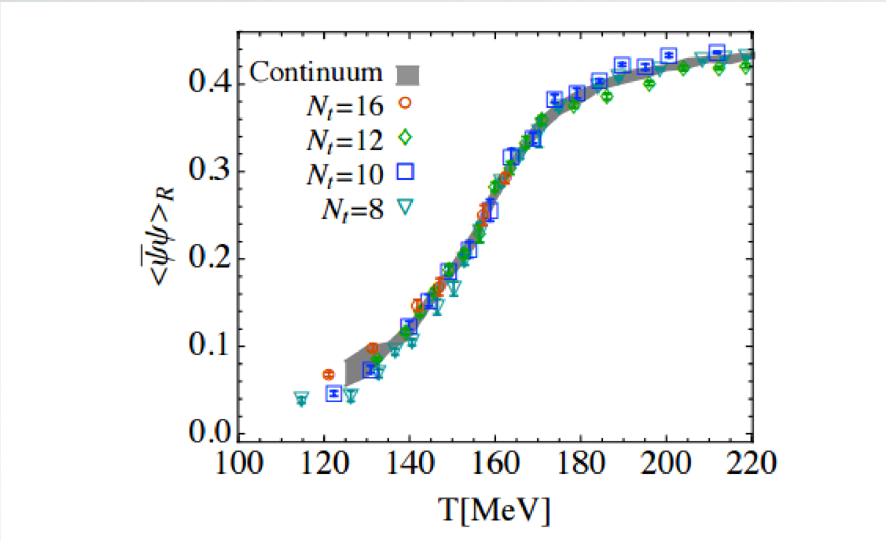
Hot QCD



RHIC - recreating conditions similar to the early Universe:

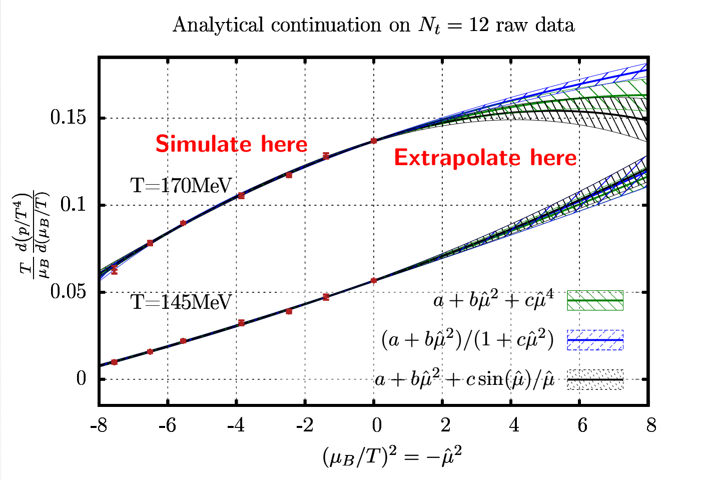
- high T - low baryon density
- LQCD has provided accurate equation-of-state,
- moving to finite baryon density
- dynamics and transport coefficients ('perfect fluid')

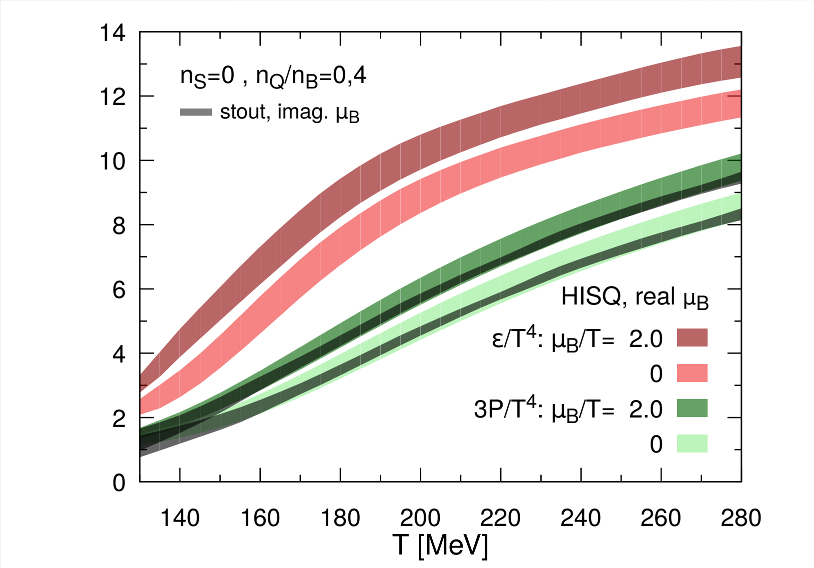
Hot QCD: Equation of State



Crossover at μ_B =0

Wuppertal-Budapest JHEP (2010)





Total energy density for finite μ_B

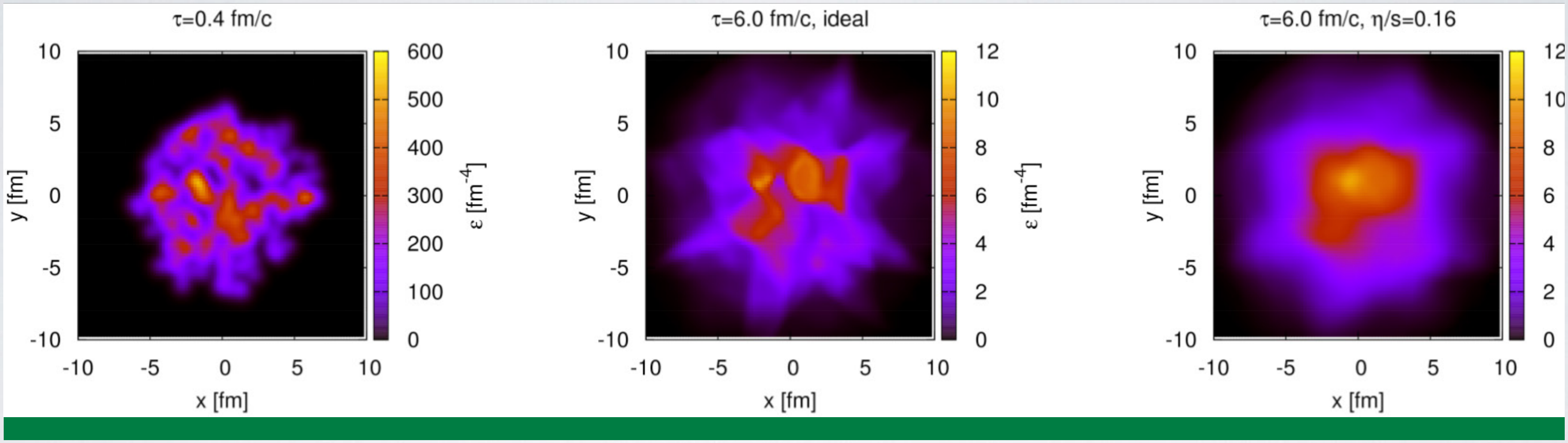
6th order taylor expansion

Hot QCD collab: PRD (2017)

Hot QCD: transport properties

Extracting shear viscosity over entropy from HI collisons:
realizing the perfect fluid

Relativistic Hydrodynamics

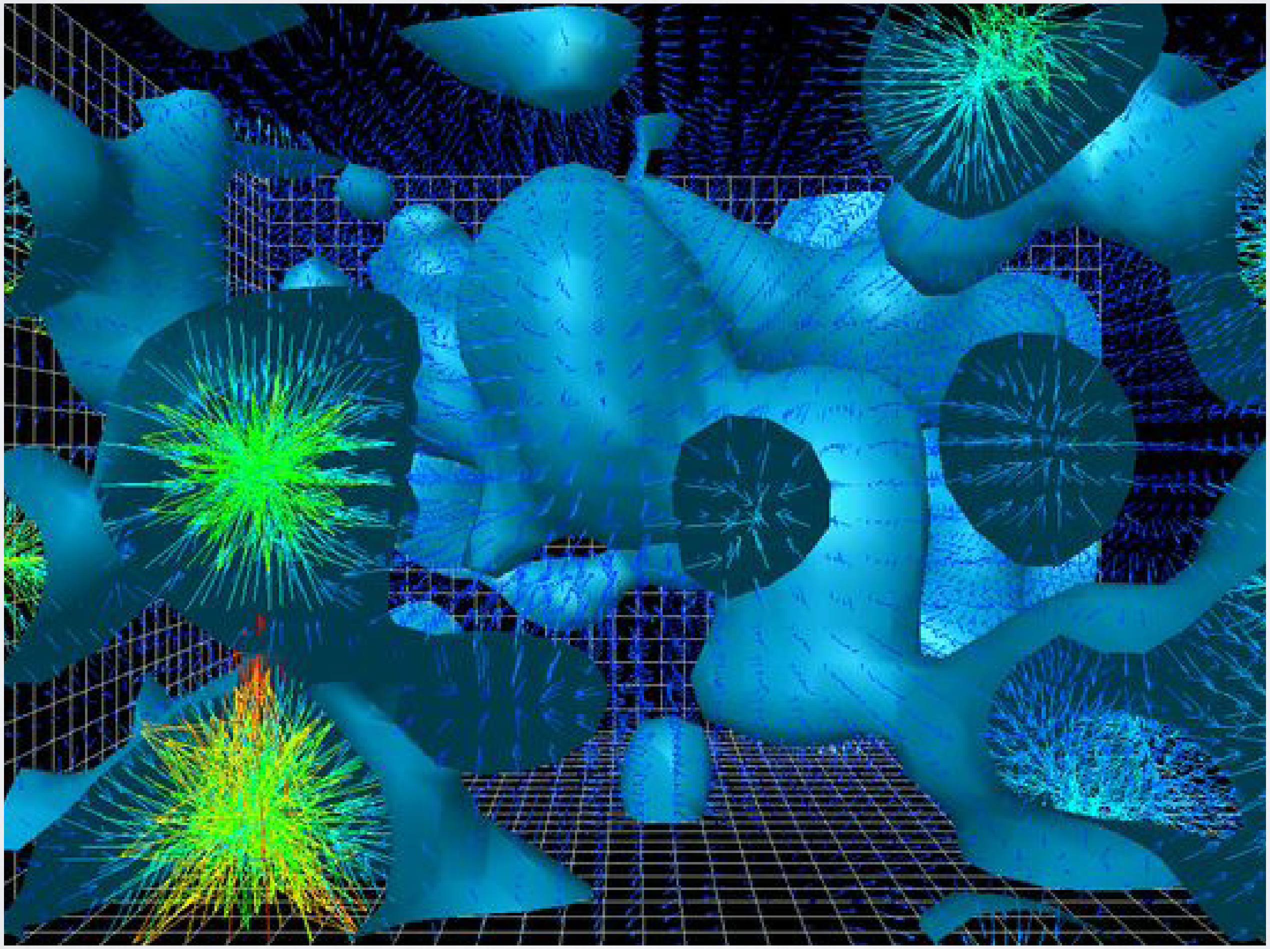


Initial energy density distribution generated in a HI collision (left), and at τ = 6 fm/c for two values of η/s = 0 (middle) and η/s = 0.16 (right).
(Images from B. Schenke.)

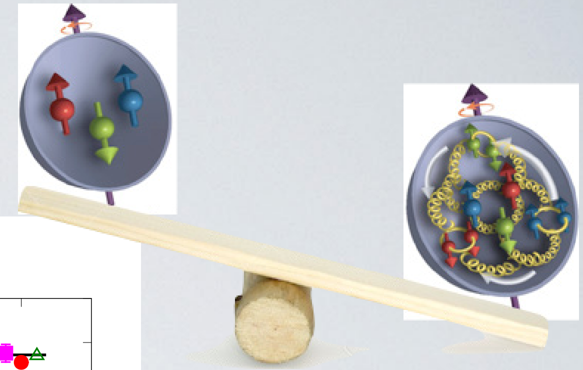
Cold QCD

- Hadron spectroscopy and structure
- Reaching towards nuclear physics from LQCD
- Fundamental symmetries and new physics

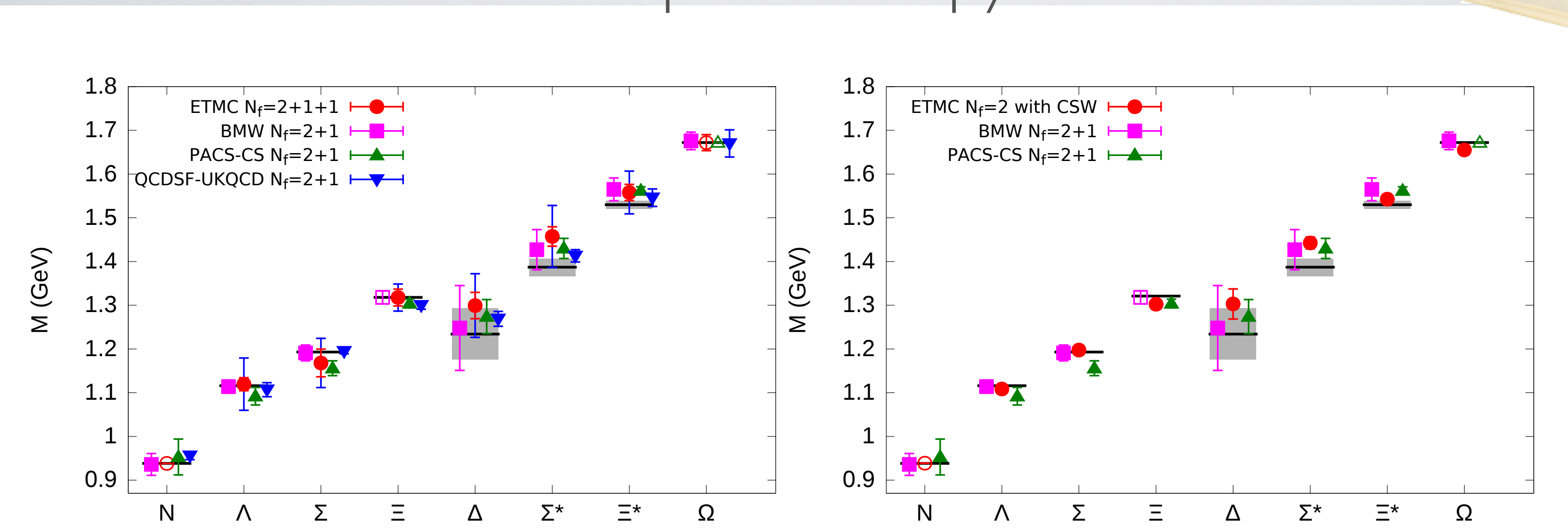
starting with gauge configurations
(computationally very demanding)



Cold QCD: Hadrons

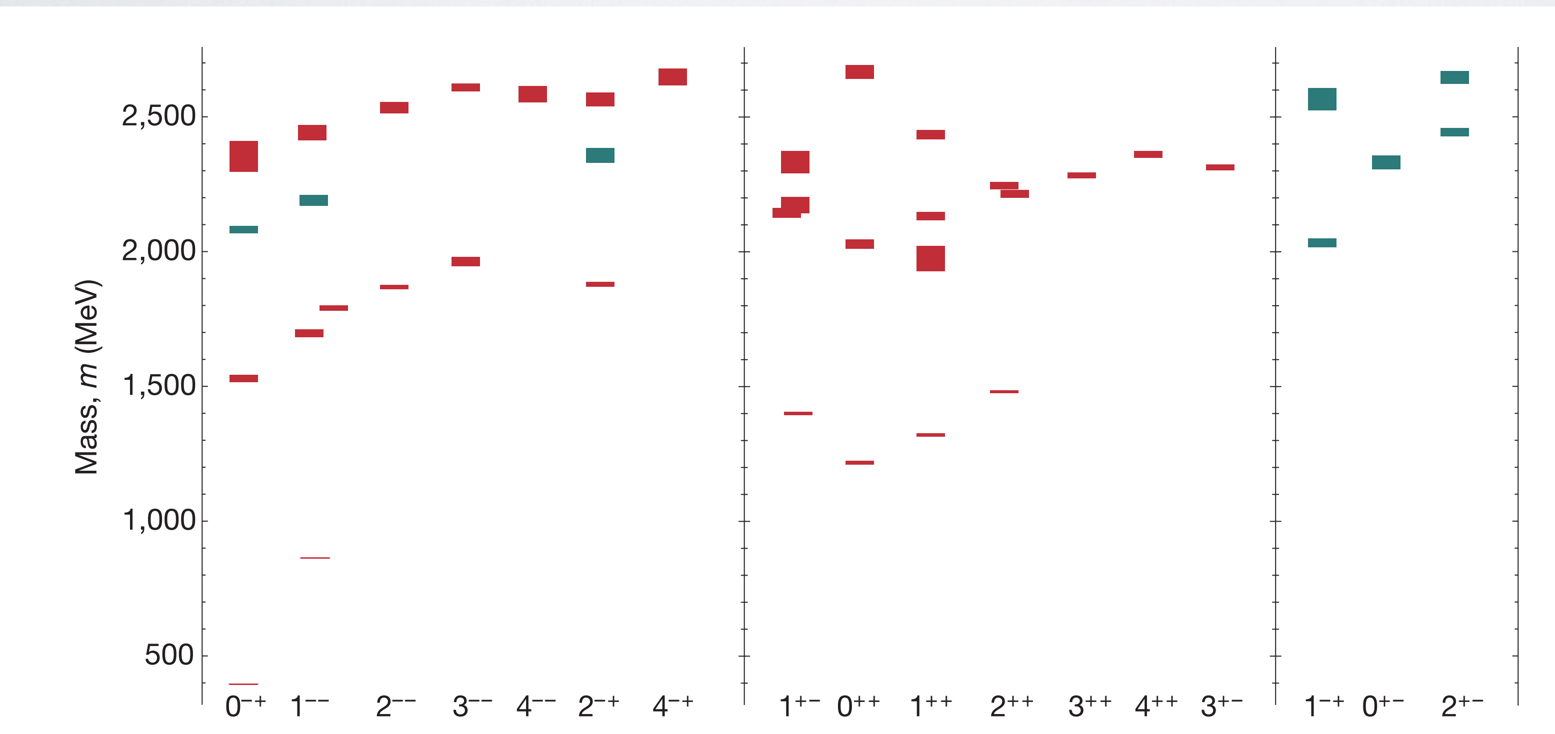


Hadron Spectroscopy



Baryon masses

Alexandrou (2014)



Meson masses (orange: glue quant. #s)

Dudek, 2013

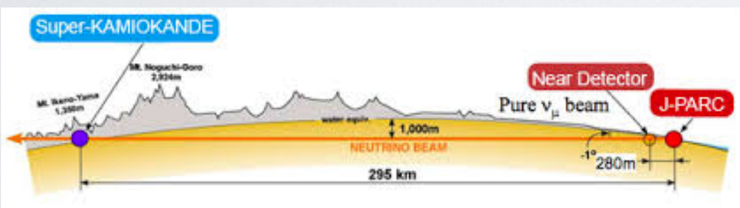
Cold QCD: Hadrons

proton radius

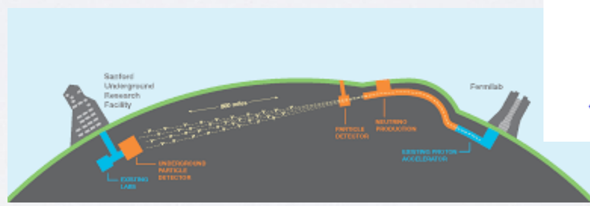
Hadronic Structure:

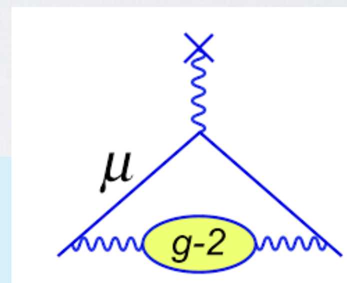
- Radii
- Form factors (e, ν scattering)
- Parton distributions and TMD
- Fundamental symmetries: g-2, nEDM

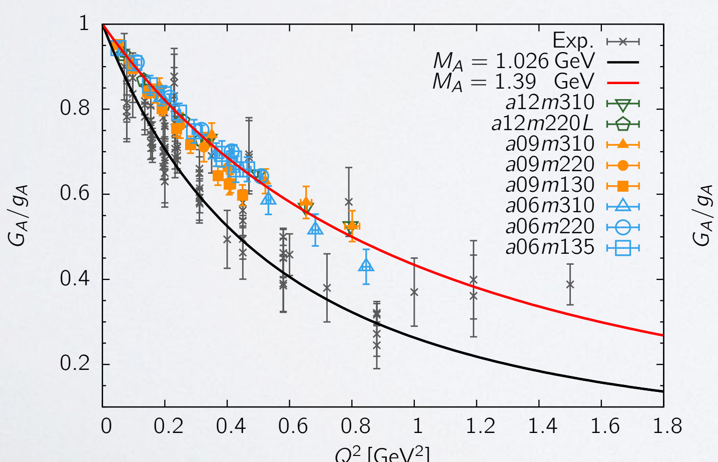
T2K



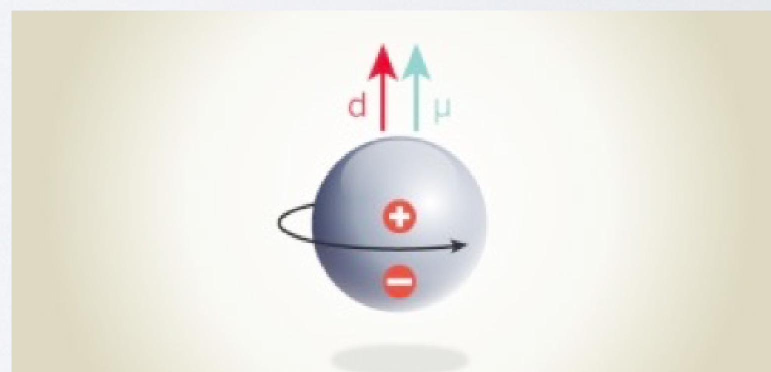
DUNE







nucleon axial form factor

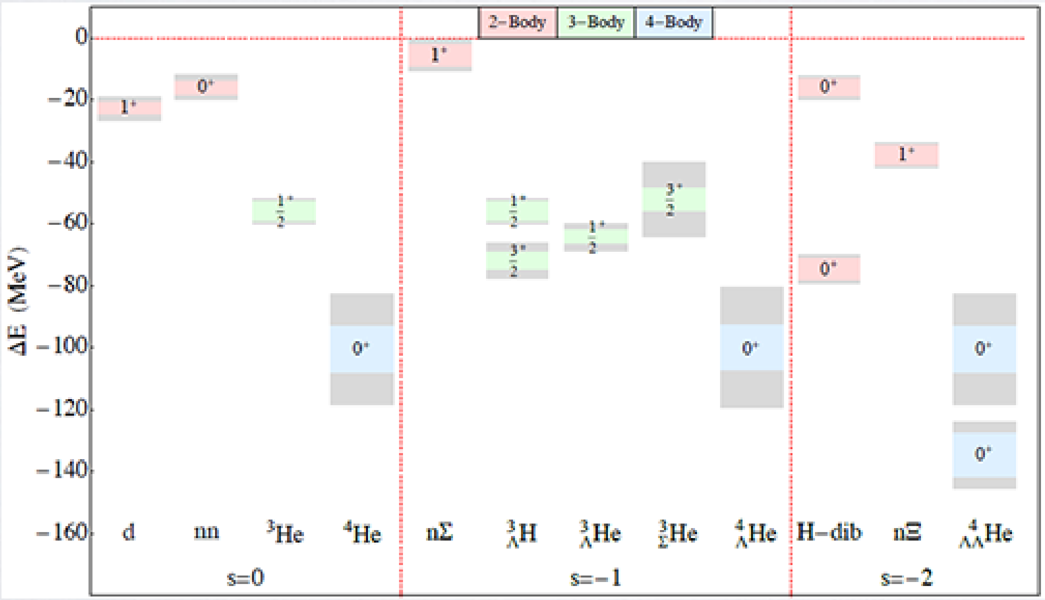


neutron EDM

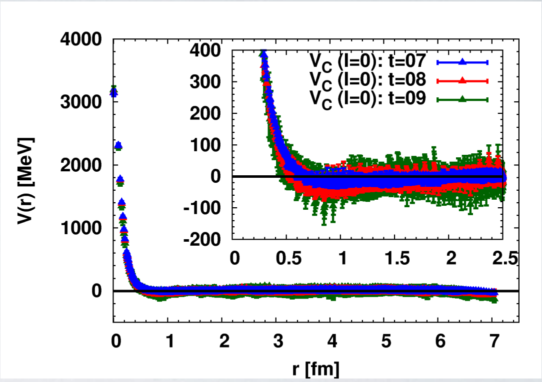
Cold QCD: towards nuclei

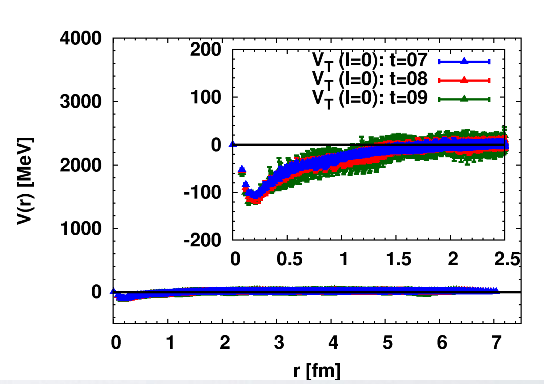
Light Nuclear Structure from LQCD:

- NN (and other) scattering
- Binding of dibaryons and light nuclei
- Magnetic moments of Light Nuclei
- NN EW matrix elements



Light Nuclear Spectra (NPLQCD)

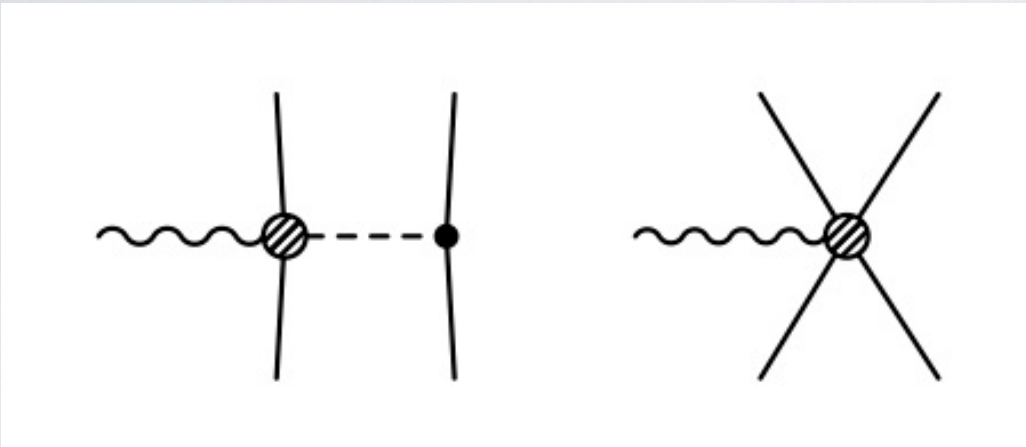


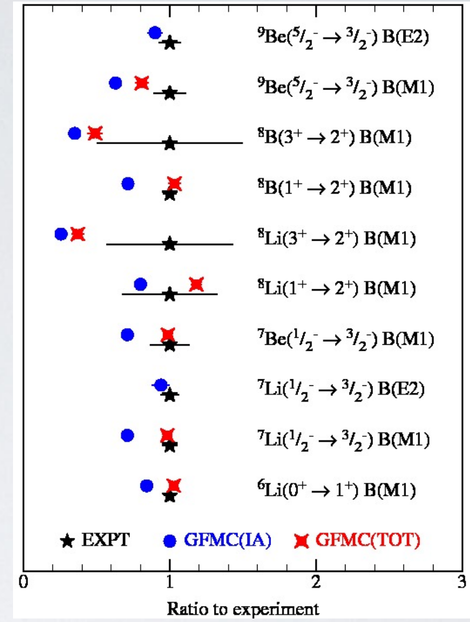


NN interaction
central, tensor
near physical point
(HAL QCD)

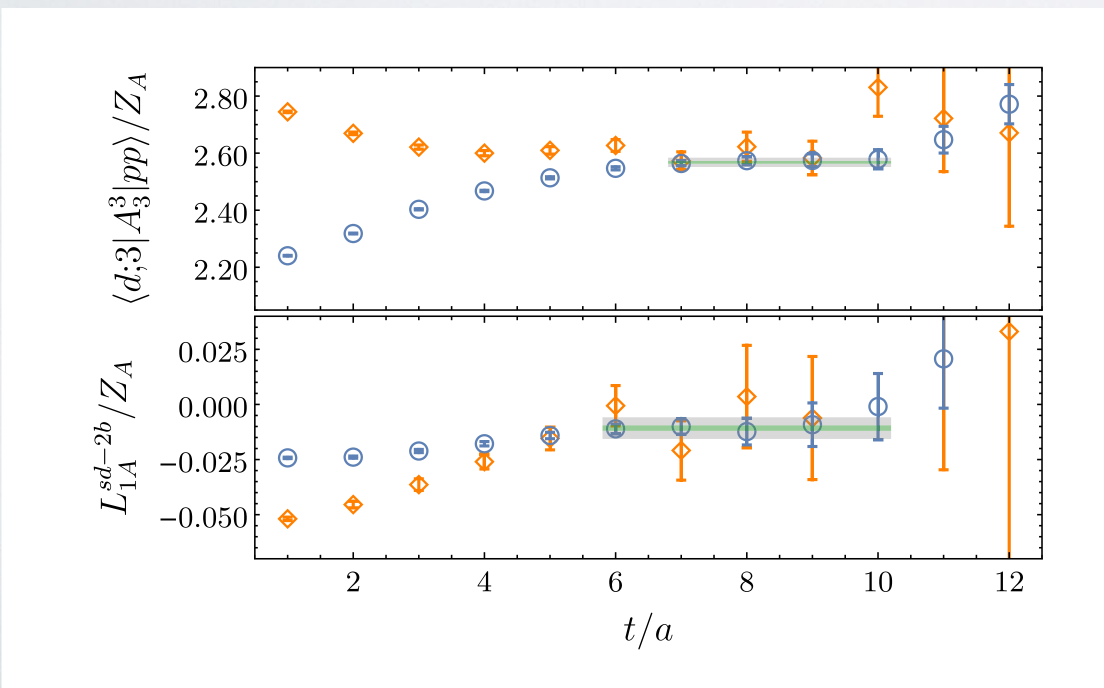
Cold QCD: towards nuclear currents

required for EM transitions





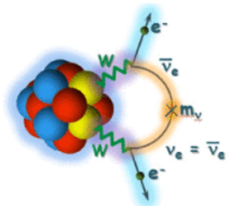
Pastore, et al, 2014



pp fusion and
tritium beta decay
NPLQCD (2017)

first efforts towards
double beta decay nn to pp

Nuclear Structure and Reactions



Nuclei from the first principles

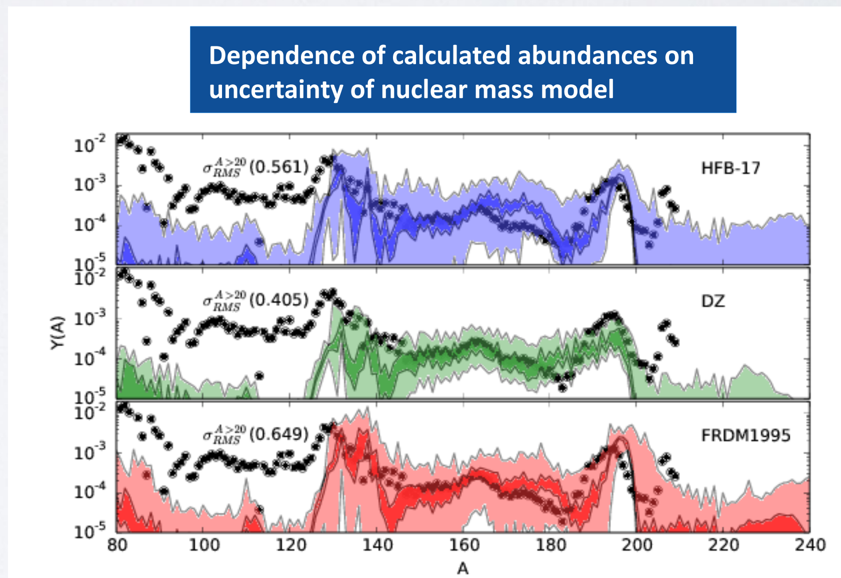
Electroweak phenomena

Light-nuclei reactions

Quantified heavy nuclei

Dense nucleonic matter

- Where do nuclei and elements originate?
- How are nuclei organized?
- How can nuclei be exploited to reveal the fundamental symmetries of nature?
- What are the practical and scientific uses of nuclei?

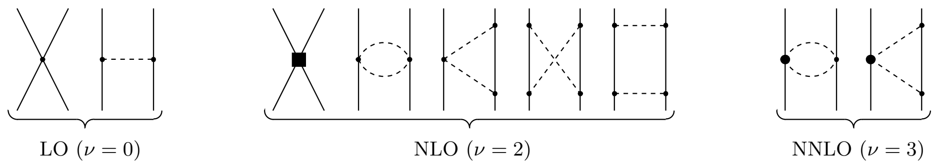


abundances vs. mass model

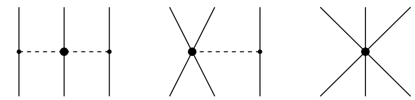
strongly-correlated quantum many-body system

Nuclear Structure and Reactions: *interactions and currents*

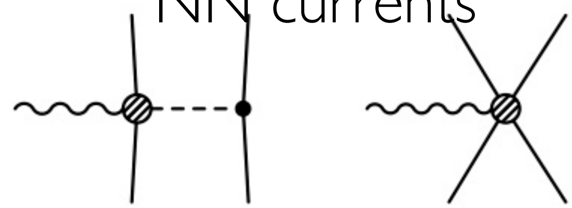
NN interactions



3N



NN currents



FRIB

NUCLEI

Nuclear Computational Low-Energy Initiative

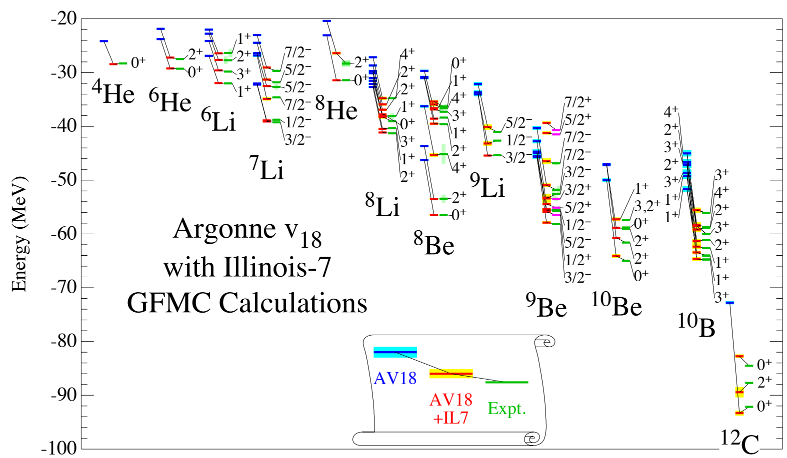
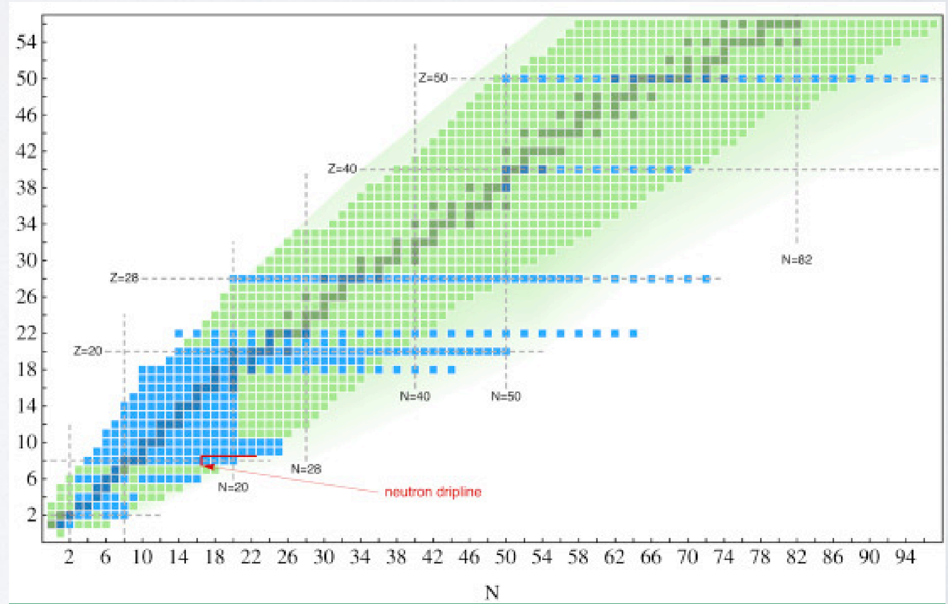


FIG. 2 GFMC energies of light nuclear ground and excited states for the AV18 and AV18+IL7 Hamiltonians compared to experiment.

Light Nuclear Spectra

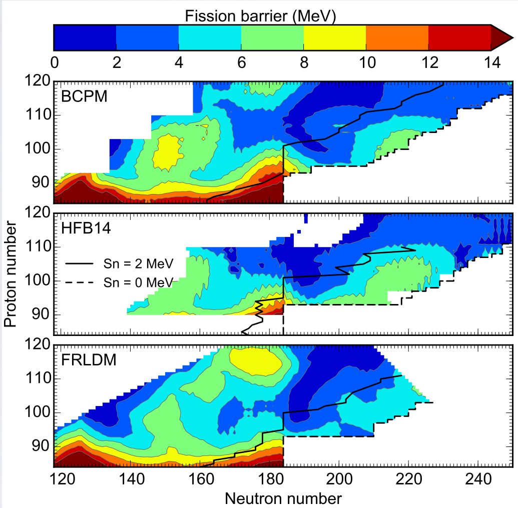


Ab Initio Methods

Nuclear Structure and Reactions: *density functional theory*

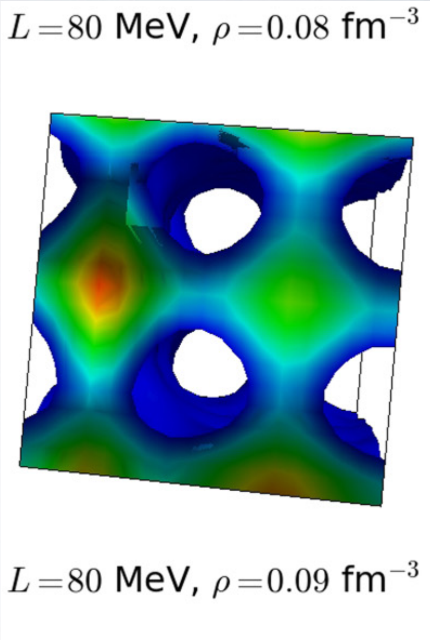
fission properties of superheavies

Samuel A. Giuliani, et al (2017)



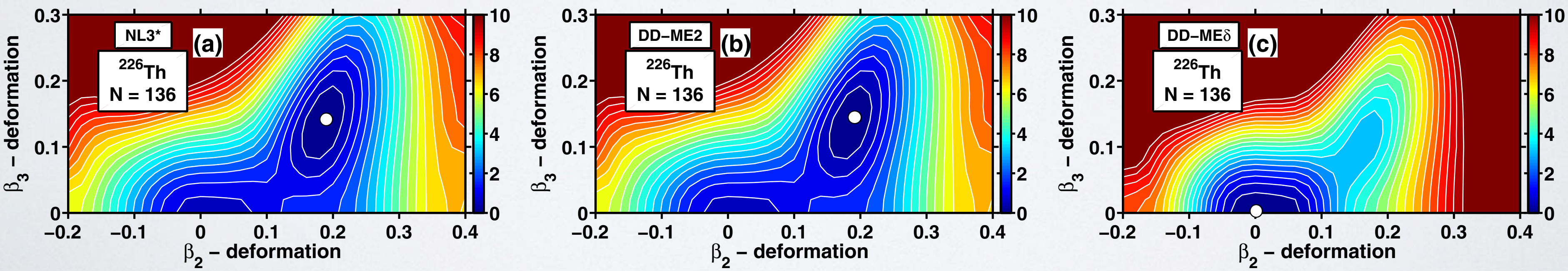
Pasta phases in dense matter

F. J. Fattoyev, et al. 2017



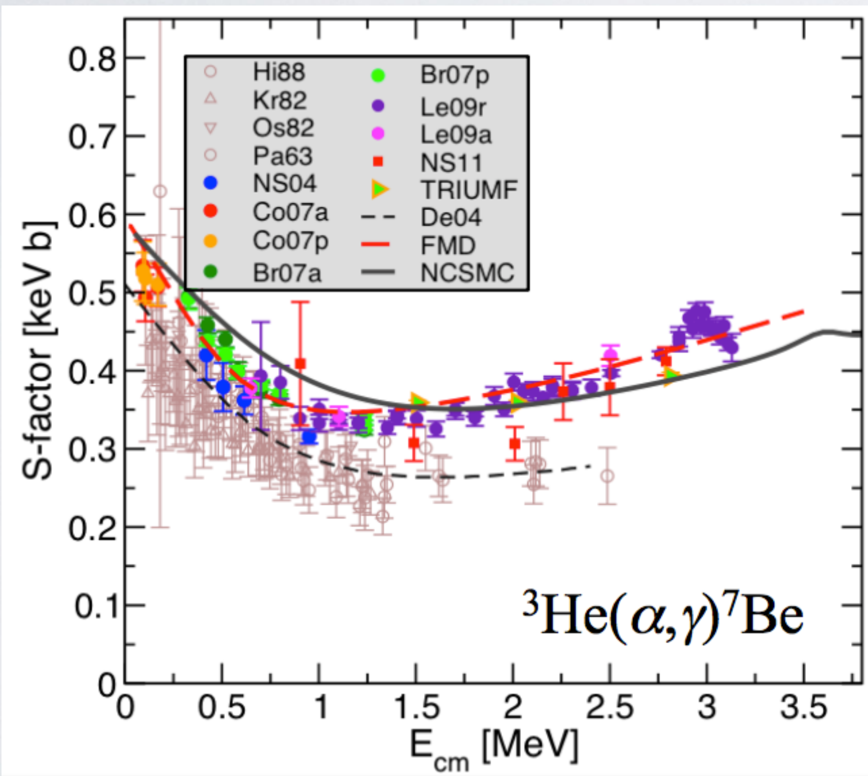
fission pathways: Th isotopes

S. E. Agbemava, et al, 2016

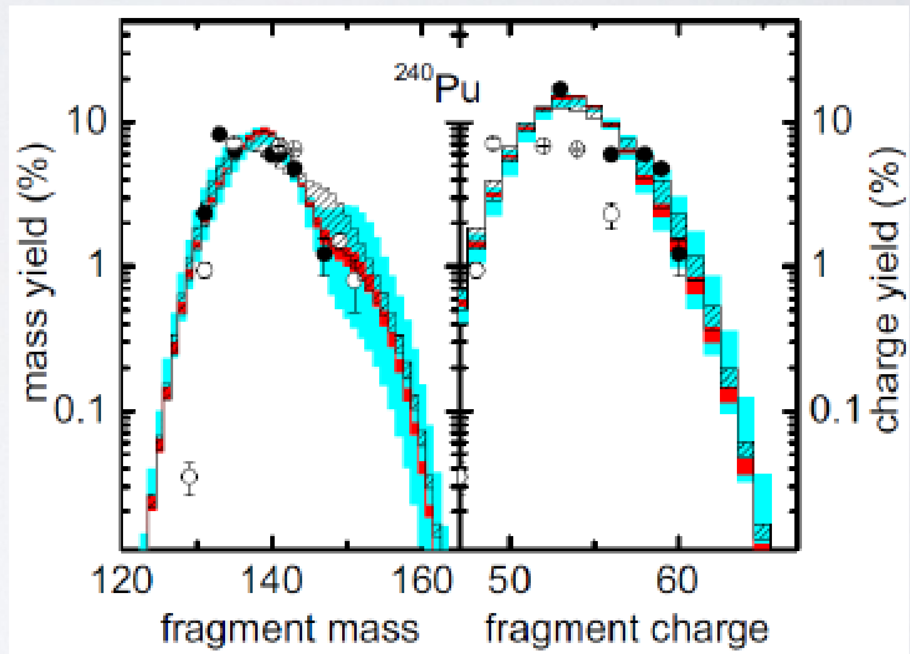


Nuclear Structure and Reactions: *low energy reactions*

Light-Ion Fusion

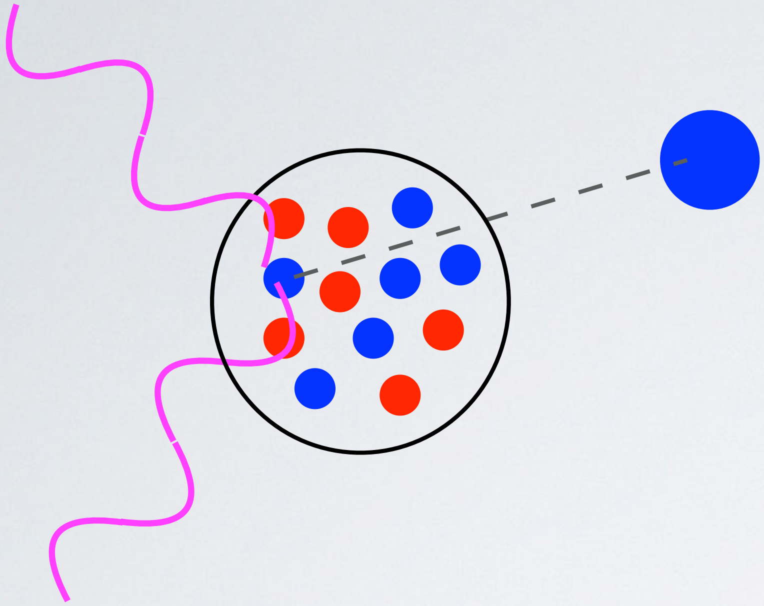


Fission Mass Distributions

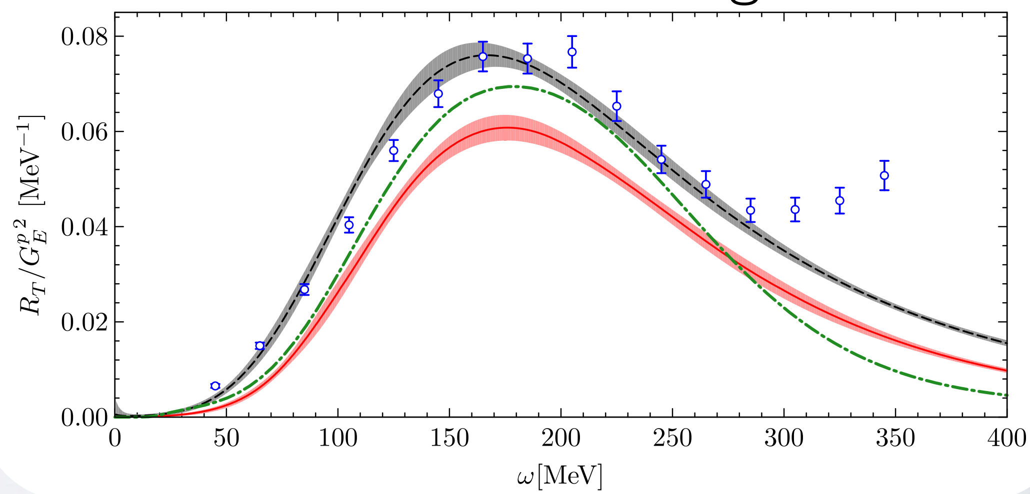


Density Functional Theory

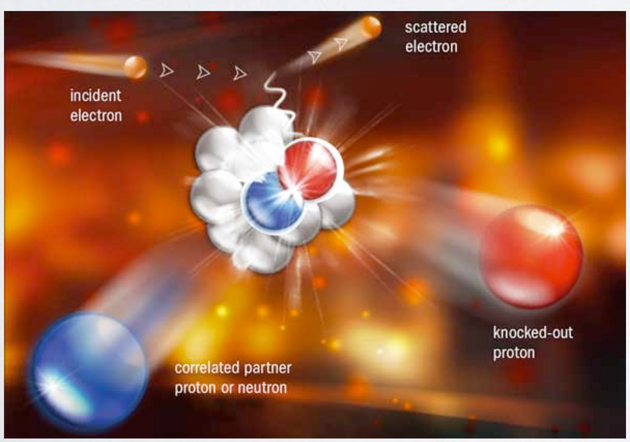
Nuclear Structure and Reactions: *high energy reactions*
electron and neutrino scattering

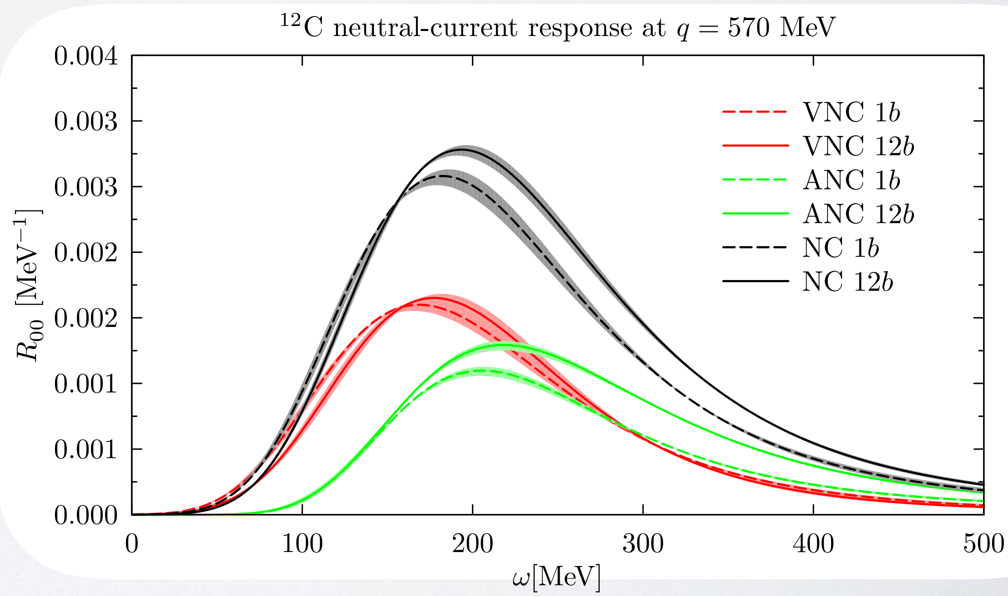


electron scattering

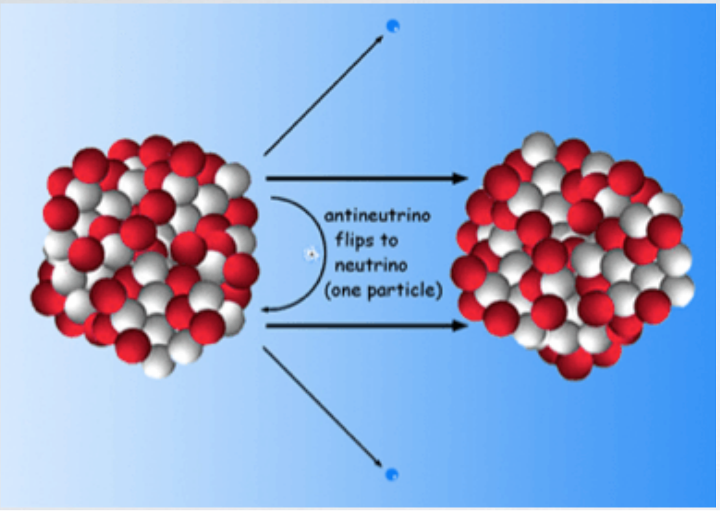


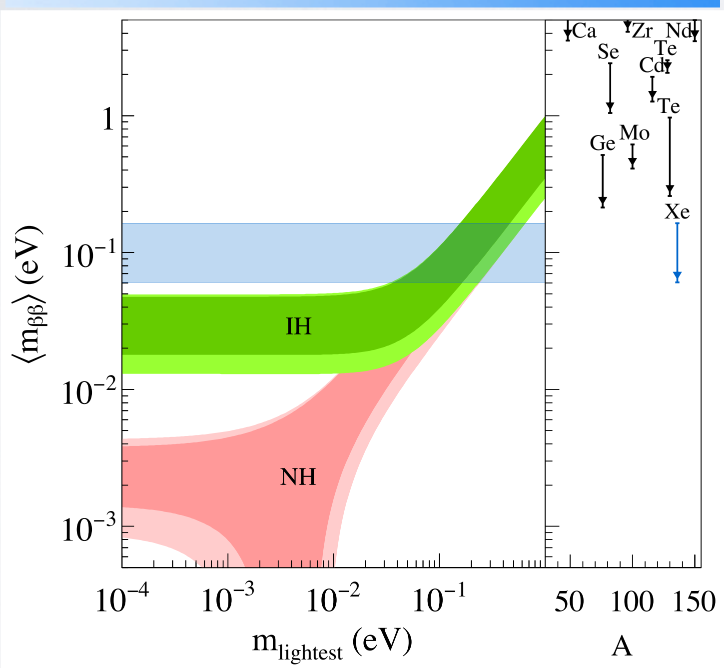
neutrino scattering

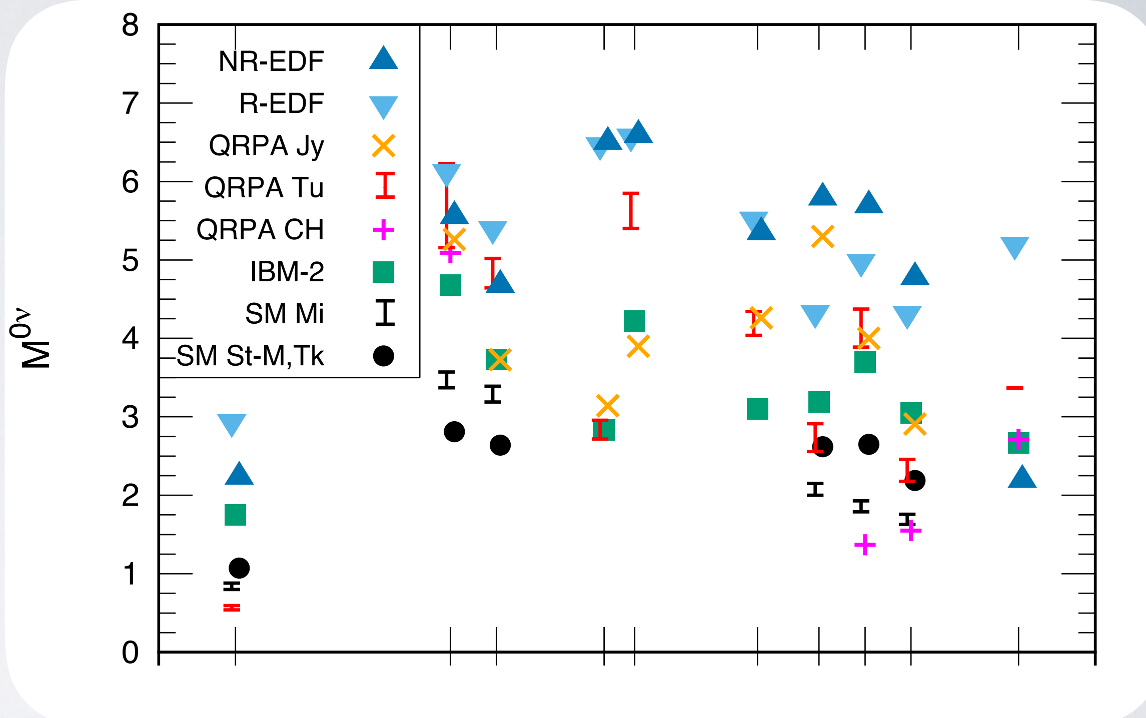


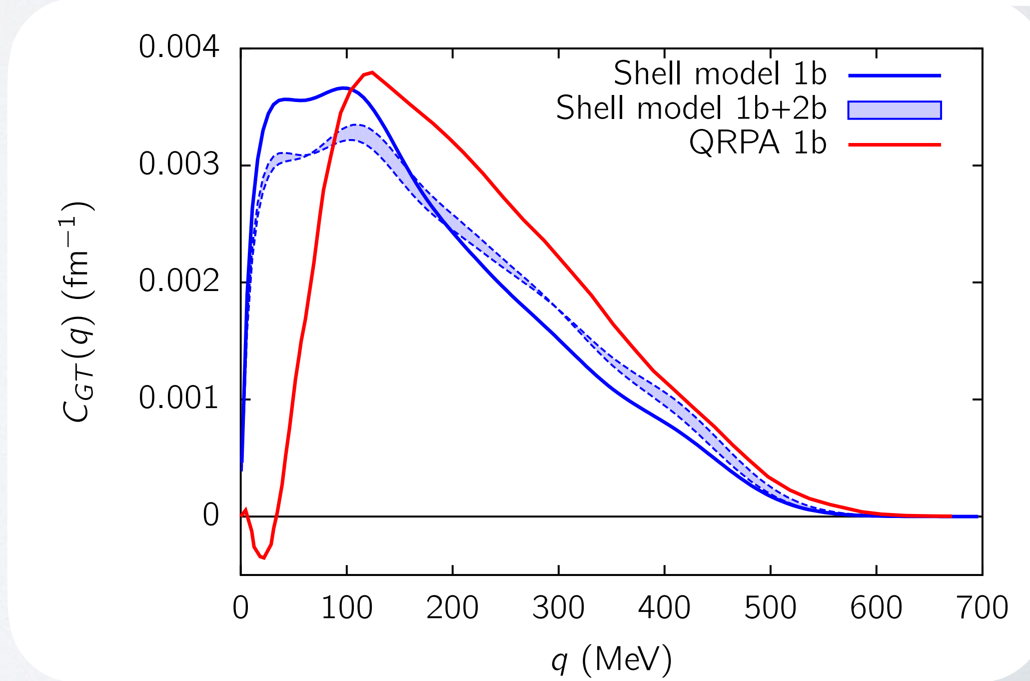


Nuclear Structure and Reactions: *double beta decay*
low energy but moderate momenta





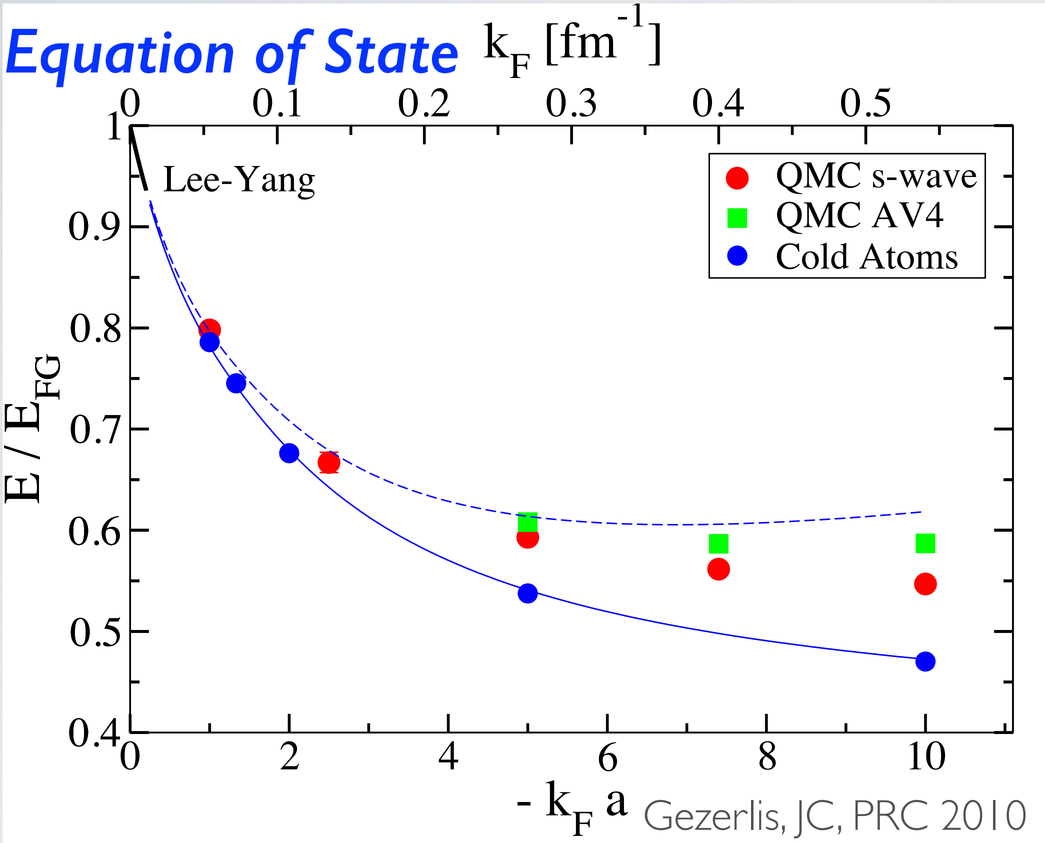




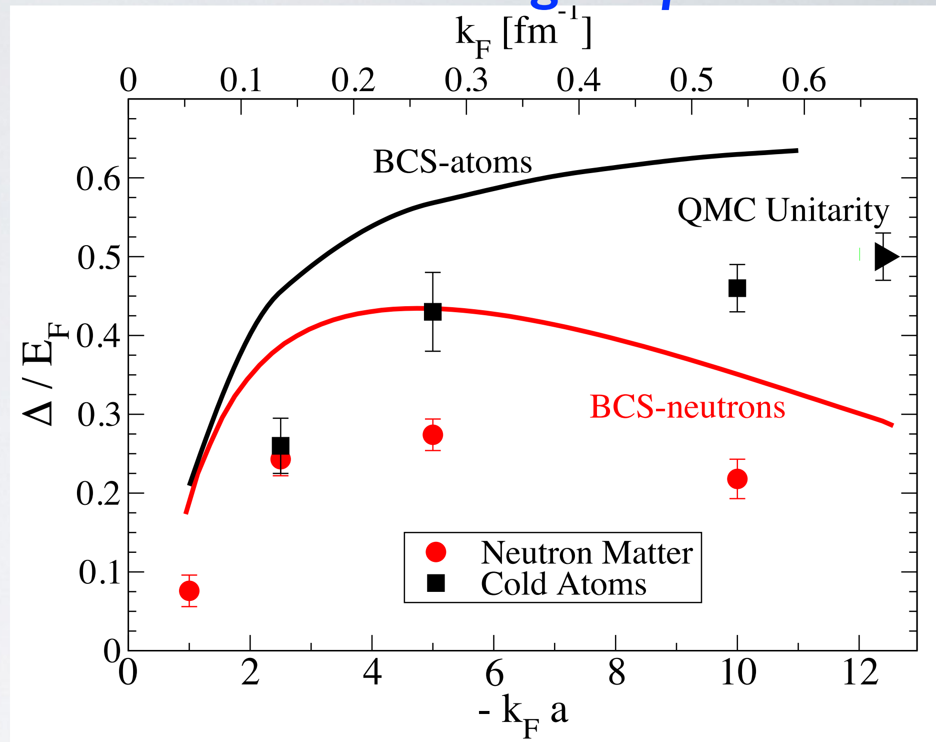
need to understand g_A 'quenching'
collective and single-particle structure

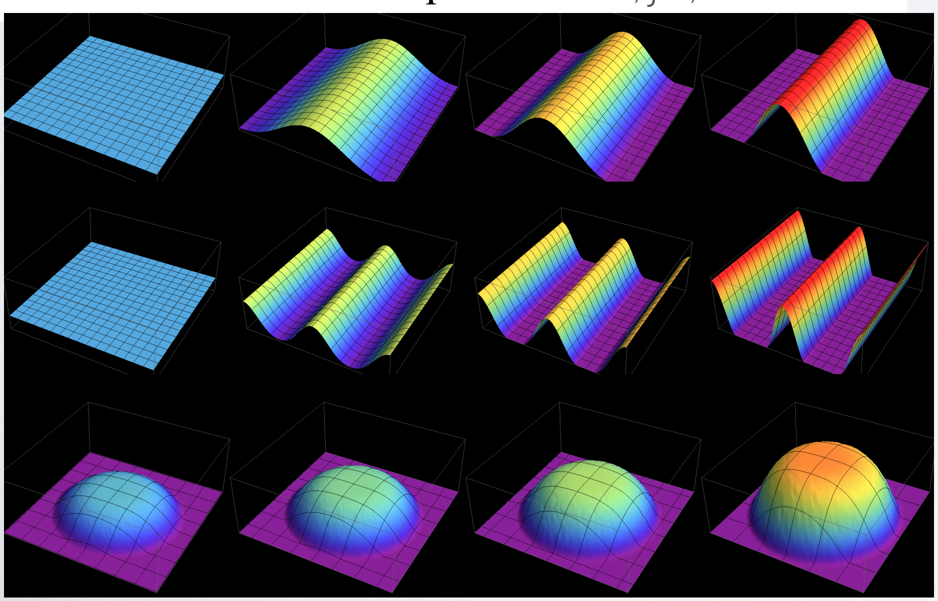
Neutron star matter: *very low density neutron matter*

Equation of State



Pairing Gap

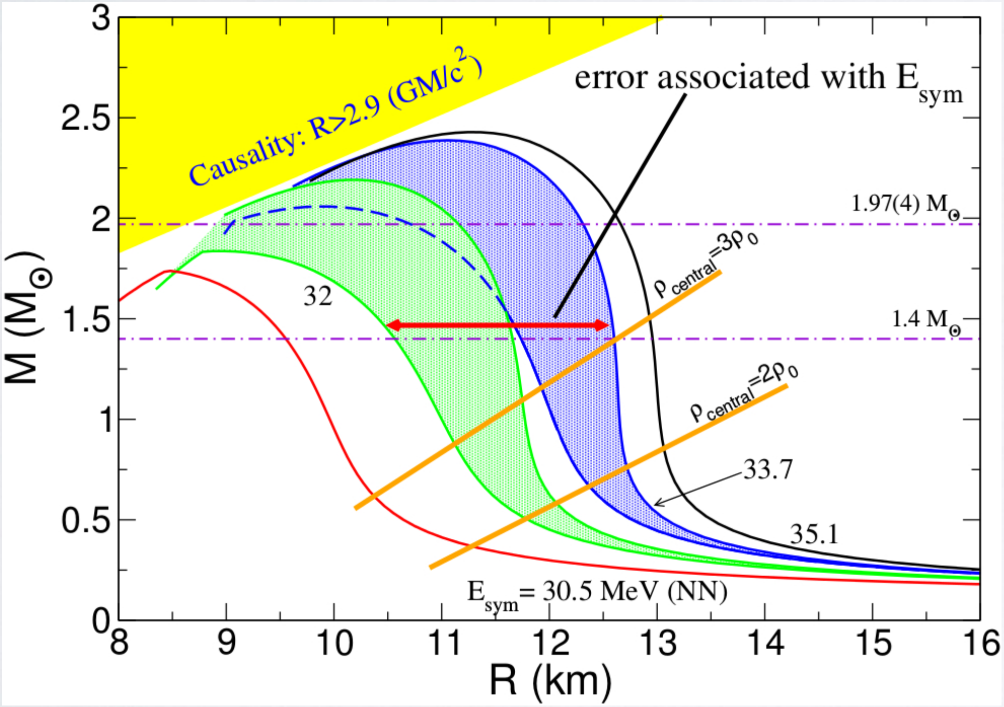




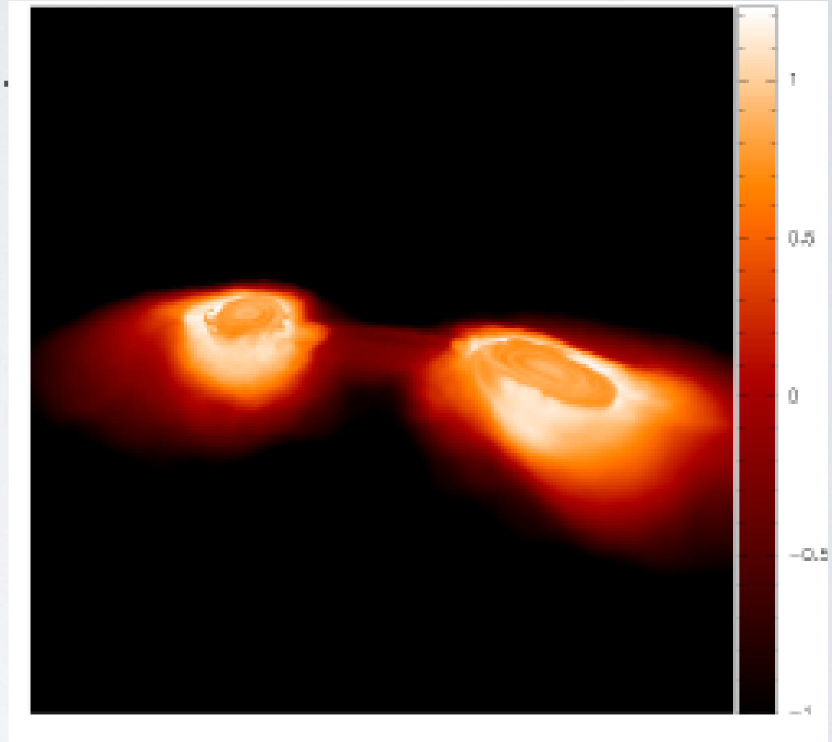
Scale-Invariance and Density Functional

Neutron star matter: *dense matter*
Neutron Star mass/radius relation, deformation

- LIGO, NICER, …
- dense matter equation of state
- are there exotic phases? (hyperons, quarks,…
- cooling and neutrino propagation



Equation of state:
dense neutron star matter

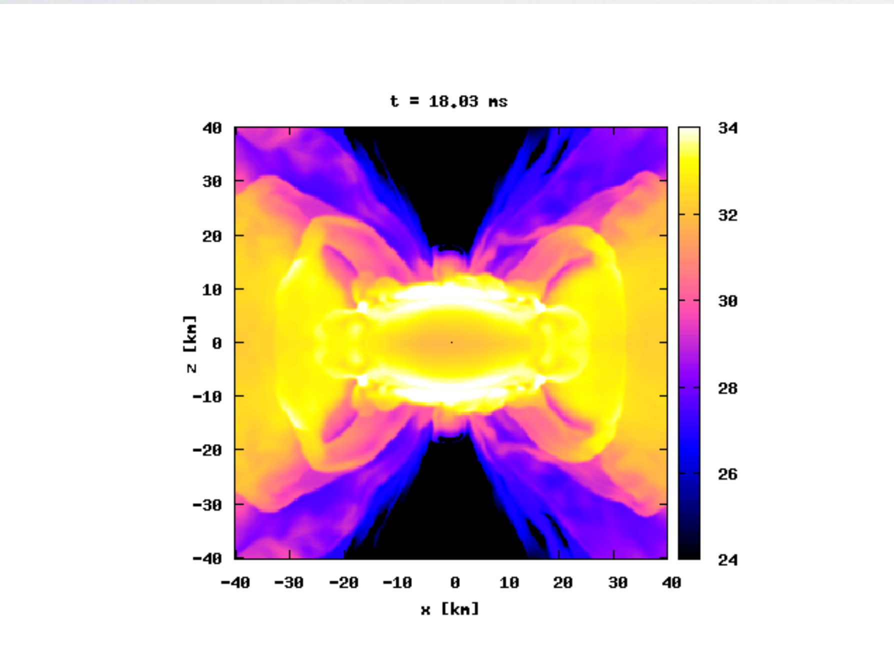


Neutron Star Merger
(Rosswog 2013)

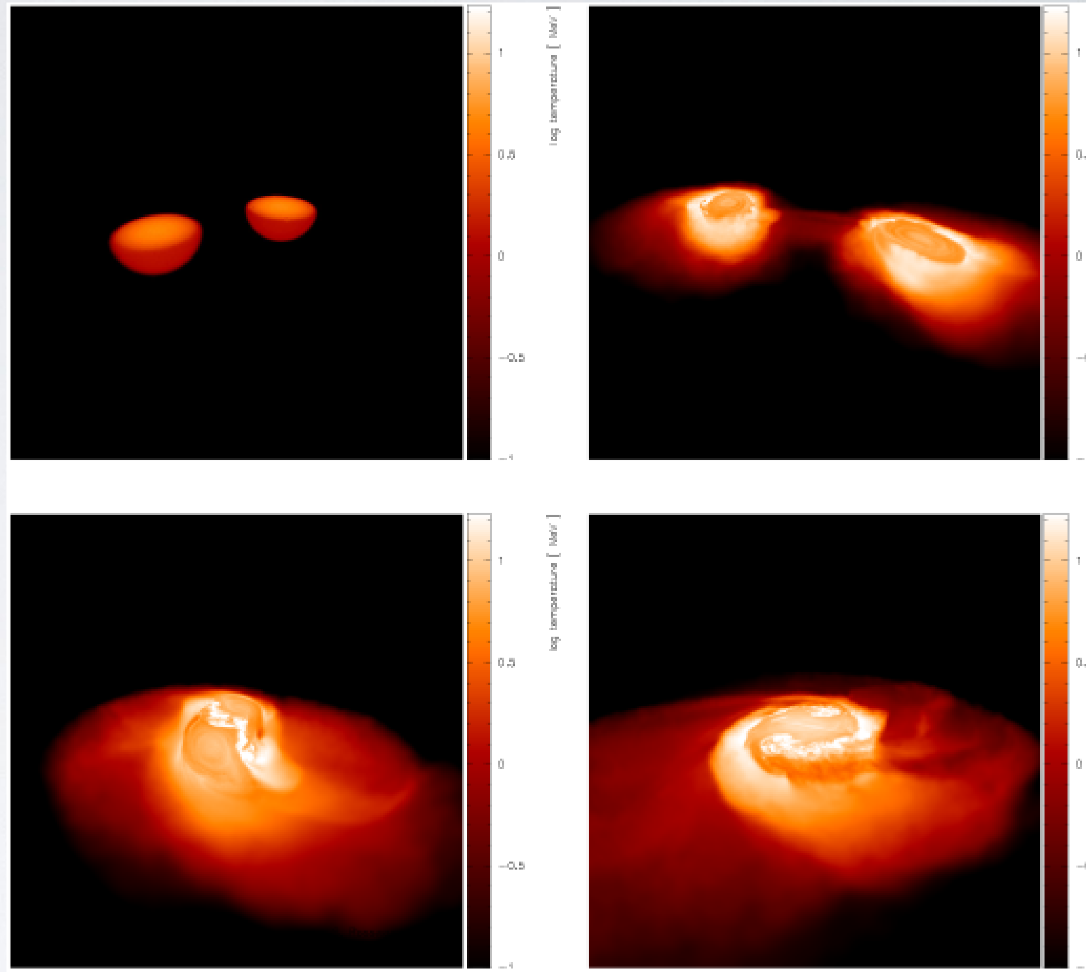
Nuclear Astrophysics

- neutron star mergers
- core-collapse supernovae

EOS
neutrino propagation
r-process nucleosynthesis

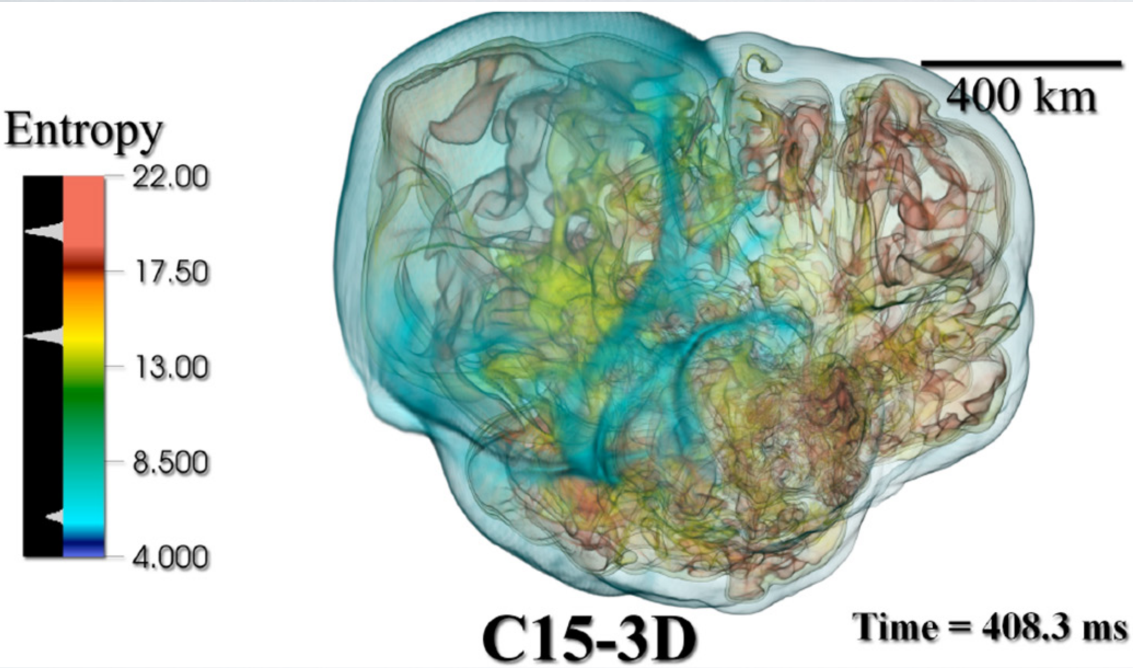


Neutrino Luminosity
Shibata, 2011

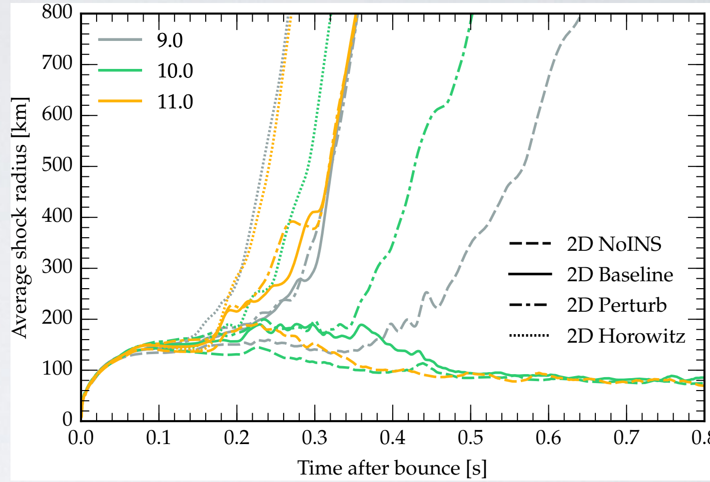


Neutron Star Merger
(Rosswog 2013)

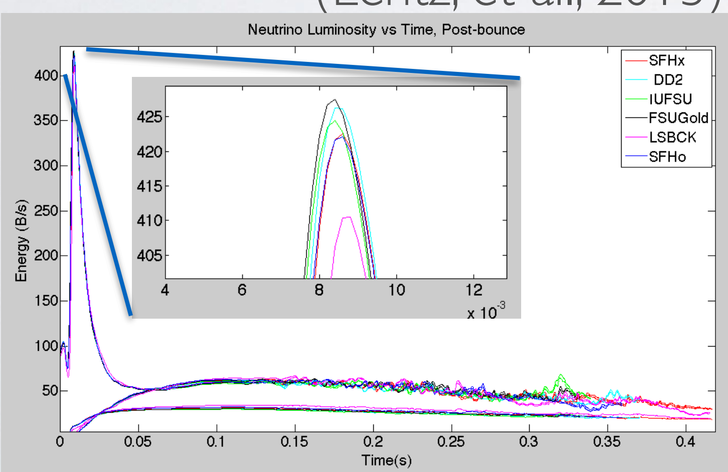
Nuclear Astrophysics: core-collapse supernovae



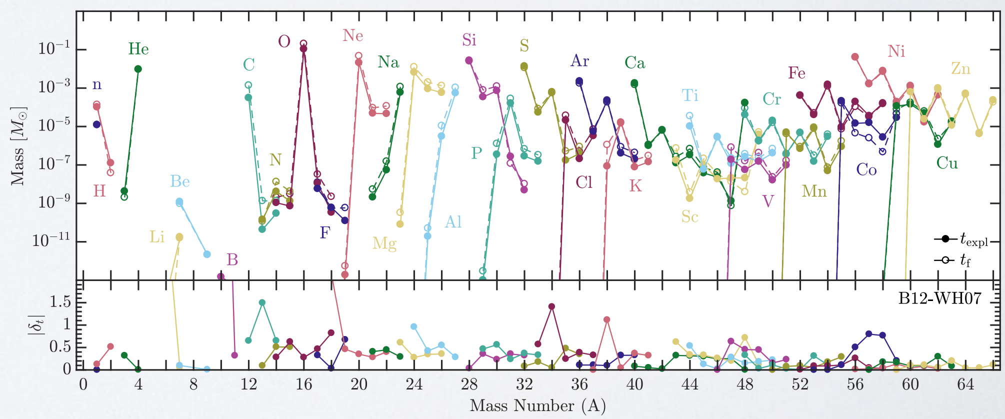
entropy in a 3D Core-collapse supernovae
(Lentz, et al., 2013)



explosion sensitivity to microphysics
(Radice, et al, 2017)

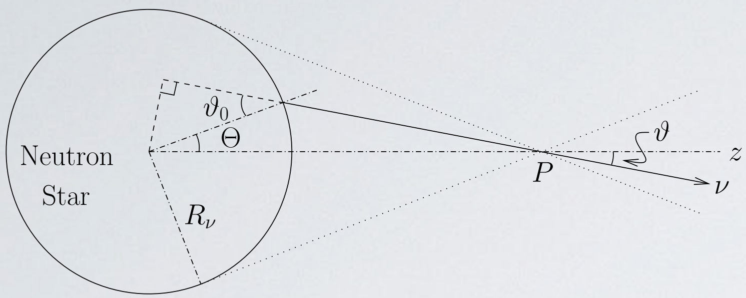


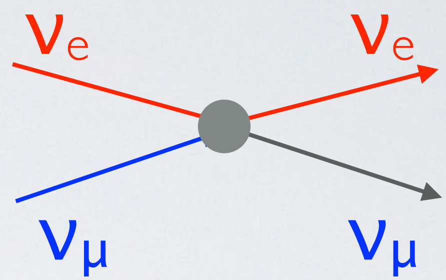
ν luminosity in neutronization burst vs. EOS
Landfield, UT thesis



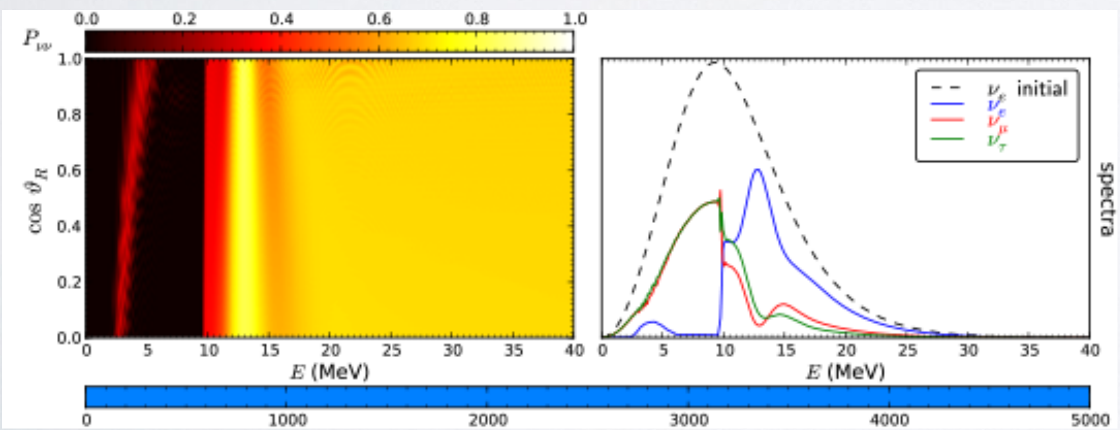
extrapolation of yields to late times
(Harris, et al., 2017)

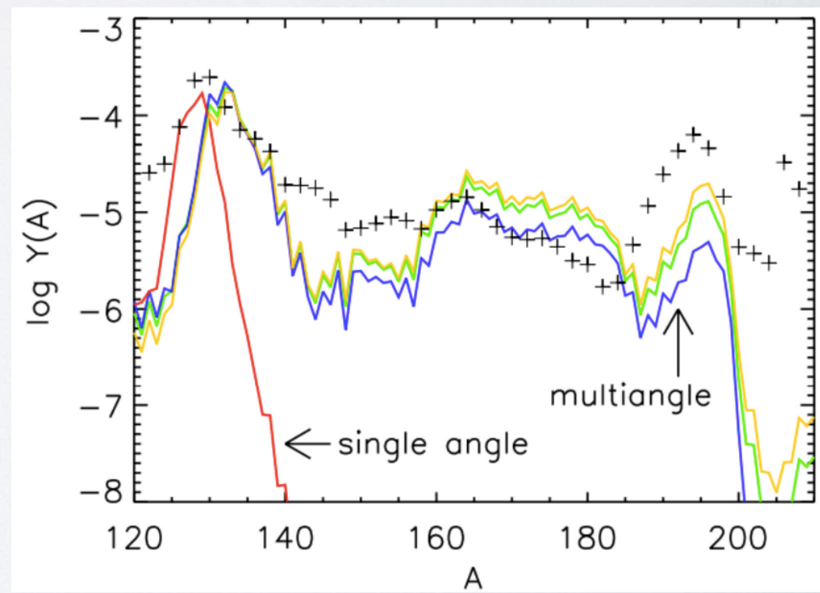
Nuclear Astrophysics: Coherent neutrino oscillations





- in early universe, NS mergers and supernovae, coherent neutrino propagation is possible
- Additional oscillations in addition to MSW-type resonances
- could impact: explosion, nucleosynthesis, …





Outlook

Nuclear physics spans a huge range of problems
exascale (classical) computing is extremely valuable

- Hot QCD
- Cold QCD
- Nuclear Structure and Reactions
- Nuclear Astrophysics

Quantum computing could have a huge impact!
many-body nuclei: limits of existence for neutron-rich
fusion of light ions
linear response (e and neutrinos)
and electroweak transitions
more general reactions

Rich future: lattice gauge theory (hot, cold, dynamics)
nuclear fission, full quantum dynamics
neutrino coherence and decoherence