

**Computational Nuclear Physics**

Summary and Whitepaper

SURA Headquarters  
Washington D.C.  
July 23-24, 2012

# Nuclear Physics Research

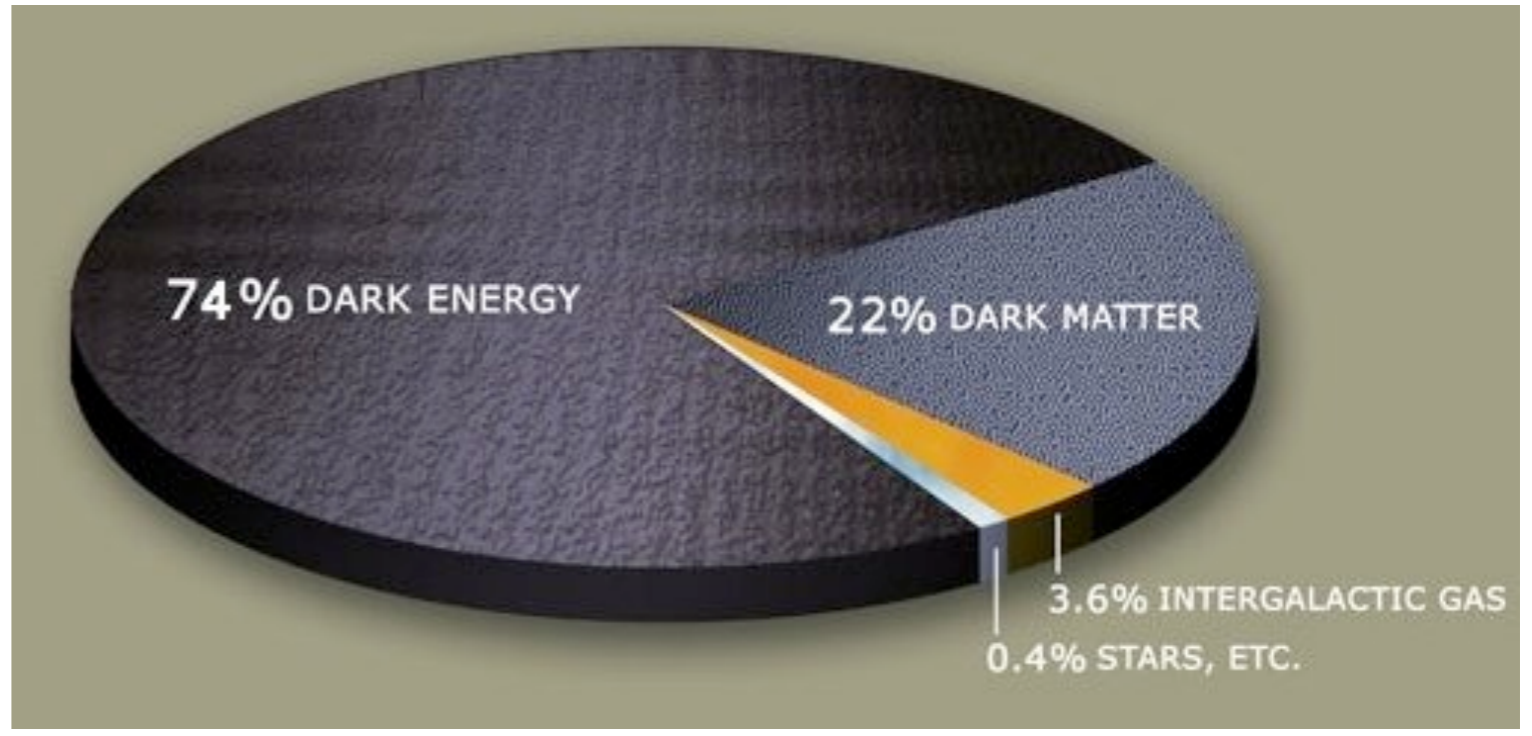
Unraveling the Origin  
and Nature of the  
Visible Matter



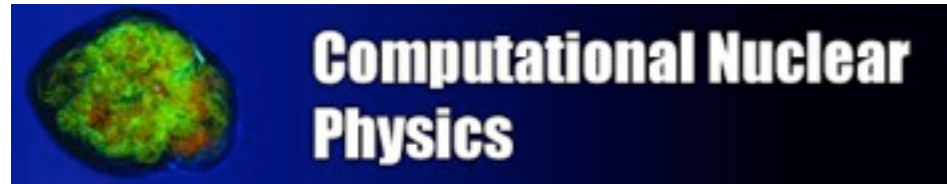
Nuclear Physics



Quantum Chromodynamics  
Electroweak Interactions

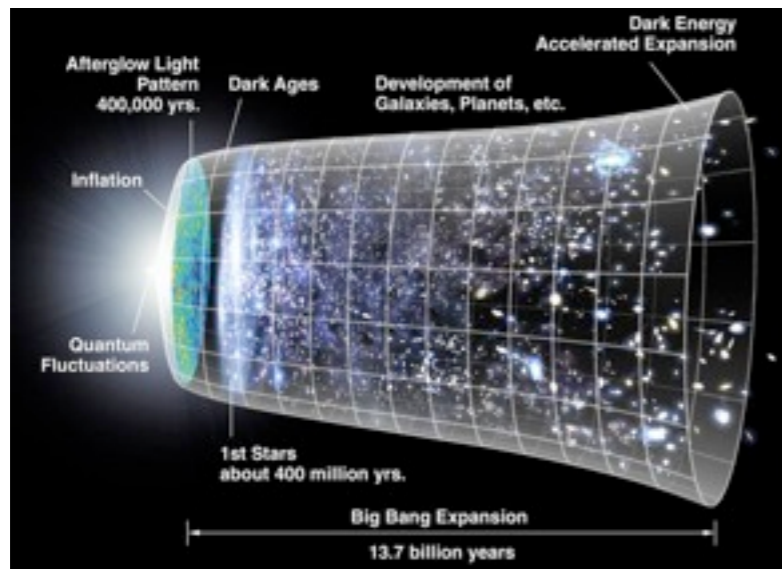


Establishing and verifying the capability to reliably predict

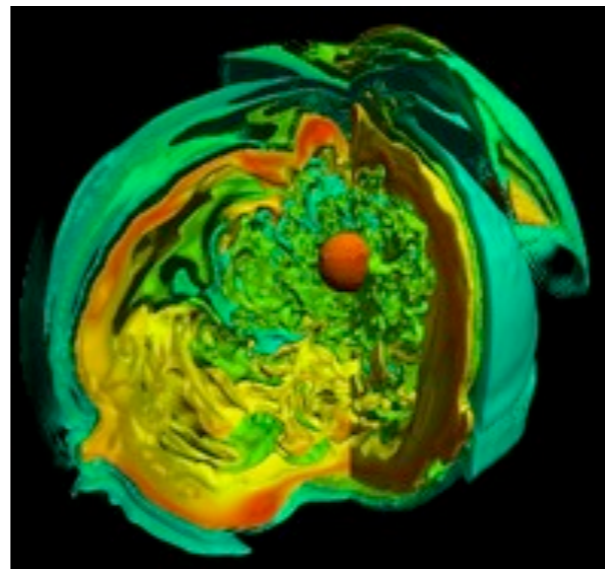


# A Broad and Balanced Nuclear Physics Agenda

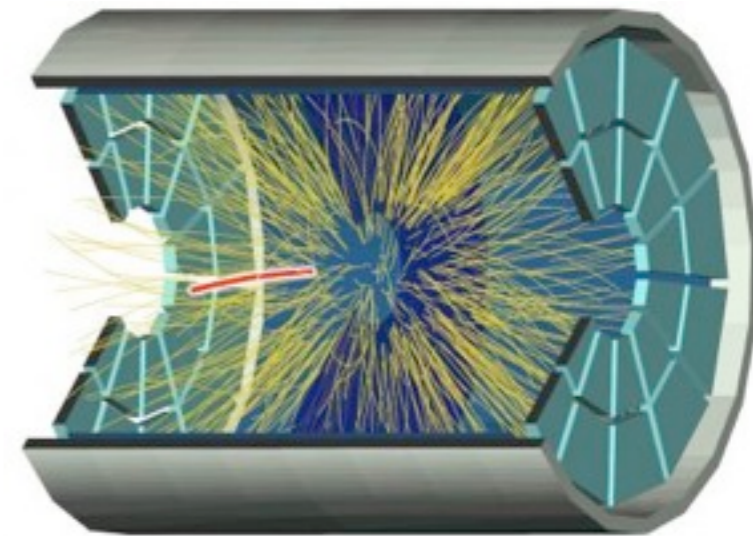
Phase transition(s) at early times,  
light sources at later times



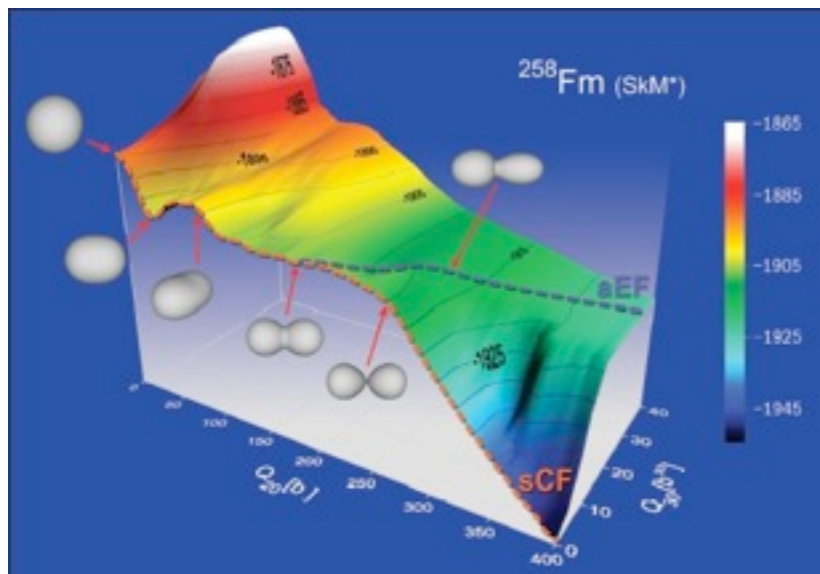
Production of most  
elements in the cosmos



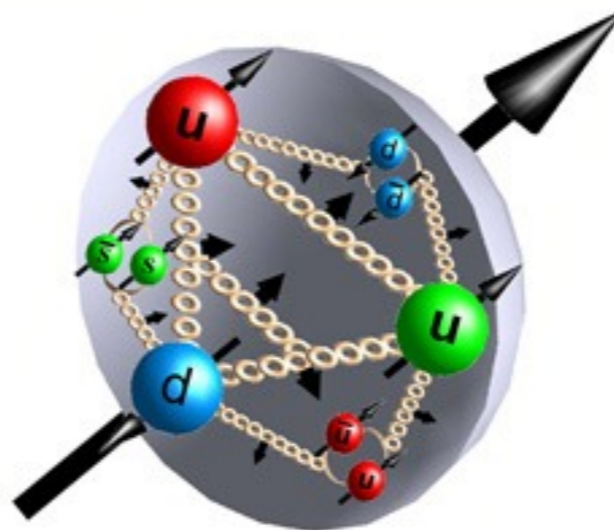
Matter under  
extreme conditions



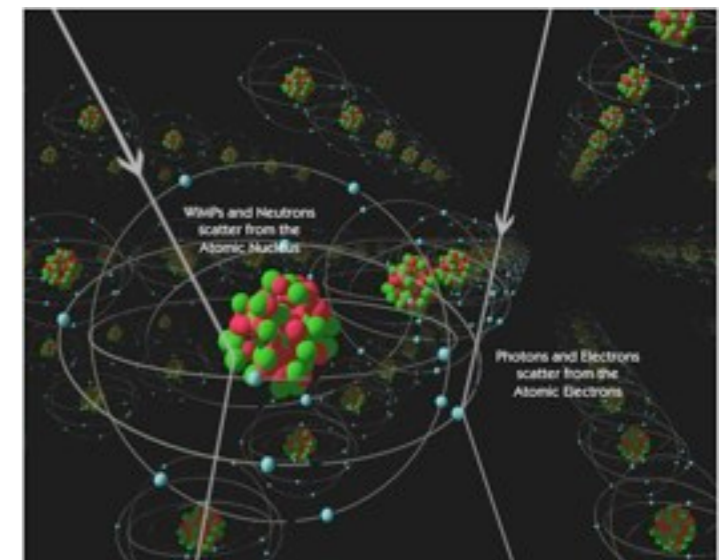
Nuclei and their reactions:  
Energy, Medical Isotopes, National Security,...



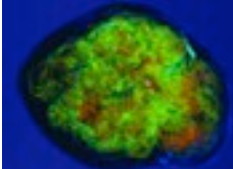
The structure of, and  
forces between, nucleons



Search for  
New Physics

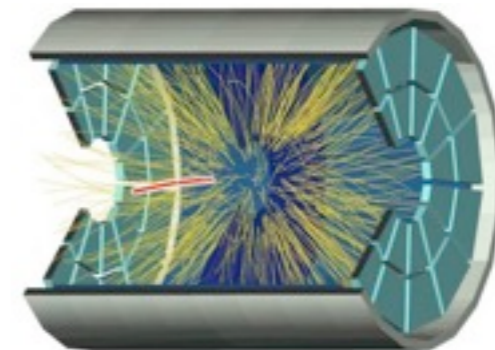
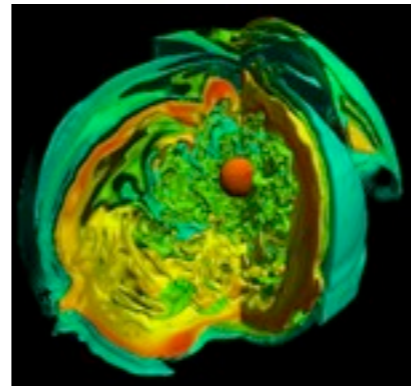
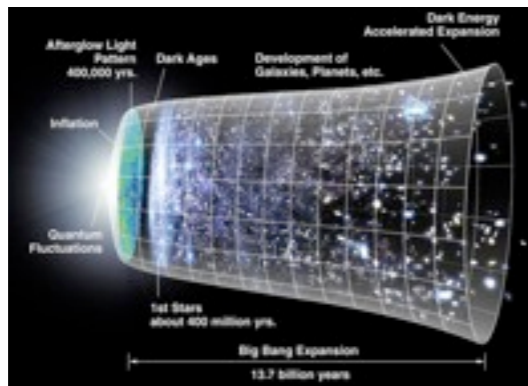
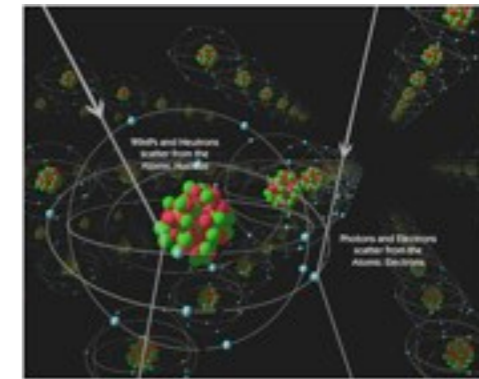
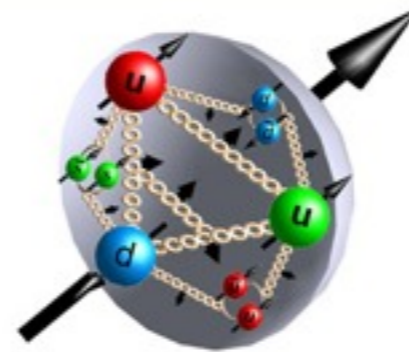
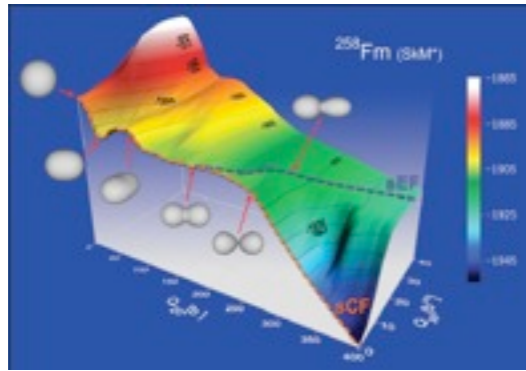


Enormous range of length scales involved



# Computational Nuclear Physics

# Computing is Essential

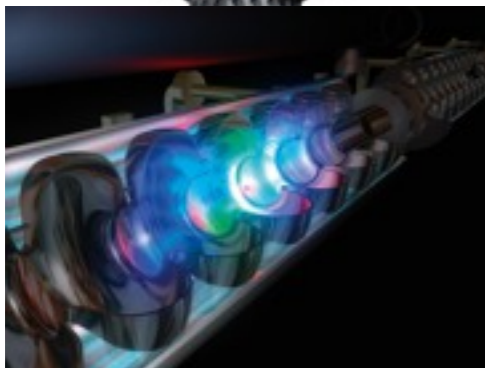


# Computing is Essential

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*High Performance Computing provides answers to questions that neither experiment nor analytic theory can address; hence, it becomes the third leg supporting the field of nuclear physics*

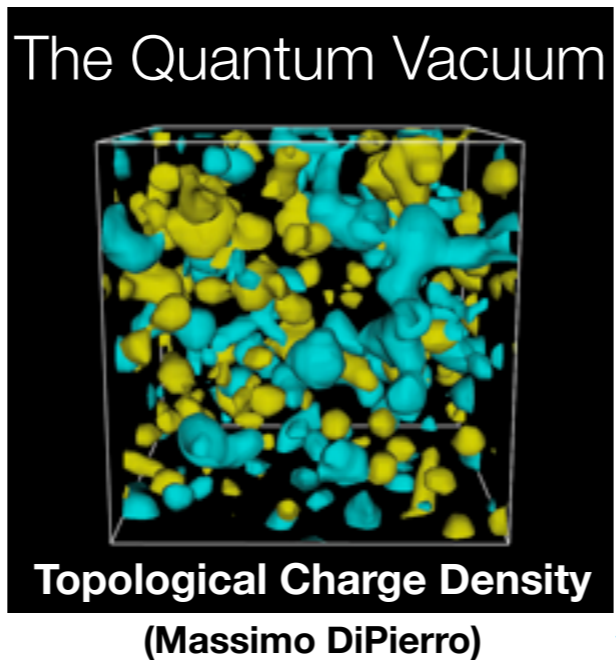
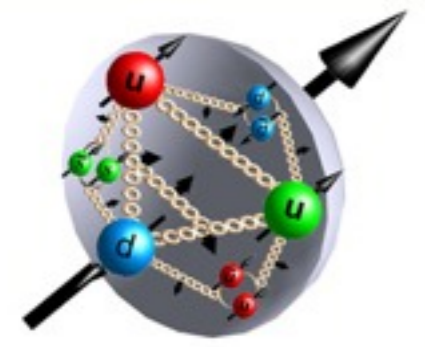
National Academy Report  
(2012)



# Cold QCD

Nature is finely tuned

capacity resources

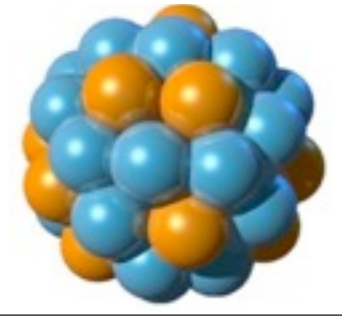
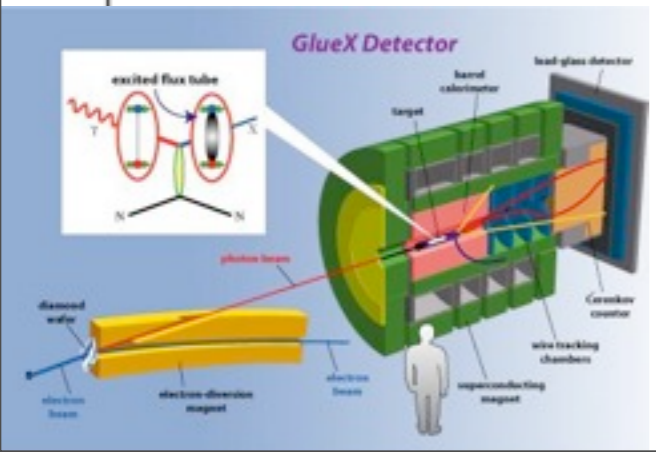
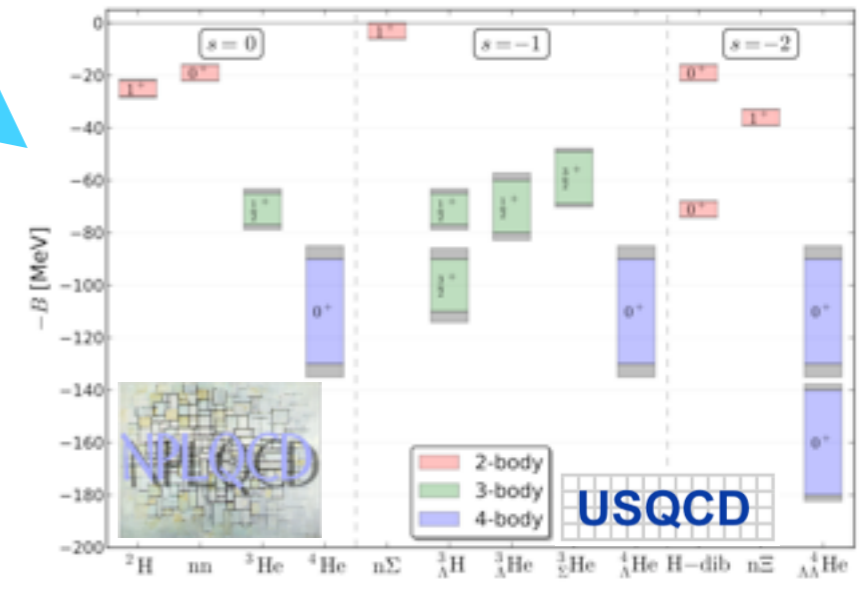
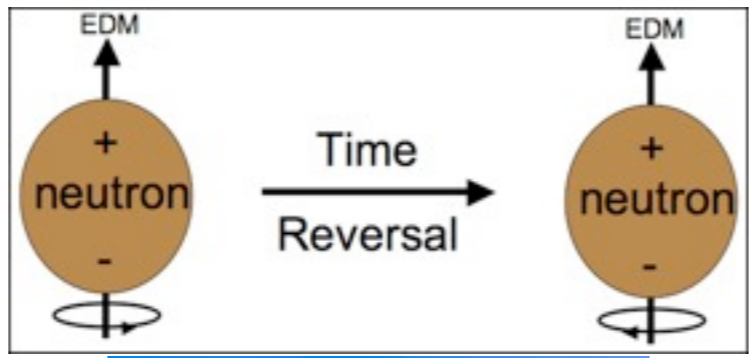
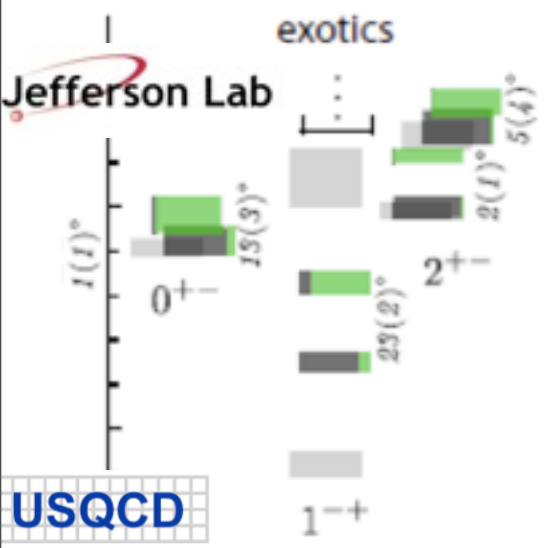


capability resources

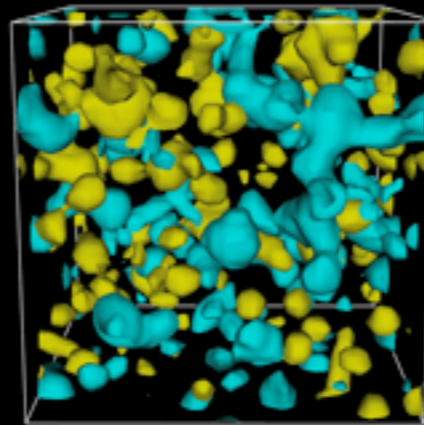
$$L \sim 4 \text{ fm}$$

$$\Delta t \sim 6 \times 10^{-24} \text{ s}$$

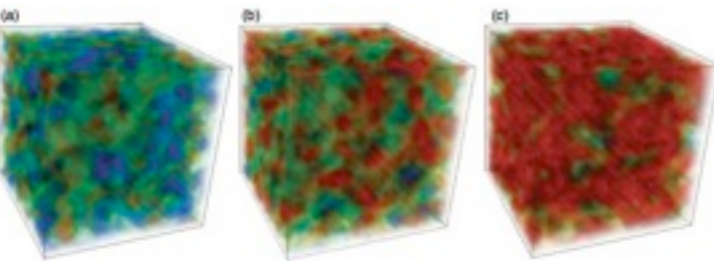
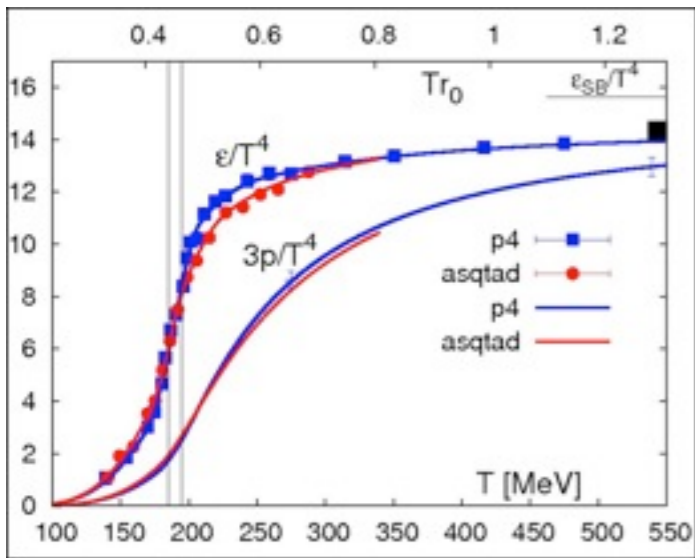
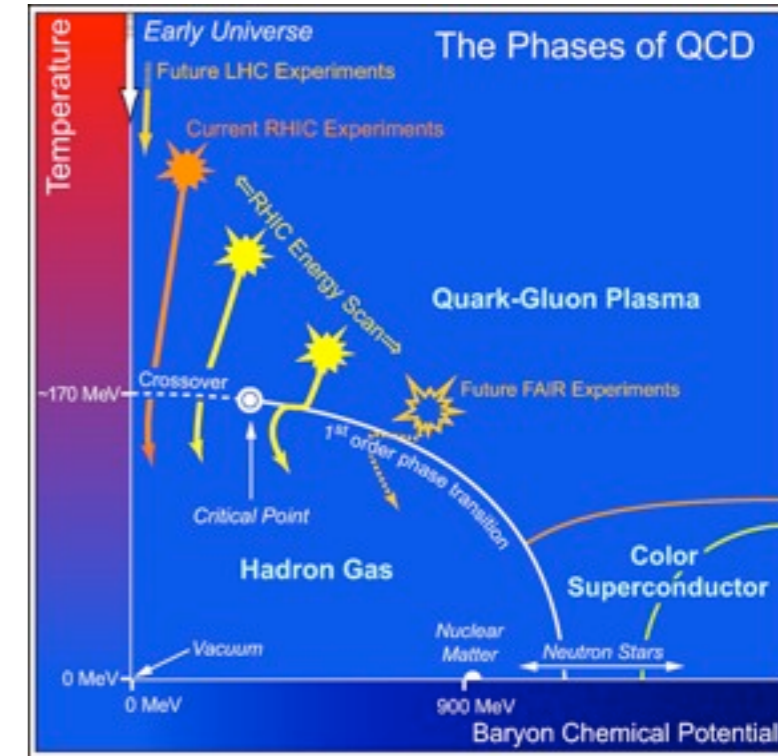
capacity resources



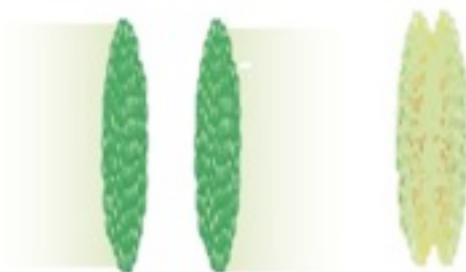
## The Quantum Vacuum



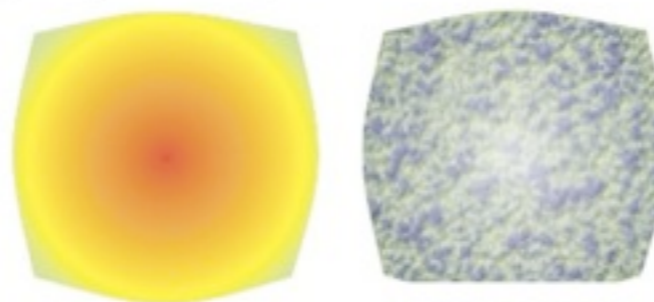
**Topological Charge Density**  
(Massimo DiPierro)



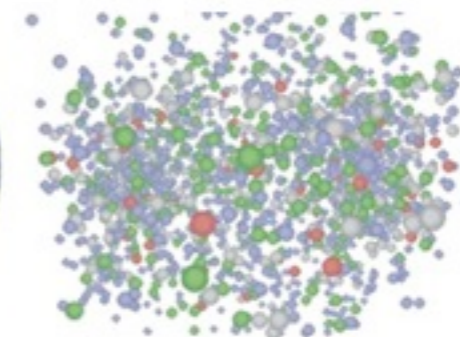
**Initial State:**  
Colliding Nuclei



**Quark Gluon Plasma & Hydrodynamic Expansion**



**Hadronic Rescattering & Freeze-out**

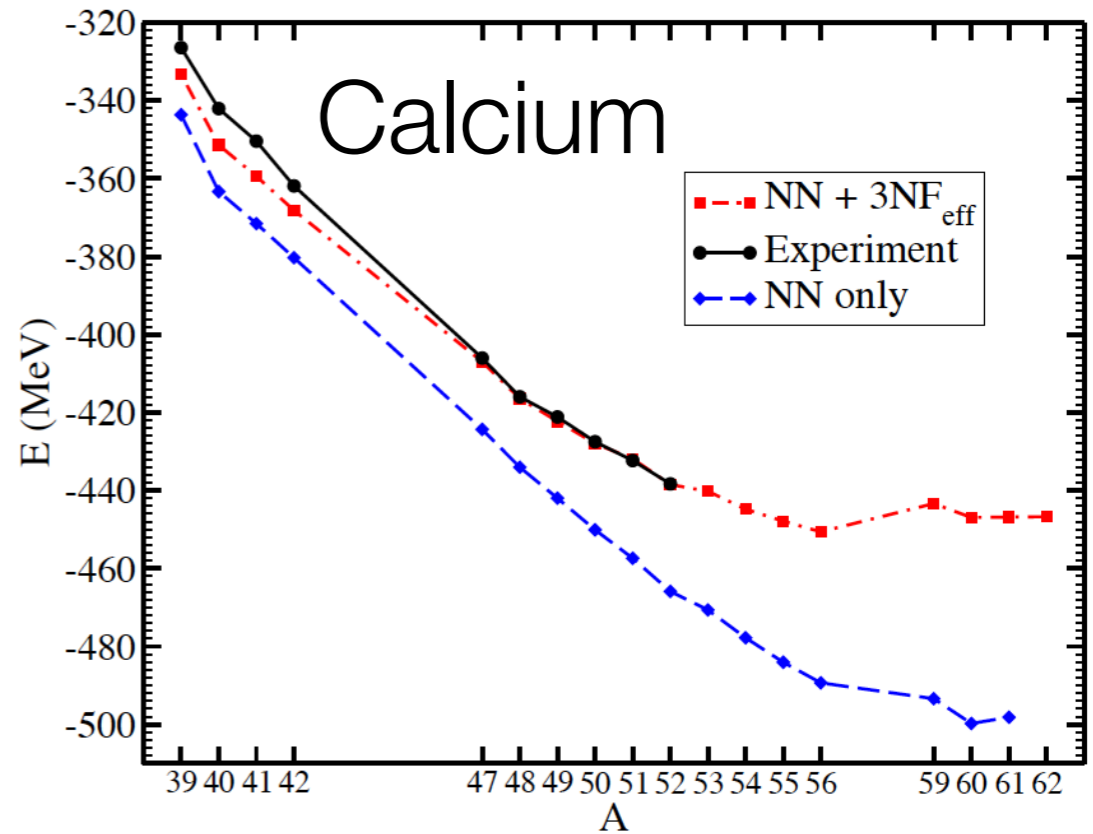
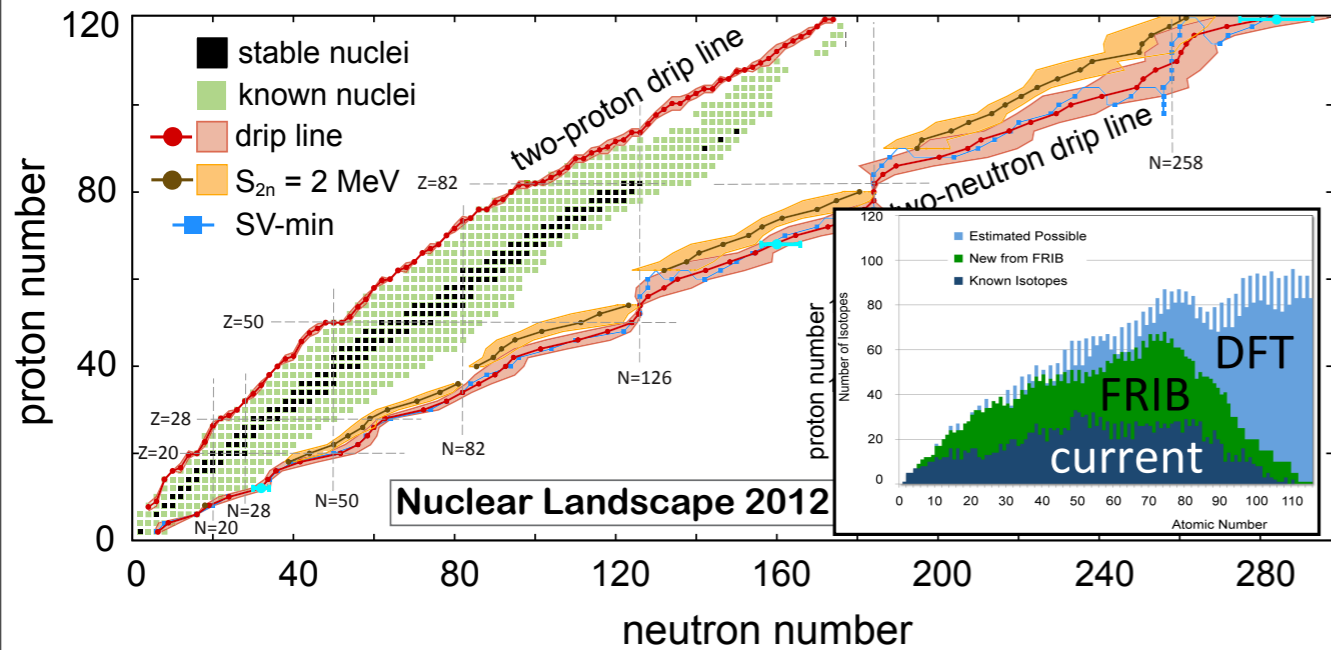
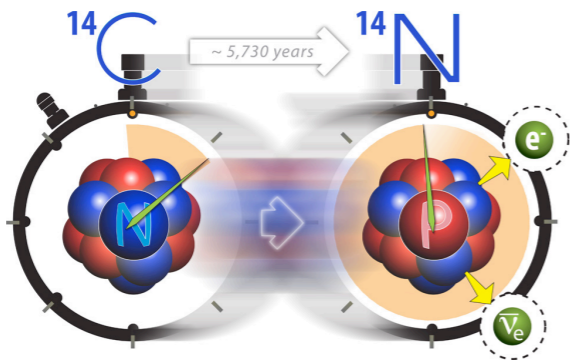
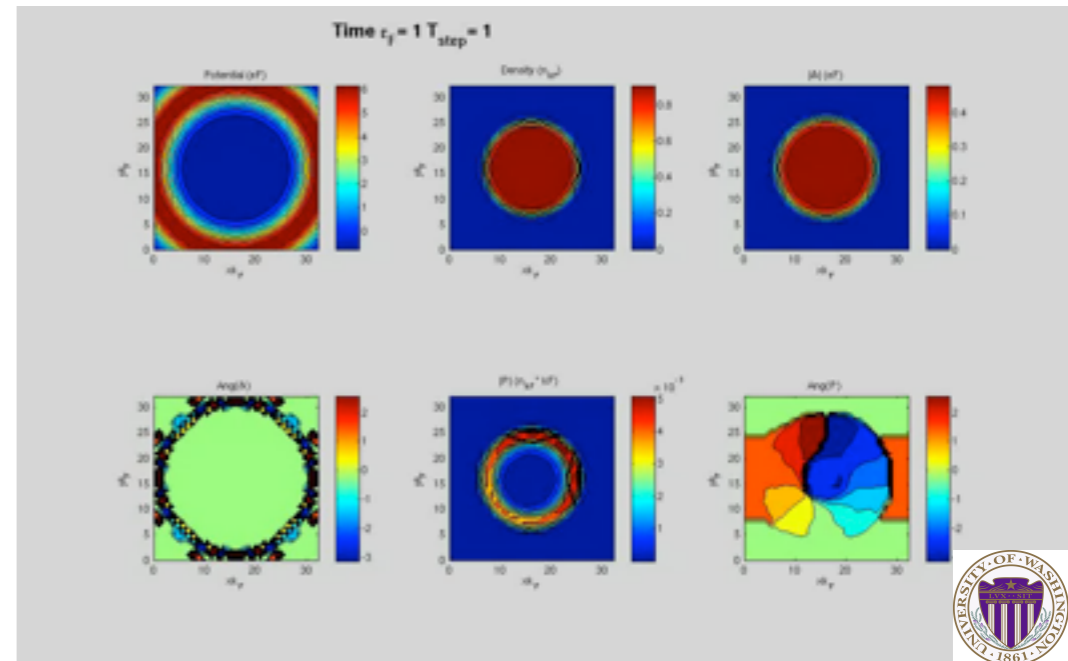
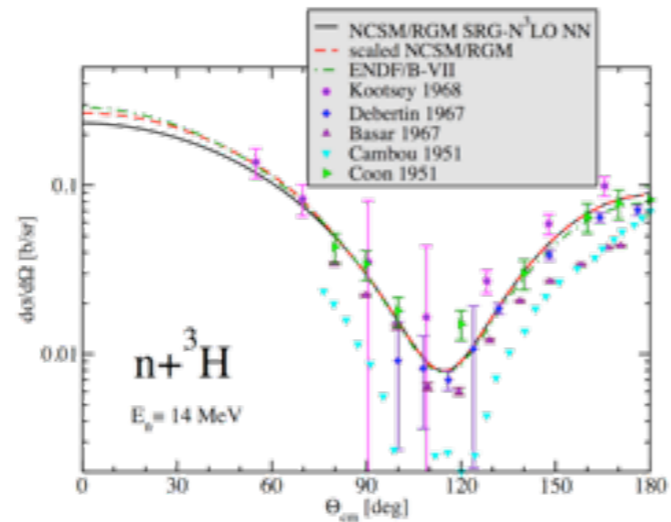


**Equilibration:**  
Turbulent Color Fields

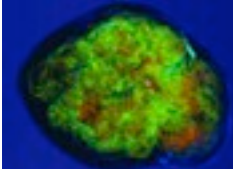
**Hadronization**

# Computational Nuclear Physics

# Nuclear Structure and Reactions

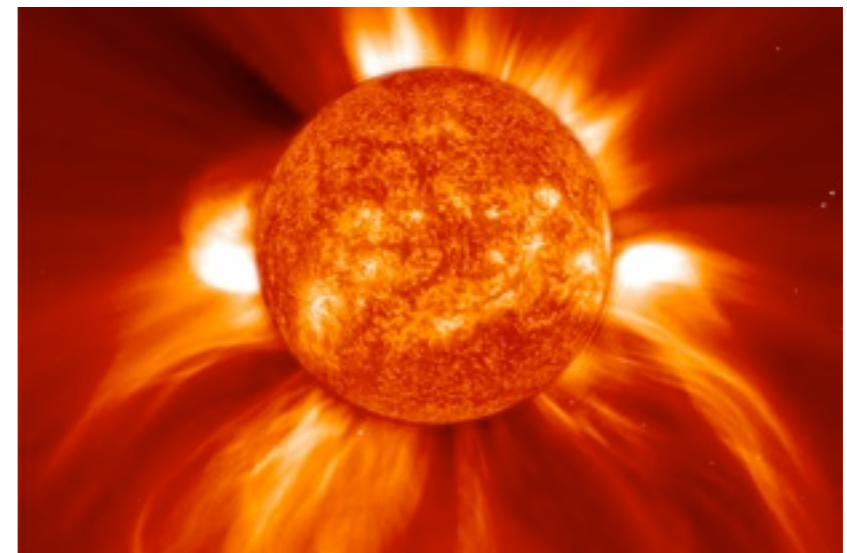
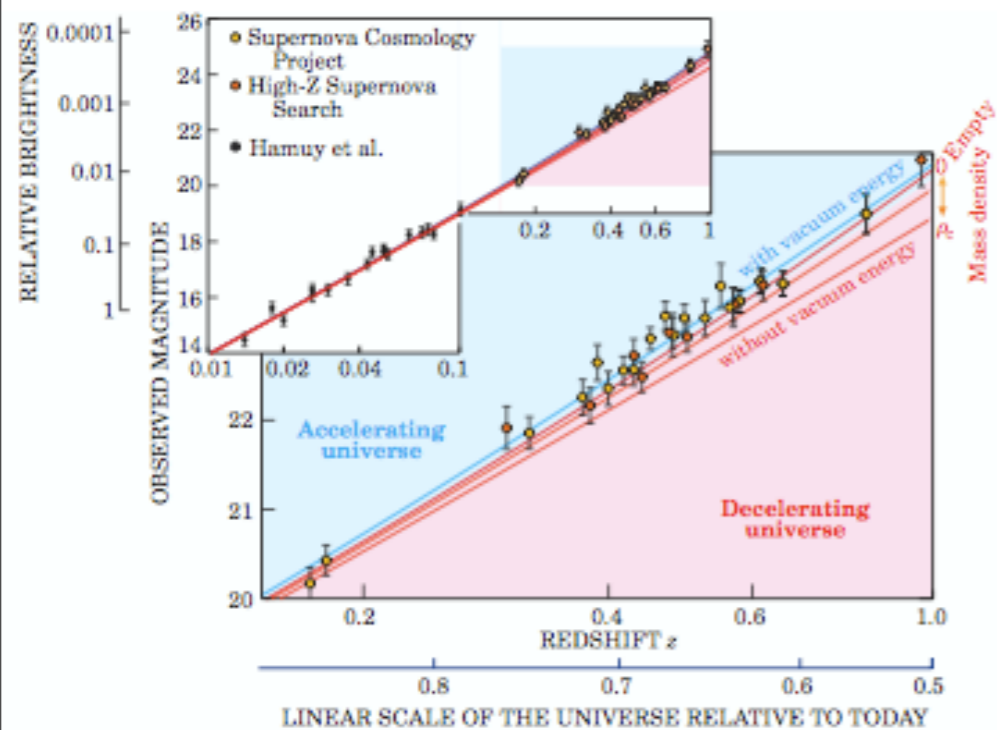
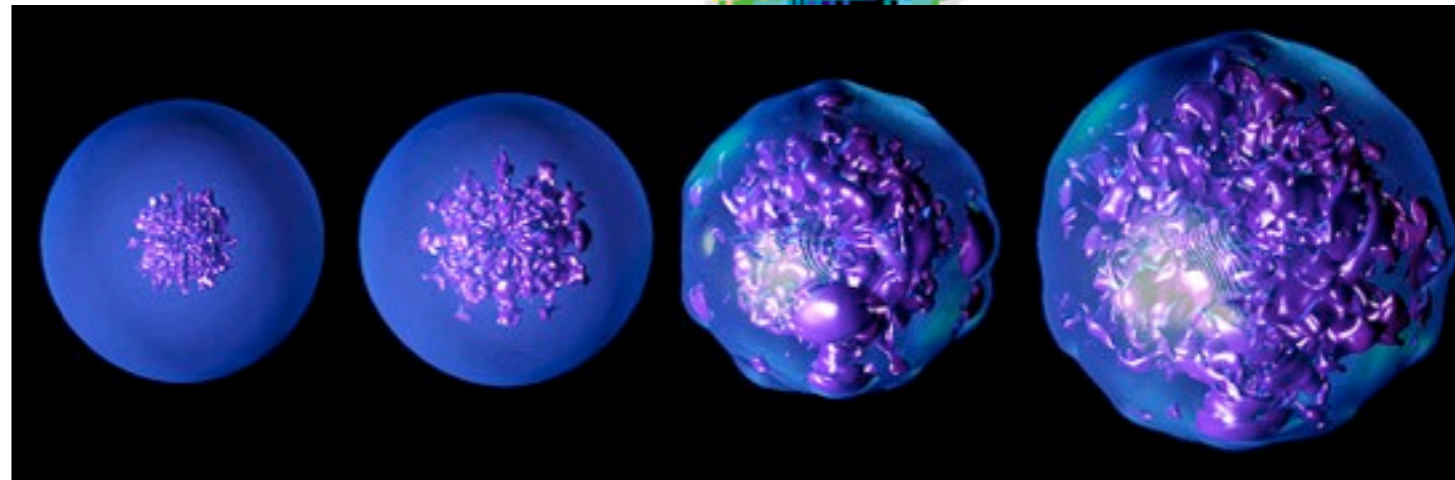
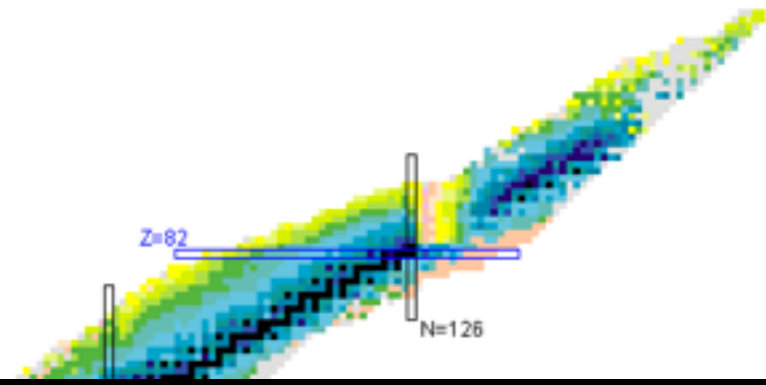
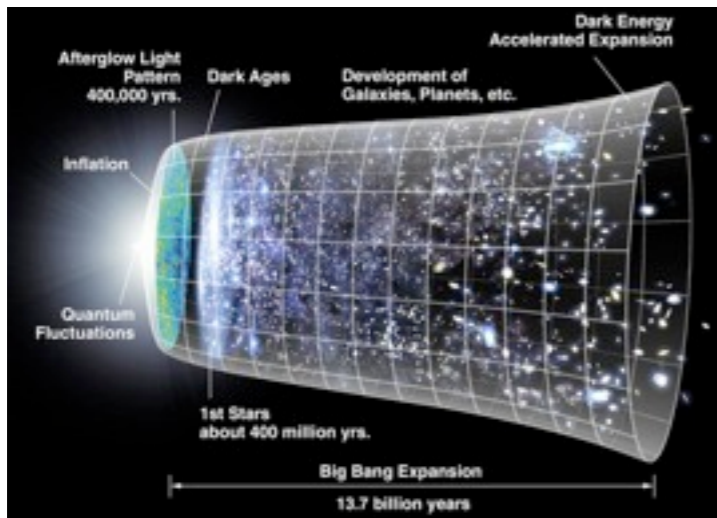






# Computational Nuclear Physics

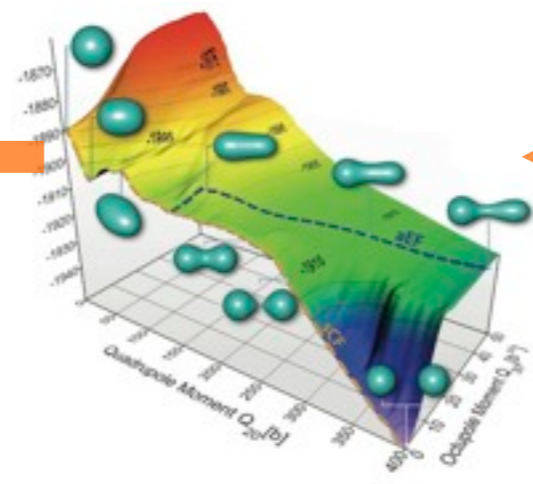
# Nuclear Astrophysics



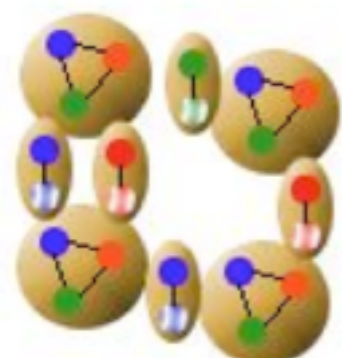
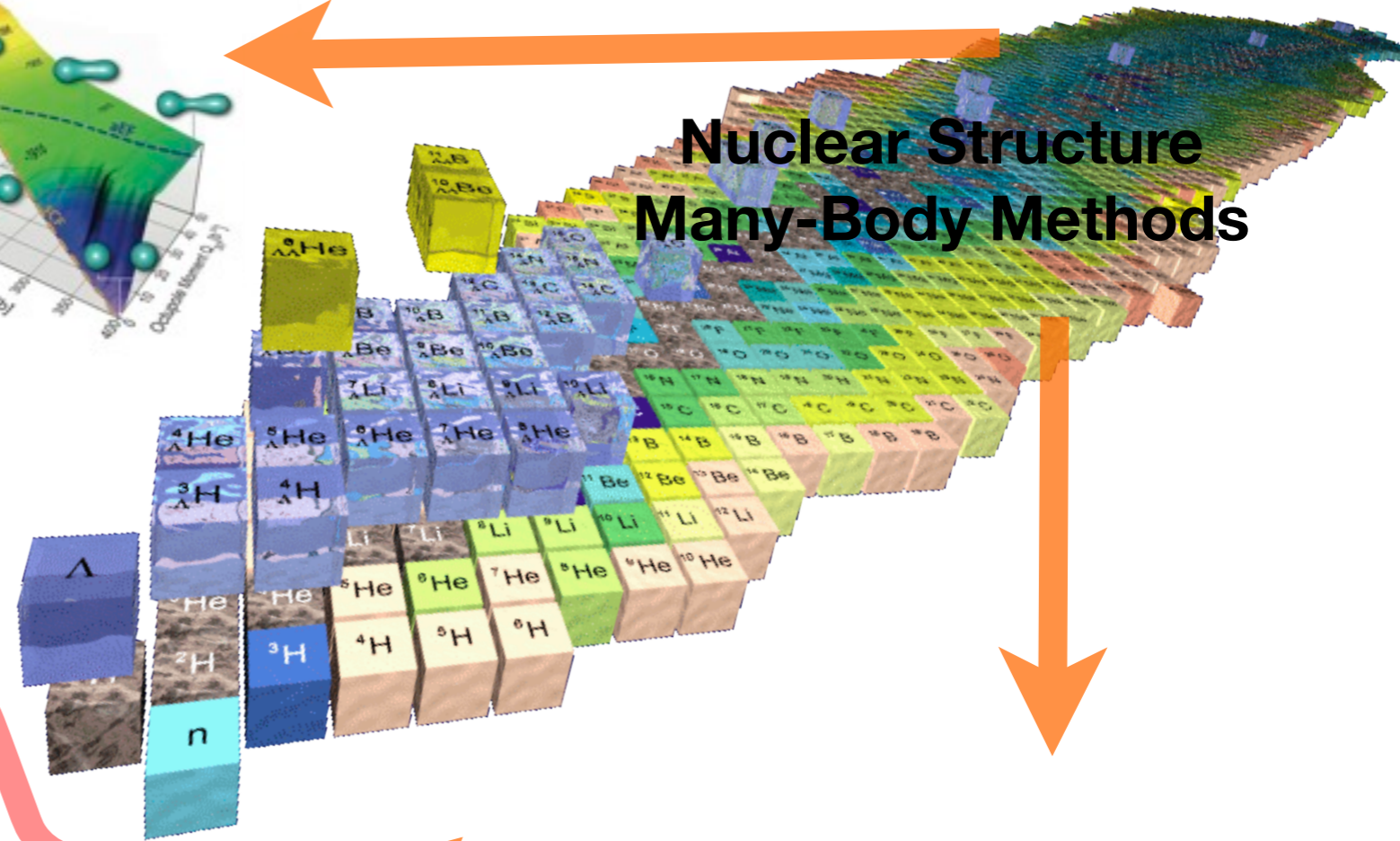
# Computational Nuclear Physics

## ( Partial ) Unification of Nuclear Physics

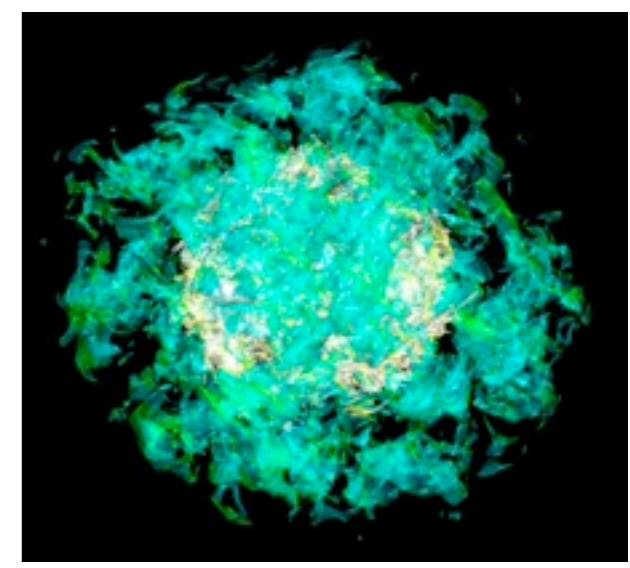
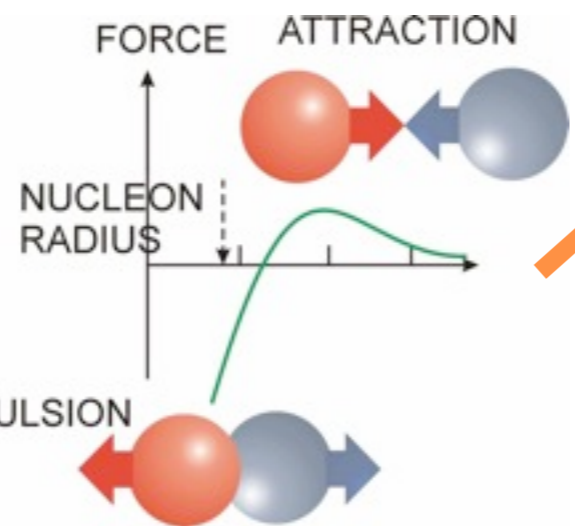
- Quantifiable Uncertainties
- Predictive Capability



Nuclear Structure  
Many-Body Methods



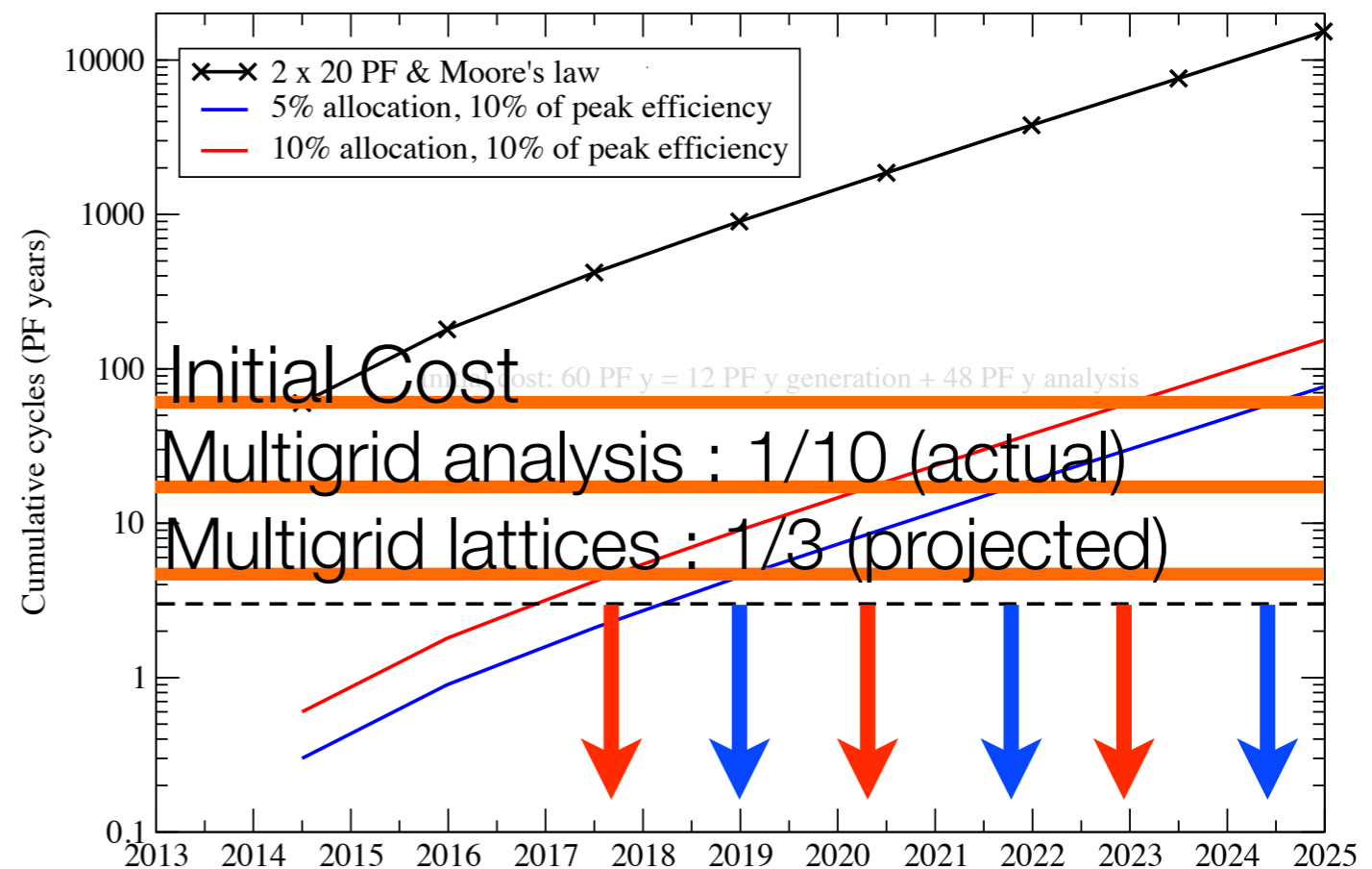
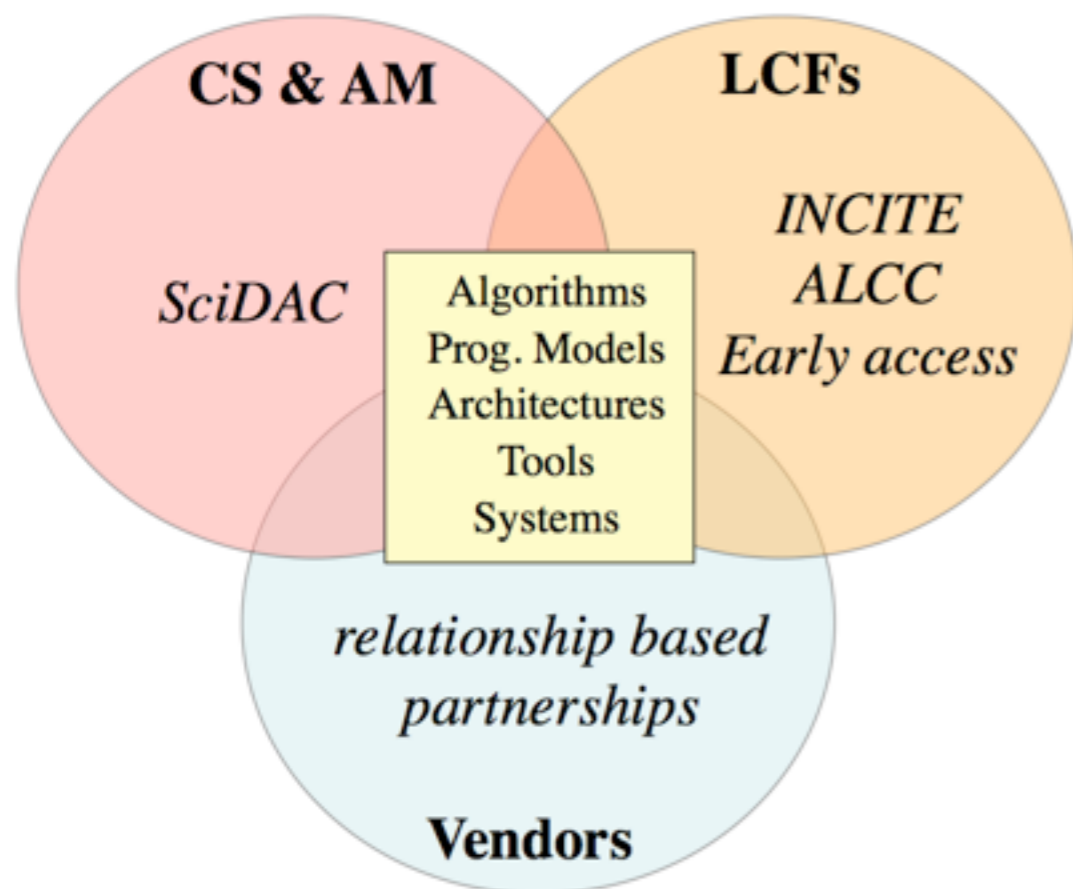
Solve QCD





**SciDAC**  
Scientific Discovery through  
Advanced Computing

SciDAC (Collaboration) has been crucial in progress



# Present Day Resources

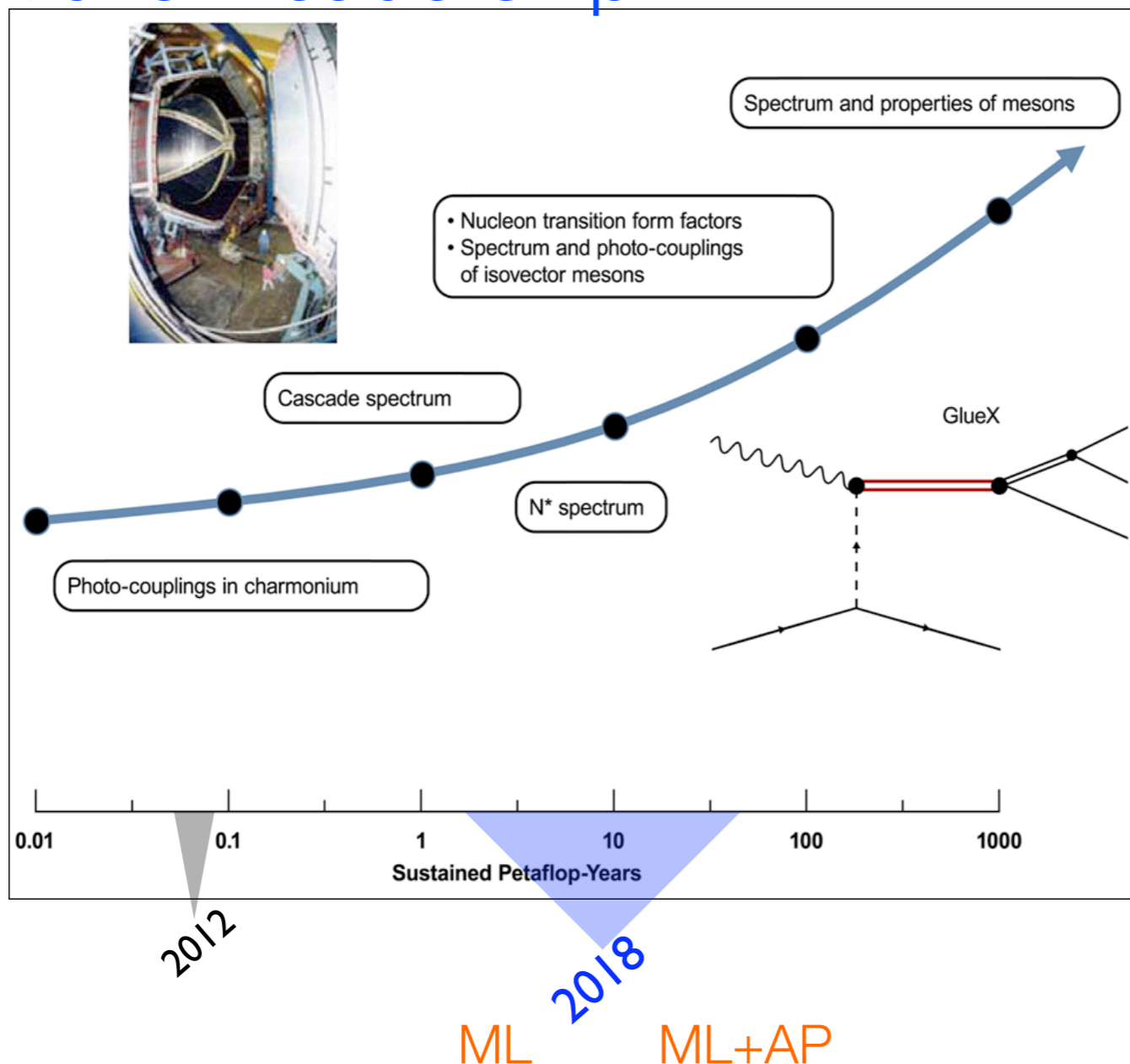


## 2011-2012 : capability and capacity

Cold QCD	~ 50 Tflops	1 : 4
HotQCD	~ 50 Tflops	
Nuclear Structure and Reactions	~ 20 Tflops	
Nuclear Astrophysics	~ 10 Tflops	
<b>Total</b>	<b>~ 130 Tflops</b>	(sustained)

Getting the job done - but when ? NSAC Milestones ?  
 Synchronized with the experimental program (+- n-years) ?  
 International Leadership ?

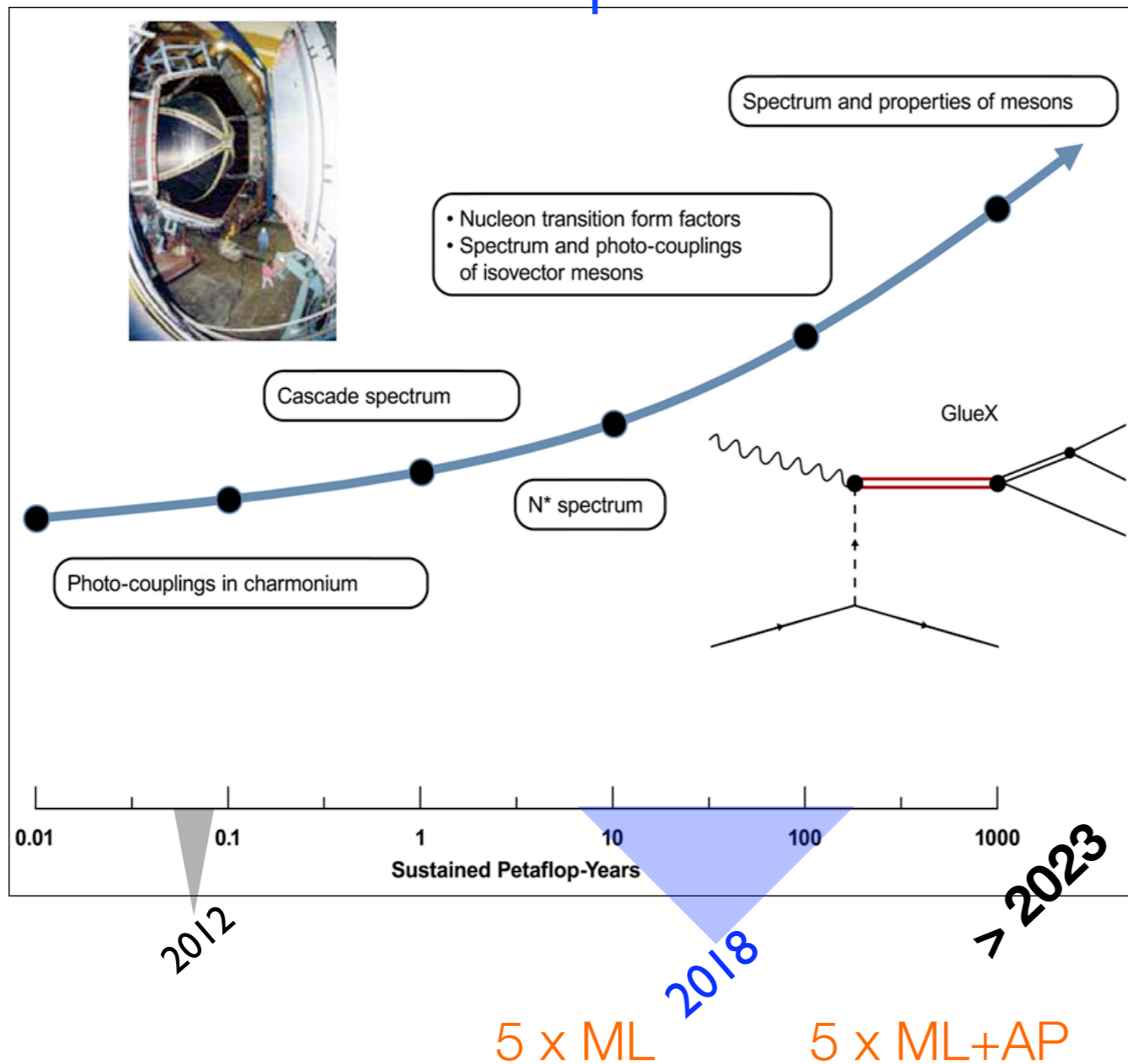
e.g.  
 Hadronic Spectroscopy



**Flat + COLA**  
 Moore's Law  
 Algorithm Potential

Getting the job done - but when ? NSAC Milestones ?  
 Synchronized with the experimental program (+- n-years) ?  
 International Leadership ?

e.g.  
 Hadronic Spectroscopy



**Viable (?)**  
 5 x Moore's Law  
 Algorithm Potential



Today : US Nuclear Physics is under-resourced

Japan :



K-Machine ~ 2 Petaflops (sustained)

Nuclear Physics allocation ~ 20% for  $\geq 1$  year

400 Tflops (sustained) = **8 x** US cold-QCD NP resource

For entertainment purposes :

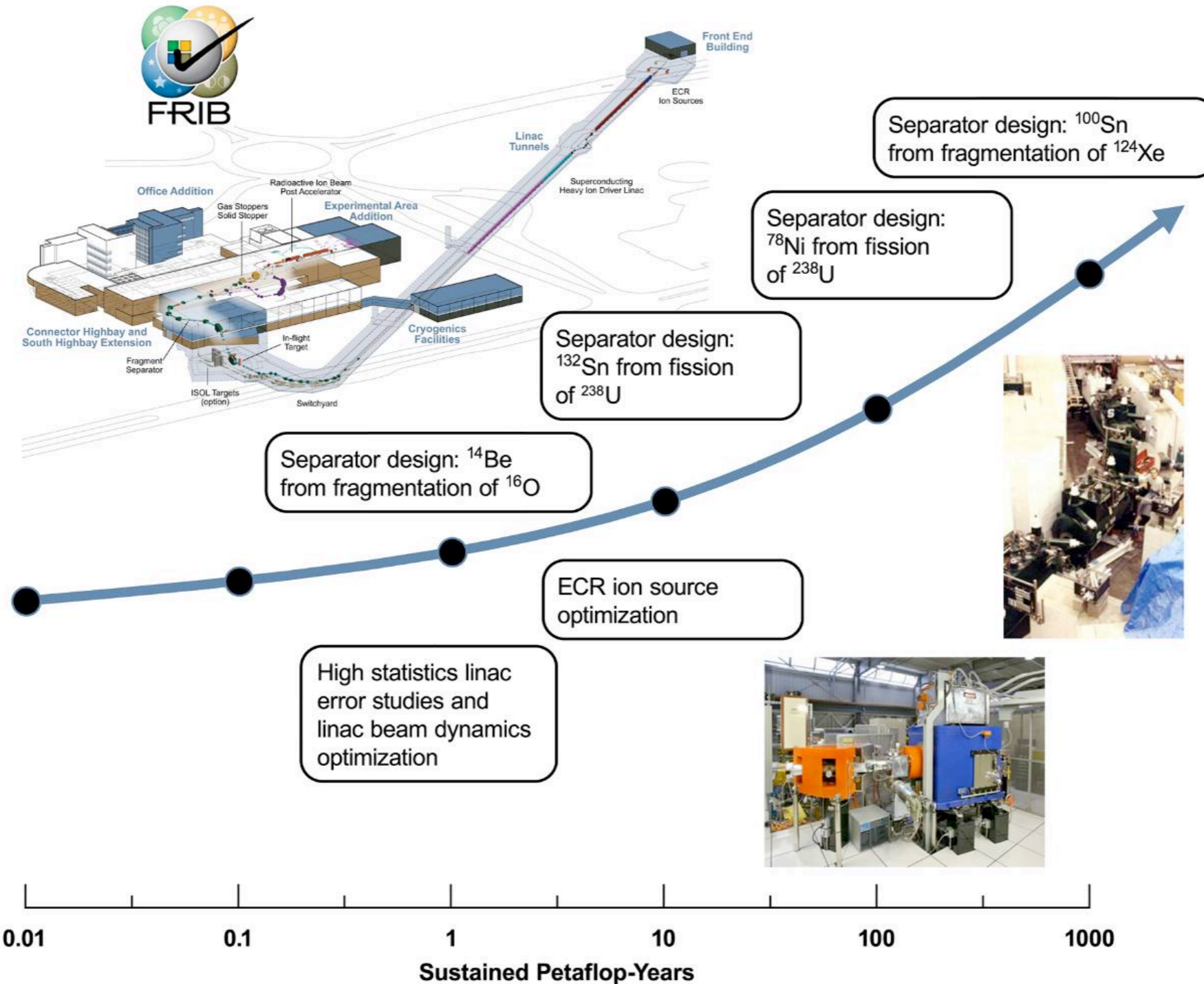
cold-QCD :

Japan : 3.2 Mflops/citizen

USA : 160 kflops/citizen

!!!

# Machine Design and Optimization



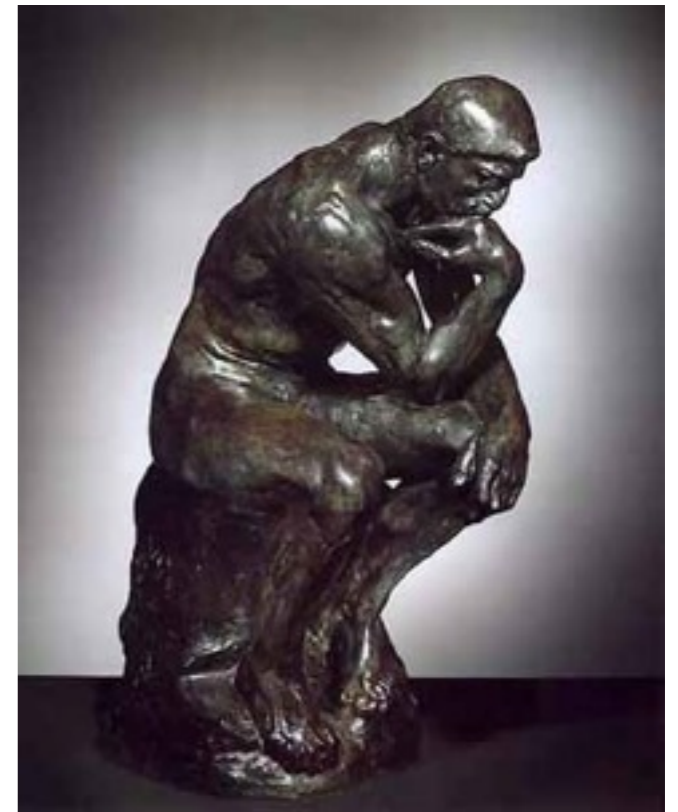
Assume facilities will present their needs separately



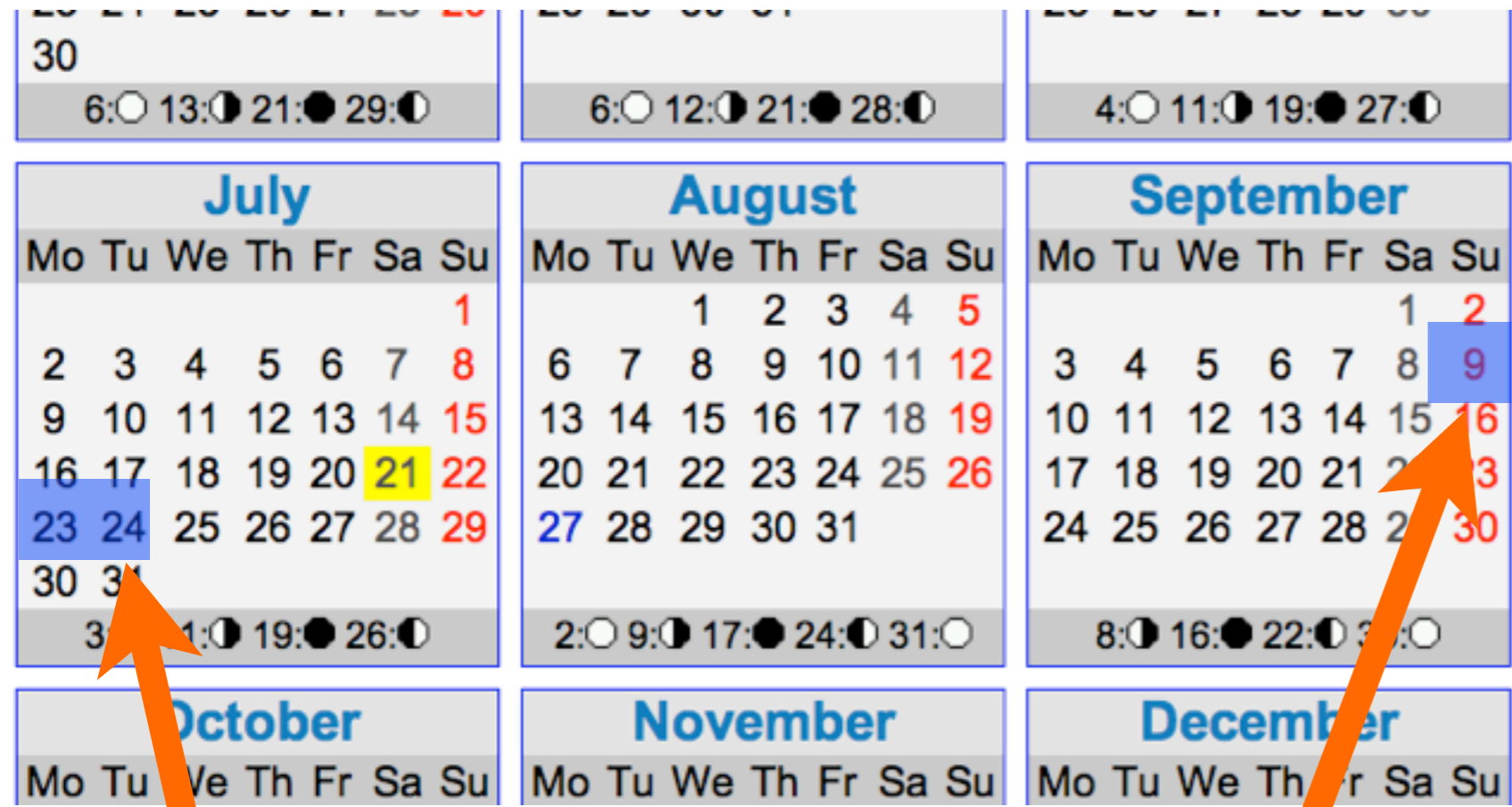
- Different areas in Nuclear Physics
  - coherent community effort - partial unification of NP
  - with Particle Physics, Plasma, Fluids, ....
- Computer Scientists
  - hardware development
  - optimizations
  - new coding paradigms
  - data management, visualization....
- Applied Mathematicians
  -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



- For viable program we need to grow HPC expertise in the NP community
  - faster than Moore's Law
  - not business as usual
- The standard interdisciplinary hiring problems exist
  - challenge at Universities (at Labs?)
  - new training models, start today for 2020?
- Broad collaborations
  - Graduate students and postdocs hired into collaboration
    - naive scaling from UNEDF programs (2009 estimate) =  
enhancement in person-power (+10+10 per project ?)
  - Organization in the Nuclear Physics community



# The Timeline



This meeting

Presentation

- ## Organizers/Writers
- Adam Burrows
  - Joe Carlson
  - Robert Edwards
  - Witek Nazarewicz
  - Peter Petreczky
  - David Richards
  - Martin Savage

Most Important :

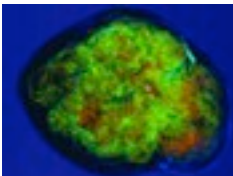
Present a compelling case for significant enhancements in resources dedicated to NP research program

(seems easy to me !)

- clearly articulate what **we** want to do
- my view : this is the right time to **go for it**
- will **lose** leadership if we don't
- will **lose** scientists if we don't
- not necessarily a scaling of present

(e.g. tighter coupling between allocations and base support?)





# Computational Nuclear Physics

## The Agenda

Monday, July 23, 2012		
8:30-8:35	Welcome	Jerry Draayer
8:35-8:45	Introduction	Martin Savage
8:45-9:45	Cold QCD	Tom Luu, Balint Joo
9:45-10:45	Hot QCD	Peter Petreczky, Swagato Mukerjee
10:45-11:15	Coffee Break	
11:15-12:15	Nuclear Structure and Reactions	Joe Carlson, Ewing Lusk
12:15-13:15	Lunch Break	
13:15-14:15	Astrophysics	Adam Burrows, Bronson Messer
14:15-14:45	Additional Opportunities for Computational Nuclear Physics-5 Minutes and Maximum of Two Transparencies From Floor	
14:45-15:15	Coffee Break	
15:15-15:35	Whitepaper: Aims and Plans	Martin Savage
15:35-	General Discussion, With Attendance by Agency Representatives	
Tuesday, July 24, 2012		
8:25-8:30	Introduction to the 2nd Day	Martin Savage
8:35-10:00	Computational Requirements Working Session	Robert Edwards (Chair)
10:00-10:30	Coffee Break	
10:30-12:00	Evolution of Computational Physics and Cross-Cutting	David Dean (Chair)
12:00-13:00	Lunch Break	
13:00-14:00	Summary, Resolutions, and Closeout	Witold Nazarewicz, David Richards
14:00-15:30	Writing Group Session	



DAQ - phase

# NSAC

## Tribble Committee Questions

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- (1) What major scientific accomplishments and discoveries have occurred in your area of high-performance computing since the 2007 LRP was drafted?
- (2a) What compelling and unique science can be carried out in the program in the next five years assuming support similar to FY13 that includes cost of living increases?
- (2b) What additional impact would flat-flat funding to FY18 have on (2a)?
- (3) What is the minimum level of support (cycles, new hardware, etc.) needed to maintain a **viable** program in computational nuclear physics?
- (4) What workforce (physicists, CS, AM, students) is needed to maintain a **viable** program?  
What will it require to take the community to the exascale era (e.g., training of students and postdocs)?
- (5) What science would you expect to pursue in the program in 2020 and beyond?  
What is needed to support this?  
What science would you expect to pursue without access to major supercomputer centers?
- (6) What is role of the science in your research area in the international context?  
If the US effort in high-performance computing were seriously curtailed, to what degree would efforts in other countries fill the gap?  
And, to what degree would US scientists be able to advance research in this area by working outside of the country?
- (7) How does high performance computing contribute to the educational mission of training the future workforce in nuclear physics and associated applied areas?

# The End, or is it the Beginning

