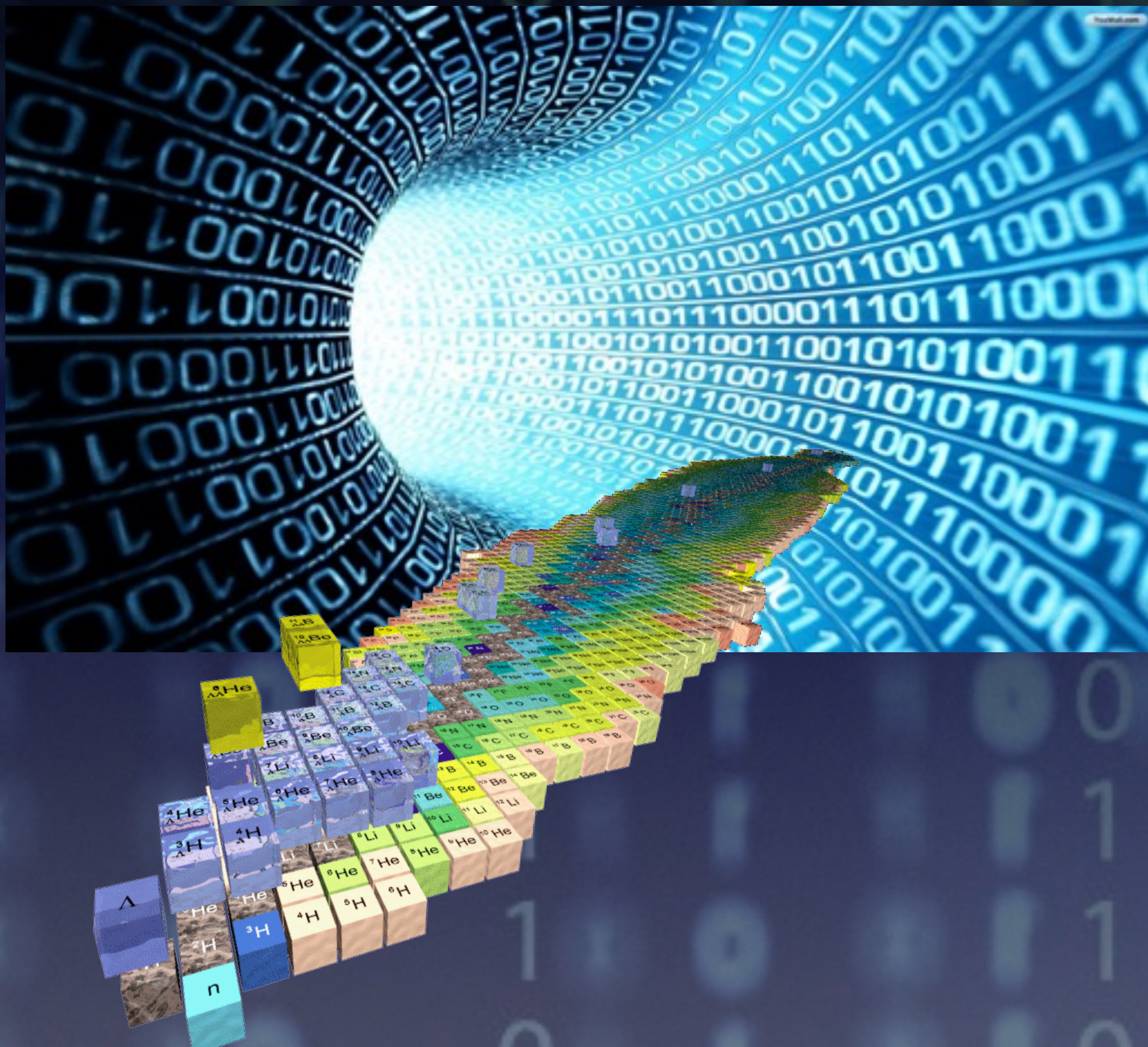
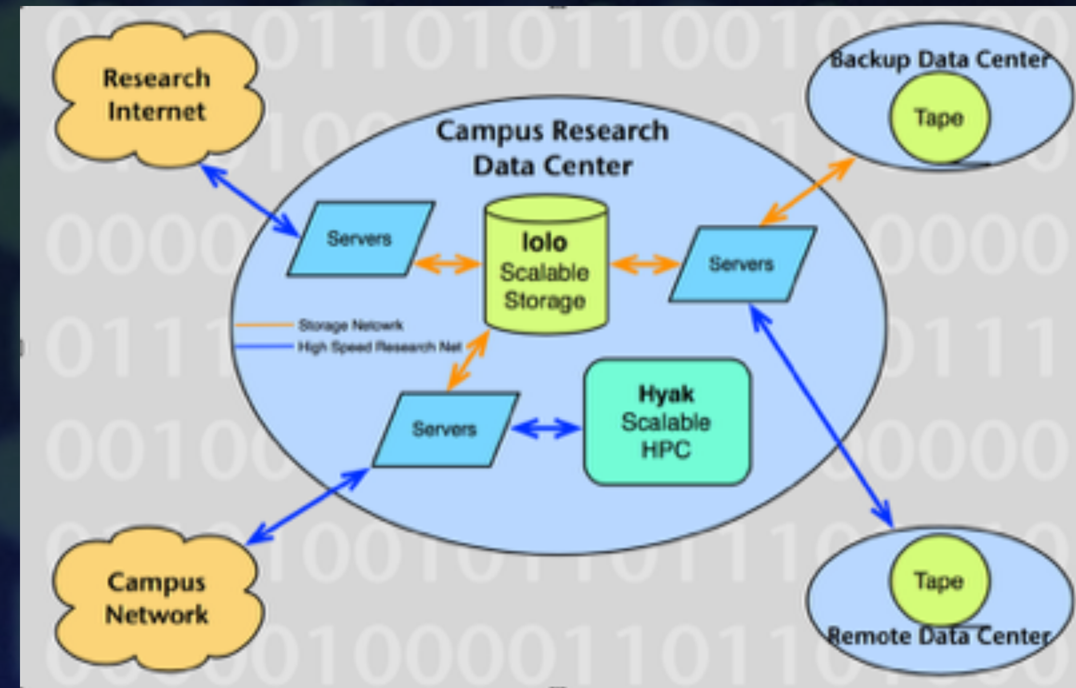




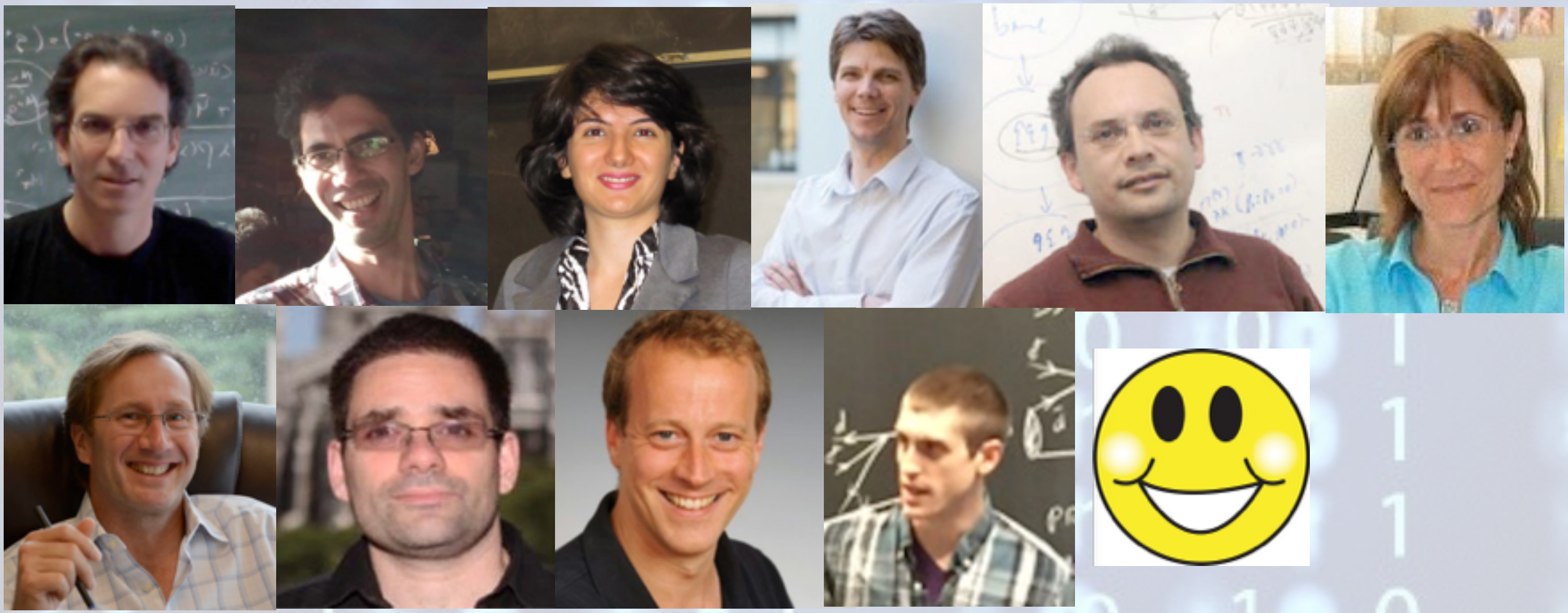
Fundamental Forces with Big Computers

Martin J. Savage

INSTITUTE for NUCLEAR THEORY

HPC club Seminar Series, May 19 (2016)

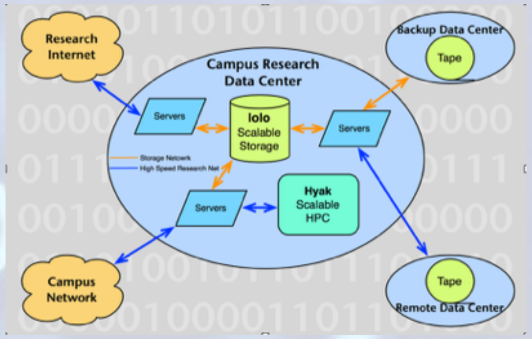
NPLQCD



Silas Beane (UW)
Zohreh Davoudi (MIT)
Kostas Orginos (WM/JLab)
Martin Savage (INT)
Frank Winter (JLab)
Jonas Wilhelm (Geissen)

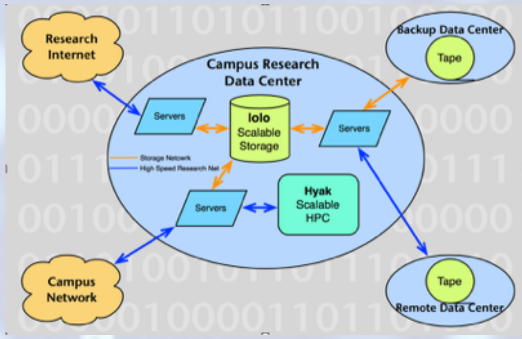
Emmanuel Chang (INT)
William Detmold (MIT)
Assumpta Parreno (Barcelona)
Brian Tiburzi (CCNY/BNL)
Michael Wagman (UW)

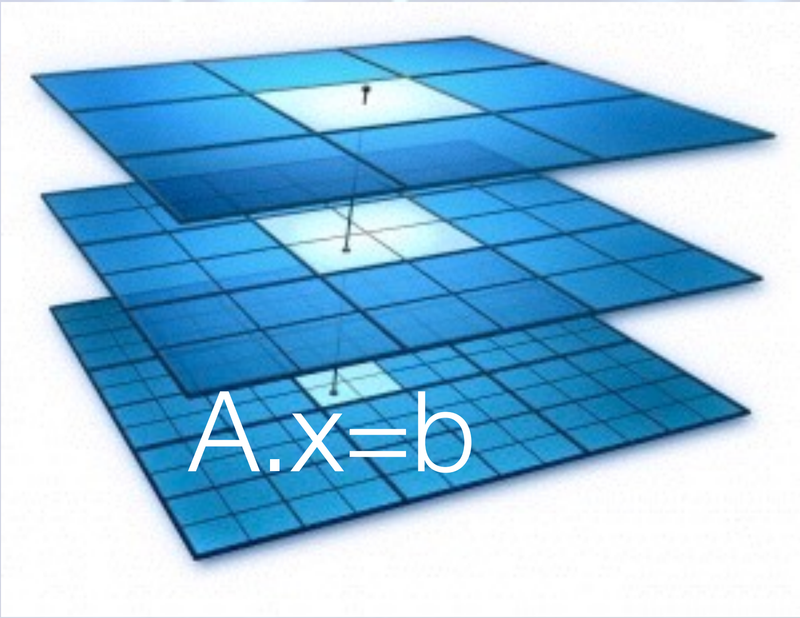
Past Collaborators
Saul Cohen
Pari Junnarkar
Huey-Wen Lin
Aaron Torok
Tom Luu
Andre Walker-Loud



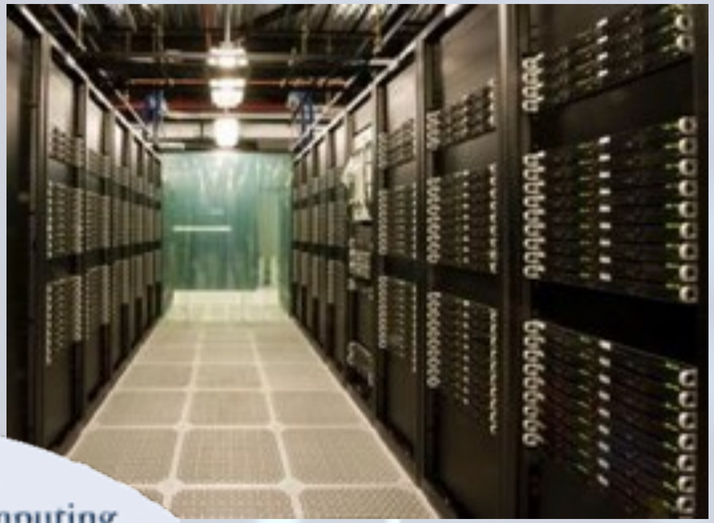
USQCD

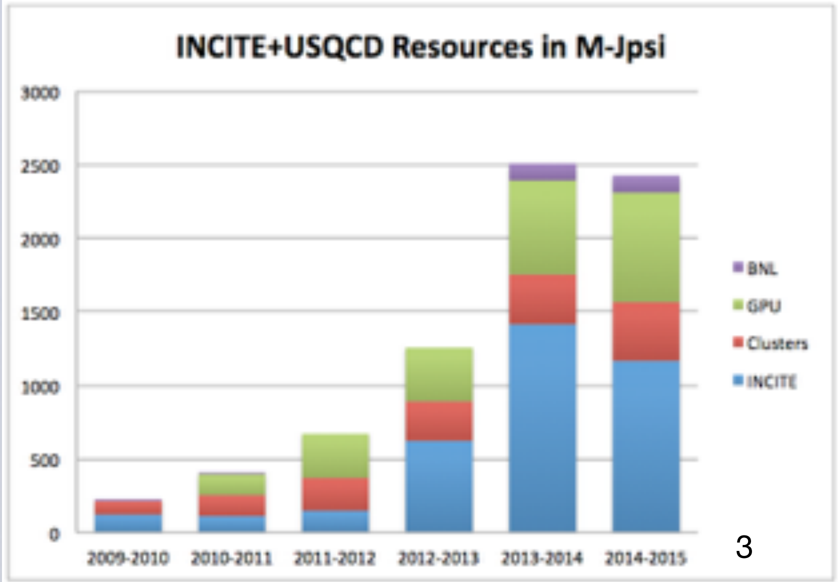
A collaboration of collaborations

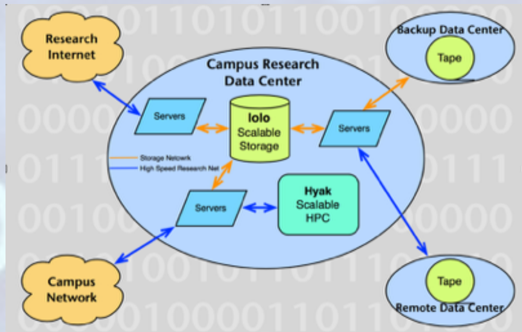




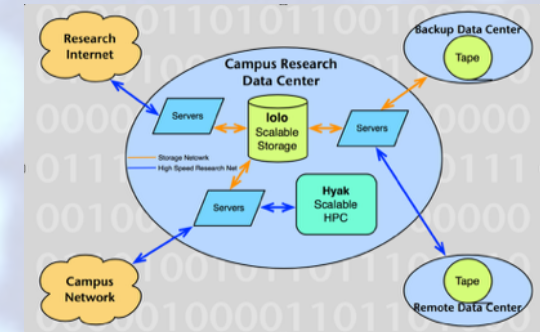
SciDAC
Scientific Discovery through Advanced Computing

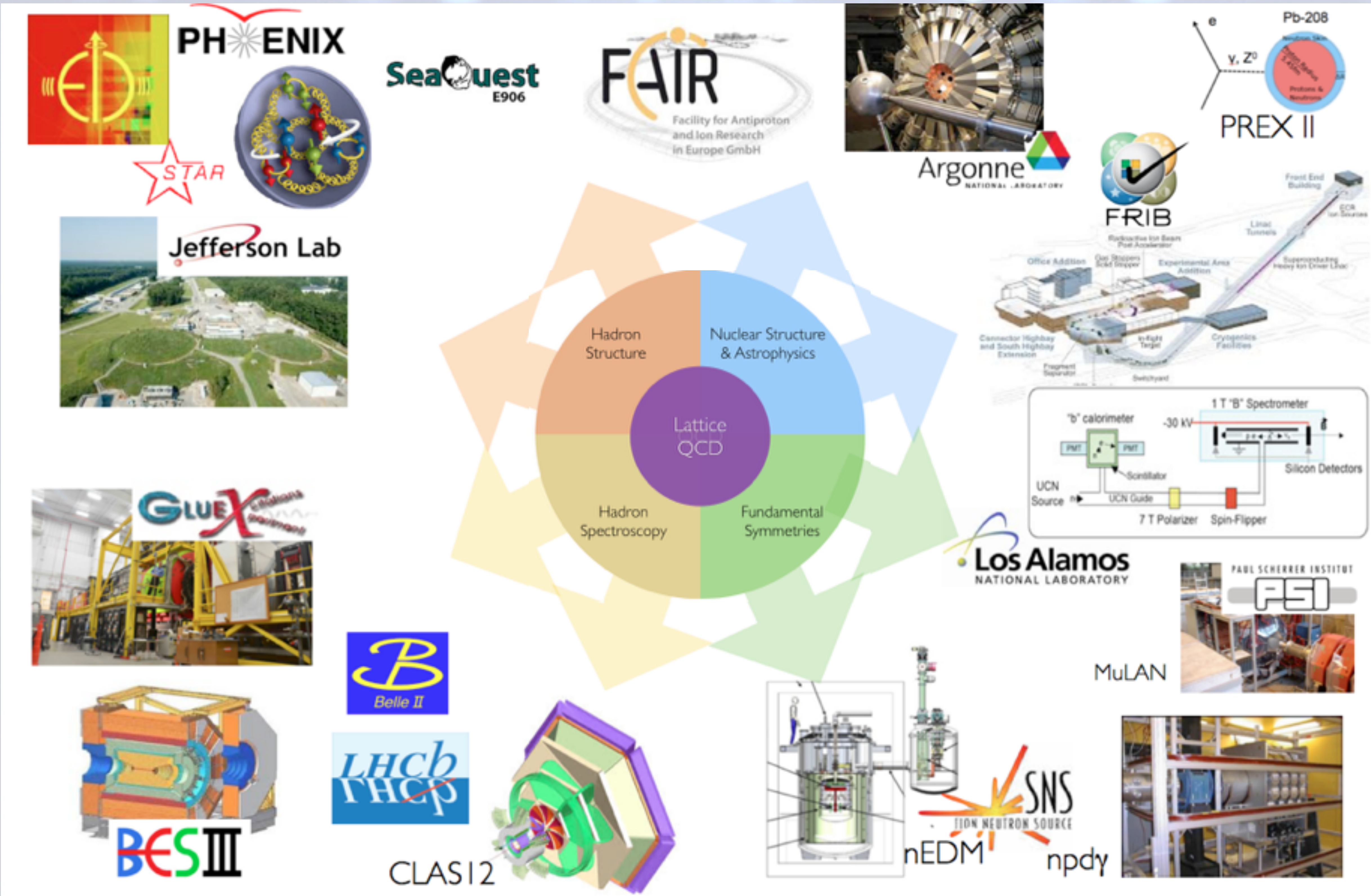


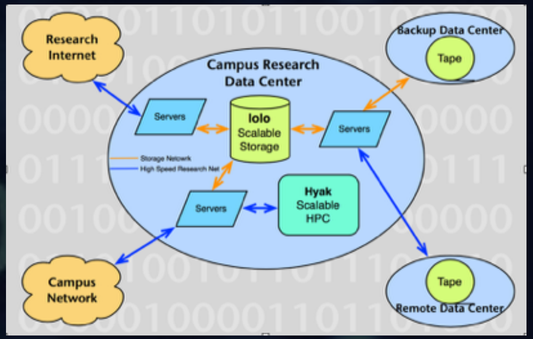




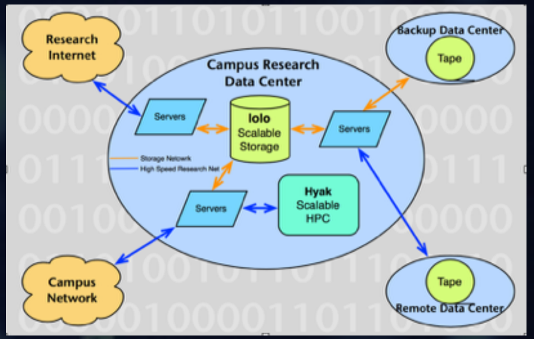
Supports NP Experimental Program



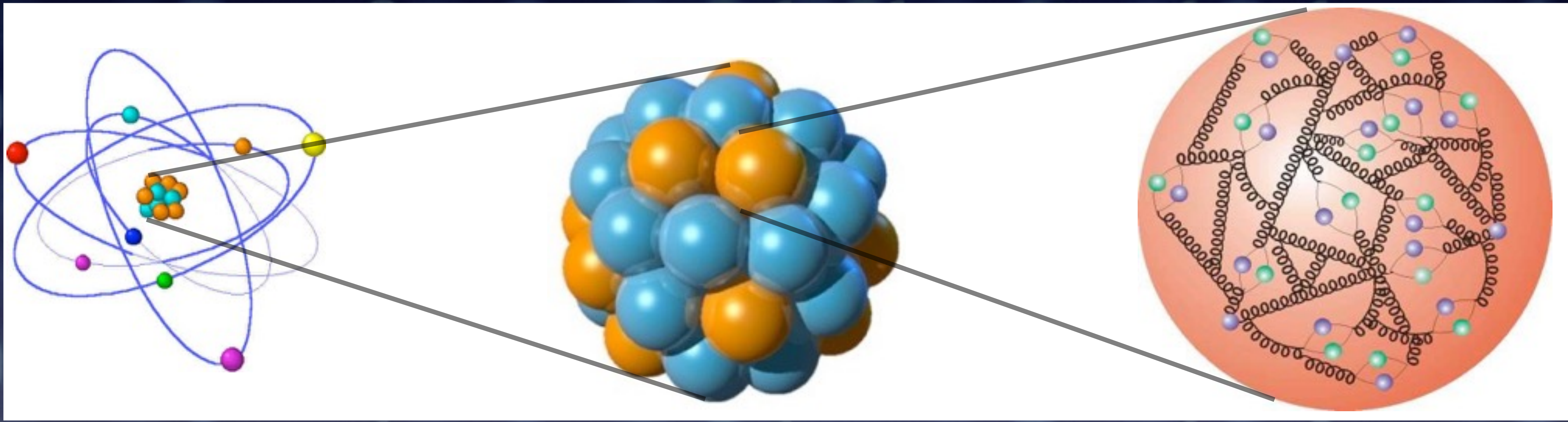




Structure of Matter



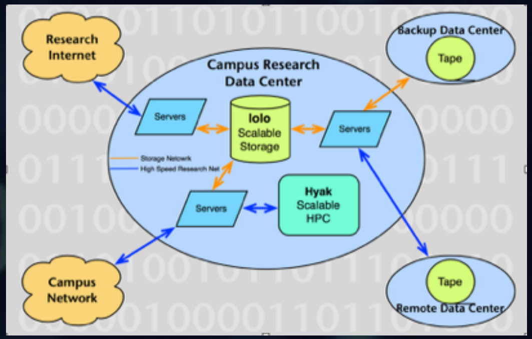
Atom | Nucleus | Proton



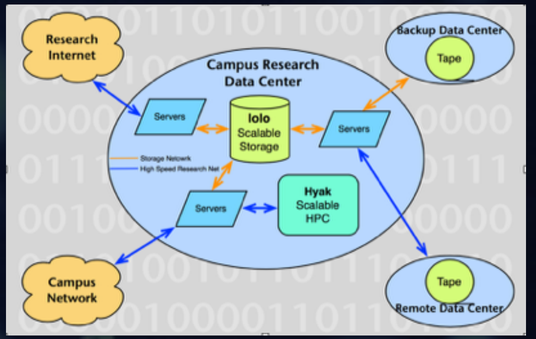
Electrons and Nuclei | Protons and Neutrons | Quarks and Gluons

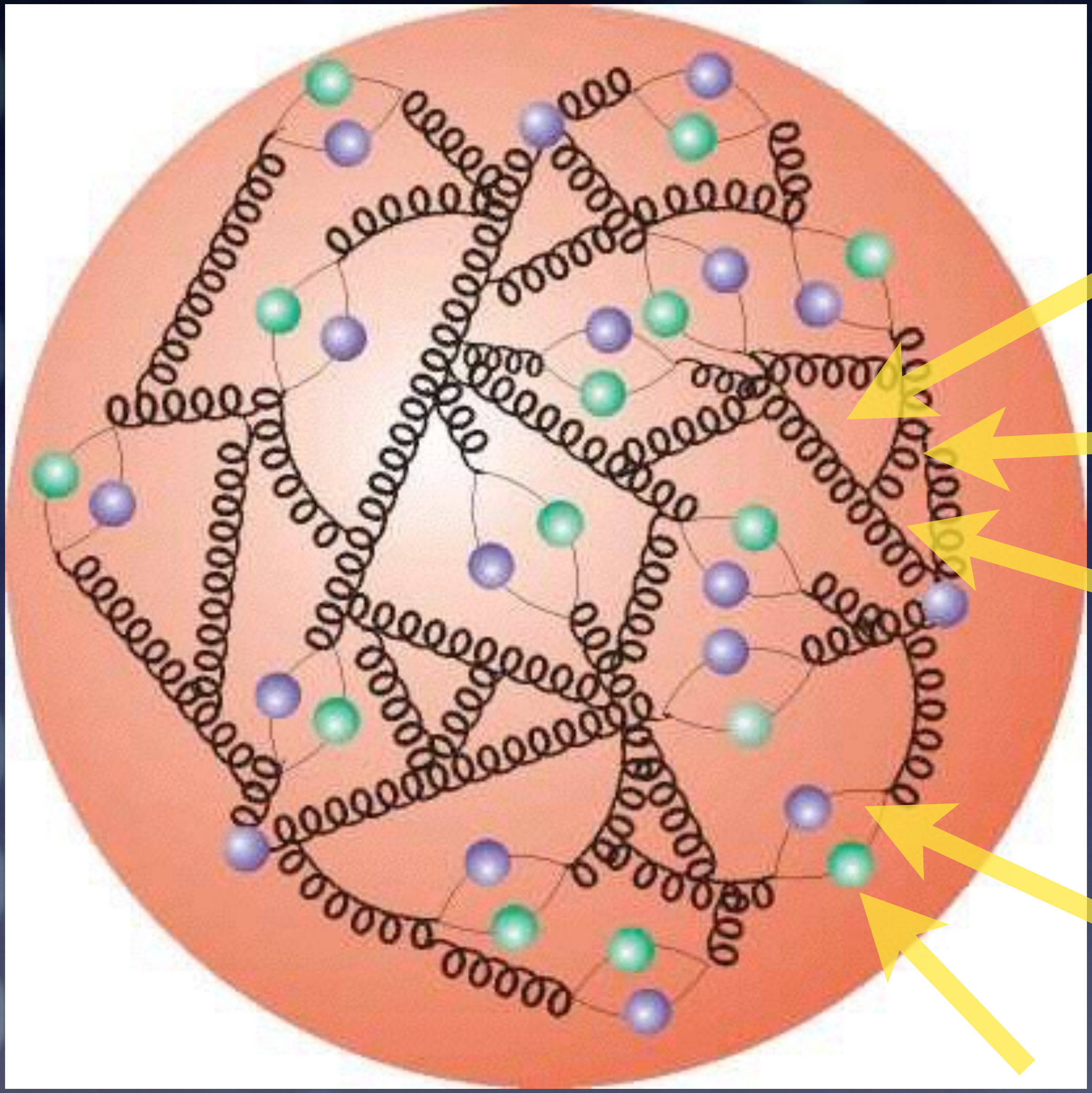
Quantum Chromodynamics

A quantum field theory describing the dynamics of gluons and quarks



At the Heart of Visible Matter


Research Internet
Campus Research Data Center
Backup Data Center
Tape
Servers
Iolo Scalable Storage
Servers
Hyak Scalable HPC
Servers
Campus Network
Tape
Remote Data Center



gluon

gluon

gluon

quark

anti-quark

Nucleon

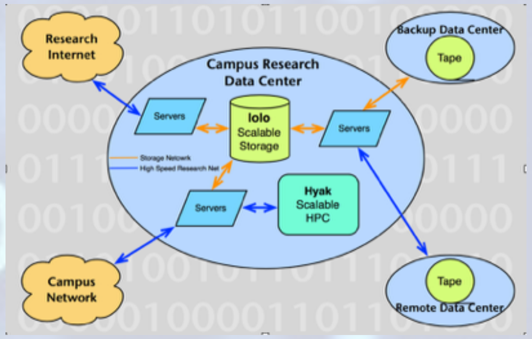
up-quark mass ~ 3 MeV

down-quark mass ~ 5 MeV

gluon mass = 0 MeV

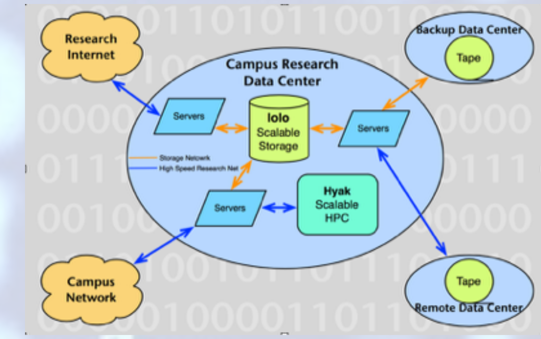
proton ~ 940 MeV

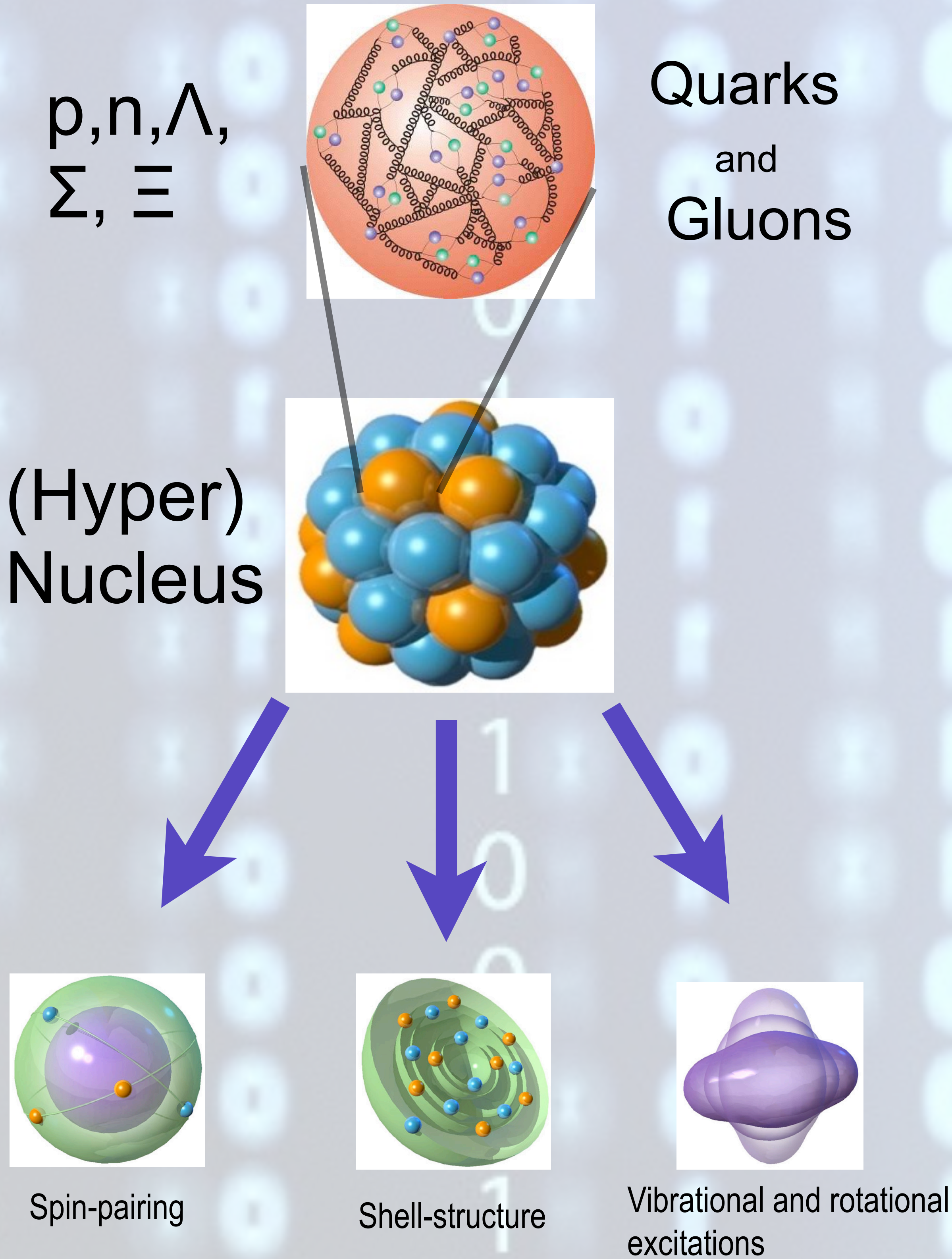
Nucleon is an entangled state of indefinite particle number with spin-1/2



QCD

Predictive Capabilities Within Reach





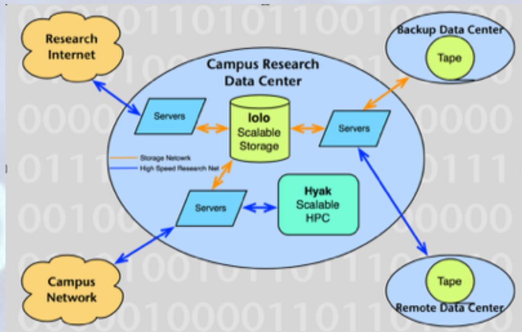
$$\Lambda_{\mathrm{QCD}}$$

$$\frac{m_u}{\Lambda_{\mathrm{QCD}}} \quad \frac{m_d}{\Lambda_{\mathrm{QCD}}} \quad \frac{m_s}{\Lambda_{\mathrm{QCD}}}$$

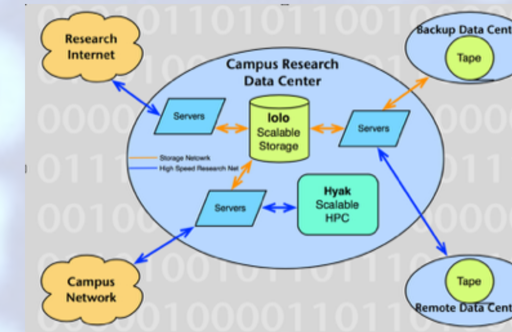
$$\alpha_e$$

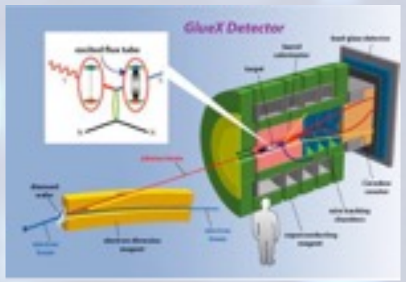
Small number of input parameters responsible for all of strongly interacting matter

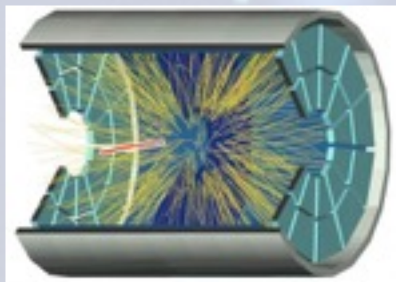
Refine predictive capabilities for low-energy nuclear physics with complete uncertainty quantification



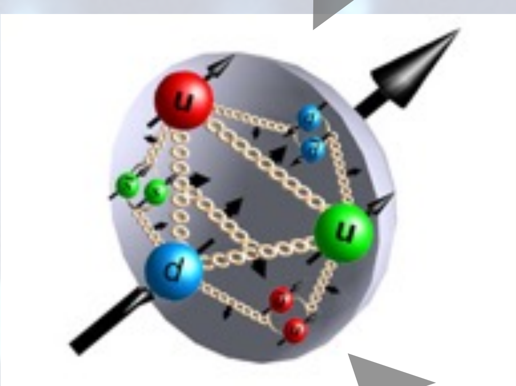
The Roadmap from QCD to Nuclear Physics

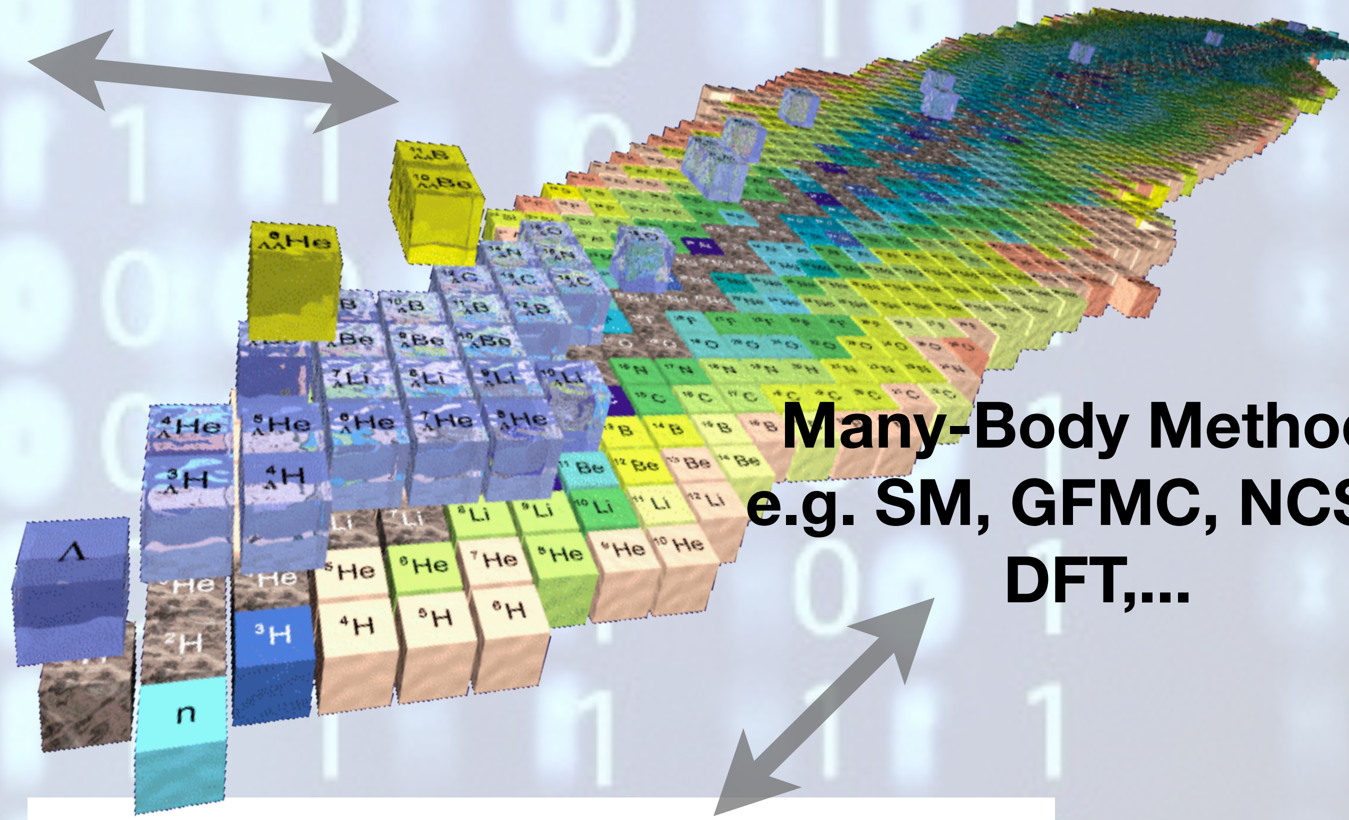




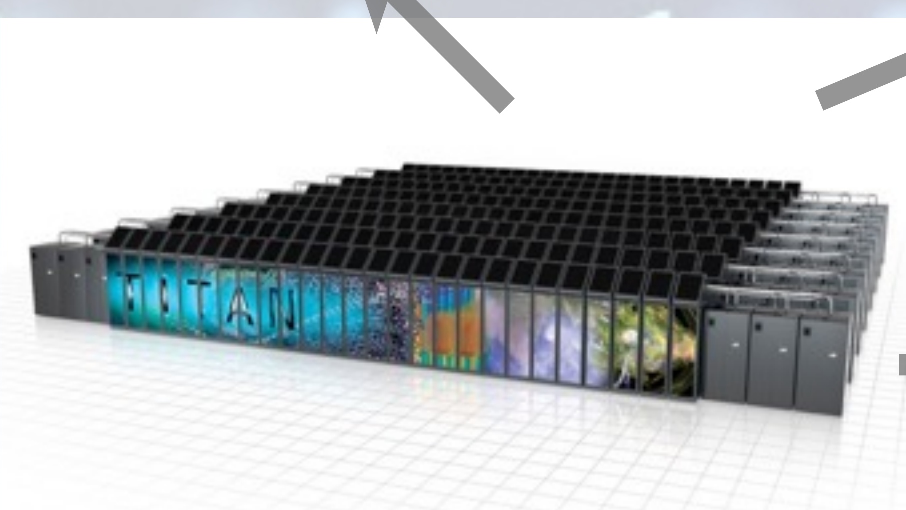


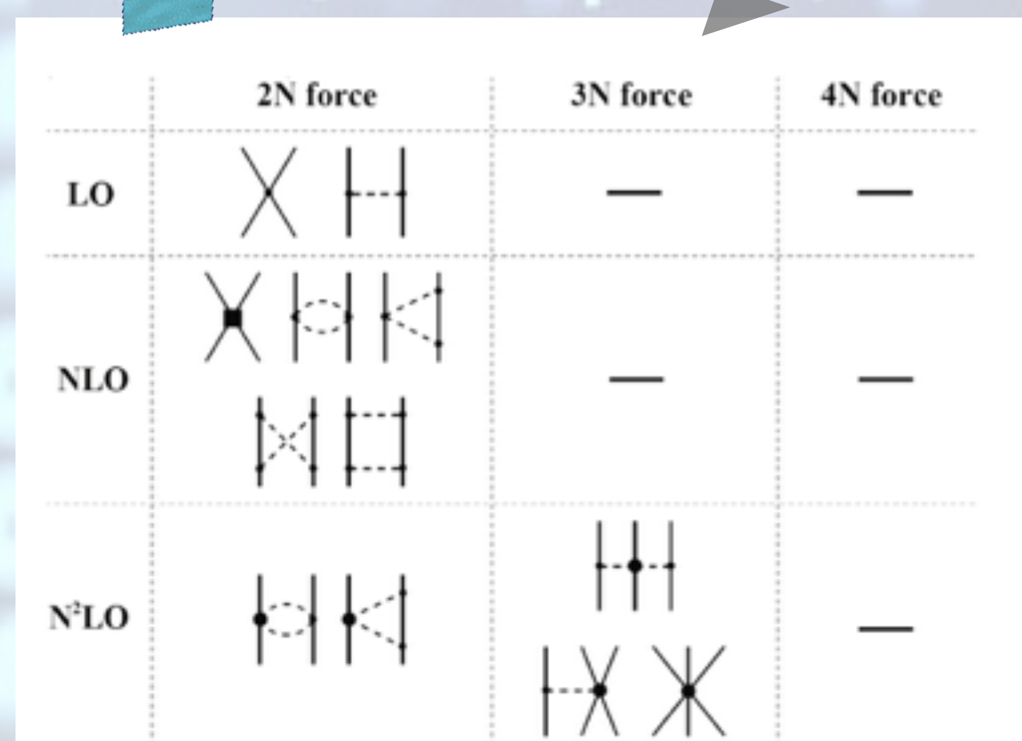
JLab RHIC FRIB



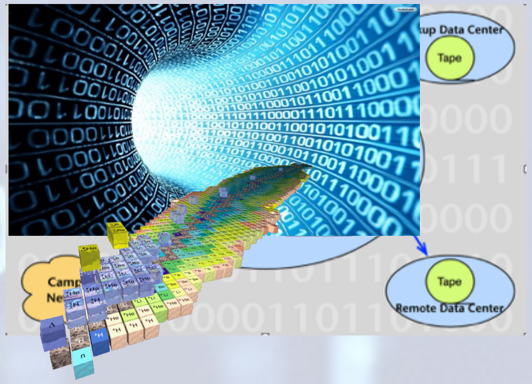


Many-Body Methods e.g. SM, GFMC, NCSM, DFT,...

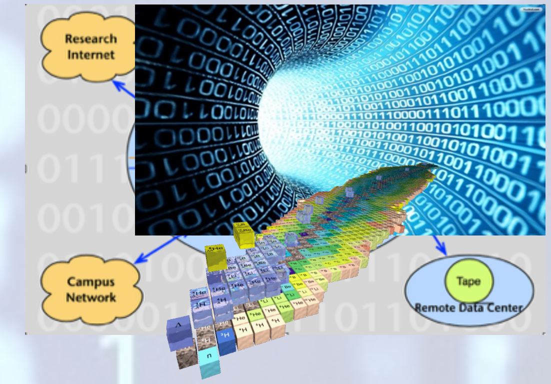


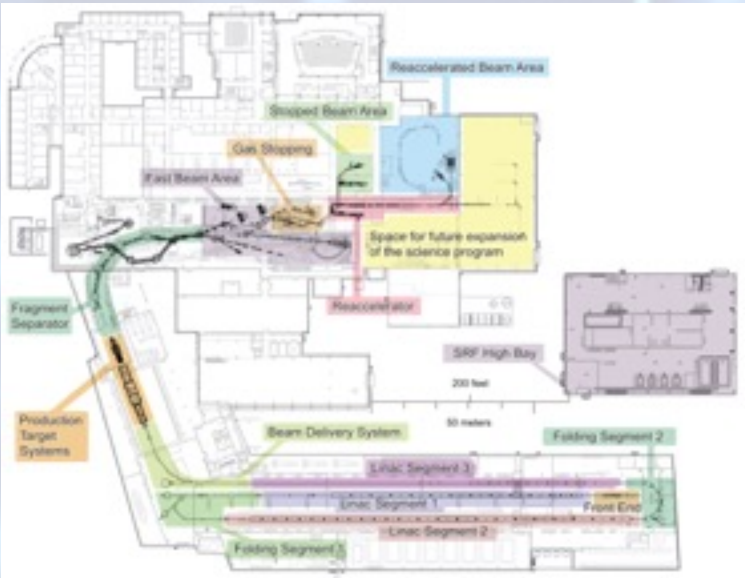


Solve QCD



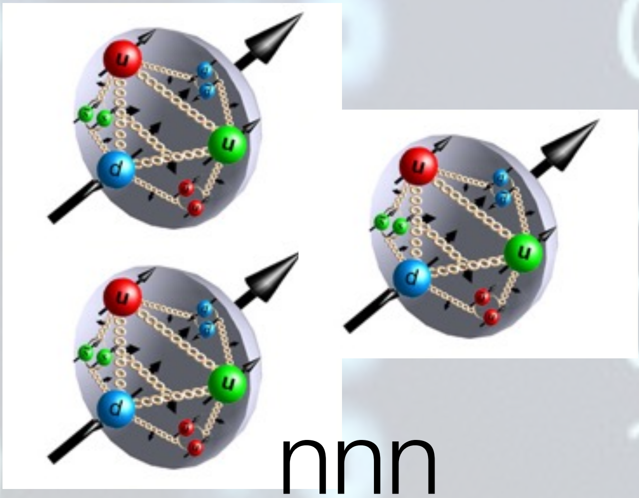
FRIB





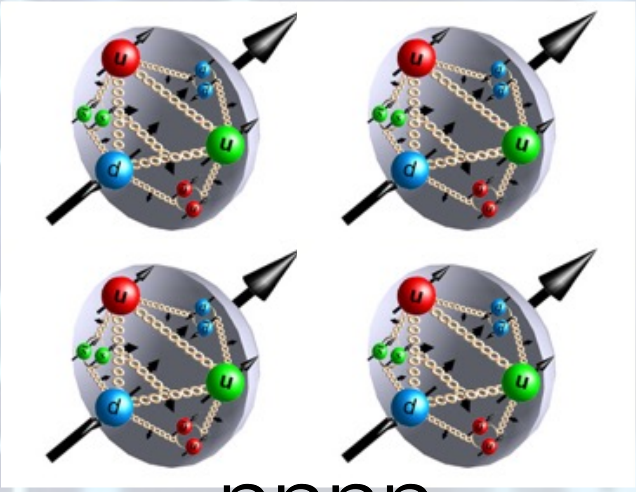
Experiment

Theory : NUCLEI

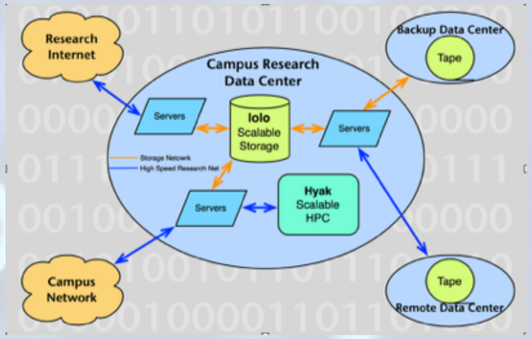


nnn

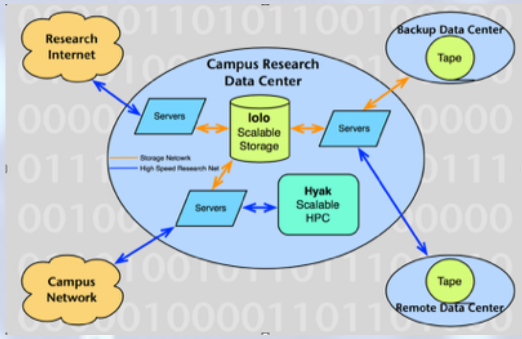
multi-neutron forces

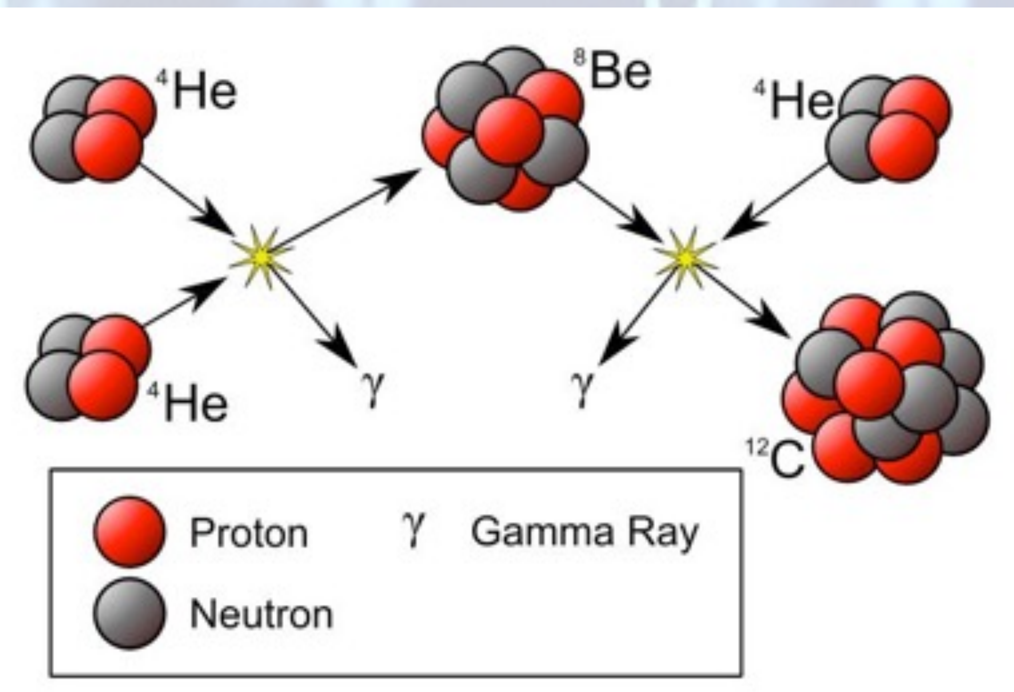


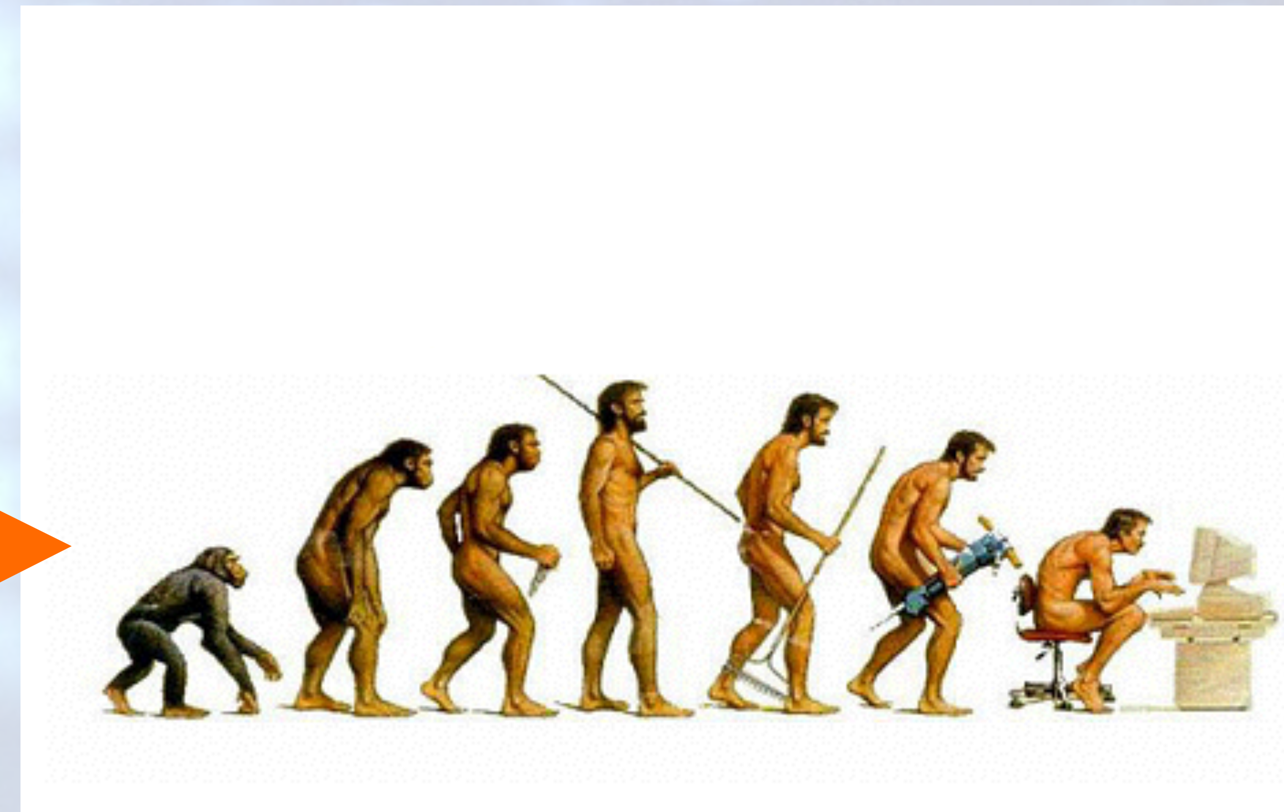
nnnn



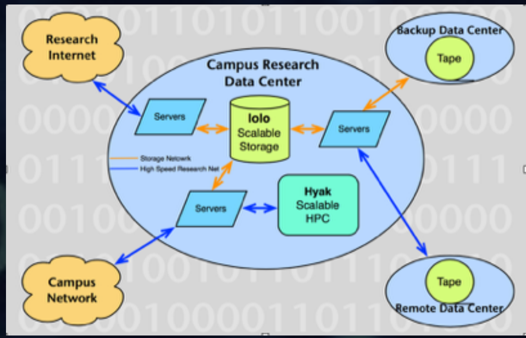
Fine-Tunings Define Our Universe



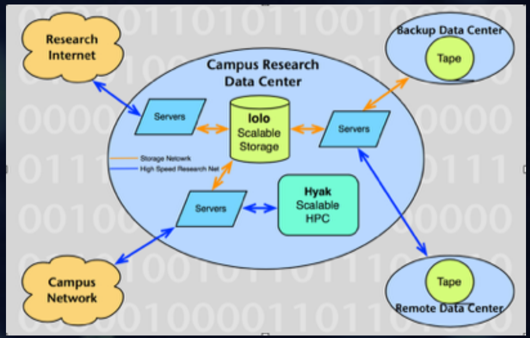




- Nuclear physics exhibits fine-tunings
  - *Why ??*
  - *Range of parameters to produce sufficient carbon ?*
  - *Large cancellation in NN interactions - weakly bound deuteron*



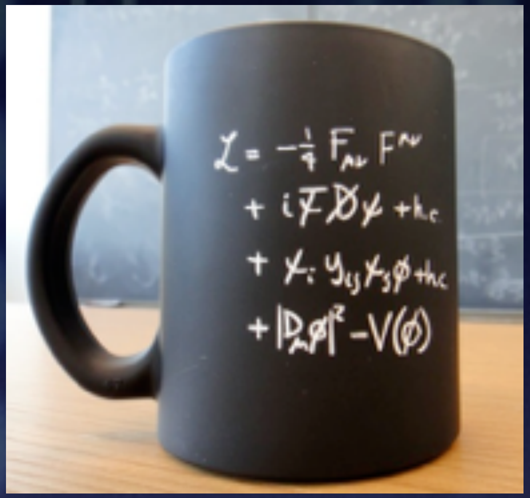
Quantum Chromodynamics



Experiment

Experiment

Thinking

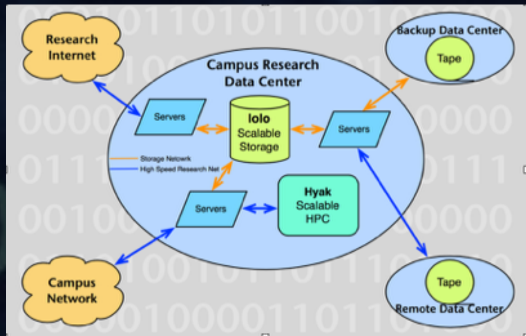


QCD

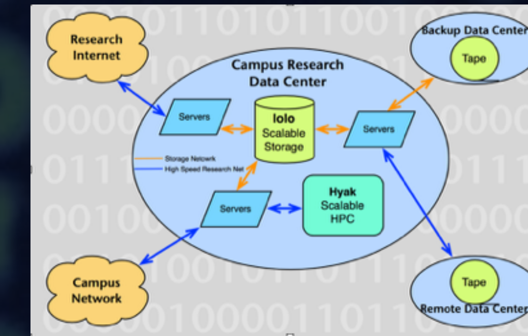
electric charges ↕ color charges

EM waves ↕ Excited Glue

QCD is Non-Linear
and essentially Quantum



Quantum Mechanics


Research Internet
Campus Research Data Center
Backup Data Center
Tape
Servers
Iolo Scalable Storage
Servers
Servers
Hyak Scalable HPC
Campus Network
Tape
Remote Data Center

Given all the interactions of the system, what is the probability for transition from A to B?

Richard Feynman

Classical

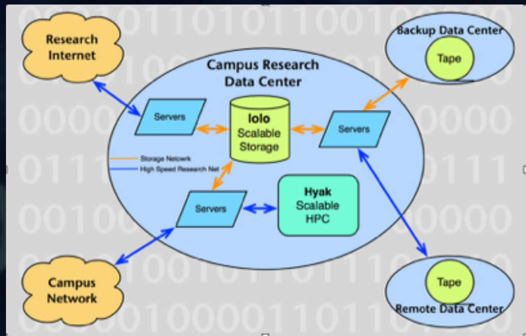
Principle of Least Action

Quantum

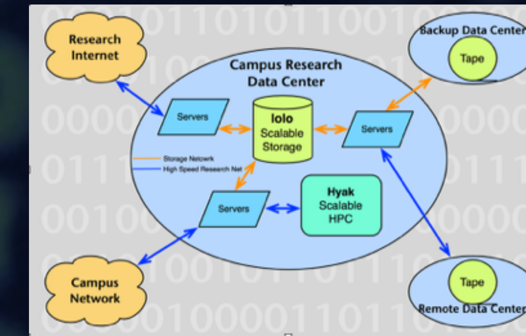
Every path contributes

Quantum probability amplitude:

1. Give each path a weight : e^{iS}
2. Sum over all paths



Quantum Field Theory on Classical Computers



Quantum

Every path contributes

Richard Feynman

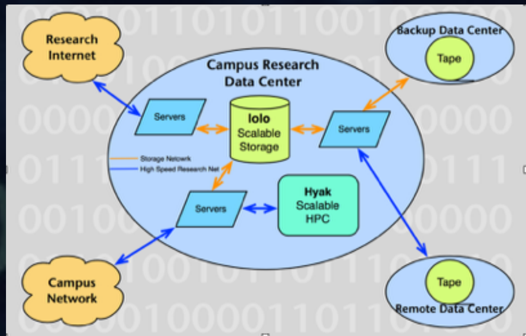
Path Integral

Integrate over the values of all fields at all points in spacetime

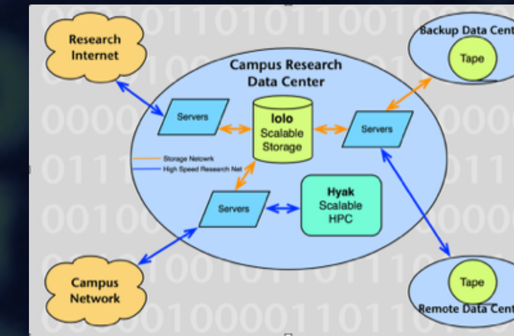
Requires infinite compute resources to numerically evaluate even subatomic volumes of spacetime

Numerically evaluated approximately using a fine grid/mesh, but in a way that can be systematically refined. Includes single precision, double precision, arbitrary precision,..

Use a classical computer to simulate a quantum system : shuffling around 0's and 1's with a well-defined algorithm

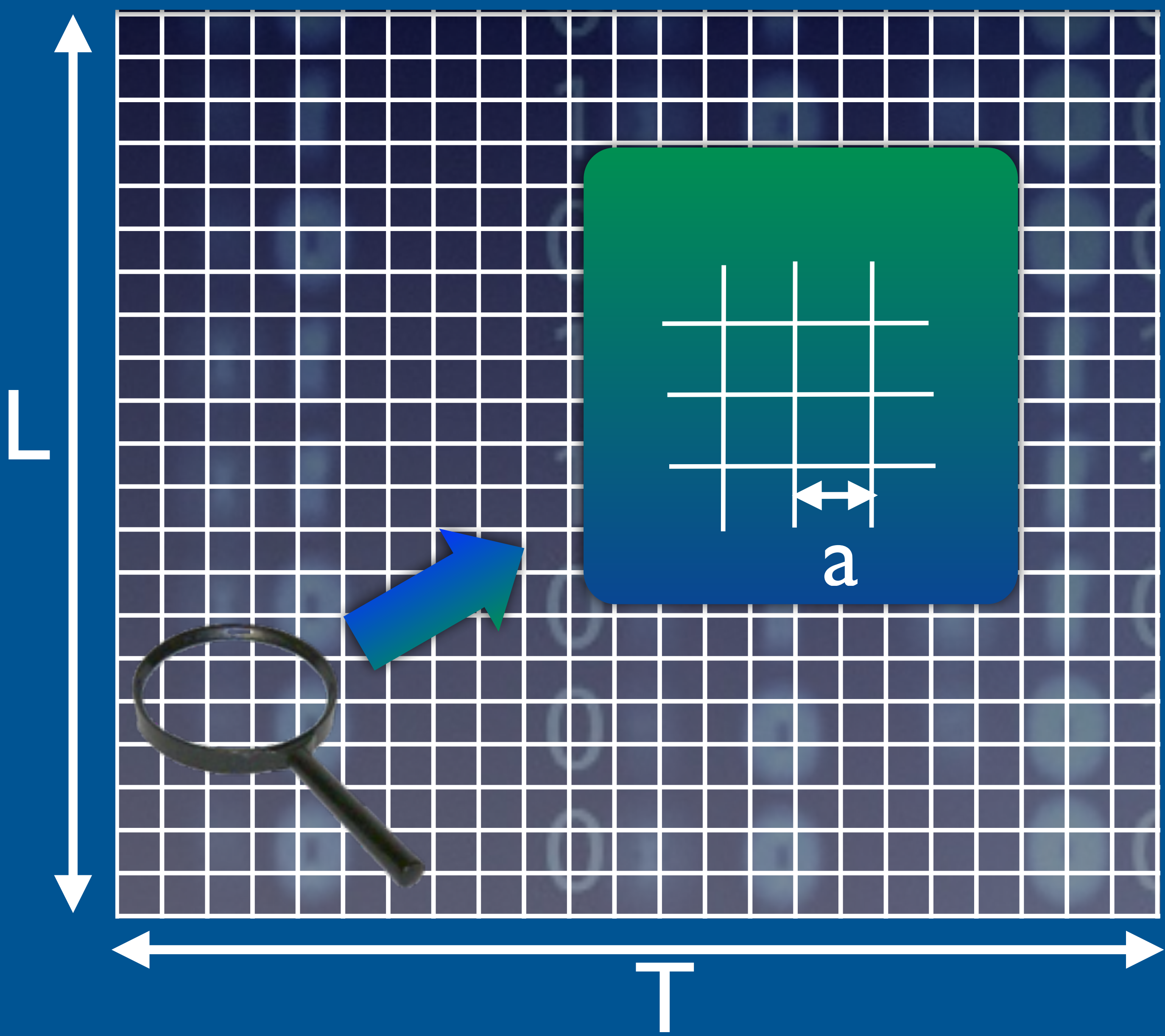


Avoid the continuum



Finite compute resources for finite number of integrals
- Renormalization group and effective field theory

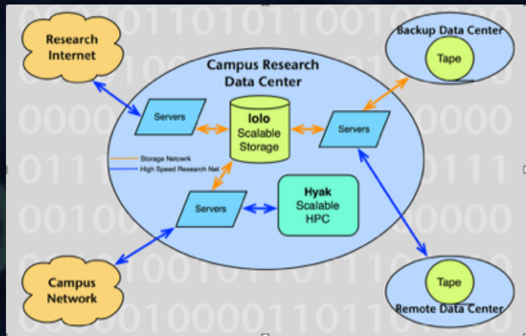
Constrained Resources



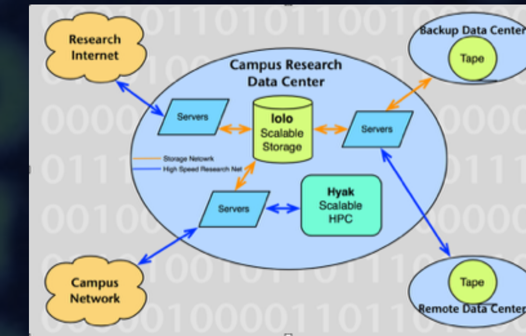
It is the ONLY way to define QCD nonperturbatively !!!!

Lattice volume: $L^3 \times T$

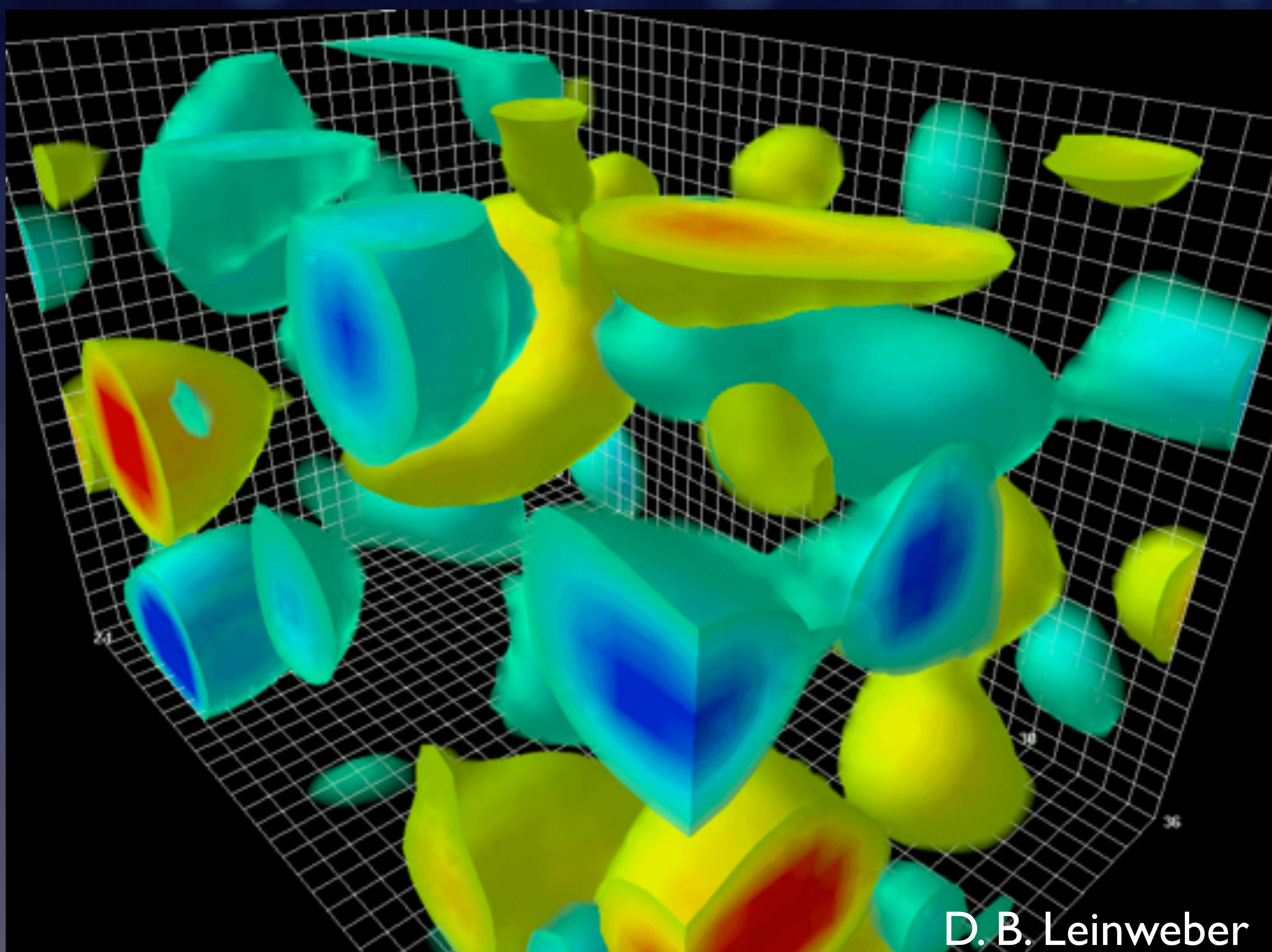
Low-energy effective field theory in powers of the lattice spacing the Symanzik action



Nuclear forces and the nature of matter - Lattice QCD



The strong vacuum is complicated and dynamic

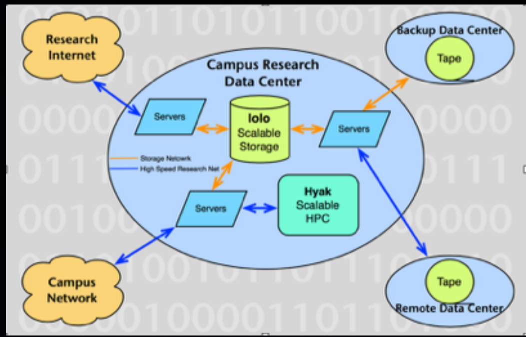

D. B. Leinweber

The cube dimension

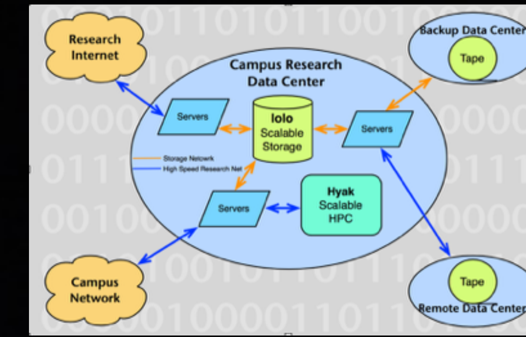
$$(4fm)^3 = (4 \times 10^{-15} m)^3$$

The time duration of one cycle

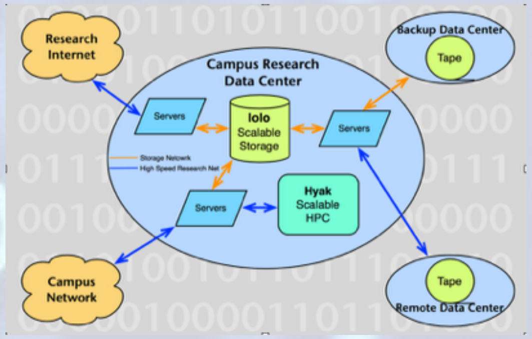
$$\sim 10^{-24} s$$



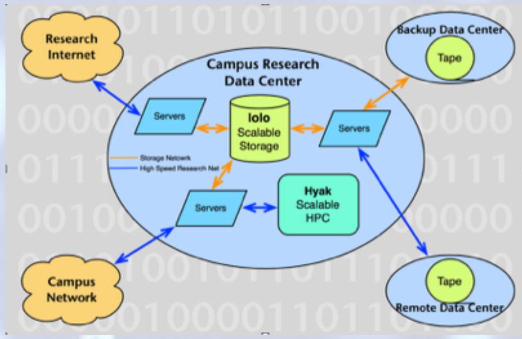
``The Cloud” Cannot Do What is Needed



- Need large partitions, scales out > 1.5 M cores
- Need fast interconnect fabric
- Need to run for MCMC for months and/or years
- Need rapid data access
- Requires World’s Supercomputers
- Why is there no Supercomputer in Seattle or at UW ?
  - a modern day mystery!



Lattice QCD:
The Mechanics



Simply do the integration over quark fields analytically

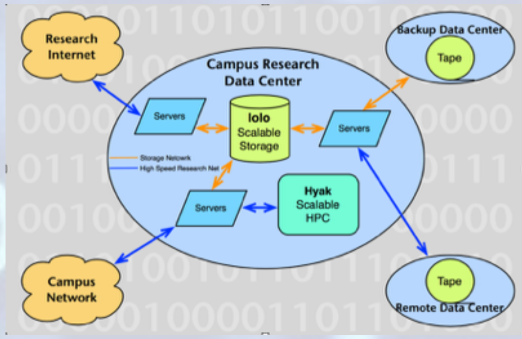
$$\int \mathcal{D}\psi\, \mathcal{D}\overline{\psi}\, e^{-\int d^4x\, \overline{\psi} K \psi} = \det(K)$$

In perfect world - would just do the integrals, but instead we sample over snapshots of the gluon fields:

$$\langle \hat{\theta} \rangle \sim \int \mathcal{D}\mathcal{U}_\mu\, \hat{\theta}[\mathcal{U}_\mu]\, \det[\kappa[\mathcal{U}_\mu]]\, e^{-S_{YM}}$$

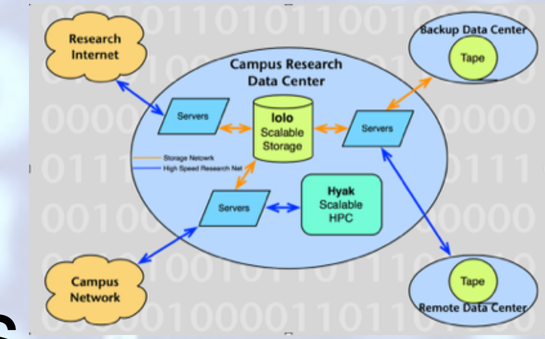
$$\rightarrow \frac{1}{N} \sum_{\text{gluon cfgs}}^{N} \hat{\theta}\left[\mathcal{U}_\mu\right]$$

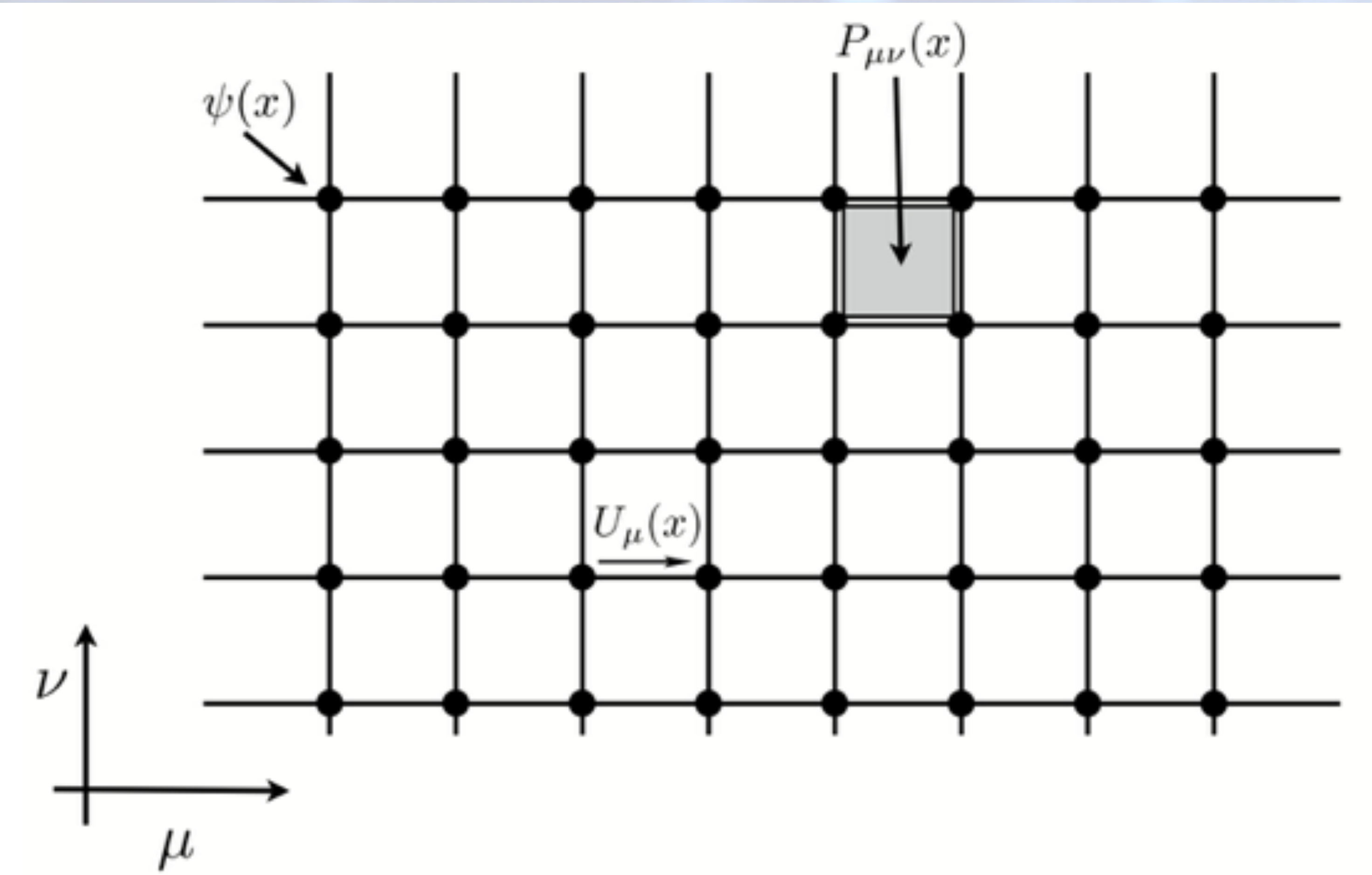
Large computing resources are required to calculate a statistically decorrelated ensemble of gauge-field configurations - snapshots of the quantum vacuum. Capability compute platforms (Leadership-class) are required for this purpose



Lattice QCD:

Simplest Discretization : Gauge Fields



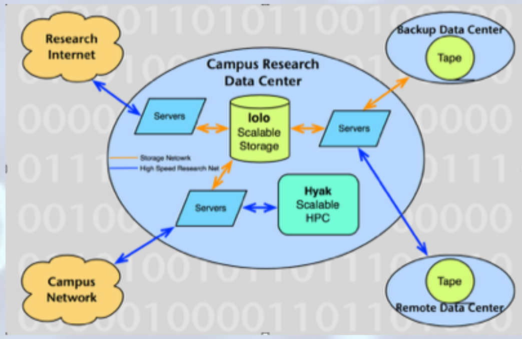


$$U_\mu(x) = \exp\left(i \int_x^{x+\hat{\mu}} dx' A_\mu(x')\right)$$

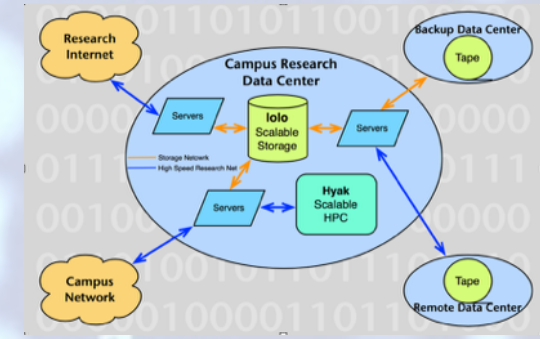
$$U_\mu(x) \rightarrow U'_\mu(x) = \Omega(x) U_\mu(x) \Omega^{-1}(x+\hat{\mu})$$

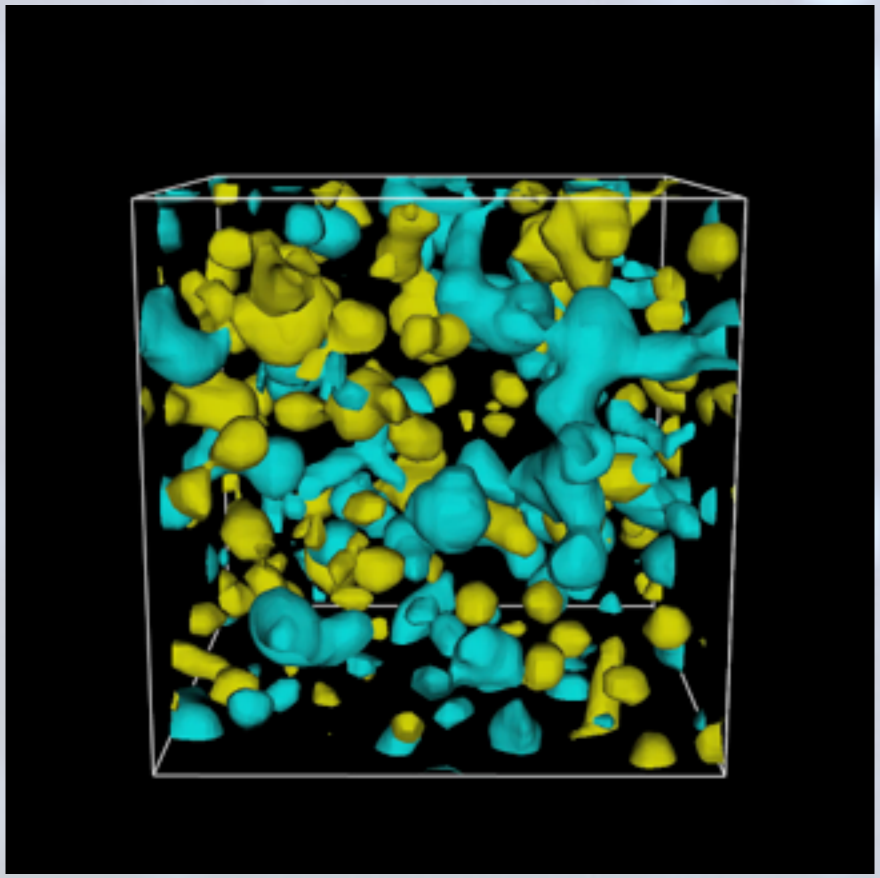
$$P_{\mu\nu} = U_\mu(x) U_\nu(x+\hat{\mu}) U^\dagger_\mu(x+\hat{\nu}) U^\dagger_\nu(x)$$

$$P_{\mu\nu} = 1 - i a^2 G_{\mu\nu} - \frac{a^4}{2} G_{\mu\nu} G_{\mu\nu} + \ldots$$

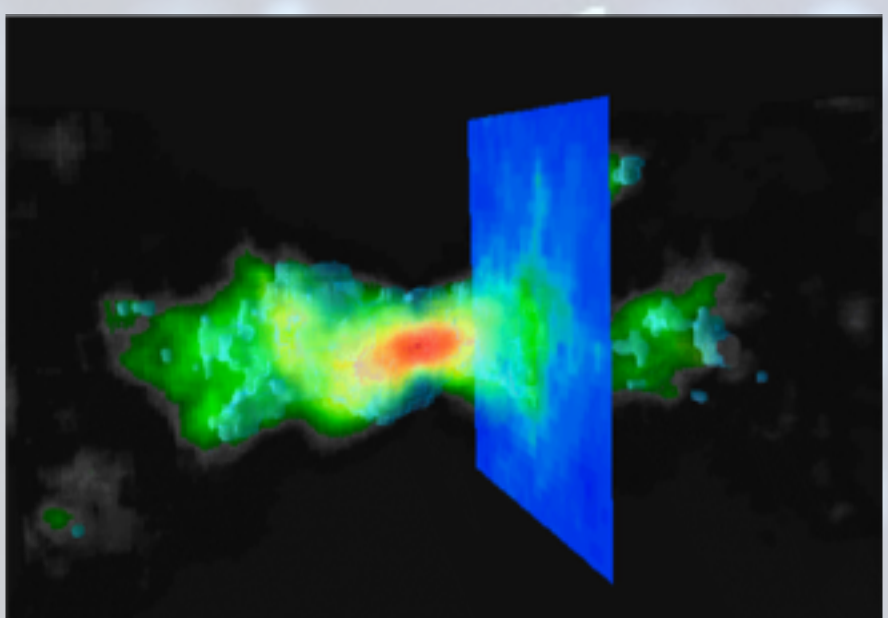


Lattice QCD:
todays typical

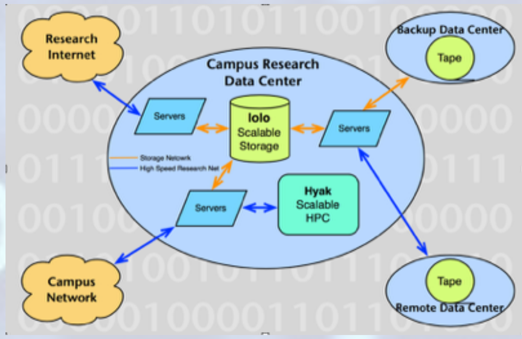




Configuration : e.g.,
Vol = 96 x 96 x 96 x 192 lattice sites
Vol x 4 x 8 = 5.4 Billion independent real numbers to define $U_\mu(x)$ (generally double precision)



Propagator : e.g.,
32 x 32 x 32 x 256 lattice sites
~ 2 Billion x 2 Billion complex sparse matrix
(to invert and take determinant)



Lattice QCD:
Configurations : HMC and Sampling

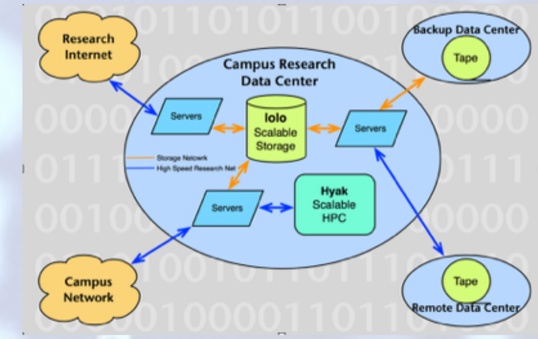
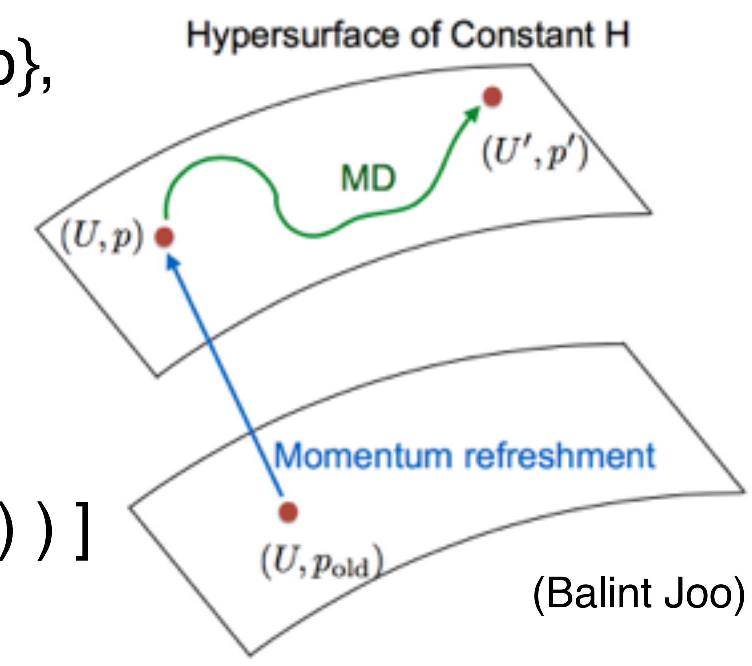


Figure from: "Improving dynamical lattice QCD simulations through integrator tuning, using Poisson Brackets and a force-gradient Integrator", M. A. Clark, B. Joo, A.D. Kennedy, P.J. Silva Phys Rev.D84,071502

HMC Algorithm:

Start with a set of links {U}
To generate one HMC trajectory:

- Assign to each link a Gaussian distributed canonical momentum {p}, hence the variable {U,p}
- Compute Hamiltonian of this system, $H = p^2/(2) + S(U)$
- Perform Molecular Dynamics evolution of the variables using Hamilton's equations to give {U',p'} (need reversible and area preserving integrators to evolve)
- Accept {U',p'} with probability min[1 , exp(-H(U',p'))/ exp(-H(U,p))] (if Hamiltonian is smaller - always accept)
- If rejected, new state is {U,p}

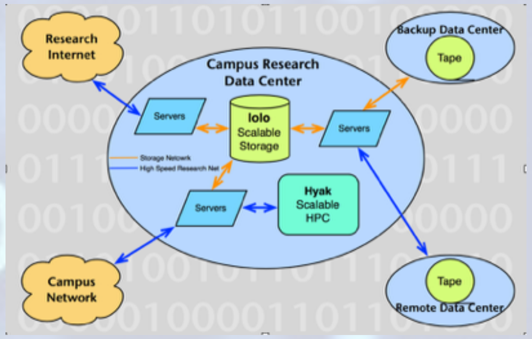


(Balint Joo)

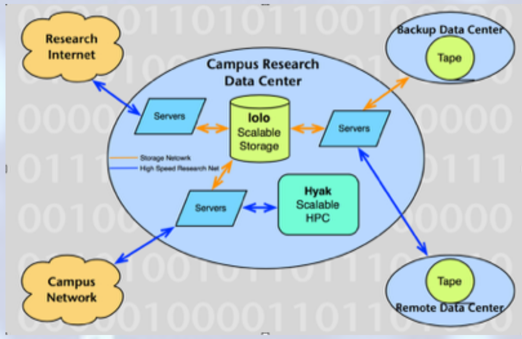
Repeat to produce another trajectory

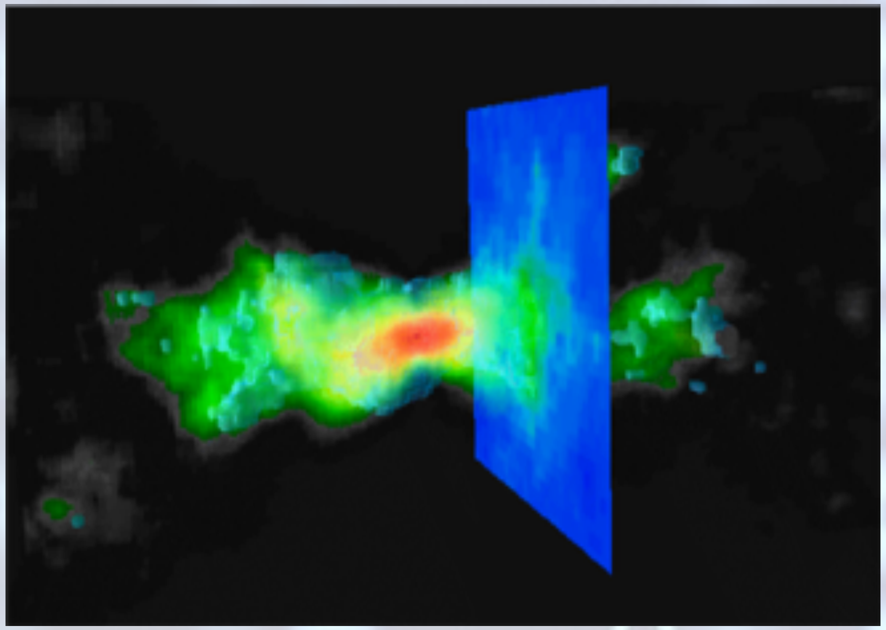
Advantage - all links updated at once through Hamiltonian evolution in fictitious time

Tuning of evolution is essential to optimize productivity



Lattice QCD:
Solvers and Quark Propagators





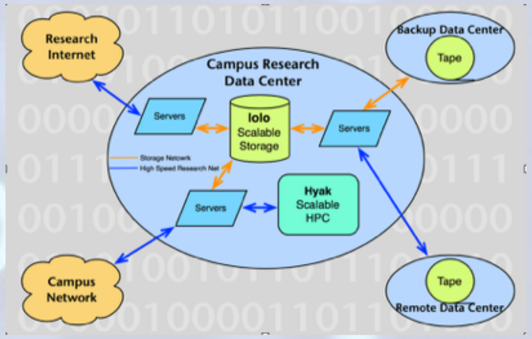
$$[D(U)]_{X,Y}[S(U)]_{Y,X_0} = G_{X,X_0}$$

light-quark propagator　　Source

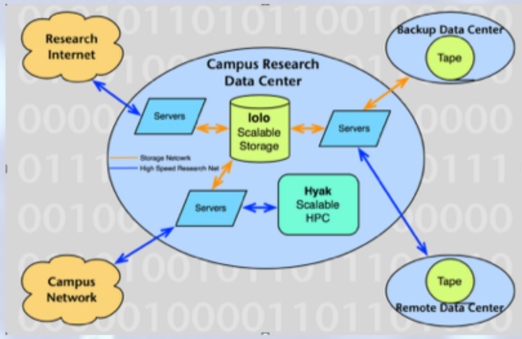
Iterative using Krylov-subspace solvers
CG, BiCGstab

Condition number of D gets larger as quark mass is reduced toward physical
- critical slowing down in convergence

Preconditioning used to improve condition number



Lattice QCD:
Solvers and Deflation



COMPUTING AND DEFLATING EIGENVALUES WHILE SOLVING MULTIPLE RIGHT HAND SIDE LINEAR SYSTEMS WITH AN APPLICATION TO QUANTUM CHROMODYNAMICS

ANDREAS STATHOPOULOS AND KONSTANTINOS ORGINOS arXiv preprint arXiv:0707.0131, 2007

SIAM J. Sci. Comput. Vol. 32, No. 1, 439--462, 2010

$$A.x = b$$

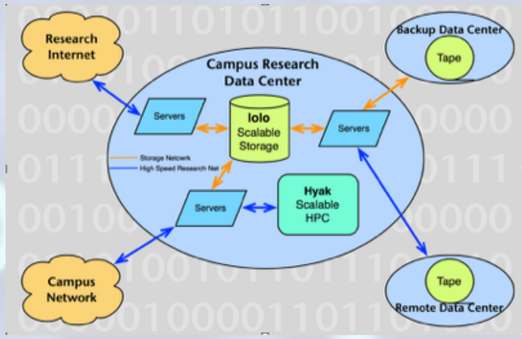
- Iteratively solve for each source location to a given tolerance. e.g. CG, BiCGstab,
- Heavy on CPU, light on memory

$$U.A.U^{-1} = \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_N \end{pmatrix}$$

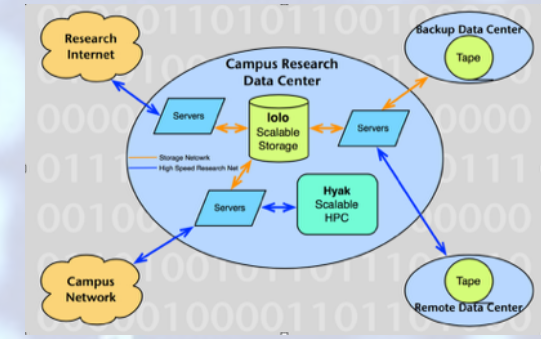
- Inversion solved exactly for all source locations
- Computationally prohibitive - cpu and memory

$$\tilde{U}.A.\tilde{U}^{-1} = \begin{pmatrix} \lambda_1 & & & \\ & \ddots & & \\ & & \lambda_p & \\ & & & \overline{A} \end{pmatrix}$$

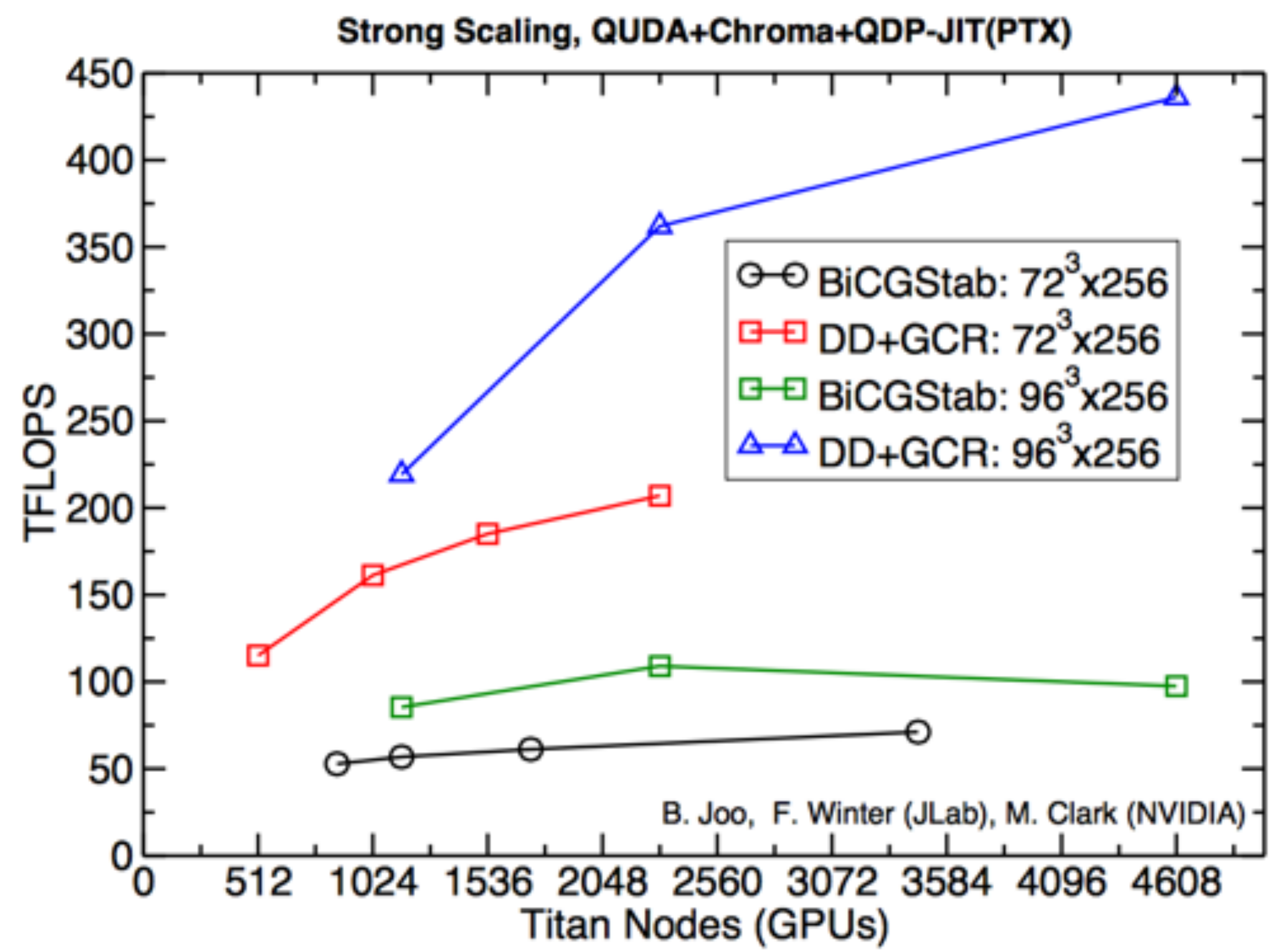
- Determine the lowest p eigenvalues and eigenvectors - tune the number p
- Re-use for all sources.
- Memory heavy - depends on p.
- Iteratively solve in reduced space.
- Better condition number.
- Set-up ``costs” recovered with large number of sources



Lattice QCD:
Solvers and Quark Propagators

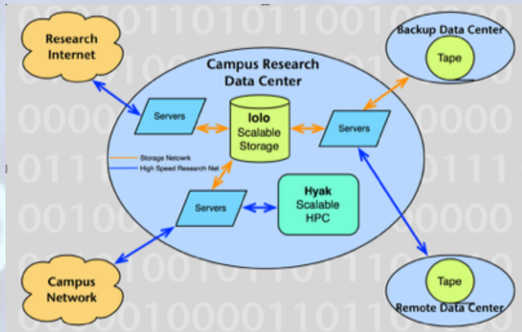


- QUDA Solver performance on Titan
  - Cray XK7 system
  - 1 NVIDIA K20X GPU per node
  - Gemini Interconnect
- The DD+GCR solver does considerably better than the standard BiCGStab
- But even DD+GCR is affected by strong scaling effects

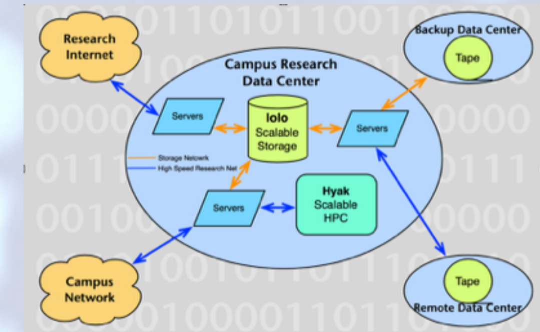


DD = Domain Decomposition Preconditioner
GCR = Generalized Conjugate Residual
multigrid only just ported to GPUs

Balint Joo (2014)

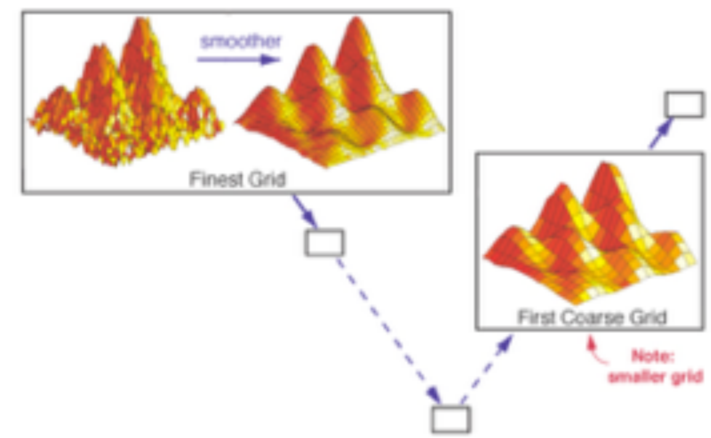


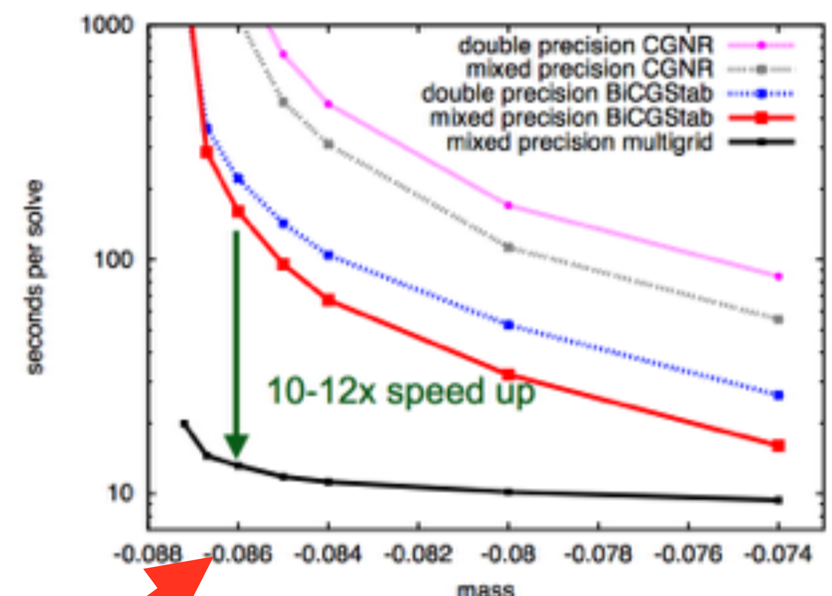
Lattice QCD:
Algebraic Multigrid and Quark Propagators



- Critical Slowing down is caused by 'near zero' modes
- Multi-Grid method
  - separate (project) low lying and high lying modes
  - solve for high lying modes with "smoother"
  - solve for low modes on coarse grid with reduced dimensional operator
  - Gauge field is 'stochastic', so no geometric smoothess on low modes => algebraic multigrid
  - Setting up restriction/prolongation operators is costly
  - Easily amortized in Analysis with O(100,000) solves

Image From: http://computation.llnl.gov/casc/sc2001_fliers/SLS/SLS01.html
Credit: LLNL, CASC

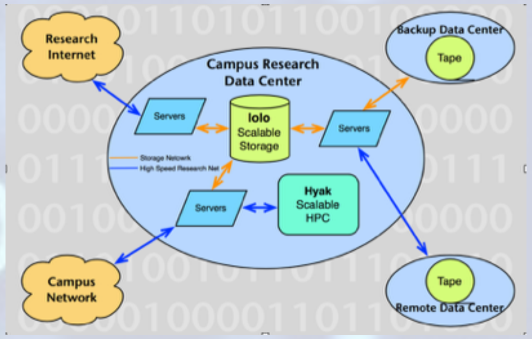


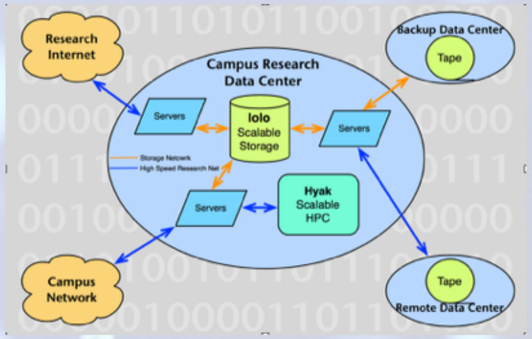


Multi-Grid. figure from J. C. Osborn et. al. PoS Lattice 2010:037,2010, R. Babich et. al. Phys. Rev. Lett, 105:201602,2010

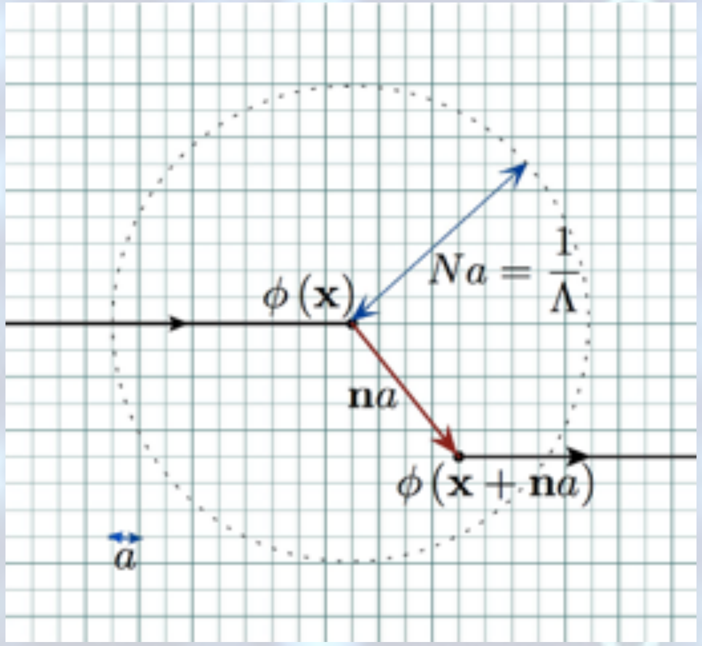
physical point

Balint Joo (2014)





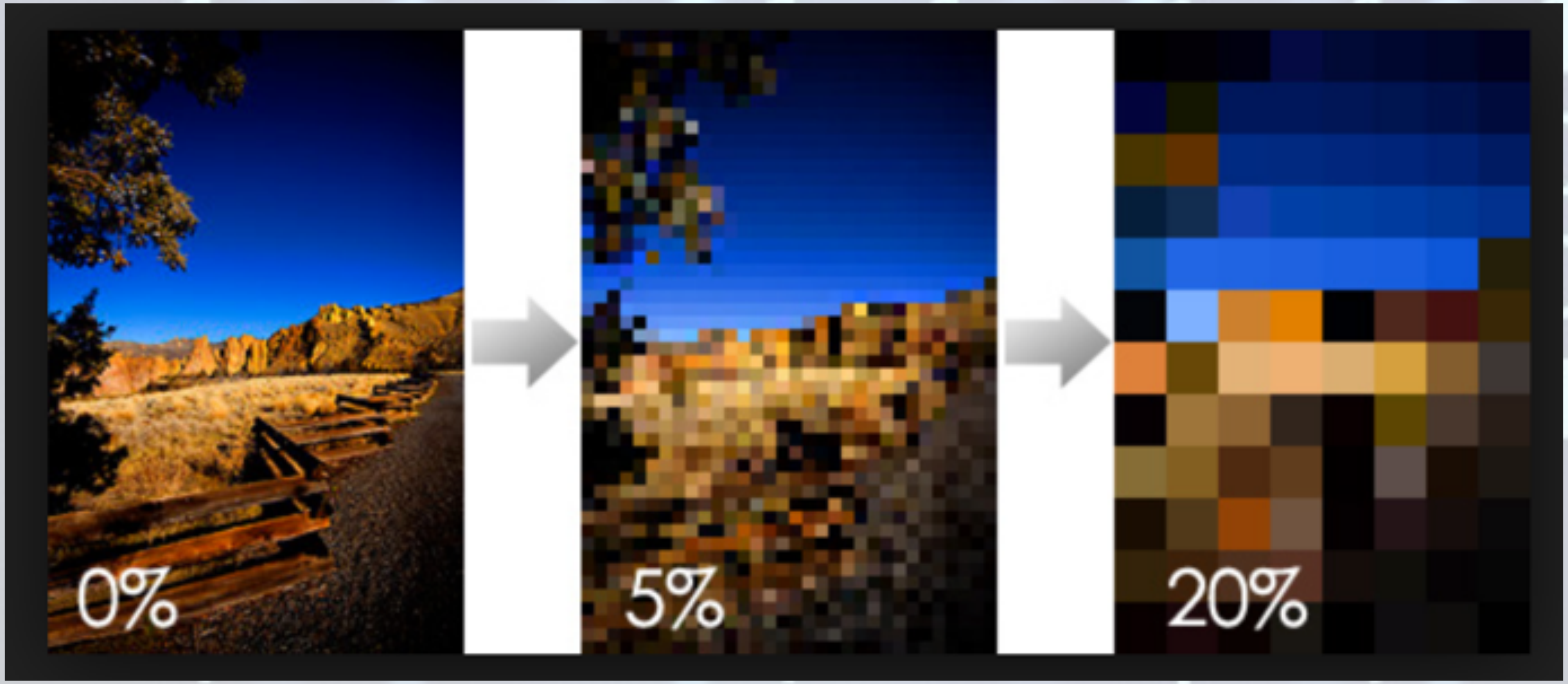
Lattice QCD:
Recovering SO(3) from H(3)

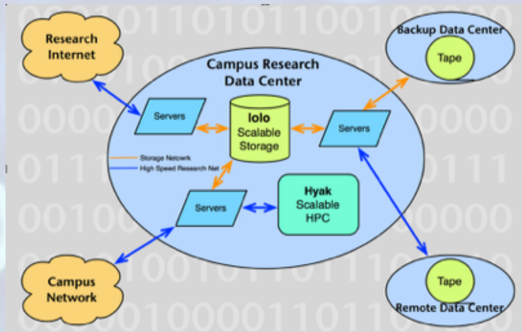


Hold all physical scales, and the renormalization scale fixed when taking lattice spacing to zero

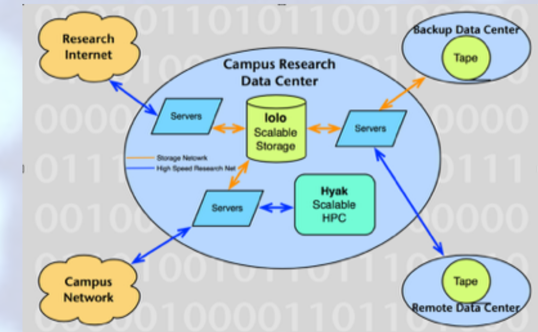
Survives at quantum level in QCD - smearing is critical so as not to ``see'' the UV cubic structure

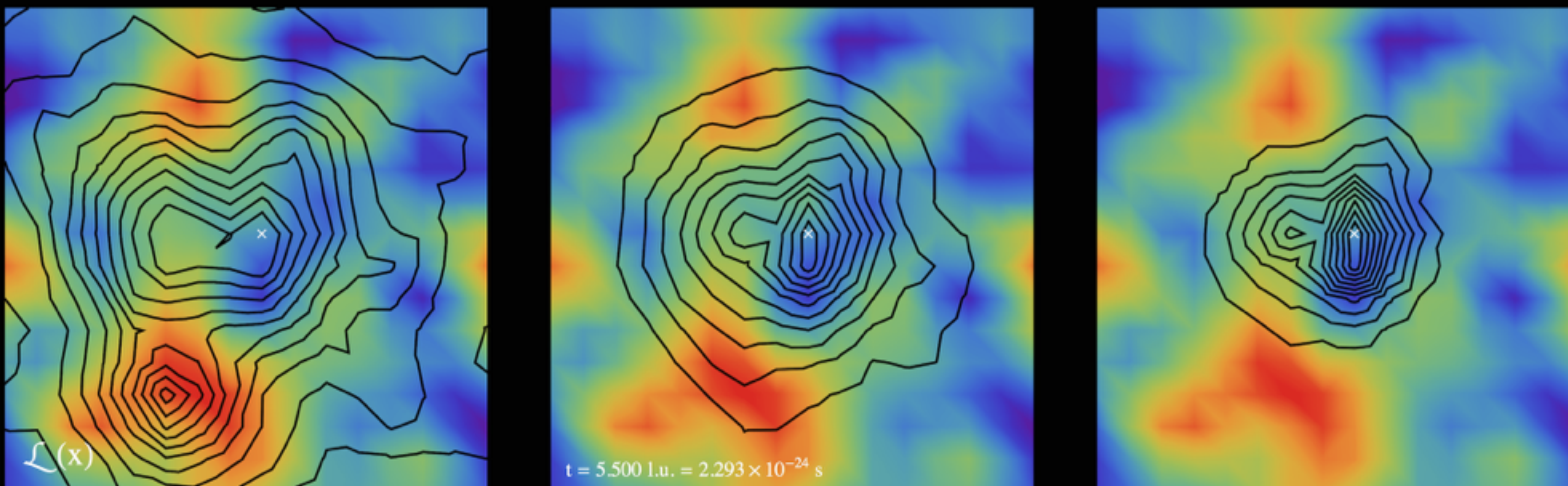
Multiplicity of irreps of H(3) allow for combinations to approach SO(3) states - both in position space (a) and momentum space (L)





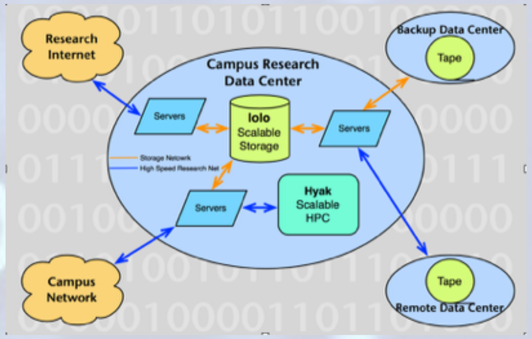
Lattice QCD:
Statistics of Correlation Functions



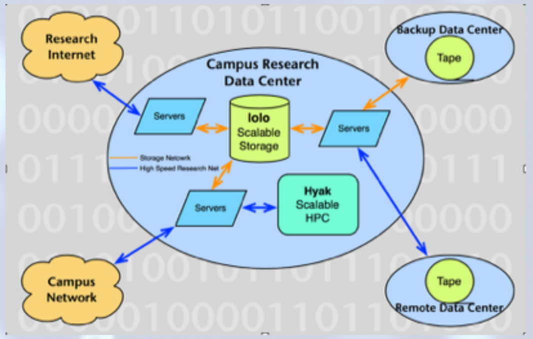


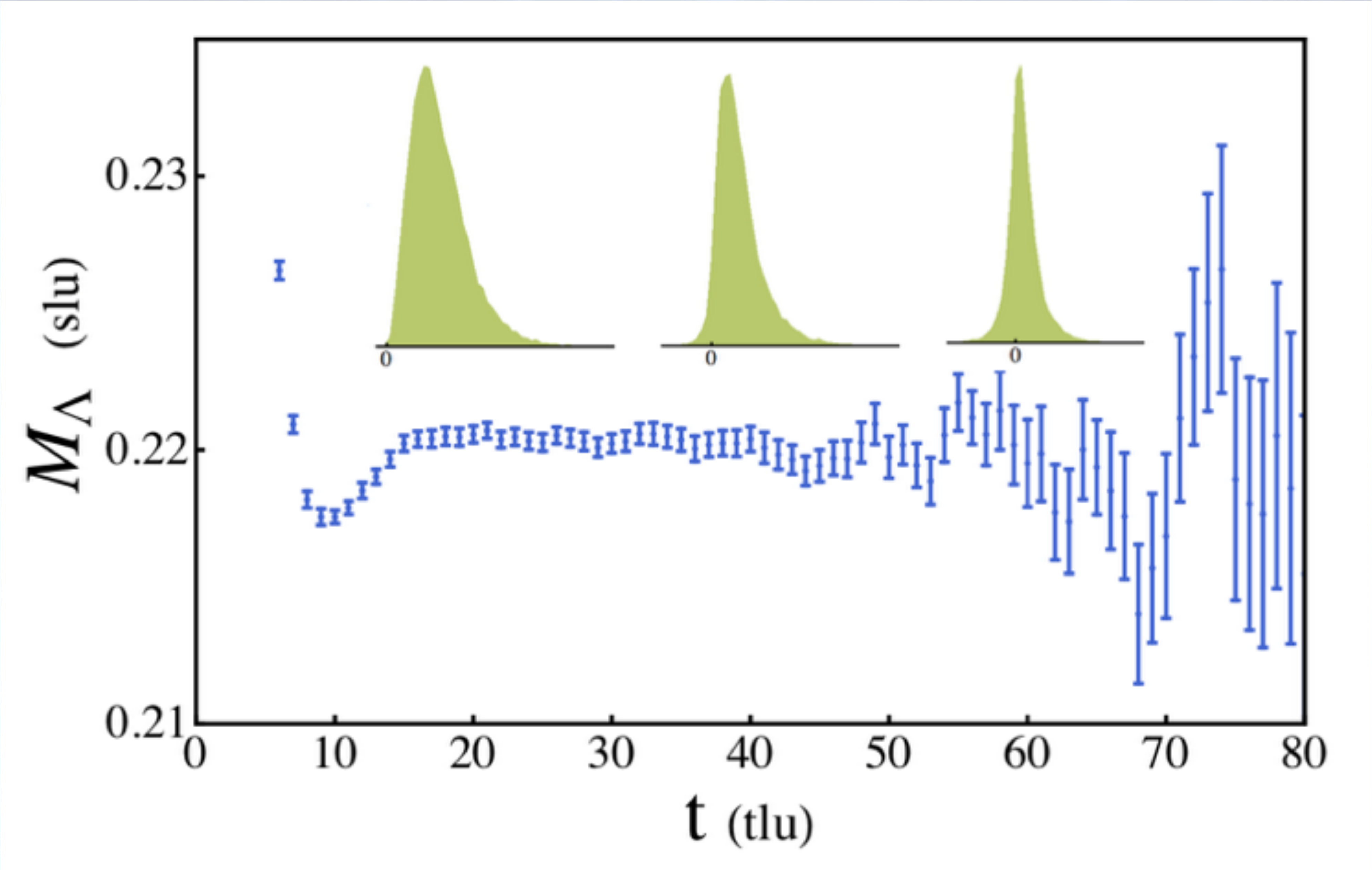
π Propagator Λ Propagator   H−dibaryon Propagator

The results of a quenched Lattice QCD calculation of the π , Λ , and H−dibaryon correlation functions. The gauge−field configuration was generated with the DBW2 gauge action on a lattice with 16 sites in each spatial direction, 32 sites in the temporal direction and a lattice spacing of approximately 0.12 fermis. The masses of the light quarks were chosen to produce a pion mass of $m_\pi \sim$ 350 MeV and a kaon mass of $m_K \sim$ 490 MeV.
The colors of the background show the (Gaussian−smeared) local action density, while the black contours are a topographical map of the given correlation function.

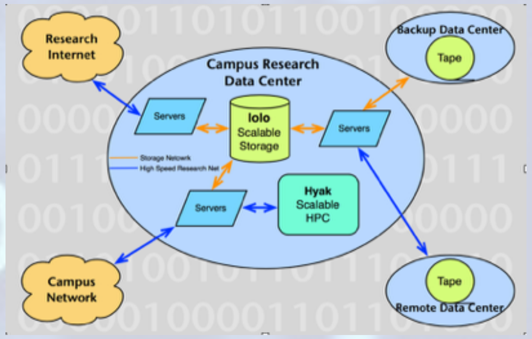


Lattice QCD:
Analysis of Correlation Functions

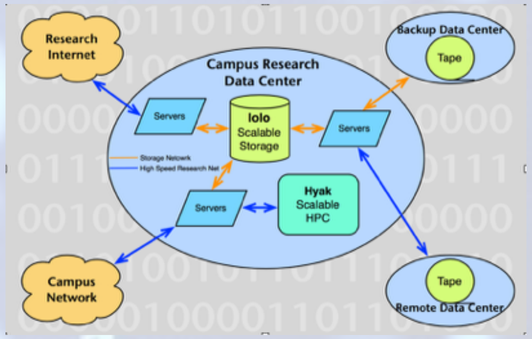


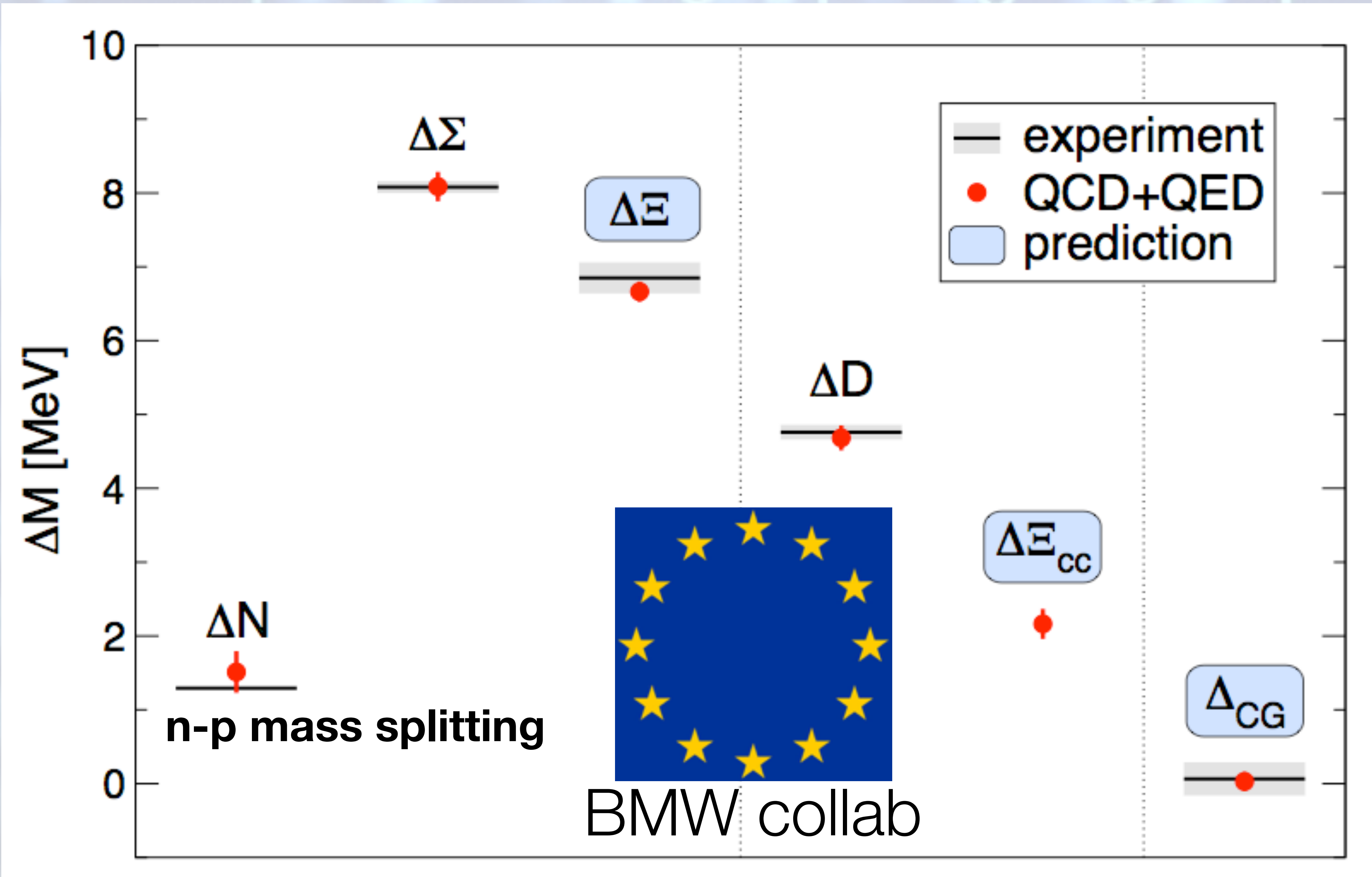


Non-Gaussian (interacting field theory) ~ Log Normal in plateau region evolves into symmetric but non-Gaussian at late times

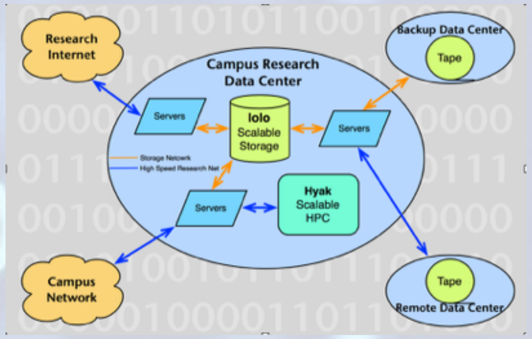


State-of-the-Art Lattice QCD

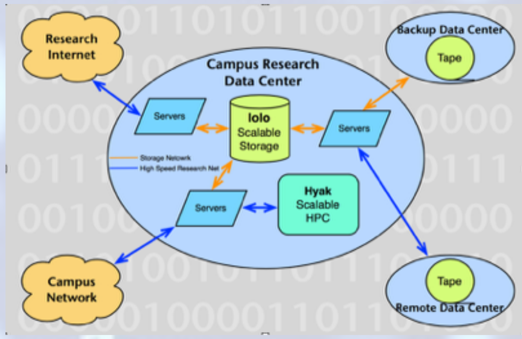




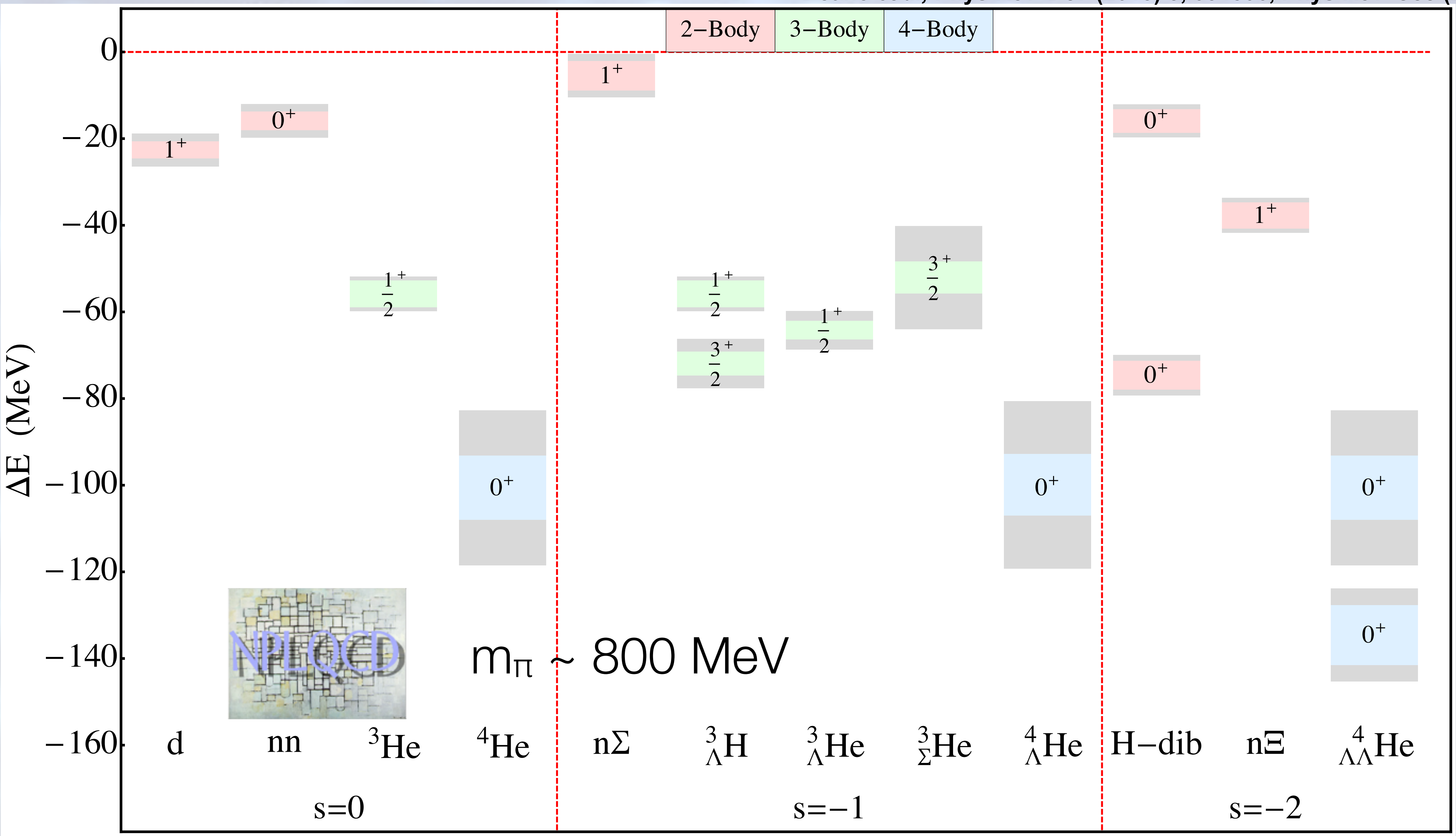
- Physical up, down, strange and charm quark masses
- Fully dynamical QCD+QED



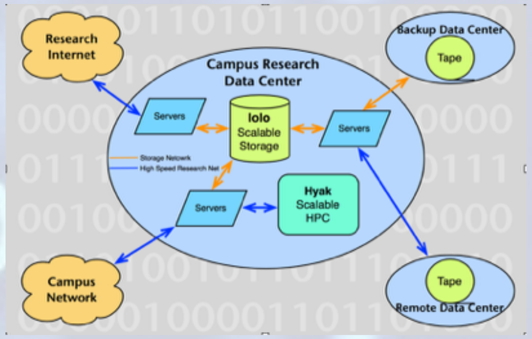
Nuclei from QCD



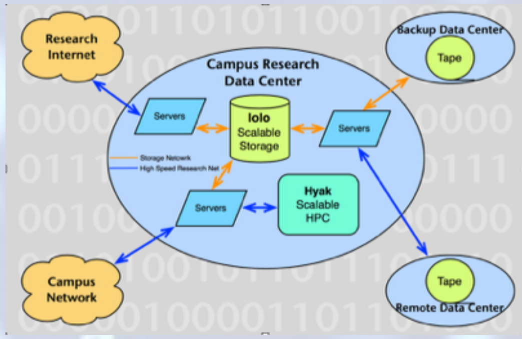
Beane *et al*, Phys.Rev. D87 (2013) 3, 034506, Phys.Rev. C88 (2013) 2, 024003

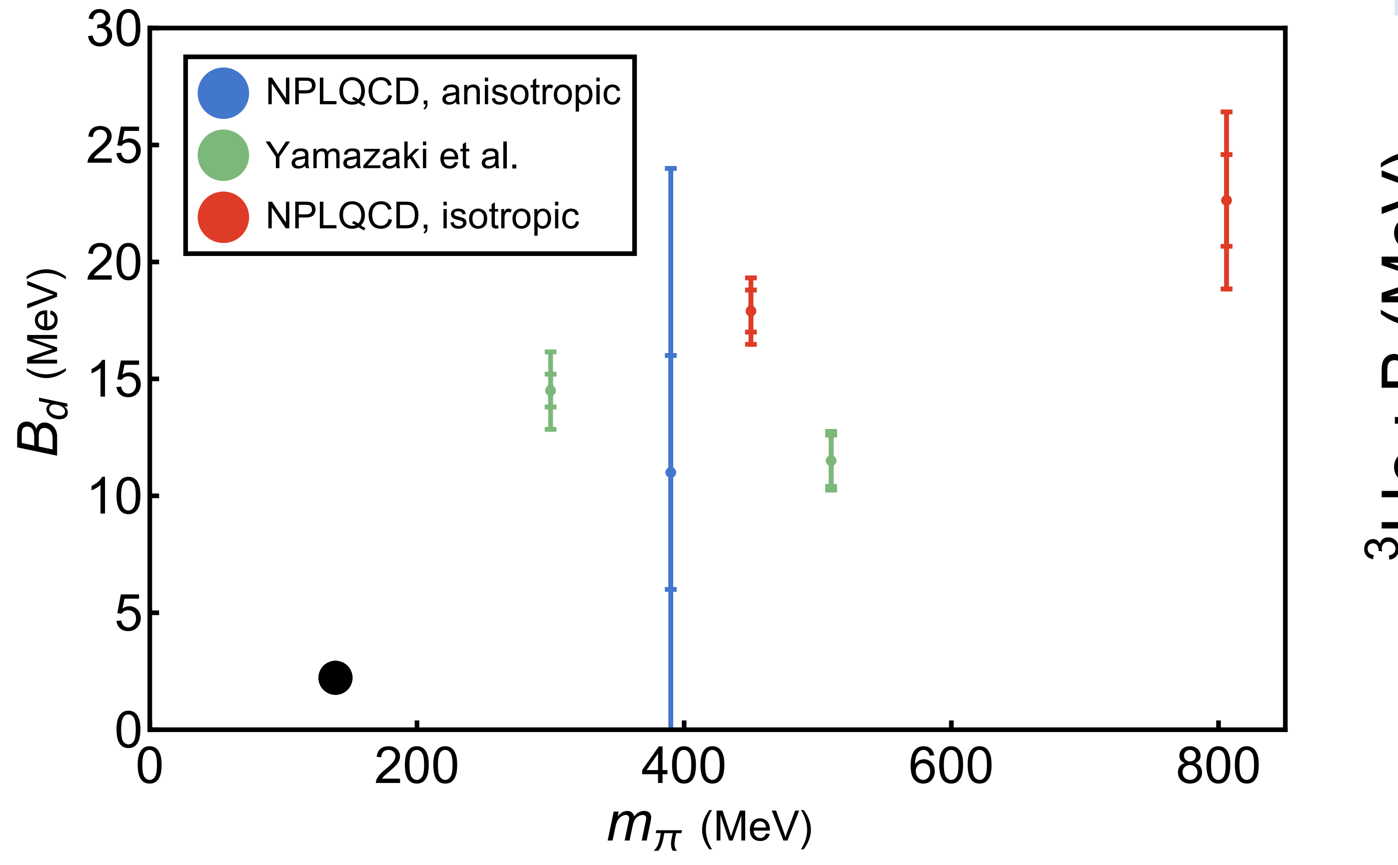


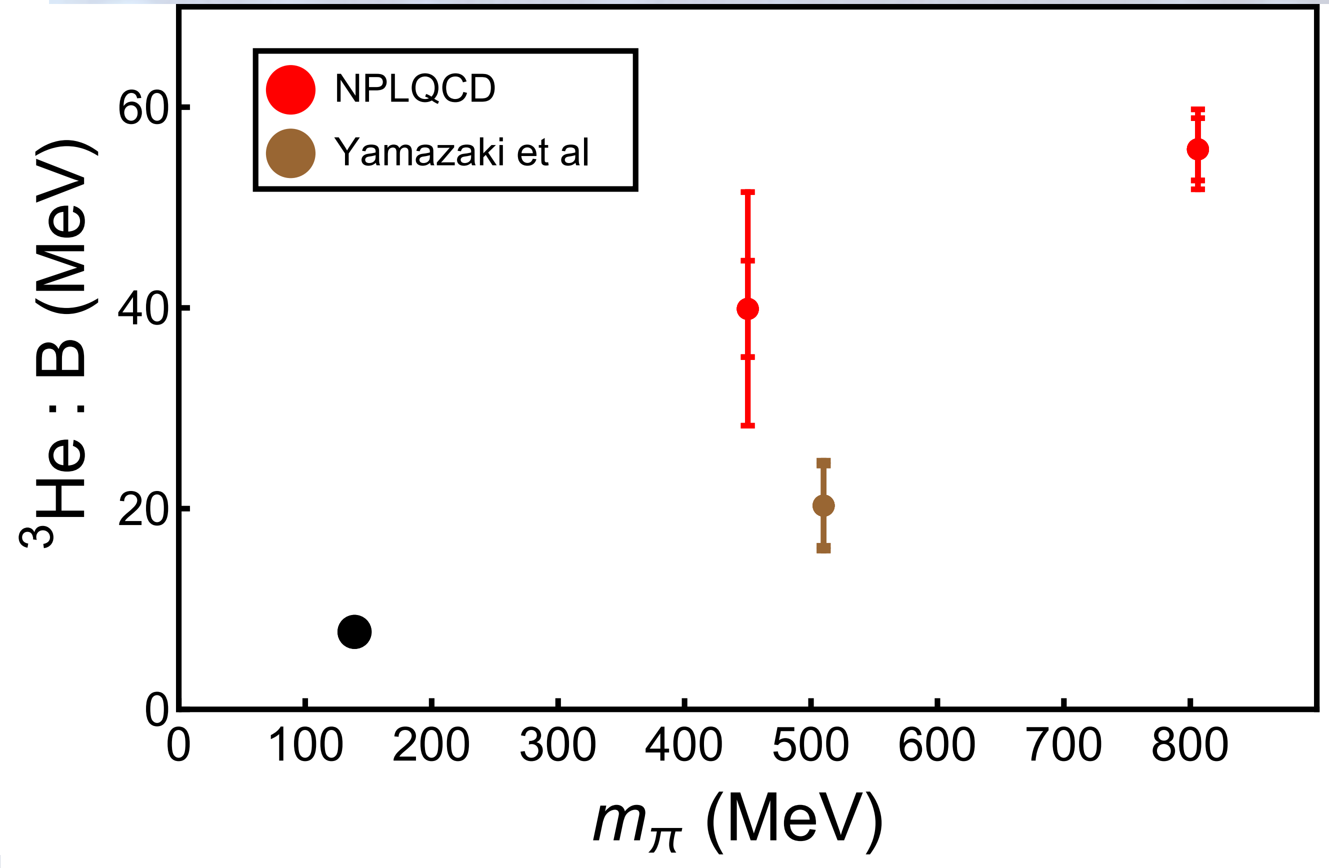
Extensive study of s-shell nuclei and hypernuclei, and baryon-baryon interactions at SU(3) symmetric point

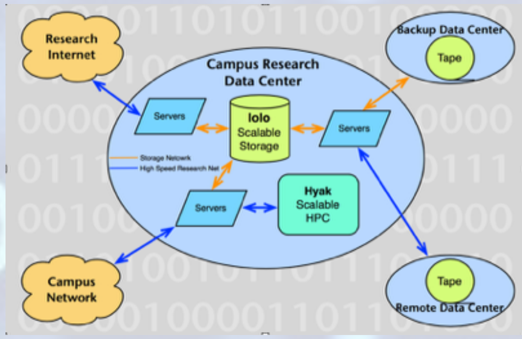


Light Nuclei : Quark Mass Effects

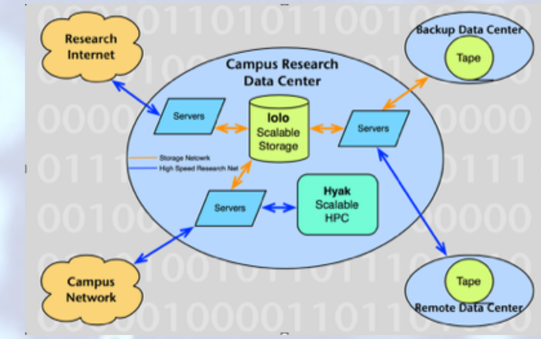




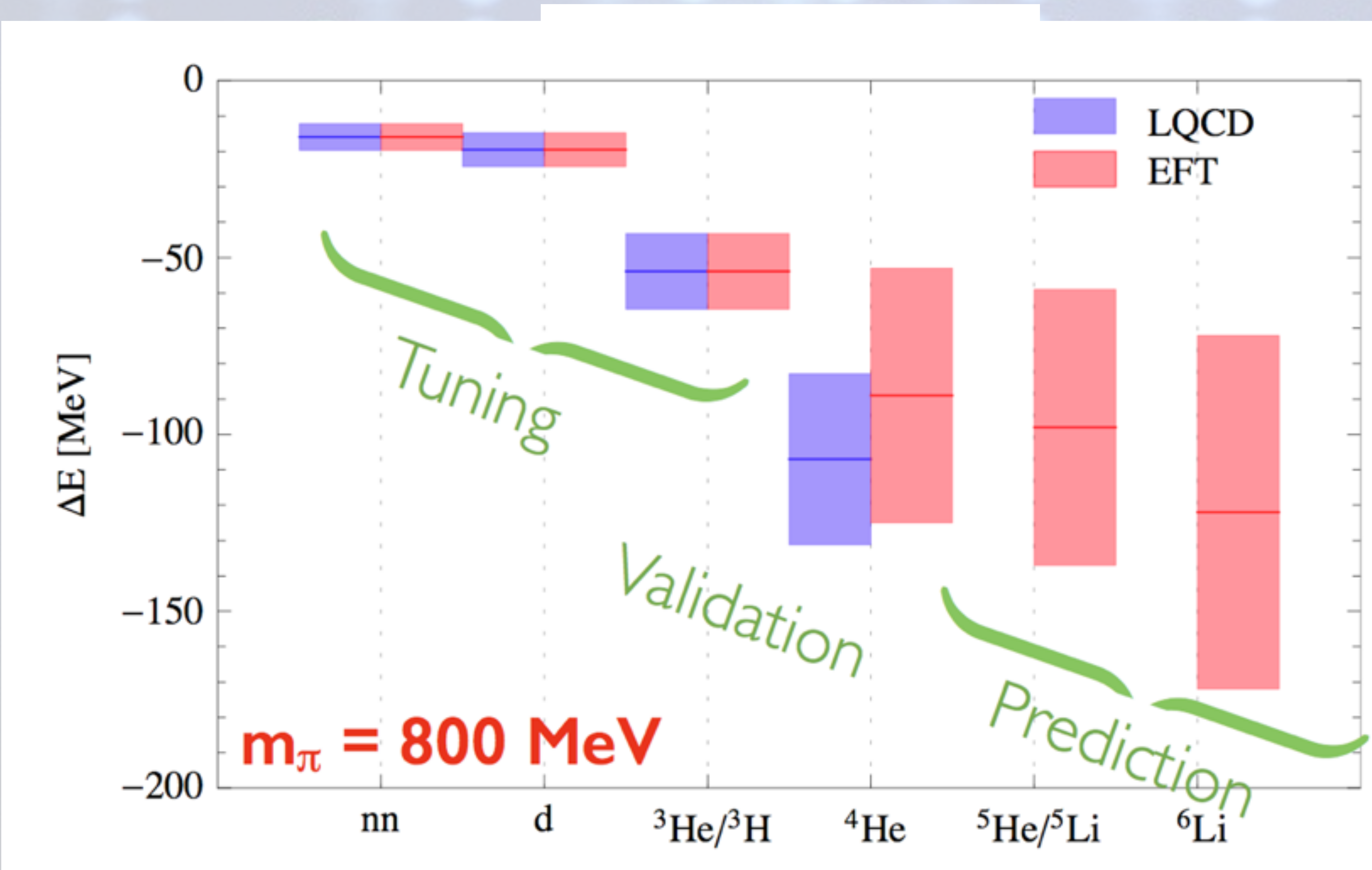


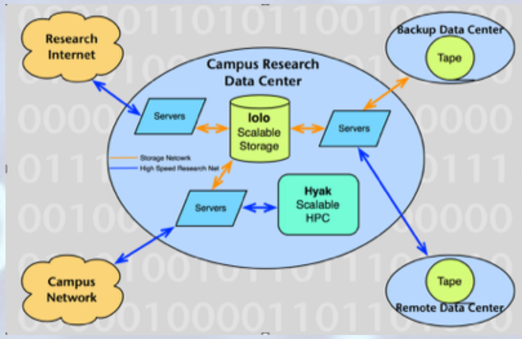


The Periodic Table as a function of the quark masses

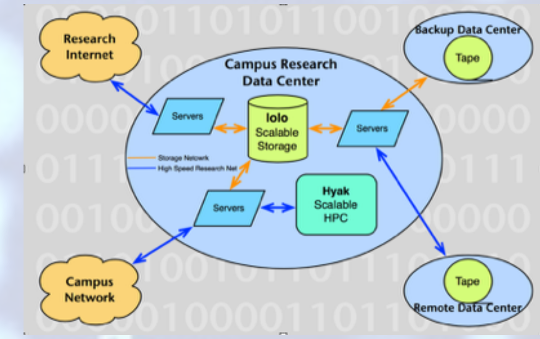


(Barnea *et al.*, Phys.Rev.Lett. 114 (2015) 5, 052501)

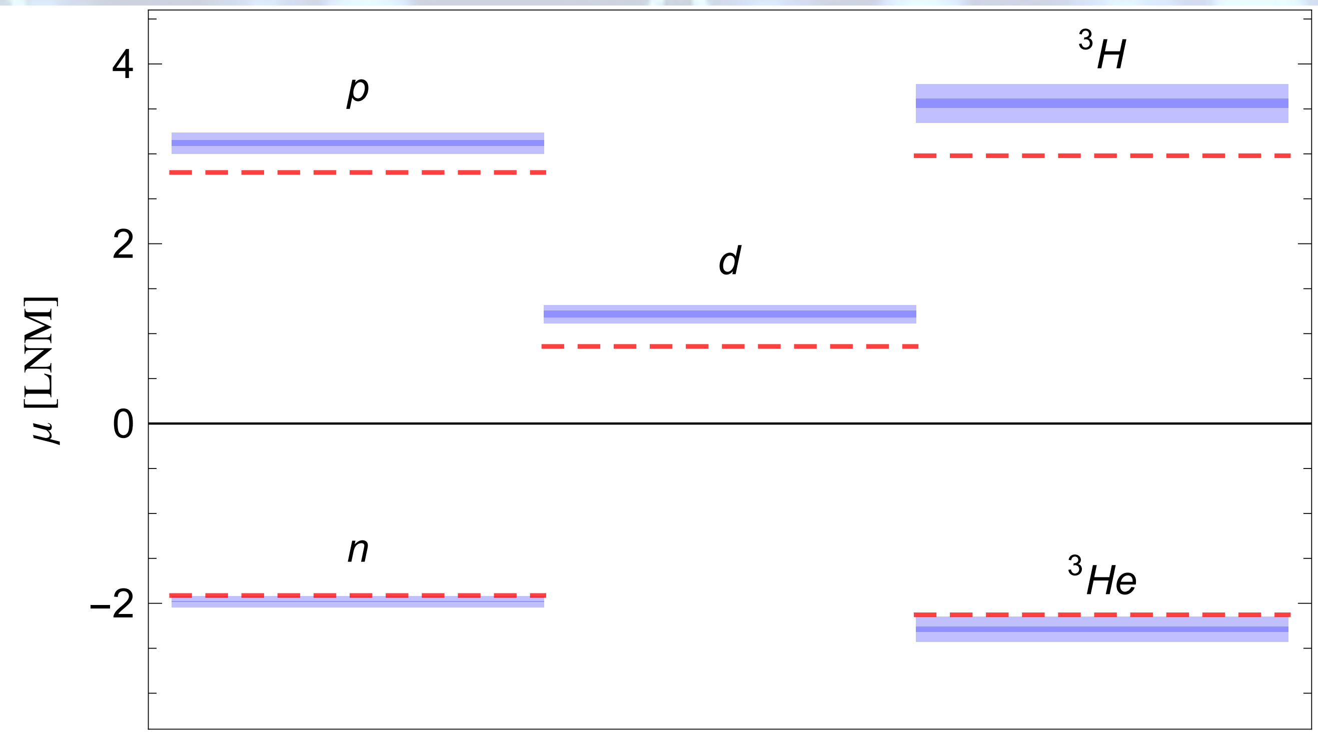


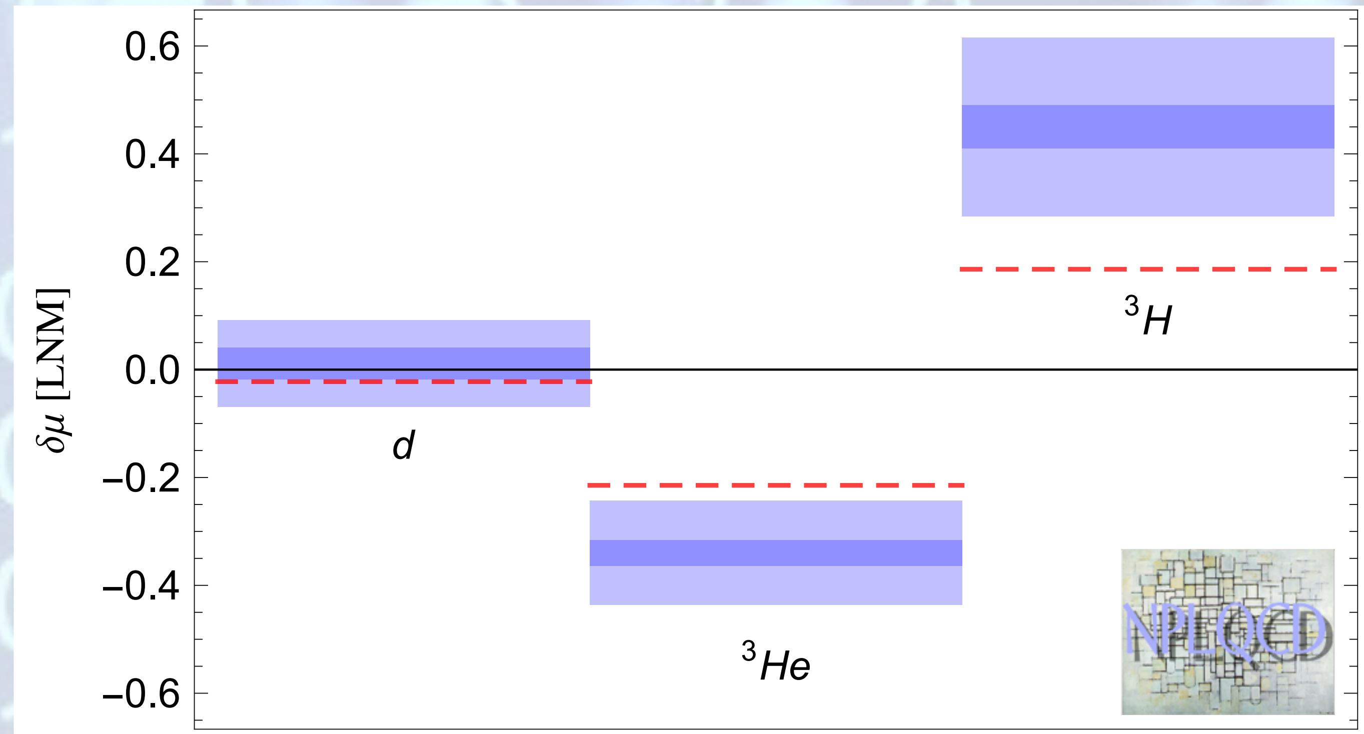


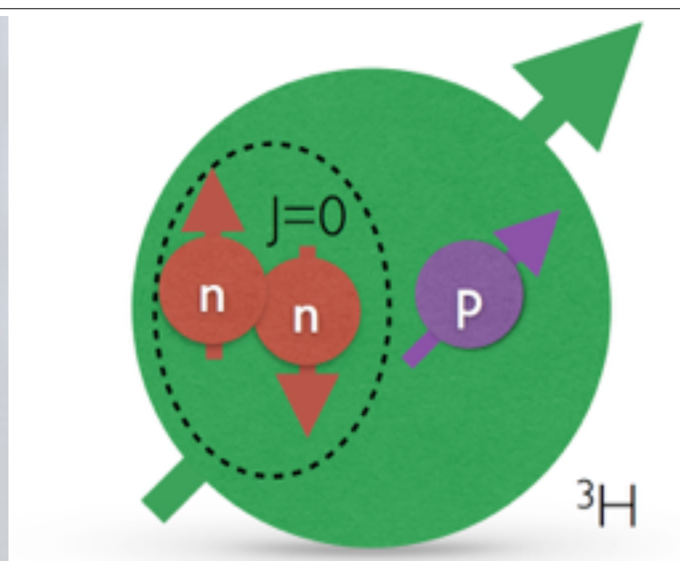
The Magnetic Structure of Nuclei : Magnetic Moments



S.R. Beane *et al.*, Phys.Rev.Lett. 113 (2014) 25, 252001

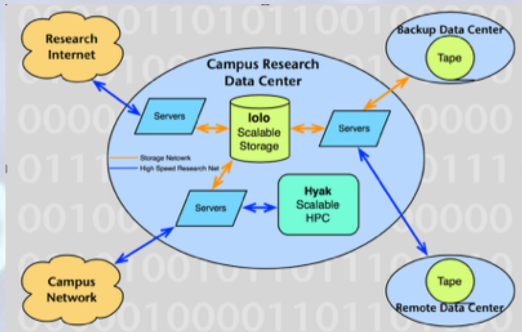




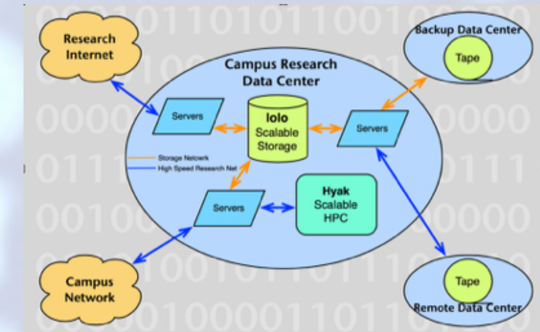


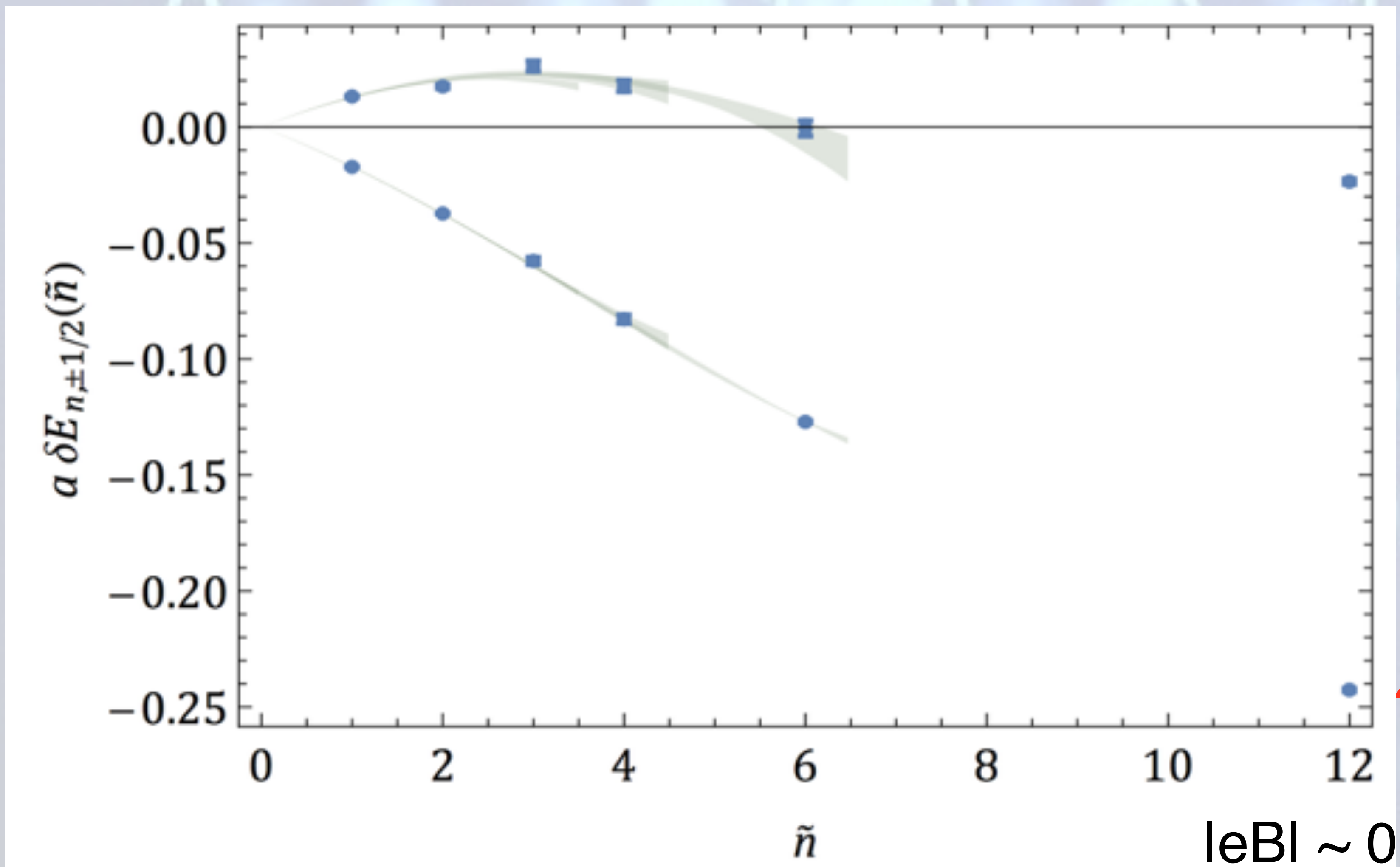
m_π ~ 800 MeV Vs Nature

Nuclei are (nearly) collections of nucleons
- shell model phenomenology!



Magnetic Moments
Neutron Spin States



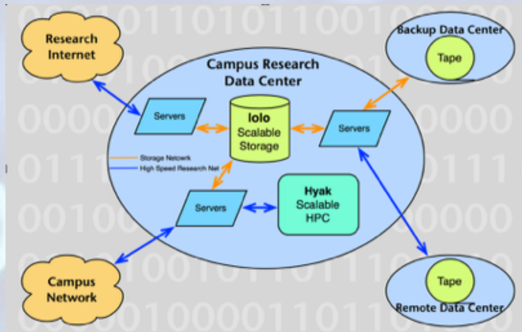


400 MeV

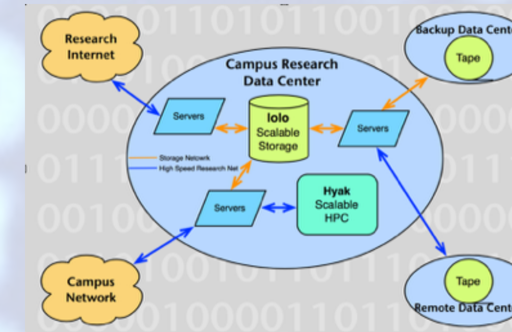
$|eB| \sim 0.7\ \text{GeV}^2$

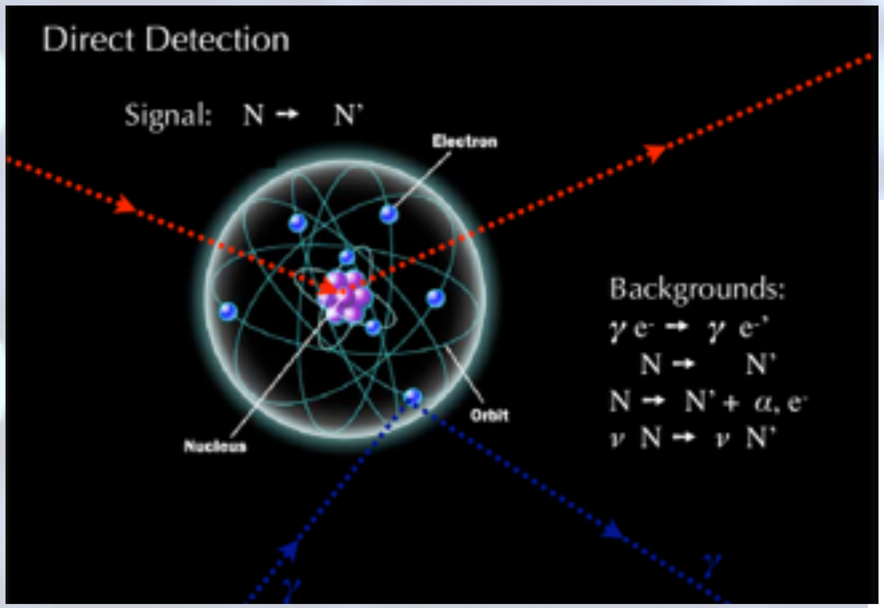
$\sim 10^{20}$ Gauss

- Lower state depends essentially linearly on B
- Polarizability results from upper level (essentially)
- Spin-dependences highly correlated



Nuclear σ-Terms and Dark Matter Interactions

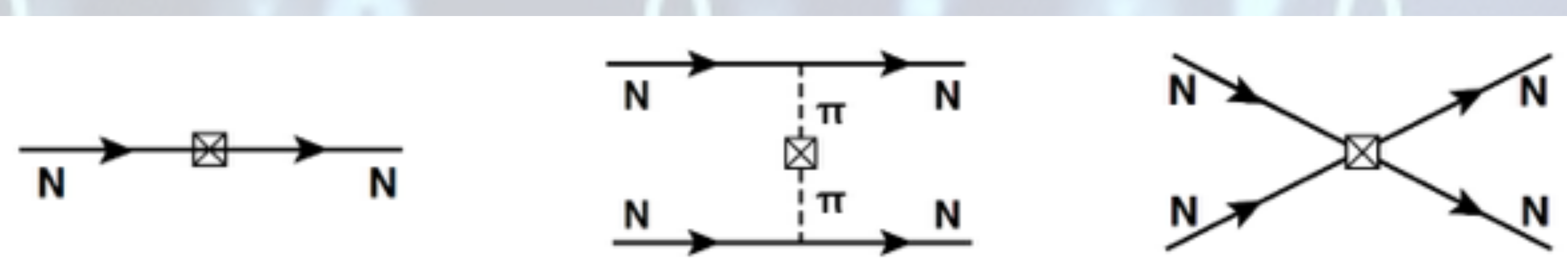


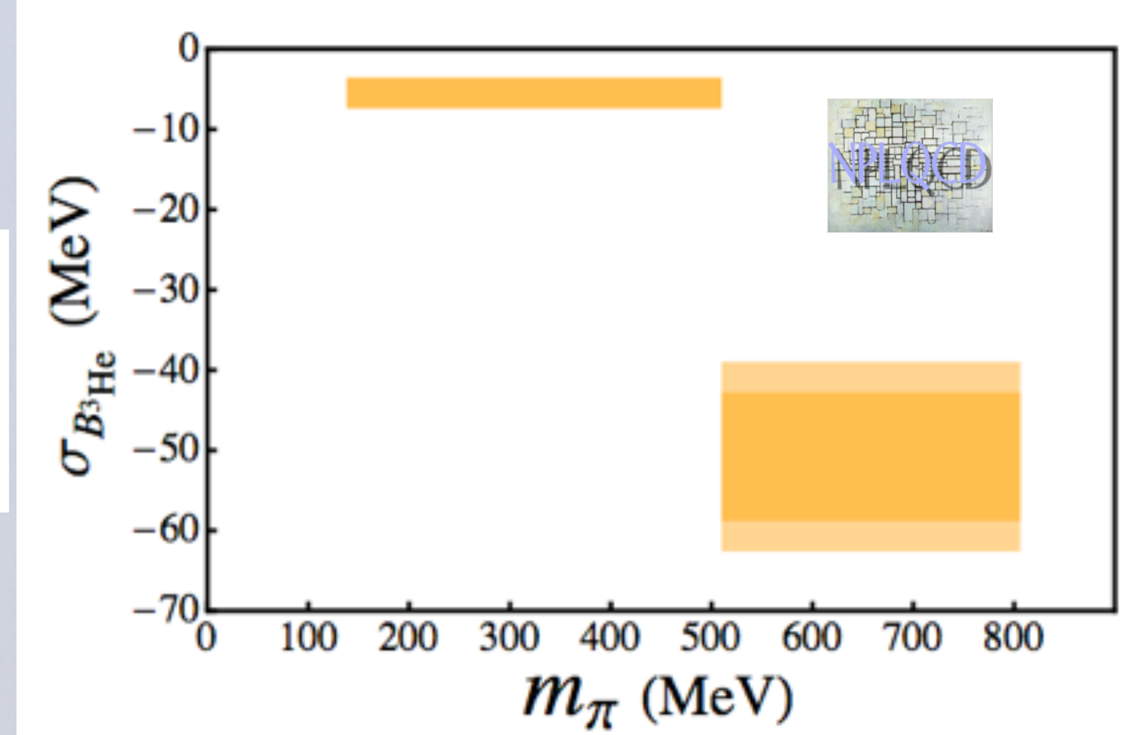


Nuclear σ-terms

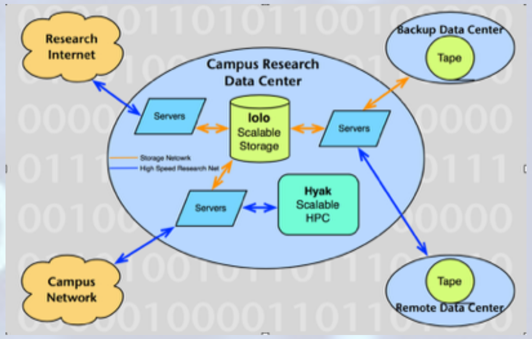
$$\sigma_{Z,N} = \overline{m}\langle Z, N(\text{gs})|\ \overline{u}u + \overline{d}d\ |Z, N(\text{gs})\rangle = \overline{m}\frac{d}{d\overline{m}}E^{(\text{gs})}_{Z,N}$$

$$= \left[\ 1\ +\ \mathcal{O}\left(m_\pi^2\right)\ \right]\frac{m_\pi}{2}\frac{d}{dm_\pi}E^{(\text{gs})}_{Z,N}$$

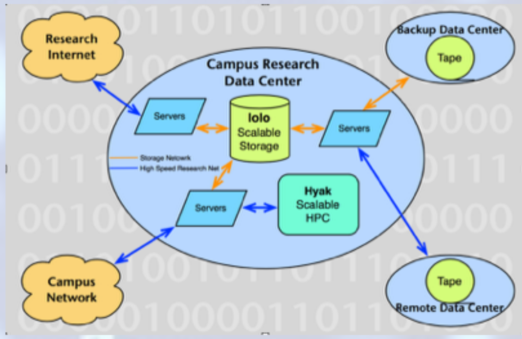


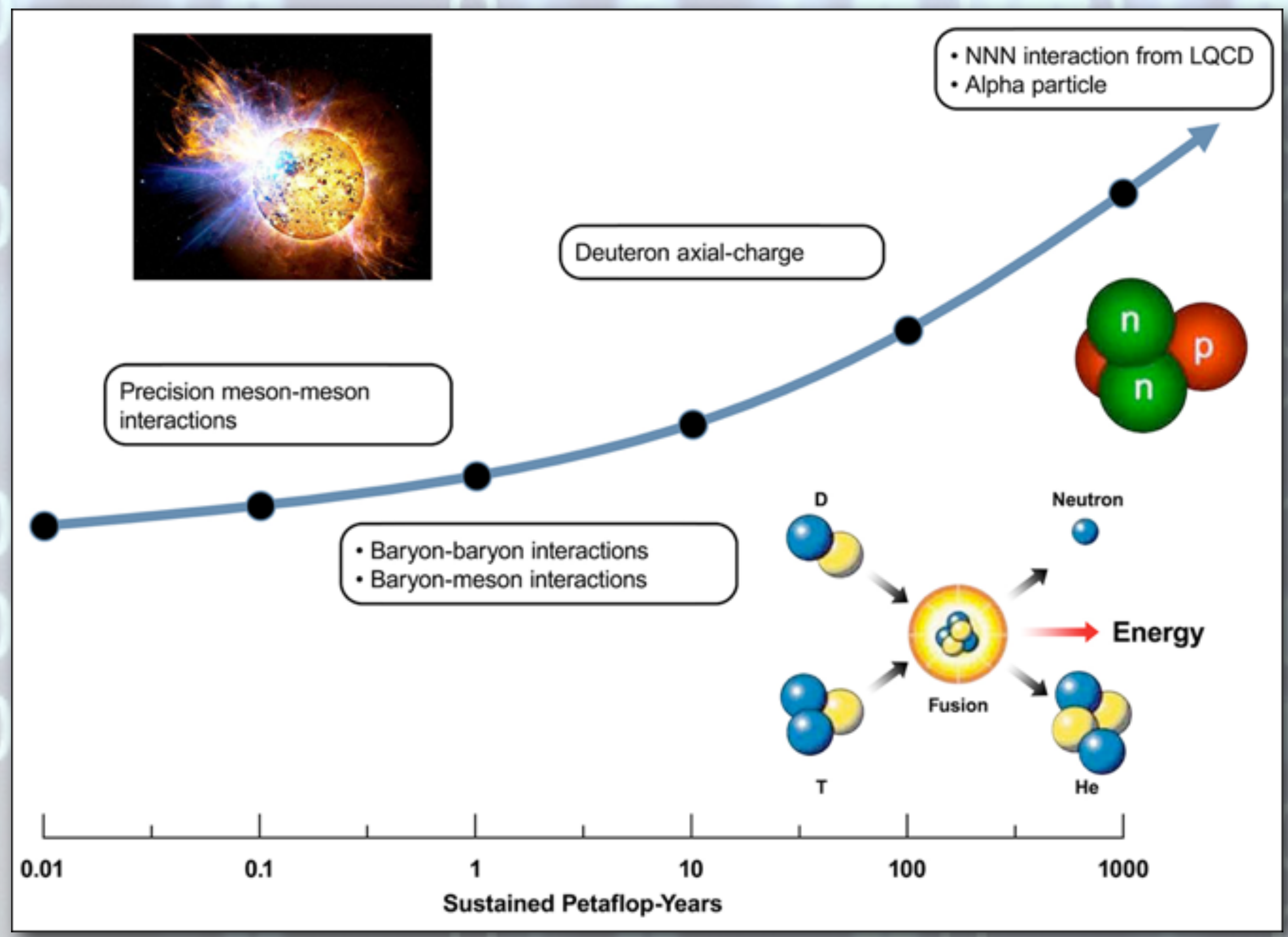


(Beane *et al*, Phys.Rev. D89 (2014) 074505)



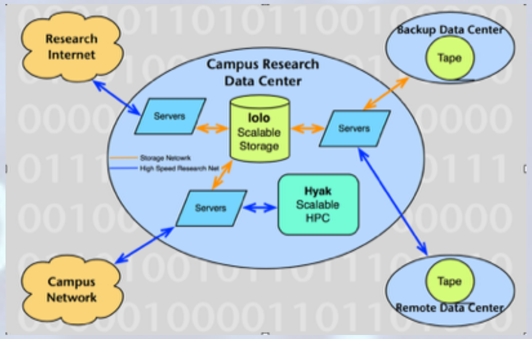
Exascale Resources Required



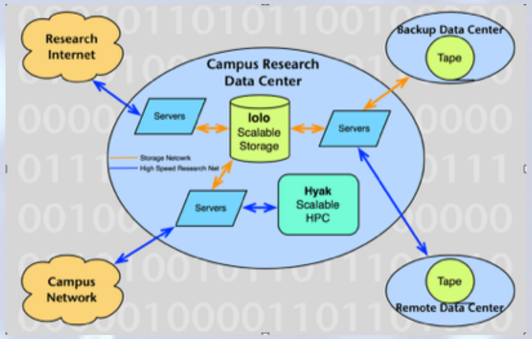


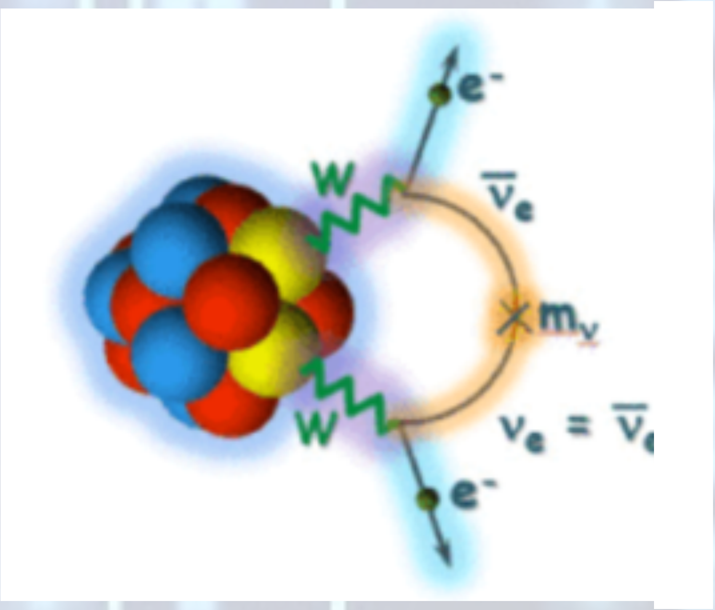
- Physical quark masses
- QED
- Continuum extrapolation
- Volume extrapolations

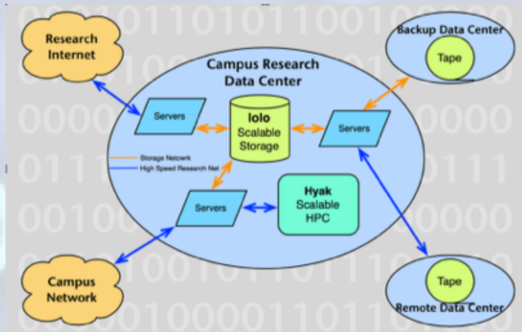
Estimates from 2009 which are in the process of being refined.



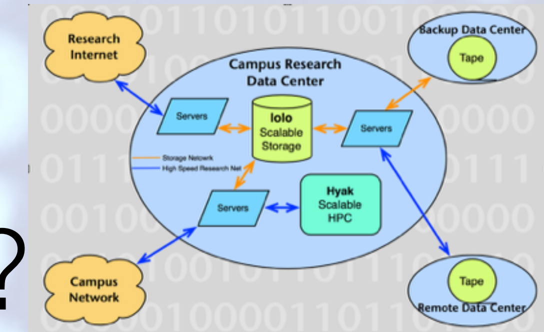
Important Things to do Next

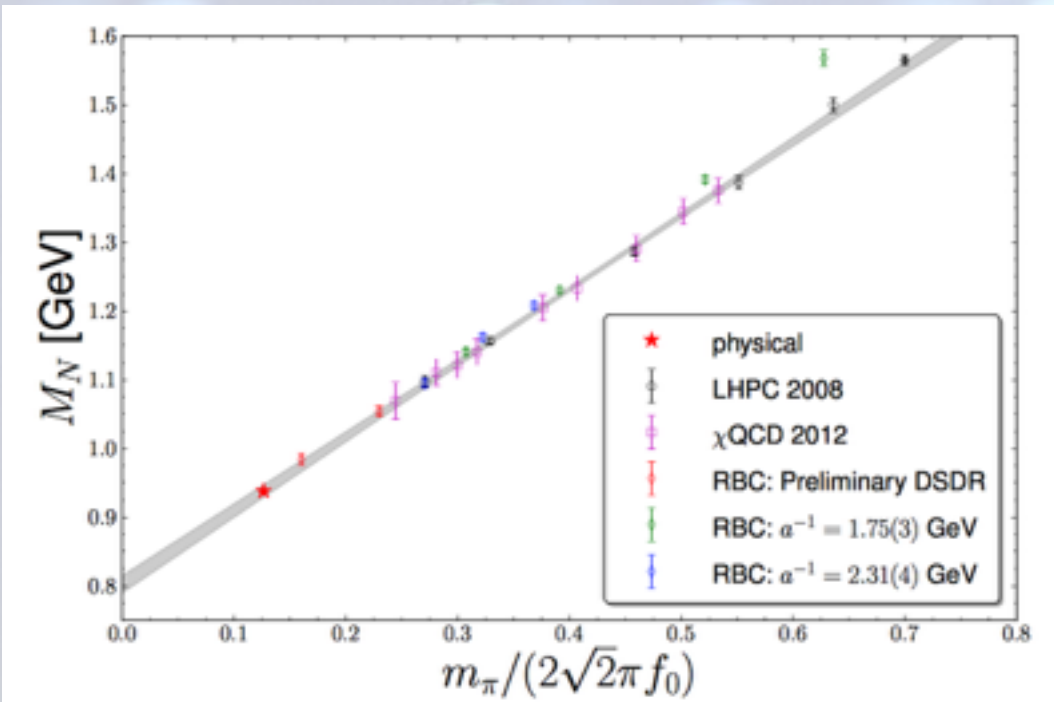


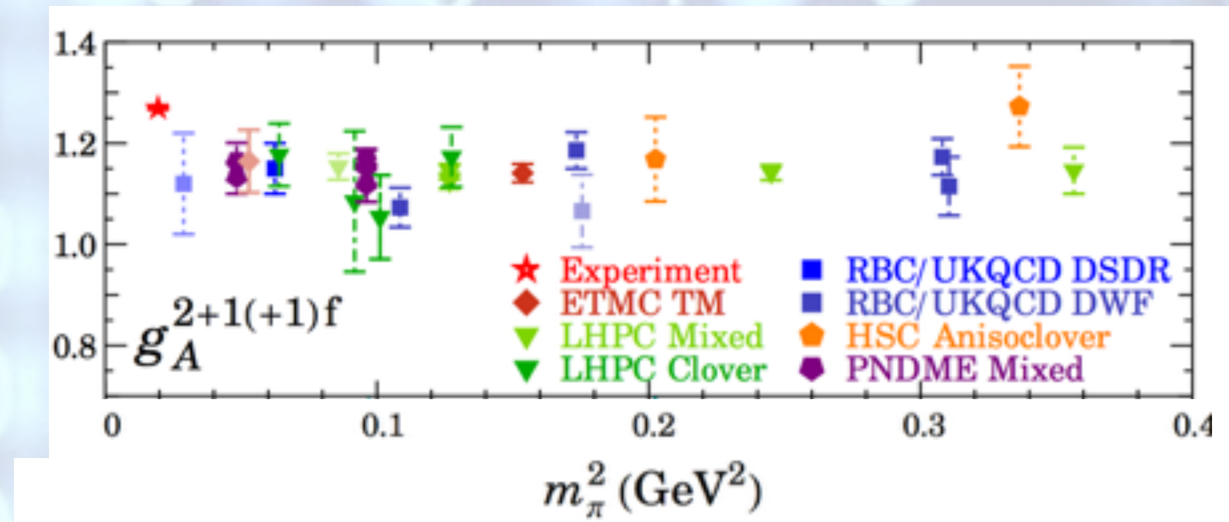


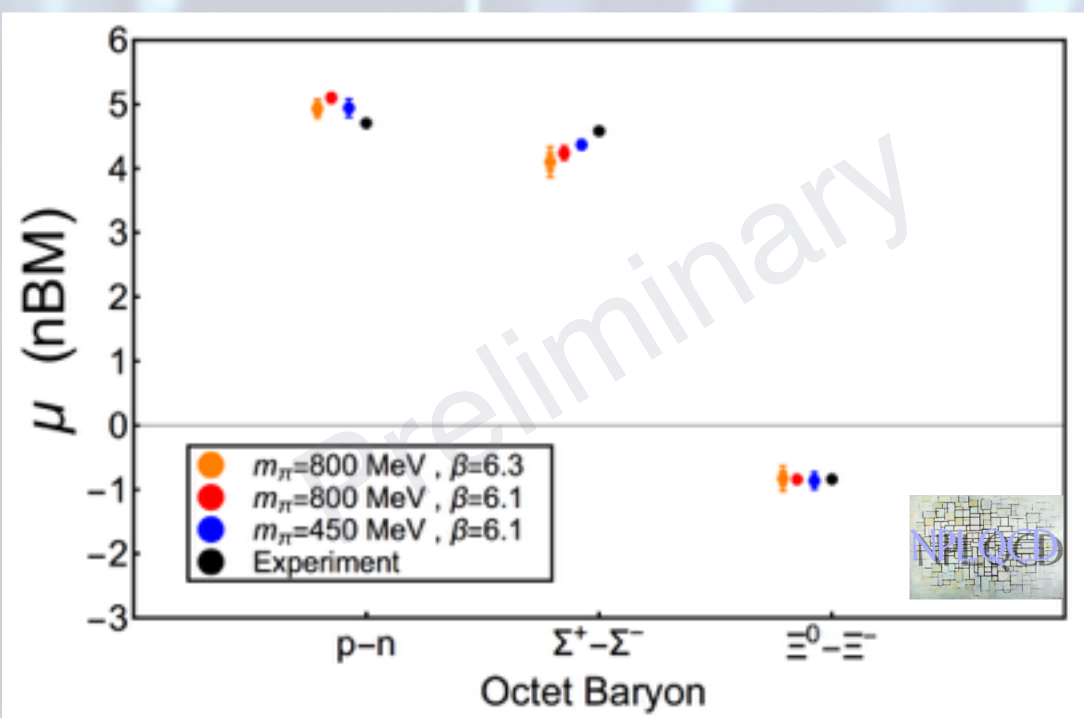


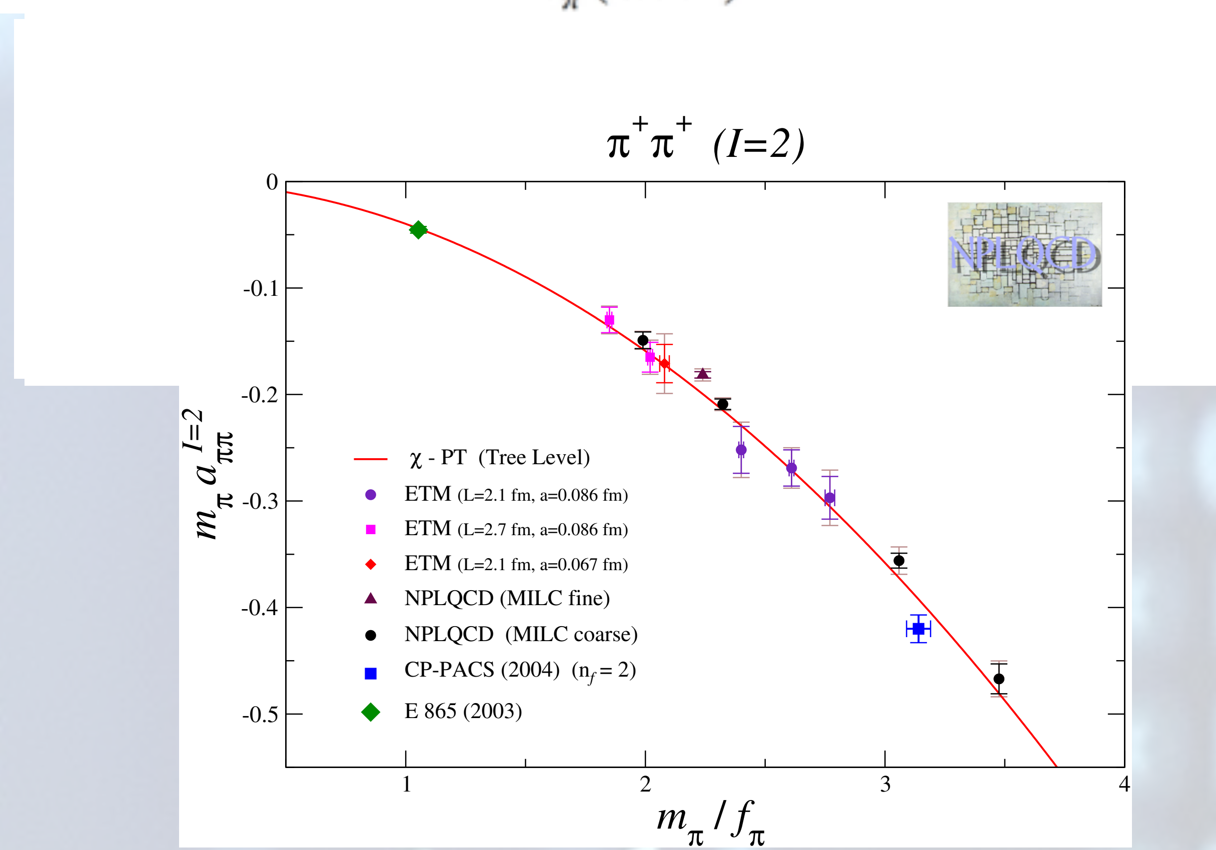
Lattice QCD: What is the Underlying Structure ?



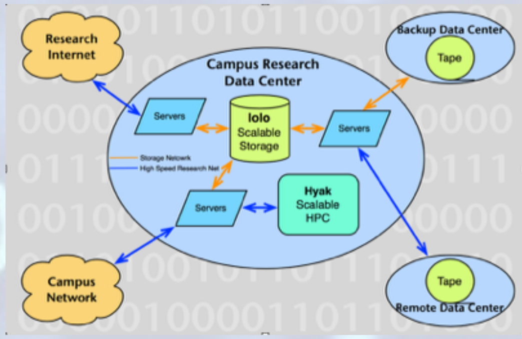




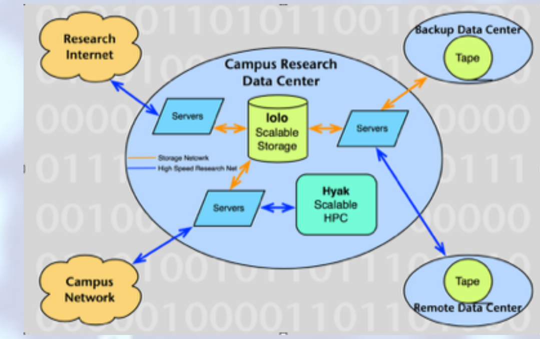




All unexpected results that Lattice QCD has revealed



Closing Remarks



Numerical Solution of Quantum Field Theory on Supercomputers is critical to subatomic physics research - presently cannot be accomplished with Cloud Computing (``the cloud” is factors of 50 too slow and factors of 10 too expensive)

Collaboration with CS/AM essential in making progress into Exascale era

Hyak continues to be essential in science, algorithm and code development, and for post processing, such data distribution and statistical analysis.