Intersection:
Quarks + multi-grid + GPUs

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Algorithms for Lattice Field Theory at Extreme Scales

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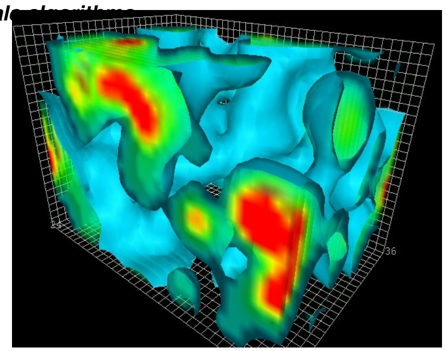
Multi-scale Challenge

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: $m_{proton}/m_{\pi} = 7$, which only recent advances in simulation are just beginning to fully resolve. As a consequence the most efficient Dirac solvers are just now becoming mult-scaled as well. Future advances will reveal more opportunities for multi-scale algorithms.



Visualization[1] of the scales in a gluonic ensemble
a(lattice) $\ll 1/m_{proton} \ll 1/m_{\pi} \ll L$ (box)

Heterogeneous Computer Architectures

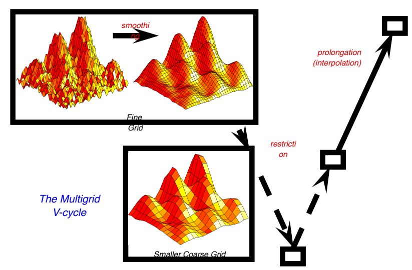
At the same time hardware suited to exascale performance is expected to become increasingly heterogeneous with O(1000) cores per node, coupled to hierarchical networks -- the GPU cluster being an early precursor of this trend. As a test of concept the Wilson multigrid inverter combined with GPU technology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

Lattice Field Theory Core Algorithms

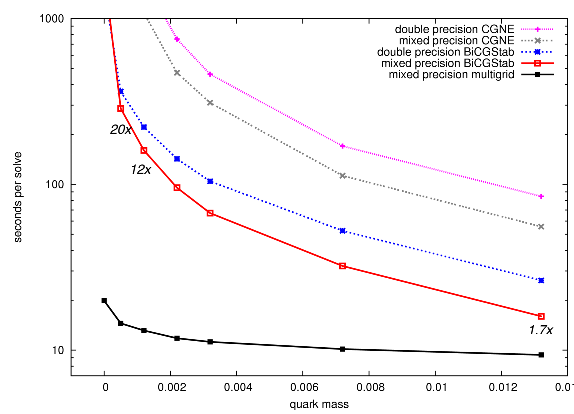
The core algorithms are

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.***

Adaptive Multigrid Inverter

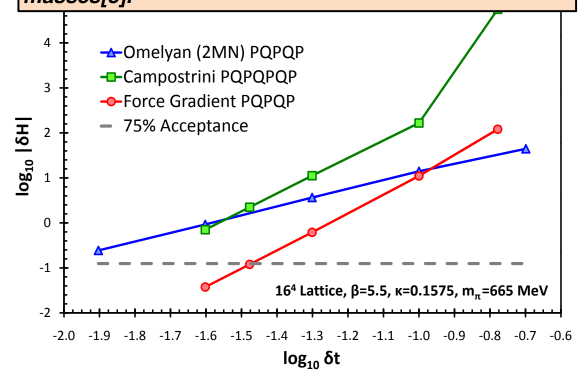


Adaptive multigrid automatically discovers the near null space to construct the coarse grid operator. Applied to the Wilson-clover Dirac inverter on 32^3x256 lattice, it outperforms single grid methods by 20x at the lightest quark mass[2]. Extensions of adaptive multigrid are under development for Domain Wall and Staggered fermions as well as to Hamiltonian evolution for lattice ensembles



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].

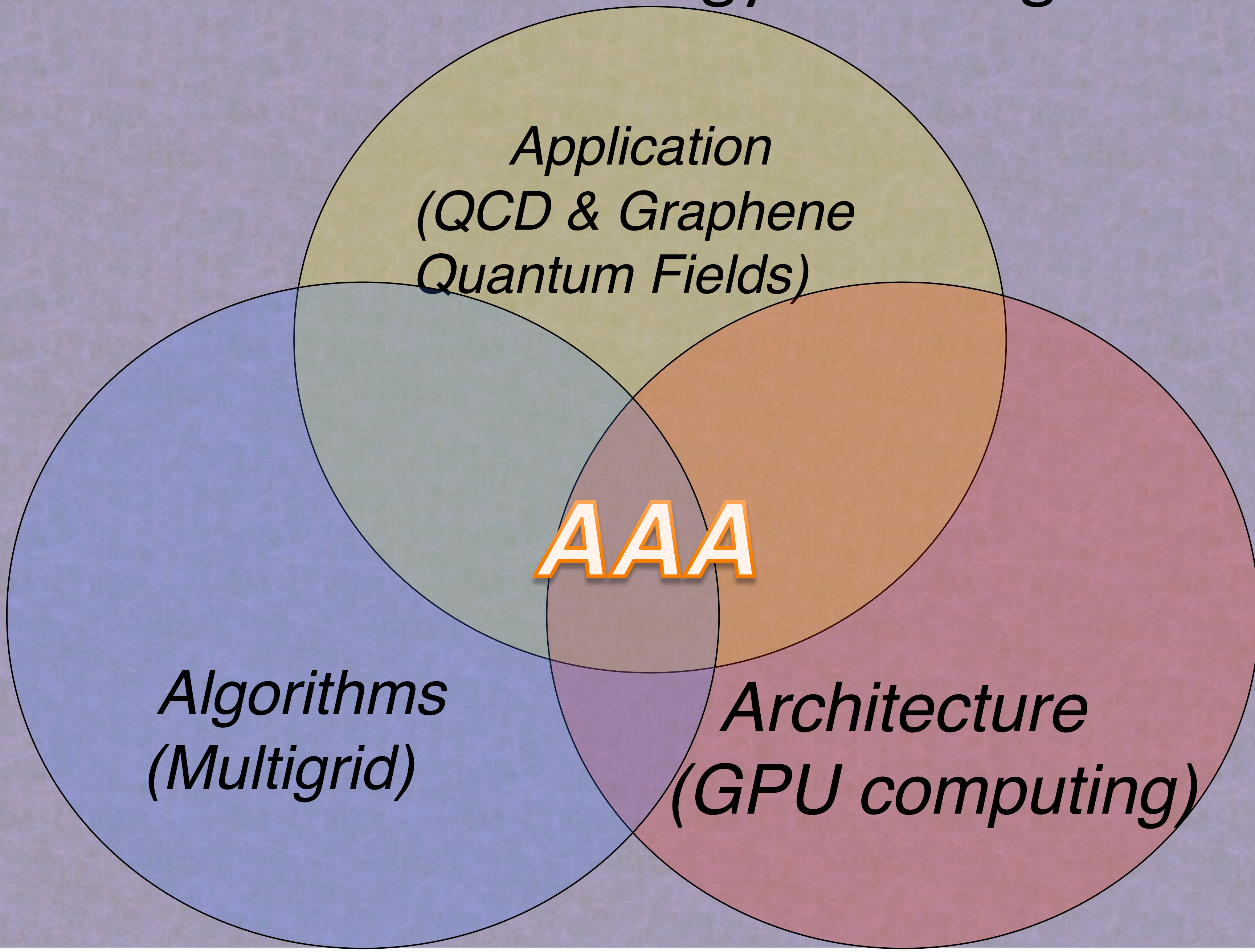


GPU Testbed and Future Directions

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.

[1] Dereck Leinweber, http://www.physics.adelaide.e

AAA Technology Challenge



Outline

I. Physics (Nature)

- Physics of QCD and Beyond SM, Higgs,..
- Graphene is lattice field theoy!

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)

MGQCD Applied Math/Physics Collaboration!

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
- Penn State
  - James Brannick
  - Ludmil Zikatanov
- Tufts
  - Scott MacLachlan
- Argonne
  - James Osborn

Harvard U

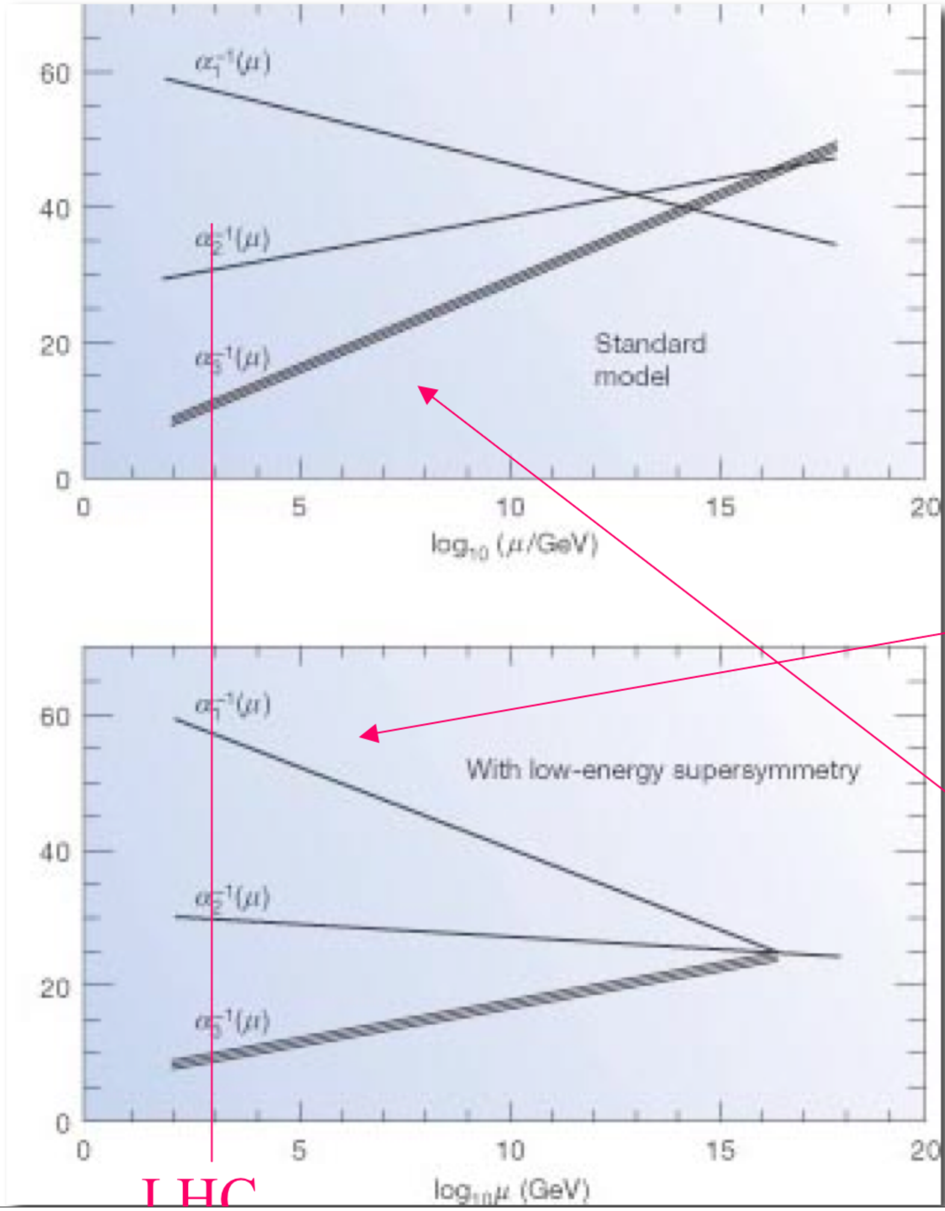
Mike Clark

Many co-authors of slide!

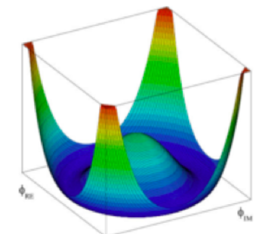
James Brannick, Ron Babich, Mike Clark, Saul Cohen, James Osborn, Claudio Rebbi et al

Part I: QCD: Exploring Quarks and Beyond

Does NATURE abhor a fundamental SCALAR ?



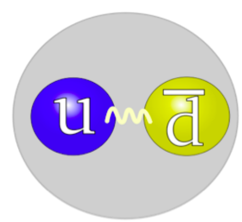
I. NO: Only a scalar Higgs



II. SORT OF: Give the Higgs a "super partner"

Spin=0&1/2

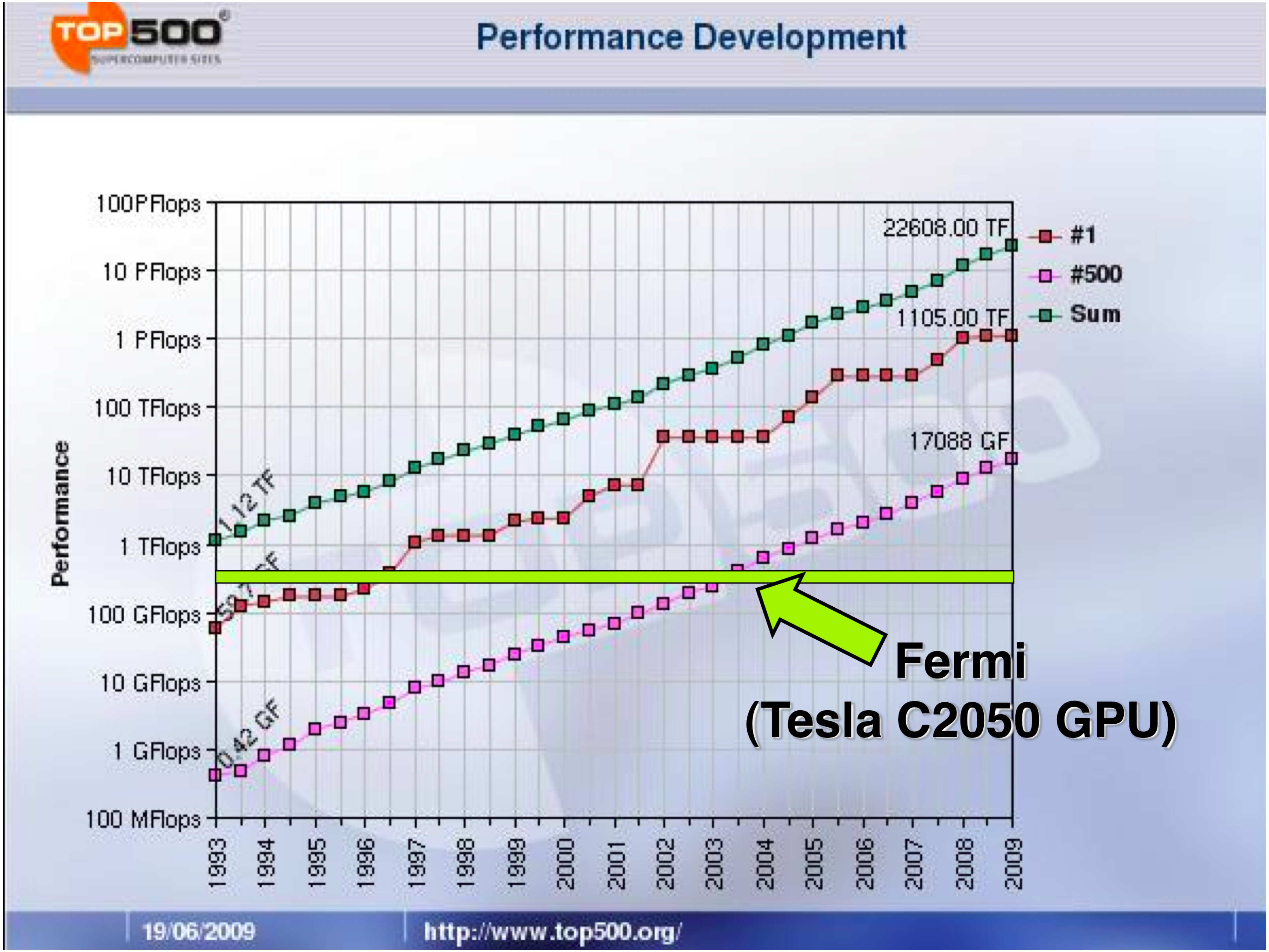
III. YES: Build at Higgs from Heavy techni-Quarks!



Problem: Theorists have propose a myriad of models for TeV physics, often dependent on *heuristics* for non-perturbative effects in gauge theories

Lattice field theory can help to

- narrow the options &
- make prediction for specific models.


TOP500
SUPERCOMPUTER SITES
Performance Development
Performance
100 PFlops
10 PFlops
1 PFlops
100 TFlops
10 TFlops
1 TFlops
100 GFlops
10 GFlops
1 GFlops
100 MFlops
1993
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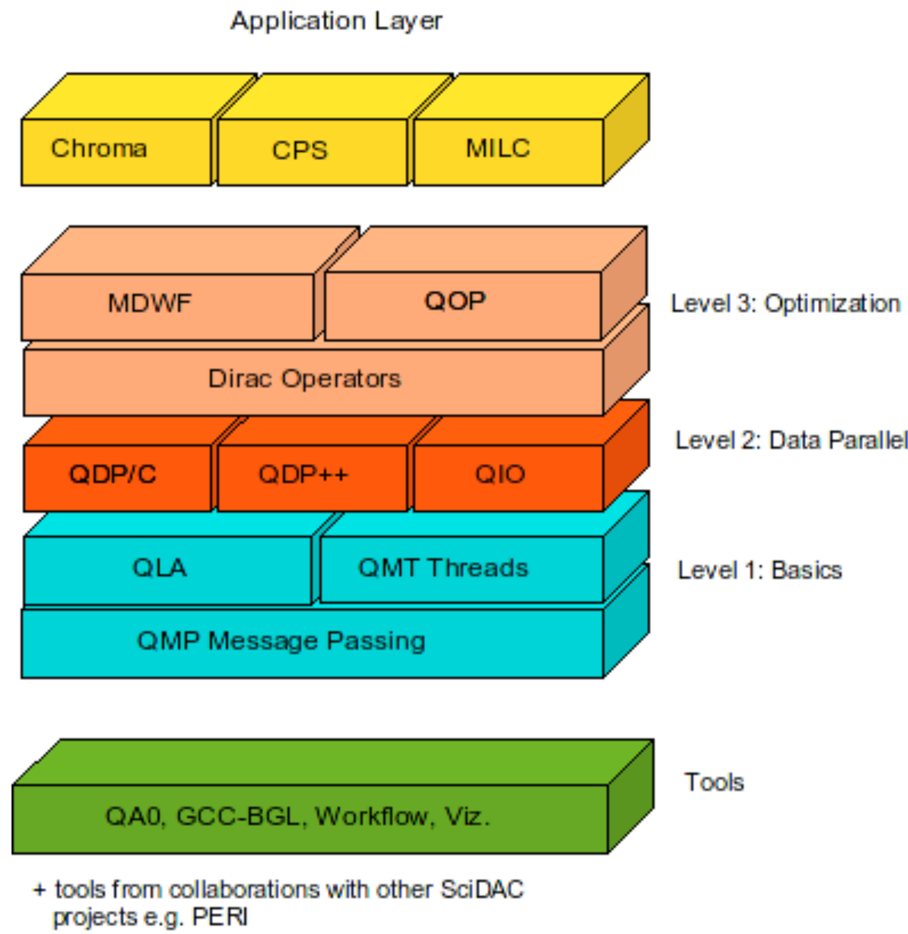
2001
2002
2003
2004
2005
2006
2007
2008
2009
22608.00 TF
1105.00 TF
17088 GF
1.12 TF
0.42 GF
#1
#500
Sum
Fermi
(Tesla C2050 GPU)
19/06/2009
http://www.top500.org/

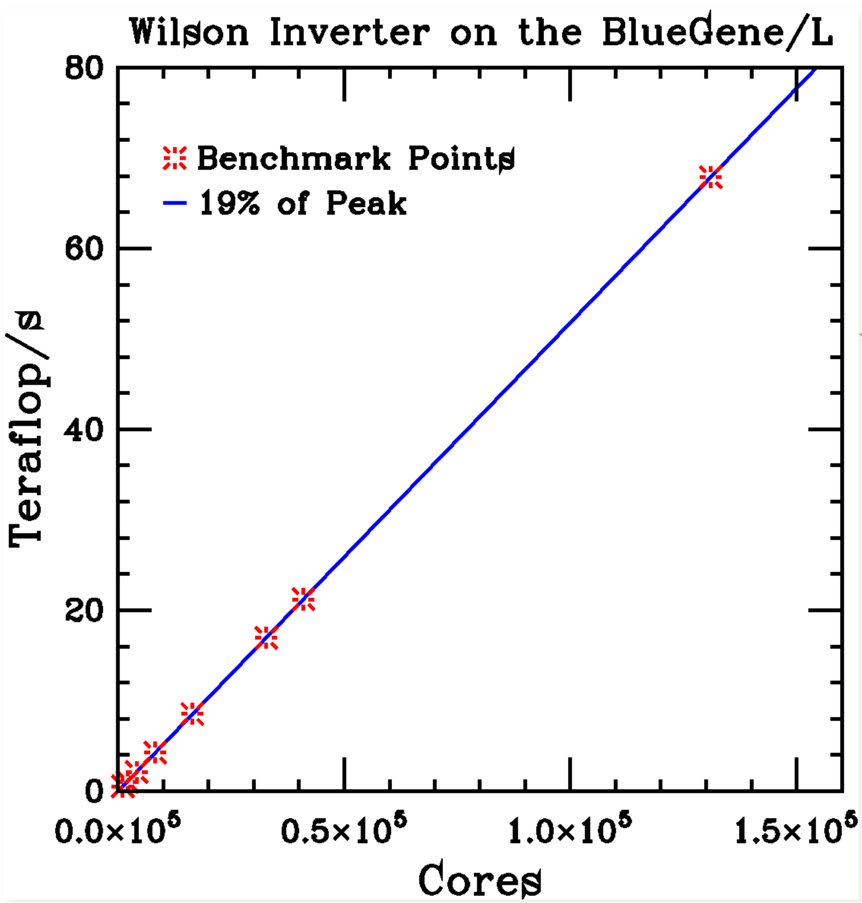
Library and Tool Dependencies

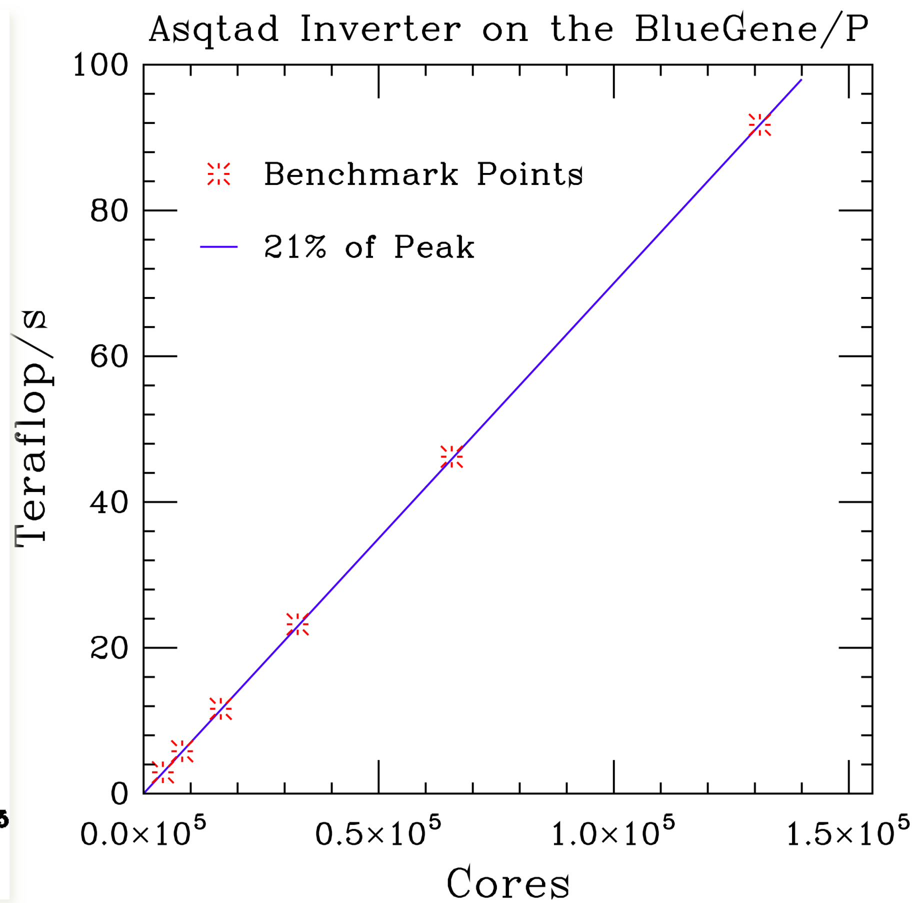
- QCD SciDAC API for Chroma/ CPS/MILC applications
- Level 3: Highly Optimized Dirac inverter, other critical kernels
- Level 2: Data Parallel Interface & IO library
- Level 1: Single core linear albebra, message passing, and threading libraries.
- Specialized code generators, workflow et al



Rich Brower SciDAC Software co-ordinator.

Parallelism and Existing Implementation





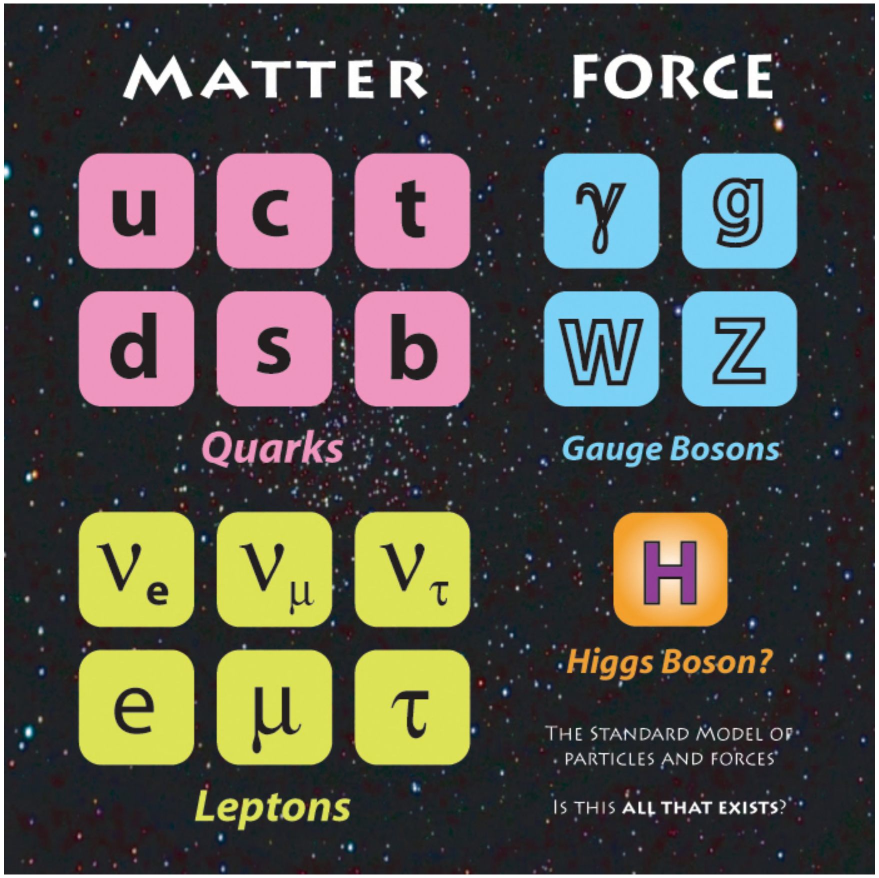
Weak scaling for Wilson Fermions on the BG/L (2006 Gordon Bell award) and for Asqtad on the BG/P, both up to 131,072 cores.

Participants in Lattice Field Theory Software Development

Arizona	Doug Toussaint	MIT	John Negele
	Alexei Bazavov		Andrew Pochinsky
BU	Rich Brower *	North Carolina	Rob Fowler*
	Ron Babich/Mike Clark		Pat Drayer
	James Osborn (ANL)	JLab	Chip Watson *
BNL	Chulwoo Jung		Robert Edwards *
	Oliver Witzel		Jie Chen
	Efstratios Efstathiadis		Balint Joo
Columbia	Bob Mawhinney *	IIT	Xien-He Sun
DePaul	Massimo DiPierro	Indiana	Steve Gottlieb
FNAL	Don Holmgren *		Subhasish Basak
	Jim Simone	Utah	Carleton DeTar *
	Jim Kowalkowski		Tommy Burch
	Amitoj Singh	Vanderbilt	Abhishek Dubey
LLNL	Pavlos Vranas*		Ted Bapty

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

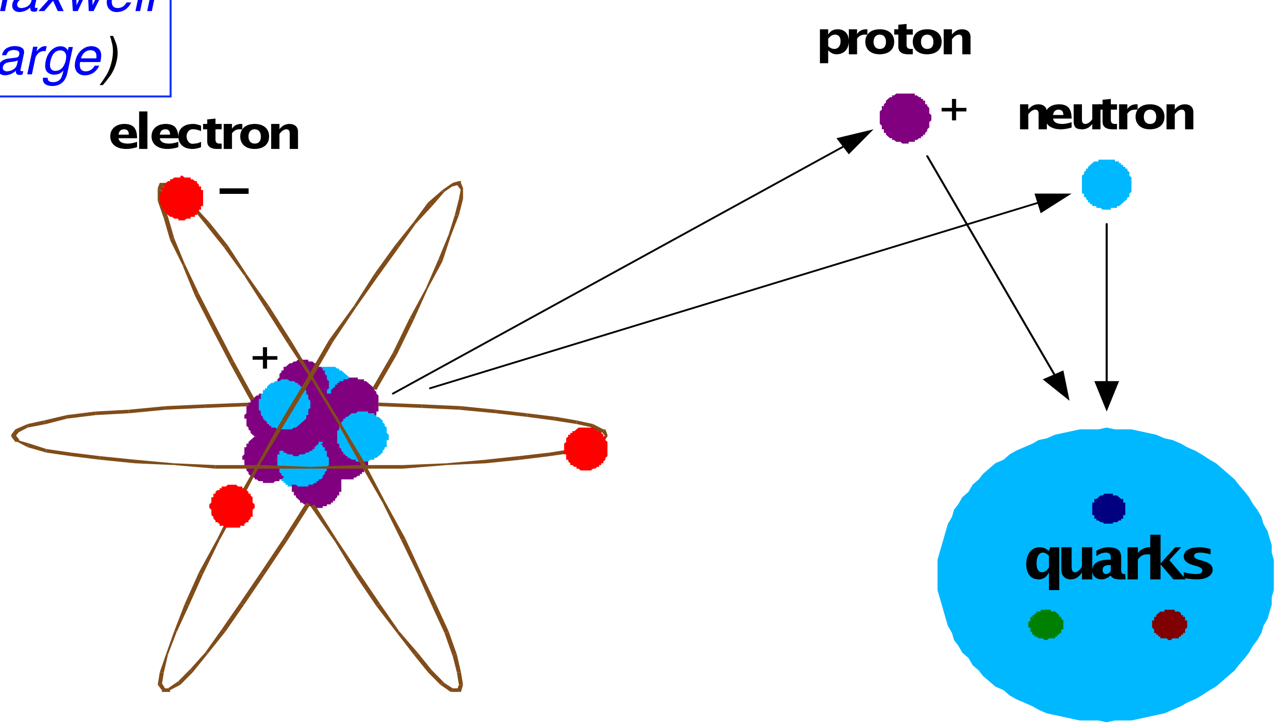
Part I Application: Quantum Field Theory



New Forces for Subatomic Particles

Nuclei: Weak
N=2 (Isospin)

Atoms: Maxwell
N=1(charge)



Standard Model: U(1) × SU(2) × SU(3)

Sub nuclear: Strong
N=3 (Color)

4 Fundamental Forces

QED *Weak* *Strong(QCD)* *Gravity (?)*

Charges: N = 1 *2* *3* *....* *∞*

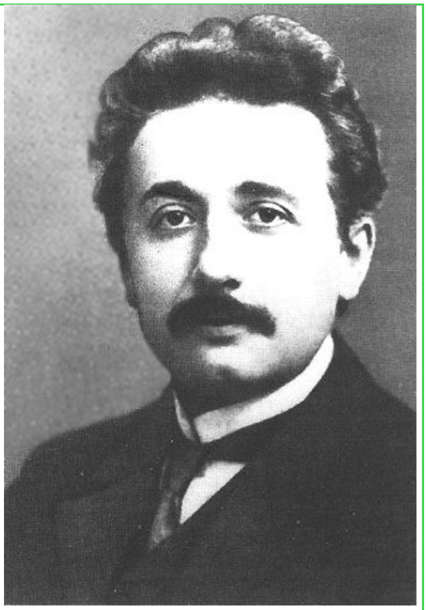
PROPERTIES OF THE INTERACTIONS

Property \ Interaction	Gravitational	Weak (Electroweak)	Electromagnetic (Electroweak)	Strong: Fundamental	Strong: Residual
Acts on:	Mass – Energy	Flavor	Electric Charge	Color Charge	See Residual Strong Interaction Note
Particles experiencing:	All	Quarks, Leptons	Electrically charged	Quarks, Gluons	Hadrons
Particles mediating:	Graviton (not yet observed)	W^+ W^- Z^0	γ	Gluons	Mesons
Strength relative to electromag for two u quarks at: 10^{-18} m	10^{-41}	0.8	1	25	Not applicable to quarks
Strength relative to electromag for two u quarks at: 3×10^{-17} m	10^{-41}	10^{-4}	1	60	
for two protons in nucleus	10^{-36}	10^{-7}	1	Not applicable to hadrons	20

All is Maxwell-Like Theories, except Gravity!

4 Maxwell Equations

100 Years Ago



- **Maxwell (E&M)**

$\nabla \cdot E = \rho, \quad \nabla \cdot B = 0,$

$\nabla \times E = J, \quad \nabla \times B = 0$

- Relativity + Quantum Mechanics

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

- Potential: $E = - e^2/r$ $\quad e^2/4\pi \simeq 1/137$

- No Mass scale $x \to \lambda x$

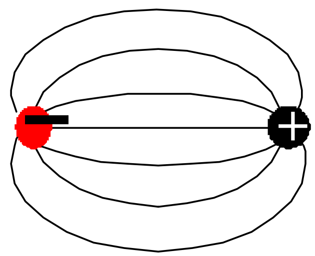
Really only One!

Maxwell's Equ: $\partial_\mu F_{\mu\nu} = J_\nu$

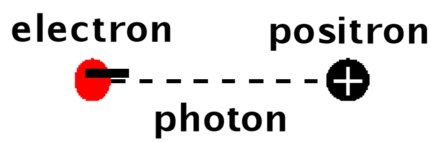
The Theory of the strong nuclear force

is Quantum Chromodynamics

Classical Electricity and Magnetism

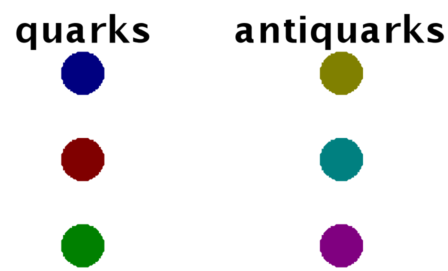


Quantum Electrodynamics

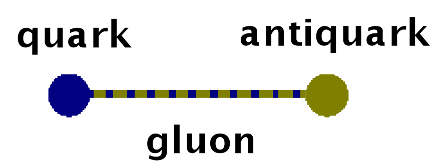


QED

3 “color” charges



QCD



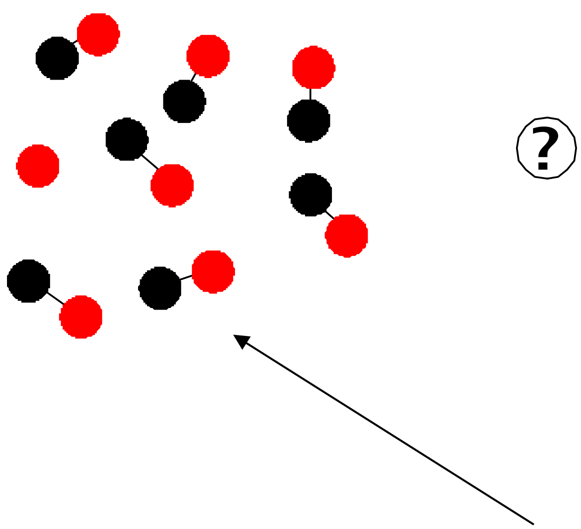
Quantum Chromodynamics

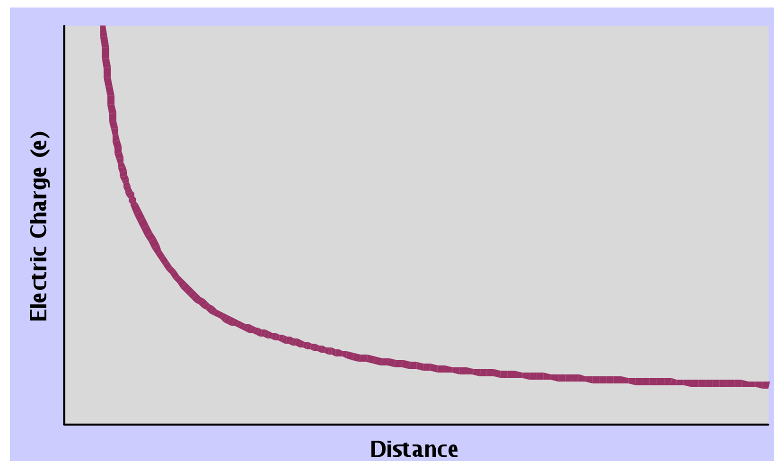
$$S_{QCD} = \frac{1}{g^2} \int d^4x \{ \, Tr[F_{\mu\nu}(x) F_{\mu\nu}(x)] + \bar{\psi}(x)[\gamma_\mu \partial_\mu + \gamma_\mu A_\mu(x) + m]\psi(x) \, \}$$

Asymptotic Freedom: Minus sign

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

QED screening





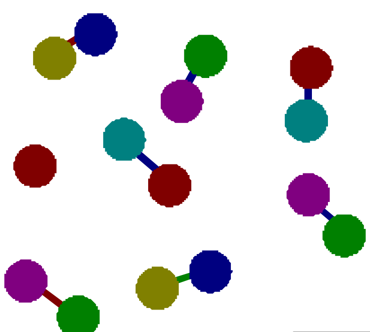
Electron – Position Pairs in Vacuum

But QCD has charged Quarks and Gluons

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

"But Gluon Act with Opposite Sign!"

QCD (anti-)screening

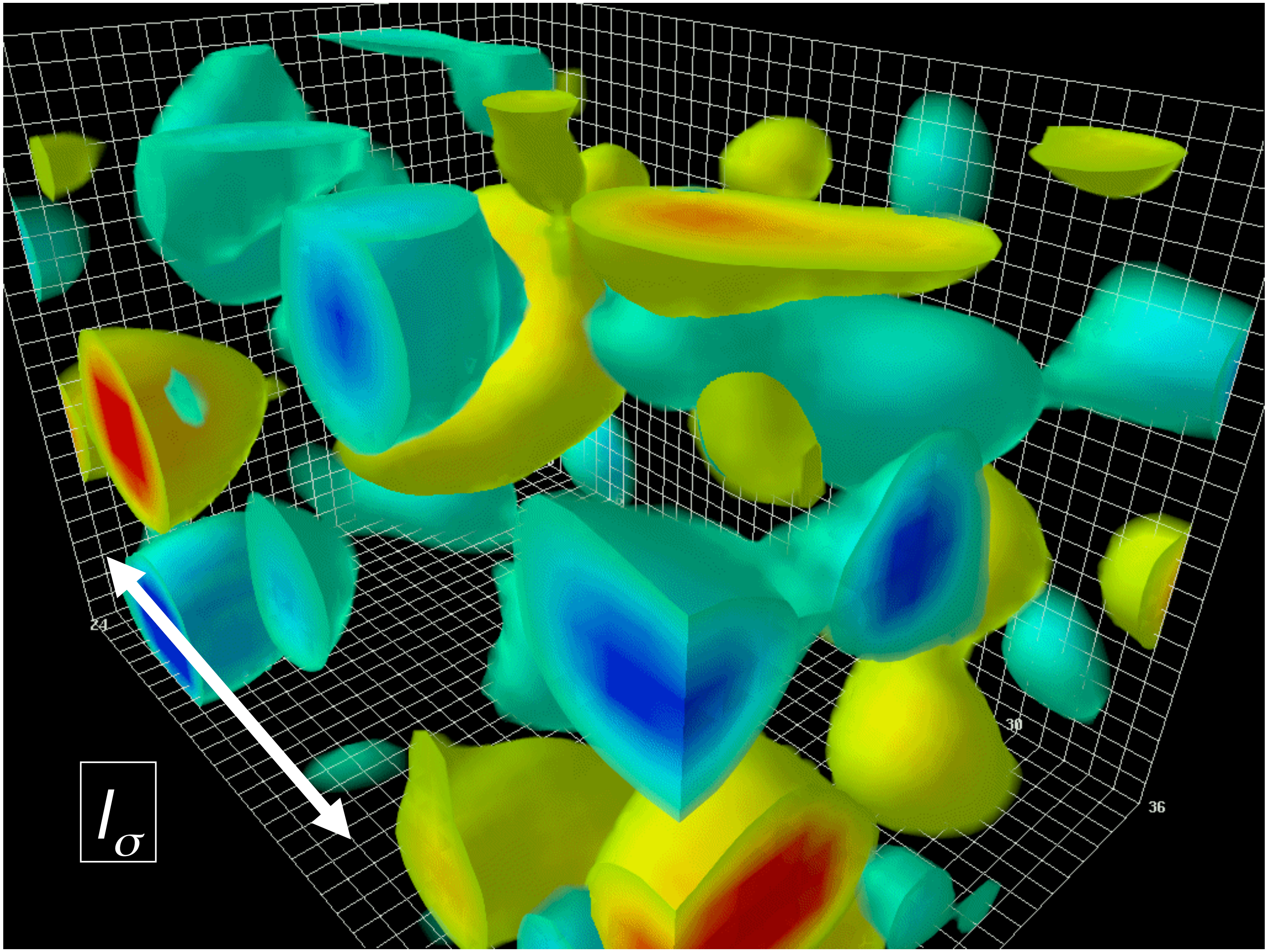


?

ΔX

$$\frac{1}{g_{eff}^2} \simeq [\frac{11N}{6} - \frac{n_f}{3}] \times \log(\frac{1}{M\Delta X})$$

Instantons, Topological Zero Modes (Atiyah-Singer index) and Confinement length l_σ



Where does MASS come from?

- QED
- Weak
- QCD

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

Masses of Proton/Neutrons come here via a quantum anomaly

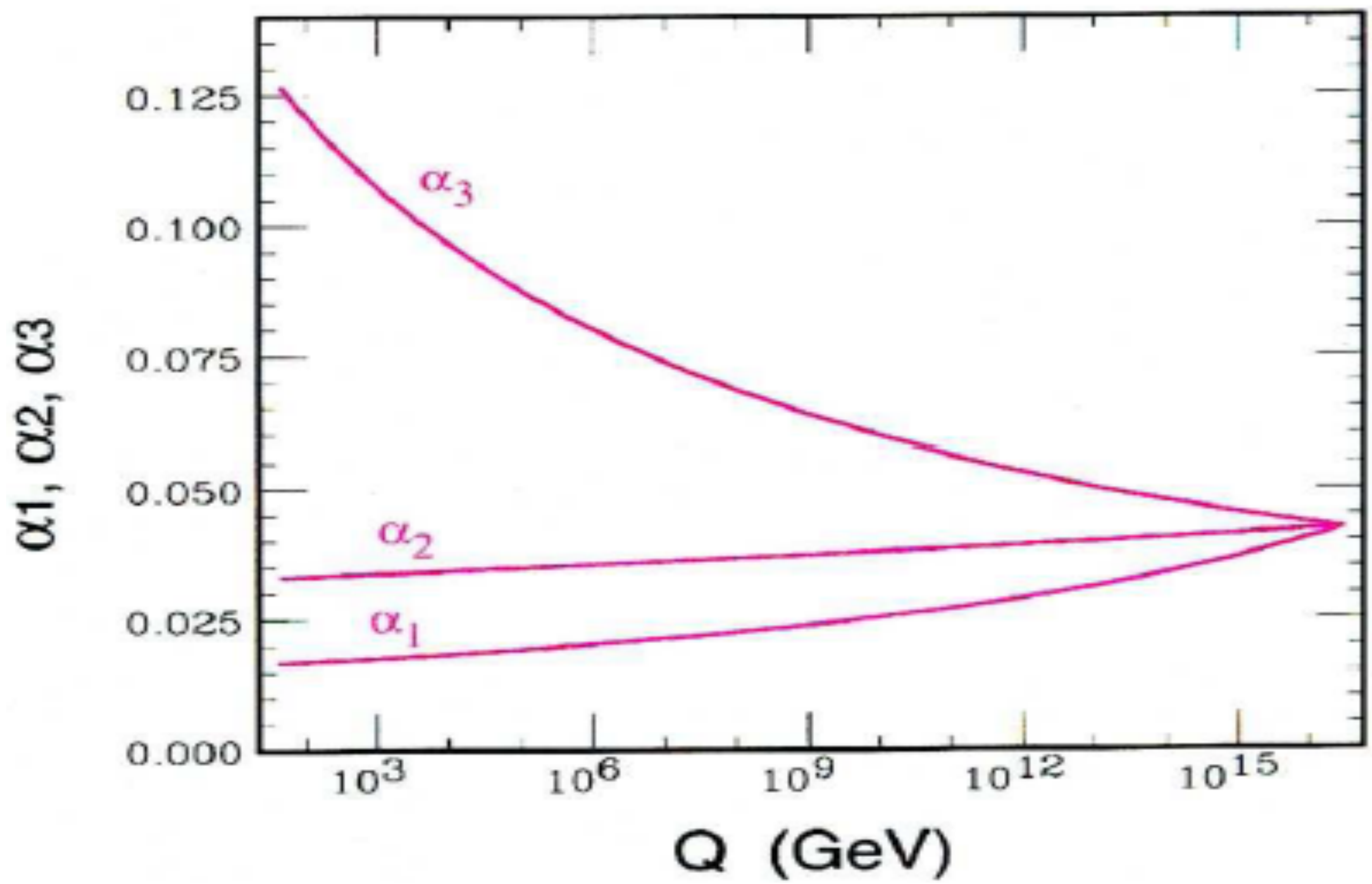
- Gravity

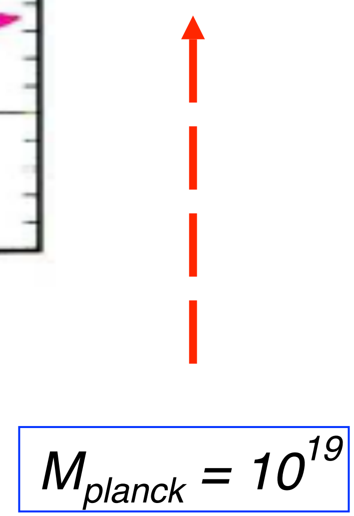
$$M_{plack} = G^{-1/2} = 1.301 \times 10^{19}\ m_{proton}$$

$$= 1.22 \times 10^{19} \text{GeV}$$

Mass scale but it is huge ➔ 21.767 microgram!

Running Coupling Unification





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)

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

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

Should use anti-symmetric tensor:

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

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

Only case where anti-sym d×d matrices looks like a (pseudo) vector

4-d Maxwell†: E(x_0, x_1, x_2, x_4) & B(x_0, x_1,x_2, x_3)

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

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

Lagrangian Density:

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

*† 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

$$x \quad \bullet\!\longrightarrow\!\bullet \quad x + a\mu = x_1$$

Finite difference:

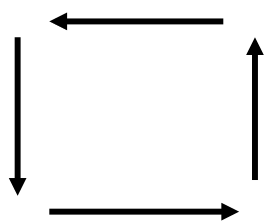
$$\frac{\partial \phi(x)}{\partial x_\mu} \to \Delta_\mu \phi(x) = \frac{\phi(x+a\mu) - \phi(x)}{a}$$

With Gauge field replace:

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

The new factor is covariant constant.

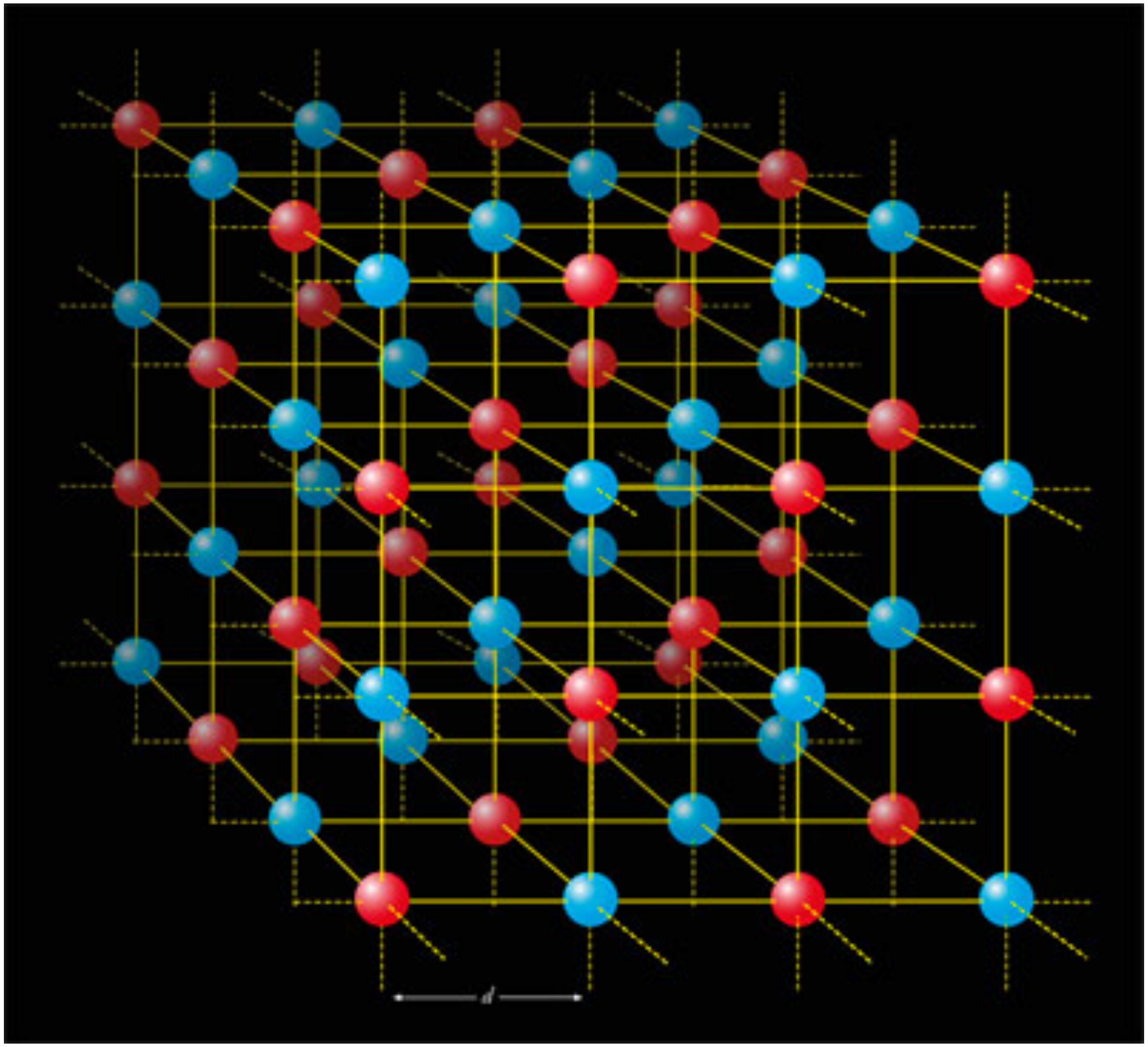
$$\boxed{\text{This is the Lattice Guage link:} \quad U(x, x+a\mu) = e^{iaA_\mu(x)}}$$



$$= e^{iaA_\mu(x)} e^{iaA_\mu(x)} e^{-iaA_\mu(x)} e^{-iaA_\mu(x)}$$

$$\simeq e^{ia^2(\partial_\nu A_\mu(x) - \partial_\mu A_\nu(x) - A_\mu(x+\nu) + i[A_\mu(x), A_\nu(x)])}$$

QCD on the Lattice: Base/Sparse vs Fiber/Dense



QCD: Theory of Nuclear Force

Anti-quark

quark

Gauge (Glue)

Partition function

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

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

$$= \int dA_\mu(x) \quad Det[D] \quad \exp[-\frac{1}{g^2} \int d^4x F^2]$$

Maxwell (Curl)

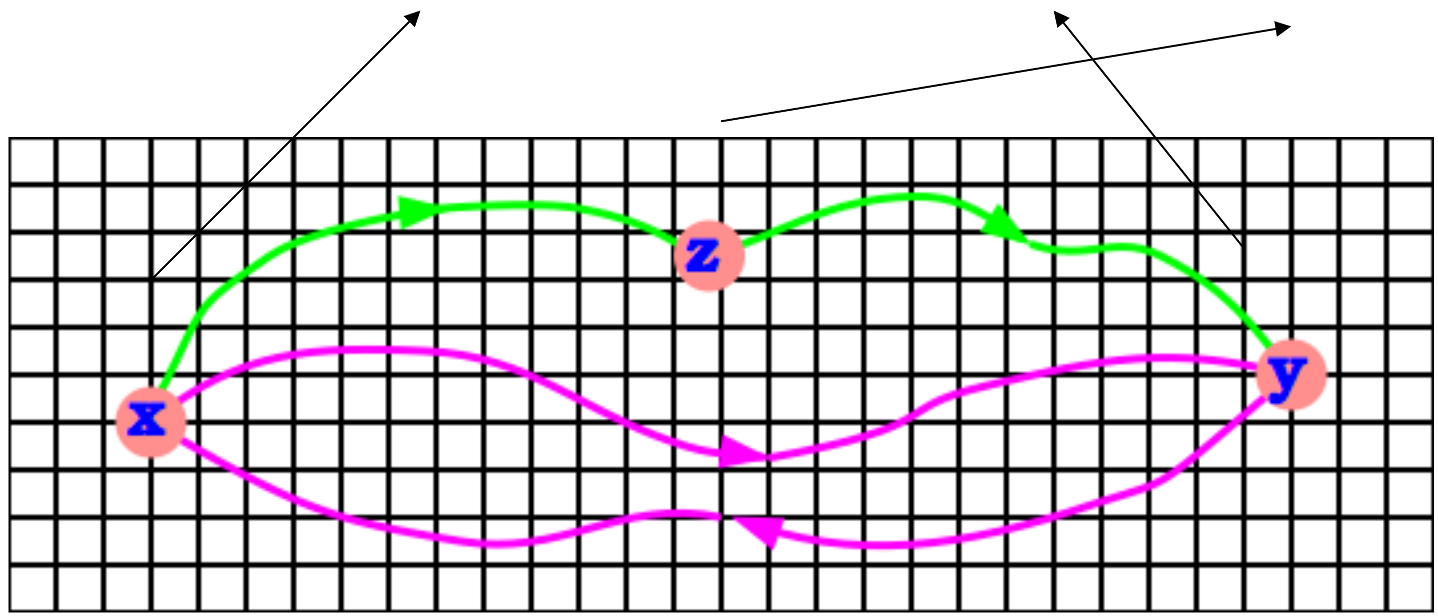
Dirac Operator

QCD Lattice Measurement

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

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

$$\int dU_\mu \; Det[D] \; [\; D^{-1}(x,y) D^{-1}(x,y) D^{-1}(x,y) \; Tr[\gamma_\mu D^{-1}(z,z) \;] e^{-S}$$

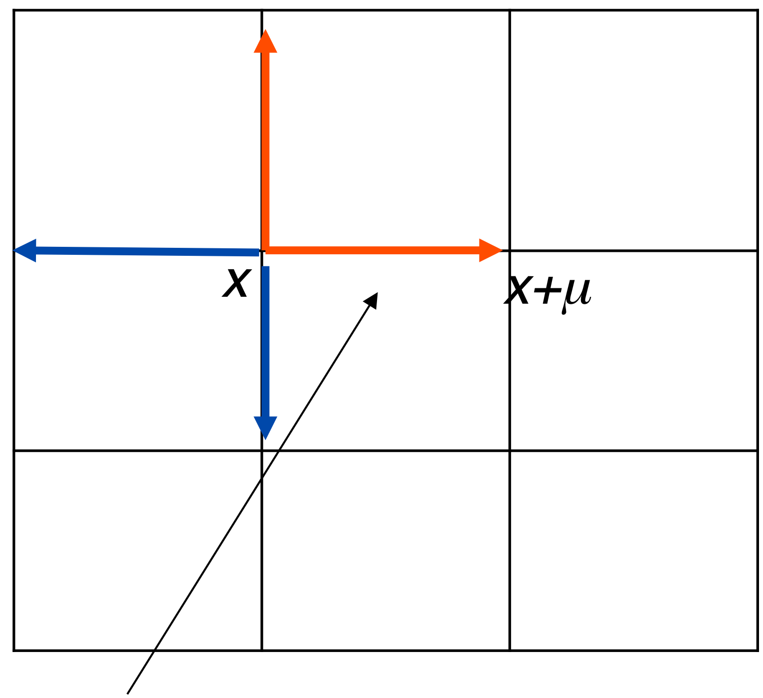


Computational Approach, Numerical Methods

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

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

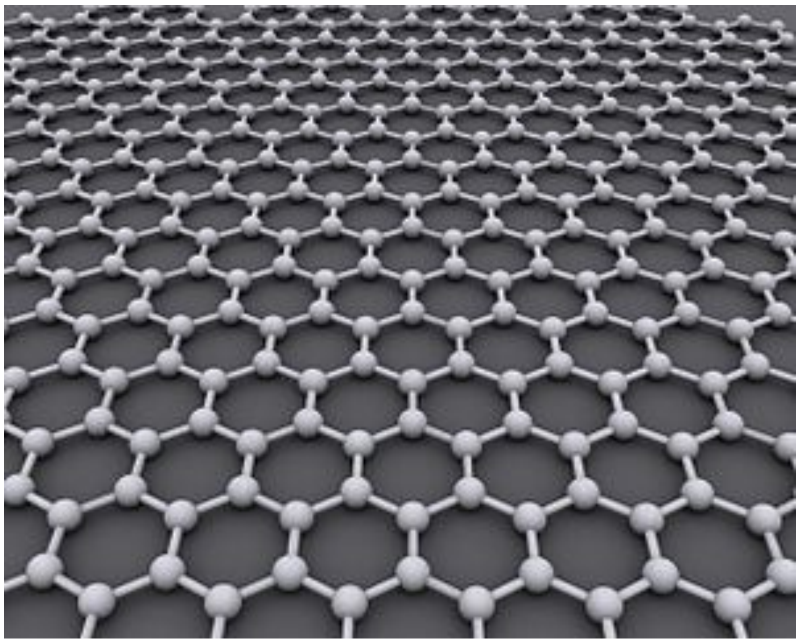
  Molecular Dynamics Algorithm:
  - Multi-time step Hamiltonian evolution in "potential": - Log(Probability).

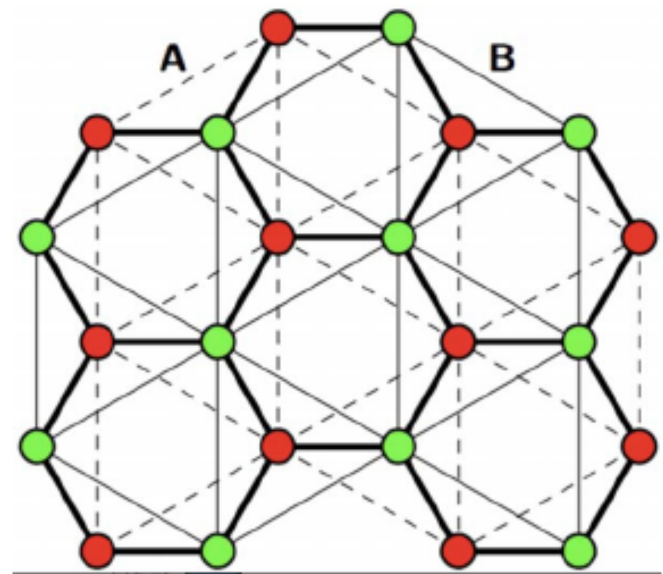


- Repeated solution of Dirac equation
  - (large sparse linear system) at each step

$$D_{quark} = m_q + \frac{1-\gamma_\mu}{2} U(x, x+\mu) + \frac{1+\gamma_\mu}{2} U(x+\mu, x)$$

Graphene





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

K. S. Novoselov, D. Jiang, F. Schedin, T. J. Booth, V. V. Khotkevich, S. V. Morozov, and A. K. Geim, *"Two-dimensional Atomic Crystals"*, *Proc. Nat. Acad. Sci.* **102**, 10451 (2005)

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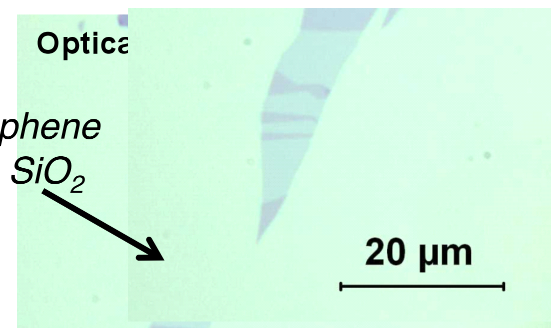


Nobel Prize
Physics
2010

"For groundbreaking experiments regarding the two-dimensional material graphene"

Geim's Graphene Superlatives

11/10

Thinnest imaginable material

Largest surface area (~3,000 m^2 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)

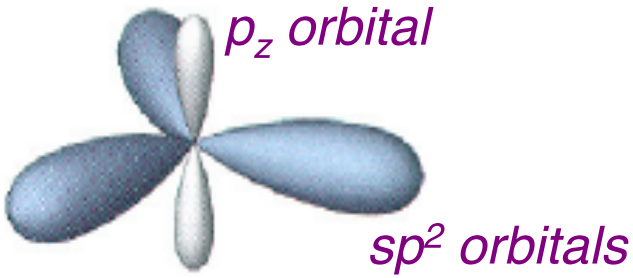
Conducts electricity in the limit of no electrons

Lightest charge carriers (zero rest mass)

Longest mean free path at room T (micron range)

sp^2 is a Unique Bonding Geometry

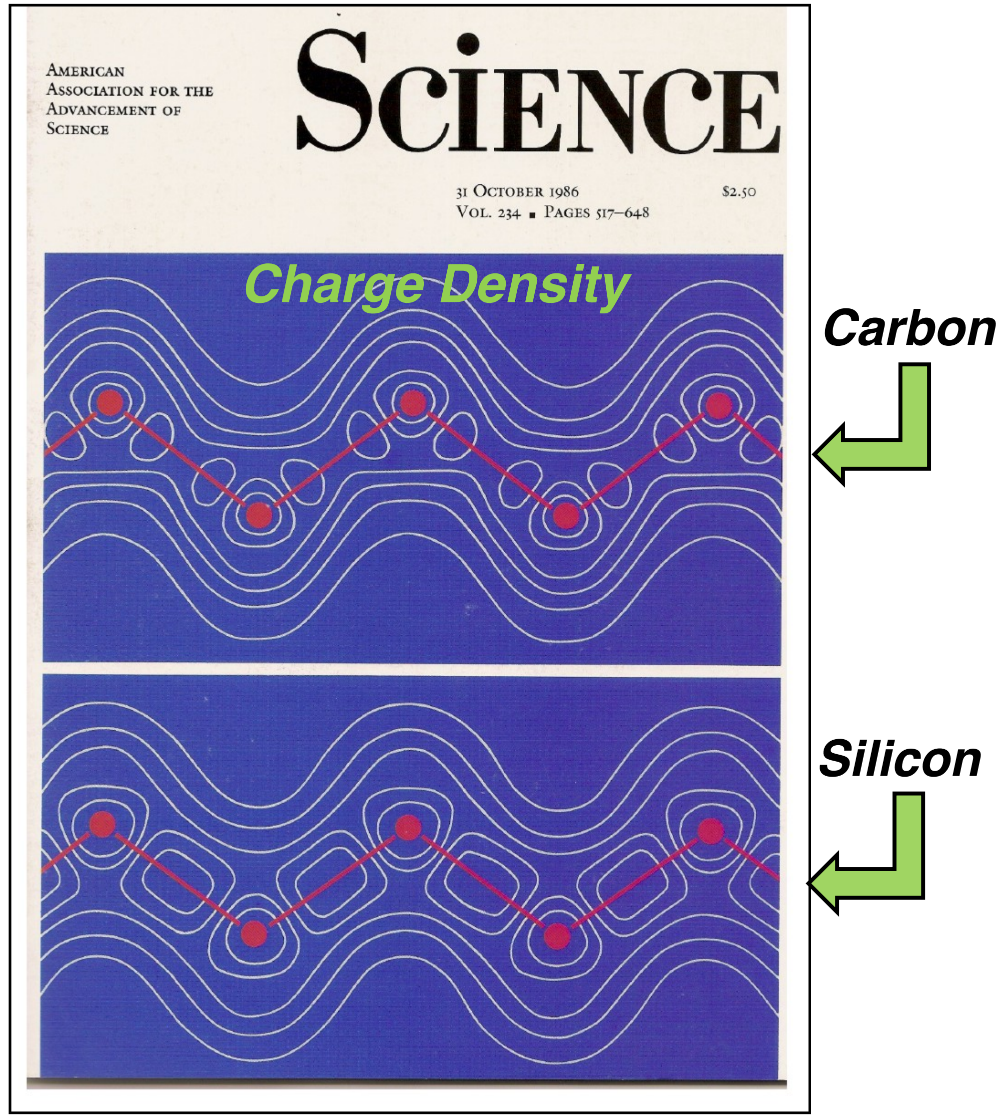
***Carbon**: $[1s^2]\ 2s^2\ 2p^2$*



Planar

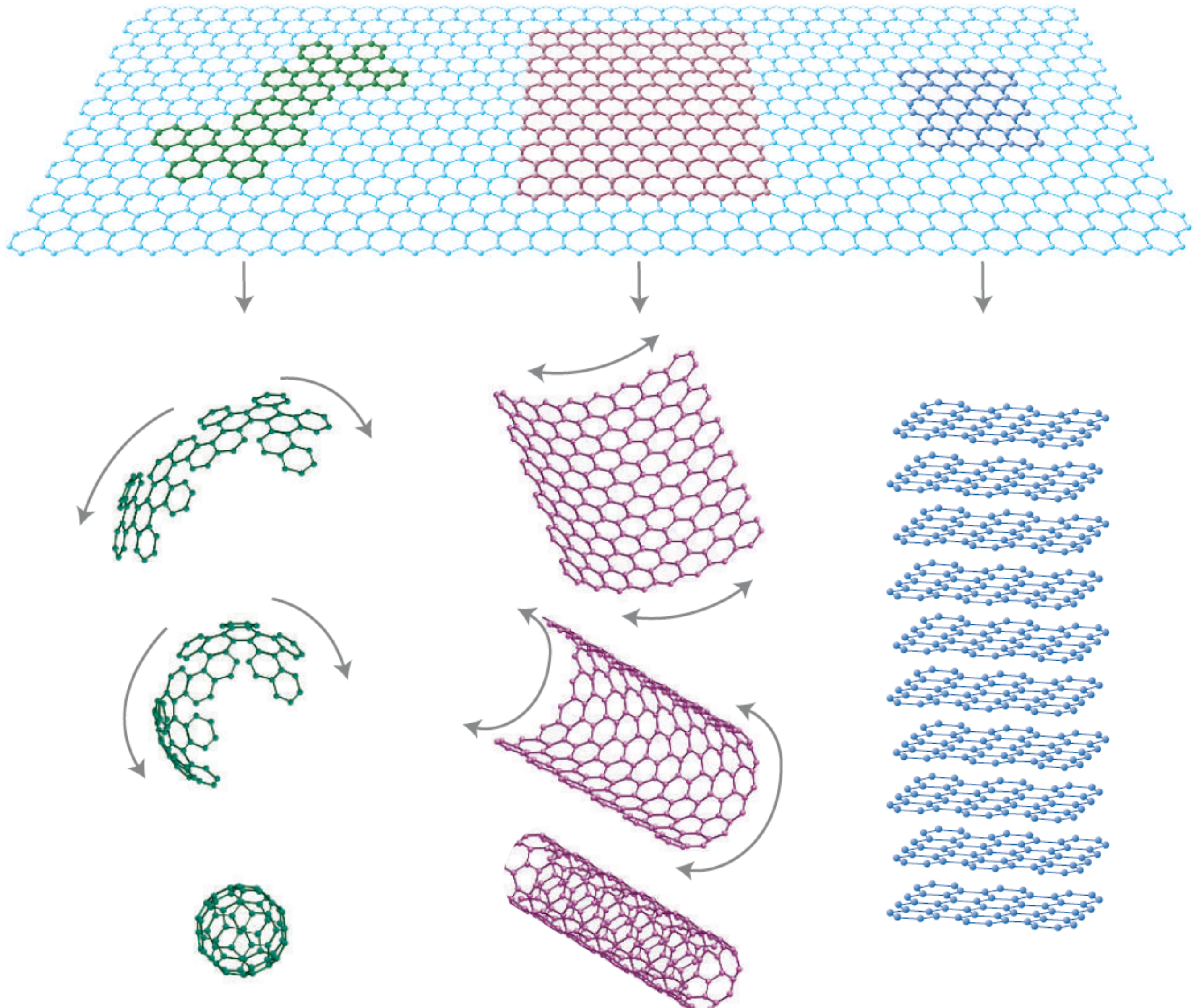
***Silicon**: $[1s^2\ 2s^2\ 2p^6]\ 3s^2\ 3p^2$*

Tetrahedral



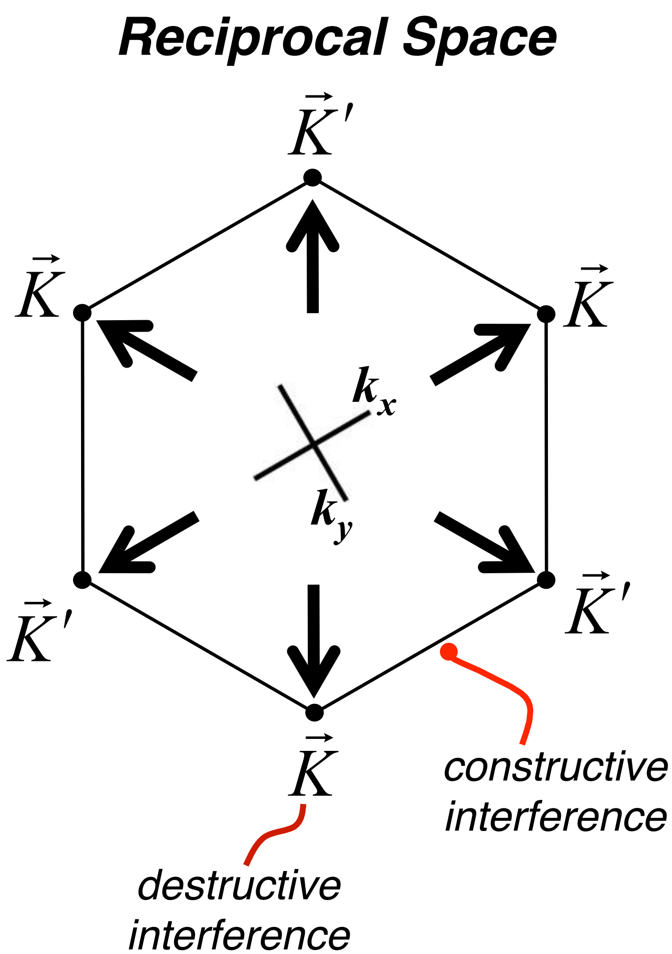
*M. L. Cohen, Science **234**, 549 (1986)*

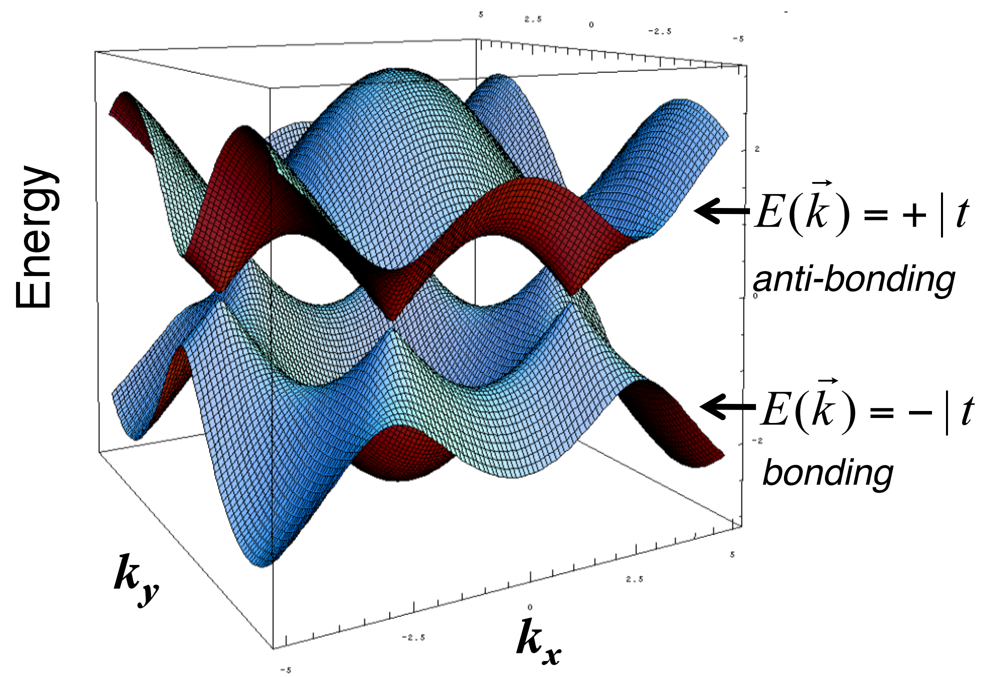
sp^2 Bonding Leads to Novel Carbon Structures



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

Graphene Bandstructure

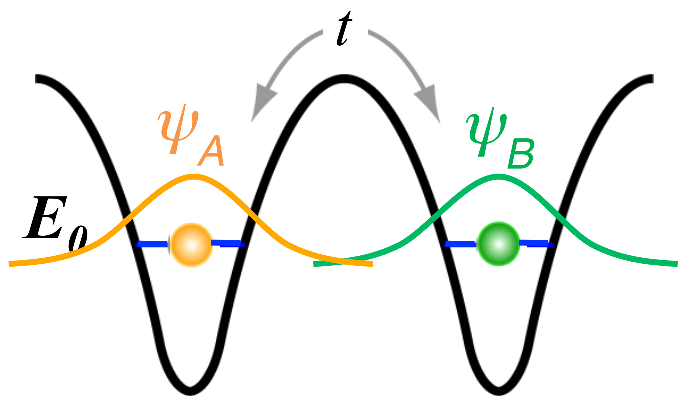




P. R. Wallace, Phys. Rev. 71, 622 (1947)

Graphene : Electronic Structure

Two Atoms (bonding)



$t \propto$ *Hopping Amplitude*

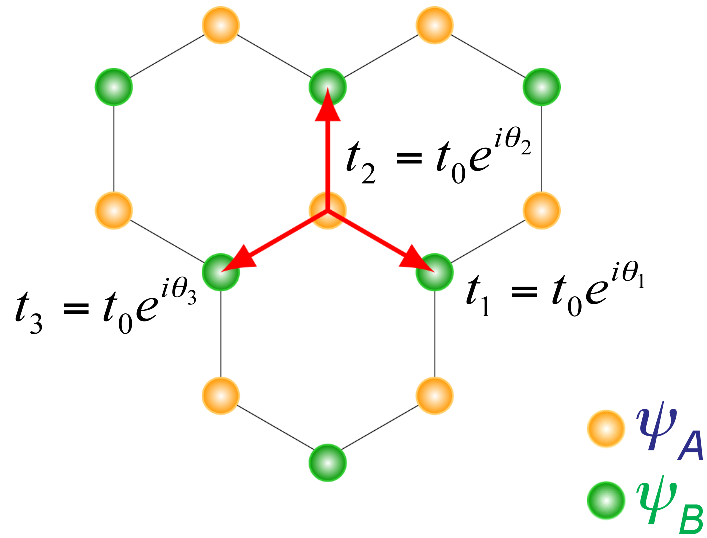
$$\hat{H}\Psi = \begin{pmatrix} 0 & t \\ t^* & 0 \end{pmatrix} \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

Atomic orbitals

$$E = \pm |t|$$

$$E_0 = 0 \quad \begin{cases} E_{anti-bonding} = +|t| \\ E_{bonding} = -|t| \end{cases}$$

Two Sub-lattices of Graphene



$$\hat{H}\Psi = \begin{pmatrix} 0 & t \\ t^* & 0 \end{pmatrix} \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

Carbon sublattices

$$E = \pm |t|$$

$$= \pm |t_0| \cdot \left| e^{i\theta_1} + e^{i\theta_2} + e^{i\theta_3} \right|$$

The Hamiltonian

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

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 $1/kT = \beta \to it/\hbar$
  - exp[- H/T] ➔ Path Integral for exp [-S/h]
- 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!