Lattice QCD on Leadership-class Machines

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QuantumChromoDynamics

- Quantum Chromodynamics is the fundamental theory of the strong nuclear force
- It explains the interactions between quarks and gluons
- Quark : fundamental constituent of matter
  Gluon : Gauge Quanta (like photon)
- Unlike photons, gluons carry color charges and self-couple
- Asymptotic Freedom : At high energies (large distances) quarks and gluons interact weakly. [D. Politzer, F. Wilczek and D. Gross, 2004 Nobel Price]
- Confinement : There are no free quarks, they always bound into hadrons (e.g., proton) or mesons.

Lattice Field Theory

- Continuous space-time is mapped onto discrete lattice (grid).
- It is a four-dimensional problem 3 space + 1 time
- Functional integral of the Quantum Field Theory

$$Z = \int [dA][d\psi][d\bar{\psi}] \exp[-S_f - S_G]$$

is evaluated on a computer by Monte Carlo techniques

Physics Goals ?

Fundamental parameters of the Standard Model

Quark-Gluon Plasma

Nucleon Structure

Beyond Standard Model (New Physics)

Lattice Calculation :

- The fermions (quarks) can be integrated out (Grassmann integration) :

$$Z = \int [dA] \det M \exp[-S_G]$$

  where M is the lattice Dirac Operator.
- Every lattice calculation requires the computation of $\det M$ and M^{-1} on suitably generated ensembles of lattice gauge fields and repeated on different lattices with different lattice spacings a.
- This comes down to solving matrix equations $M \cdot x = y$. Standard tool to solve these systems for x is to use *conjugate gradient algorithm* for given y and M .
- Computation slows down as the quark mass m_q gets smaller and requires higher performance computers
- Repeated solution of the Dirac equation is required in Lattice QCD computations.
- Kraken (NSF), BGP/Intrepid (Argonne), Jaguar/Cray-XT5 (ORNL)

SciDAC Software:

The DOE SciDAC project : “A National Computational Infrastructure for Lattice Gauge Theory” has developed community software specialized for LGT might be useful elsewhere.

- Level 1 : message passing (QMP) linear algebra (QLA) and (QIO) for I/O
- Level 2 : data parallel operations (QDP)
- Level 3 : high optimized, computationaly intensive algorithms (QOP)
  http://www.usqcd.org/usqcd-sofware/
  MILC code has been modified to use this code

  For a tutorial and simple examples
  http://web.mit.edu/ bgl/scidac-2007/

Wilson Dslash with QOP/QOP

$$\text{Continuum :} \qquad \not{D}\psi(x) = \gamma_\mu(\partial^\mu - igA_\mu(x))\psi(x)$$

$$\text{Lattice :} \sum_{\mu=0}^{3} U_\mu(x)(1-\gamma_\mu)\psi(x+a\hat{\mu}) + \sum_{\mu=0}^{3} U_\mu(x-a\hat{\mu})(1+\gamma_\mu)\psi(x-a\hat{\mu})$$

QDP allows to one to shift operators easily. We have a 4d problem Shifts :

```
QDP_DiracFermion *psi_up[4];*psi_dw[i];
QDP_DiracFermion *tempf,*source;
QDP_GaugeField   *u[4];
for(i=0;i<4;i++){
 QDP_D_eq_M_times_sD(psi_up[i],u[i],source,QDP_neighbor[i],QDP_forward,
                    QDP_all);
 QDP_D_eq_Ma_times_D(tempf,u[i],source,QDP_all);
 QDP_D_eq_sD(psi_dw[i],tempf,QDP_neighbor[i],QDP_backward,QDP_all);
}
.
.
```

then it communicates at the boundaries for the next-neigbor sites.

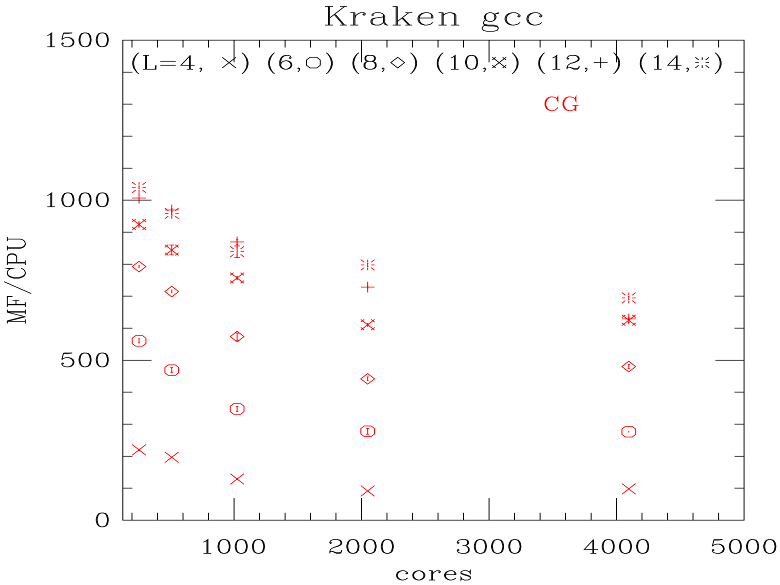
Application Bottlenecks (I)

- Data distribution is uniform among the nodes : conjugate gradient message passing between nodes : Certain amount of message passing has to be done
- Scaling :
  - Strong : Size of the problem is fixed and number of processors is varied
  - Weak : Size/processor is fixed. We would like constant speed per processor

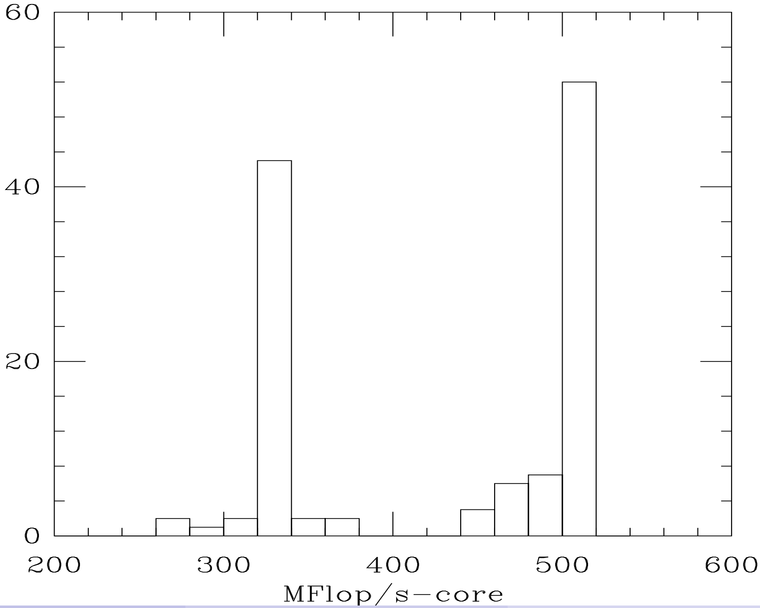
  Bottleneck :
  - Balancing communication and computation ?

  Solution :
  - Long computations so that the communication is not a big loss. (Our code is better for a large size/processor problem)
  - Increase the problem size per processor. Surface/Volume ratio

Scaling


Kraken gcc
(L=4, ×) (6,○) (8,◇) (10,×) (12,+) (14,⁜)
CG
MF/CPU
1500
1000
500
0
1000
2000
3000
4000
5000
cores

Performance



Application Bottlenecks (II)

Bottleneck :

- Double precision takes twice as much memory. Local memory bandwidth problem.

Solution :

- Multi-precision inverter : Double precision accuracy is reached using only a single-precision solver. The algorithm alternates single precision solves for the improvement of the solution with double precision accumulation of the improvement.

Solution :

- Desing algorithms to use the data in the cache. Single precision calculations.

BlueGene & Cray-XT5 : Bottlenecks and Solutions

Bottleneck :

- Lots of I/O slows down the computation

Solution :

- BlueGene (GPFS) system. %30 of job time is I/O. Faster I/O is required. Single precision is used. Cray-XT5 has fast I/O (LUSTRE)

Bottleneck :

- Fourier Transform is slow. There are too much communication.

Solution :

- We developed a new FFT algorithm that uses a combination of data remapping. There is a big improvement over the old algorithm.

BlueGene & Cray-XT5 : Bottlenecks and Solutions

Bottleneck :

- Partition Count :

Solution :

- Restriction on the partition count on BlueGene (2^n) but not on Cray-XT5, e.g., $56^3 \times 144$ lattices.

Bottleneck(?) :

- Memory management

Solution :

- It may have memory management problem performance fluctuates between 150 mflops and 300 mflops