U.S. DEPARTMENT OF ENERGY | Office of Science

NP-NERSC Meeting on:

Large Scale Computing and Storage Requirements for Nuclear Physics (NP): Target 2017

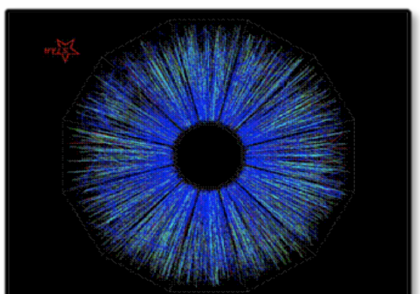
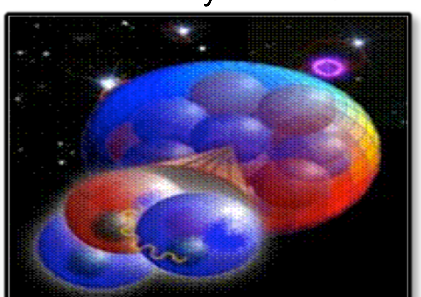
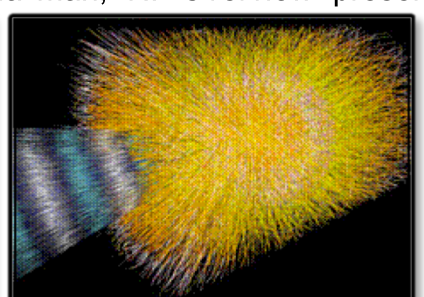
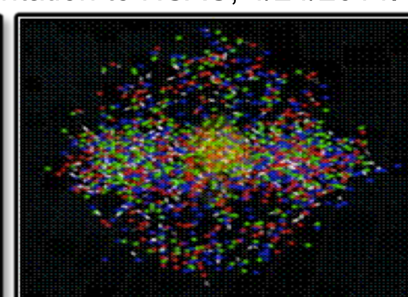
April 29-30, 2014   Bethesda, MD

NP Program Office Research Directions

Ted Barnes DOE/NP

Program Manager, Nuclear Data & Nuclear Theory Computing

n.b. Many slides c/o T. Hallman, “NP Overview” presentation to NSAC, 4/24/2014.

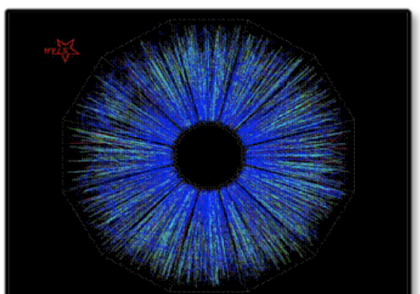





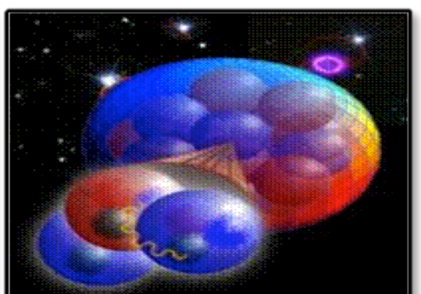
DOE Nuclear Physics Mission Statement

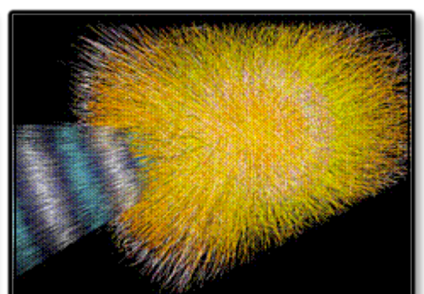
Discovering, exploring, and understanding all forms of nuclear matter

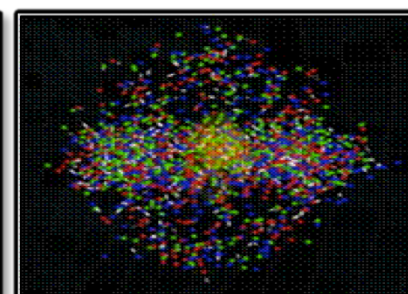
The Scientific Challenges

- The existence and properties of nuclear matter under extreme conditions, including that which existed at the beginning of the universe
- The exotic and excited bound states of quarks and gluons, including new tests of the Standard Model
- The ultimate limits of existence of bound systems of protons and neutrons [nuclei]
- Nuclear processes that power stars and supernovae, and synthesize the elements
- The nature and fundamental properties of neutrinos and neutrons and their role in the matter-antimatter asymmetry of the universe









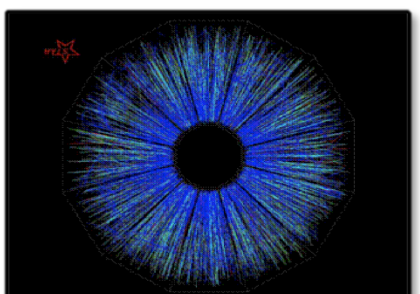
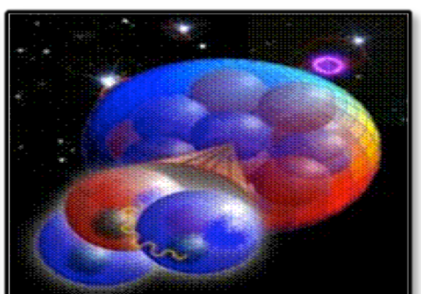
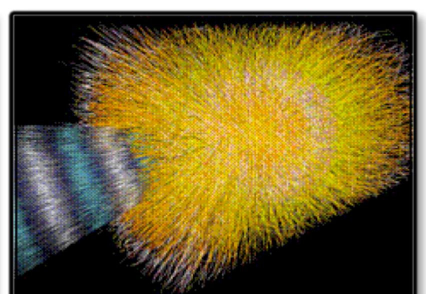
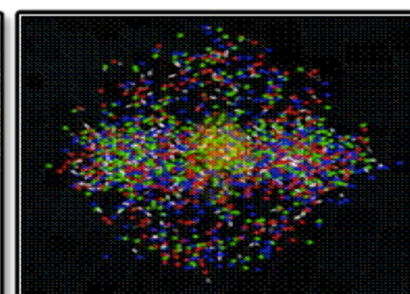
DOE Nuclear Physics Mission Statement

Discovering, exploring, and understanding all forms of strong int. (QCD) matter

~ The strong interaction (QCD) r US

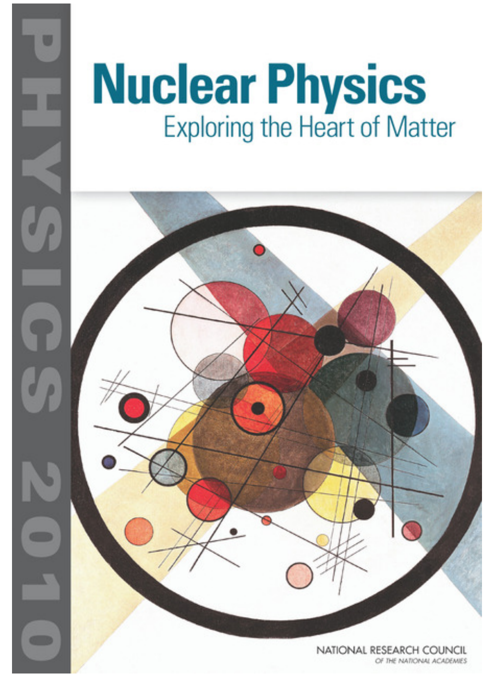
The Scientific Challenges

- The existence and properties of nuclear matter under extreme conditions, including that which existed at the beginning of the universe [phase diagram, EOS]
- The exotic and excited bound states of quarks and gluons, including new tests of the Standard Model [FSI. BSM? νs]
- The ultimate limits of existence of bound systems of protons and neutrons [nuclei]
- Nuclear processes that power stars and supernovae, and synthesize the elements
- The nature and fundamental properties of neutrinos and neutrons and their role in the matter-antimatter asymmetry of the universe [fund symms & ints = growth area]

SC NP is a Primary Federal Steward of U.S. Nuclear Science

DOE/NP is the largest supporter of nuclear physics in the U.S. and operates large National User Facilities



Responsible for Strategic Planning and Funding

- Identify the scientific opportunities for discoveries and advancements
- Build and operate forefront facilities to address these opportunities
- Develop and support a research community that delivers significant outcomes
- Work with other agencies/countries to optimize use of U.S. resources

Goals

- **World-class facility research capabilities**
  - to make significant discoveries/advancements
- **A strong, sustainable research community**
  - to deliver significant outcomes
- **Forefront advanced technologies, capabilities**
  - for next-generation capabilities
- **A well-managed and staffed, strategic sustainable program**
  - that ensures leadership/optimizes resources

Deliverables

- New insights and advancements in the fundamental nature of matter and energy
- New and accumulated knowledge, developed and cutting-edge technologies, and a highly-trained next-generation workforce that will underpin the Department's missions and the Nation's nuclear-related endeavors
- Isotopes for basic and applied sciences

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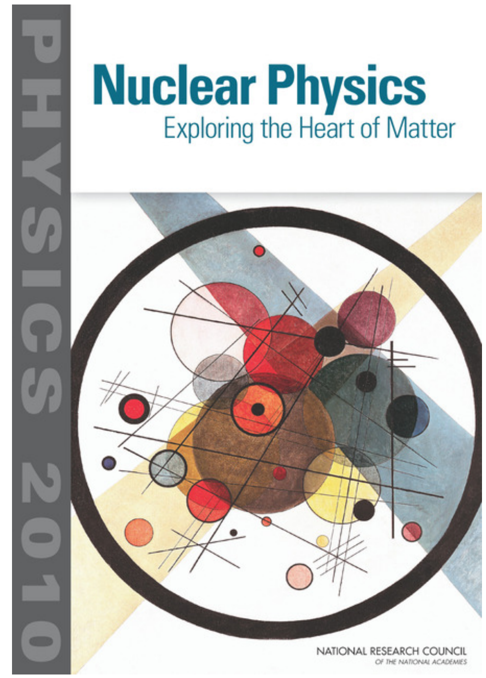

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3 NP Research Areas, 3 Major DOE/NP Facilities

&

a few examples of HPC applications

NP Research Programs and Associated **Major Facilities**

- *Heavy Ion Physics* (**RHIC@BNL**, LHC@CERN)
  - QCD thermodynamics, phase diagram (QCD EOS)
  - HPC *e.g.*: finite temperature lattice QCD (pref. theor. method)
- *Medium Energy NP* (**CEBAF@TJNAF@Newport News**, RHIC)
  - physics of hadrons; exotics, hadron structure
  - HPC *e.g.*: zero temperature lattice QCD (pref. theor. method); GPUs!
- *Low Energy NP* (**FRIB@MSU**, ATLAS@ANL)
  - nuclei, nuclear matrix elements
  - HPC *e.g.*: QMC; shell models; DFT

(*) *LENP (& MENP) incl. nuclear astrophysics*, *fund. symms. & ints*. (νs)

HPC *e.g.*: Type II SNe; n stars (QCD EOS); weak int. nucl. MEs

⇨ HPC can directly address most of the NP expt. program!

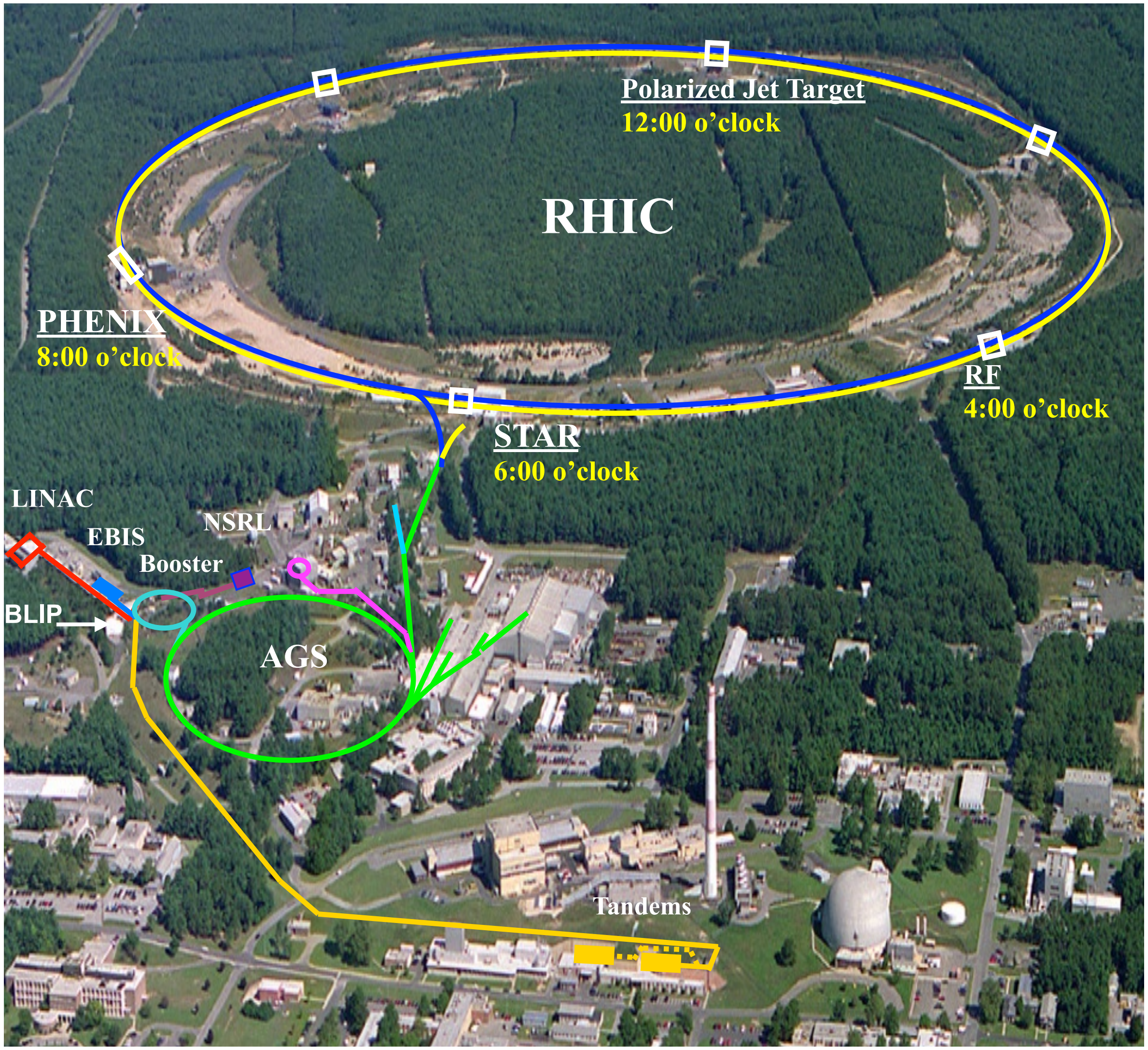
HINP

Continuing Scientific Discovery at the Relativistic Heavy Ion Collider

RHIC discovered a completely new state of matter - a ~ perfect quark-gluon liquid. The RHIC science campaigns planned in the next 3-5 years will:

- determine, with precision, the properties of this perfect liquid (QGP)
- search for new discoveries such as the postulated Critical Point in the phase diagram of QCD
- explore the gluon and sea quark contributions to the spin of the proton using RHIC, the only collider with polarized beams ["proton structure" – parton distns.]
- explore and develop intellectual connections and broader impacts to other subfields

No other facility worldwide, existing or planned, can rival RHIC in range and versatility.



HINP QCD phase diagram (calc. at $\mu_B = 0$) with physical light quark masses

"The QCD phase transition with ***physical-mass****, chiral quarks."* (hotQCD Collab.)

arXiv:1402.5175v1 (21 Feb. 2014)

No phase transition at physical m_q . (μ=0)

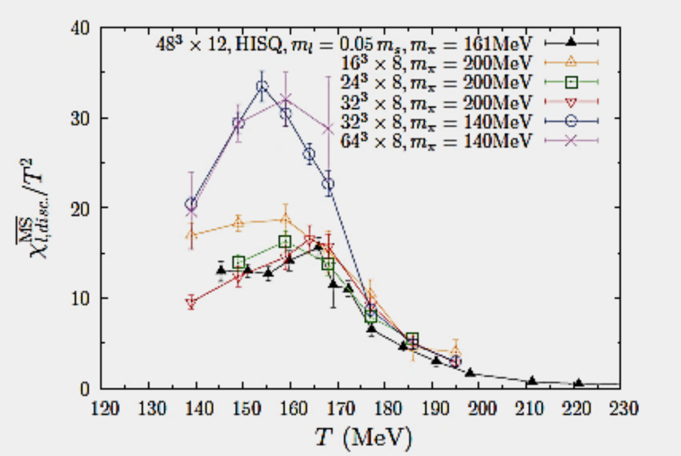


FIG. 1. The dependence of the disconnected chiral susceptibility on temperature for $m_\pi = 135$ and 200 MeV. The $m_\pi = 135$ MeV data shows a near $2\times$ increase over that for $m_\pi = 200$ MeV. HISQ results for $m_\pi = 161$ MeV [7, 11] are also plotted.

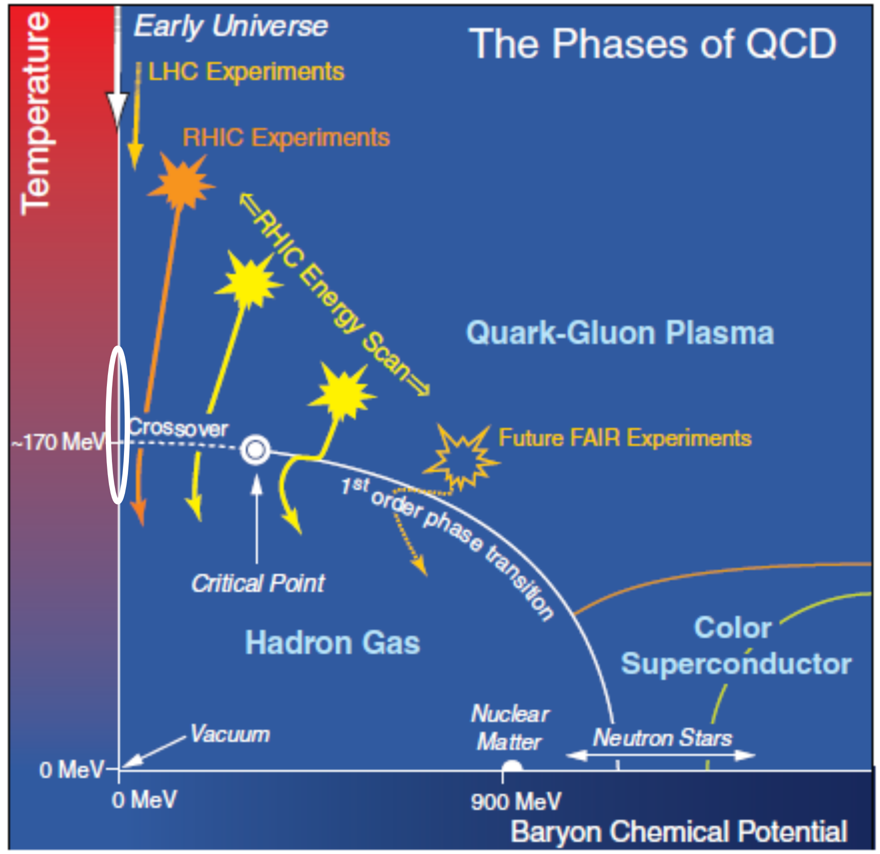


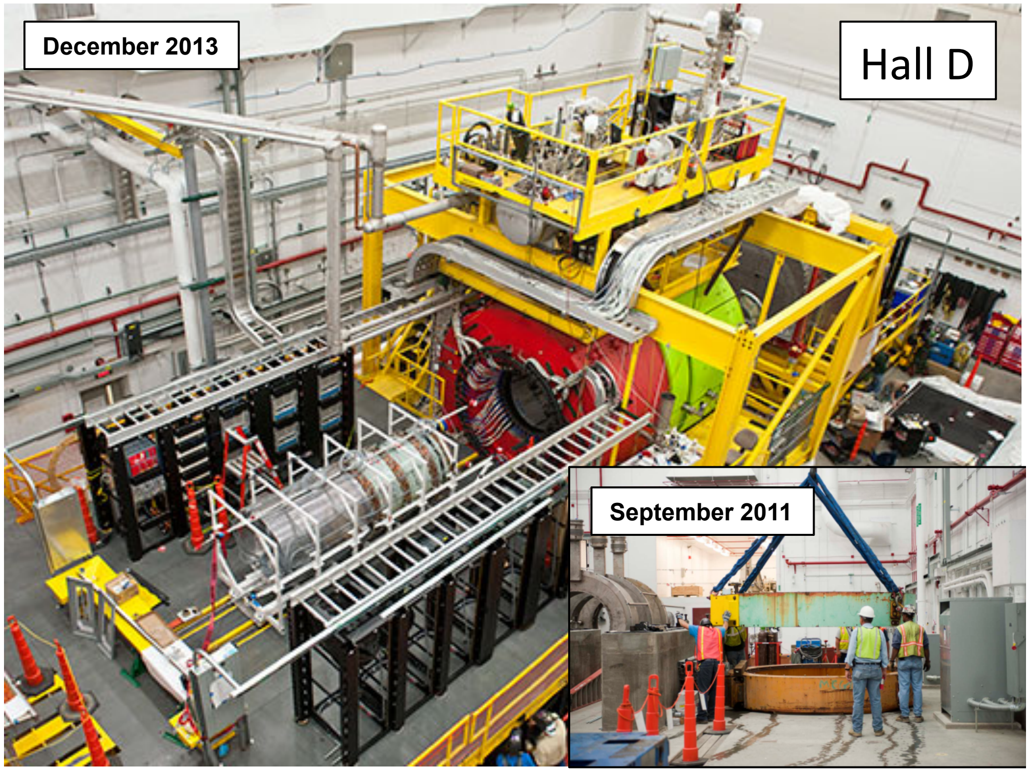
FIGURE 2.25 The phase diagram of QCD is shown as a function of baryon chemical potential (a measure of the matter to antimatter excess) and temperature. A prominent feature in this landscape is the location of the critical point, which indicates the end of the first-order phase transition line in this plane. SOURCE: DOE/NSF, Nuclear Science Advisory Committee, 2007, *The Frontiers of Nuclear Science: A Long Range Plan.*

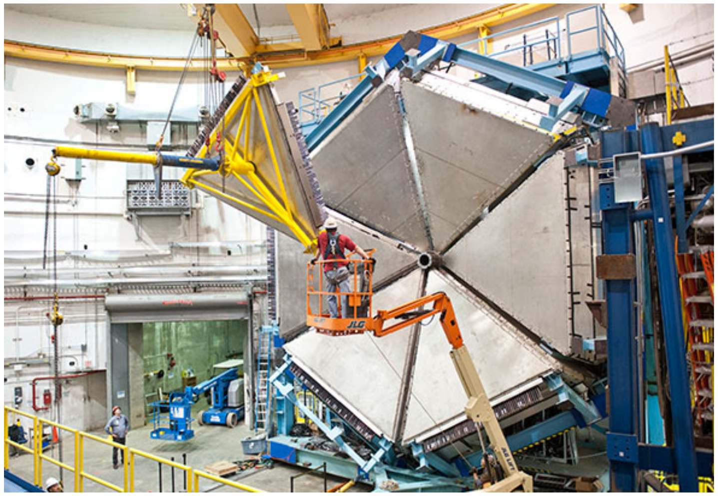
MENP

The 12 GeV CEBAF Upgrade at TJNAF is 87% Complete

With the completion of the 12 GeV CEBAF Upgrade, researchers will address:

- The search for exotic mesons (not quark-antiquark) to advance our understanding of the strong force [GlueX, @ new Hall D]
- Evidence of new physics from sensitive searches for violations of nature's fundamental symmetries [e.g. PVES]
- A detailed microscopic understanding of the internal structure of the proton, including the origin of its spin, and how this structure is modified when the proton is inside a nucleus

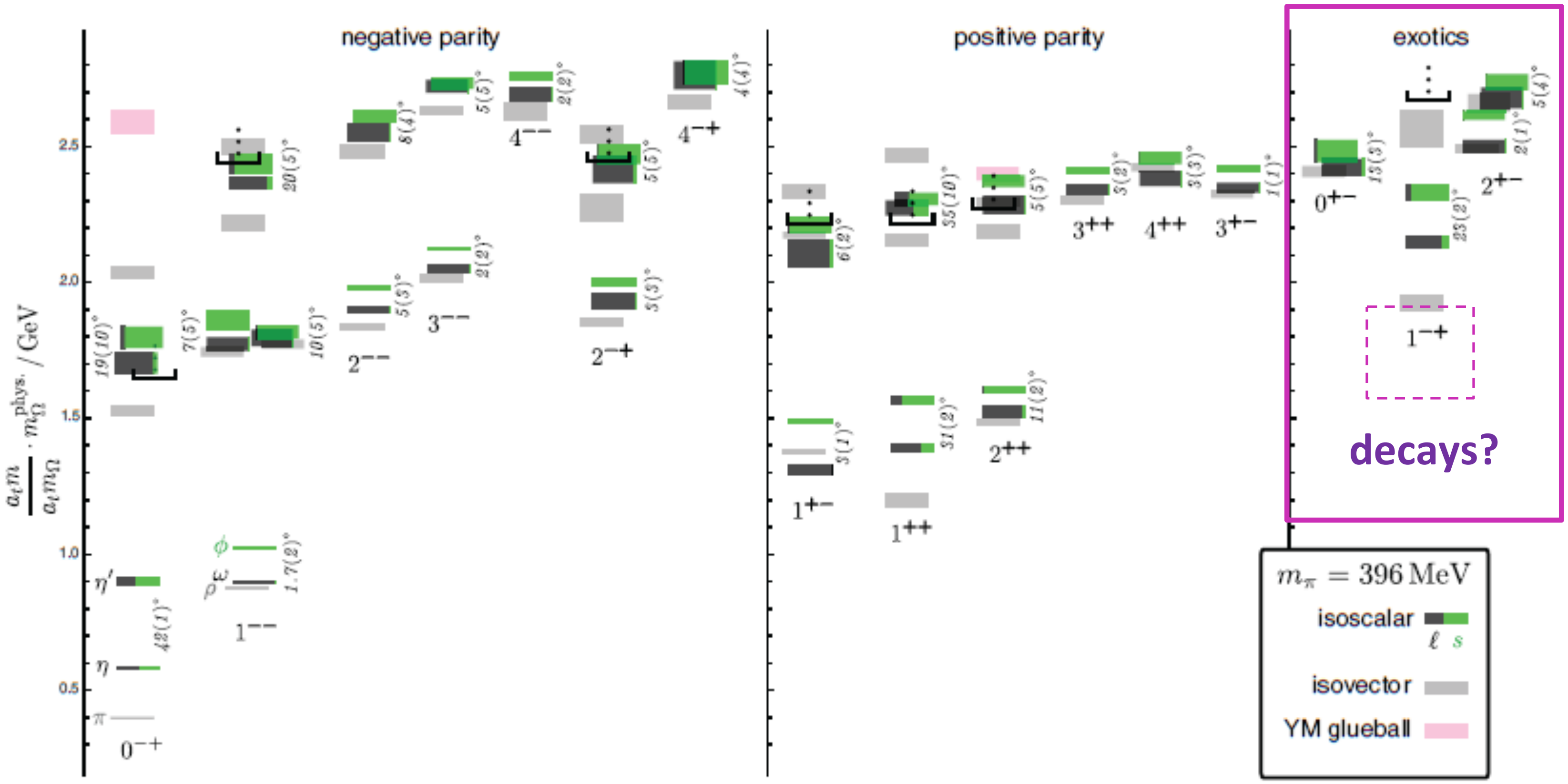




Mounting of the Forward Time-of-Flight detector arrays onto the forward carriage in Hall B

Project was re-baselined in Sept. 2013 with a Total Project Cost of **$338M** and completion in Sept. 2017 [early science?]

MENP Famous <u>2011</u> JLAB LQCD exotic meson spectrum prediction. However at **m_π = 396 MeV**.



R. Edwards: <u>Now</u> running at **m_π = 230 MeV (expt. avg. (GOAL!) = 138 MeV)**. (No figure yet.)

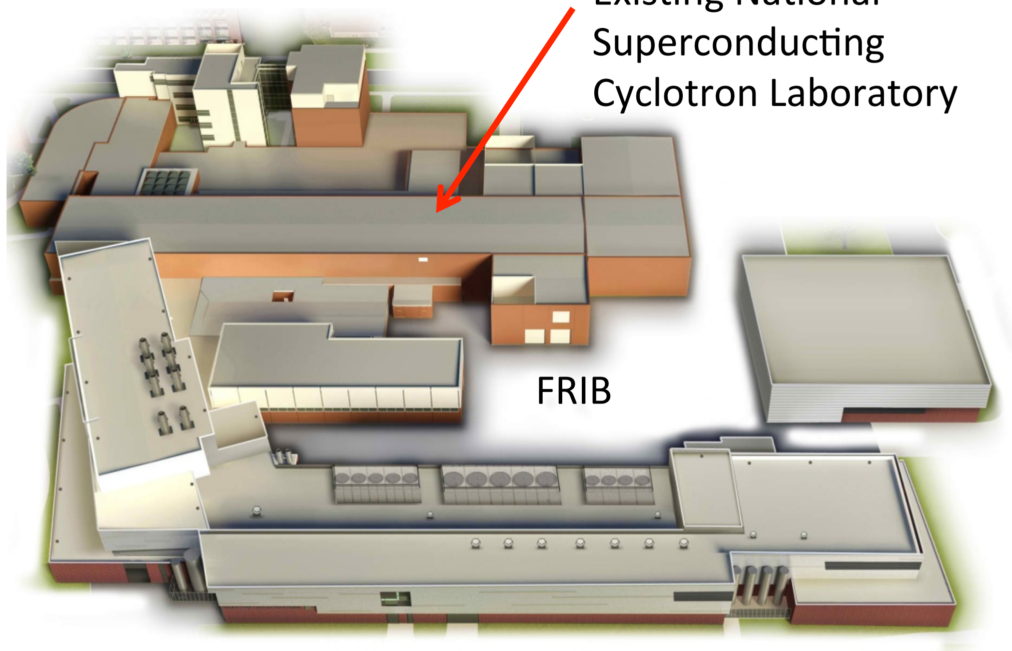
Not Moore's law (need 1000x > 10 yrs.); <u>technique</u>! (*multigrid*). SciDAC: Brower -> pdf -> JLAB.

FIGURE 2.34 Results from a lattice QCD calculation of the meson spectrum. The first two panels show the masses of states predicted by the quark model. For comparison the mass of a purely gluonic excitation is plotted in pink. The third panel shows the masses of states that involve excitations of both quarks and gluons and are not predicted by the quark model (exotics). The calculations were performed at unphysical quark masses that result in a pion mass of 390 MeV. However, they suggest the presence of many exotics in the region accessible by the GlueX experiment at JLAB. SOURCE: J.J. Dudek, R.G. Edwards, B. Joo, M.J. Peardon, D.G. Richards, and C.E. Thomas, 2011, Isoscalar meson spectroscopy from lattice QCD, *Physical Review D* 83:111502, Figure 4. Copyright 2011, American Physical Society. Courtesy of D.G. Richards, JLAB.

LENP

FRIB: Facility for Rare Isotope Beams

"On August 1, 2013, the Department of Energy's Office of Science approved Critical Decision-2 (CD-2), Approve Performance Baseline, and Critical Decision-3a (CD-3a), Approve Start of Civil Construction and Long Lead Procurements, for the Facility for Rare Isotope Beams (FRIB) construction project, which will be located at Michigan State University.



As with other DOE Office of Science construction projects, CD-2 formally establishes the cost and schedule for the FRIB project. The Total Project Cost for FRIB is **$730M**, of which $635.5M will be provided by DOE and $94.5M will be provided by Michigan State University. The project will be completed by **2022**.

The CD-3a decision allows the project to proceed with long lead procurements. Commencement of the start of civil construction is subject to a Fiscal Year 2014 appropriation.

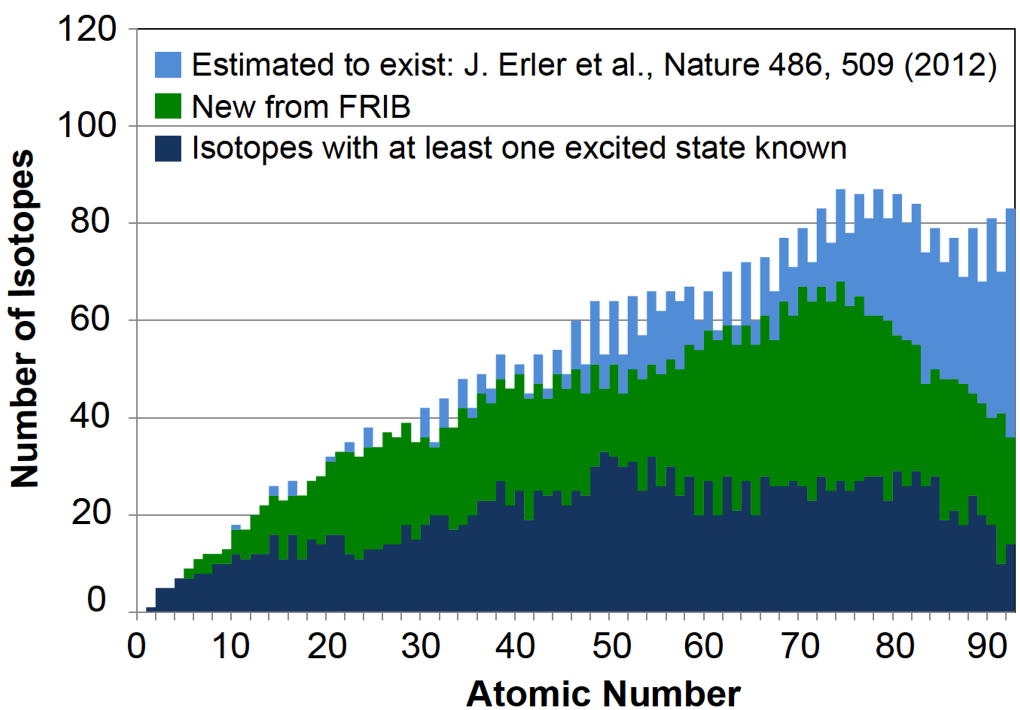
FRIB will be constructed under a Cooperative Agreement between MSU and DOE

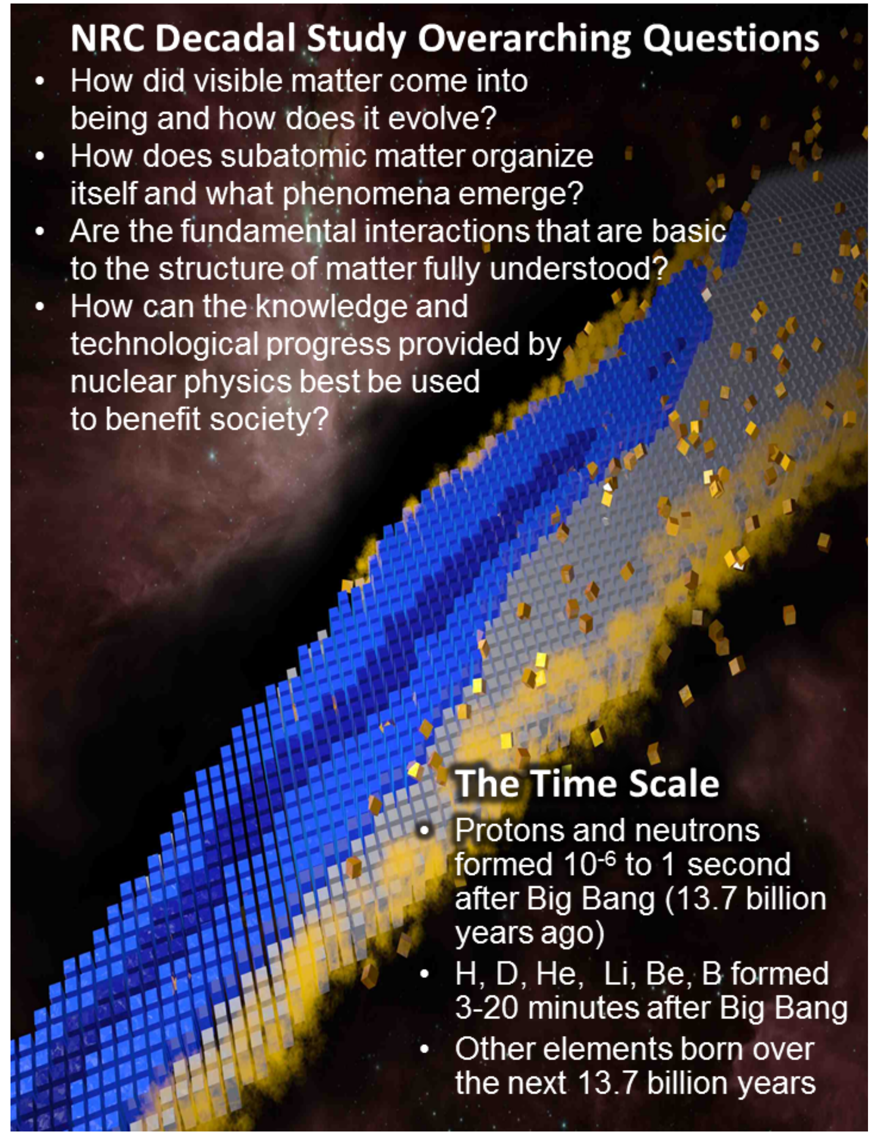
LENP

FRIB: 21st Century Science Questions

- FRIB physics is at the core of nuclear science: "To understand, predict, and use"
- FRIB provides access to a vast unexplored terrain in the chart of nuclides

[*ca.* 7000 nuclei exist (NUCLEI SciDAC-3 project)]

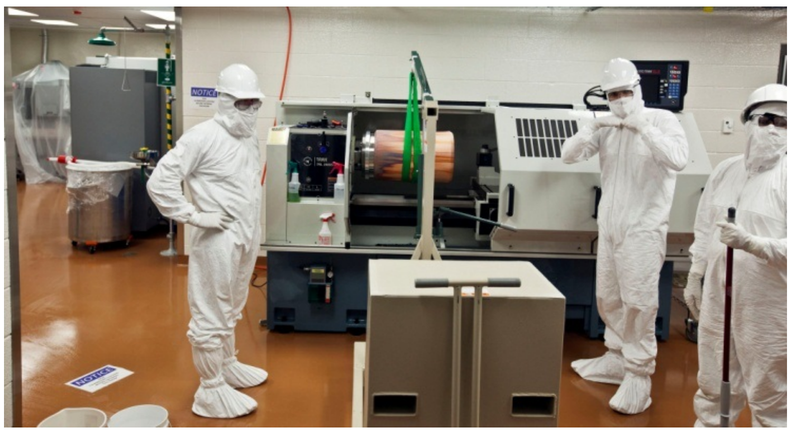




LENP

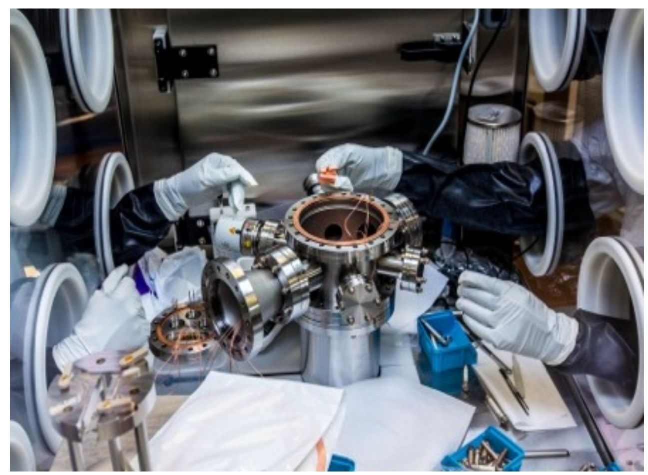
Preparations for NP Stewarded Neutrino-less Double Beta Decay Experiments

R&D on one of several approaches by U.S. scientists is ongoing at Lead, South Dakota



4800 feet below ground, the copper needed for a cryostat to cool sensitive Germanium detectors is being electroformed to avoid induced backgrounds caused by cosmic rays

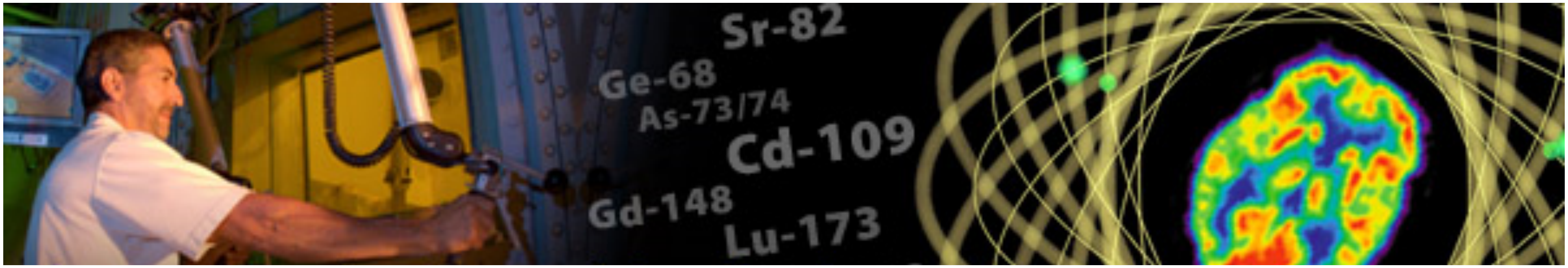
With techniques that use nuclear isotopes inside cryostats, often made of ultra-clean materials, scientists are “tooling up” to study whether neutrinos are their own anti-particle. The answer could help determine why the matter/anti-matter ratio today is far different than in the early cosmos.
[Future HPC: $0\nu\beta\beta$ nuclear MEs !] (Ge, Xe, Te)



The cyrostat, made from some of the purest copper in the world, is also prepared 4800 ft underground

Isotopes

Isotope Program Mission



The mission of the DOE Isotope Program is threefold

- Produce and/or distribute radioactive and stable isotopes that are in short supply, associated byproducts, surplus materials and related isotope services.
- Maintain the infrastructure required to produce and supply isotope products and related services.
- Conduct R&D on new and improved isotope production and processing techniques which can make available new isotopes for research and applications.

Produce isotopes that are in short supply only;
The Isotope Program does not compete with industry

More than 225 customer orders in FY2013

More than 470 shipments in FY2013

The FY2015 SC Budget Request

	FY 2013 Current (prior to SBIR/STTR)	FY 2013 Current Approp.	FY 2014 Enacted Approp.	FY 2015 President's Request	FY15 President's Request vs. FY14 Enacted Approp.	
Advanced Scientific Computing Research	417,778	405,000	478,093	541,000	+62,907	+13.2%
Basic Energy Sciences	1,596,166	1,551,256	1,711,929	1,806,500	+94,571	+5.5%
Biological and Environmental Research	578,294	560,657	609,696	628,000	+18,304	+3.0%
Fusion Energy Sciences	385,137	377,776	504,677	416,000	-88,677	-17.6%
High Energy Physics	748,314	727,523	796,521	744,000	-52,521	-6.6%
Nuclear Physics	**519,859**	**507,248**	**569,138**	**593,573**	**+24,435**	**+4.3%**
Workforce Development for Teachers and Scientists	17,486	17,486	26,500	19,500	-7,000	-26.4%
Science Laboratories Infrastructure	105,673	105,673	97,818	79,189	-18,629	-19.0%
Safeguards and Security	77,506	77,506	87,000	94,000	+7,000	+8.0%
Program Direction	174,862	174,862	185,000	189,393	+4,393	+2.4%
Subtotal, Office of Science	**4,621,075**	**4,504,987**	**5,066,372**	**5,111,155**	**+44,783**	**+0.9%**
SBIR/STTR	...	176,208	...	...	...	...
Total, Office of Science	**4,621,075**	**4,681,195**	**5,066,372**	**5,111,155**	**+44,783**	**+0.9%**

Nuclear Physics
FY 2015 President's Request by Subprogram

Budget Structure/ Subprogram ($ in 000s)	FY 2013 Approp (w/SBIR/STTR)	FY 2014 Enacted	FY 2015 Request	FY 2015 vs. FY 2014
Medium Energy	128,328	148,695	149,892	+1,197
Heavy Ions	193,229	199,693	198,966	-727
Low Energy*	100,190	75,704	75,269	-435
Nuclear Theory	39,057	45,142	43,096	-2,046
Isotope Program	18,483	19,404	19,850	+446
Construction	40,572	80,500	106,500	+26,000
TOTAL NP	**519,859**	**569,138**	**593,573**	**+24,435**

* FRIB included in Low Energy in FY 2013 ($22M)

Increase in the FY 2015 budget request for NP is dominated by the construction profile of FRIB

Finally: the 2014 NP NERSC Portfolio

2014 NP Allocation (T+OT) = 258M [MPP hrs] ☺ **NP loves "cycles"**

(was 114M in 2013) *n.b.* rough conversion 1B [MPP hrs] ~ 1 [Pf-yr]

2014: 48 NP NERSC proposals (multiusers / repos):

Props. & area	~ alloc.
5 NP Accel.	4M
13 Nucl. Astro.	60M
7 LQCD (1 thermo, 4 structure, 1 baryon spec.)	164M
23 general "NP Theory" [wide range of topics, incl. expt. sim.]	9M

Request(T)/Alloc.(T+OT) = 1.18 [8% reserves].

Vast improvement over previous years. R/A ~ 3 was typical.

3 OT projects nom. by NP (1 LQCD, 2 nucl. astro.); all approved "upstairs"

n.b. Majority of LQCD and LENP comp time fm. INCITE, ALCC, and LQCD-ext.

END