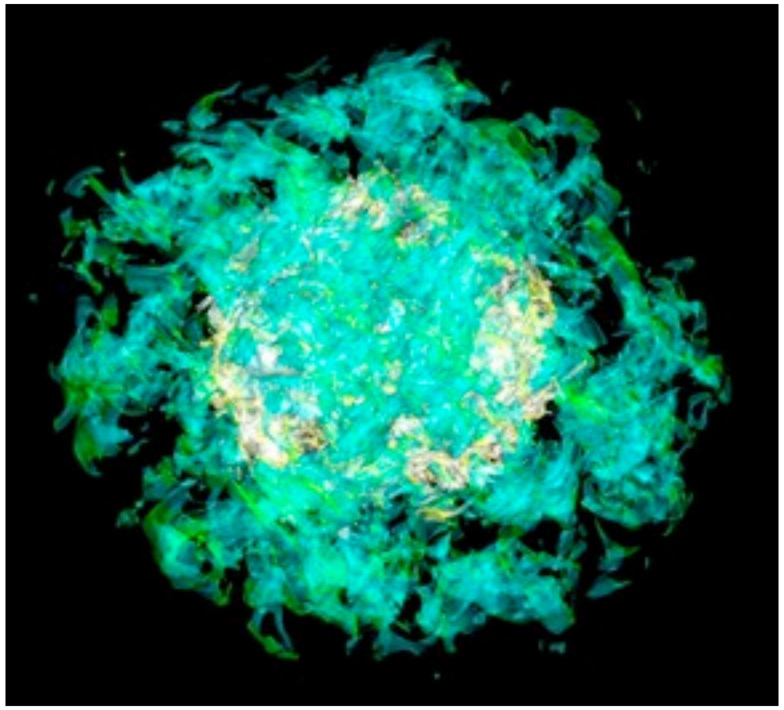
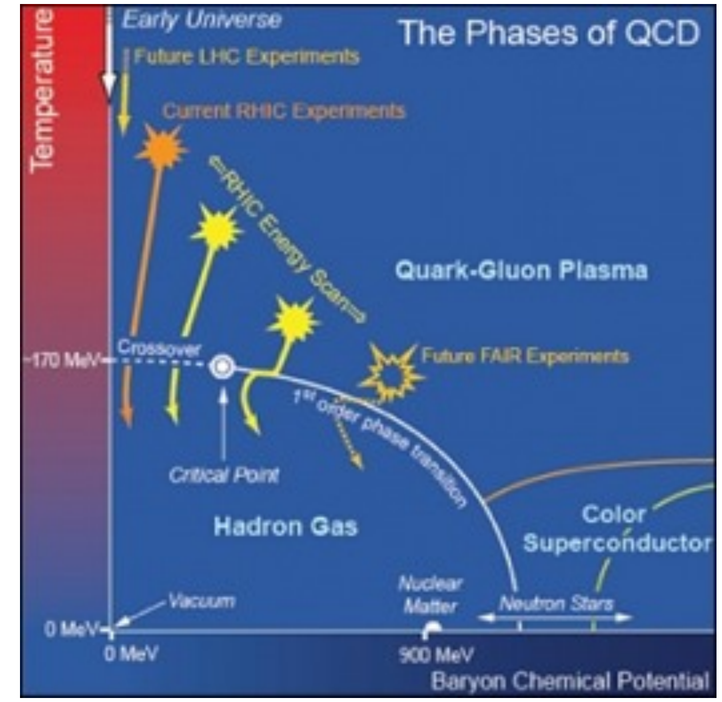
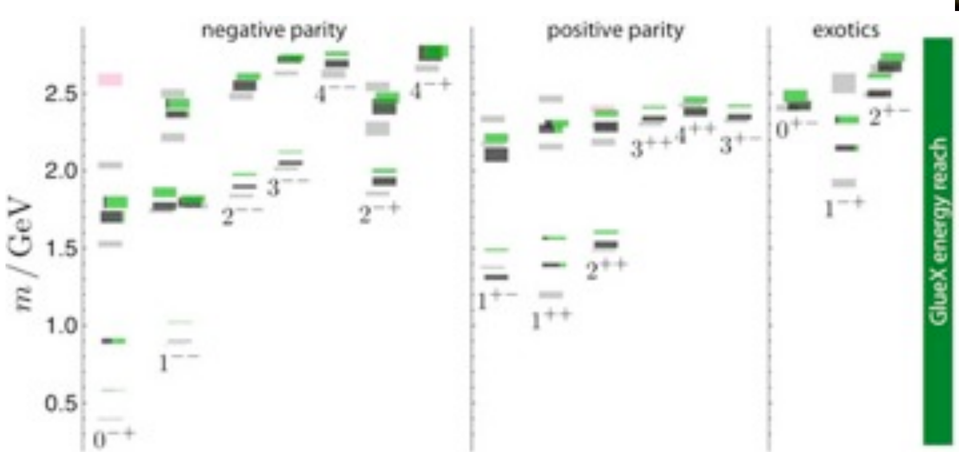
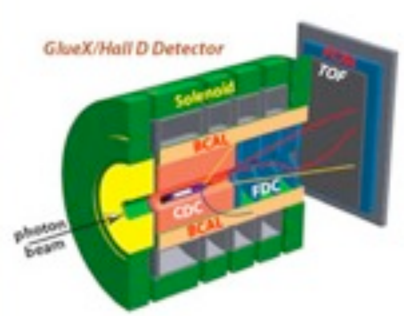
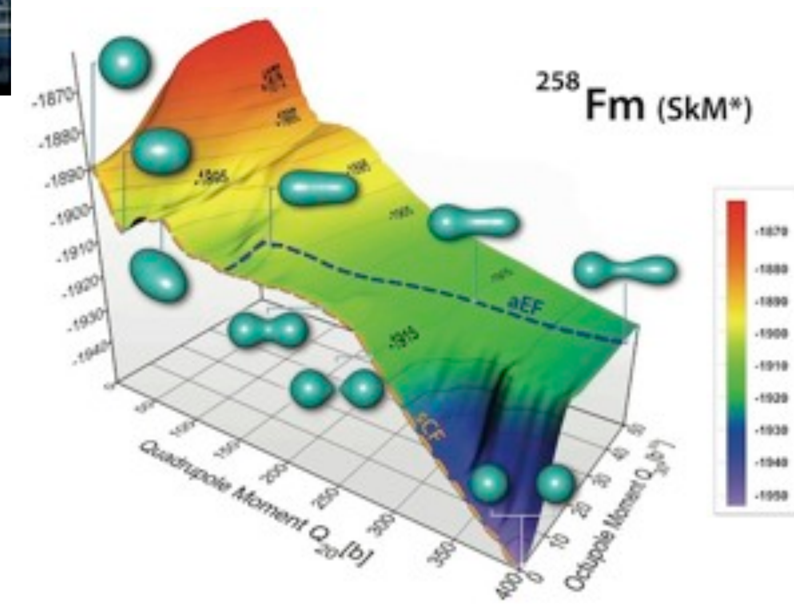





# Extreme Computing Trilogy: Nuclear Physics


Martin J. Savage
University of Washington

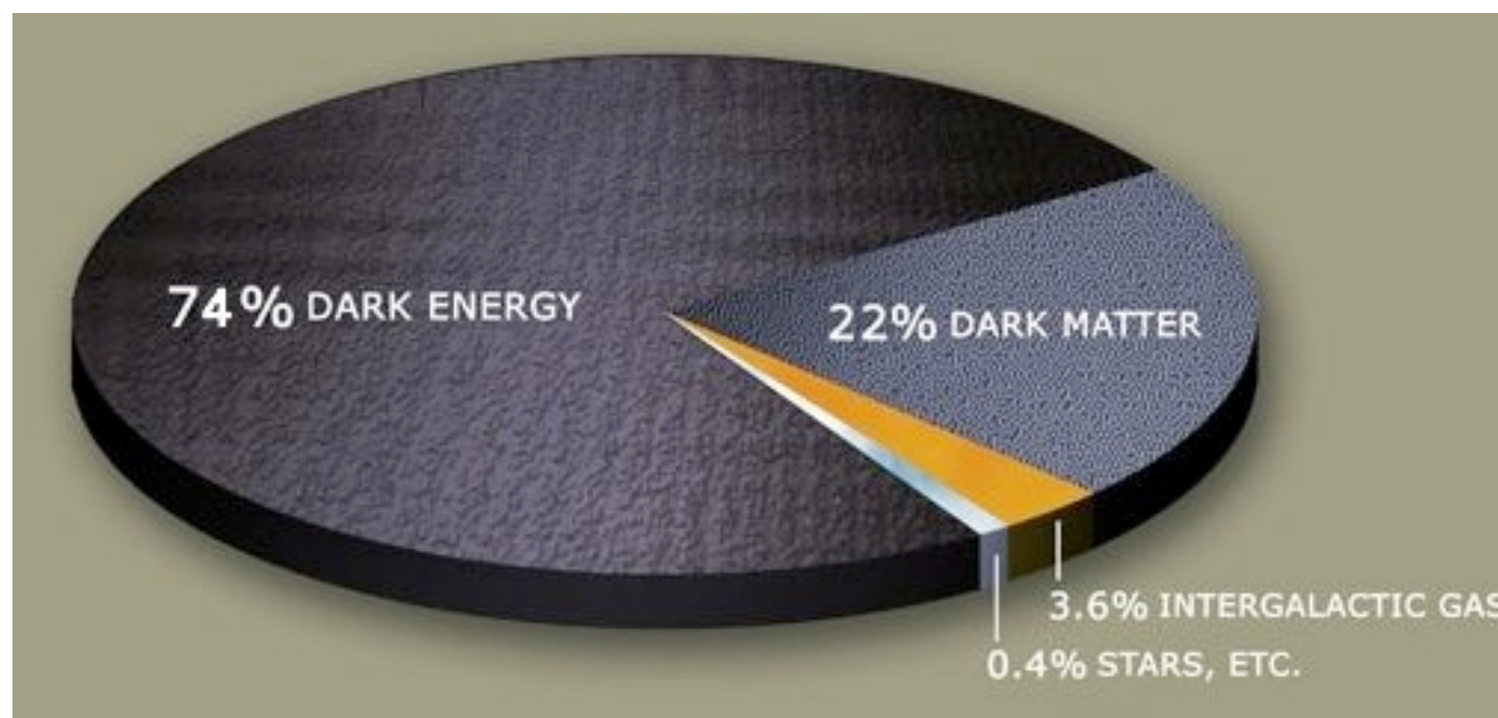

**August 2012,**
**Lattice Summer School**

Computational Nuclear Physics

# Nuclear Physics Research

Unraveling the Origin and Nature of the Visible Matter ⟷ Nuclear Physics

Nuclear Physics ↑ Quantum Chromodynamics Electroweak Interactions

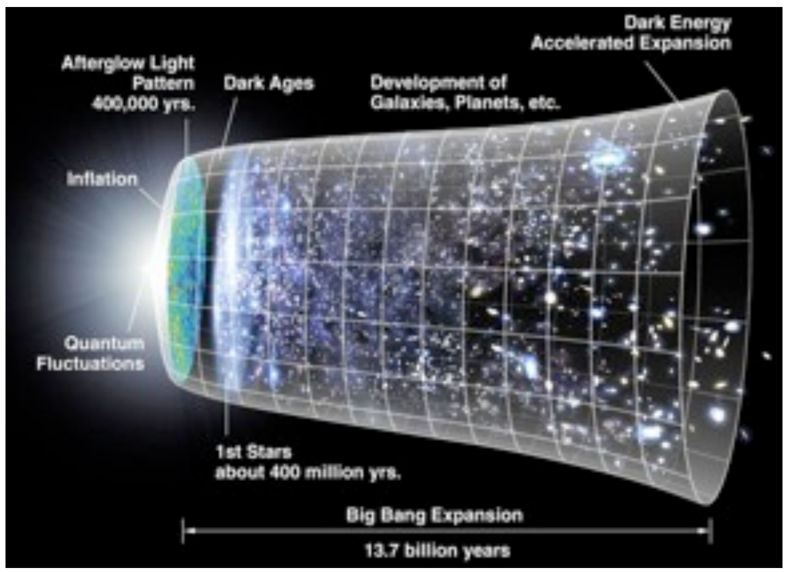



Establishing and verifying the capability to reliably predict

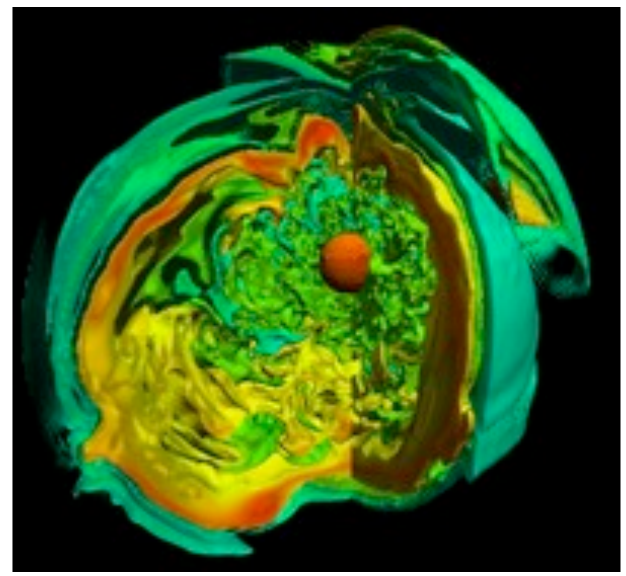
Computational Nuclear Physics

# A Broad and Balanced Nuclear Physics Agenda

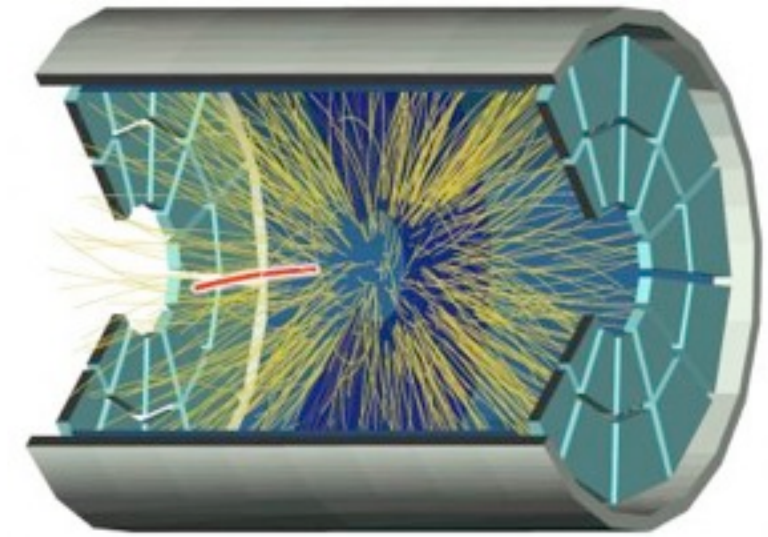
Phase transition(s) at early times, light sources at later times



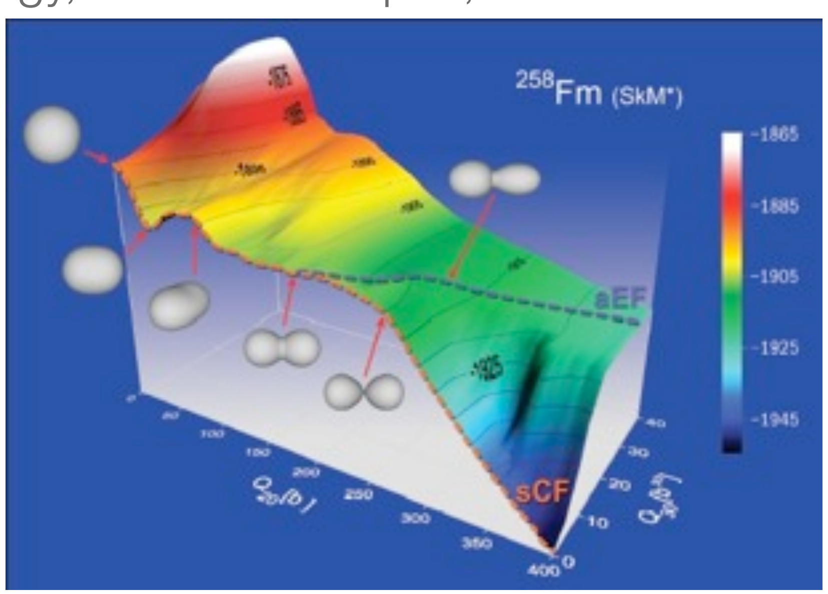

Production of most elements in the cosmos



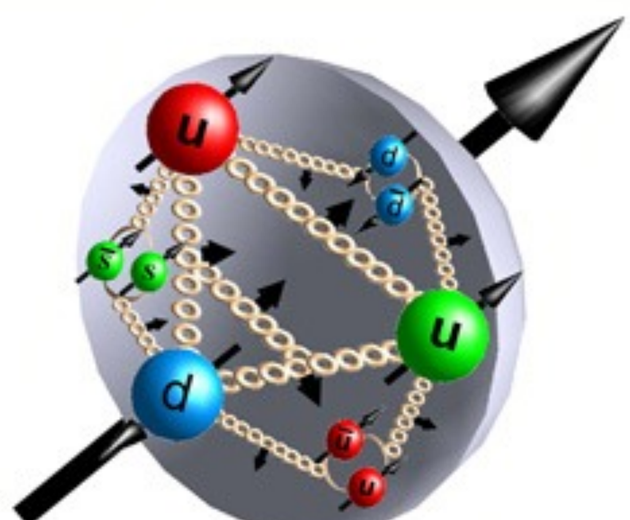
Matter under extreme conditions



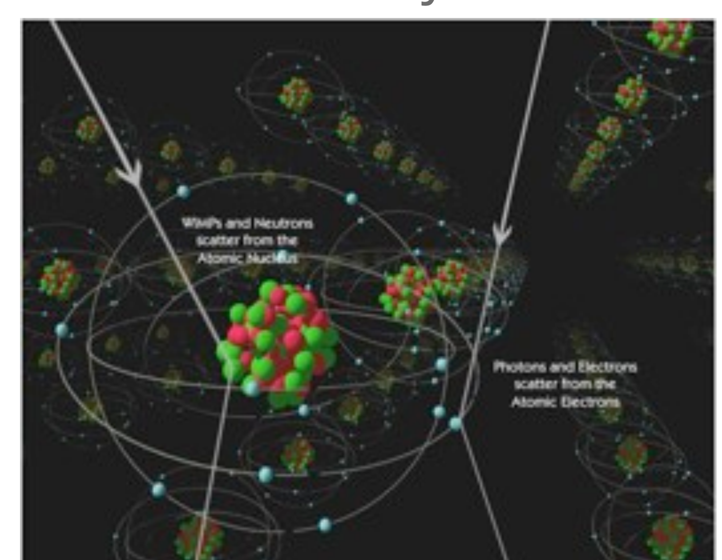
Nuclei and their reactions:
Energy, Medical Isotopes, National Security,...




The structure of, and forces between, nucleons




Search for New Physics




Enormous range of length scales involved !

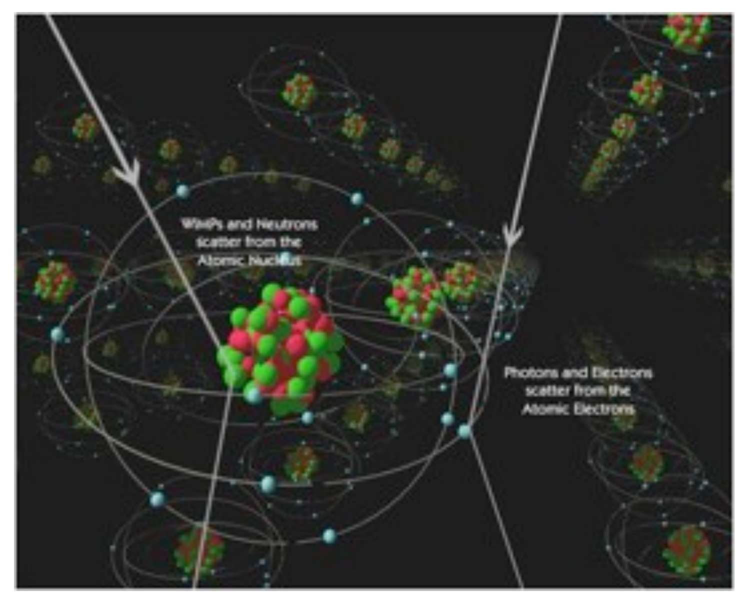
# Nuclear Physics is Diverse in Application and Impact

Proton Therapy

Radiation Detection

Training Future Generations

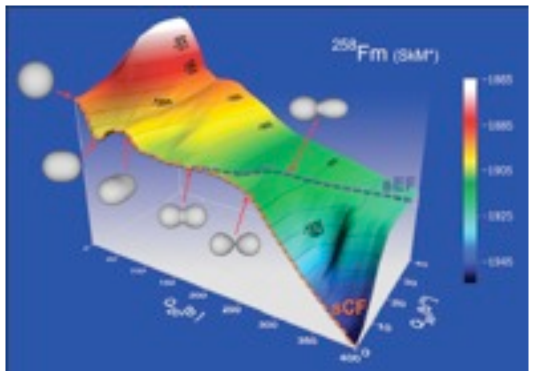
NMR
(Magnetic Resonance Imaging)

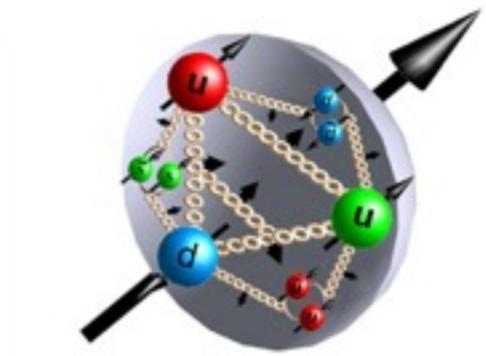


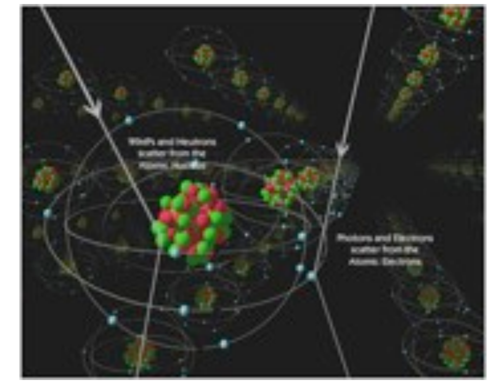

Search for New Physics,
e.g. dark matter, neutrino properties

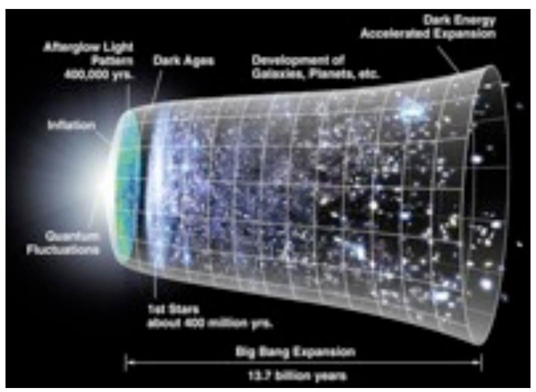
**Computational Nuclear Physics**

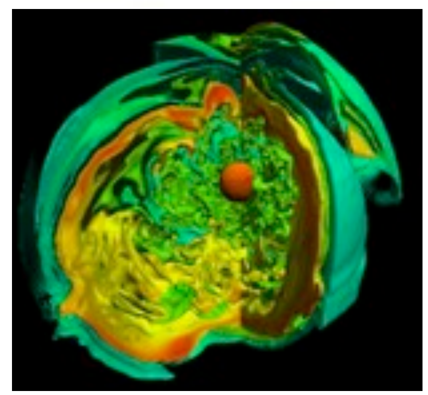
# Computing is Essential in Nuclear Physics Research

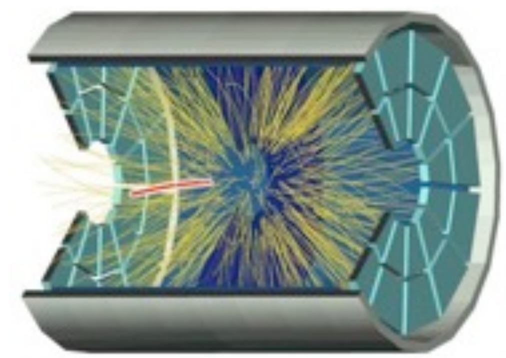










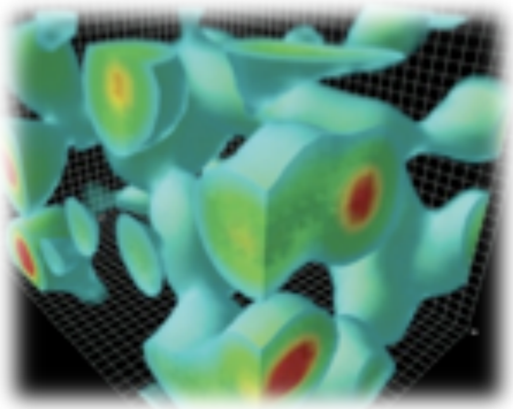


**Experiment**

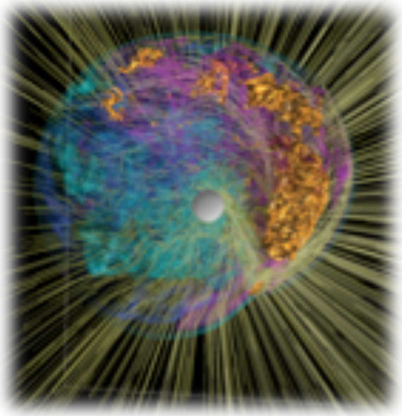
**Human Creativity**

**Computation**

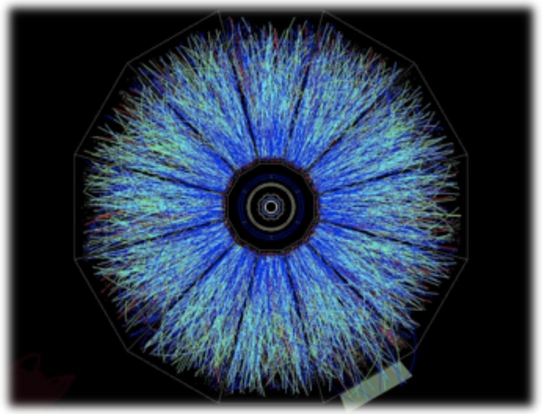
# Nuclear Physics HPC Thrusts



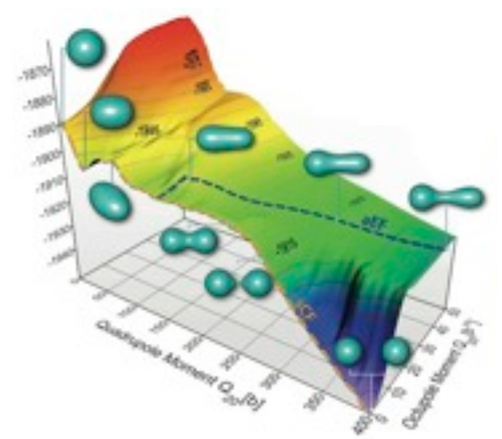
Cold QCD
(lattice QCD)



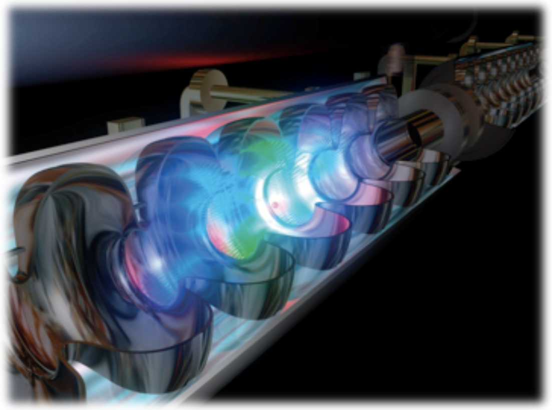
Astrophysics



Hot QCD

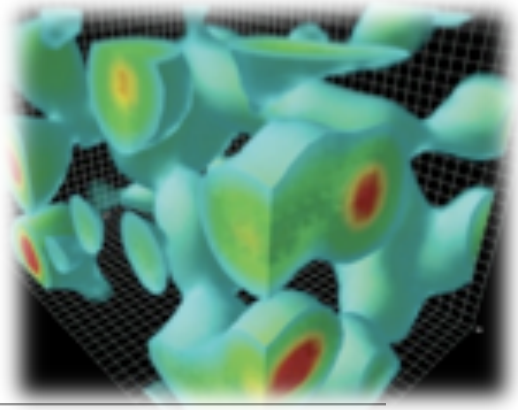


Nuclear Structure
and Reactions

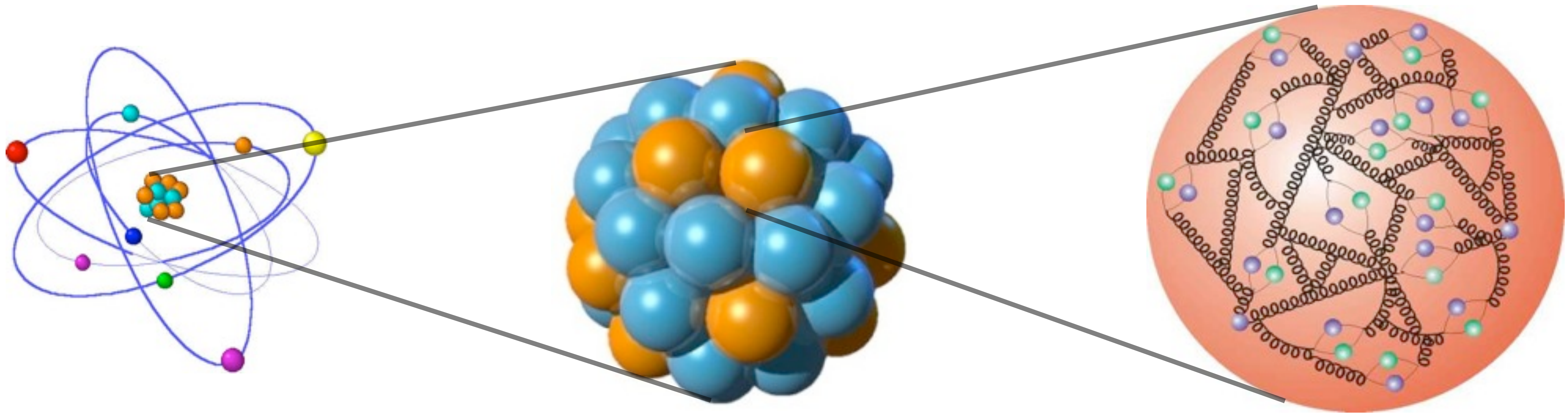


Accelerators

# At the Heart of Visible Matter



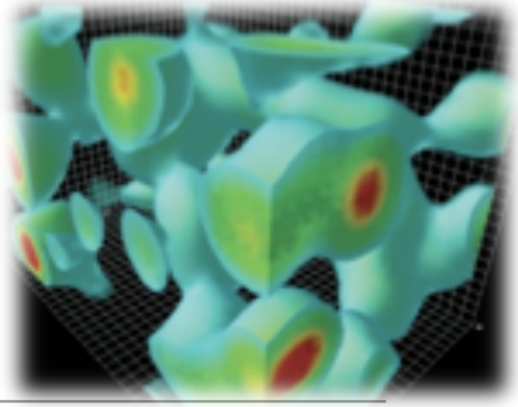
Atom | Nucleus | Proton

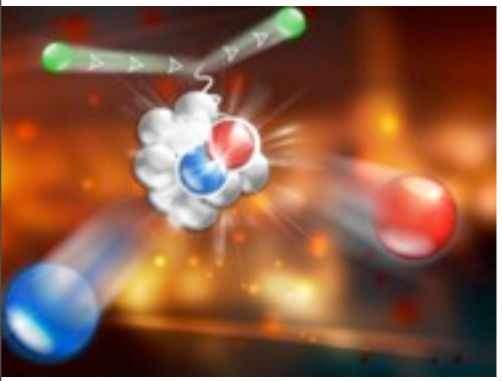


Electrons and Nuclei | Protons and Neutrons | Quarks and Gluons

## Quantum Chromodynamics

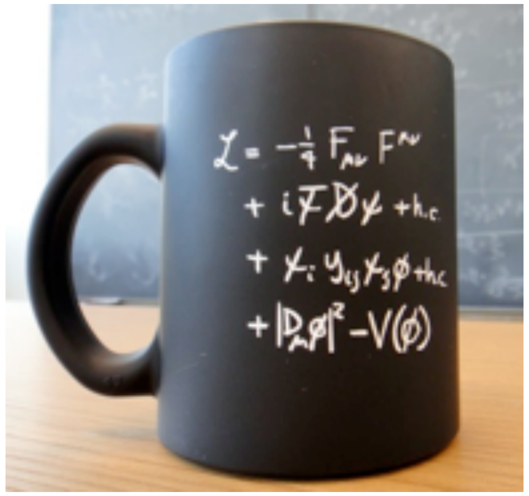
# Quantum Chromodynamics:
# The Underlying Theory of Nuclear Physics





Experiment

Thinking




QCD

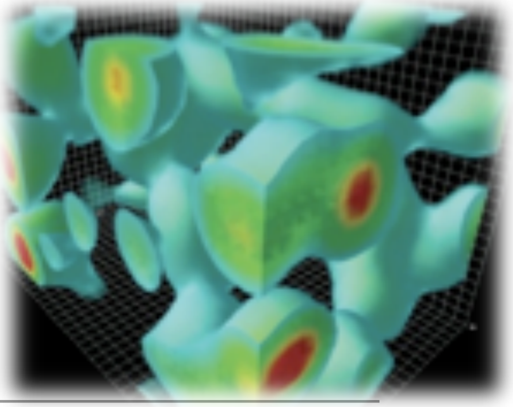
Experiment

electric charges ↔ color charges

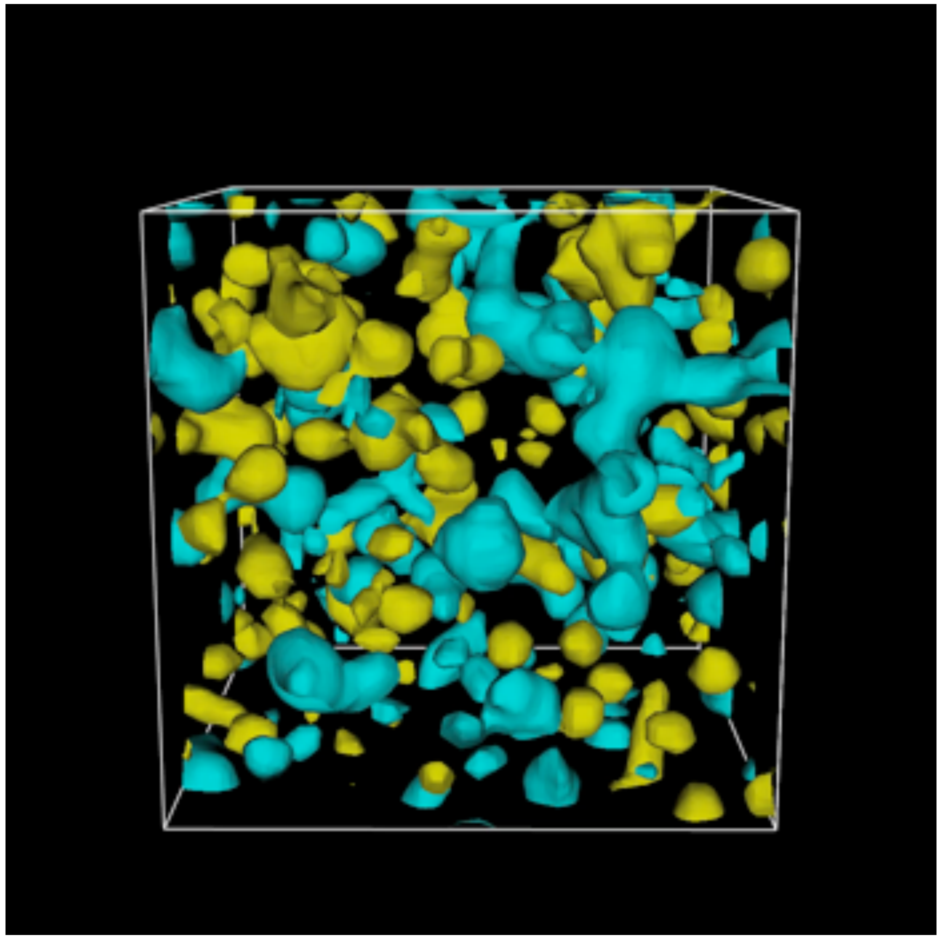
EM waves ↔ Excited Glue

QCD is Non-Linear
and essentially Quantum

# Quantum Fluctuations and Quark and Gluon Confinement



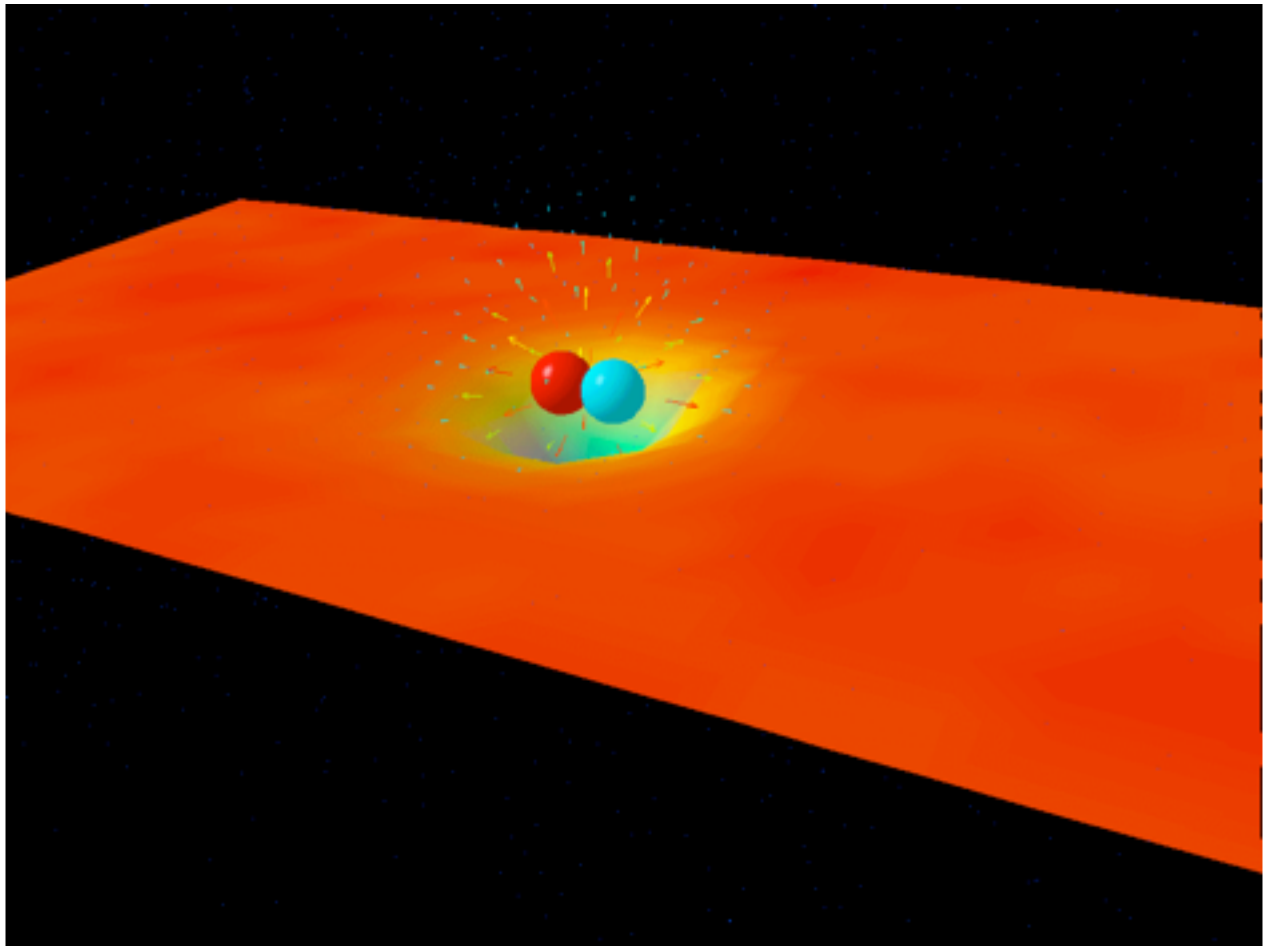
$F \sim 2 \times 10^5$ N



**The Quantum Vacuum**

**Topological Charge Density**

**(Massimo DiPierro)**



**Gluon Energy Density**

**Flux-Tubes between color charges**

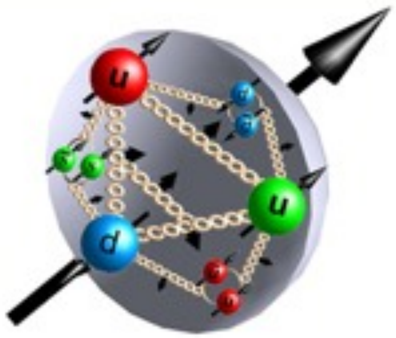
**(Derek Leinweber)**

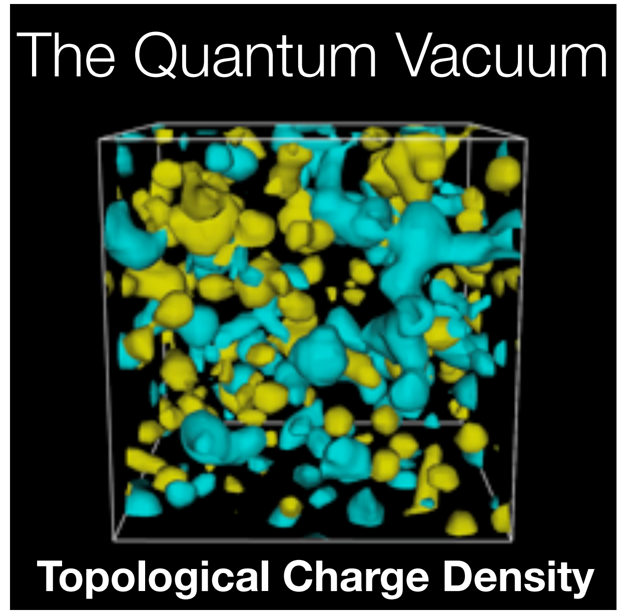
Computational Nuclear Physics

# Cold QCD

## Nature is finely tuned

capacity
resources

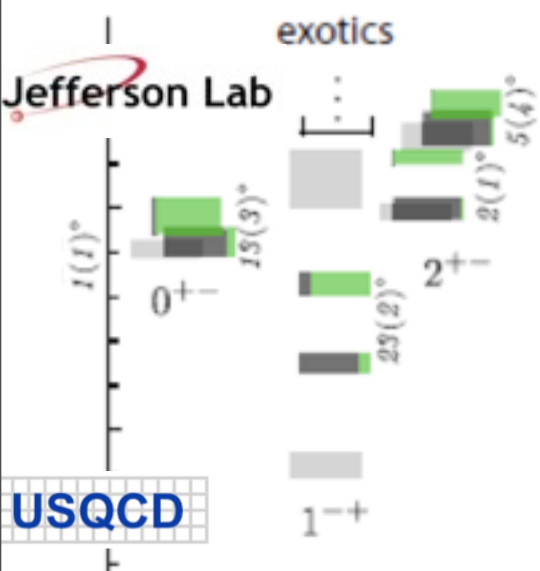


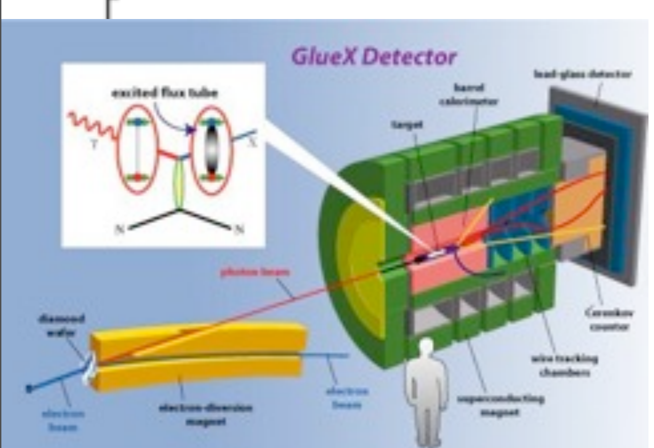


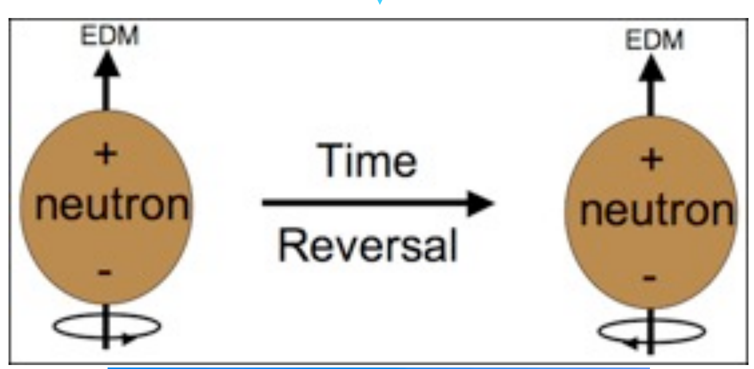

(Massimo DiPierro)

capability
resources

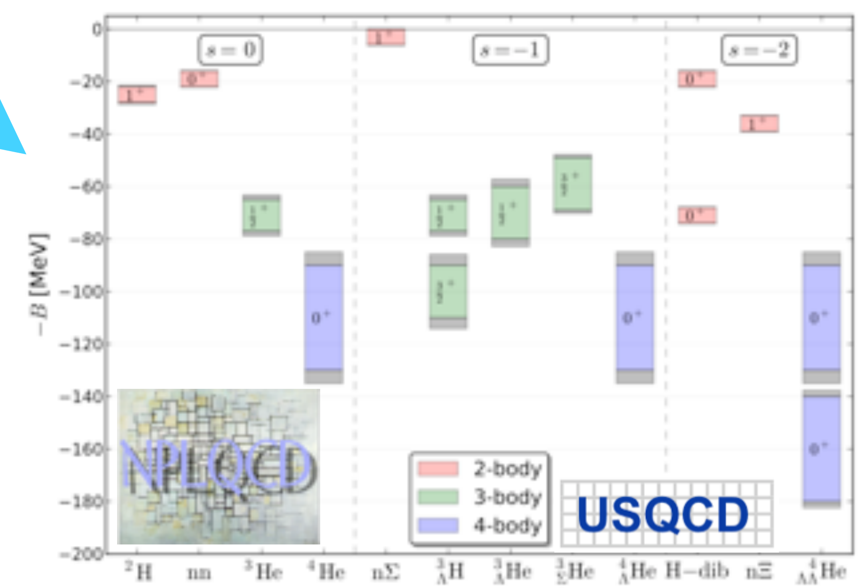
$$L \sim 4 \text{ fm}$$
$$\Delta t \sim 6 \times 10^{-24} \; s$$



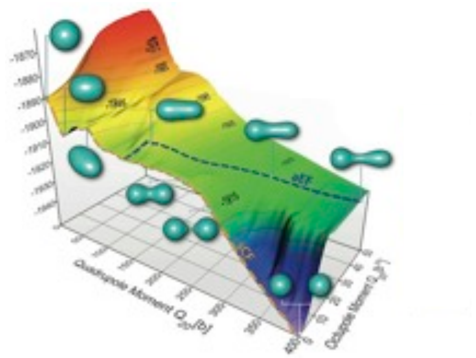



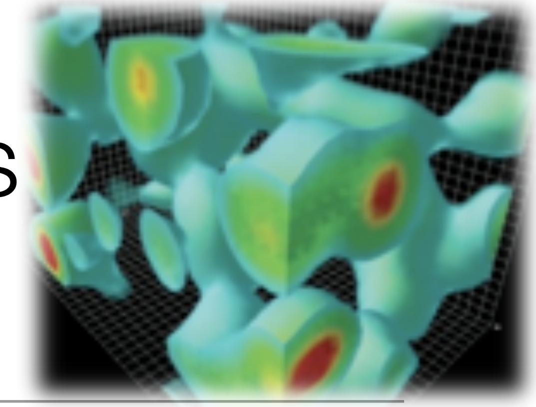



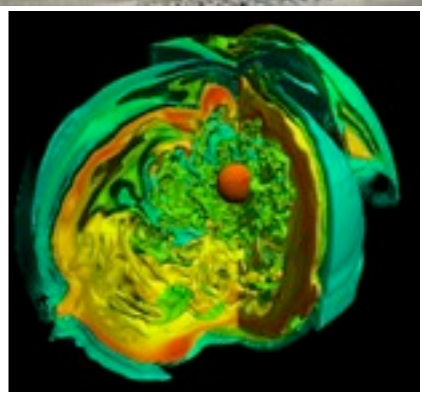

capacity
resources

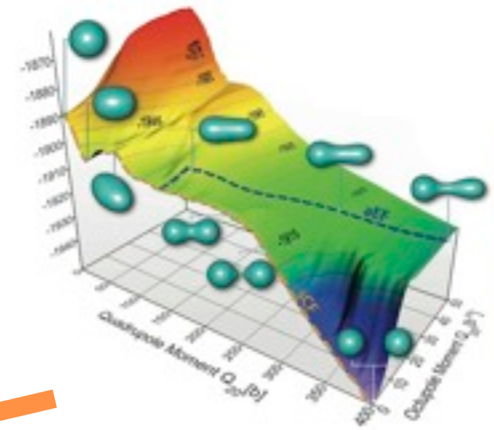


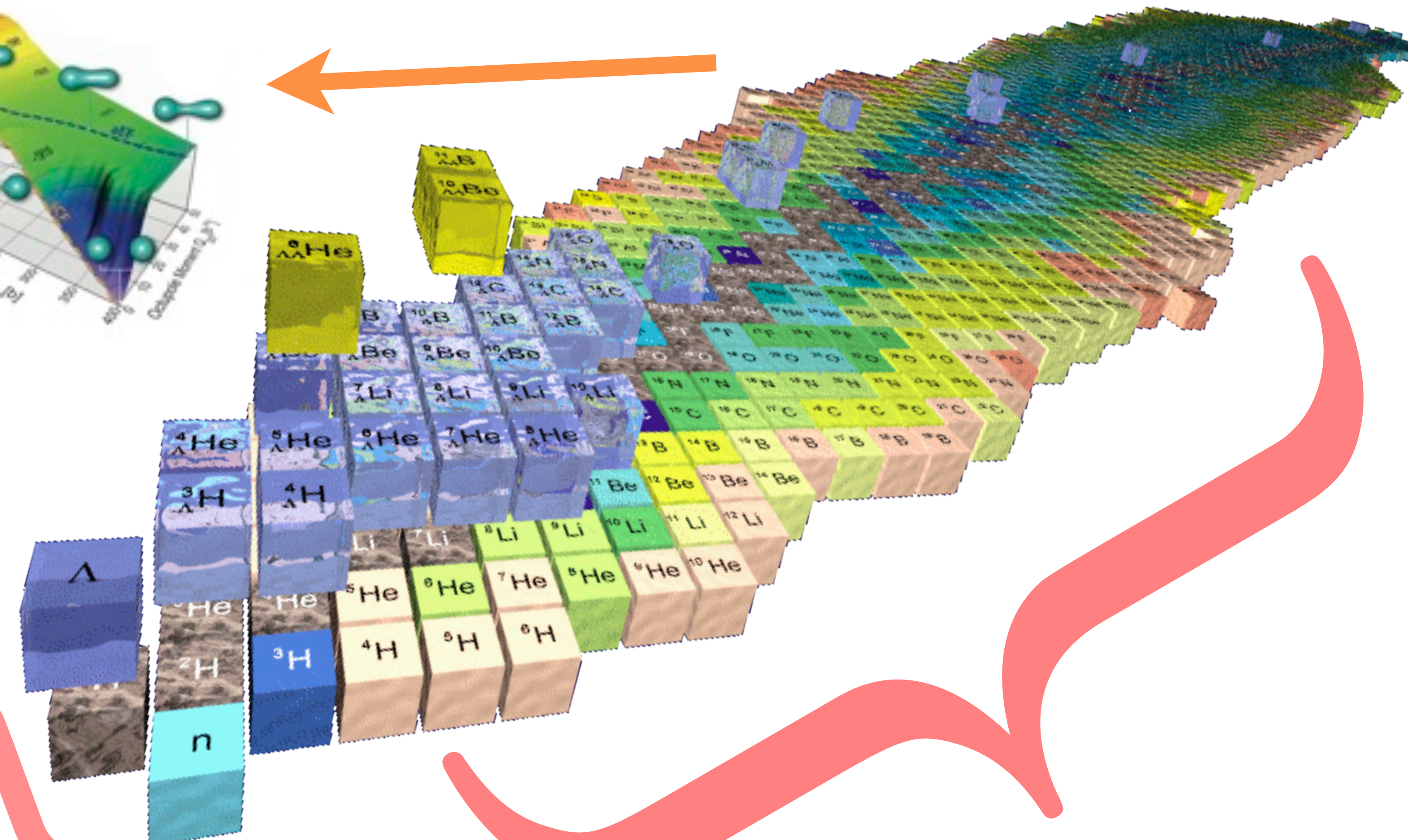

# ( Partial ) Unification of Nuclear Physics - Quantifiable Uncertainties

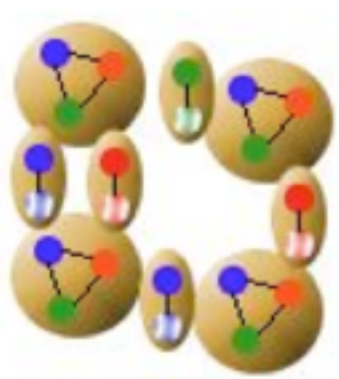




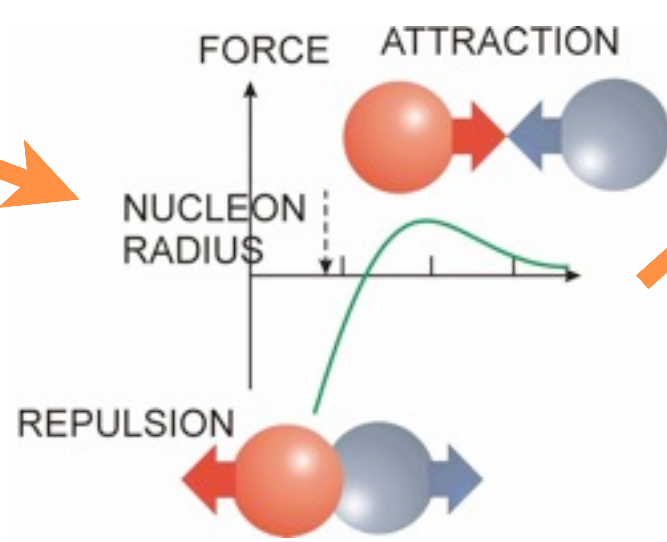






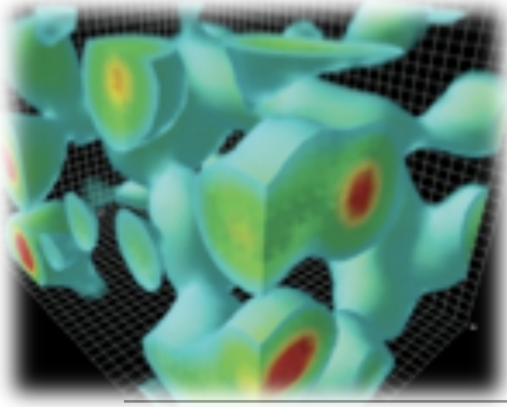


Solve QCD

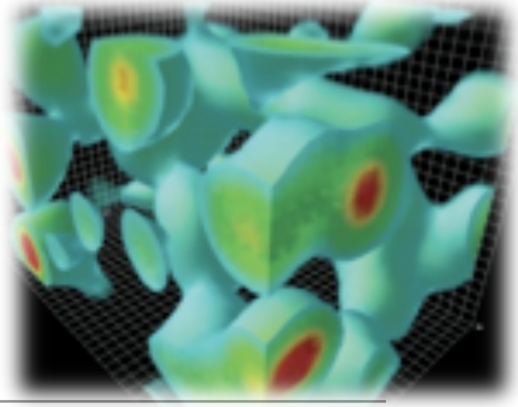


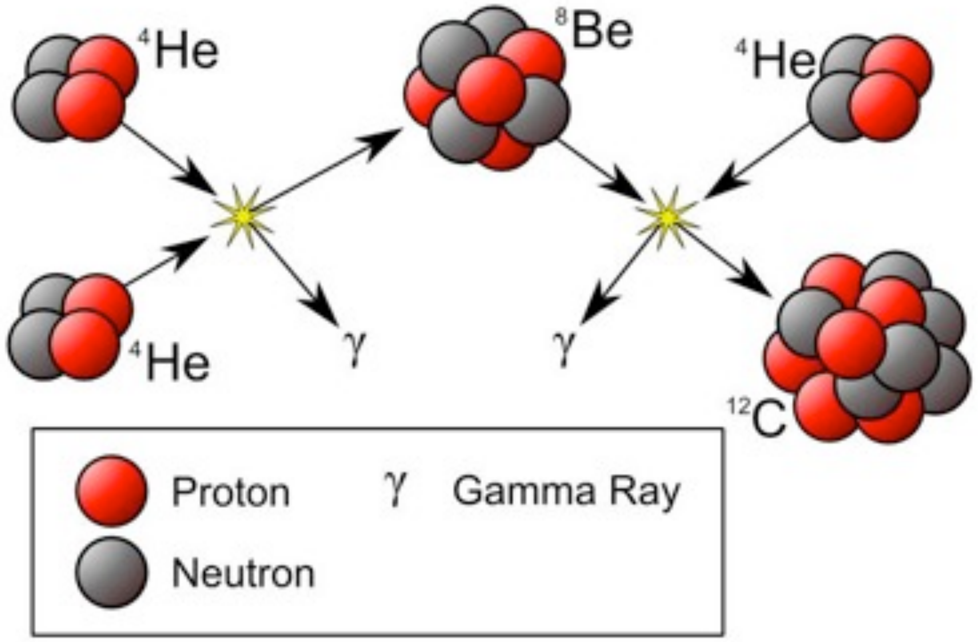

**Many-Body Methods**
**EFT, LatticeEFT,**
**GFMC, NCSM**

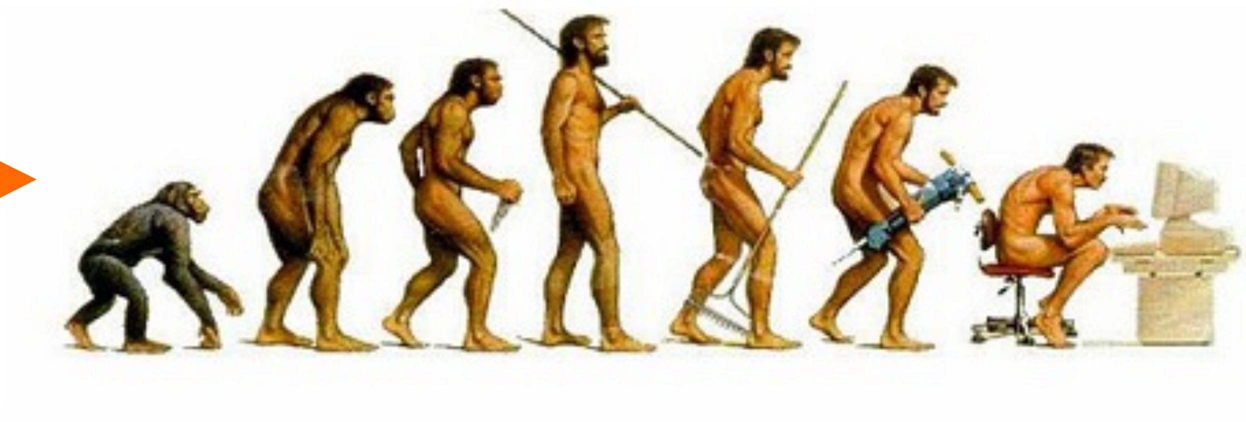
Predictions with Quantifiable Uncertainties



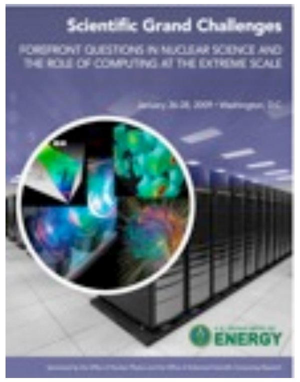
# Fine-Tunings define our Universe



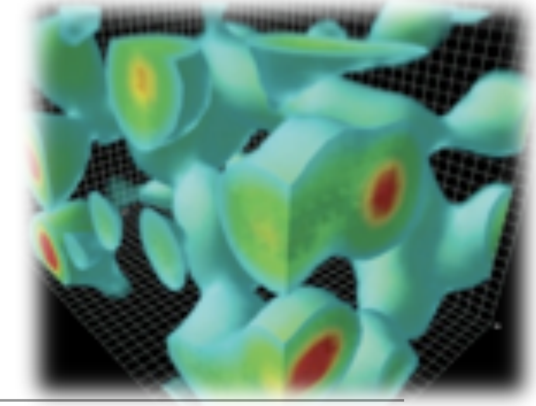



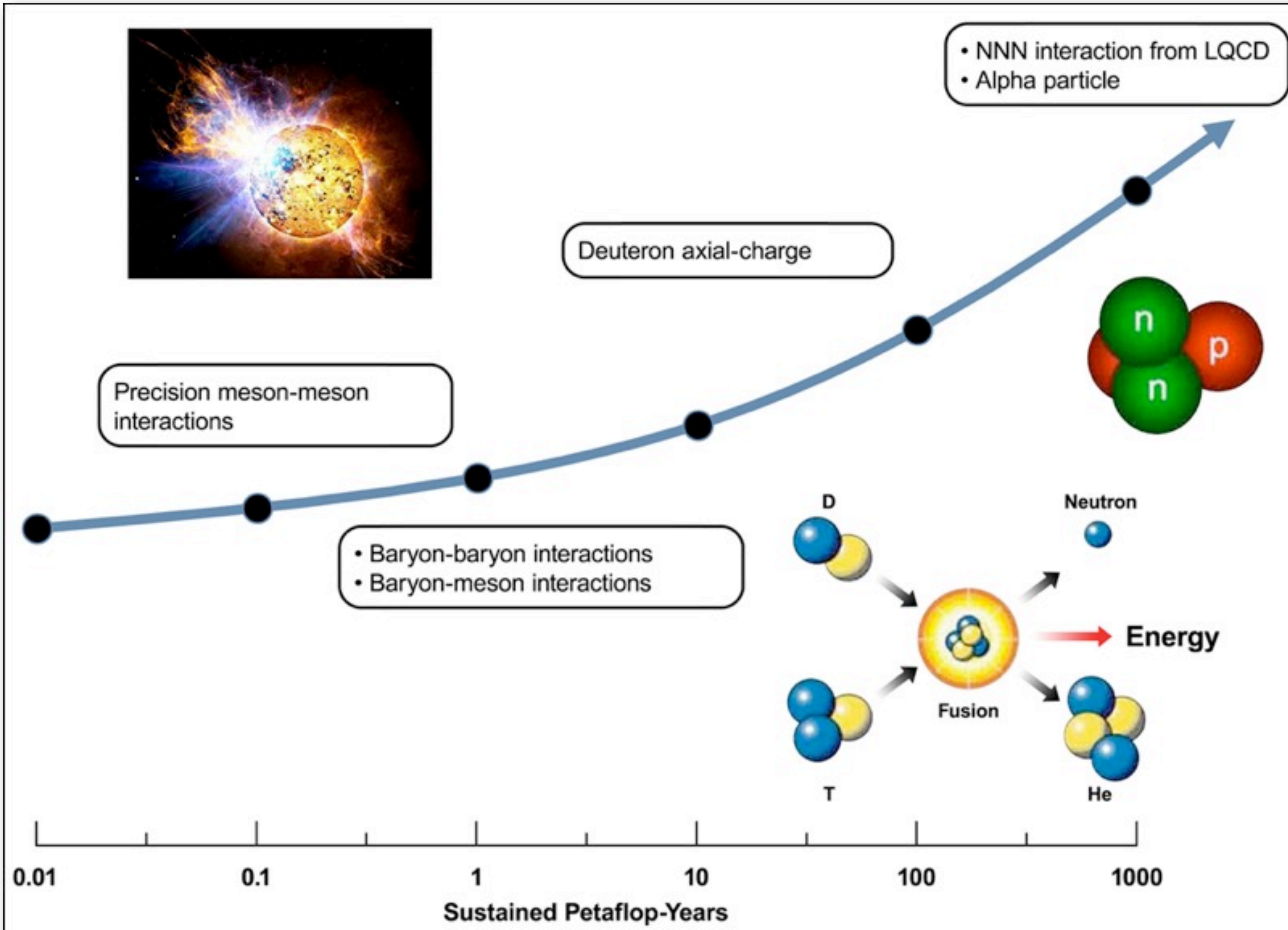
- Nuclear physics exhibits fine-tunings
  - *Why ??*
  - *Range of parameters to produce sufficient carbon ?*

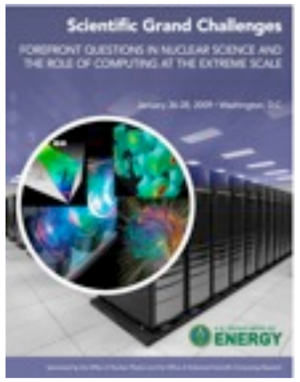



# Computational Requirements

## From QCD to Nuclei

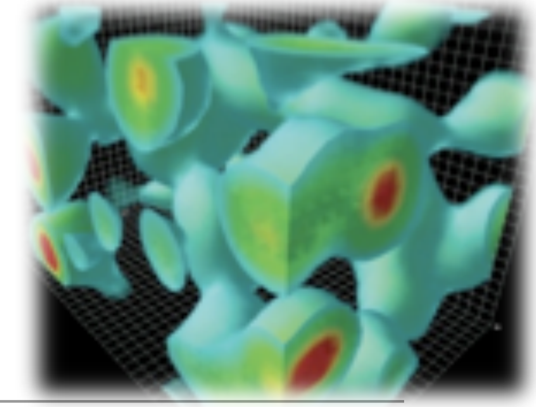


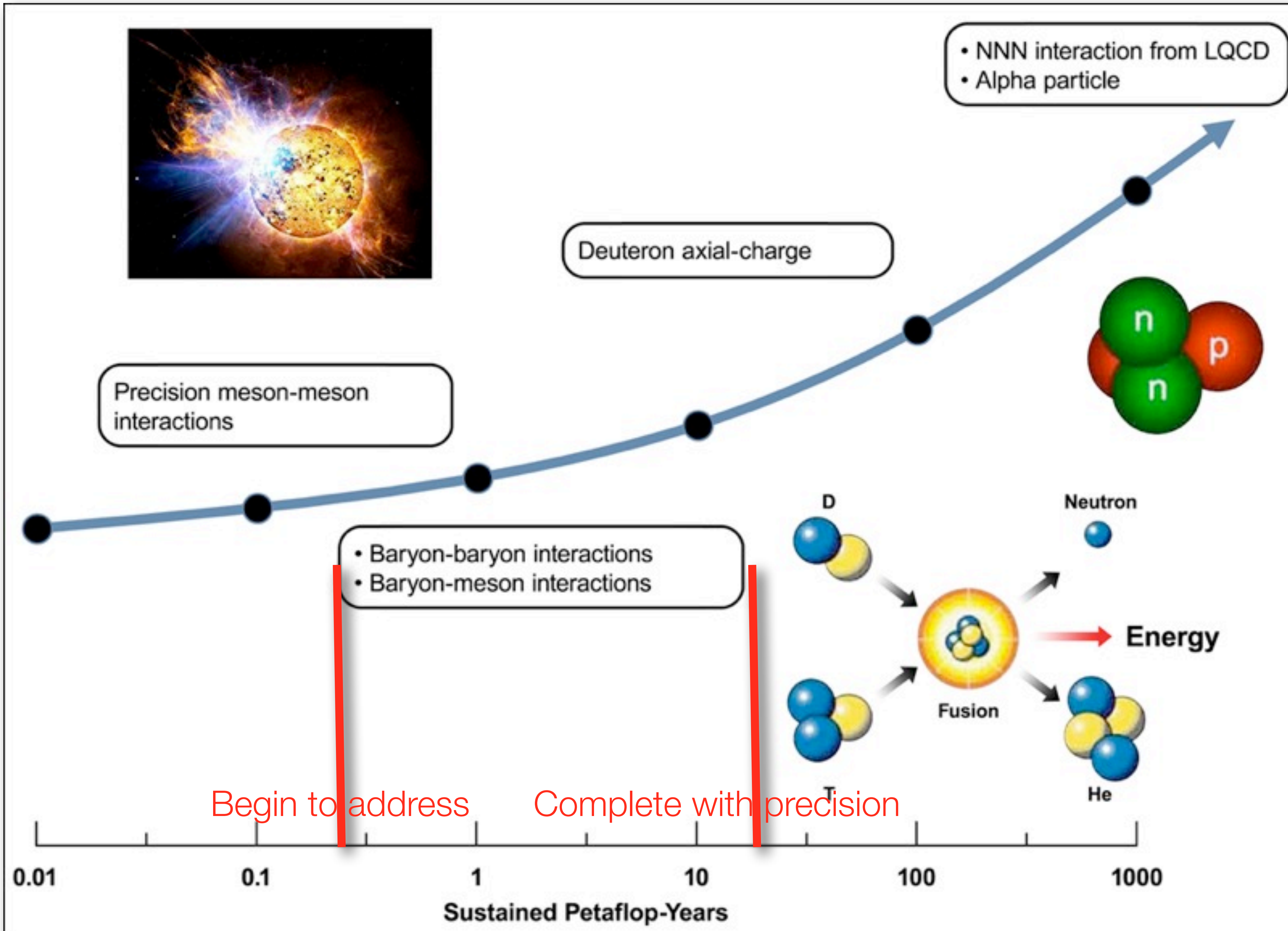




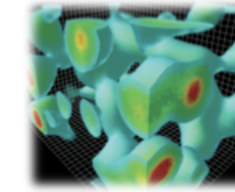

# Computational Requirements

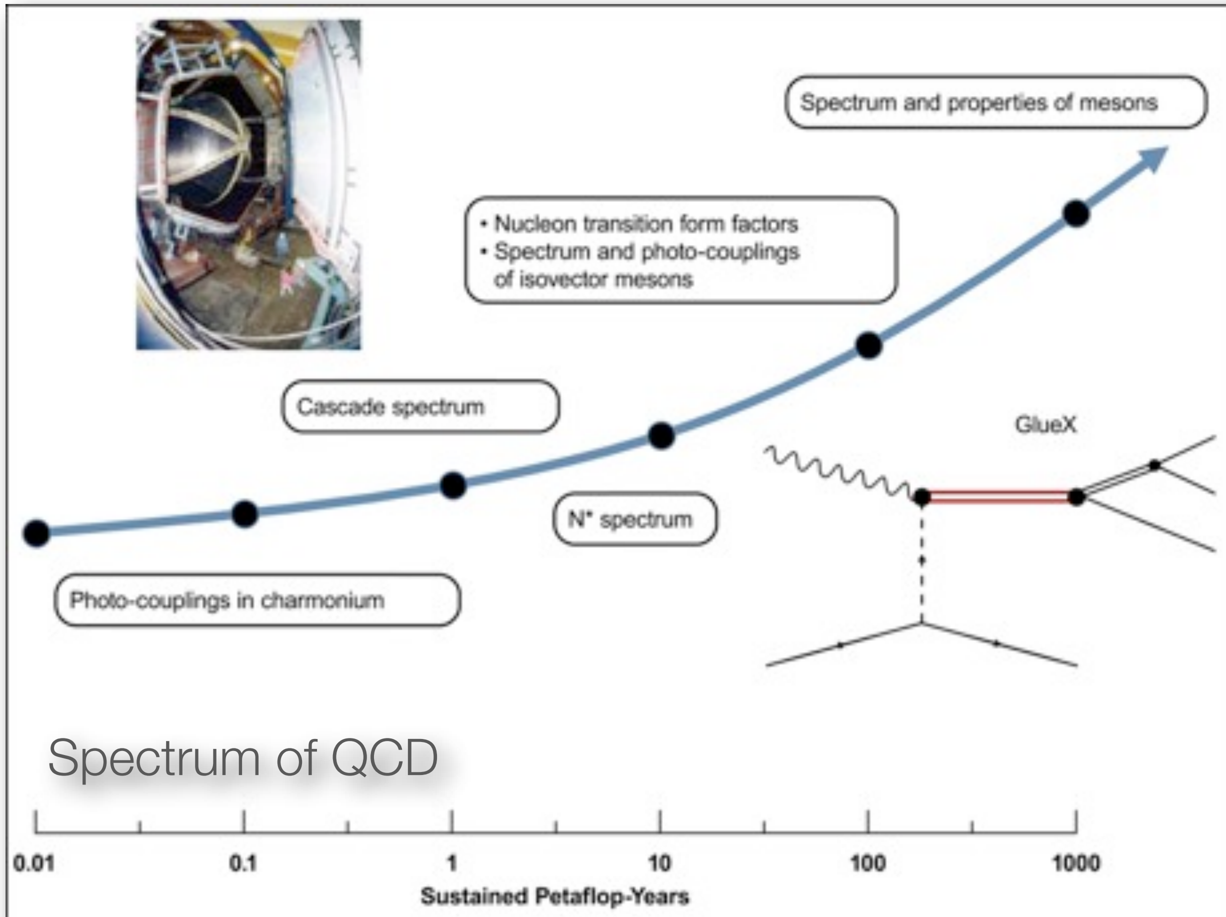
## From QCD to Nuclei

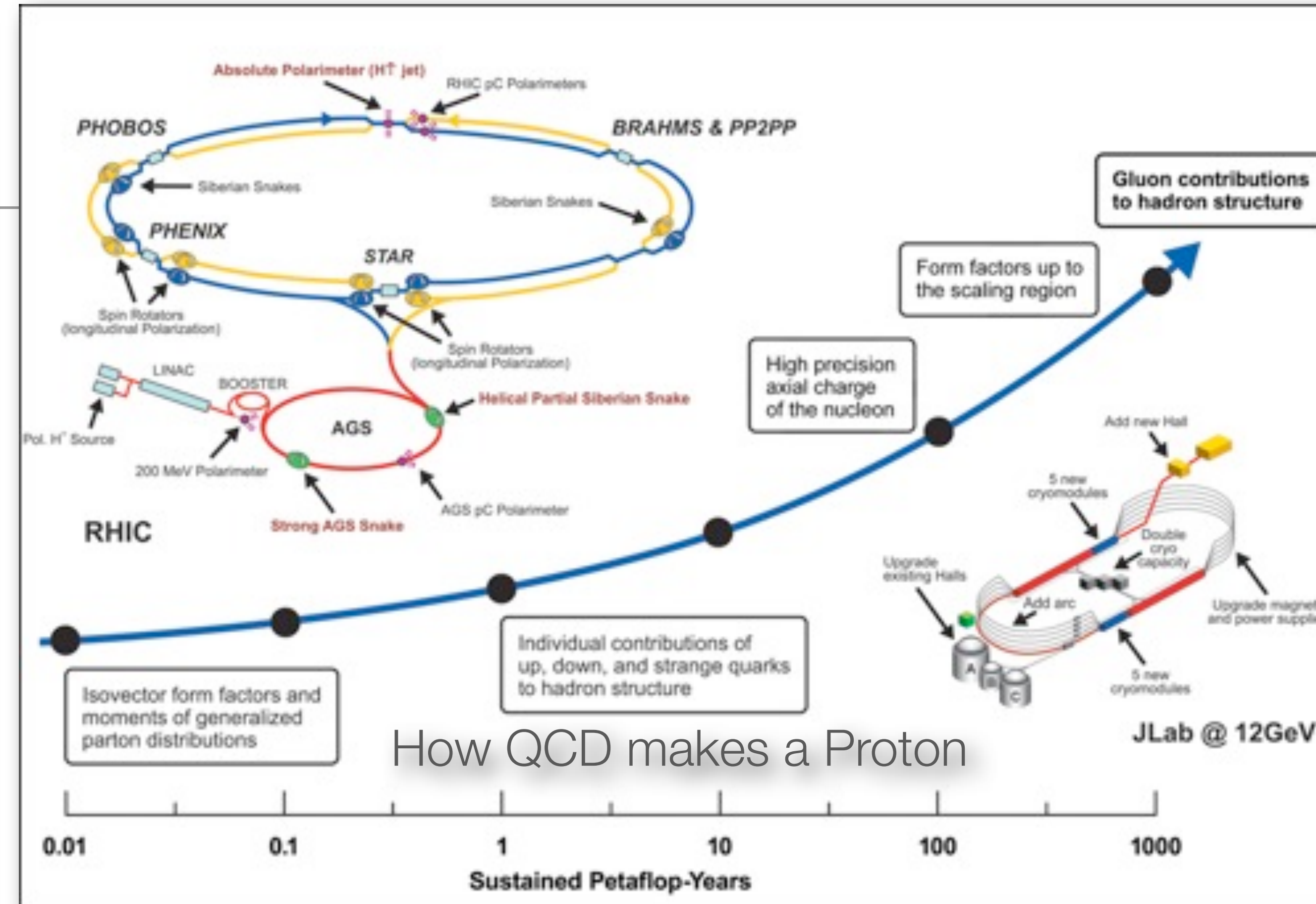


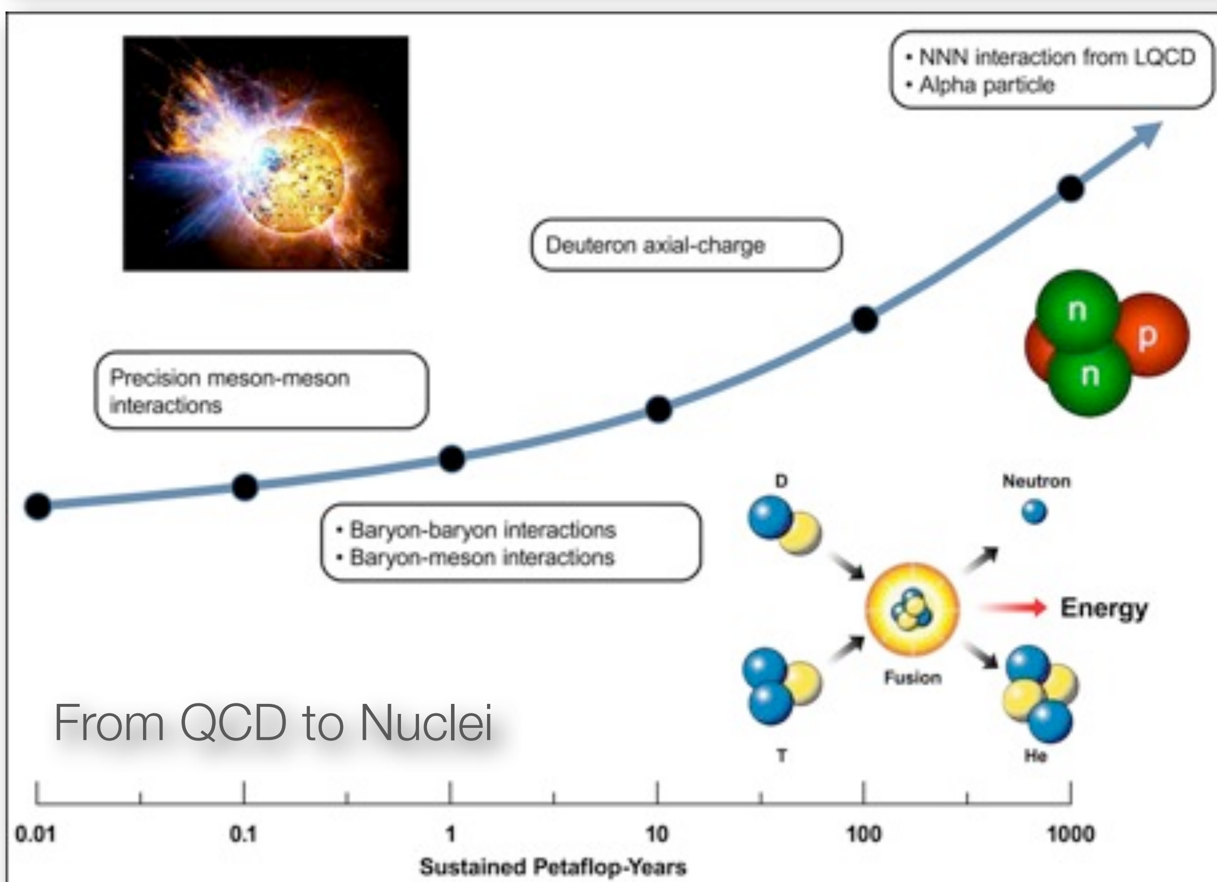


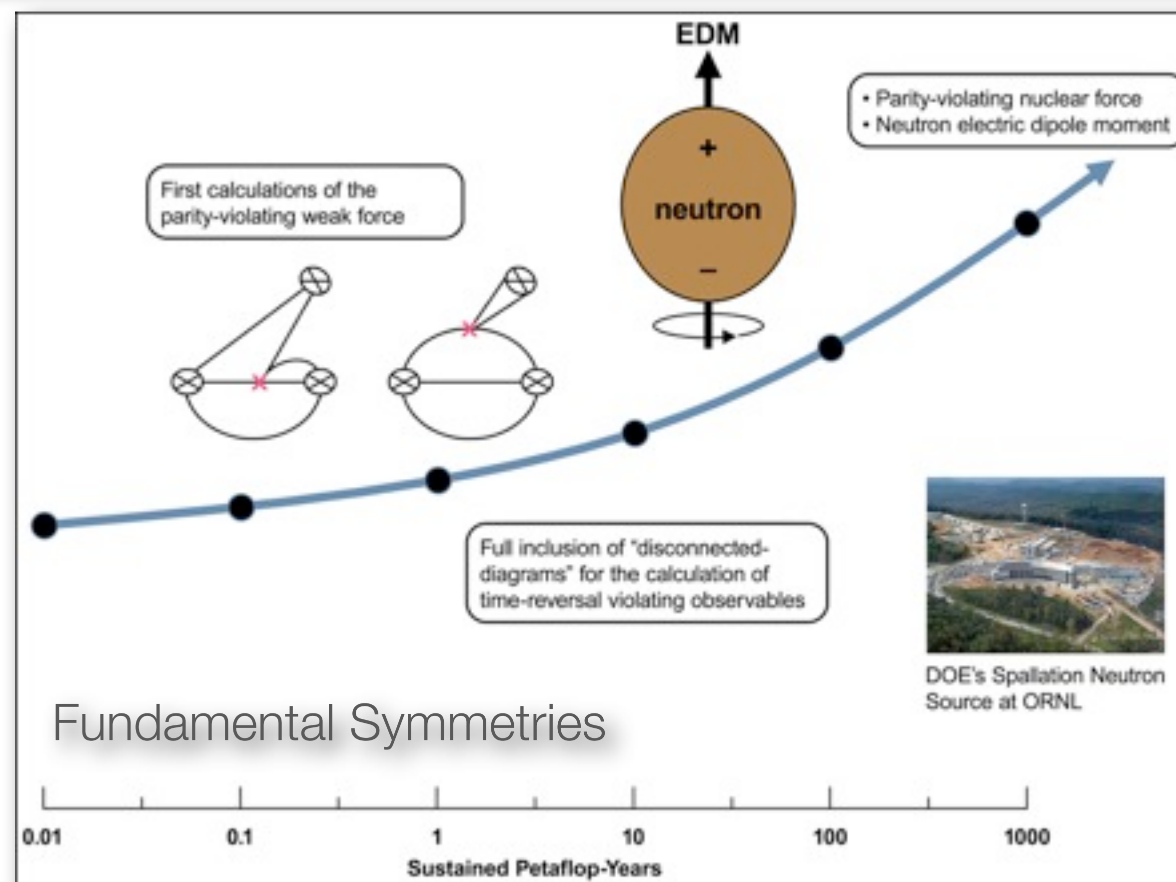
# Computational Requirements

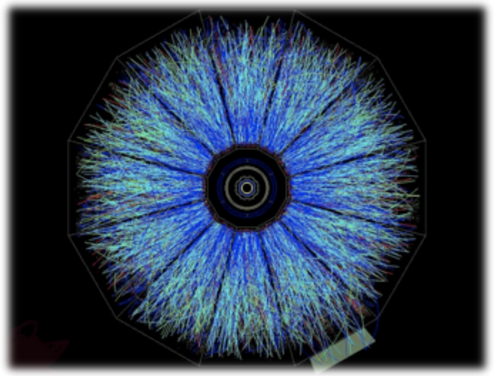




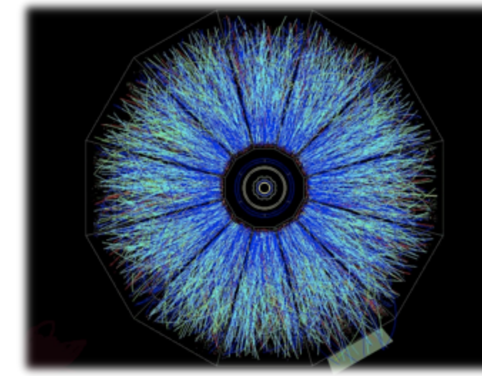



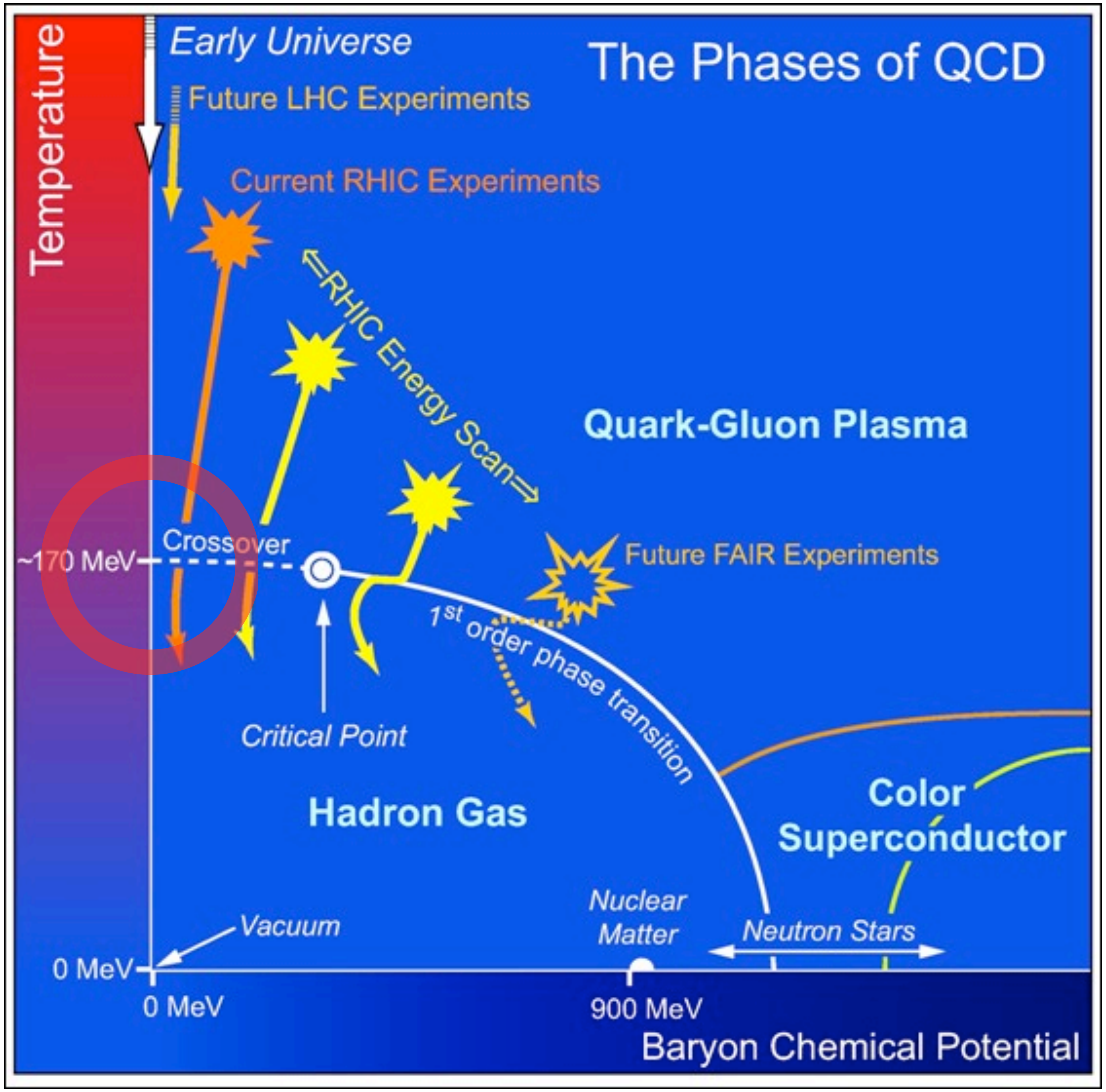



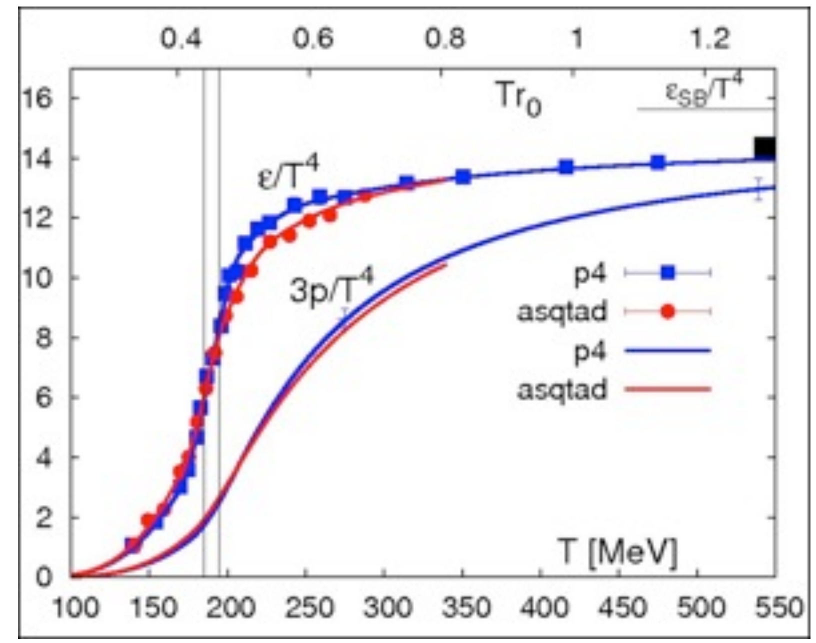



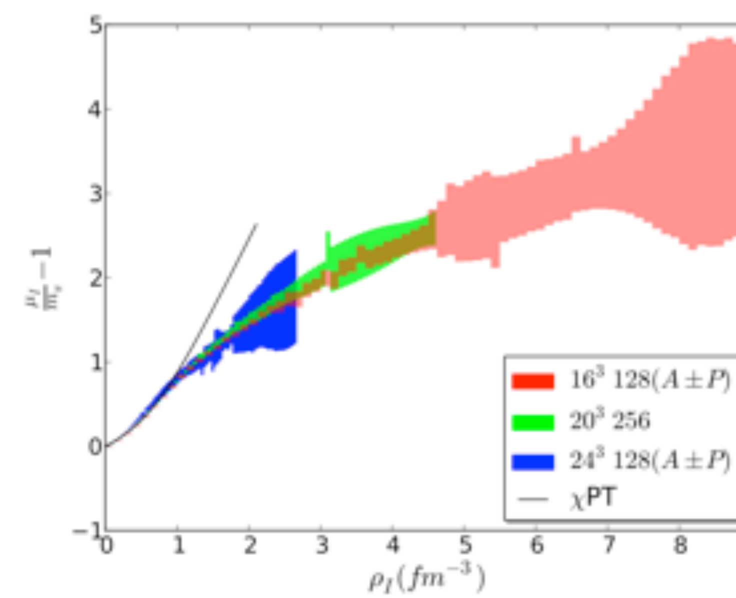


# The Phase Structure of QCD : Heating-up Nuclear Matter

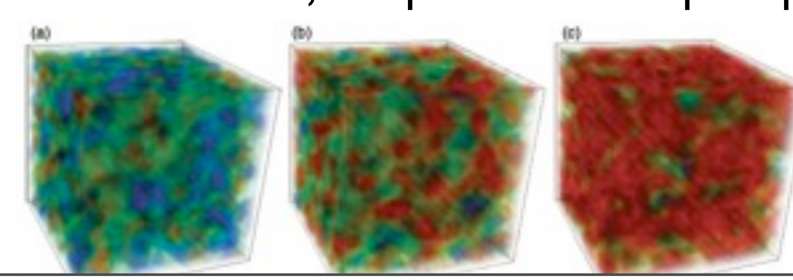


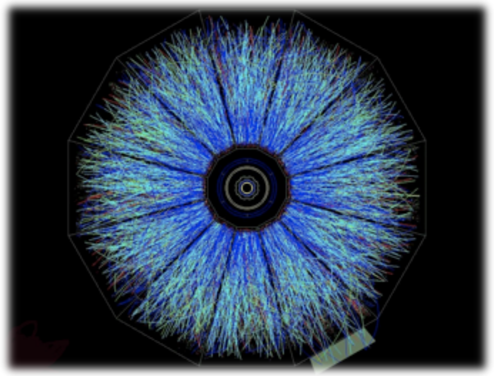


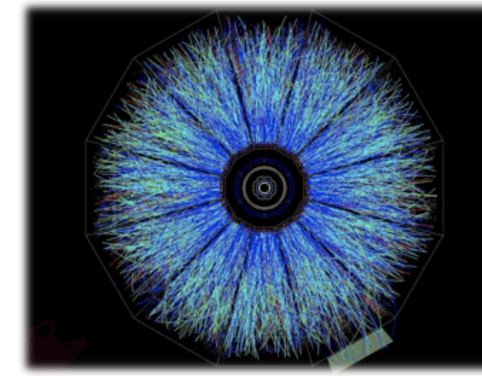



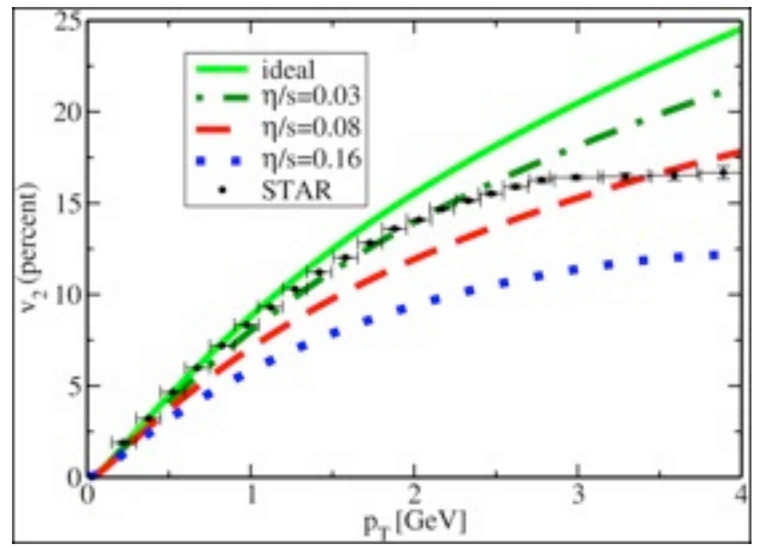

LQCD: Static, equilibrium properties

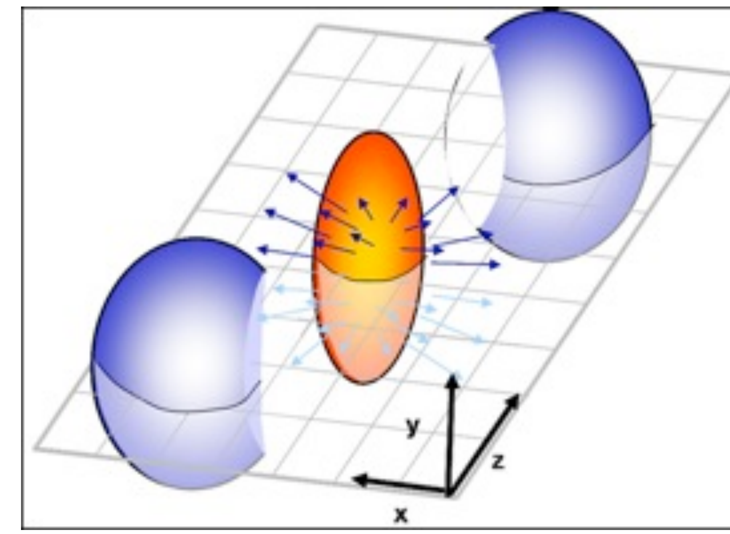


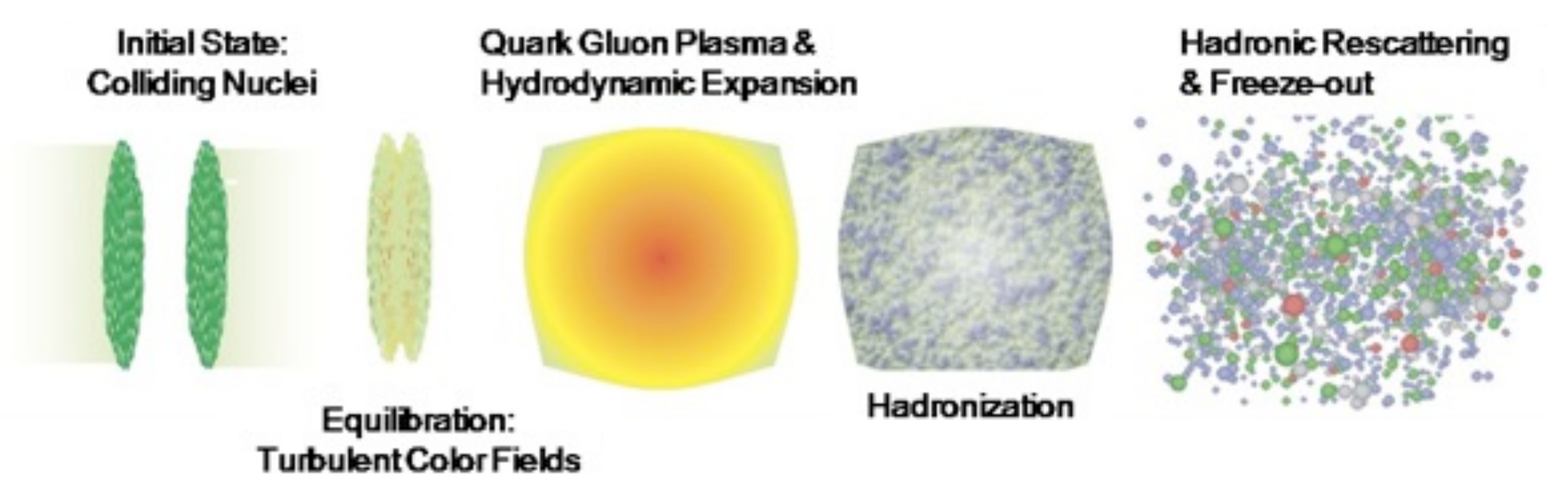


# Evolution of Matter in Collision

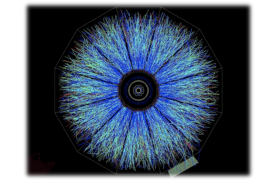


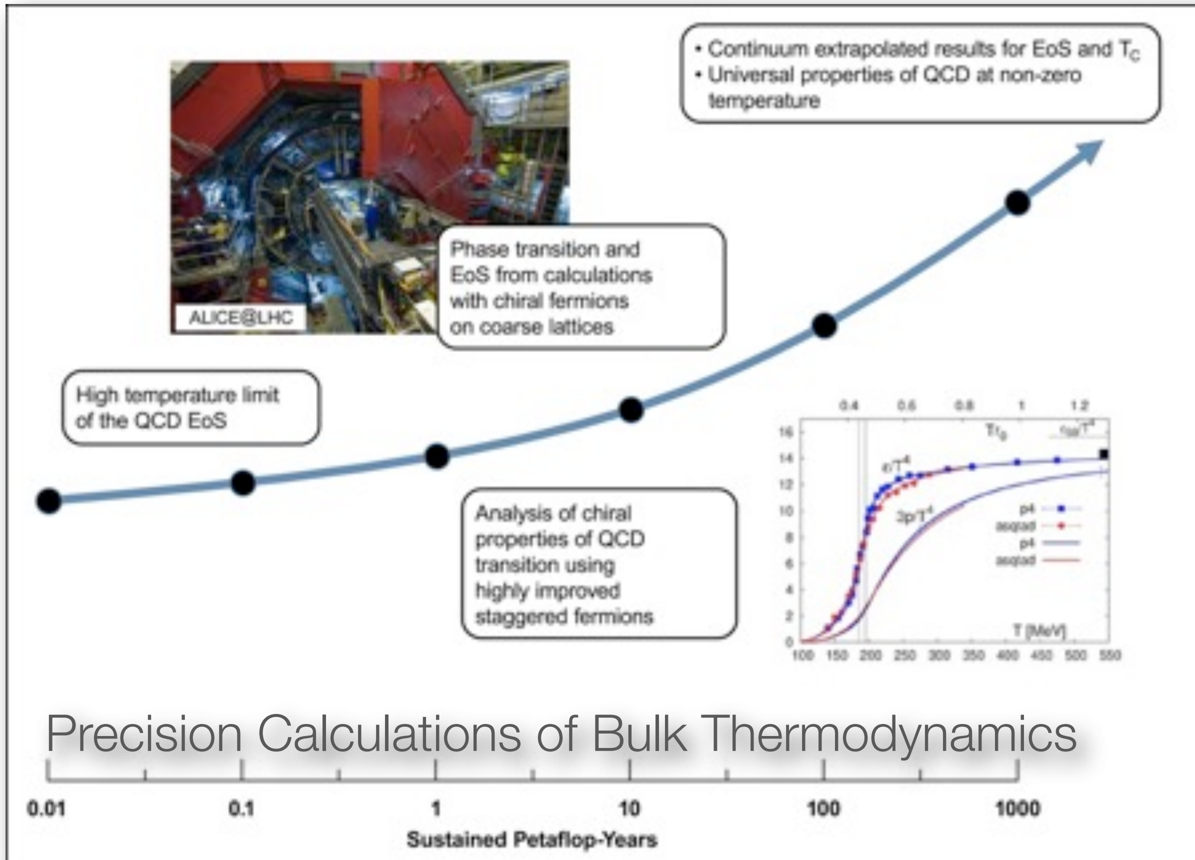



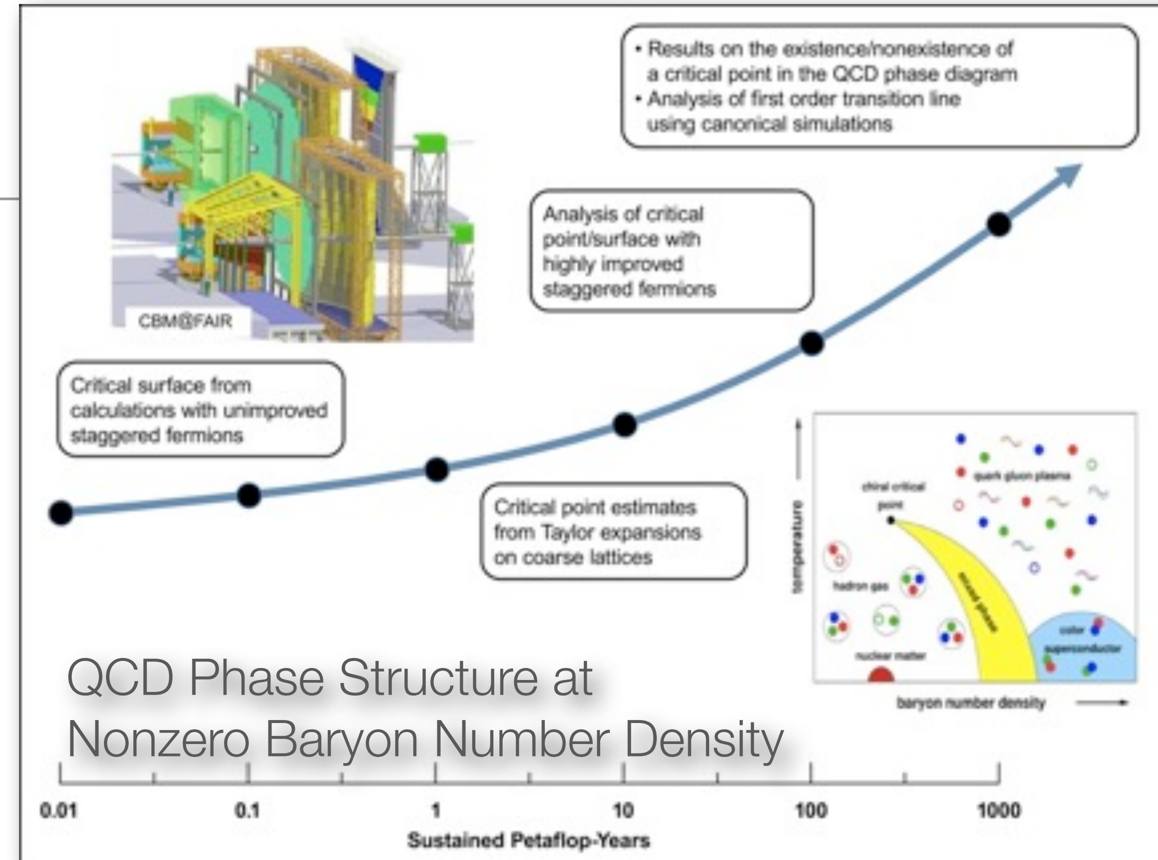



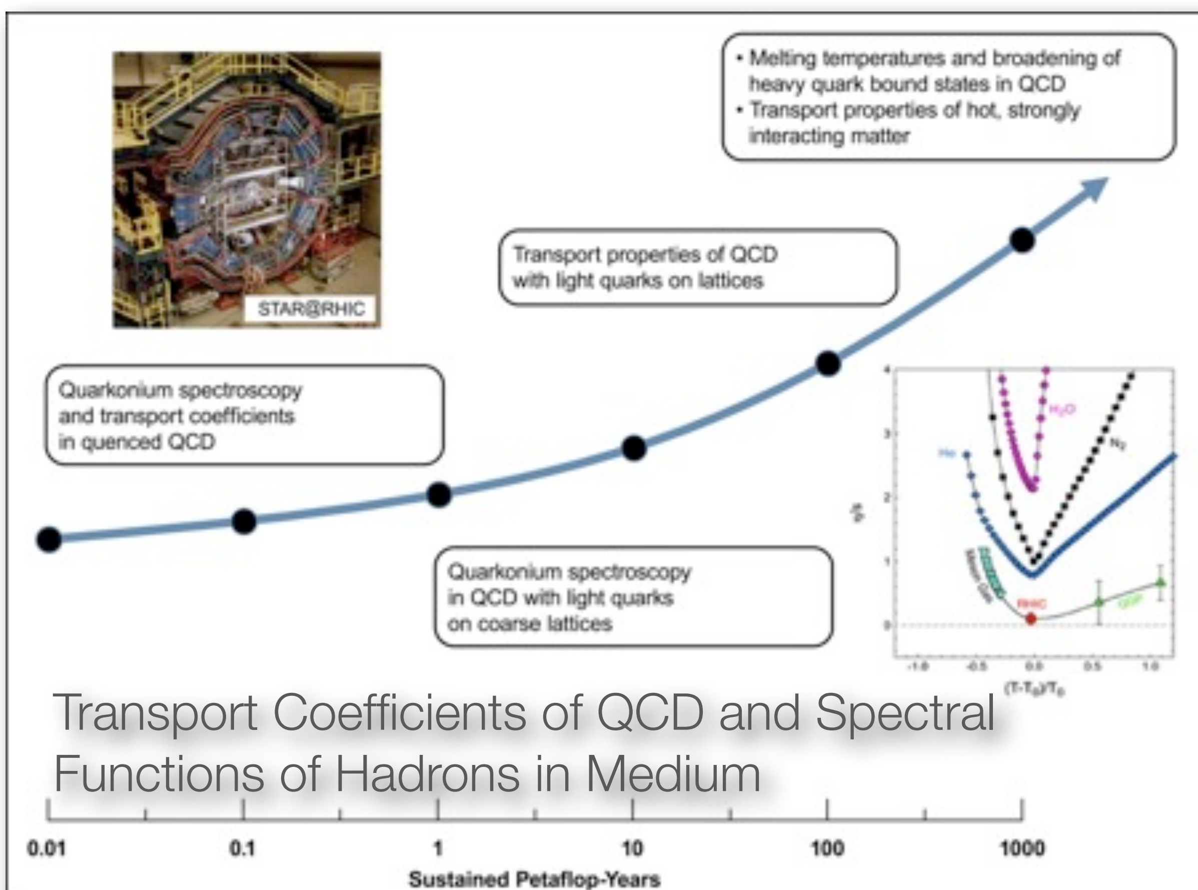



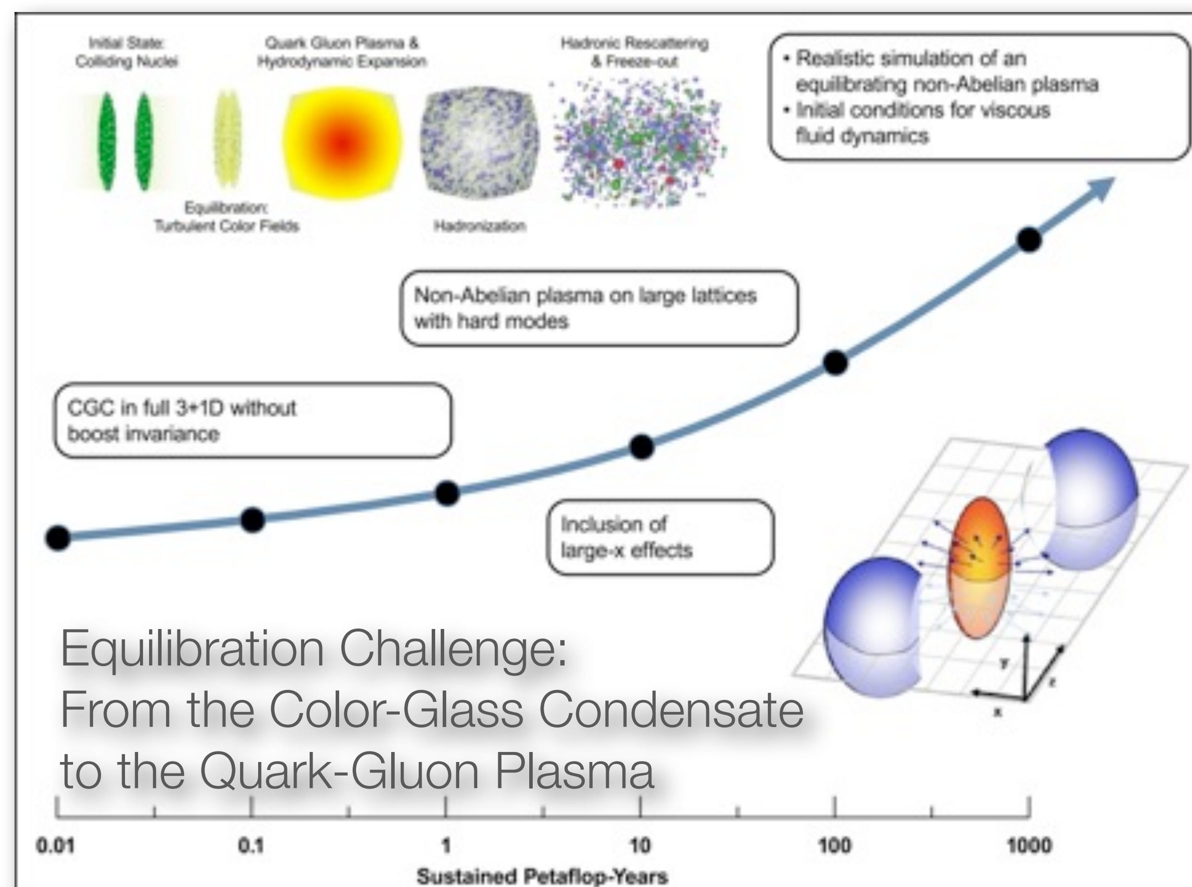
# Computational Requirements

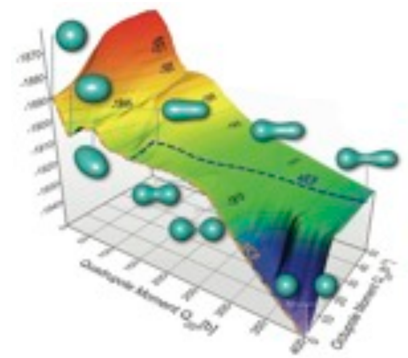




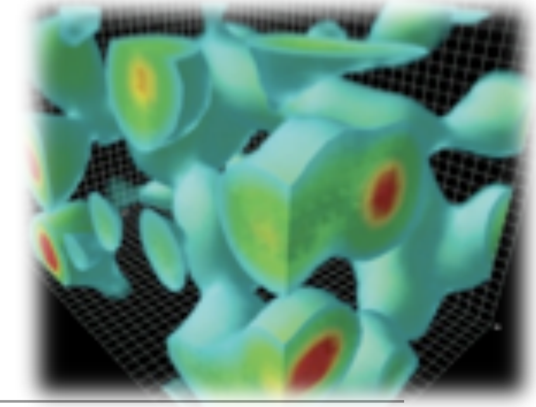



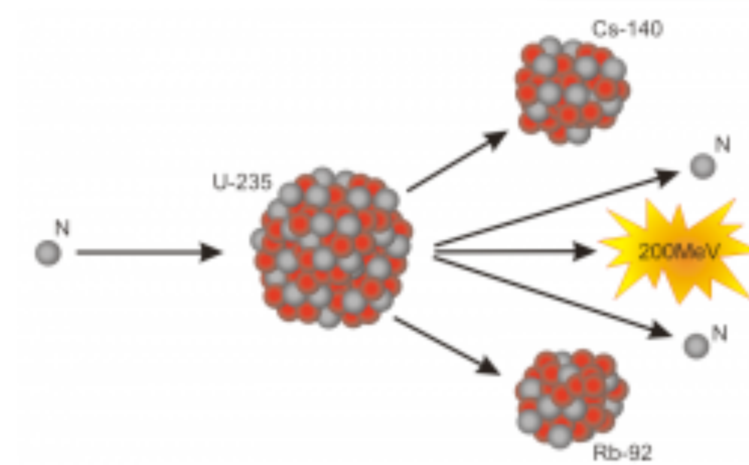



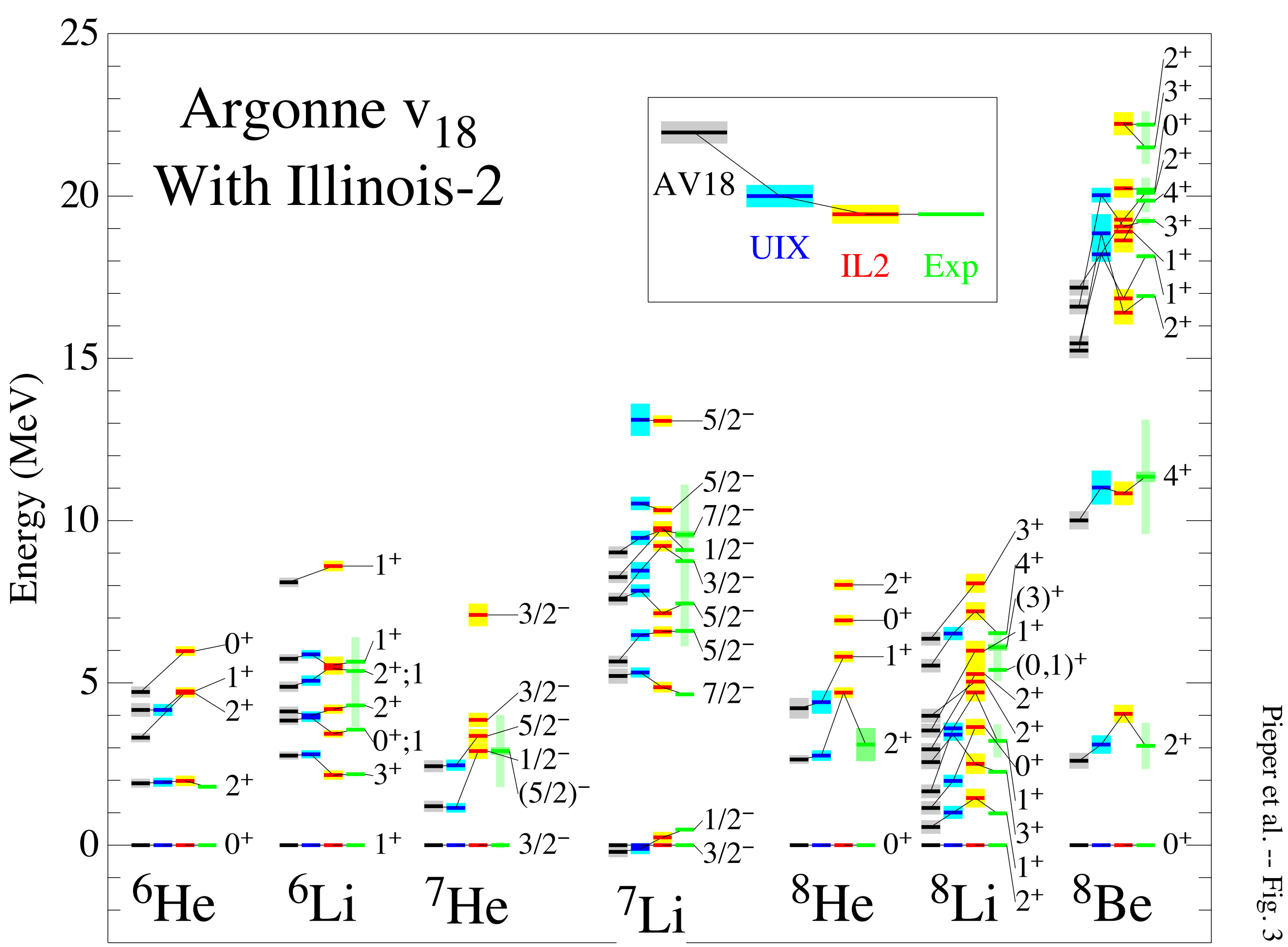



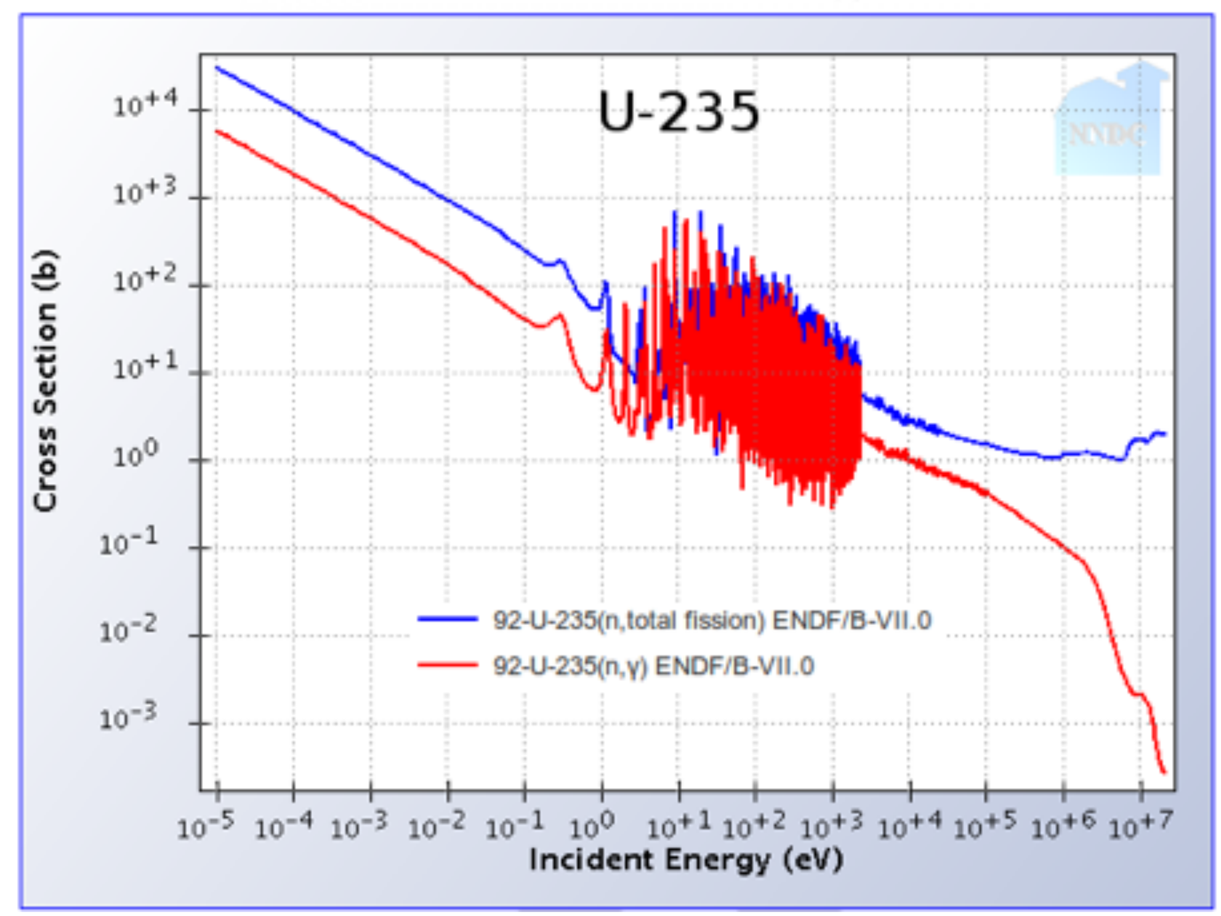


# Nuclear Energy Scales from QCD



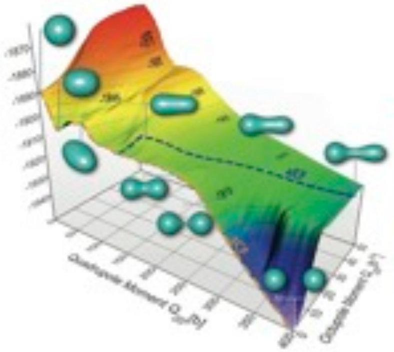


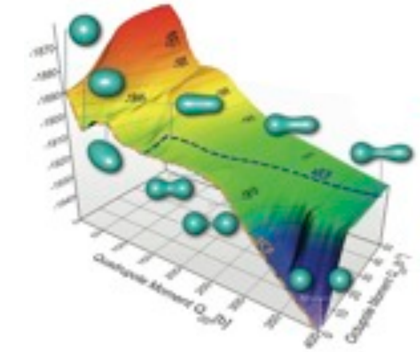

Mass $_{8Be}$ ~ 7 500 MeV

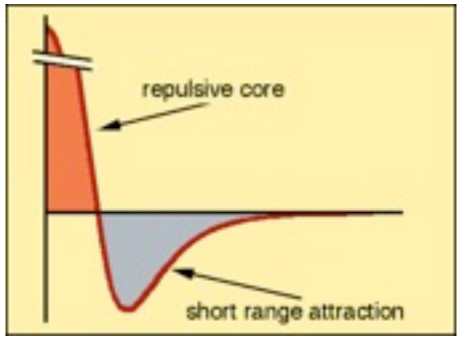
Mass $_{235U}$ ~ 220 900 MeV

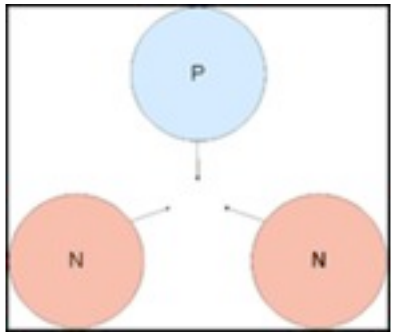


# Light and Medium Nuclei, Fusion

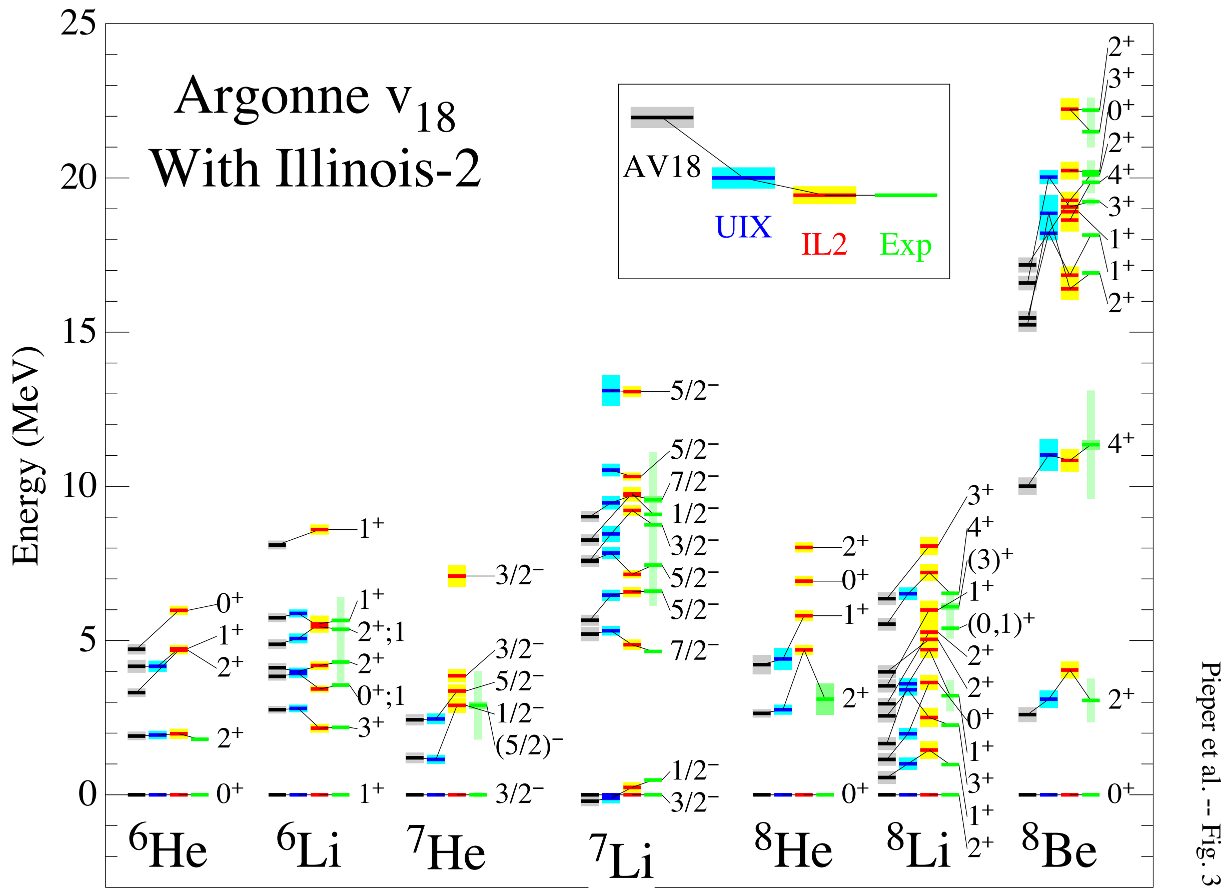
## e.g. GFMC and NCSM



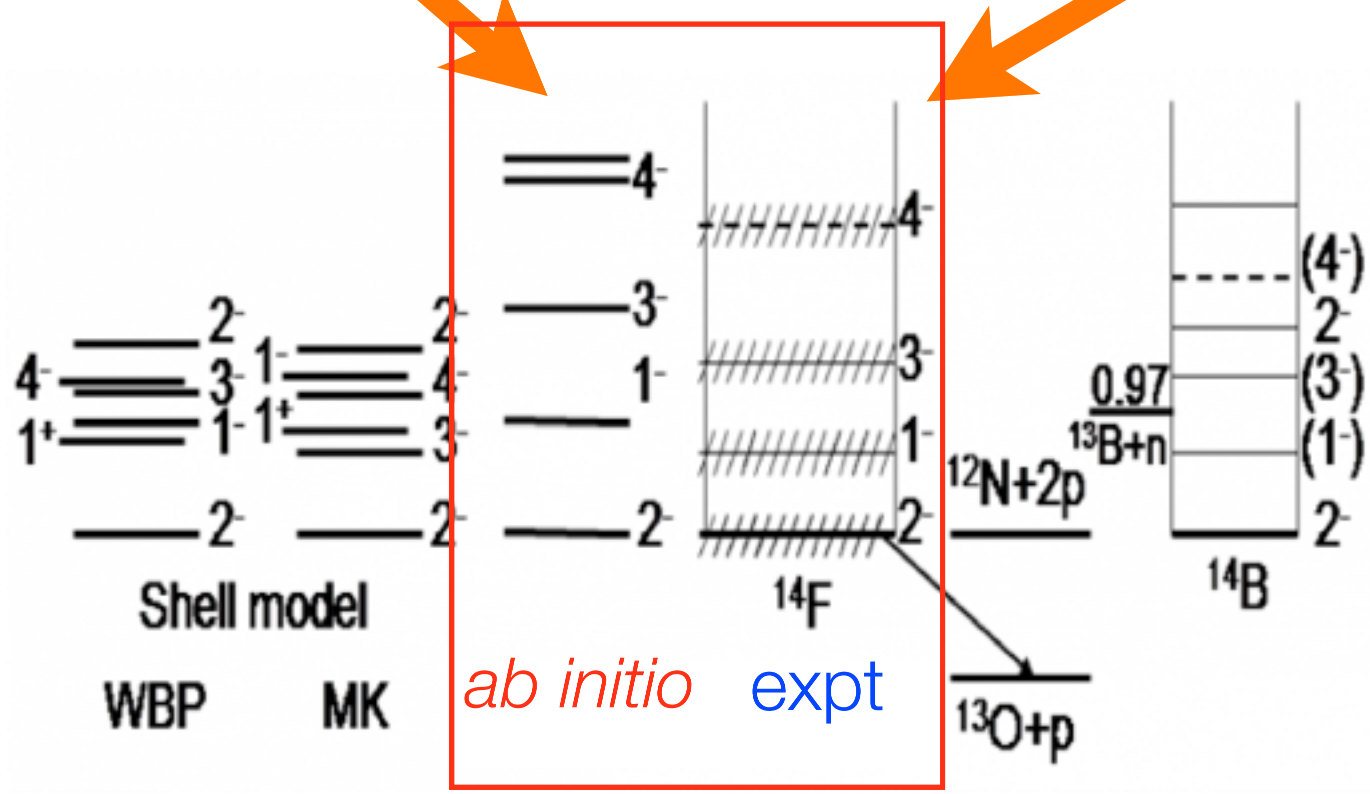


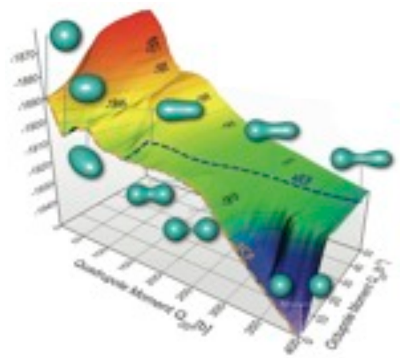

Predicted 6 months before expt



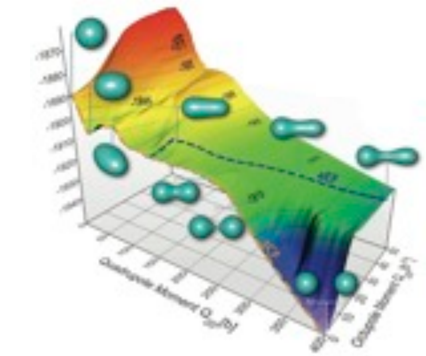

**(Carlson, Pieper, Wiringa)**




**(Maris, Vary *et al*)**



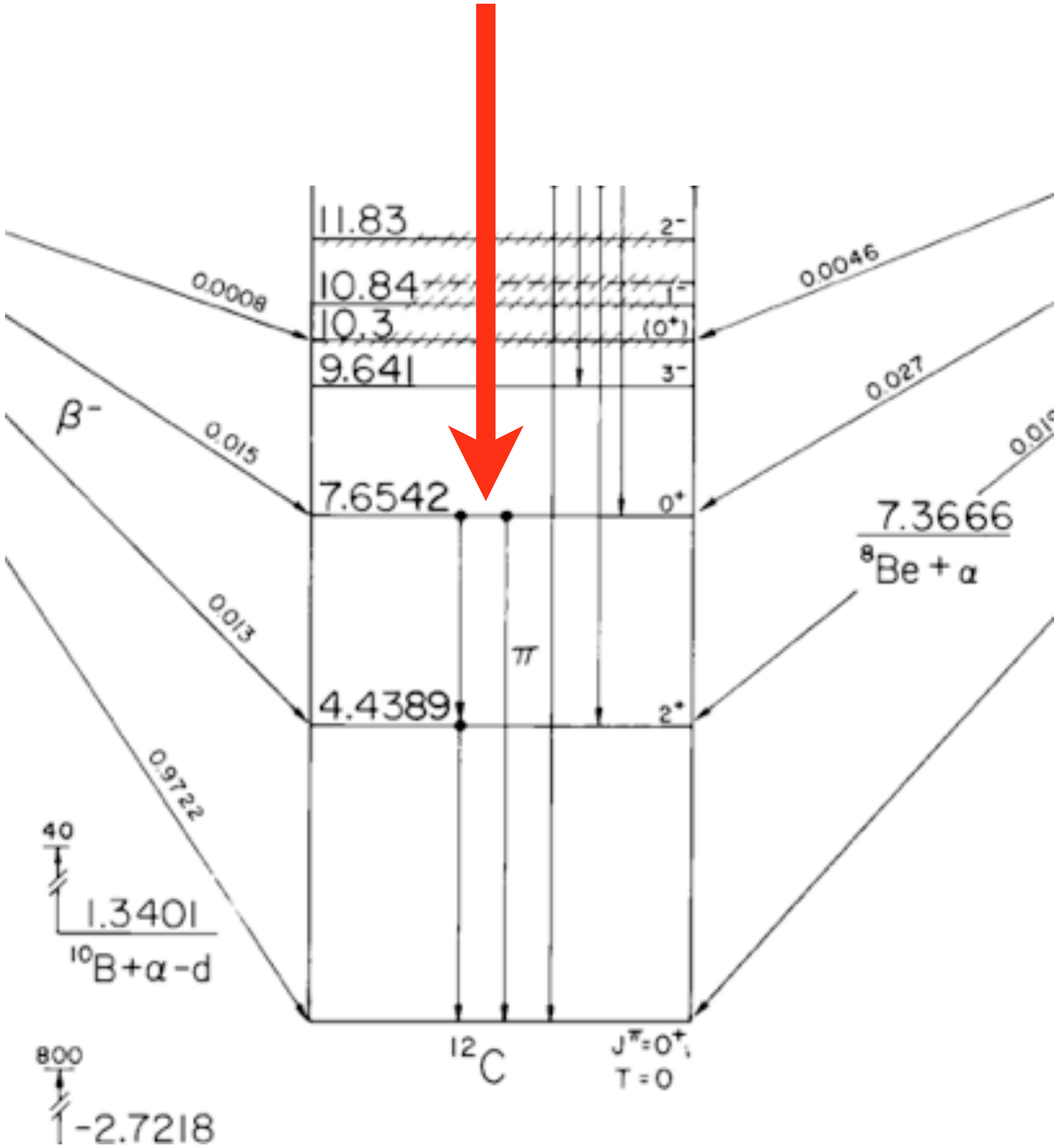
# Important Progress in Nuclear Many-Body Physics in 2011

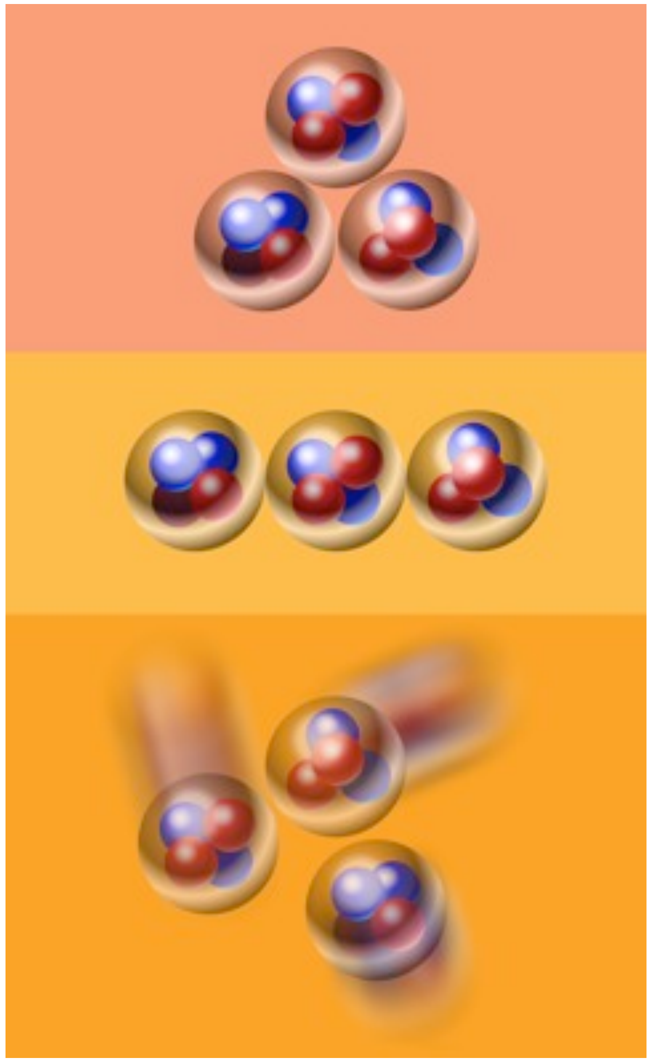


Epelbaum, Krebs, Lee, Meissner

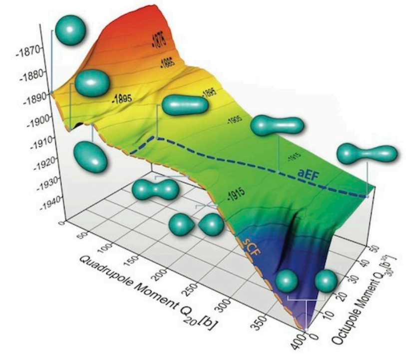
universitätbonn

## The Hoyle State

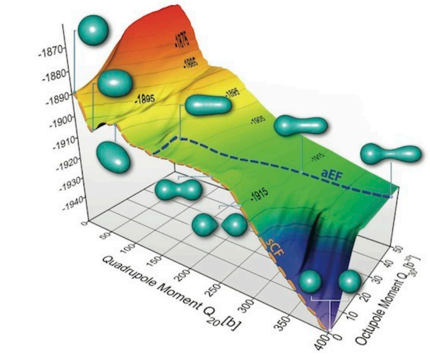


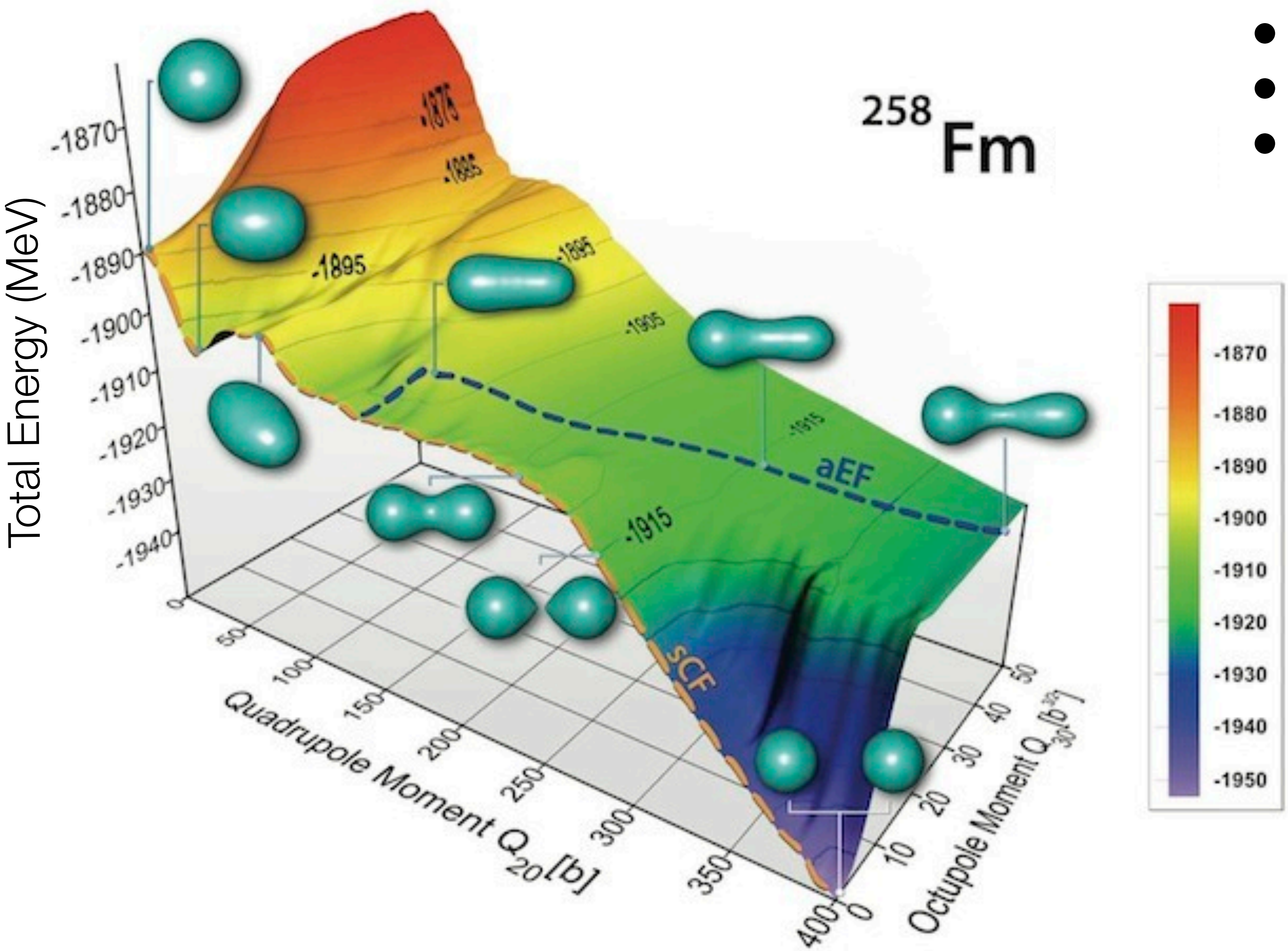



Lattice EFT

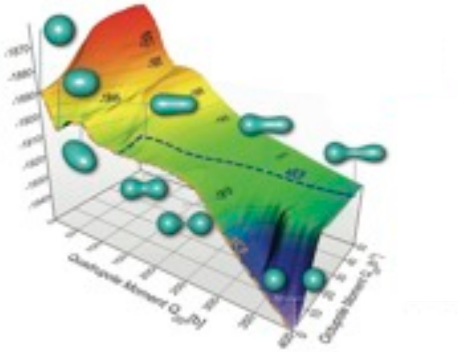


# Shape Deformations and Fission

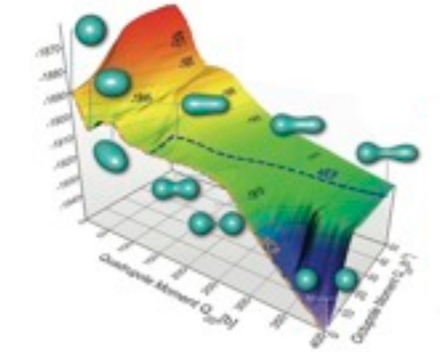





- non-central nuclear forces
- electromagnetism
- fermions
- surface effects



# Fission Barriers



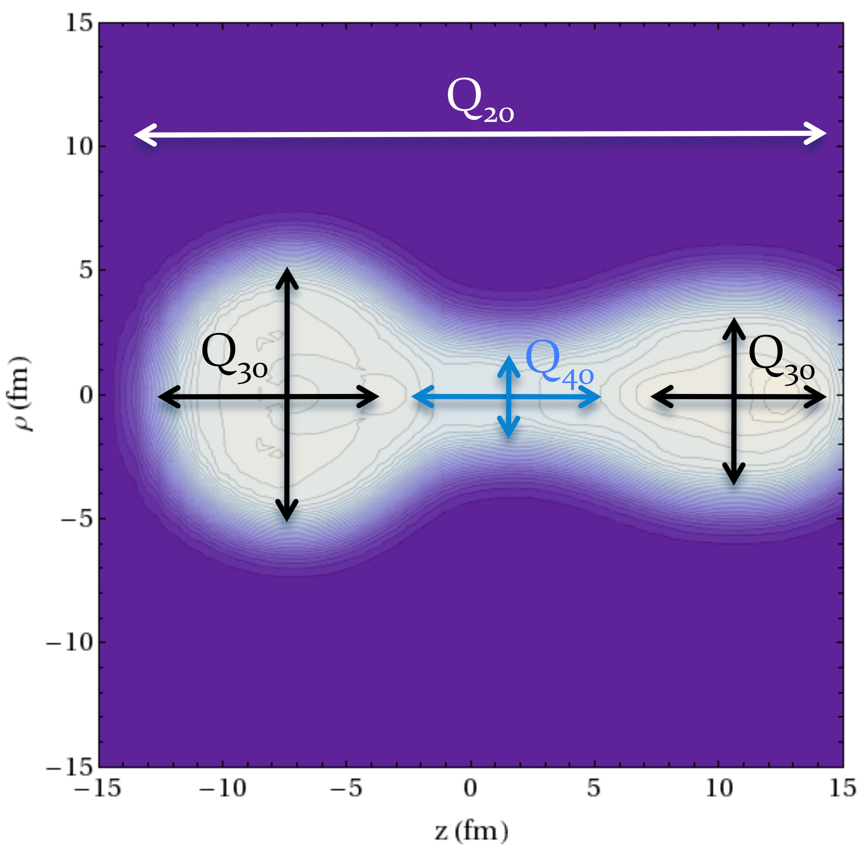
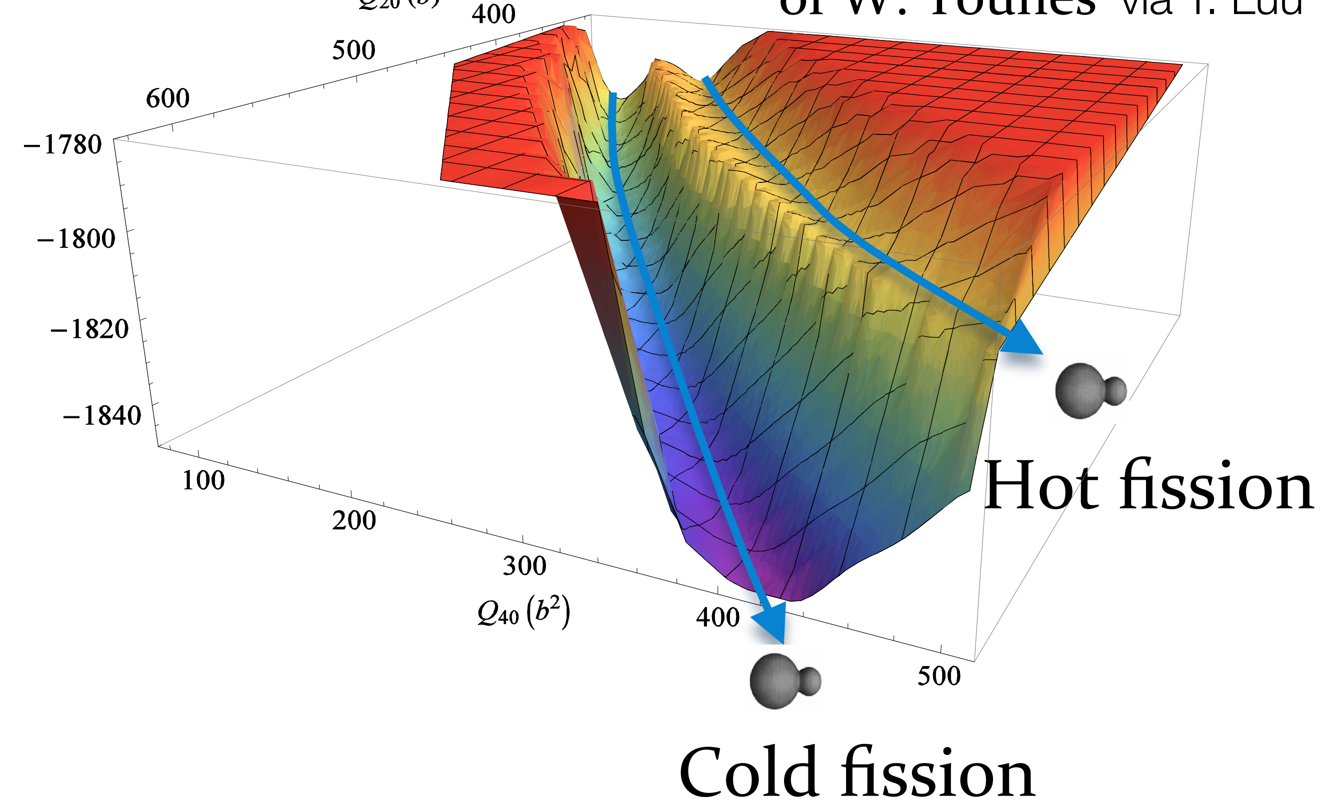



Figure courtesy of W. Younes via T. Luu

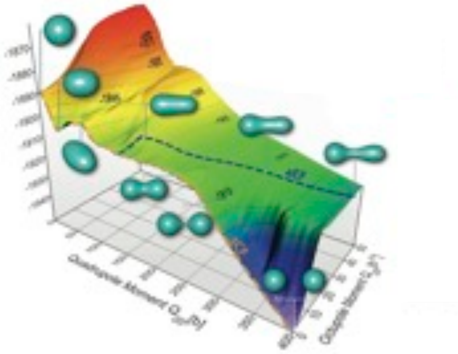
Figure and data courtesy of W. Younes via T. Luu



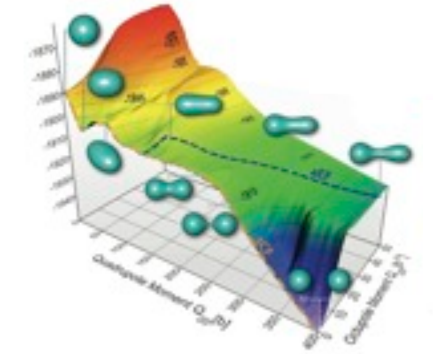

Naïve scaling of resources

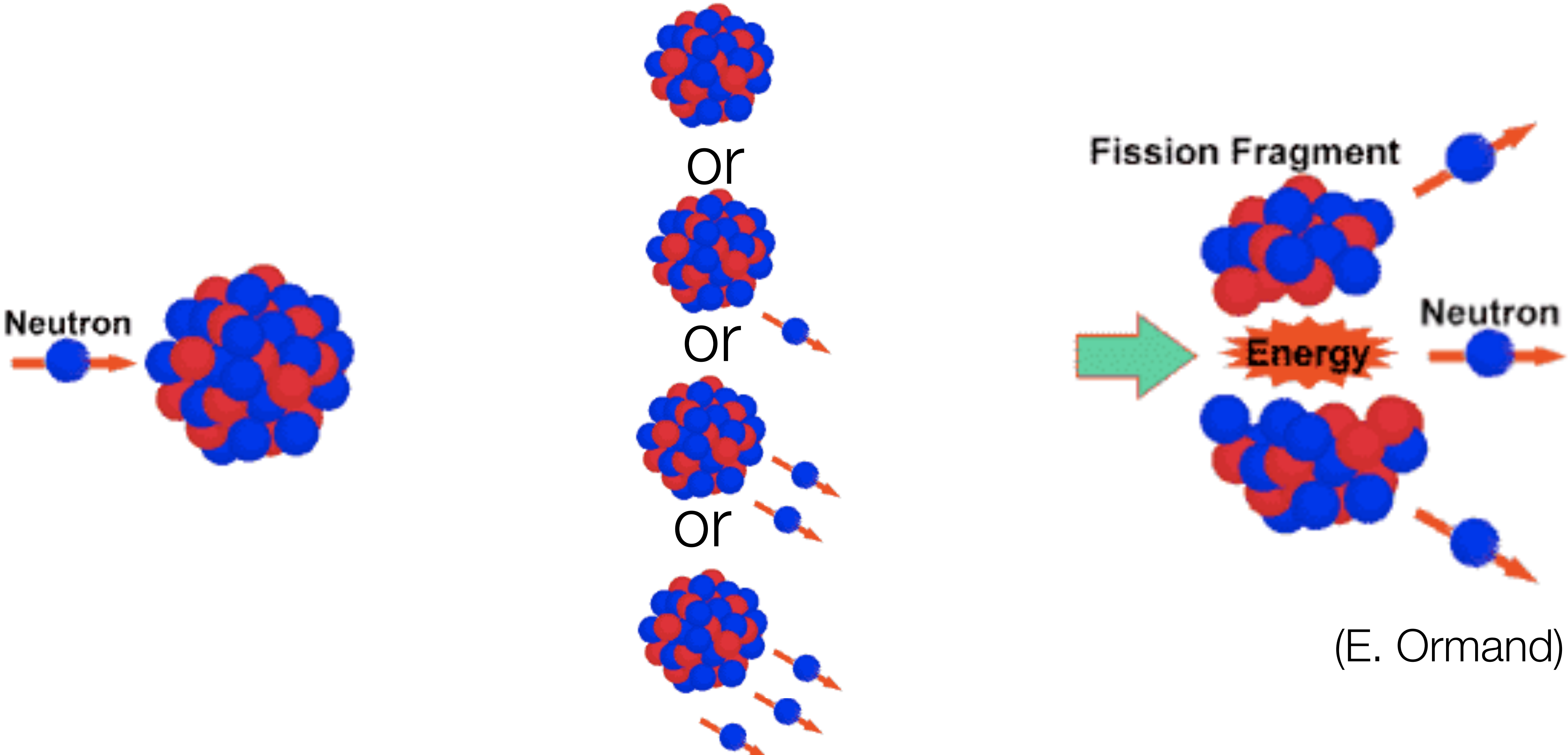
| Coordinate | Physics | Grid points |
|---|---|---|
| $Q_{20}$ | Basic fission | 50 |
| + $Q_{22}$ | Triaxiality | 2500 |
| + $Q_{30}$ | Asymmetry | 125000 |
| + $Q_{40}$ | Hot-to-cold fission | $6.25\times10^{6}$ |
| + $Q_{N}$ | Scission points | $3.125\times10^{8}$ |

- Each new constraint/coordinate  new physics
- Assume 5 hrs/config on 1 CPU (at  5 GFLOP/s)
  - 1 PetaFLOP/s  1 year (too long for 1 nucleus)
  - 1 ExaFLOP/s  8 hours (reasonable)



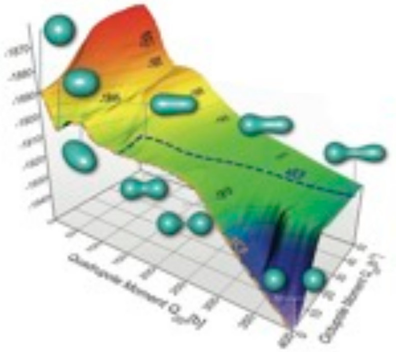
# Heavy Nuclei and Fission



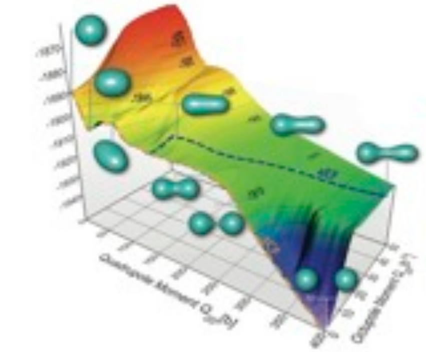


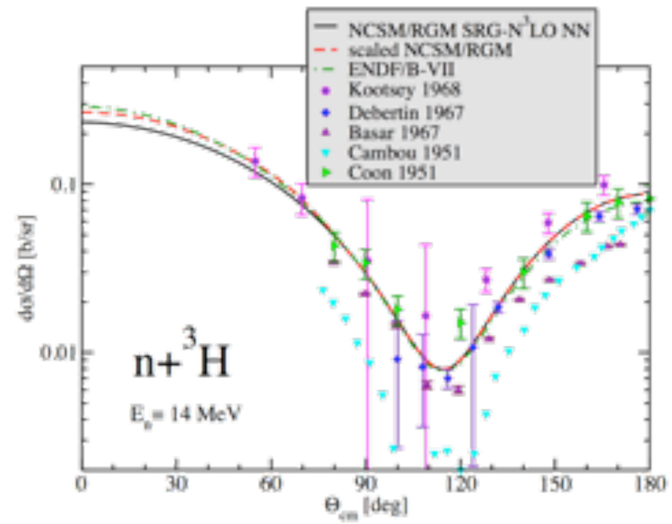

(E. Ormand)

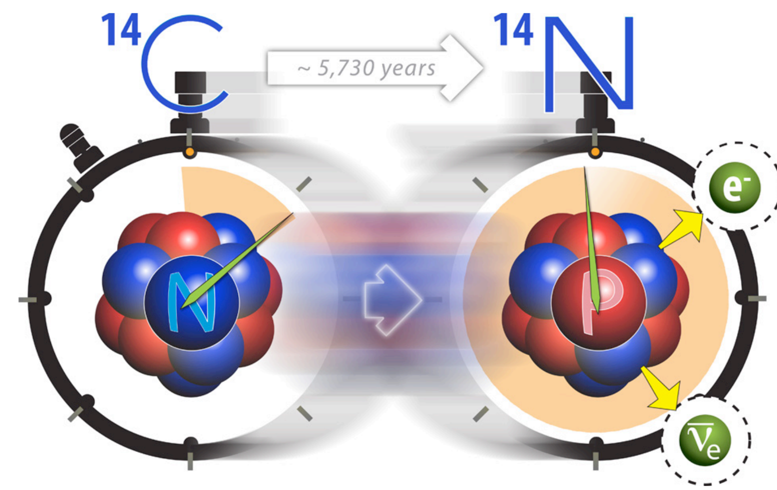
- Data not sufficient
- Need yield neutron distributions
- Microscopic interactions with Extreme-Scale Computing

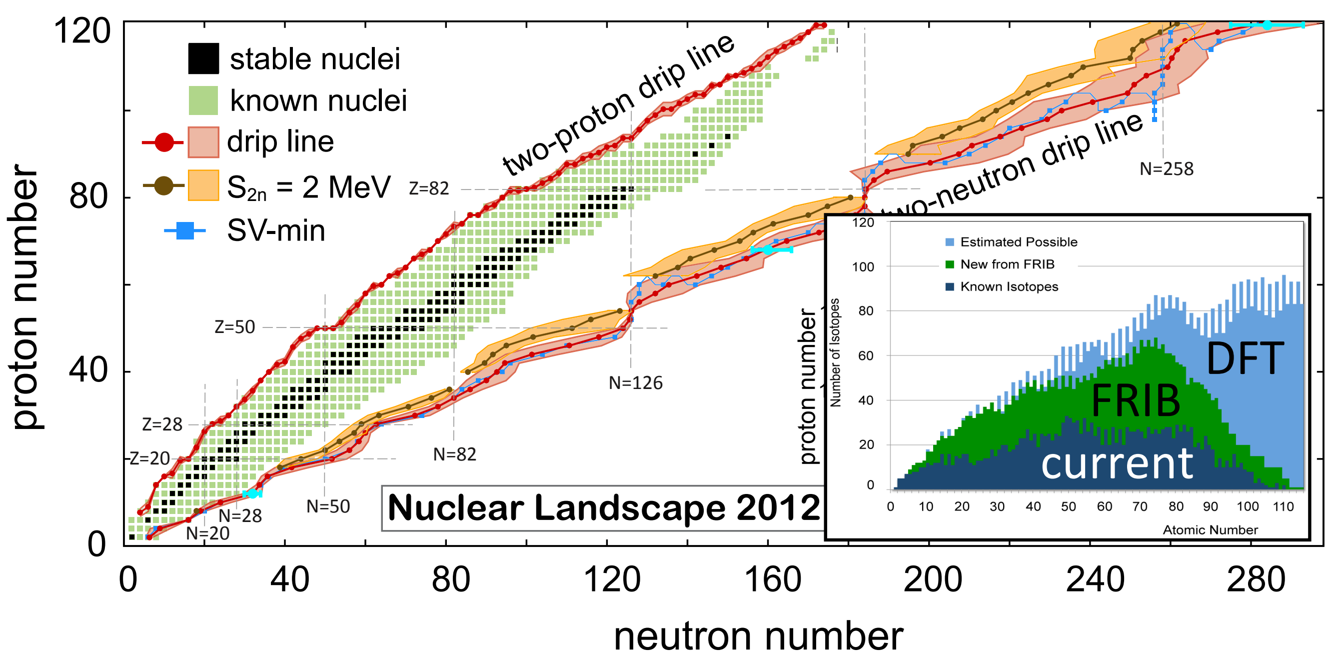


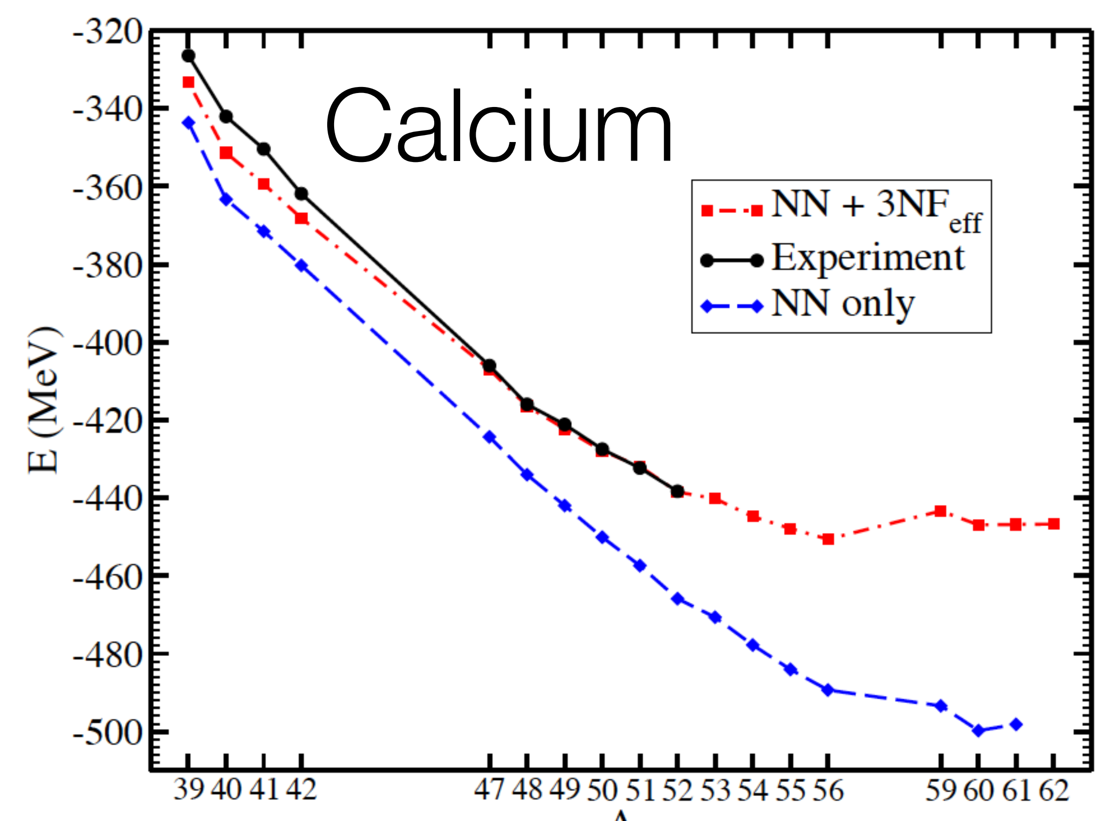
# Nuclear Structure and Reactions

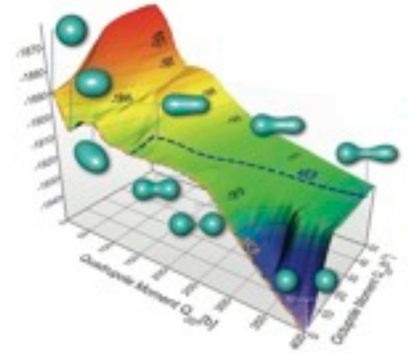




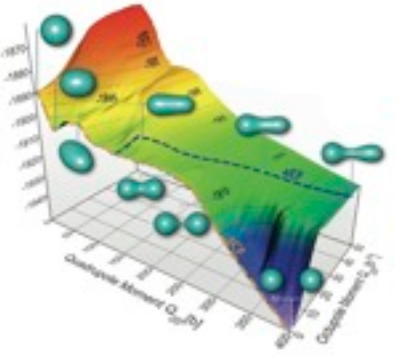



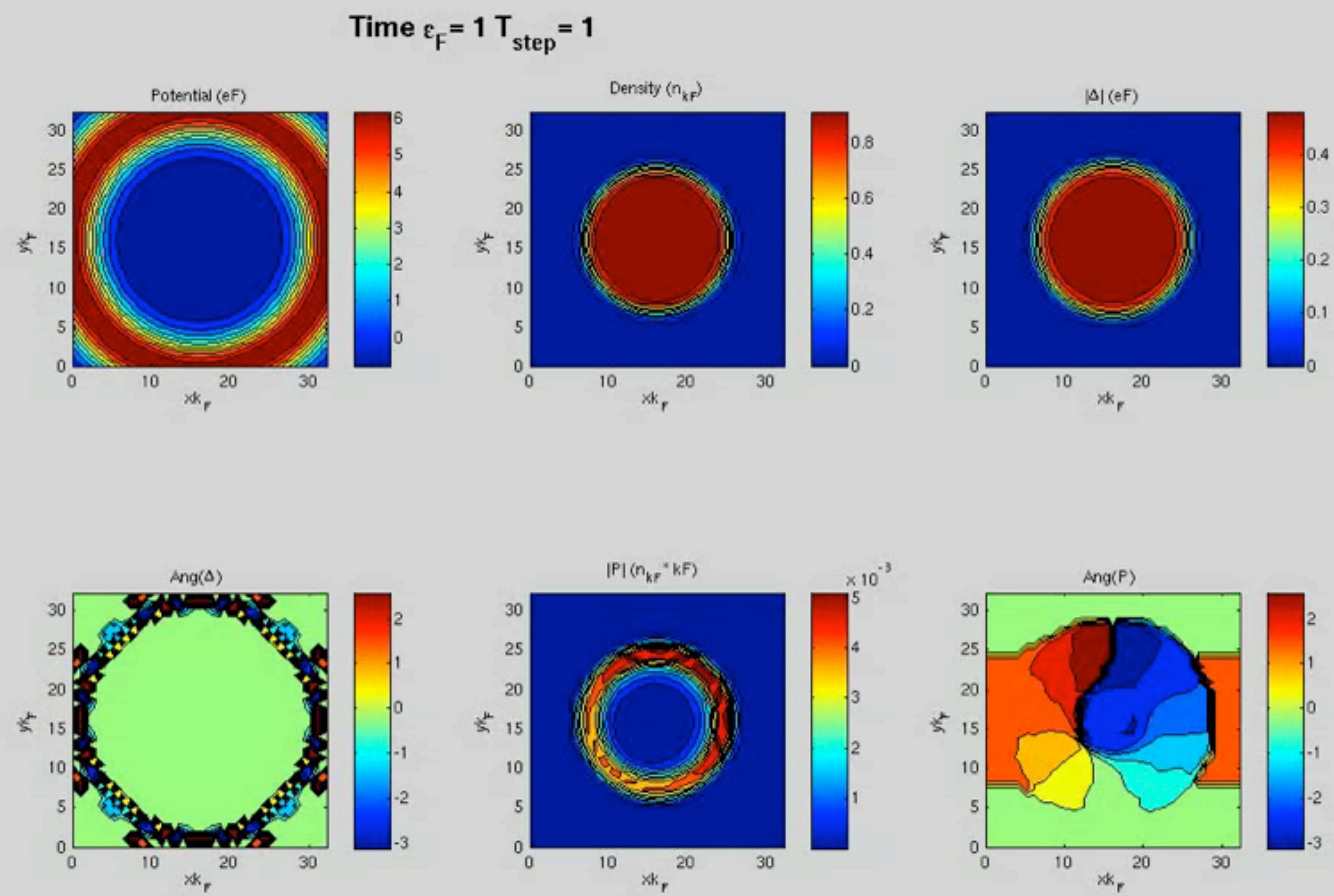





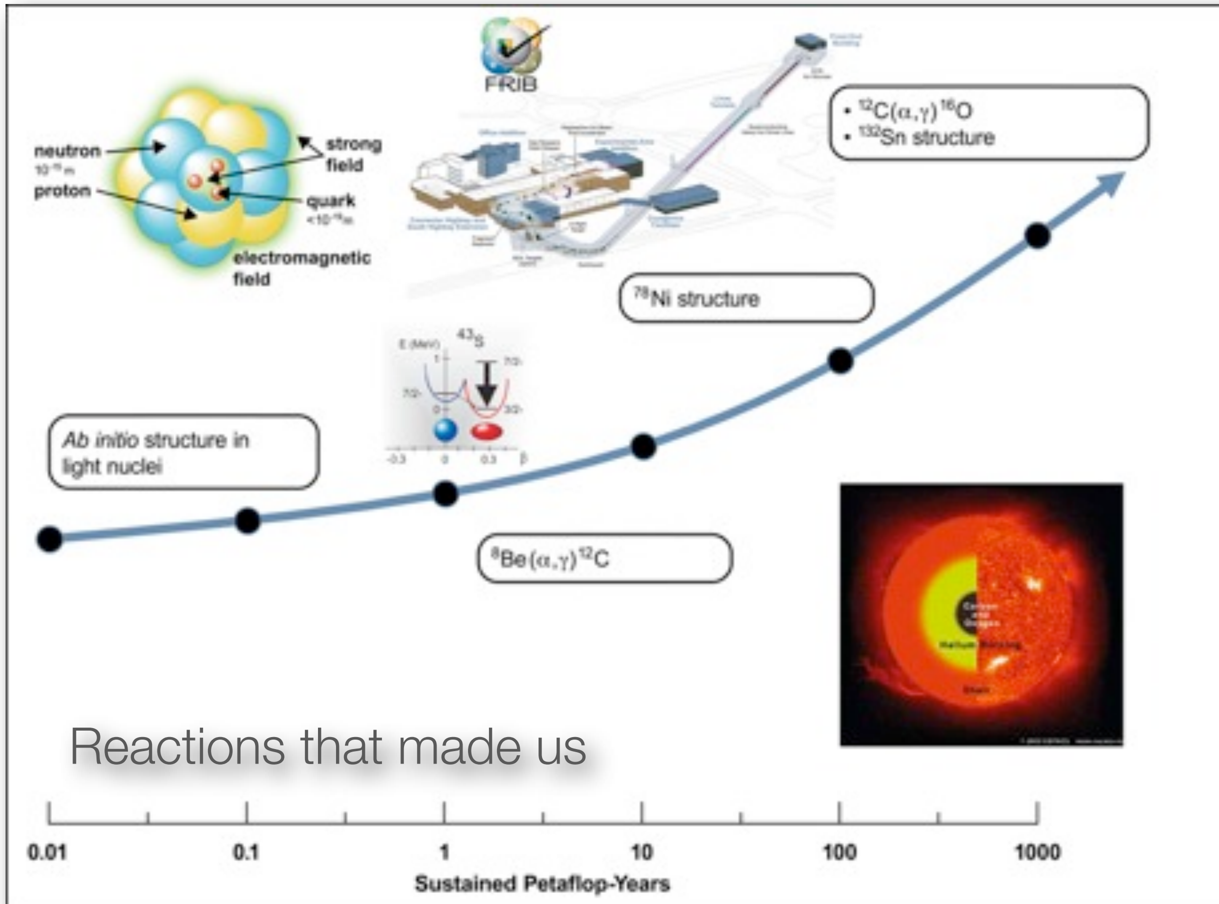
# HPC Simulations of Unitary Systems

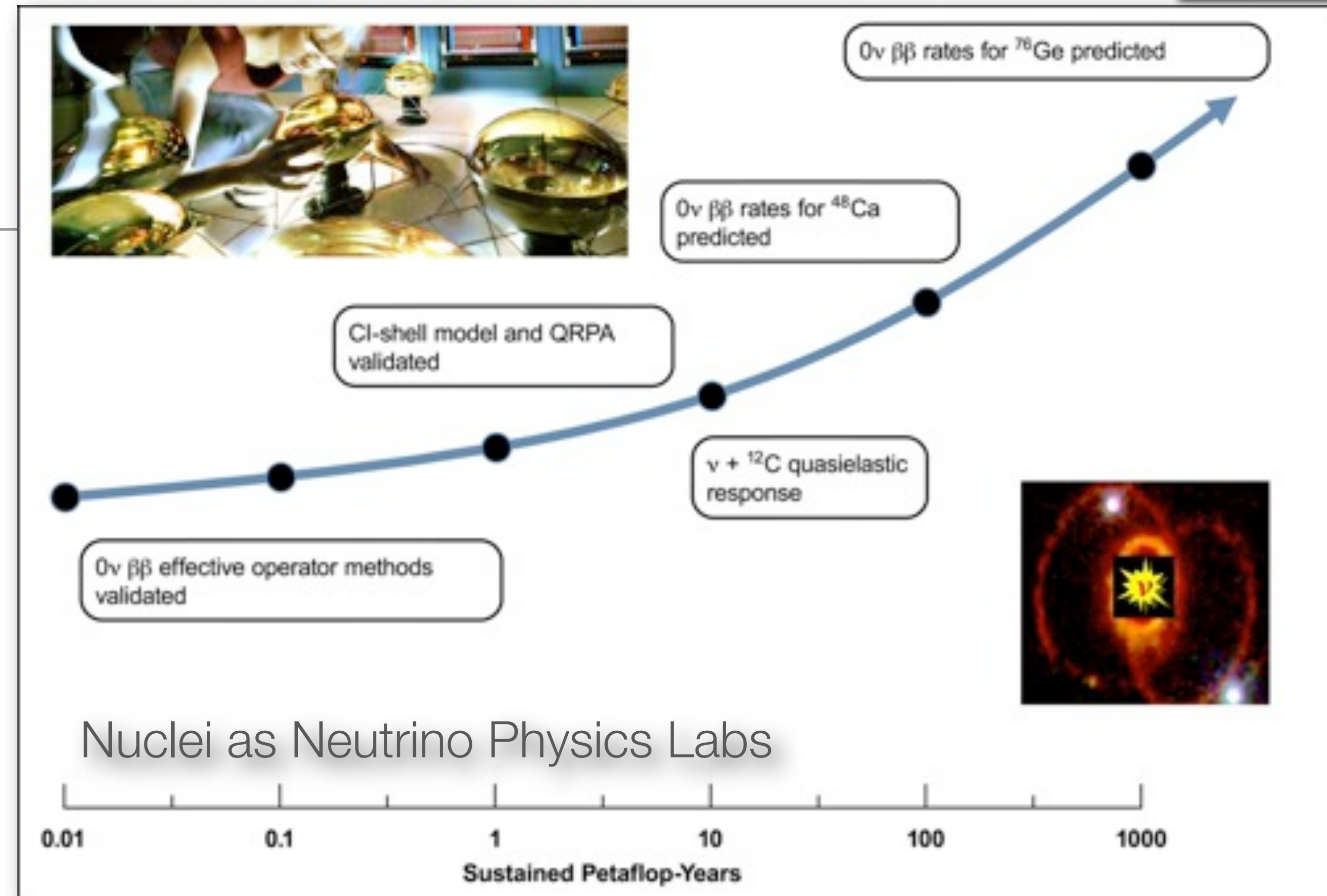


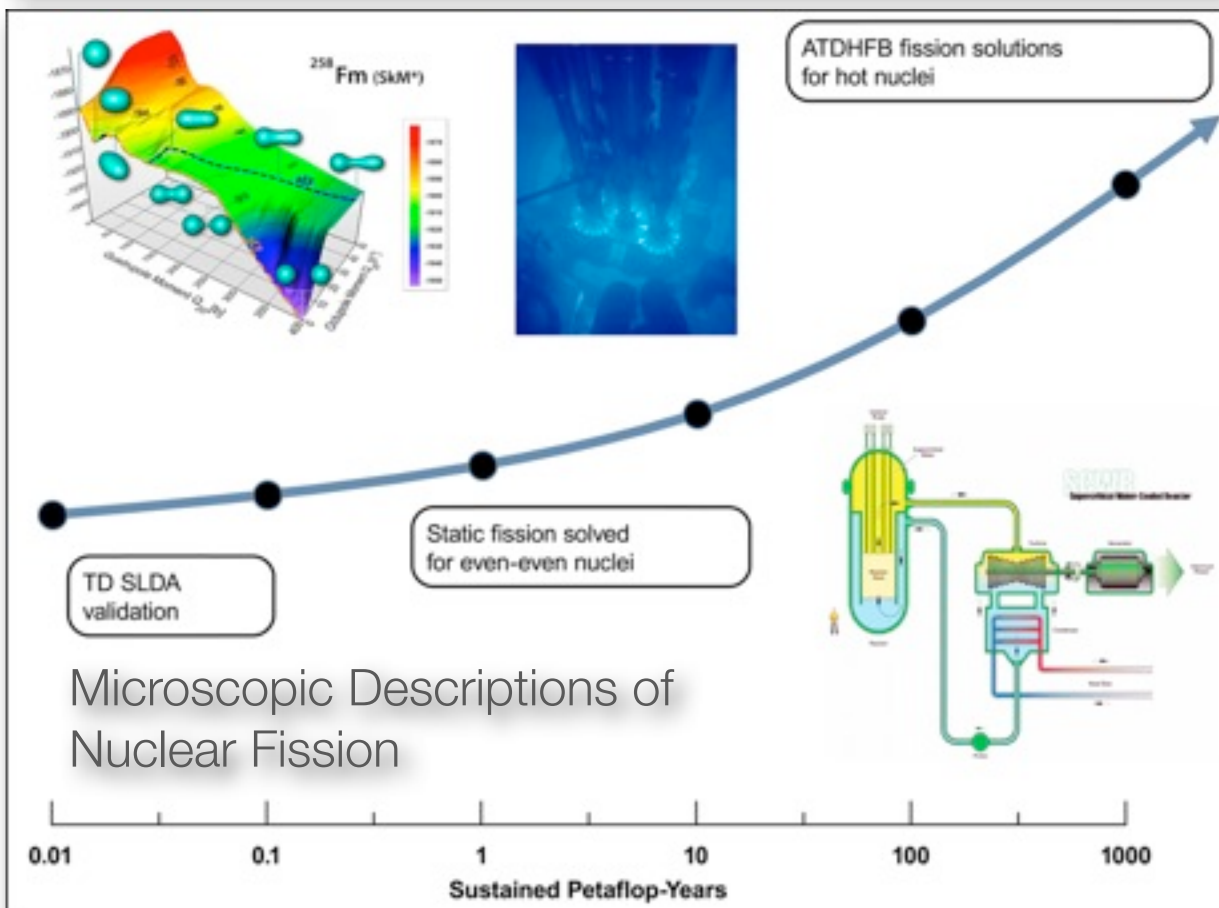


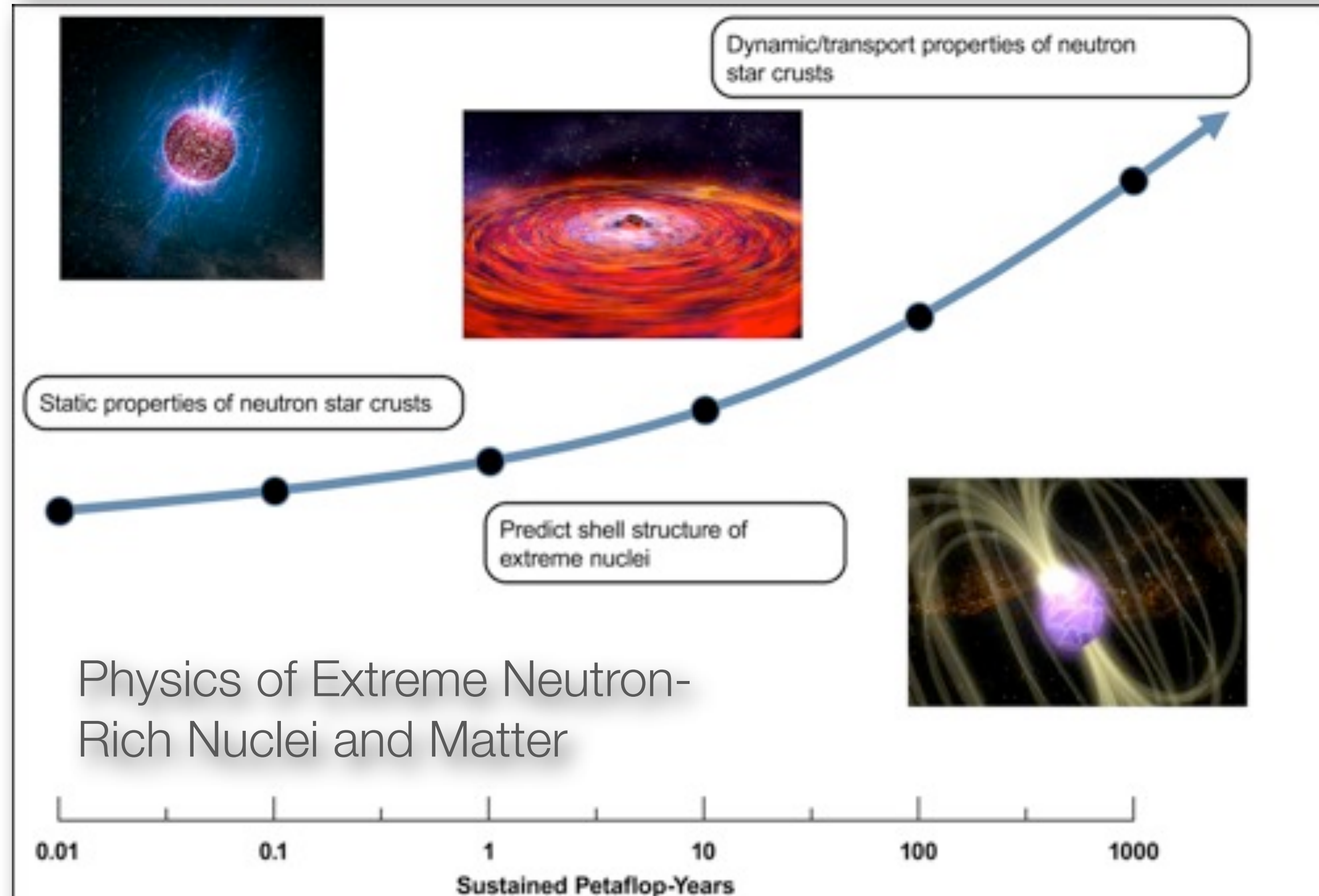

**(by Bulgac, Luo, Roche, Yoon, Yu)**

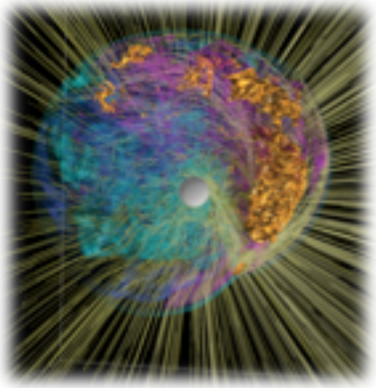
# Computational Requirements



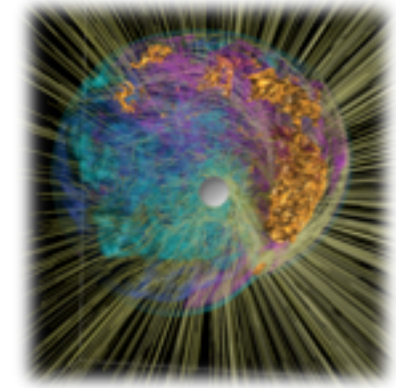



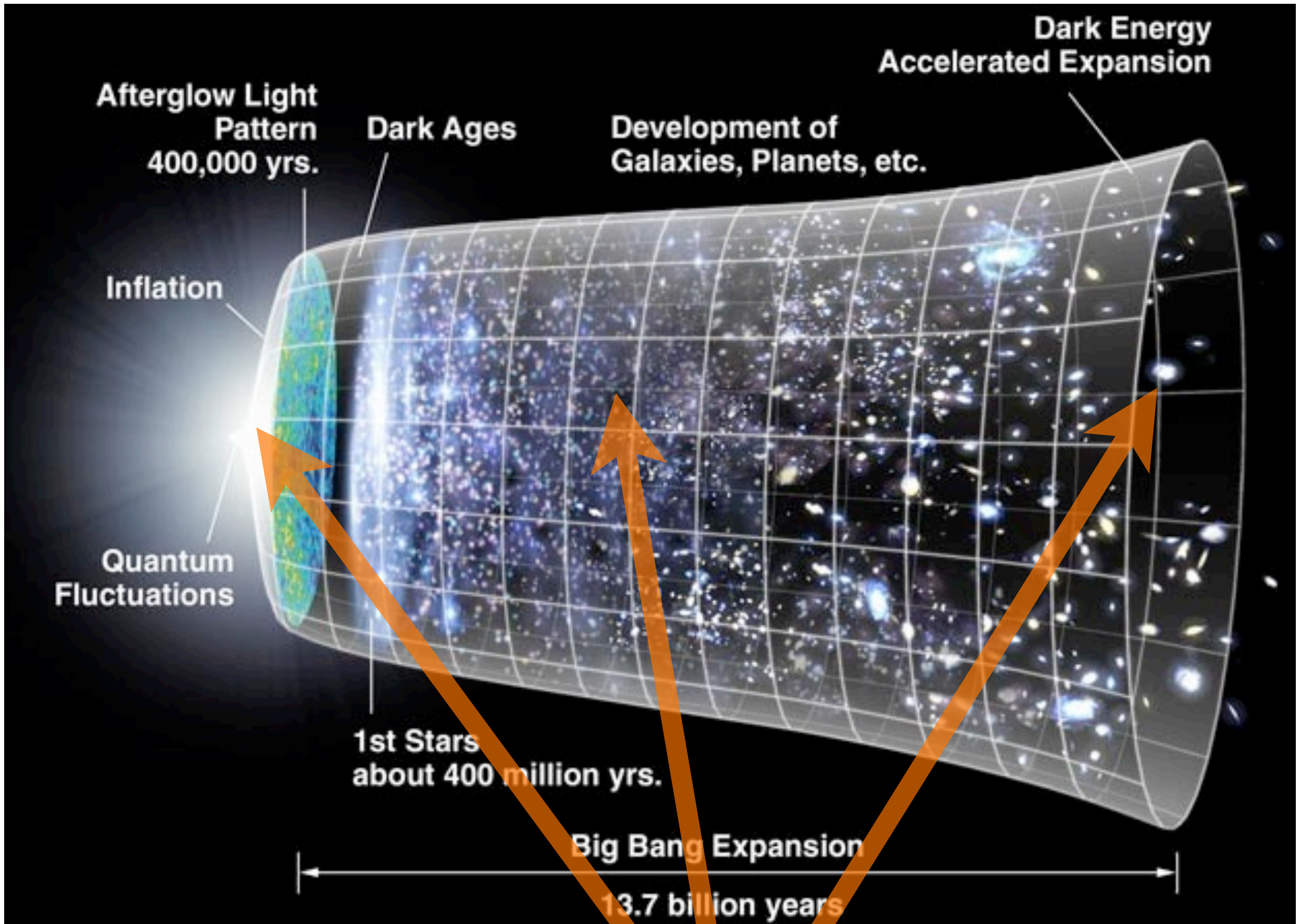



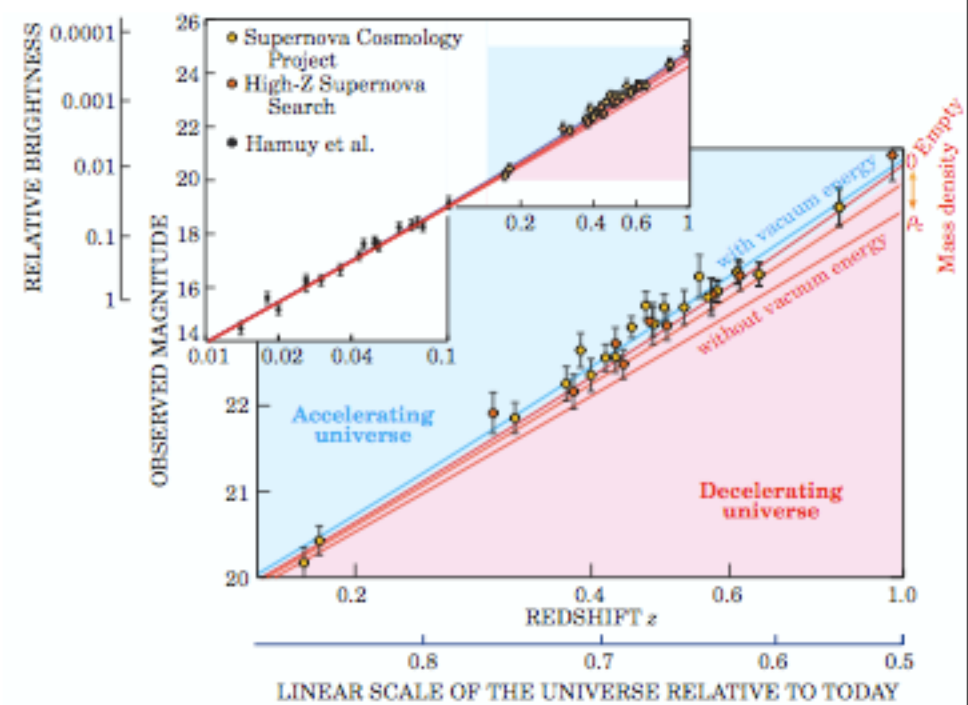





# Nuclear Astrophysics



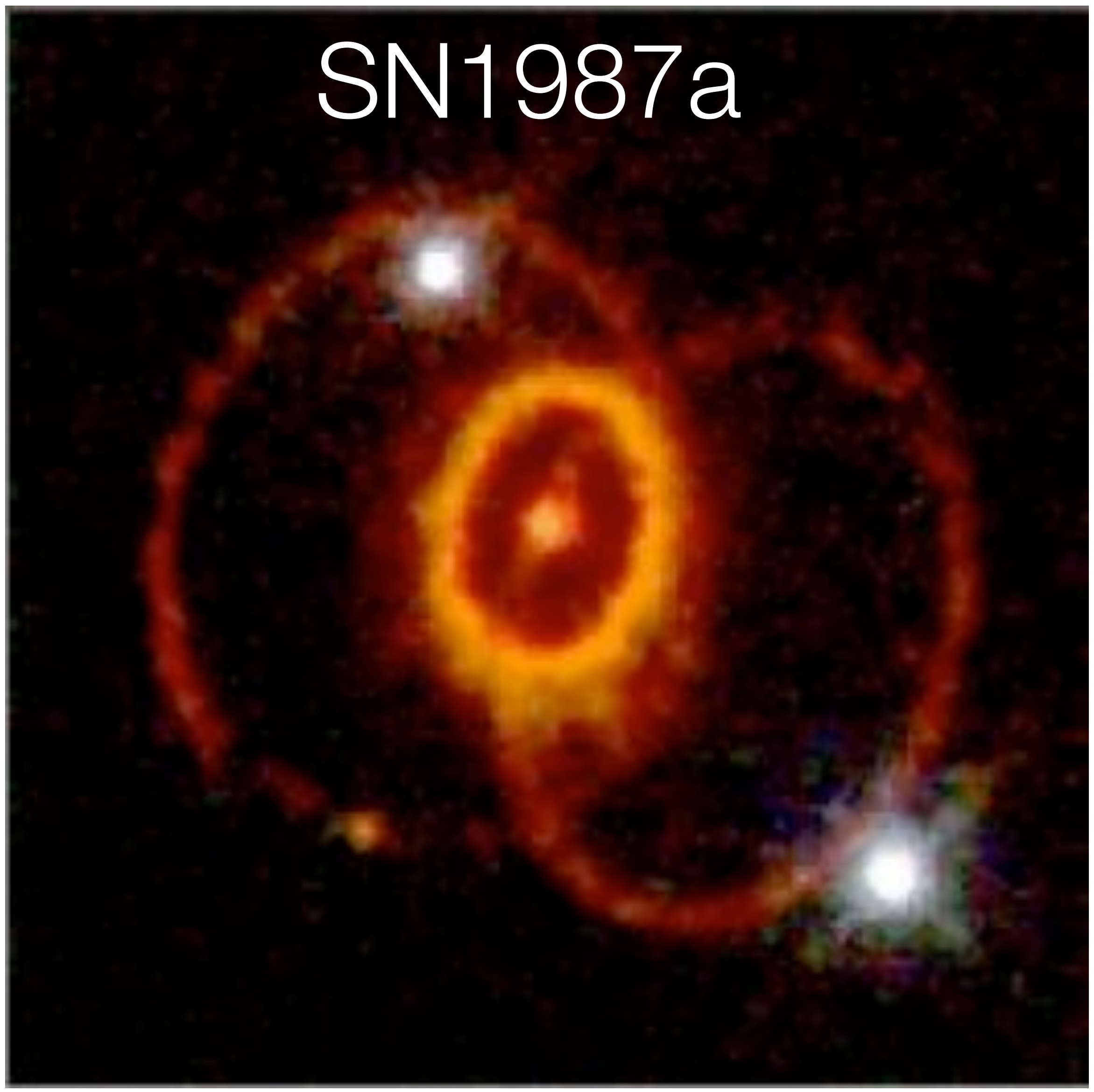



Type 1A Supernovae are Standard Candles in the Universe

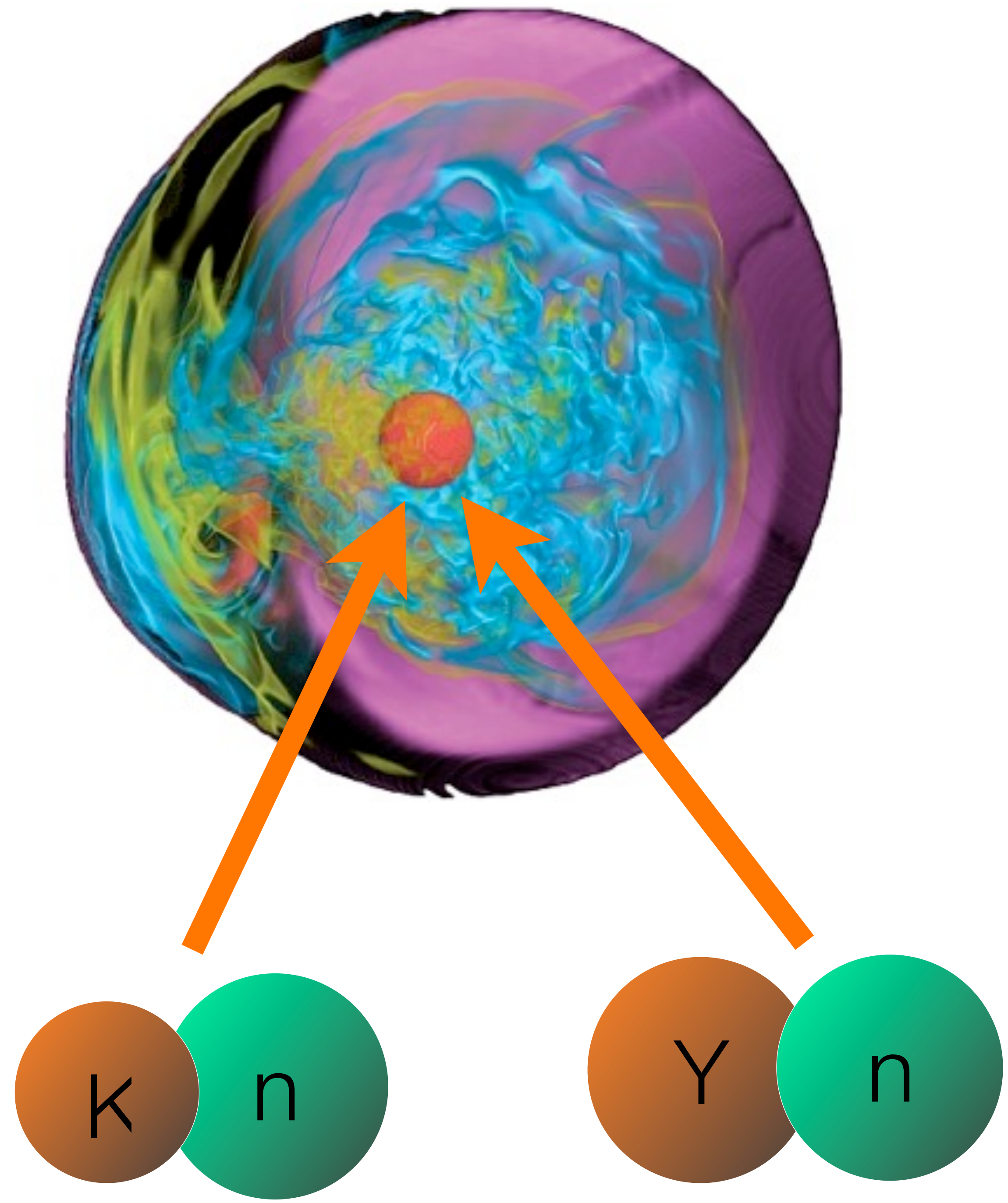
$t > 10^{-6}$ s : Hadrons, Big Bang Nucleosynthesis, Nuclear Astrophysics

# Core-Collapse Supernova and the Heavy Elements

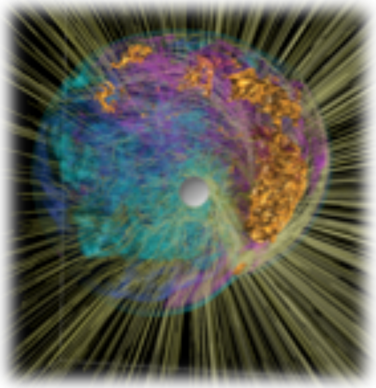



Black-Hole or Neutron Star ?

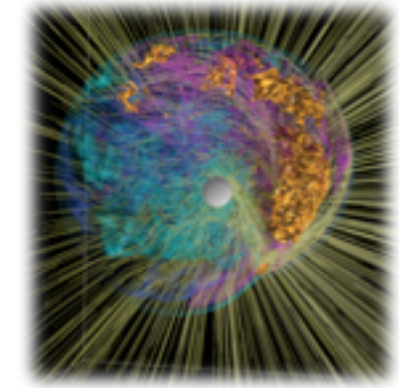
**(Mezzacappa *et al*)**




Nuclear EoS



# Computational Status : Supernovae



## Three Major Code Lines

GenASiS

50K, >65K cores

**Exascale**

Multi-frequency and Multi-angle
Neutrino Transport
2D/3D

- Theoretical foundations laid.
- MHD SASI studies completed.
- Full GR (BSSN) hydrodynamics with AMR nearly complete.
- Boltzmann transport modules under development.

CHIMERA

12K, 18K, 132K cores

**Petascale**

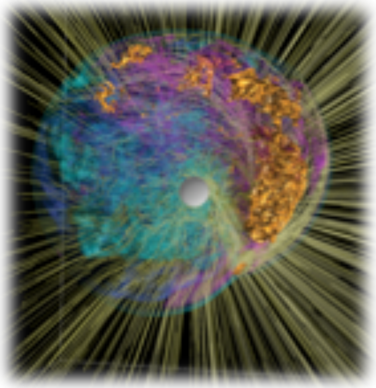
Multi-frequency Neutrino Transport
2D/3D

- First neutrino-driven explosions in 2D models with multi-frequency neutrino transport and first for progenitor masses >15 Solar masses.
- First 3D models with multi-frequency neutrino transport.

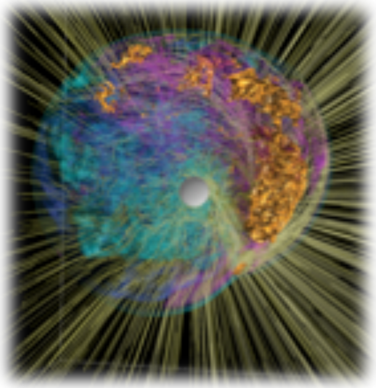
***Agile BOLTZTRAN***

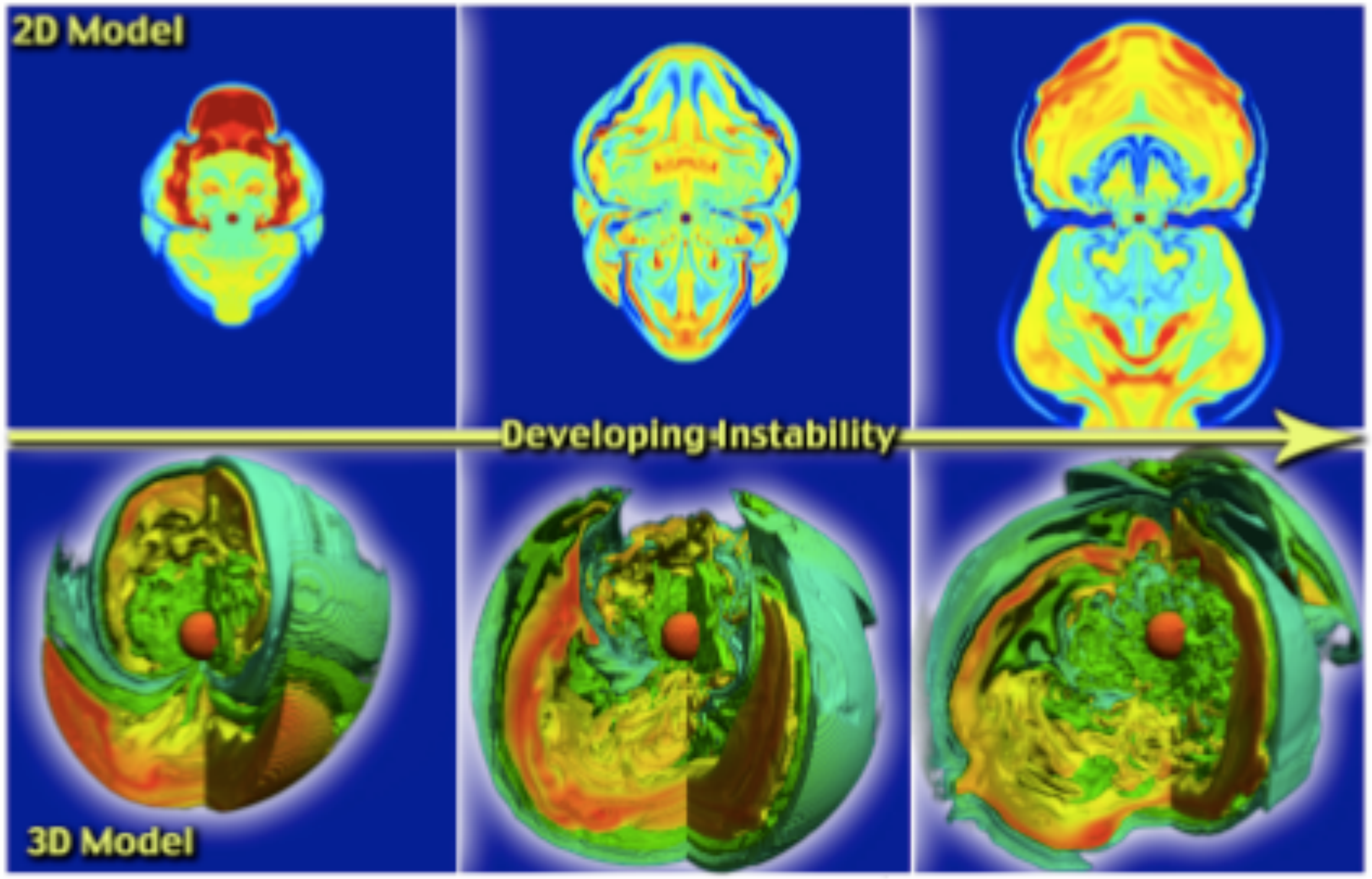
Multi-frequency and Multi-angle
Neutrino Transport
1D

- Remains industry standard in 1D.
- Primary tool for the exploration of new weak interaction and EOS physics.
- Critical validation for 2D/3D codes.
- Critical interpretation of 2D/3D models.

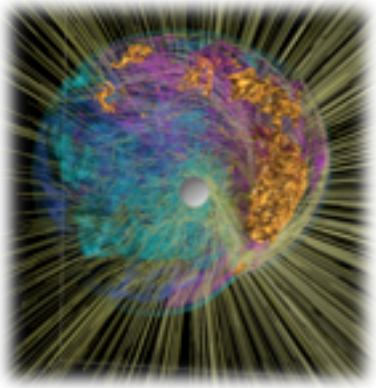


# Computational Status

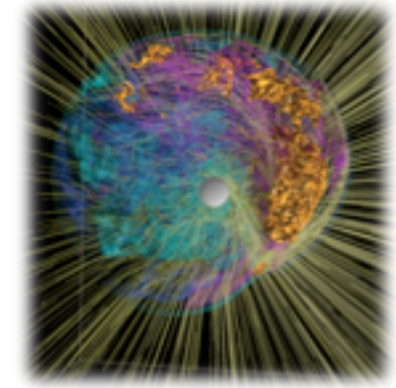


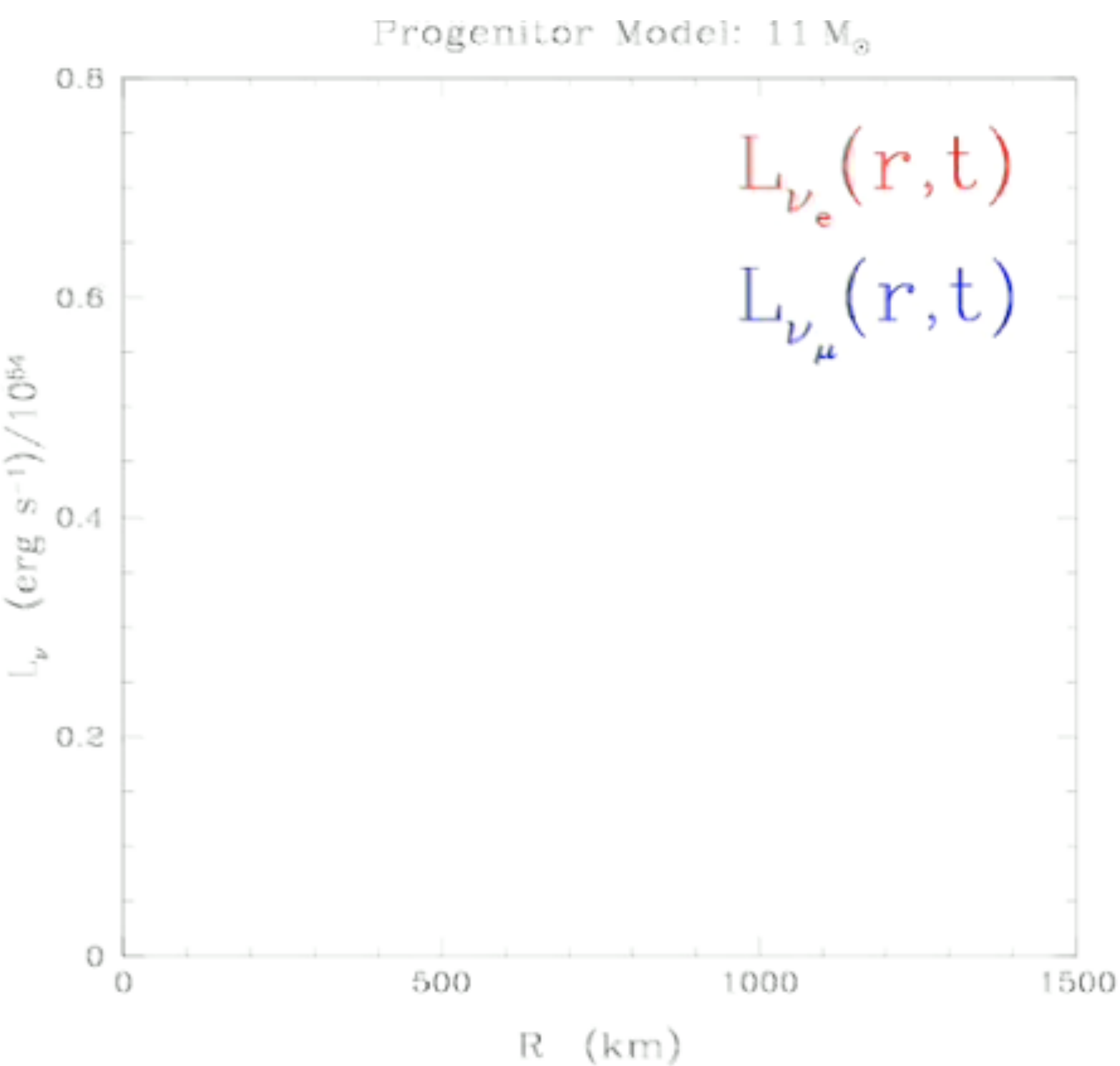


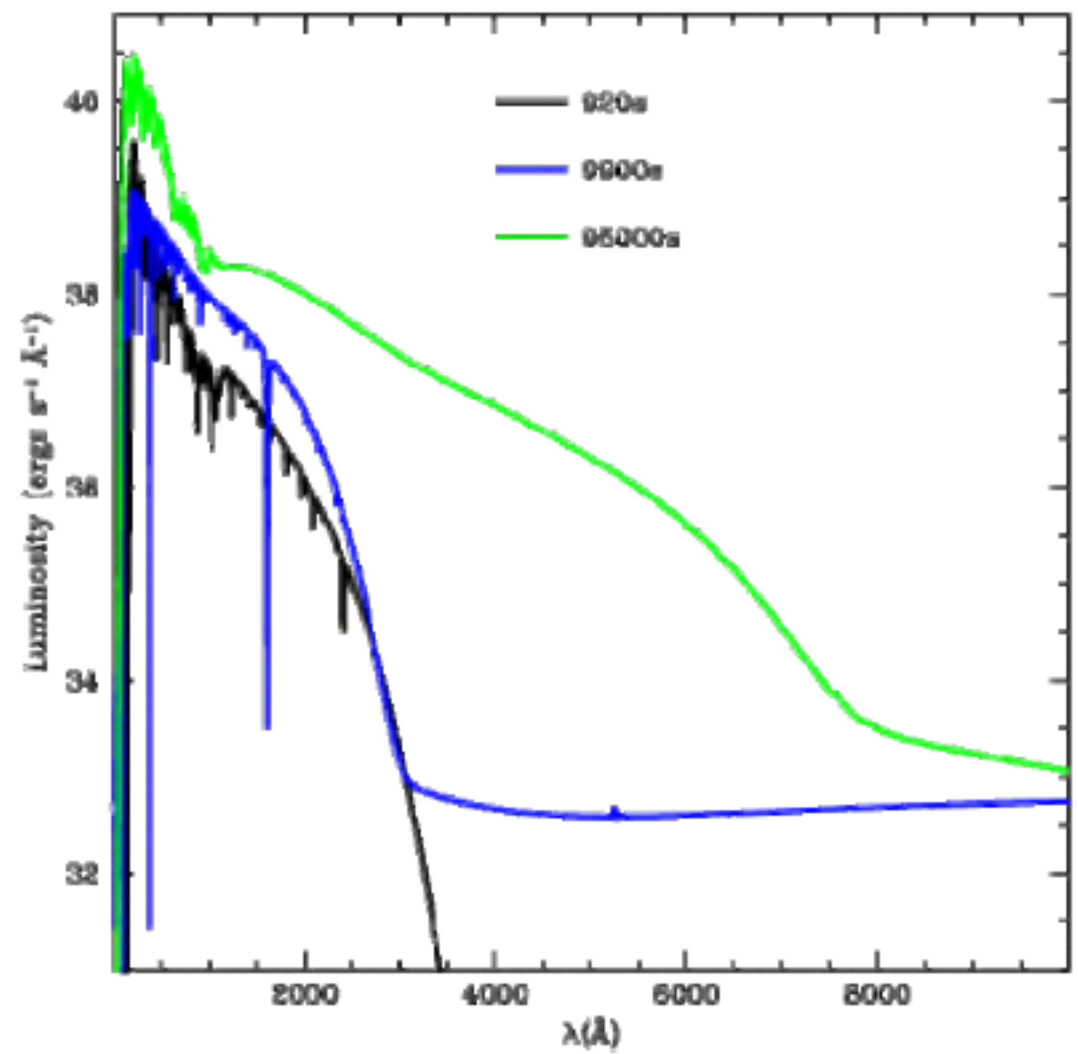

- typical : 50M-100M core hrs



# Observables from Core-Collapse

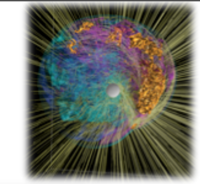


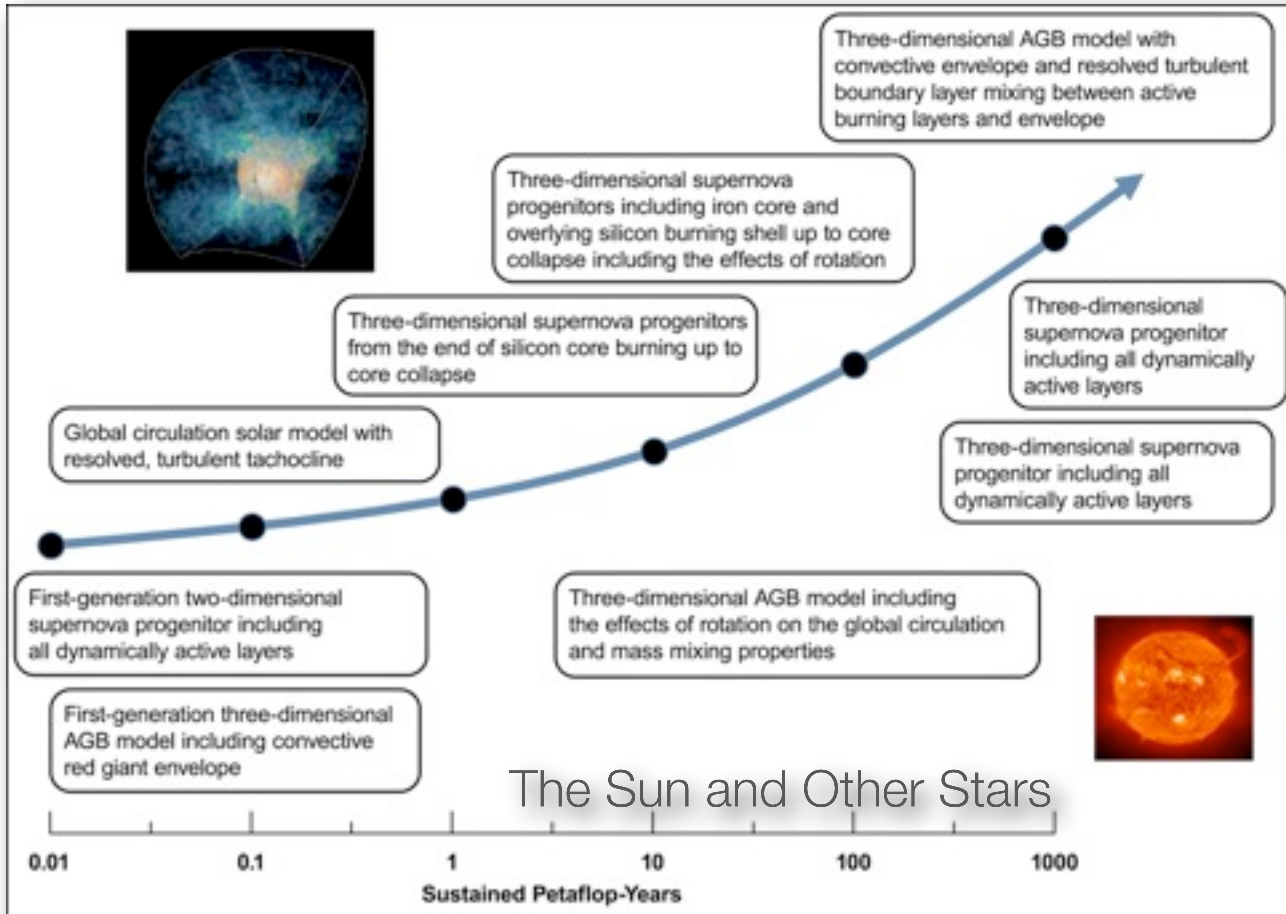


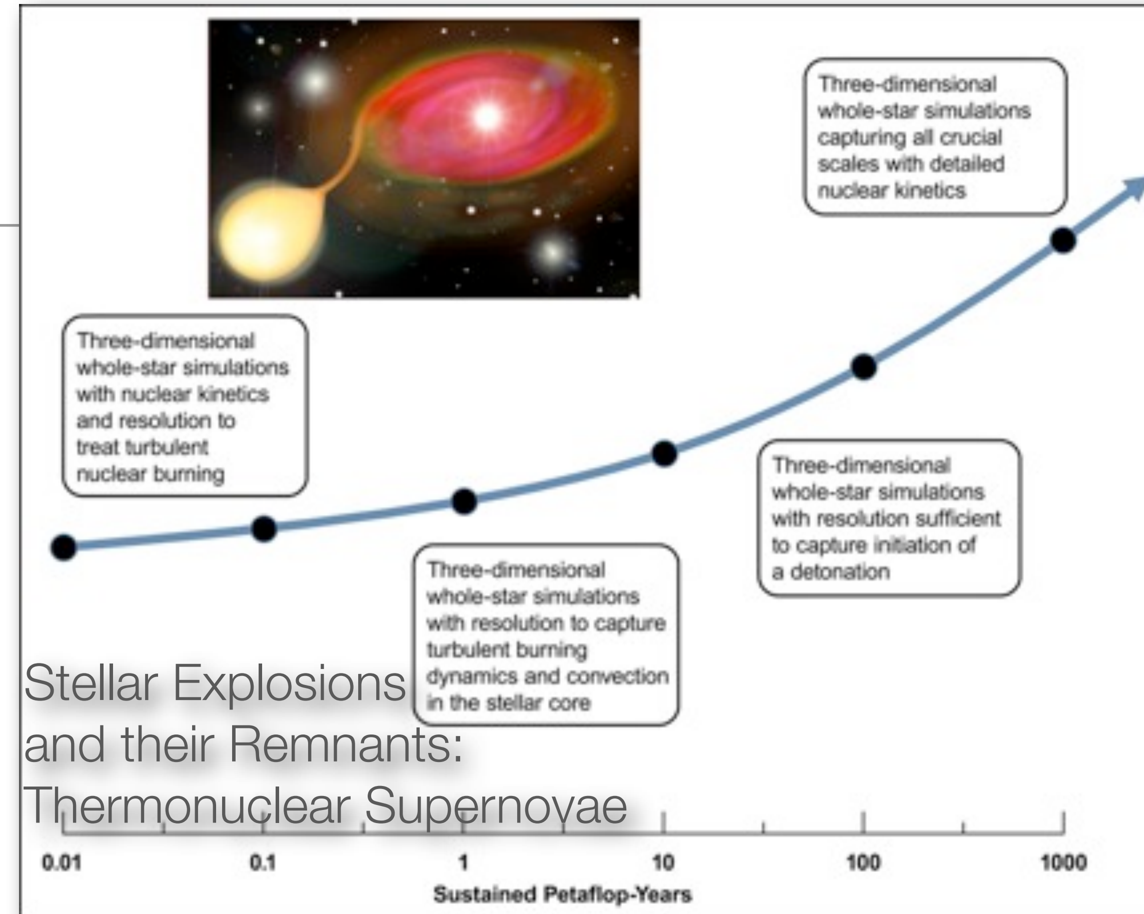



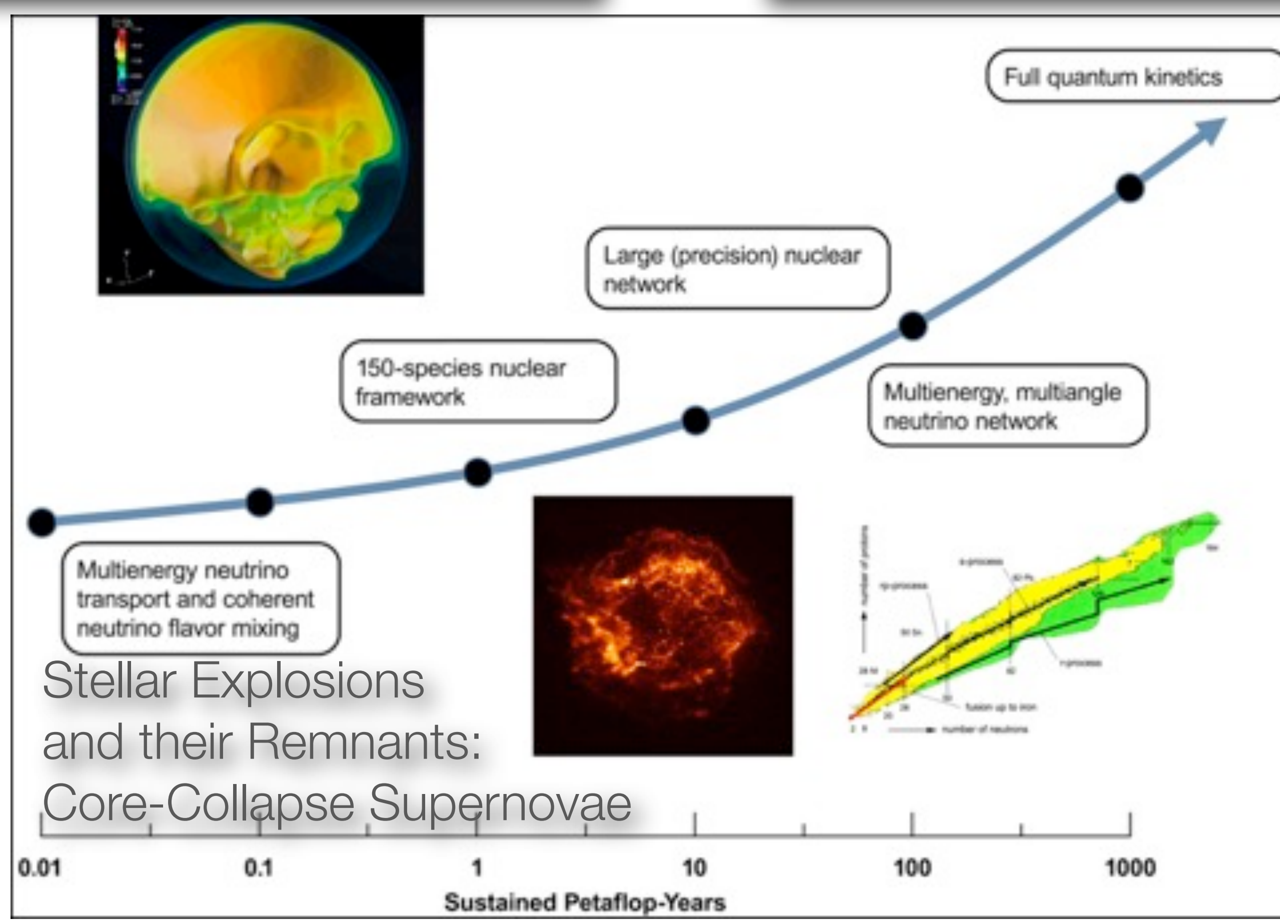

Source: Frey et al. (2009).

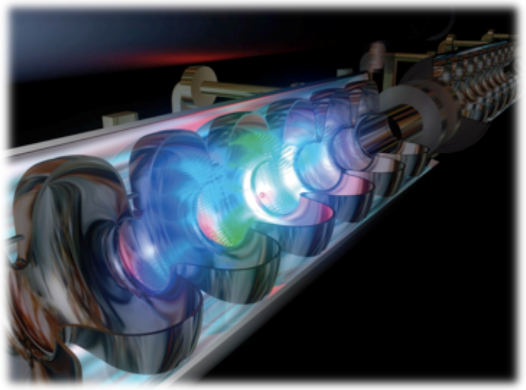
# Computational Requirements



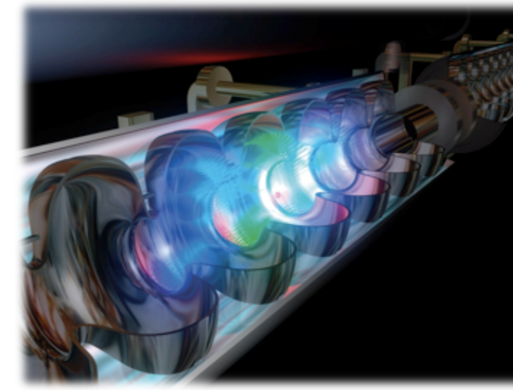


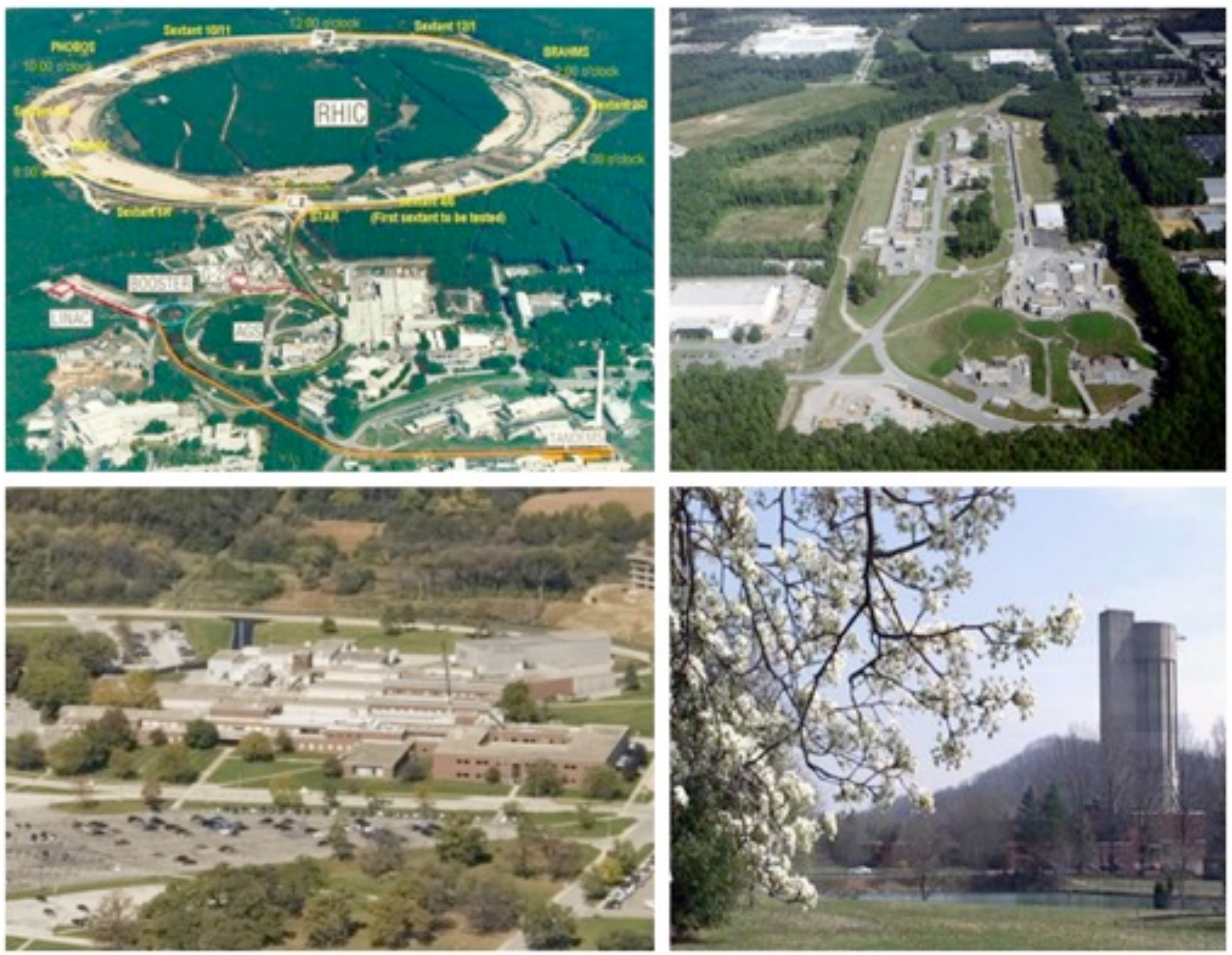



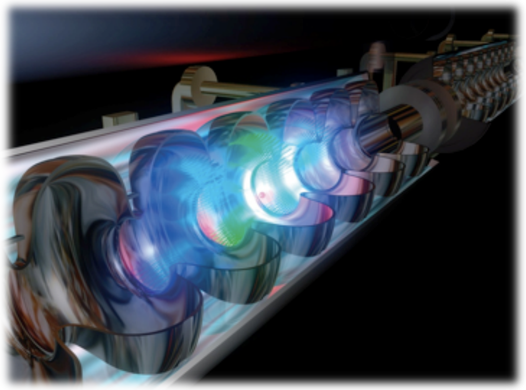


# Accelerators : Research Facilities

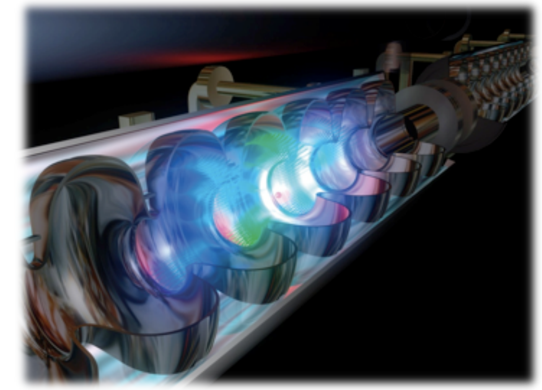




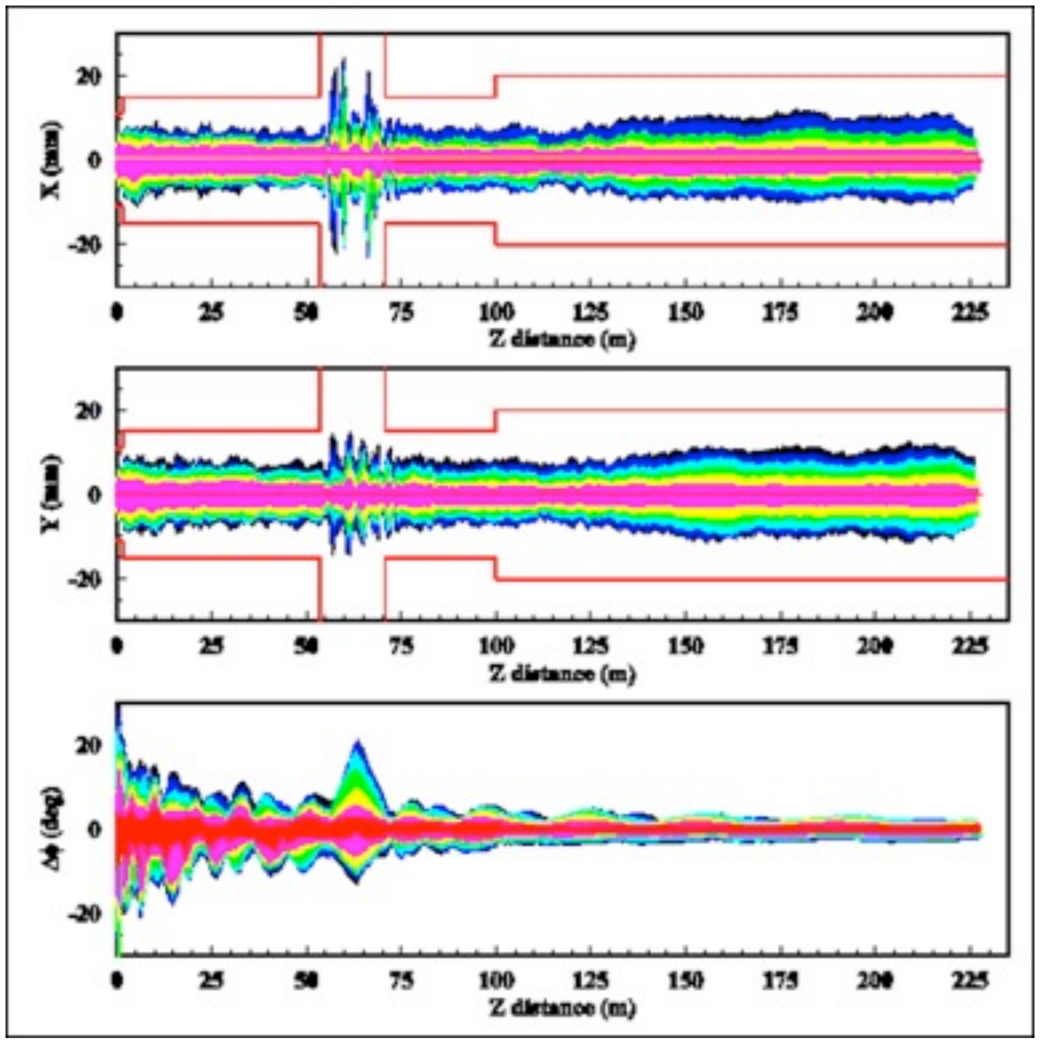

Sophisticated Design, Construction and Operation
Expensive to Build, Expensive to Operate



# Accelerators :
# Design Optimization

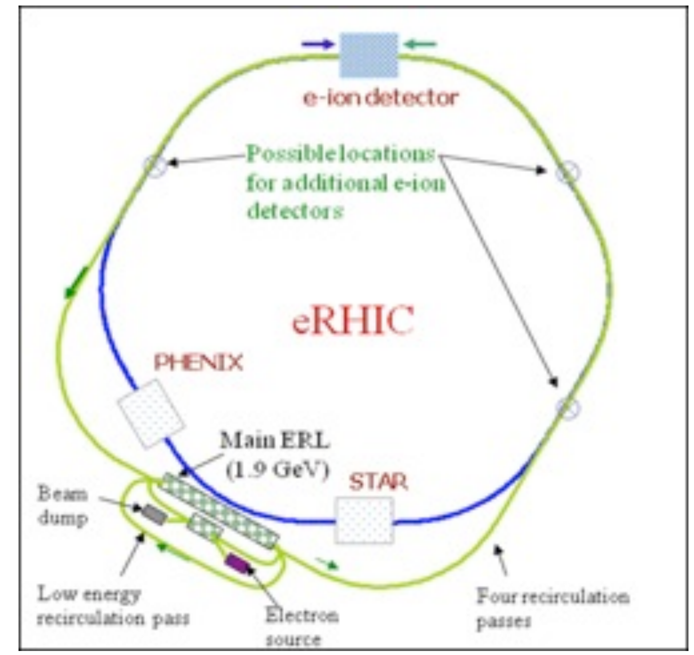


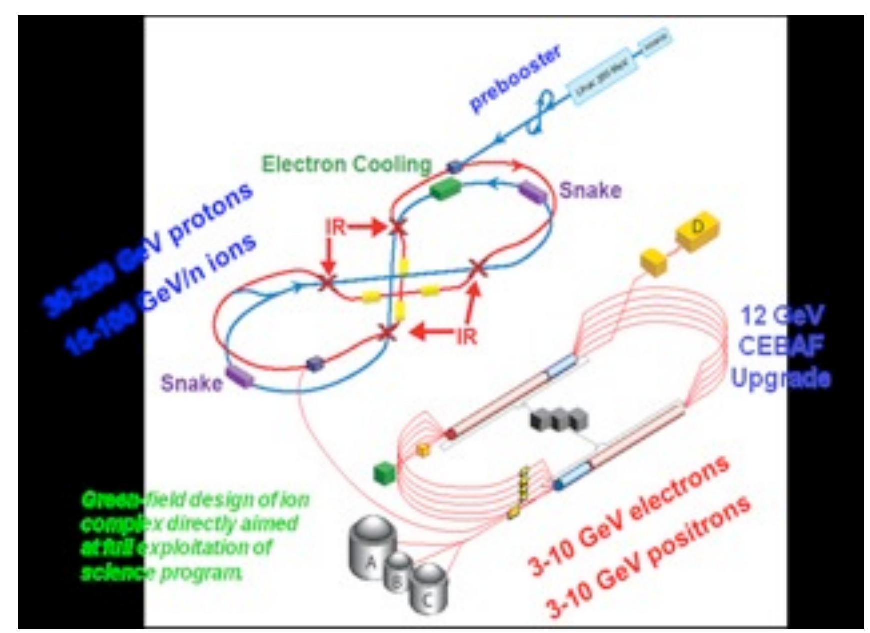
## Design for Facility for Rare Isotope Beams (FRIB)

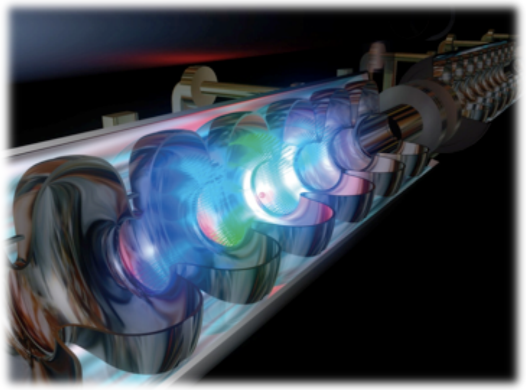



- Uranium Beam
- 2 x $10^5$ particles,
- 100 seeds

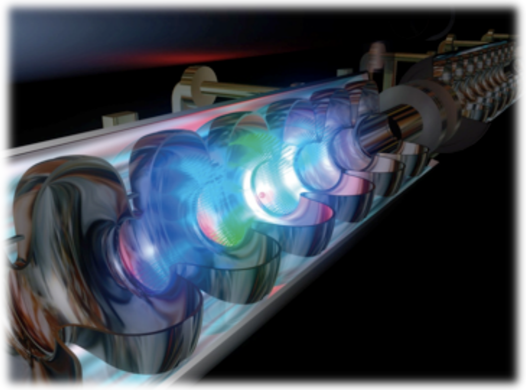
## Design for electron-Ion collider

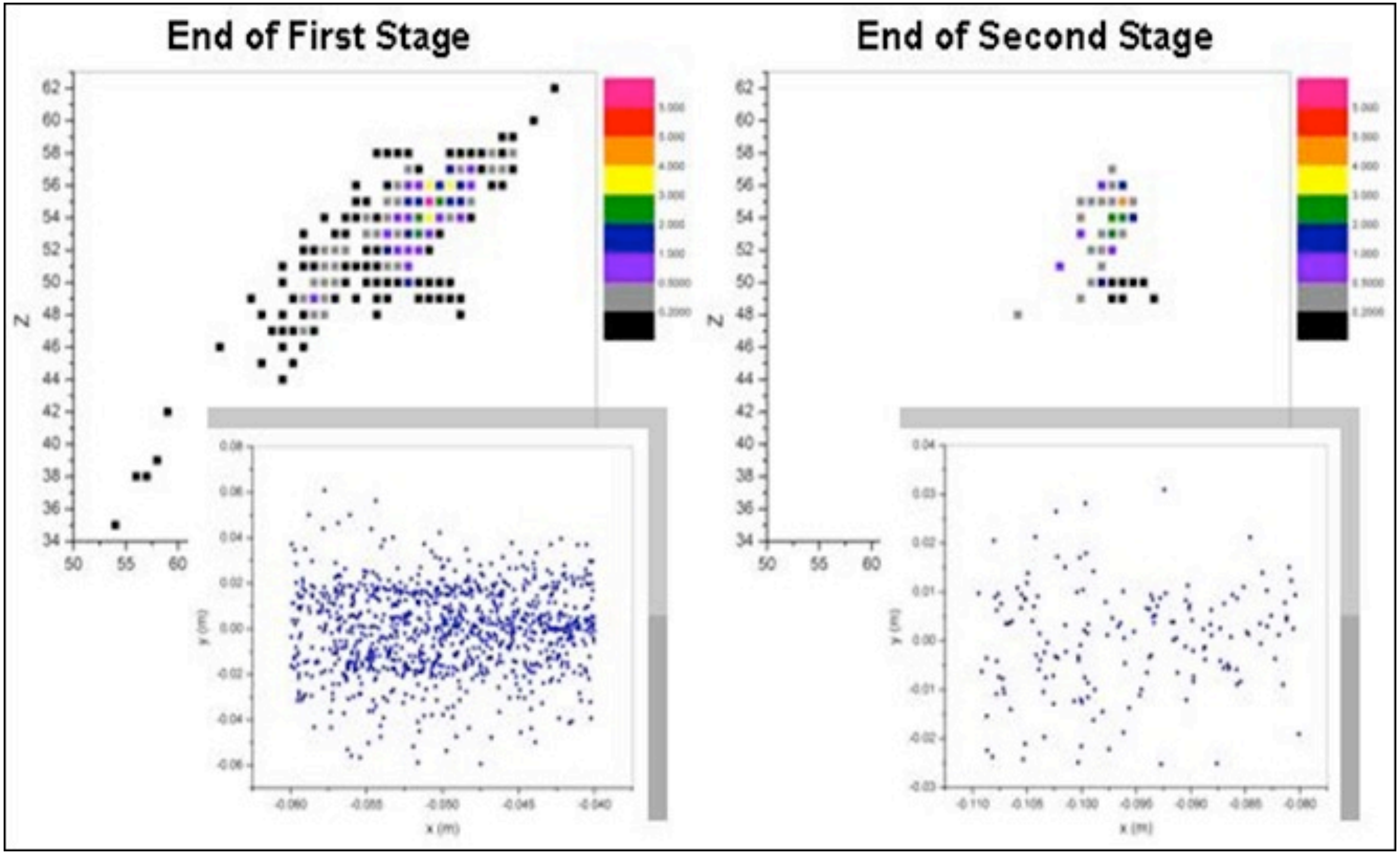




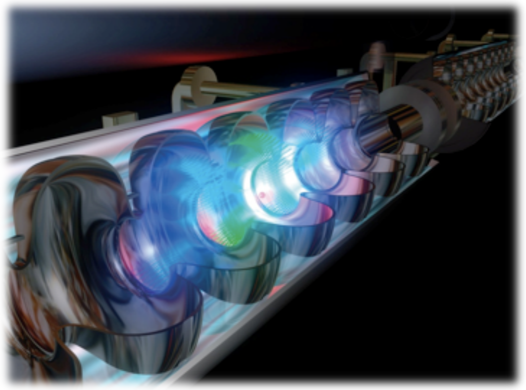
# Accelerators : Design Optimization



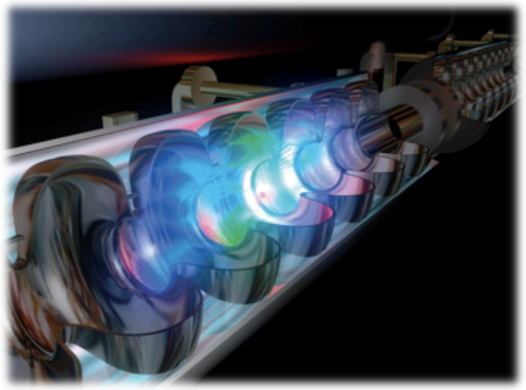



Proposed Two-Stage Separator : $^{132}Sn$

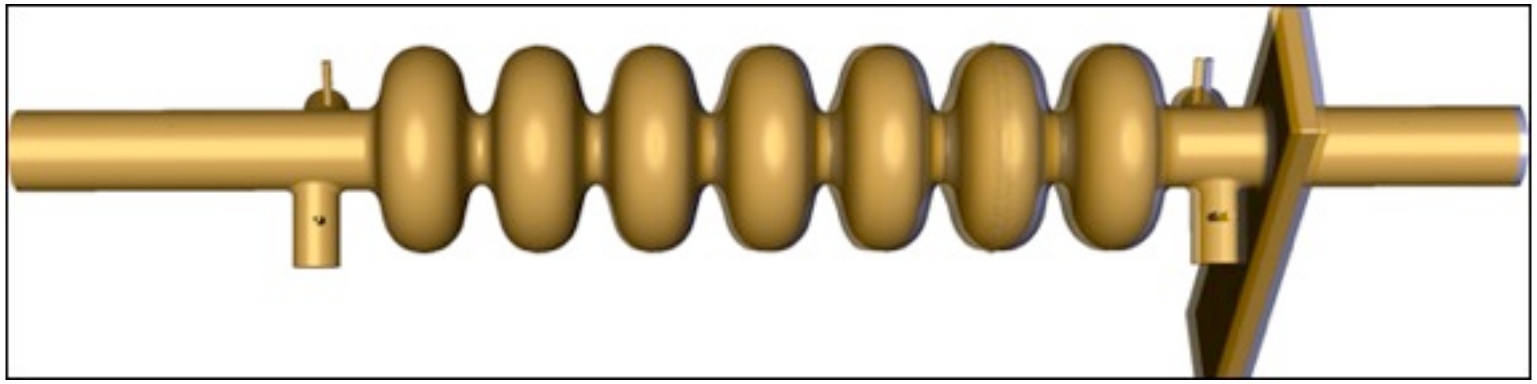
Doubly magic and radioactive **(n,p = 2, 8, 20, 28, 50, 82, 126)**



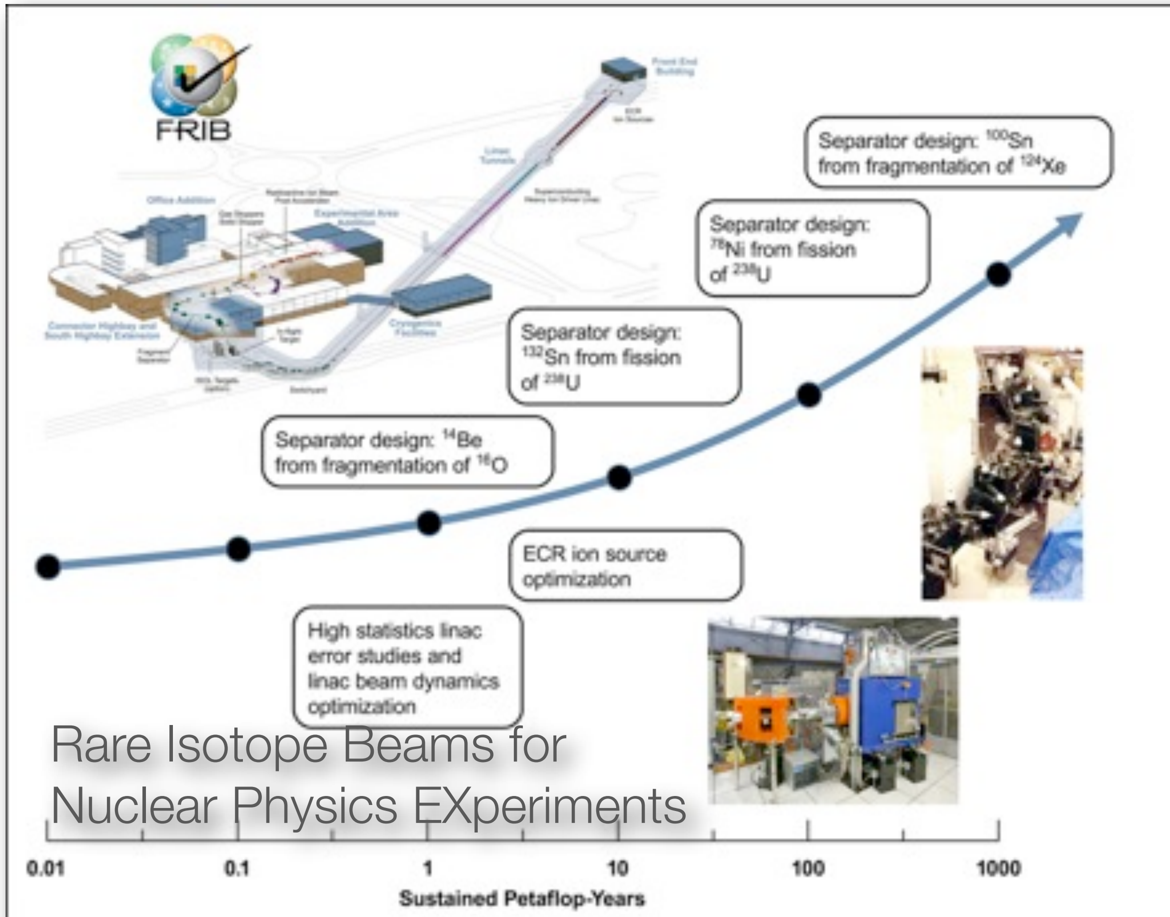
# Accelerators : Research facilities

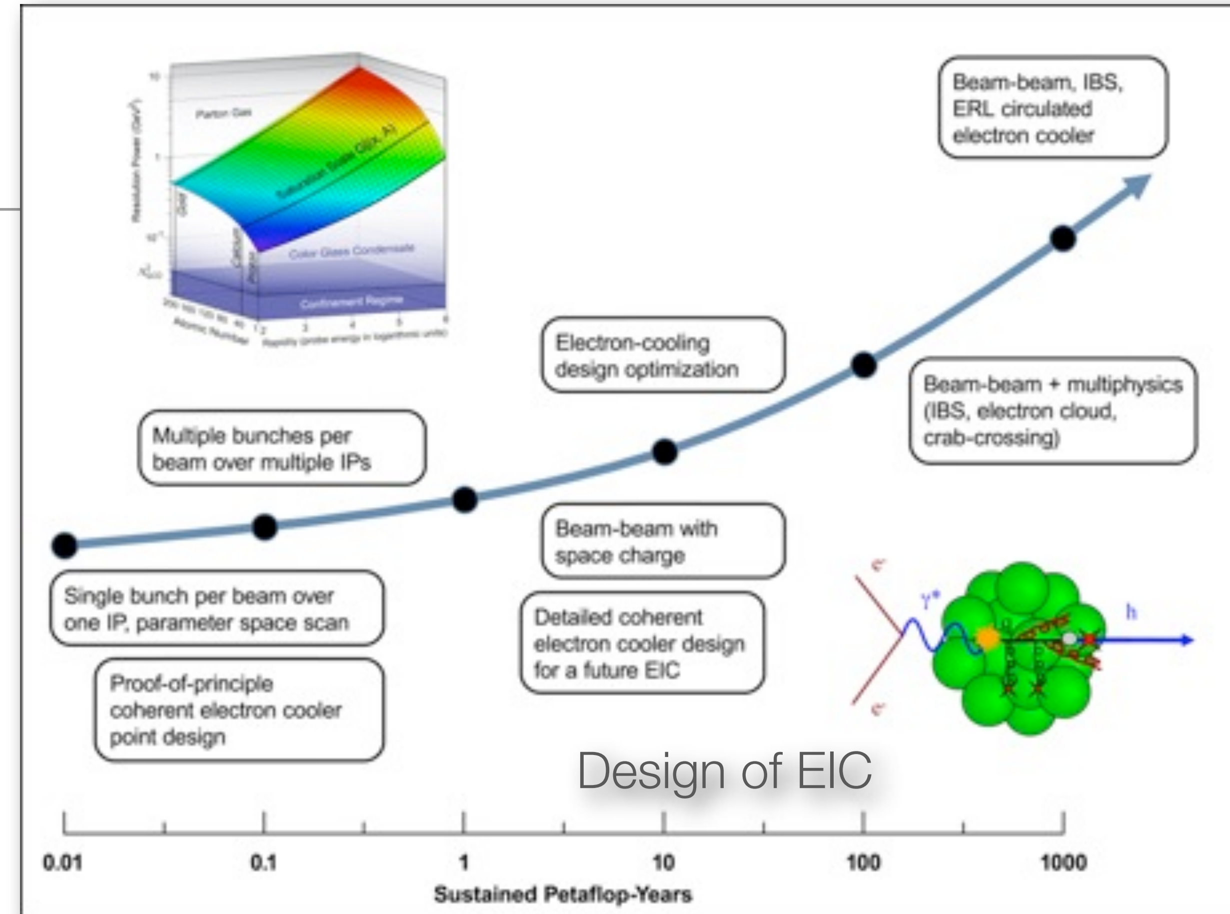


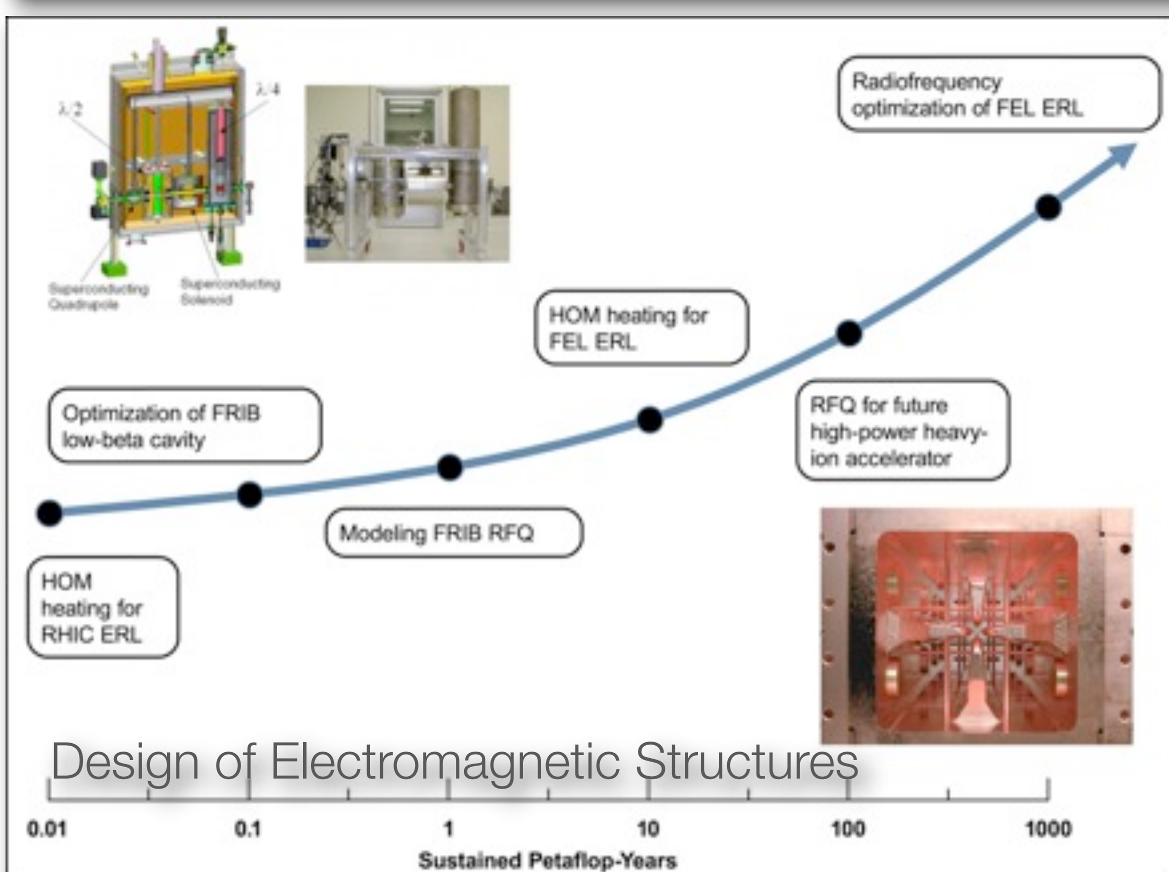
- FRIB design
- Isotope Separator
- EIC
- Beam-Beam at RHIC
- Beam Break-up at TJNAF
- Electron Cooling
- Stability of Non-Linear Dynamics in Synchrotrons

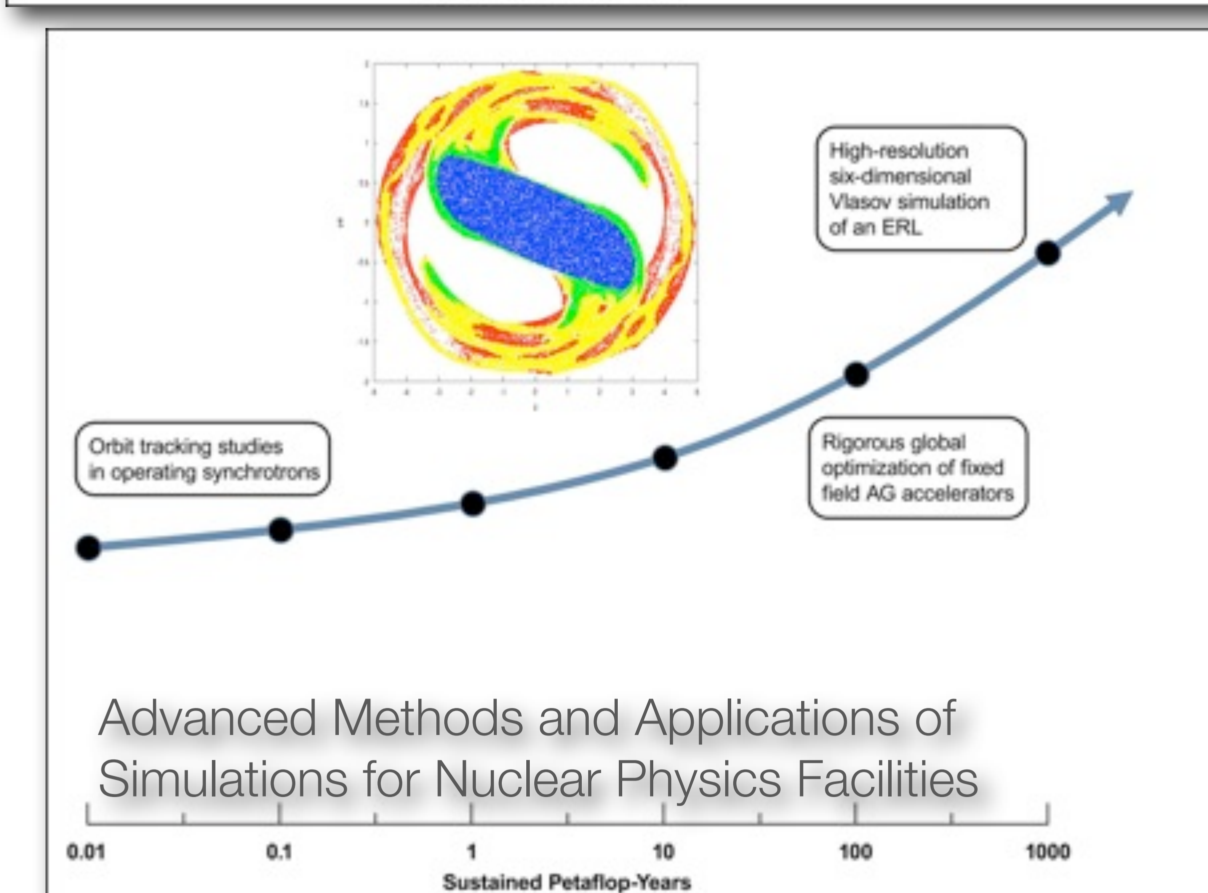


# Computational Requirements



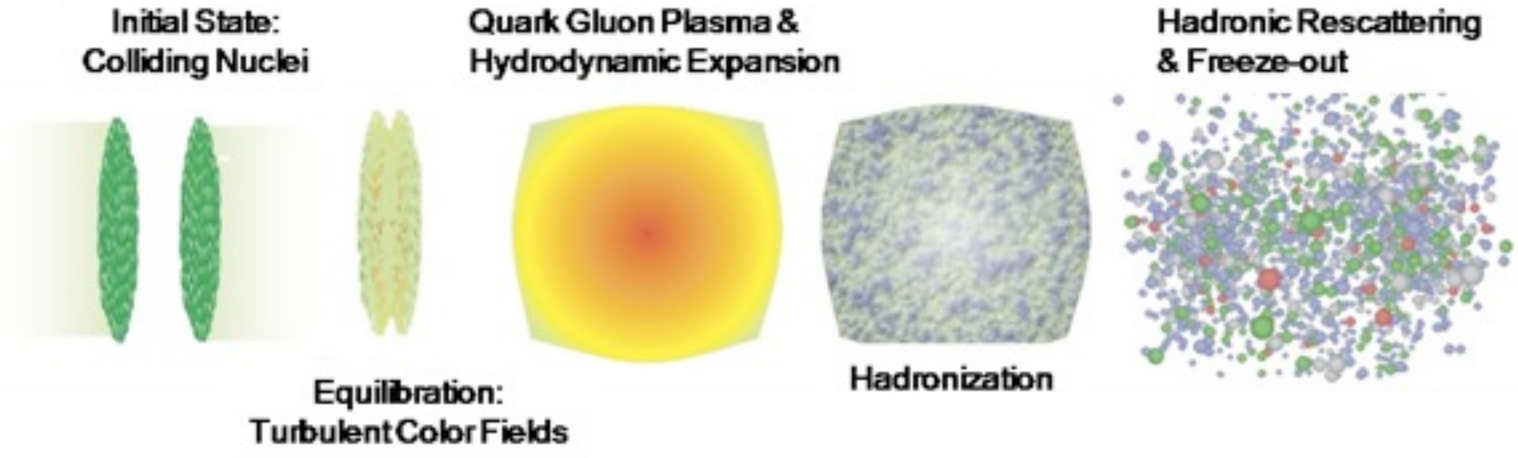



# Beyond Computational Requirements: Number of Formal Issues, e.g.

How to deal with the sign-problem at finite density?

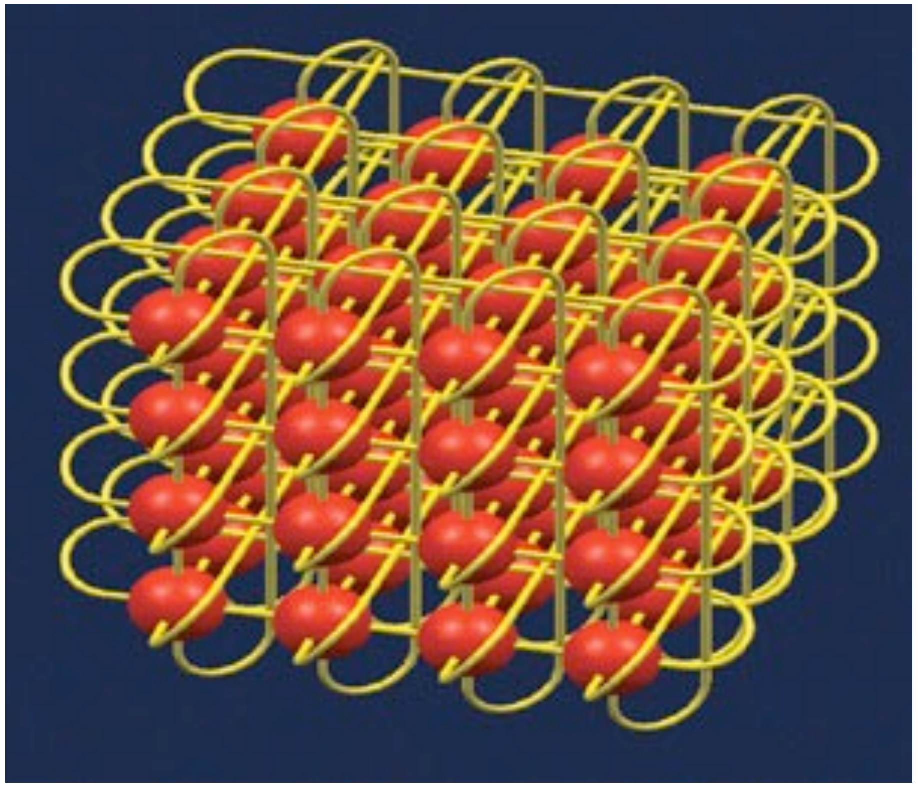

How to invert heavy-ion data to constrain critical point?



# How Much Computing is that?

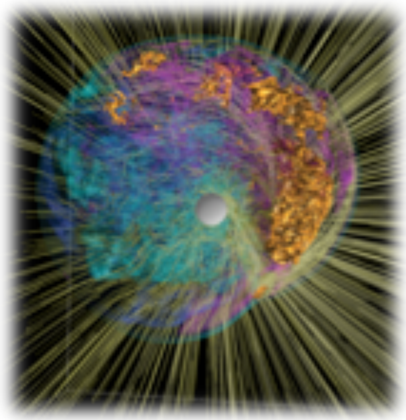
~ 1 Gigaflop
~ 9 thousand core-hours/year

1 Exaflop = $10^3$ Petaflops = $10^6$ Teraflops = $10^9$ Gigaflops

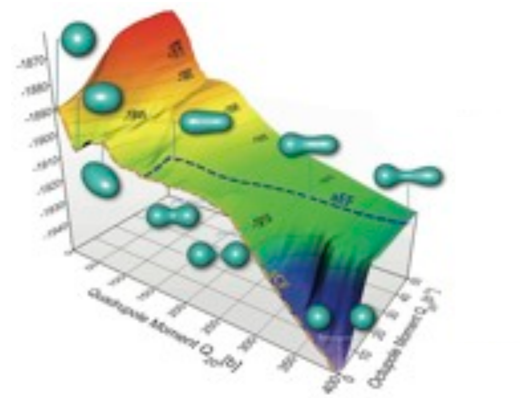



~10 Petaflops, 2.2 Gflops/Watt
~700 000 compute cores


# Different Hardware Requirements

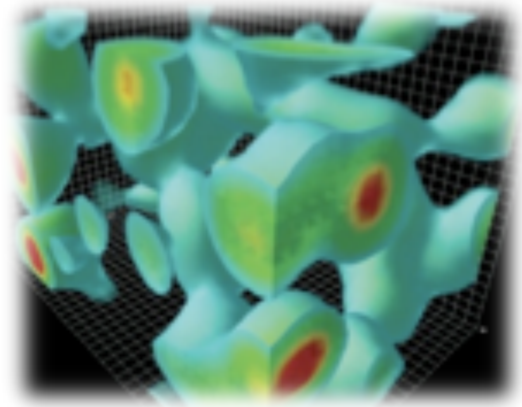


Nuclear Astrophysics

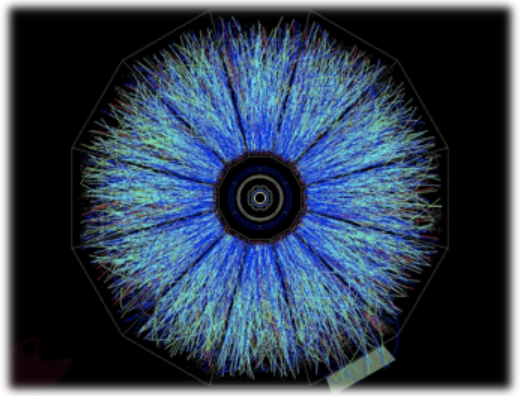


Nuclear Structure and Reactions

- Significant memory/core
- Fast memory access
- somewhat conflicts with present machine design ?
- low efficiency
- in current design : 4 GB/core preferred
- IO



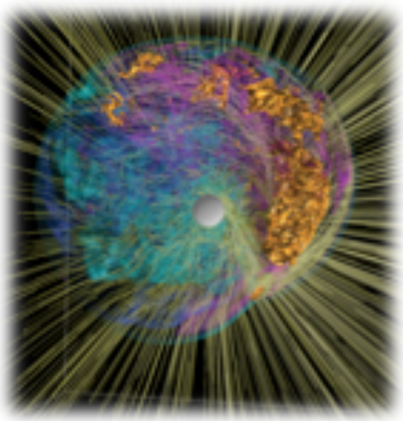
Cold QCD and Nuclear Forces



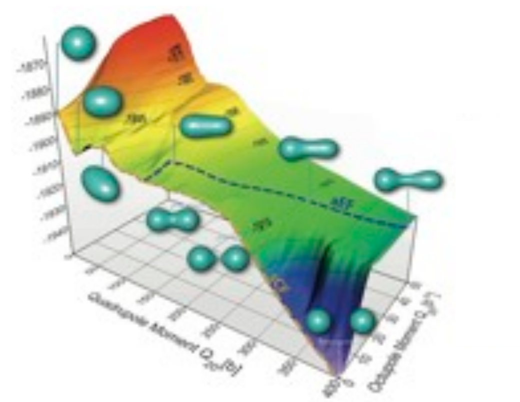
Hot and Dense QCD

- Modest memory per core
- Large number of cores
- Range of Partitions
- Fast network
- low latency
- IO

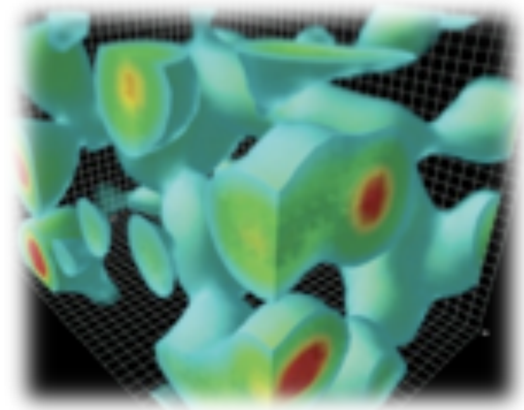

# Different Hardware Requirements



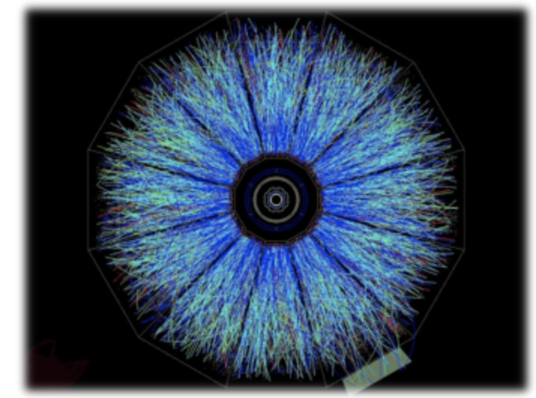
Nuclear Astrophysics



Nuclear Structure and Reactions



Cold QCD and Nuclear Forces



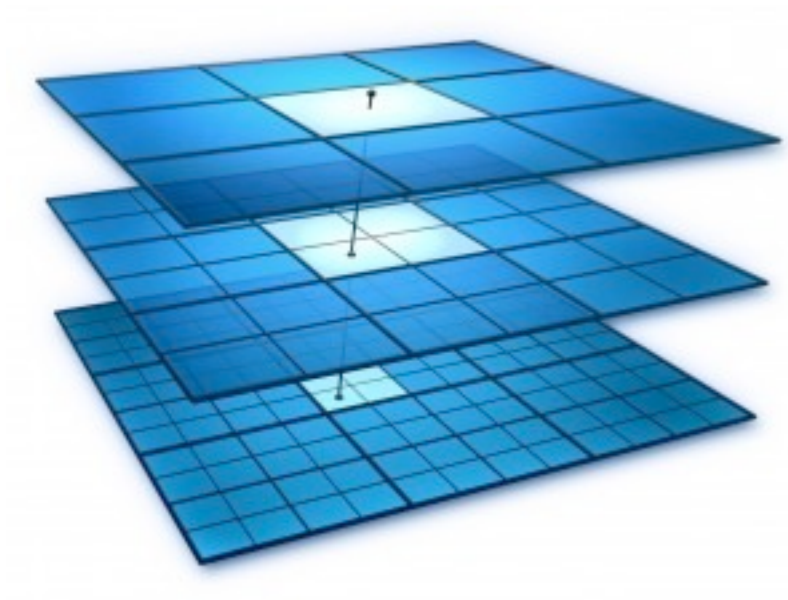
Hot and Dense QCD

Require a distribution of capacity and capability computing resources

# Algorithms and Applied Mathematics

## e.g. How to solve **optimally** ?

A.x=b



- Multigrid is current (new)  technology...
- What is next ?
- Requires talking/collaboration with CS and AM researchers

SciDAC
Scientific Discovery through
Advanced Computing

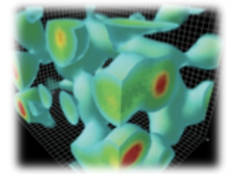
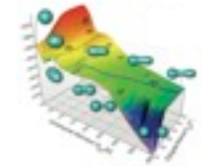
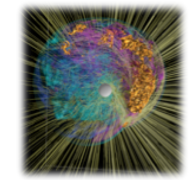
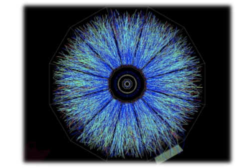
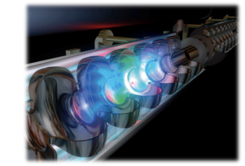

# Cross Cutting Challenges

- Scaling - algorithms and codes
  - Adapting to new architectures
    - GPU's - well underway in some areas, but not all
      - people-power issue - i.e. it costs money to have someone do it !
    - memory and communications use
- asynchronous I/O and load balancing across millions of cores
  - adaptive-mesh and MC
- Fault tolerance and checkpointing
- Memory/core likely less on extreme facilities - memory management
- Large data sets to be held during calculation,
  - e.g. supernova calculations -- new algorithms

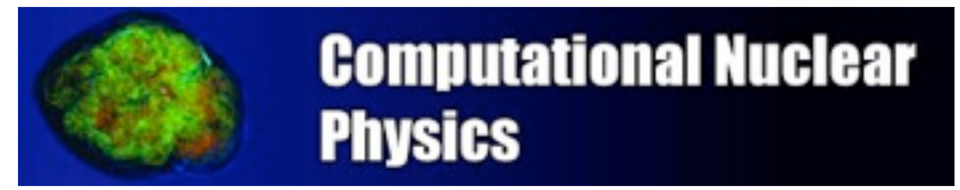

# Cross Cutting Challenges

- Large outputs - large post-processing facilities -
  - capacity issue
  - Visualization and data handling/science extraction
- Data management among large collaborations distributed around US/world
- Arbitrary precision calculations (> double precision) - already being implemented
- Improved linear algebra techniques for large matrices
  - sparse-matrix eigensolvers
- global nonlinear optimization for nonlinear constraints
- improved programming environments
- verification and validation issues for extreme-scale computing


# Collaboration in the Exa-Scale Era

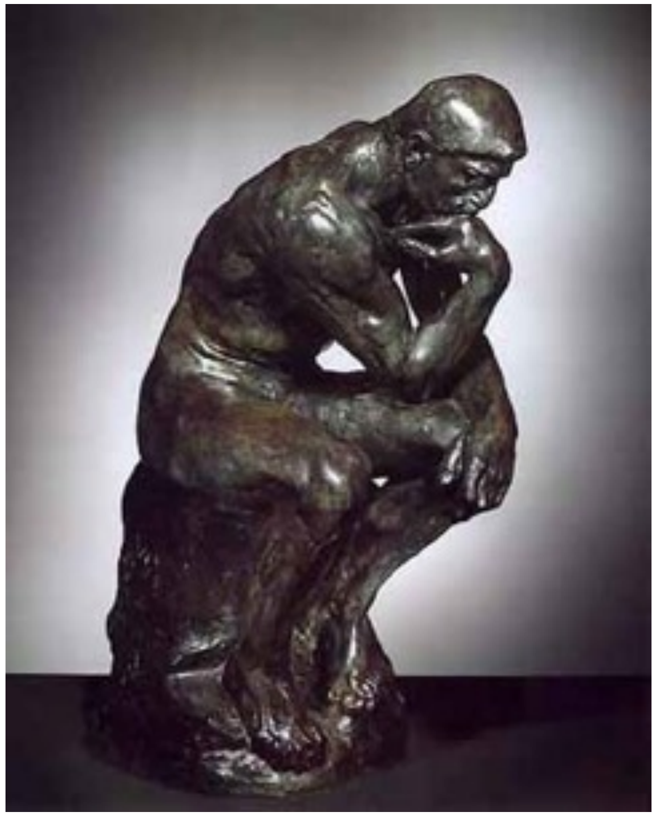
- Different areas in Nuclear Physics
  - coherent community effort
  - with Particle Physics, Plasma, Fluids, ....
- Computer Scientists
  - hardware development
  - optimizations
  - new coding paradigms
  - data management, visualization....
- Applied Mathematicians
  - algorithm development
- Statisticians
  - Monte Carlo
- Many collaborations currently exist
  - embraced and strengthened
  - requires support mechanism
  - International and multi-Institutional




# Human Resources

- Extreme-scale by 2020 (?) :  need to further grow expertise in the NP community
    - resource growth substantial - faster than Moore's Law
    - algorithms/code evolution should follow growth curve



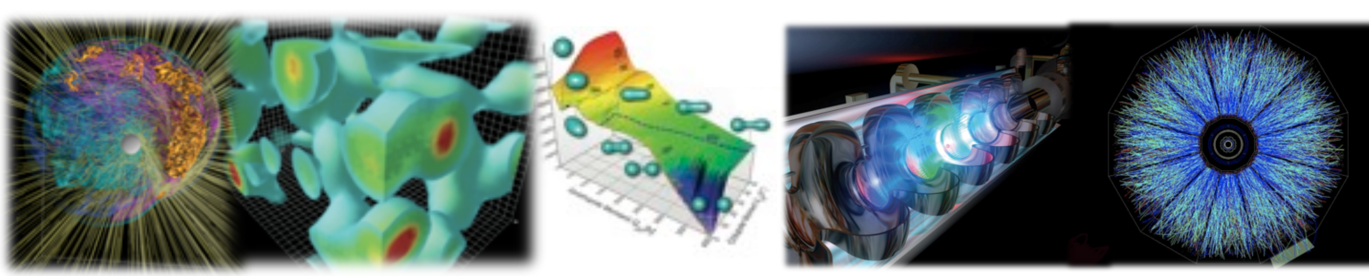
- The standard interdisciplinary hiring problems exist
    - challenges to the current system
    - new training models

- Broad collaborations
    - Graduate  students and postdocs hired into collaboration
        - naive scaling from RHIC and UNEDF programs  =
          SIGNIFICANT enhancement in person-power  (+10+10 per project ?)

    - Organization  in the Nuclear Physics community


# Further Enhanced Nuclear Physics Program

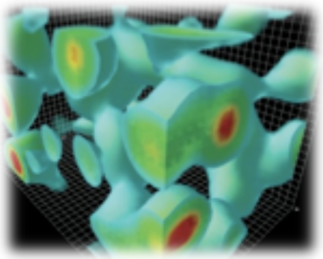
- New (Nuclear) Physics areas will likely emerge through Extreme-Scale research
- Additional Nuclear Physics goals during evolution to Extreme-scale
- Deeper cross-fertilization between sub-fields
- Nuclear Physics drive to Extreme-scale will spawn research in Computer Science, Applied Math, High Energy Physics, Statistics, ....

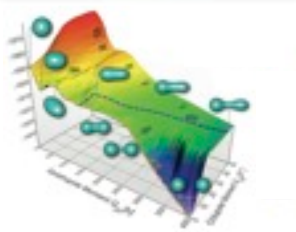


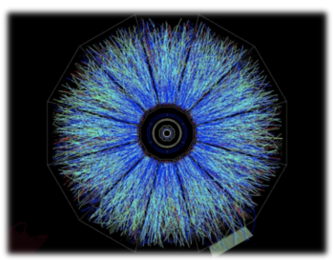
| ? | ? | ? | ? |
|---|---|---|---|

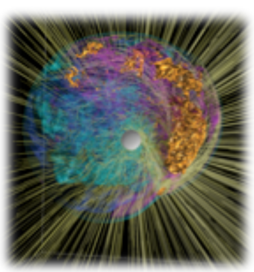
# Concluding Remarks

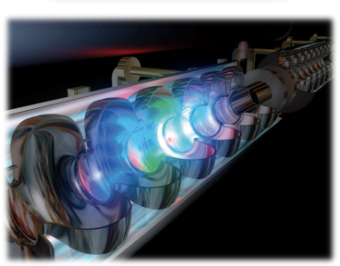
INT











- Extreme-scale computing is required to accomplish the scientific goals of nuclear physics.
- The field will be enormously transformed/unified by such resources
- The community is eager for such resources and is preparing for them
- Answer long-standing nuclear physics questions that will impact
  - Basic Science
  - Energy
  - Security

**Thanks to organizers**

# End