BGL for high energy physics

— QCD (Quantum Chromodynamics) simulation

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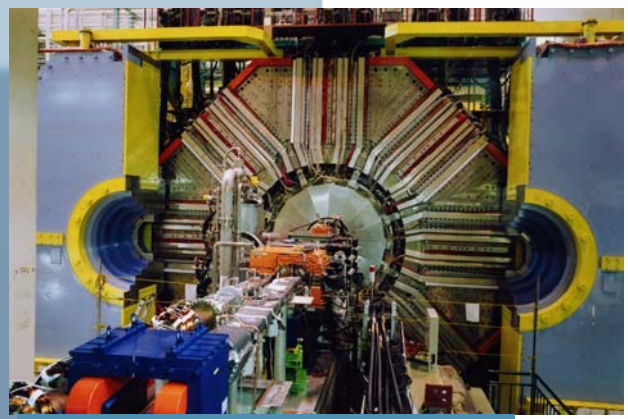
@ BG/L Systems Software and Applications Workshop,

at CBRC, Apr. 19, 2006

KEK is ...

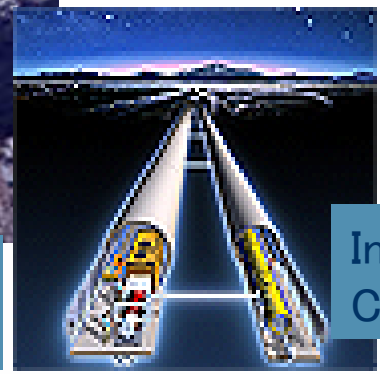
High Energy Accelerator Research Organization (KEK), located in Tsukuba

- Particle and nuclear physics, material sciences, etc. using accelerators

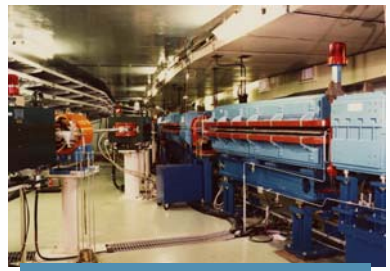


KEK B Factory (KEKB)

Japan Proton Accelerator Research Complex (J-PARC)



International Linear Collider (ILC) project



Photon Factory

KEK supercomputer

Leading computing facility in that time

• 1985	Hitachi S810/10	350 MFlops
• 1989	Hitachi S820/80	3 GFlops
• 1995	Fujitsu VPP500	128 GFlops
• 2000	Hitachi SR8000 F1	1.2 TFlops
• 2006	Hitachi SR11000	2.15 TFlops
	IBM Blue Gene/L	57 TFlops

Machine is for ...

- To be shared by Japanese groups on (theoretical) particle and nuclear physics
- “KEK Large Scale Simulation Program” : call for proposals of project to be performed on the supercomputer.
  - Program Advisory Committee (PAC) decides the approval and machine time allocation.
- 60~80% of the computer time has been allocated for lattice QCD.
- Other big users include accelerator design.

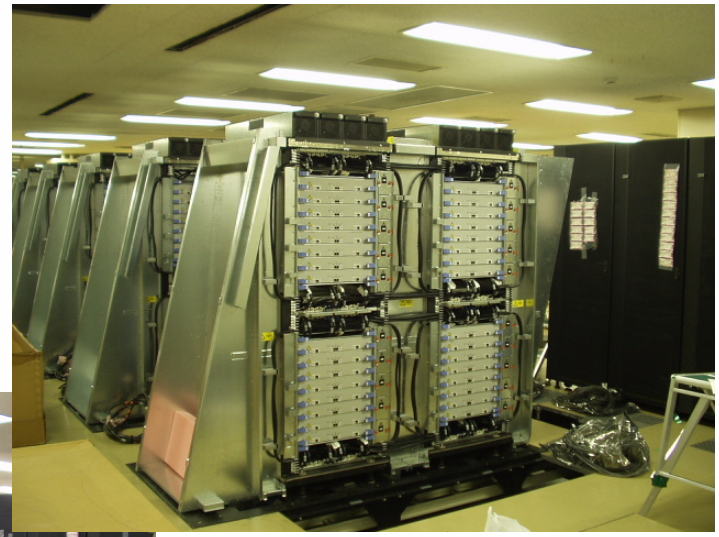
Installation

Dec. 26, 2005

Installation

Dec. 27, 2005

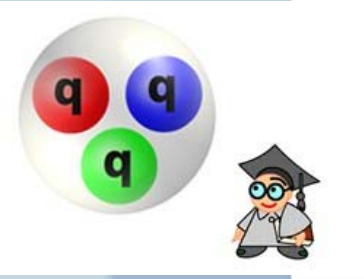
Jan. 11, 2006



Jan. 13, 2006

Now under operation

- 10 racks (4+4+2)
  - 5 1024-node queues
  - 8 512-node queues
  - some small test queues
- Fully operational since March 1st, 2006.
  - saturated by lattice QCD jobs

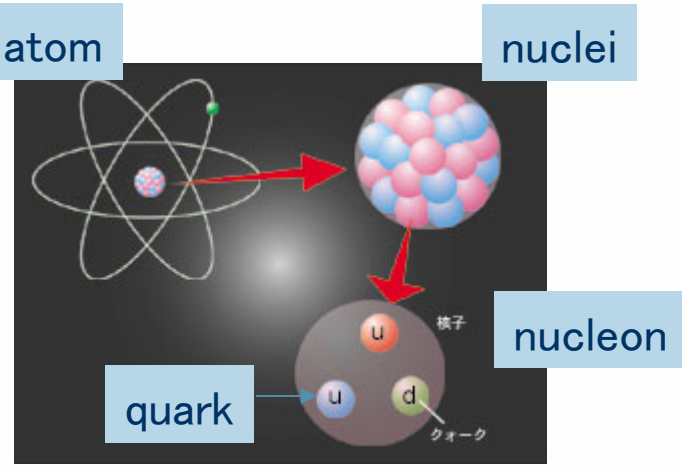


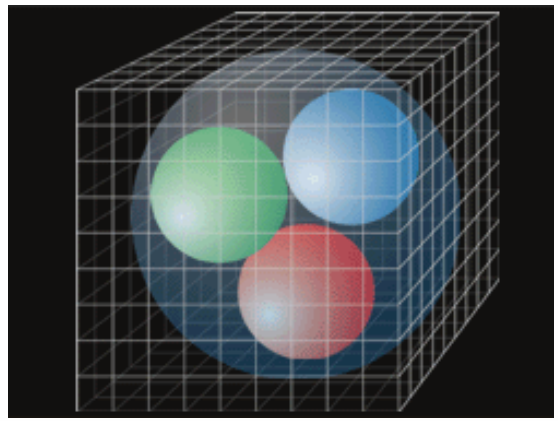
Lattice QCD

- Quantum Chromodynamics (QCD) = theory of strong interation
- Forces binding quarks and gluons to form proton/neutron, mesons, etc.
- Chiral symmetry breaking: origin of masses of matters

“strong” nonlinear interaction

⇒ Needs numerical simulation on the lattice

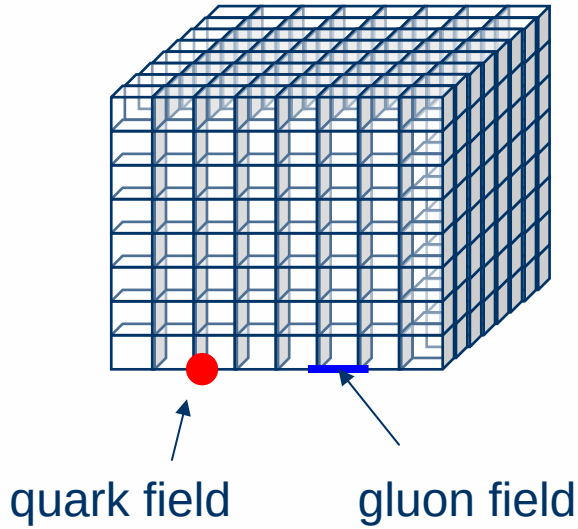




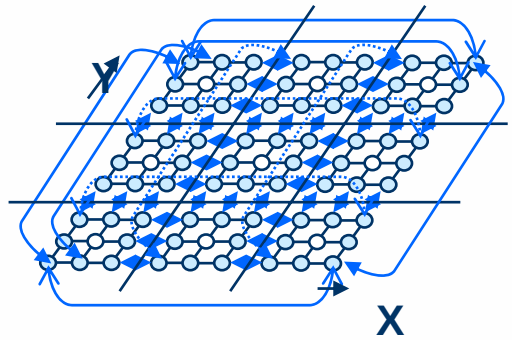
Lattice QCD simulation

Fields on the lattice

- Quark fields (3 color and 4 spin degrees of freedom) on 4D lattice sites
- Interaction with nearest neighbors
- Pickup effects of gluons on links



- 4D lattice naturally mapped on 3D torus; extra 1D on 2 cores inner node (VN mode)



Optimization for BGL

Done by IBM Japan (J. Doi and H. Samukawa)

- Use of Dual FPU by hand-written assembly language
  - 3x3 complex matrix times vector
  - Efficient use of registers
  - Most recent compiler can do a comparable job??
- Low-level communication API
  - MPI is too rich for NN communications.
  - Direct access to send/recv FIFO
  - Small packet (< 256 bytes); no temporal buffer needed

Jun Doi

Optimization result of our lattice QCD program

Sustained performance per peak performance:

global lattice size	8x8x8x16	12x12x12x24
1 node card 4x4x2x2 = 64 CPUs	25.45%	29.84%

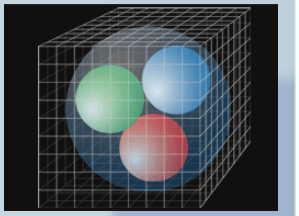
weak scaling

global lattice size	16x16x16x32	24x24x24x48
1/2 rack (2.8 TFLOPS) 8x8x8x2 = 1024 CPUs	24.33% (0.68 TFLOPS)	29.23% (0.82 TFLOPS)
1 rack (5.6 TFLOPS) 8x8x16x2 = 2048 CPUs	22.78% (1.28 TFLOPS)	28.57% (1.60 TFLOPS)

strong scaling

For comparison:

inline assembly with MPI (using buffer to send at once) (1/2 rack 24x24x24x48)	17.88%



Physics goals

Limitations in lattice QCD

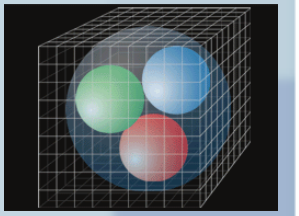
- finite lattice spacing a
- finite lattice volume L
- quark masses heavier than those in nature

Need extrapolations in each directions

Lattice simulation with *exact* chiral symmetry

Exact chiral symmetry

- ***was*** difficult to realize on the lattice
- now formulation is available, but numerically very demanding (need Blue Gene)
- Essential to prove the chiral symmetry breaking (source of mass generation)



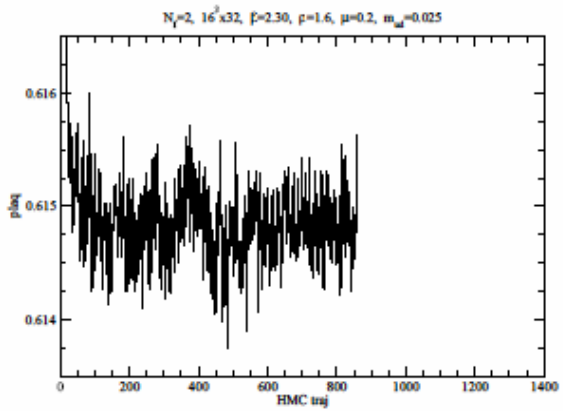
Why so hard

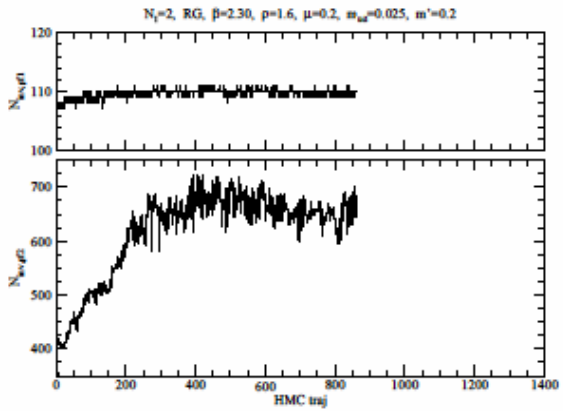
- Molecular dynamics type evolution
- Large matrix inversion using CG at each step
- The matrix contains sign function

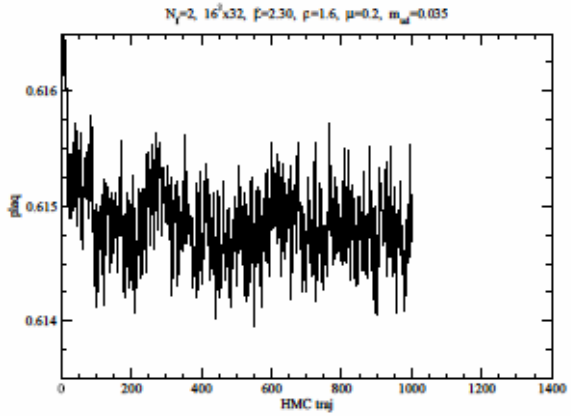
$$D \propto 1+\gamma_5 \,\mathrm{sgn}(H_W),$$

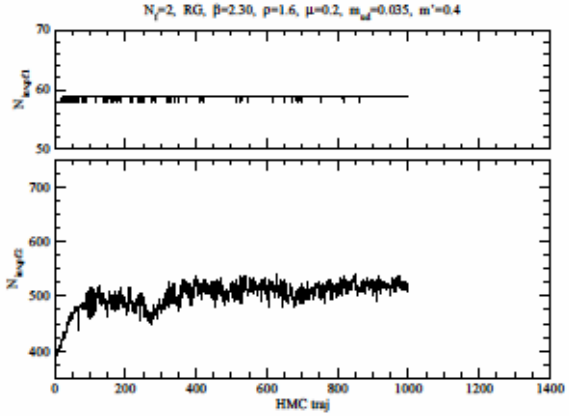
  approximated by a rational function of a large sparse matrix H_W.
- Need inner CG to obtain the rational function (nested CG!)
  - $O(10^5)$ MV operation at each step
  - Becomes harder towards small quark masses

Simulations ongoing









Summary

- 10 racks of BG/L installed at KEK; working for 50 days without major problems.
- BG/L fits perfectly for lattice QCD applications.
  - In fact, several installations of BG/L (mainly) for lattice QCD around the world (BU, MIT, Edinburgh, Julich, KEK)
  - A workshop was held in Boston (Jan 2006): http://super.bu.edu/~brower/qcd-bgl/

New powerful engine for lattice QCD!