**Lattice Field Theory Core Algorithms**

The core algorithms are:

1. Sparse matrix solvers for the quark propagating in a "turbulent" chromo-electromagnetic background field.
2. Symplectic integrators for the Hamiltonian evolution to produce an stochastic ensemble of these fields.

**Hamiltonian Integrators**

The Force Gradient integrator is an optimized 4th order multi-time step algorithm for Hybrid Monte Carlo (HMC) sampling of the gauge field ensemble. The error in the true Hamiltonian plotted as function of step size demonstrates its superiority for light quark masses[3].

**GPU Testbed and Future Directions**

The exascale era promises to dramatically expand the ability of lattice field theory to investigate the multiple scales in nuclear physics, the quark-gluon plasma as well as possible dynamics beyond the standard model. Increasingly complex scale-aware QCD algorithms are a challenge to software engineering and the co-design of heterogeneous architectures to support them. At present the multi-GPU cluster offers a useful preview of the challenge at the level of 100’s of cores per node with a relatively low bandwidth interconnect.

Development of new algorithms to meet this challenging architecture include communication reduction by (Schwarz) domain decomposition, multi-precision arithmetic, data compression and on the fly local reconstruction. The QUDA library[4] developed at Boston University is being used as a software platform for these early investigation.

---

**Multi-scale Challenge**

Current state of the art QCD algorithms exploit the simplicity of a uniform space-time hypercubic lattice grid mapped onto a homogenous target architecture to achieve nearly ideal scaling. Nonetheless, this single grid paradigm is very likely to be modified substantially at extreme scales. Neither the lattice physics nor computer hardware are intrinsically single scaled.

For example in QCD, uniquely non-perturbative quantum effects spontaneously break conformal and chiral symmetry giving rise to a ratio of length scales: \( m_{\text{proton}}/m_q \approx 7 \), which only recent advances in simulation are just beginning to fully resolve. As a consequence the most efficient Dirac solvers are just now becoming multi-scaled as well. Future advances will reveal more opportunities for multi-scale algorithms.

**Adaptive Multigrid Inverter**

Adaptive multigrid automatically discovers the near null space to construct the coarse grid operator. Applied to the Wilson-clover Dirac inverter on \( 32^3 \times 256 \) lattice, it outperforms single grid methods by 20x at the lightest quark mass[2]. Extensions of adaptive multigrid are under development for Domain Wall and Staggered fermions as well as to Hamiltonian evolution for lattice ensembles.

**Visualization[1] of the scales in a gluonic ensemble**

\( a(lattice) \ll \frac{1}{m_{\text{proton}}} \ll \frac{1}{m_q} \ll L \) (box)

**Heterogeneous Computer Architectures**

At the same time hardware suited to exascale performance is expected to become increasingly heterogeneous with O(1000) cores per node, coupled to hierarchical networks -- the GPU cluster being an early precursor of this trend. As a test of concept the Wilson multigrid inverter combined with GPU technology is estimated to reduce the cost per Dirac solve by O (100).

---

AAA Technology Challenge

Application (QCD & Graphene Quantum Fields)

Algorithms (Multigrid)

Architecture (GPU computing)
Outline

I. Physics (Nature)
   – Physics of QCD and Beyond SM, Higgs,..
   – Graphene is lattice field theory!

II. Math (Algorithms)
   – Scales and Multigrid inverters
   – (Ax = b Not F.E. not Stored)
   – MD: Muti-time step time sym Symplectic Integrators

III. Computer (Architecture)
   – GPUs and Heterogeneous computing
   – Multi-precision and data compression
Word from our NSF/DOE sponsors!

- NSF PetaApp project on Multi-grid QCD (Brower & Rebbi + PSU + Colorado)
- NSF Experimental GPU cluster for fund Phys. (Brower, Barba, Rebbi)
- DOE SciDAC QCD software co-ordinator (Brower et al)
- DOE INCITE and NSF TeraGrid time BG/L-P-Q, Cray XT#, et al. (USQCD)
- NSF project to combine MG+GPU (BU+Harvard)
Many different people (TOPS, QCD) and institutions involved in the collaboration

- CU Boulder
  - Tom Manteuffel
  - Steve McCormick
  - Marian Brezina
  - John Ruge
  - James Brannick
  - Christian Ketelsen
  - Scott MacLachlan
- Lawrence Livermore
  - Rob Falgout
- Columbia
  - David Keyes
- Boston University
  - Rich Brower
  - Claudio Rebbi
  - Mike Clark
  - James Osborn
- Harvard U
  - Mike Clark
- Penn State
  - James Brannick
  - Ludmil Zikatanov
- Tufts
  - Scott MacLachlan
- Argonne
  - James Osborn
Many co-authors of slide!

James Brannick, Ron Babich, Mike Clark, Saul Cohen, James Osborn, Claudio Rebbi et al
Does NATURE abhor a fundamental SCALAR?

I. **NO:** Only a scalar Higgs

II. **SORT OF:** Give the Higgs a “super partner”

III. **YES:** Build at Higgs from Heavy techni-Quarks!

---

*Spin = 0 & 1/2*
Problem: Theorists have propose a myriad of models for TeV physics, often dependent on *heuristics* for non-perturbative effects in gauge theories.

Triage is needed!

Experimental data is needed!

Lattice field theory can help to
  - narrow the options &
  - make prediction for specific models.
Library and Tool Dependencies

- QCD SciDAC API for Chroma/CPS/MILC applications
- Level 3: Highly Optimized Dirac inverter, other critical kernels
- Level 2: Data Parallel Interface & IO library
- Level 1: Single core linear algebra, message passing, and threading libraries.
- Specialized code generators, workflow et al

Parallelism and Existing Implementation

Weak scaling for Wilson Fermions on the BG/L (2006 Gordon Bell award) and for Asqtad on the BG/P, both up to 131,072 cores.

ALCF Early Science Program
### Participants in Lattice Field Theory Software Development

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* **Software Committee: Participants funded in part by SciDAC-1 & 2**

ALCF Early Science Program
Part I  Application: Quantum Field Theory
New Forces for Subatomic Particles

Atoms: Maxwell
\(N=1\) (charge)

Nuclei: Weak
\(N=2\) (Isospin)

Sub nuclear: Strong
\(N=3\) (Color)

Standard Model: \(U(1) \times SU(2) \times SU(3)\)
4 Fundamental Forces

QED          Weak                  Strong (QCD)                  Gravity (?)

Charges: N = 1   2   3   ....

All is Maxwell-Like Theories, except Gravity!
4 Maxwell Equations
100 Years Ago

- **Maxwell (E&M)**
  \[ \nabla \cdot \mathbf{E} = \rho, \quad \nabla \cdot \mathbf{B} = 0, \\
  \nabla \times \mathbf{E} = \mathbf{J}, \quad \nabla \times \mathbf{B} = 0 \]

- **Relativity + Quantum Mechanics**

  Units: \( c = \hbar = 1 \) so \( m = E = p = 1/x = 1/t \)

- **Potential:** \( E = - \frac{e^2}{r} \) \( \quad e^2/4 \pi \approx 1/137 \)

- **No Mass scale** \( x \rightarrow \lambda x \)
Really only One!

Maxwell’s Equ: $\partial_\mu F_{\mu\nu} = J_\nu$
The Theory of the strong nuclear force is Quantum Chromodynamics

Classical Electricity and Magnetism

Quantum Electrodynamics

3 "color" charges
- quarks
- antiquarks

QCD
- quark
- antiquark
- gluon

Quantum Chromodynamics

\[ S_{QCD} = \frac{1}{g^2} \int d^4x \{ Tr[F_{\mu\nu}(x)F^{\mu\nu}(x)] + \bar{\psi}(x)[\gamma_{\mu}\partial_{\mu} + \gamma_{\mu}A_{\mu}(x) + m] \psi(x) \} \]
Asymptotic Freedom: Minus sign

Dielectric Effect: “In good old Electrodynamics (or water)
Charged pairs polarize to reduce the effective charge

QED screening

Electron – Position Pairs in Vacuum
But QCD has charged Quarks and Gluons

Quark-Antiquarks polarize just like $e^+ - e^-$ pairs

“But Gluon Act with Opposite Sign!”

QCD (anti-)screening

\[
\frac{1}{g_{\text{eff}}^2} \approx \left[ \frac{11N}{6} - \frac{n_f}{3} \right] \times \log\left( \frac{1}{M \Delta X} \right)
\]
Instantons, Topological Zero Modes (Atiyah-Singer index) and Confinement length $l_\sigma$
Where does MASS come from?

- **QED**
- **Weak**
- **QCD**
- **Gravity**

All Maxwell Like theories have no apparent mass scale: Higgs instability cause some Masses by fakery:

Masses of Proton/Neutrons come here via a quantum anomaly

\[
M_{\text{plack}} = G^{-1/2} = 1.301 \times 10^{19} \text{ m}_{\text{proton}}
\]

\[
= 1.22 \times 10^{19}\text{GeV}
\]

Mass scale but it is huge ➔ 21.767 microgram!
Running Coupling Unification

\[ M_{\text{planck}} = 10^{19} \]
Part I

• Putting Multi-fermion Field Theory on that Lattice. (LFT algorithms)

• QCD

• Graphene

(All h bar physics: Super conductivity etc.)
3-d Maxwell: $B(x_1, x_2, x_3)$

Replace

$$\vec{\nabla} \cdot \vec{B} = 0 \quad \text{and} \quad \vec{\nabla} \times \vec{B} = \vec{J}$$

$$\vec{B} = \vec{\nabla} \times \vec{A} \quad \text{and} \quad -\vec{\nabla}^2 \vec{A} + \vec{\nabla}(\vec{\nabla} \cdot \vec{A}) = \vec{J}$$

Should use anti-symmetric tensor:

$$F_{ij} = \begin{bmatrix}
0 & B_3 & -B_2 \\
-B_3 & 0 & B_1 \\
B_2 & -B_1 & 0
\end{bmatrix} = \frac{\partial}{\partial x_i} A_j(x_1, x_2, x_3) - \frac{\partial}{\partial x_j} A_i(x_1, x_2, x_3)$$

Note: $d(d-1)/2 = d$ for $d = 3$

Only case where anti-sym $d \times d$ matrices looks like a (pseudo) vector
4-d Maxwell\(^\dagger\): \(E(x_0, x_1, x_2, x_4) \& B(x_0, x_1, x_2, x_3)\)

\[
F_{\mu\nu} = \begin{bmatrix}
0 & E_1 & E_2 & E_3 \\
-E_1 & 0 & B_3 & -B_2 \\
-E_2 & -B_3 & 0 & B_1 \\
-E_3 & B_2 & -B_1 & 0
\end{bmatrix} = \frac{\partial}{\partial x_\mu} A_\nu(x) - \frac{\partial}{\partial x_\nu} A_\mu(x)
\]

or \(F_{\mu\nu} = i \left[ \frac{\partial}{\partial x_\mu} - iA_\mu(x) , \frac{\partial}{\partial x_\nu} - iA_\nu(x) \right] \)

**Lagrangian Density:**

\[
\frac{1}{4} \sum_{\mu,\nu} F_{\mu\nu} F^{\mu\nu} = \frac{1}{2} (E^2 - B^2) = \frac{1}{2} \partial_\mu \vec{A} \cdot \partial_\nu \vec{A} - \frac{1}{2} (\vec{\nabla} \times \vec{A})^2
\]

\(^\dagger\) Now \(d(d-1)/2 = 4*3/2 = 6\) elements!
Lesson: Symmetries are Critical

- **Gauge Invariance:**
  - Finite elements doesn’t work
- **Euclidean O(4) “Lorentz” group**
  - The H4 subgroup of Hypercubic grid is nice
- **Almost conformal sym O(4,1)**
  - Asymptotic freedom and relevant terms
- **Zero mass Fermions have chiral sym**
  - Solutions: **Good, Bad and the Ugly**
QCD is Maxwell on SU(3) lattice

Finite difference:

\[
\frac{\partial \phi(x)}{\partial x_\mu} \rightarrow \Delta_\mu \phi(x) = \frac{\phi(x + a\mu) - \phi(x)}{a}
\]

With Gauge field replace:

\[
\Delta_\mu \phi(x) = \frac{e^{i \int_{x+\alpha_\mu}^x A_\mu \, dx_\mu} \phi(x + a\mu) - \phi(x)}{a}
\]

The new factor is **covariant constant**.

This is the Lattice Guage link: \( U(x, x + a\mu) = e^{i a A_\mu(x)} \)

\[
= e^{i a A_\mu(x)} e^{i a A_\mu(x)} e^{-i a A_\mu(x)} e^{-i a A_\mu(x)} \\
\sim e^{i a^2 (\nabla_\nu A_\mu(x) - \nabla_\mu A_\nu(x) - A_\mu(x + \nu) + i[A_\mu(x), A_\nu(x)])}
\]
QCD on the Lattice: Base/Sparse vs Fiber/Dense
QCD: Theory of Nuclear Force

Partition function

\[ \int d\bar{\Psi}(x)d\Psi(x)dA_\mu(x) \]  [Probability Density]

\[ \int d\bar{\Psi}(x)d\Psi(x)dA_\mu(x) \quad \exp[-\int d^4x \bar{\Psi}D\Psi - \frac{1}{g^2} \int d^4xF^2] \]

\[ \int dA_\mu(x) \quad Det[D] \quad \exp[-\frac{1}{g^2} \int d^4xF^2] \]
QCD Lattice Measurement

\[ \int dU_\mu d\bar{\Psi} d\Psi \left[ \Psi(x)^3 \bar{\Psi}(z)\gamma_\mu \Psi(x) \bar{\Psi}(y)^3 \right] e^{-S} = \]

\[ \int dU_\mu \ Det[D] \left[ D^{-1}(x, y)D^{-1}(x, y) D^{-1}(x, z)\gamma_\mu D^{-1}(z, y) \right] e^{-S} + \]

\[ \int dU_\mu \ Det[D] \left[ D^{-1}(x, y)D^{-1}(x, y)D^{-1}(x, y) Tr[\gamma_\mu D^{-1}(z, z) \right] e^{-S} \]
Computational Approach, Numerical Methods

\[ \text{Prob}[U, \phi] = Z^{-1} e^{\beta \text{Tr}[U_{\text{glue}} + U_{\text{glue}}^\dagger]} + \bar{\phi}(D_{\text{quark}} \dagger D_{\text{quark}})^{-1}\phi \]

- **Monte Carlo importance sampling of gauge configurations:**
  - Generate Quark Gluon background ensemble in Probability:

- **Hybrid Monte Carlo:**
  - Molecular Dynamics Algorithm:
    - Multi-time step Hamiltonian evolution in “potential”: - Log(Probability).

- Repeated solution of Dirac equation
  - (large sparse linear system) at each step

\[ D_{\text{quark}} = m_q + \frac{1 - \gamma_\mu}{2} U(x, x + \mu) + \frac{1 + \gamma_\mu}{2} U(x + \mu, x) \]
Graphene is 2+1 dimension Carbon sheet with Dirac fields: But lattice is real Hexagonal structure. Couple to coulomb potential and phones act like gauge fields! Ideal for Lattice field theory, MG and GPU! (Brower, Rebbi and Schaich)
Isolating A Single Crystal of Graphene


Andre Geim
Kostya Novoselov

Nobel Prize Physics 2010

“For groundbreaking experiments regarding the two-dimensional material graphene”
Geim’s Graphene Superlatives

Thinnest imaginable material
Largest surface area (~3,000 m² per gram)
Strongest material ‘ever measured’ (theoretical limit)
Stiffest known material (stiffer than diamond)
Most stretchable crystal (up to 20% elastically)
Record thermal conductivity (outperforming diamond)

Highest current density at room $T$ (1,000s times of Cu)
Completely impermeable (even He atoms cannot squeeze through)
Highest intrinsic mobility (100 times more than in Si)
Conducts electricity in the limit of no electrons
Lightest charge carriers (zero rest mass)
Longest mean free path at room $T$ (micron range)
sp$^2$ is a Unique Bonding Geometry

**Carbon:** \([1s^2] 2s^2 \, 2p^2\)

- \(p_z\) orbital
- Planar

**Silicon:** \([1s^2 \, 2s^2 \, 2p^6] 3s^2 \, 3p^2\)

- \(sp^3\) orbitals
- Tetrahedral

---

$sp^2$ Bonding Leads to Novel Carbon Structures

Geim and Novoselov Nat. Matr. 6, 183 (2007)
Graphene Bandstructure

Reciprocal Space

\[ \text{constructive interference} \]

\[ \text{destructive interference} \]

\[ E(\vec{k}) = + |t| \]

\[ E(\vec{k}) = - |t| \]

P. R. Wallace, Phys. Rev. 71, 622 (1947)
Graphene: Electronic Structure

Two Atoms (bonding)

\[ \Psi_A \xrightarrow{t} \Psi_B \]

\[ E_0 = 0 \quad E_{\text{bonding}} = -|t| \quad E_{\text{anti-bonding}} = +|t| \]

\[ \hat{H}\Psi = \begin{pmatrix} 0 & t \\ t^* & 0 \end{pmatrix} \begin{pmatrix} \Psi_A \\ \Psi_B \end{pmatrix} \]

\[ E = \pm |t| \]

Two Sub-lattices of Graphene

\[ t_1 = t_0 e^{i\theta_1}, \quad t_2 = t_0 e^{i\theta_2}, \quad t_3 = t_0 e^{i\theta_3} \]

\[ \hat{H}\Psi = \begin{pmatrix} 0 & t \\ t^* & 0 \end{pmatrix} \begin{pmatrix} \Psi_A \\ \Psi_B \end{pmatrix} \]

\[ E = \pm |t| \]

\[ = \pm |t_0| \cdot (e^{i\theta_1} + e^{i\theta_2} + e^{i\theta_3}) \]
The Hamiltonian

\[ H = \sum_{\langle x, y \rangle, s} \kappa (a^\dagger_{x,s} a_{y,s} + \text{h.c.}) + e^2 \sum_{x,y} V_{x,y} q(x) q(y) \]

where \( \langle x, y \rangle \) stands for nearest neighbors and

\[ q(x) = a^\dagger_{x,\uparrow} a_{x,\uparrow} + a^\dagger_{x,\downarrow} a_{x,\downarrow} - 1 \]

The \(-1\) stands for the charge of the nucleus and insures neutrality at half filling. We demand that \( V \) be positive definite. (Both will be important for the MC formulation.)
Finite T Graphene = 3d Lattice Gauge Theory!

- Finite Temp \( \frac{1}{kT} = \beta \rightarrow it/\hbar \)
  - \( \exp[ - H/T] \rightarrow \) Path Integral for \( \exp[ - S/\hbar] \)
- Staggering in “time” give spin
  - NO sign problem!
- Real spatial lattice with DW fermion at edge
- FFT on Hexagonal lattice
  - (2 triangular Bravais lattices)
- Phonons are Gauge fields
  - Perfect for MG and GPUs
- etc.
Part II Algorithms for Multiscale

• Fundamental problem is to construct a solver for a elliptic partial derivative operators!