Simulation of QCD with a GPU cluster

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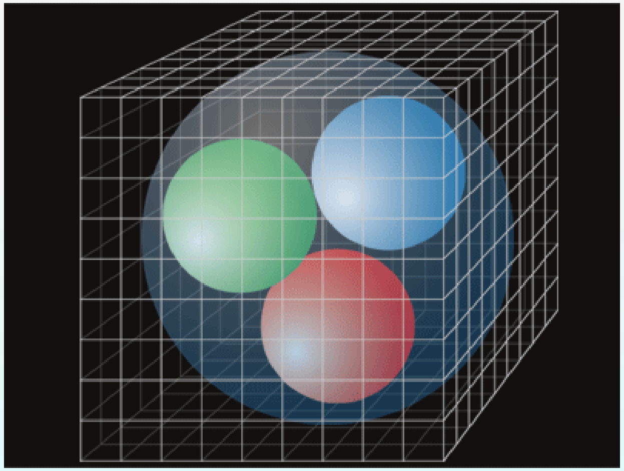


GPU Computing Seminar
January 22, 2010

High Energy Physics

Goal: To understand the fundamental constituents of matter and their fundamental interactions

Fundamental Interactions: Gravitational Force
Electromagnetic Force
Weak Interaction
Strong Interaction

Fundamental Particles: Atom $\longrightarrow$ Electron, Nucleus

$\Downarrow$

Proton, Neutron

$\Downarrow$

Quarks

Standard Model of

FUNDAMENTAL PARTICLES AND INTERACTIONS

The Standard Model is a quantum theory that summarizes our current knowledge of the physics of fundamental particles and fundamental interactions (interactions are manifested by forces and by decay rates of unstable particles).

FERMIONS
matter constituents
spin = 1/2, 3/2, 5/2, ...

Leptons spin =1/2

Flavor	Mass GeV/c^2	Electric charge
ν_L lightest neutrino*	$(0-0.13)\times10^{-9}$	0
e electron	0.000511	–1
ν_M middle neutrino*	$(0.009-0.13)\times10^{-9}$	0
μ muon	0.106	–1
ν_H heaviest neutrino*	$(0.04-0.14)\times10^{-9}$	0
τ tau	1.777	–1

*See the neutrino paragraph below.

Quarks spin =1/2

Flavor	Approx. Mass GeV/c^2	Electric charge
u up	0.002	2/3
d down	0.005	–1/3
c charm	1.3	2/3
s strange	0.1	–1/3
t top	173	2/3
b bottom	4.2	–1/3

Spin is the intrinsic angular momentum of particles. Spin is given in units of ħ, which is the quantum unit of angular momentum where $\hbar = h/2\pi = 6.58\times10^{-25}$ GeV s $=1.05\times10^{-34}$ J s.

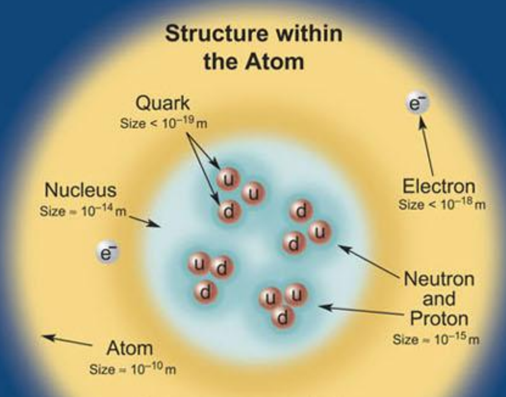
Electric charges are given in units of the proton's charge. In SI units the electric charge of the proton is 1.60×10^{-19} coulombs.

The energy unit of particle physics is the electronvolt (eV), the energy gained by one electron in crossing a potential difference of one volt. **Masses** are given in GeV/c^2 (remember $E = mc^2$) where 1 GeV = 10^9 eV $=1.60\times10^{-10}$ joule. The mass of the proton is 0.938 GeV/c^2 = 1.67×10^{-27} kg.

Neutrinos
Neutrinos are produced in the sun, supernovae, reactors, accelerator collisions, and many other processes. Any produced neutrino can be described as one of three neutrino flavor states ν_e, ν_μ, or ν_τ, labelled by the type of charged lepton associated with its production. Each is a defined quantum mixture of the three definite mass neutrinos ν_L, ν_M, and ν_H for which currently allowed mass ranges are shown in the table. Further exploration of the properties of neutrinos may yield powerful clues to puzzles about matter and antimatter and the evolution of stars and galaxy structures.

Matter and Antimatter
For every particle type there is a corresponding antiparticle type, denoted by a bar over the particle symbol (unless + or – charge is shown). Particle and antiparticle have identical mass and spin but opposite charges. Some electrically neutral bosons (e.g., Z^0, γ, and $\eta_c = c\bar{c}$ but not $K^0 = d\bar{s}$) are their own antiparticles.

Structure within the Atom



If the proton and neutrons in this picture were 10 cm across, then the quarks and electrons would be less than 0.1 mm in size and the entire atom would be about 10 km across.

BOSONS
force carriers
spin = 0, 1, 2, ...

Unified Electroweak spin = 1

Name	Mass GeV/c^2	Electric charge
γ photon	0	0
W^-	80.39	–1
W^+ W bosons	80.39	+1
Z^0 Z boson	91.188	0

Strong (color) spin =1

Name	Mass GeV/c^2	Electric charge
g gluon	0	0

Color Charge
Only quarks and gluons carry "strong charge" (also called "color charge") and can have strong interactions. Each quark carries three types of color charge. These charges have nothing to do with the colors of visible light. Just as electrically-charged particles interact by exchanging photons, in strong interactions, color-charged particles interact by exchanging gluons.

Quarks Confined in Mesons and Baryons
Quarks and gluons cannot be isolated – they are confined in color-neutral particles called **hadrons**. This confinement (binding) results from multiple exchanges of gluons among the color-charged constituents. As color-charged particles (quarks and gluons) move apart, the energy in the color-force field between them increases. This energy eventually is converted into additional quark-antiquark pairs. The quarks and antiquarks then combine into hadrons; these are the particles seen to emerge.

Two types of hadrons have been observed in nature **mesons** $q\bar{q}$ and **baryons** qqq. Among the many types of baryons observed are the proton (uud), antiproton ($\bar{u}\bar{u}\bar{d}$), neutron (udd), lambda Λ (uds), and omega Ω^- (sss). Quark charges add in such a way as to make the proton have charge 1 and the neutron charge 0. Among the many types of mesons are the pion π^+ ($u\bar{d}$), kaon K^- ($s\bar{u}$), B^0 ($d\bar{b}$), and η_c ($c\bar{c}$). Their charges are +1, –1, 0, 0 respectively.

Properties of the Interactions

The strengths of the interactions (forces) are shown relative to the strength of the electromagnetic force for two u quarks separated by the specified distances.

Property		Gravitational Interaction	Weak Interaction (Electroweak)	Electromagnetic Interaction	Strong Interaction
Acts on:		Mass – Energy	Flavor	Electric Charge	Color Charge
Particles experiencing:		All	Quarks, Leptons	Electrically Charged	Quarks, Gluons
Particles mediating:		Graviton (not yet observed)	W^+ W^- Z^0	γ	Gluons
Strength at	10^{-18} m	10^{-41}	0.8	1	25
	3×10^{-17} m	10^{-41}	10^{-4}	1	60

Visit the award-winning web feature *The Particle Adventure* at

ParticleAdventure.org

This chart has been made possible by the generous support of:
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Lawrence Berkeley National Laboratory

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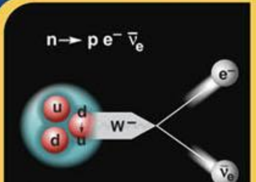
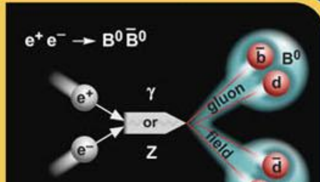
Particle Processes

These diagrams are an artist's conception. Blue-green shaded areas represent the cloud of gluons.



A free neutron (udd) decays to a proton (uud), an electron, and an antineutrino via a virtual (mediating) W boson. This is neutron β (beta) decay.



An electron and positron (antielectron) colliding at high energy can annihilate to produce $\bar{B}^0$ and B^0 mesons via a virtual Z boson or a virtual photon.

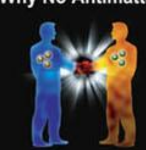
Unsolved Mysteries

Driven by new puzzles in our understanding of the physical world, particle physicists are following paths to new wonders and startling discoveries. Experiments may even find extra dimensions of space, mini-black holes, and/or evidence of string theory.

Universe Accelerating?

The expansion of the universe appears to be accelerating. Is this due to Einstein's Cosmological Constant? If not, will experiments reveal a new force of nature or even extra (hidden) dimensions of space?

Why No Antimatter?



Matter and antimatter were created in the Big Bang. Why do we now see only matter except for the tiny amounts of antimatter that we make in the lab and observe in cosmic rays?

Dark Matter?

Invisible forms of matter make up much of the mass observed in galaxies and clusters of galaxies. Does this dark matter consist of new types of particles that interact very weakly with ordinary matter?

Origin of Mass?

In the Standard Model, for fundamental particles to have masses, there must exist a particle called the Higgs boson. Will it be discovered soon? Is supersymmetry theory correct in predicting more than one type of Higgs?

Fundamental Interactions

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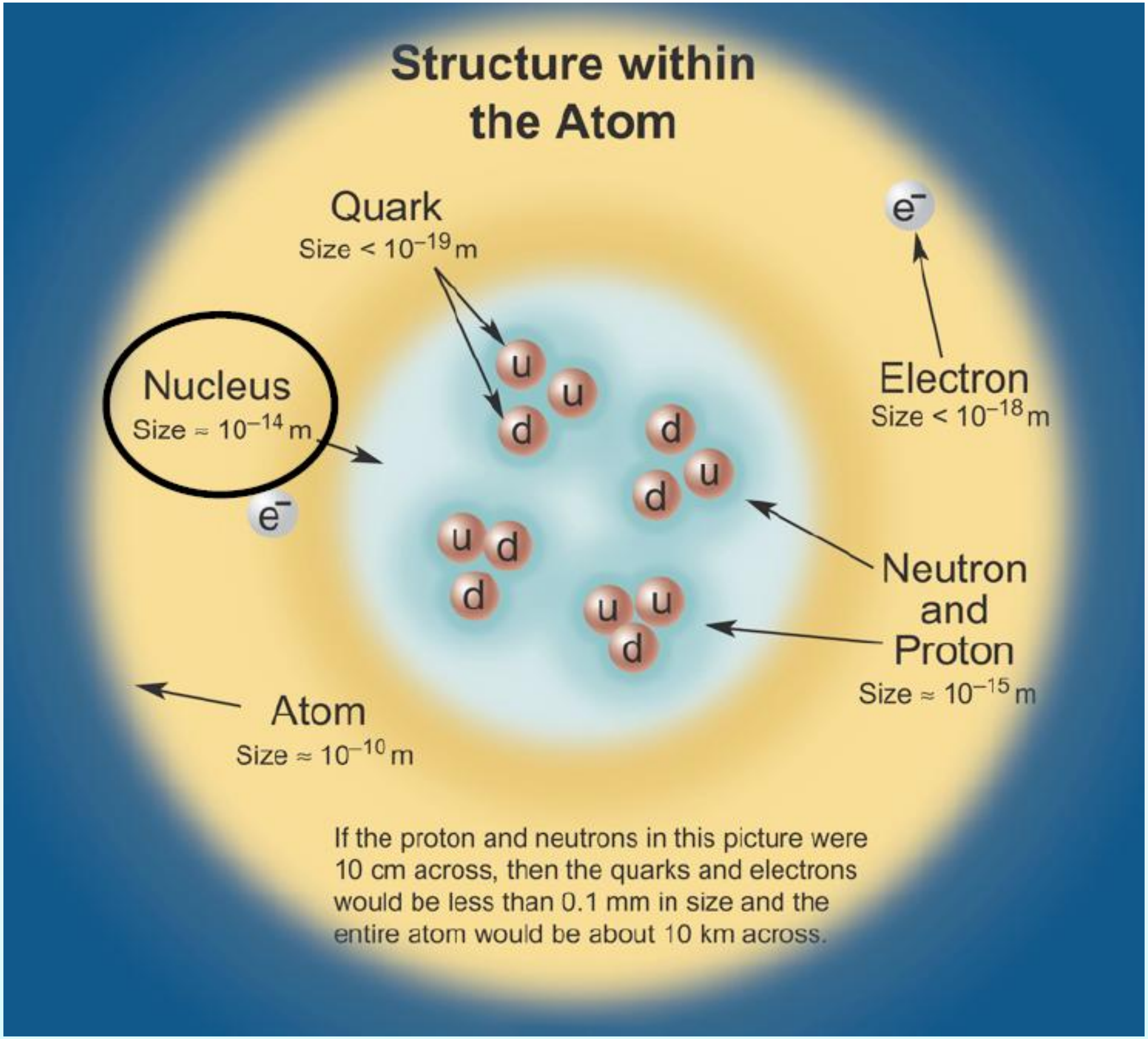
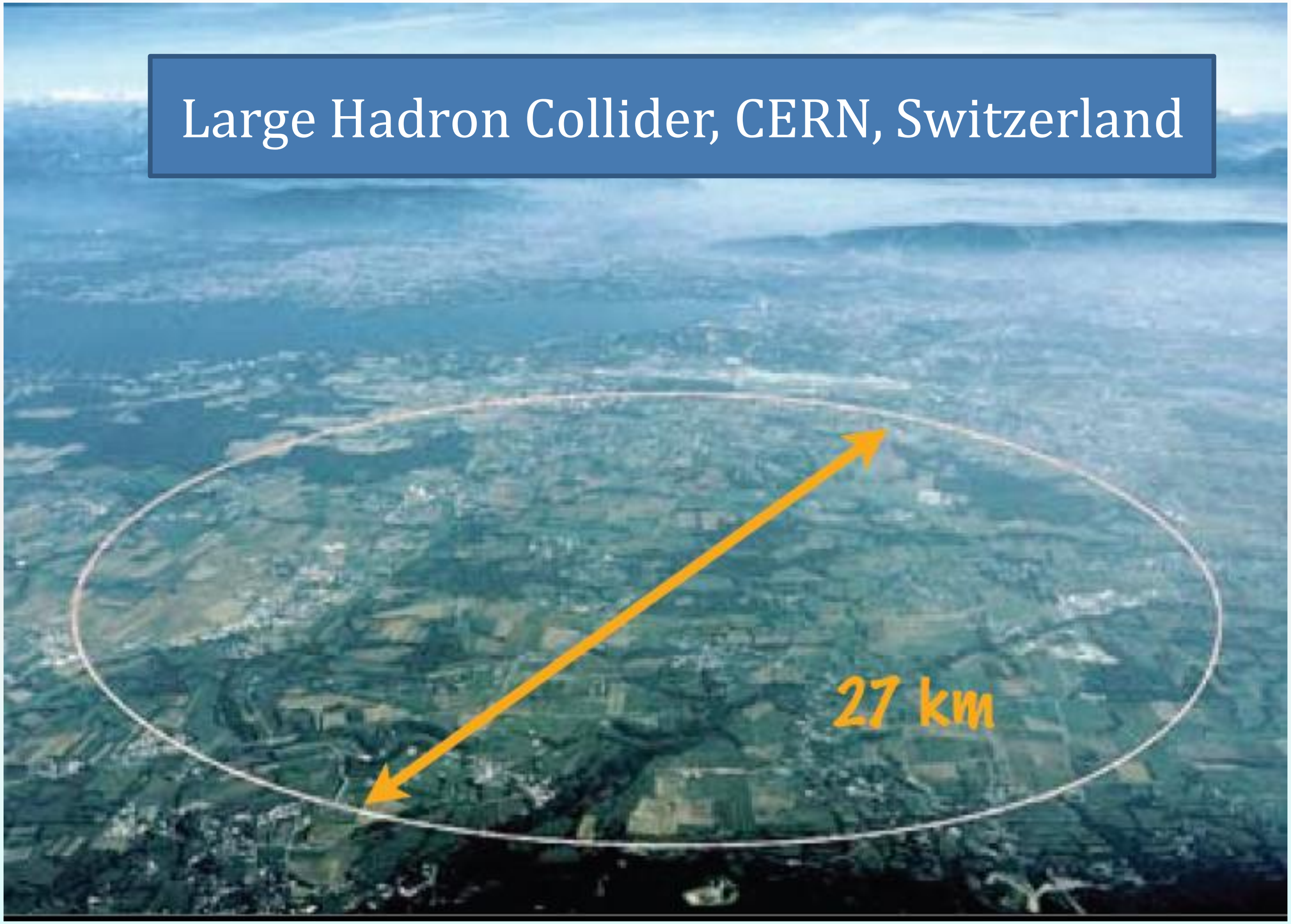

Structure within the Atom
Quark
Size < 10⁻¹⁹ m
e⁻
Nucleus
Size ≈ 10⁻¹⁴ m
Electron
Size < 10⁻¹⁸ m
u
u
d
d
d
u
e⁻
u
d
d
u
u
d
Neutron and Proton
Size ≈ 10⁻¹⁵ m
Atom
Size ≈ 10⁻¹⁰ m
If the proton and neutrons in this picture were 10 cm across, then the quarks and electrons would be less than 0.1 mm in size and the entire atom would be about 10 km across.

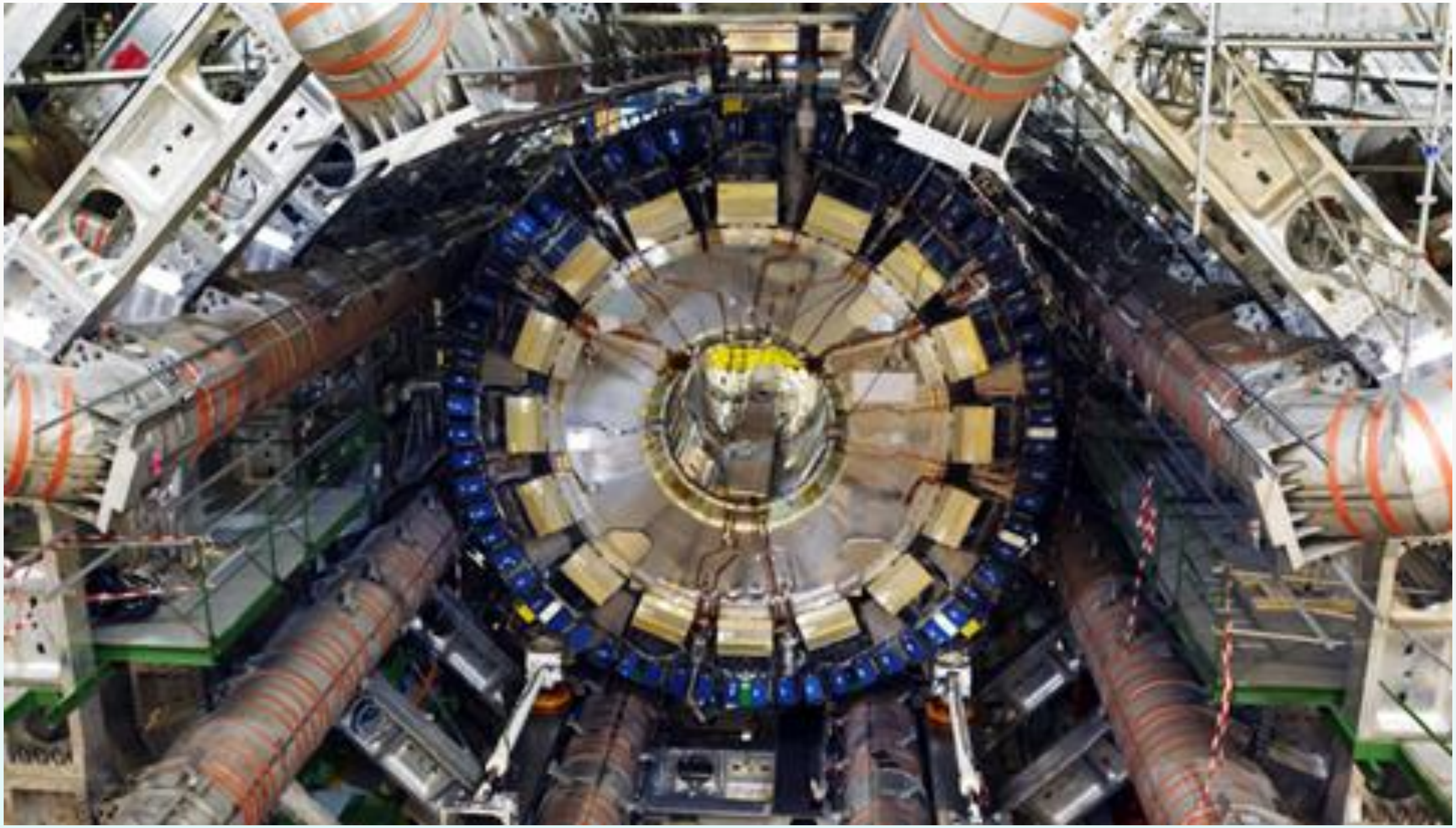
HEP Experiments ➡ Huge Accelerator



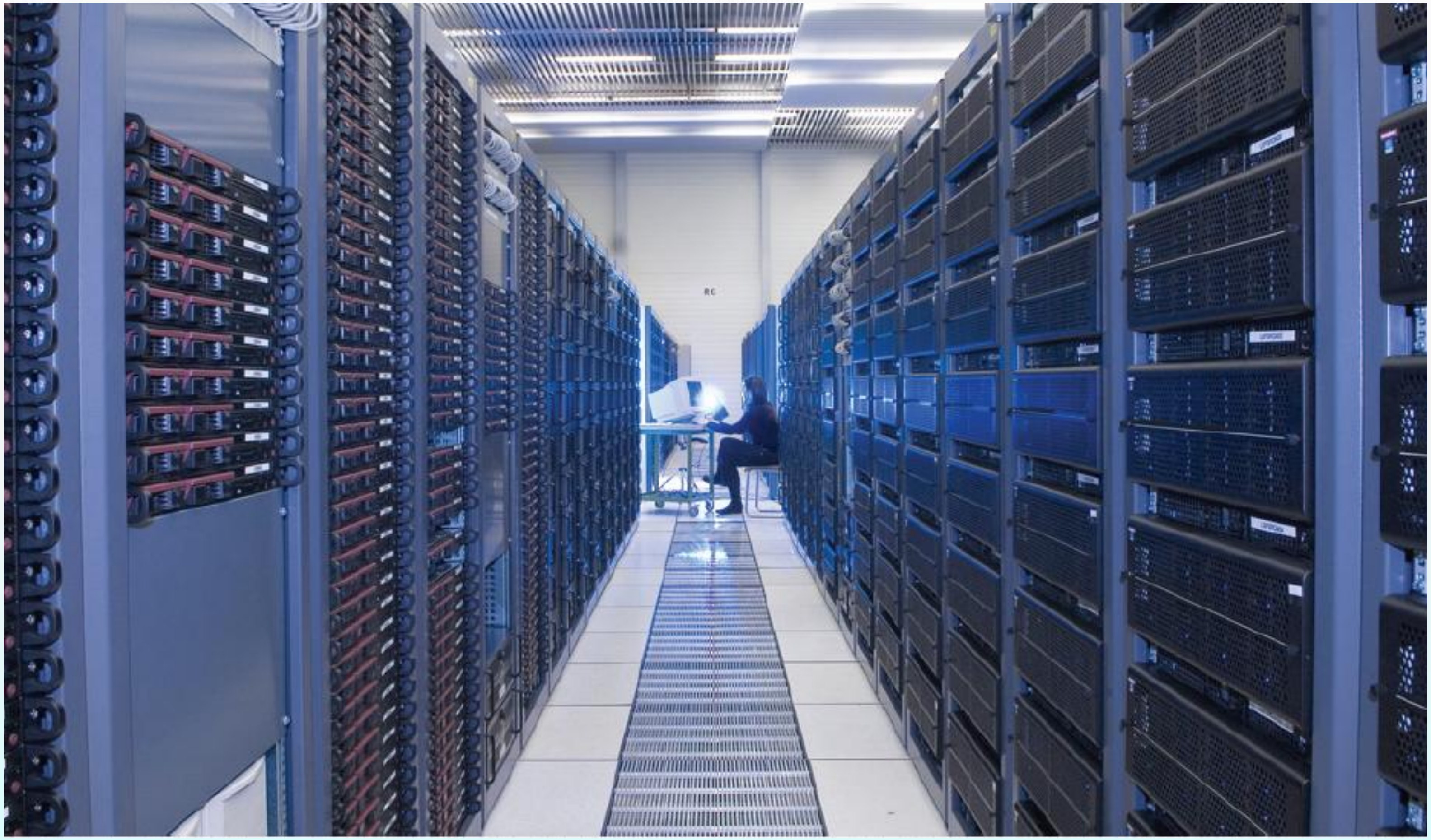
Tunnel of the Large Hadron Collider

The tunnel is buried around 50 to 175 m. underground

ATLAS Detector



LHC experiments will produce roughly 15 petabytes of data annually. CERN is collaborating with institutions in 33 different countries (including Taiwan) to operate a distributed computing and data storage infrastructure known as the LHC Computing Grid



ABSTRACT

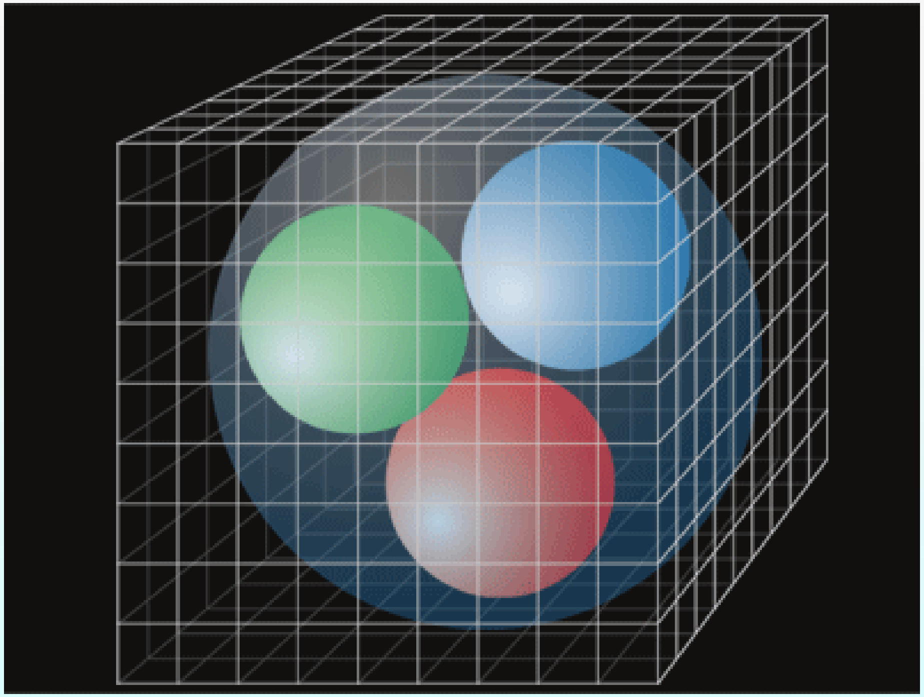
◆ Quantum Chromodynamics (**QCD**) is the quantum field theory of the strong interaction, describing the interactions of the quarks and gluons making up hadrons (e.g., proton, neutron, and pion).

◆ Quantum Chromodynamics (**QCD**) accounts for the nuclear energy inside an atom, and plays an important role in the evolution of the early universe.

◆ To solve **QCD** is a grand challenge among all sciences. The most promising approach to solve **QCD** nonperturbatively is to discretize the continuum space-time into a 4 dimensional lattice (lattice **QCD**), and to compute physical observables with Monte Carlo simulation.

ABSTRACT(cont)

◆ To solve QCD is a grand challenge among all sciences. The most promising approach to solve QCD nonperturbatively is to discretize the continuum space-time into a 4 dimensional lattice (lattice QCD), and to compute physical observables with Monte Carlo simulation.



ABSTRACT (cont)

◆ For lattice QCD with exact chiral symmetry, it often requires supercomputers (e.g., 10 racks of IBM BlueGene supercomputer) to perform the simulations.

10 racks of IBM BG/L at KEK, Japan (57 TFLOPS peak)

ABSTRACT (cont)

◆ TWQCD Collaboration is the first lattice **QCD** group around the world to use a GPU cluster (128 TFLOPS) to perform large-scale unquenched simulations of lattice **QCD** with exact chiral symmetry.

Outlines

- Introduction
- Optimal Domain-Wall Fermion
- HMC Simulation with ODWF
- GPU Strategies
- Research Highlights
- Conclusion and Outlook

Quantum Chromodynamics (QCD)

QCD is the quantum field theory for the strong interaction, describing the interactions of the quarks and gluons making up hadrons (e.g. proton, neutron, and pion). It accounts for the nuclear energy inside the nucleus of an atom, and plays an important role in the evolution of the early universe.

Salient features:

- Gauge group $SU(3) \Rightarrow$ gluons have self-interactions.
- Asymptotic freedom: $g(r) \to 0$ as $r \to 0$.
- IR slavory: $g(r) \simeq 1$ at $r \simeq 10^{-15}\,\mathrm{m} \Rightarrow$ quark/color confinement
- No exact analytic solutions

Quarks

Quarks are spin $\frac{1}{2}$ fermions carrying color,
and there are 6 species (flavors) of quarks.

u	c	t	u	c	t	u	c	t
d	s	b	d	s	b	d	s	b

Hadrons are color singlets composed of quarks

$$P = uud + \text{antisym. in color,} \qquad \text{Proton}$$

$$N = udd + \text{antisym. in color,} \qquad \text{Neutron}$$

$$\pi^{+} = \bar{d}u + \bar{d}u + \bar{d}u, \qquad \text{Pion}$$

The nuclear force between nucleons emerges as
residual interactions of QCD

The Challenge of QCD

At the hadronic scale, $g(r) \simeq 1$, perturbation theory is incapable to extract any quantities from **QCD**, nor to tackle the most interesting physics, namely, the **spontaneously chiral symmetry breaking** and the **color confinement**

To extract any physical quantities from the first principles of **QCD**, one has to solve **QCD** nonperturbatively.

A viable nonperturbative formulation of **QCD** was first proposed by **K. G. Wilson** in 1974.

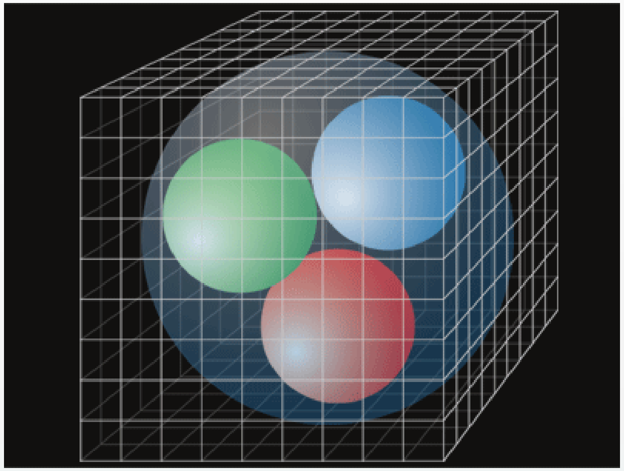
But, the problem of lattice fermion, and how to **formulate exact chiral symmetry on the lattice had not been resolved until 1992-98** **[Kaplan, Neuberger, Narayanan,…]**, i.e., **Lattice QCD with exact chiral symmetry.**

Basic notions of Lattice QCD

1. Perform Wick rotation: $t \to -ix_4$, then $\exp(iS) \to \exp(-S_E)$, and the expectation value of any observable O

$$\langle O \rangle = \frac{1}{Z} \int [dA][d\psi][d\bar{\psi}] O(A,\psi,\bar{\psi}) e^{-S_E}$$

$$Z = \int [dA][d\psi][d\bar{\psi}] e^{-S_E}$$



2. **Discretize the space-time as a 4-d lattice** $L^4 = (Na)^4$ with lattice spacing a. Then the path integral in QFT becomes a well-defined multiple integral which can be evaluated via Monte Carlo

$$\langle O \rangle = \frac{1}{Z} \int \prod_i dA_i \prod_j d\psi_j \prod_k d\bar{\psi}_k \, O(A,\psi,\bar{\psi}) e^{-S_E}$$

Gluon fields on the Lattice

The $SU(3)$ color gluon field $A_\mu(x)$ are defined on each link connecting x and $x+a\hat{\mu}$, through the link variable

$$U_\mu(x) = \exp\left[iagA_\mu\left(x + \frac{a}{2}\hat{\mu} \right) \right]$$

Then the gluon action on the lattice can be written as

$$S_g[U] = \frac{6}{g^2} \sum_{\text{plaquette}} \left[1 - \frac{1}{3} \operatorname{Re}\ tr\left(U_p\right) \right] \xrightarrow{a \to 0} \int d^4x \frac{1}{2} tr\left[F_{\mu\nu}(x) F_{\mu\nu}(x) \right]$$

where $\quad U_p = U_\mu(x) U_\nu(x+a\hat{\mu}) U_\mu^\dagger(x+a\hat{\nu}) U_\nu^\dagger(x)$

$$\begin{tikzcd}
x+a\hat{\nu} \arrow[d] & x+a\hat{\mu}+a\hat{\nu} \arrow[l] \\
x \arrow[r] & x+a\hat{\mu} \arrow[u]
\end{tikzcd}$$

Lattice QCD

The QCD action $S = S_G(U) + \bar{\psi} D(U) \psi$

where $S_G(U)$ is the action of the gluon fields

$$\bar{\psi} D(U) \psi \equiv \bar{\psi}^f_{a\alpha x} D_f(U)_{a\alpha x, b\beta y} \psi^f_{b\beta y}$$

$f = u, d, s, c, b, t$	flavor index
$a, b = 1, 2, 3$	color index
$\alpha, \beta = 1,2,3,4$	Dirac index
$x, y = 1, \cdots, N_{\text{sites}} = N_x N_y N_z N_t$	site index

For example, on the $16^3 \times 32$ lattice, D is a complex matrix of size $1,572,864 \times 1,572,864$

$$\langle \mathcal{O}(\bar{\psi}, \psi, U) \rangle = \frac{\int dU d\bar{\psi} d\psi \, \mathcal{O}(\bar{\psi}, \psi, U) e^{-S}}{\int dU d\bar{\psi} d\psi \, e^{-S}} = \frac{\int dU \, \Theta(D^{-1}, U) \det(D) e^{-S_G}}{\int dU \det(D) e^{-S_G}}$$

The Challenge of Lattice QCD

- To have lattice volume large enough such that $m_\pi L \gg 1$.

  So far, the lightest u/d quark cannot be put on the lattice.

  Rely on ChPT to extrapolate lattice results to physical ones.

- To have lattice spacing small enough such that $m_q a \ll 1$.

- To meet the above two conditions:

  The lattice size should be at least $100^3 \times 200$.

  The computing power should be at least $\text{Petaflops} \times \text{year}$

The Hardware

One unit (1U) of Tesla S1070

4 GPUs, each with 4 GB

# of Tesla GPUs	4
# of Streaming Processor Cores	960 (240 per processor)
Frequency of processor cores	1.296 to 1.44 GHz
Single Precision floating point performance (peak)	3.73 to 4.14 TFlops
Double Precision floating point performance (peak)	311 to 345 GFlops
Floating Point Precision	IEEE 754 single & double
Total Dedicated Memory	16GB
Memory Interface	512-bit
Memory Bandwidth	408GB/sec
Max Power Consumption	800 W
System Interface	PCIe x16 or x8
Software Development Tools	C-based CUDA Toolkit

Two GTX285 on one motherboard

The Hardware (cont)

- **16 units of Nvidia Tesla S1070** (total **64 GPUs, 64 x 4 GB**) connected to **16 servers** (total **32 Intel QC Xeon, 16 x 32 GB**)
- **64 Nvidia GTX285** (total **64 GPUs, 64 x 2/1 GB**), connected to **32 servers** (total **32 Intel i7**, **32 x 12 GB**)
- Hard disk storage > **300 TB**, **Lustre** cluster file system
- Peak performance is **128 TFLOPS**
- Developed efficient **CUDA** codes for unquenched lattice QCD.

  140/100 Gflops per each GTX285/T10
- Attaining **15 TFLOPS (sustained) with a price $220,000.**

Optimal Domain-Wall Fermion

[TWC, Phys. Rev. Lett. 90 (2003) 071601]

$$A_{\text{odwf}} = \sum_{s,s'=1}^{N_s} \sum_{x,x'} \bar{\psi}_{x,s} \left[\left(I + \omega_s D_w \right)_{x,x'} \delta_{s,s'} - \left(I - \omega_s D_w \right)_{x,x'} \left(P_- \delta_{s',s+1} + P_+ \delta_{s',s-1} \right) \right] \psi_{x',s'}$$

$$\equiv \bar{\Psi} D_{\text{odwf}} \Psi$$

$$D_w = \sum_{\mu=1}^{4} \gamma_\mu t_\mu + W - m_0, \quad m_0 \in (0,2)$$

$$t_\mu(x,x') = \frac{1}{2}\left[U_\mu(x) \delta_{x',x+\mu} - U_\mu^\dagger(x') \delta_{x',x-\mu} \right]$$

$$W(x,x') = \sum_{\mu=1}^{4} \frac{1}{2}\left[2\delta_{x,x'} - U_\mu(x) \delta_{x',x+\mu} - U_\mu^\dagger(x') \delta_{x',x-\mu} \right]$$

with boundary conditions

$$P_+ \psi(x,0) = -\frac{m_q}{2m_0} P_+ \psi(x,N_s)$$

$$P_- \psi(x,N_s+1) = -\frac{m_q}{2m_0} P_- \psi(x,1)$$

Optimal Domain-Wall Fermion (cont.)

The weights $\{\omega_s\}$ are fixed such that the effective 4D Dirac operator possesses the optimal chiral symmetry,

$$\omega_s = \frac{1}{\lambda_{\min}} \sqrt{1 - \kappa'^2 sn^2(v_s;\kappa')}, \quad s = 1, \cdots, N_s$$

where $sn(v_s;\kappa')$ is the Jacobian elliptic function with argument v_s and modulus $\kappa' = \sqrt{1 - \lambda_{\min}^2 / \lambda_{\max}^2}$,
$\lambda_{\min}^2$ and $\lambda_{\max}^2$ are lower and upper bounds of the eigenvalues of H_w^2

The action for Pauli-Villars fields is similar to A_{odwf}

$$A_{PV} = \sum_{s,s'=1}^{N_s} \sum_{x,x'} \bar{\phi}_{x,s} \left[(I + \omega_s D_w)_{x,x'} \delta_{s,s'} - (I - \omega_s D_w)_{x,x'} \left(P_- \delta_{s',s+1} + P_+ \delta_{s',s-1} \right) \right] \phi_{x',s'}$$

but with boundary conditions: $P_+\phi(x,0) = -P_+\phi(x,N_s), \quad m_{\mathrm{PV}} = 2m_0$

$$P_-\phi(x,N_s+1) = -P_-\phi(x,1)$$

Optimal Domain-Wall Fermion (cont.)

$$\int [d\bar{\psi}][d\psi]\left[d\bar{\phi}\right][d\phi]\exp\left(-A_{\text{odwf}} - A_{\text{PV}}\right) = \det D\left(m_q\right)$$

The effective 4D Dirac operator

$$D\left(m_q\right) = m_q + \left(m_0 - m_q/2\right)\left[1 + \gamma_5 S_{opt}\left(H_w\right)\right]$$

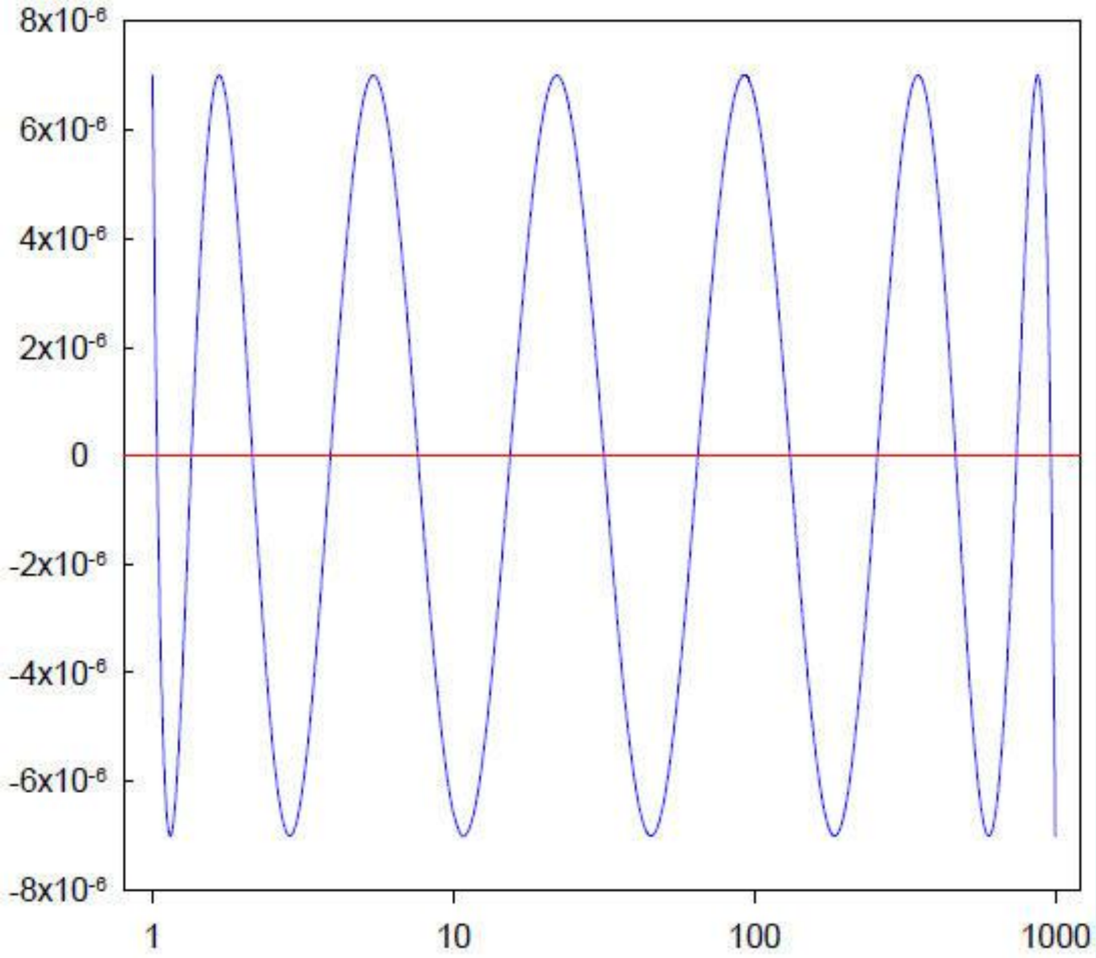
(1847 – 1878)

$$S_{opt}\left(H_w\right) = \begin{cases} H_w R_Z^{(n,n)}\left(H_w^2\right), & N_s = 2n+1 \\ H_w R_Z^{(n-1,n)}\left(H_w^2\right), & N_s = 2n \end{cases}$$

Zolotarev optimal rational approx. for $\dfrac{1}{\sqrt{H_w^2}}$
(1877)

The salient feature of optimal rational approximation

$$1-\sqrt{x}R_Z^{(n,m)}(x)$$



$\log(x)$

Has $(n+m+2)$ alternate change of sign in $[x_{\min}, x_{\max}]$, and attains its max. and min. (all with equal magnitude)

In the figure, $n=m=6$, it has 14 alternate change of sign in [1,1000]

Even-Odd Preconditioning of ODWF Matrix

$$\left[D_{\text{odwf}}\right]_{x,s;x',s'} = \left(I + \omega_s D_w\right)_{x,x'} \delta_{s,s'} - \left(I - \omega_s D_w\right)_{x,x'} \left(P_- \delta_{s',s+1} + P_+ \delta_{s',s-1}\right)$$

$$= \begin{pmatrix} X & D_w^{eo} Y \\ D_w^{oe} Y & X \end{pmatrix}$$

$$Y_{s,s'} = \omega_s (I + L)_{s,s'}$$

$$X_{s,s'} = (4 - m_0)\omega_s (I + L)_{s,s'} + (I - L)_{s,s'}$$

$$L_{s,s'} = P_- \delta_{s',s+1} + P_+ \delta_{s',s-1}$$

with boundary conditions: $P_- L_{N_s,s'} = -\dfrac{m_q}{2m_0} P_- \delta_{s',1}$

$$P_+ L_{1,s'} = -\frac{m_q}{2m_0} P_+ \delta_{s',N_s}$$

Even-Odd Preconditioning of ODWF Matrix (cont)

$$\begin{pmatrix} X & D_w^{eo}Y \\ D_w^{oe}Y & X \end{pmatrix} = \begin{pmatrix} I & 0 \\ D_w^{oe}YX^{-1} & I \end{pmatrix} \begin{pmatrix} X & 0 \\ 0 & X - D_w^{oe}YX^{-1}D_w^{eo}Y \end{pmatrix} \begin{pmatrix} I & X^{-1}D_w^{eo}Y \\ 0 & I \end{pmatrix}$$

Schur complement

$$\det D_{\mathrm{odwf}} \Rightarrow \det(I - D_w^{oe}YX^{-1}D_w^{eo}YX^{-1}) = \det C$$

$$C \equiv I - D_w^{oe}YX^{-1}D_w^{eo}YX^{-1}$$

For 2-flavor QCD, the pseudofermion action is

$$A_{PF} = \phi^\dagger C_{PV}^\dagger (CC^\dagger)^{-1} C_{PV}\phi$$

$$C_{PV} \equiv C(m_q = 2m_0)$$

Hybrid Monte Carlo (HMC) for 2 flavor QCD

1. Initial gauge configuration $\{U_l\}$
2. Generate $\{P_l^a\}$ with probability distribution $\propto \exp[-(P_l^a)^2/2]$
3. Generate ξ with probability distribution $\propto \exp(-\xi^\dagger \xi)$

   Recall: $\exp[-\phi^\dagger C_{PV}^\dagger (CC^\dagger)^{-1} C_{PV} \phi] = \exp[-\xi^\dagger \xi]$
4. Fixing the pseudofermion field $\phi = C_{PV}^{-1} C \xi \equiv D\xi$
5. Molecular dynamics (Omelyan integrator with multiple-time scale)

   $\boxed{\eta(\tau) = \left(DD^\dagger(U(\tau))\right)^{-1}\phi}$ $\leftarrow$ the most expensive part of HMC

   $\dot{U}_l(\tau) = iP_l(\tau)U_l(\tau), \quad P_l(\tau) \equiv P_l^a(\tau)T^a$

   $\dot{P}_l^a(\tau) = -D_l^a\left[A_{\text{gauge}}\left(U(\tau)\right)\right] + \eta^\dagger(\tau) D_l^a\left[DD^\dagger\left(U(\tau)\right)\right]\eta(\tau)$
6. Accept $\{U_l'\}$ with the probability $P_A = \min\left[1, \exp(-H' + H)\right]$
7. Go to 2.

Conjugate Gradient algorithm $(CC^\dagger)\eta' = \phi'$

$$Ax = b, \quad A \equiv CC^\dagger$$

$$x_0 = 0, \quad r_0 = b - Ax_0, \quad p_0 = r_0$$

$$\alpha_k = \frac{(r_k, r_k)}{(p_k, Ap_k)} = \frac{(r_k, r_k)}{(Cp_k, Cp_k)}$$

$$r_{k+1} = r_k - \alpha_k A p_k$$

If $|r_{k+1}| < \varepsilon |b|$, then stop

$$x_{k+1} = x_k + \alpha_k p_k$$

$$\beta_k = \frac{(r_{k+1}, r_{k+1})}{(r_k, r_k)}$$

$$p_{k+1} = r_{k+1} + \beta_k p_k$$

$$\phi' = C_{PV}\phi$$

$$\eta = C_{PV}^\dagger \eta'$$

* The most time-consuming operations are the matrix-vector multiplications $C(C^\dagger p_k)$
* GPU computes in SP $\gg$ DP

CG Algorithm with Mixed Precision

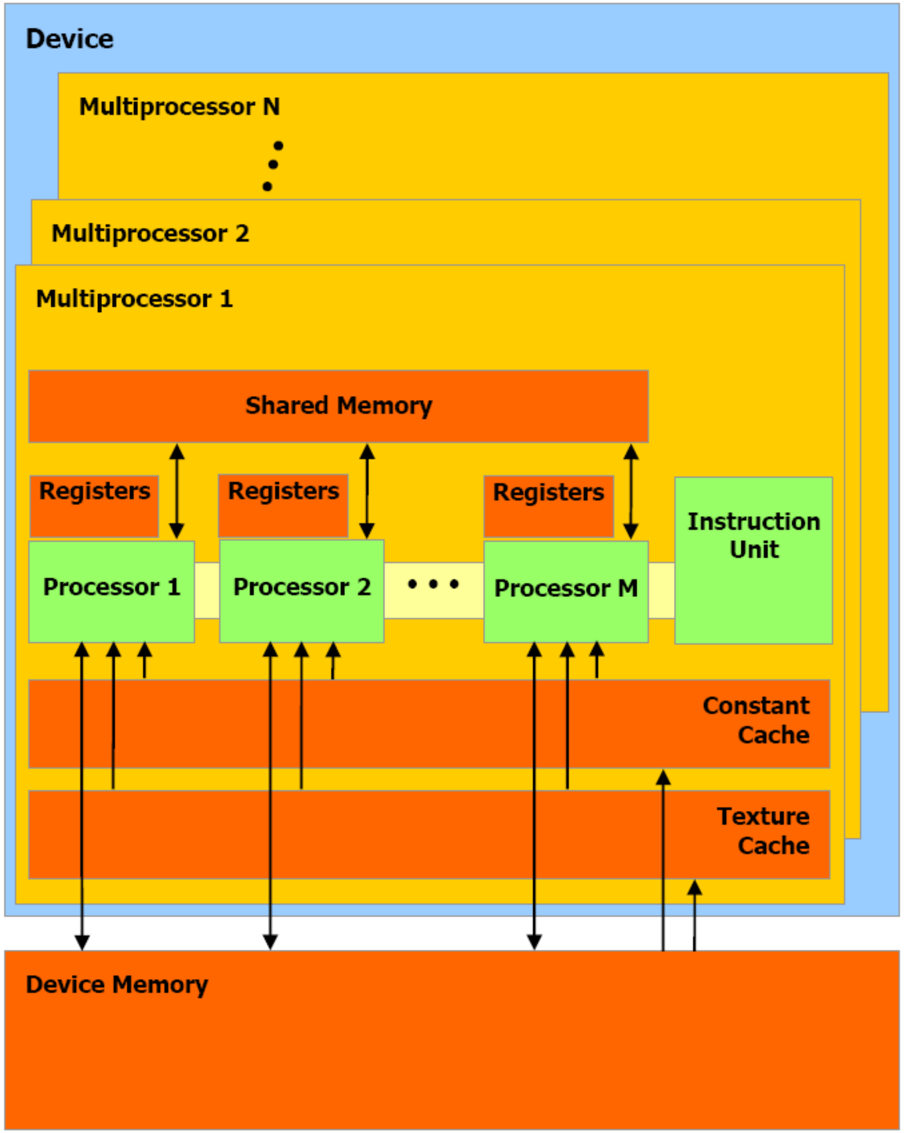
1. $r_k = b - Ax_k$
2. If $|r_k| < \varepsilon |b|$, then stop
3. Solve $At_k = r_k$ in single precision to an accuracy $\varepsilon_1 < 1$
4. $x_{k+1} = x_k + t_k$
5. Go to 1.

Proof of convergence:

Let $s_k = r_k - At_k, \quad |s_k| < \varepsilon_1 |r_k|$

then $|r_{k+1}| = |b - Ax_{k+1}| = |b - Ax_k - At_k| = |s_k| < \varepsilon_1 |r_k| < |r_k|$

Hardware Model



A set of SIMT multiprocessors with on-chip shared memory.

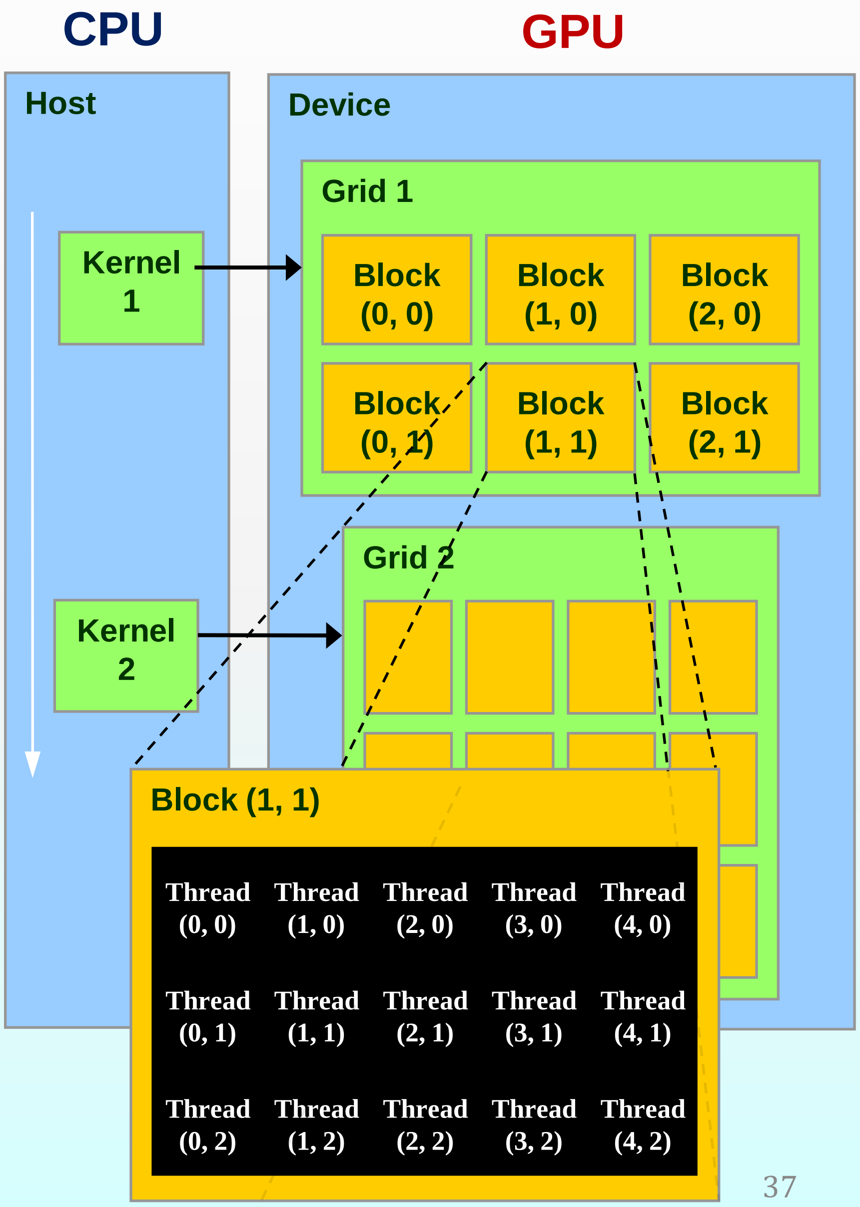
T10/ GTX285

Global memory:	4/1/2 Gbytes
# of multiprocessors:	30
# of cores:	240
Constant memory:	65536 bytes
Shared memory/block:	16384 bytes
# of registers/block:	16384
Warp size:	32
Max. # threads/block:	512
Block-size limits x,y,z:	512, 512, 64
Grid-size limits in x,y:	65535, 65535

CUDA Programming Model

A kernel is executed by a grid of thread blocks

- A thread block is a set of threads that can cooperate with each other by:
  - Sharing data through shared memory
  - Synchronizing their execution
- Threads from different blocks cannot cooperate



Features of CG Kernel for ODWF

$$(CC^{\dagger})\eta' = \phi'$$

$$C \equiv I - D_w^{oe} Y X^{-1} D_w^{eo} Y X^{-1}$$

One thread takes care of all computations at each (s, x, y, z) with a loop going over all t (even/odd).

- 1-dim Grid $\quad Nthread_X \times Nthread_Y \times Nblock = N_s N_x{}^3$
- 2-dim Block $\quad Nthread_X = N_s = 16 \times (1, 2, \ldots)$

$$Nthread_X \times Nthread_Y = 64$$

Tuning the CG Kernel for ODWF

- $M \equiv YX^{-1}$ in constant memory space
- Use texture memory for link variables and vectors
- Reorder data in the device memory
  (coalescing; Ns threads share the same link variables)
- Reuse forward/backward data (in t) for neighboring sites
- Unroll short loops
- …

Attaining 140/120/100 Gflops for GTX285/GTX280/T10

Salient Features of TWQCD's HMC Simulation

- HMC with Multiple Time Scale Integration and Mass Preconditioning
- Even-Odd Preconditioning for the 4D Quark Matrix
- Omelyan Integrator for the Molecular Dynamics
- Conjugate Gradient with Mixed Precision
- New Algorithm for (2+1)-flavor QCD
- Chiral Symmetry is preserved exactly with ODWF
- All Topological Sectors are sampled ergodically.
- The First Large-Scale Simulation of Unquenched Lattice QCD with Exact Chiral Symmetry using a GPU Cluster.

Technical Breakthrough

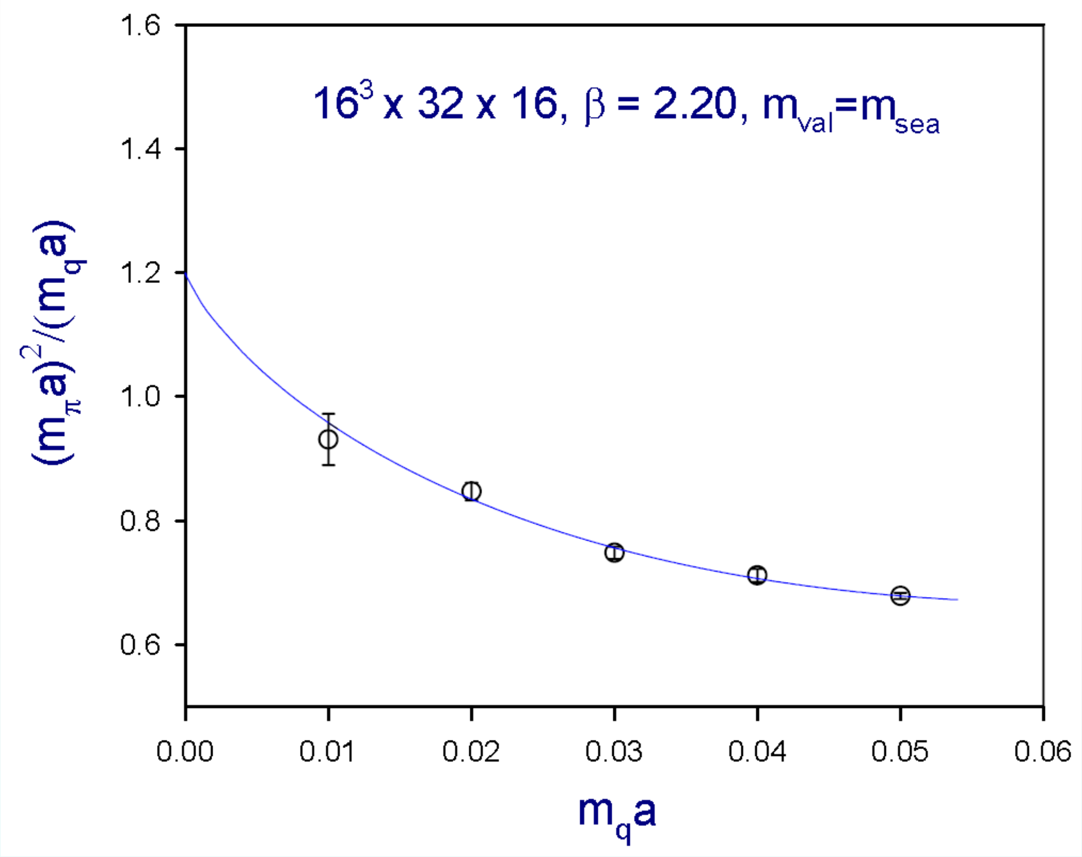
- **The First Large-Scale Dynamical Lattice QCD Simulation with a GPU Cluster**

The lattice QCD group (TWQCD) based at NTU is the first group around the world to use a GPU cluster to perform large-scale simulations of lattice QCD with exact chiral symmetry. [T.W. Chiu et al., PoS (LAT2009) 034, arXiv:0911.0529].

Currently, there are only 3 groups (RBC/UKQCD, JLQCD, and TWQCD) around the world who are capable to perform large scale simulation of lattice QCD with exact chiral symmetry.

Research Highlights

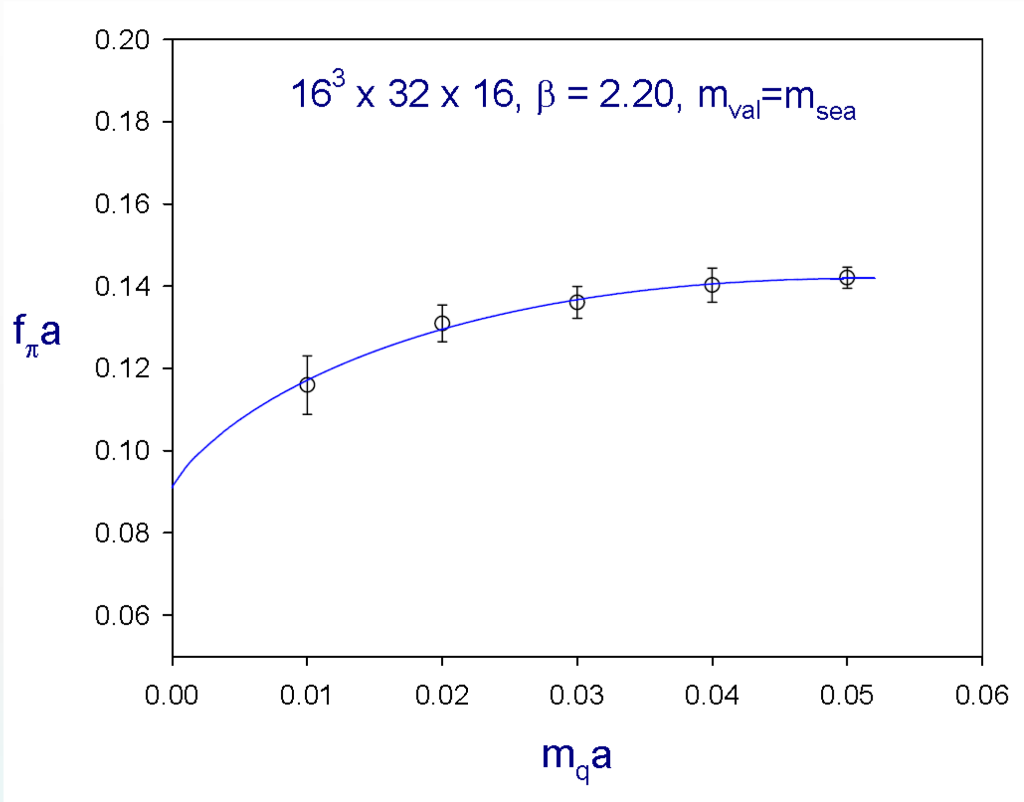
➢ Zero Temperature QCD $(N_f = 2)$



ChPT to NLO

$$\frac{m_\pi^2}{m_q} = 2B\left(1+\frac{1}{2}x\ln x\right)+c_3 x, \quad x = \frac{4Bm_q}{(4\pi f)^2}$$

Research Highlights (cont)



Fitting data to $f_\pi = f\left(1 - x \ln x\right) + c_4 x \;\Rightarrow\; f\,a = 0.091(6)$

Using $f = 131$ MeV as input $\Rightarrow a^{-1} = 1.45(9)$ GeV

Research Highlights (cont)

➢ Topological structure of the QCD vacuum

- The vacuum (ground state) of QCD constitutes various quantum fluctuations, which are the origin of many interesting and important nonperturbative physics

- In QCD, each gauge configuration possesses a well-defined topological charge Q with integer value.

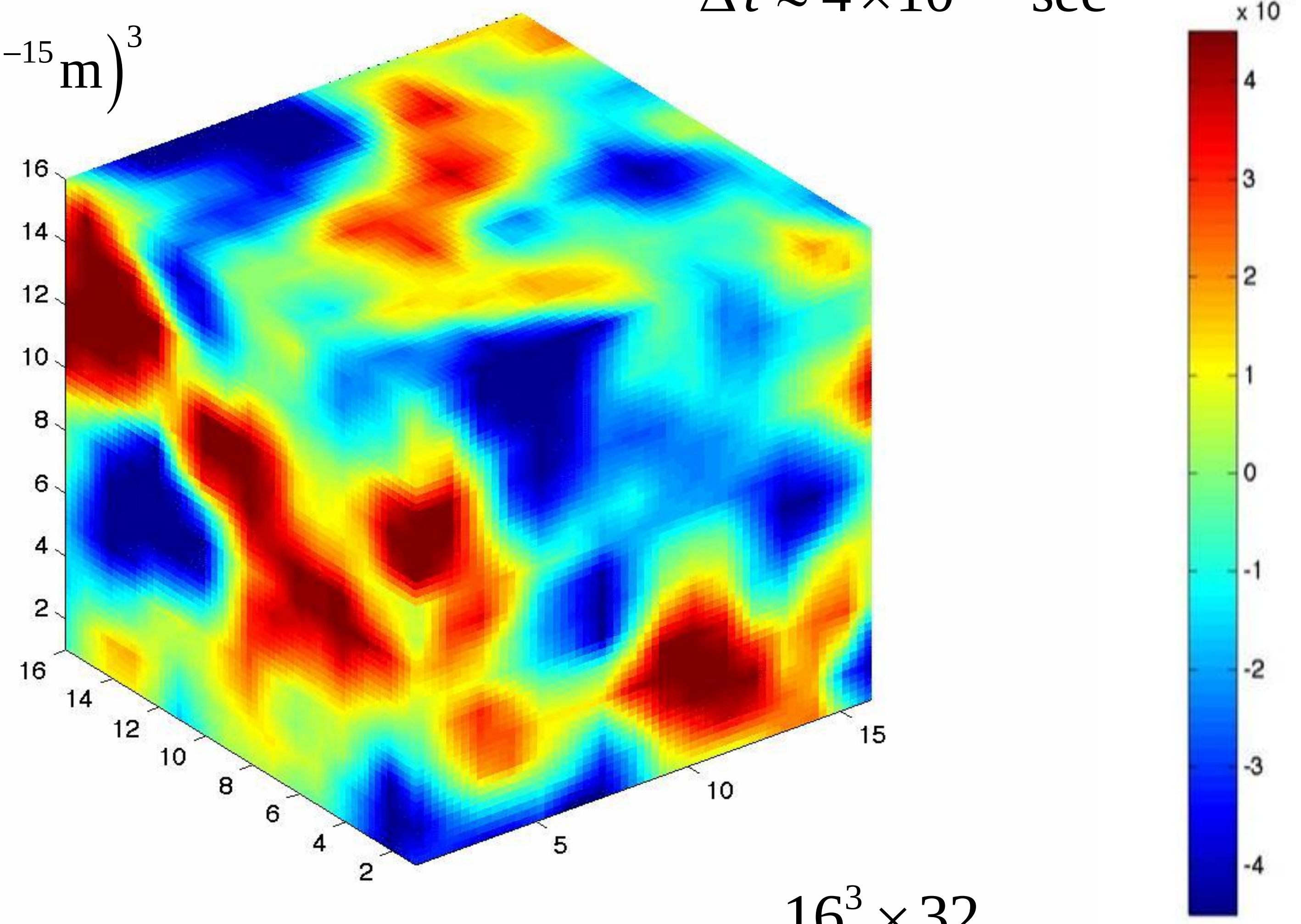
- It is important to determine the topological charge fluctuations in the QCD vacuum. One of the outstanding problems is to identify the vacuum fluctuations which are crucial to the mechanism of color confinement

Quantum fluctuations in the QCD vacuum

$\Delta x = a \approx 1.4 \times 10^{-16}\,\mathrm{m}$

$L^3 \approx \left(2.2 \times 10^{-15}\,\mathrm{m}\right)^3$

$\Delta t \approx 4 \times 10^{-24}$ sec



$Q_t = -1$

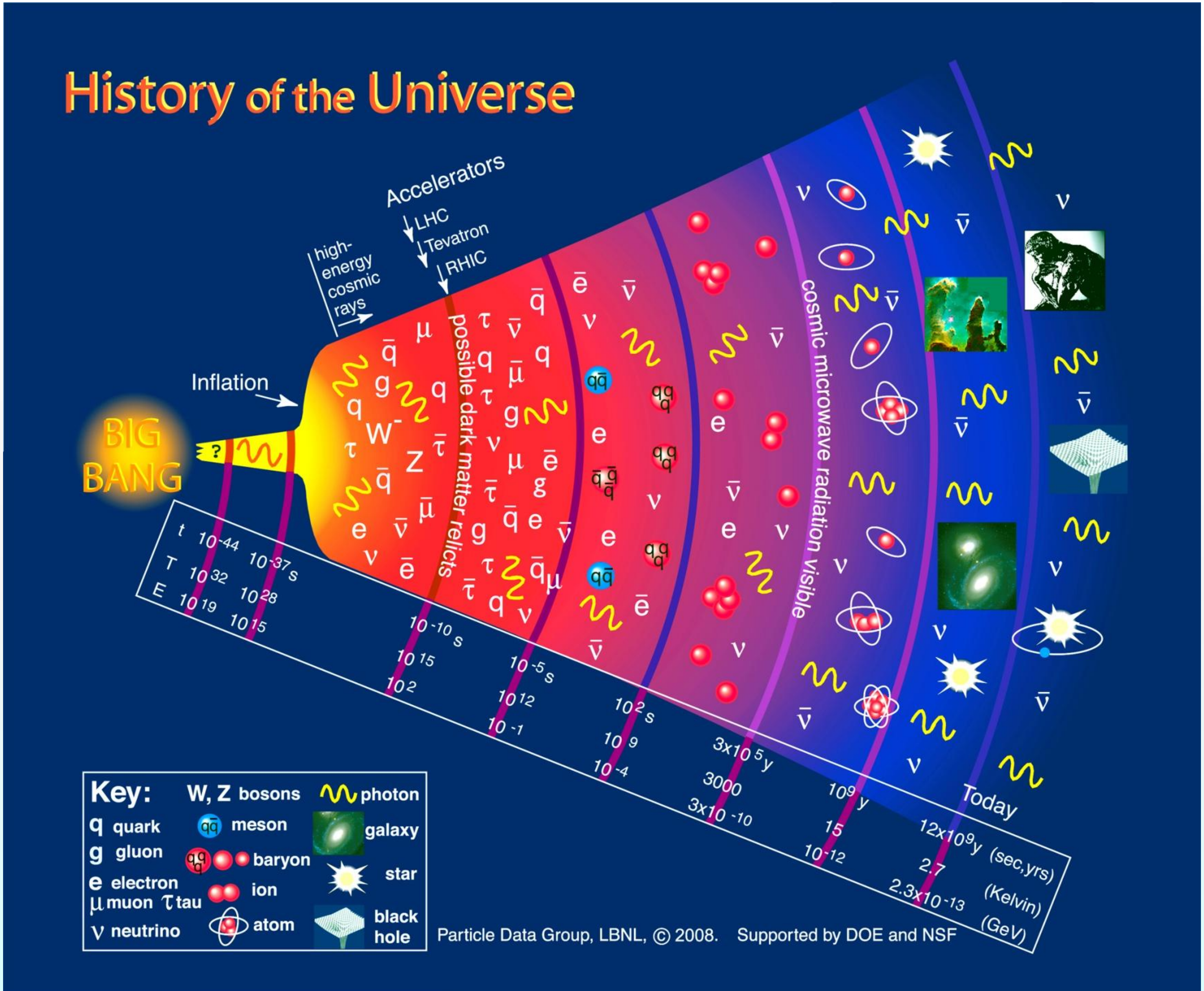
$16^3 \times 32$

Research Highlights (cont)

- **Finite Temperature QCD**

The nature of finite temperature phase transition in QCD is relevant to the evolution of the early universe from the **quark-gluon plasma** to the **hadrons**.

However this issue has remained controversial for many years. The Wuppertal group finds the deconfining transition [170(7) MeV] and the chiral transition [146(5) MeV] are at widely separated temperatures. On the other hand,the Brookhaven/Bielefeld collaboration claims that both temperatures coincide at 196(3) MeV. Since both groups used the staggered fermion, it is vital to resolve this issue in the framework of lattice QCD with exact chiral symmetry. We are in a good position to resolve this problem.


History of the Universe
Accelerators
LHC
Tevatron
RHIC
high-energy cosmic rays
Inflation
BIG BANG
possible dark matter relicts
cosmic microwave radiation visible
t 10^-44 10^-37 s
T 10^32 10^28
E 10^19 10^15
10^-10 s
10^15
10^2
10^-5 s
10^12
10^-1
10^2 s
10^9
10^-4
3x10^5 y
3000
3x10^-10
10^9 y
15
10^-12
Today
12x10^9 y (sec,yrs)
2.7 (Kelvin)
2.3x10^-13 (GeV)
Key:
W, Z bosons
photon
q quark
meson
galaxy
g gluon
baryon
star
e electron
ion
μ muon τ tau
black hole
ν neutrino
atom
Particle Data Group, LBNL, © 2008. Supported by DOE and NSF

Big Bang Timeline

Time	Era	Temperature	Characteristics of the Universe
0 to 10^{-43} s	Big Bang	infinite	infinitely small, infinitely dense Primeval fireball 1 force in nature - Supergravity
10^{-43} s	Planck Time	10^{32} K	Earliest known time that can be described by modern physics 2 forces in nature, gravity, GUT
10^{-35} s	End of GUT	10^{27} K	3 forces in nature, gravity, strong nuclear, electroweak Quarks and leptons form (along with their anti-particles)
10^{-35} to 10^{-33} s	Inflation	10^{27} K	Size of the Universe drastically increased, by factor of $10^{30}$to 10^{40}
10^{-12} s	**End of unified forces**	**10^{15} K**	**4 fundamental forces in nature, protons and neutrons start forming from quarks**
10^{-7} s	Heavy Particle	10^{14} K	proton, neutron production in full swing
10^{-4} s	Light particle	10^{12} K	electrons and positrons form
100 s (a few minutes)	Nucleosynthesis era	10^{9} - 10^{7} K	helium, deuterium, and a few other elements form
380,000 years	Recombination (Decoupling)	3000 K	Matter and radiation seperate End of radiation domination, start of matter domination of the Universe
500 million yrs	Galaxy formation	10 K	galaxies and other large structures form in the universe
14 billion years or so	Now	3 K	You are reading this table, that's what's happening.

Conclusion and Outlook

- GPU has emerged as a revolutionary device for lattice QCD as well as any computational science. It is crucial to TWQCD's dynamical DWF project.

- Currently, there are many lattice QCD groups around the world building large GPU clusters dedicated to QCD. This will have significant impacts to lattice QCD, leading to new discoveries in the strong interaction physics.