Lattice QCD on Leadership-class Machines

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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.
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?

<table>
<thead>
<tr>
<th>Fundamental parameters of the Standard Model</th>
<th>Nucleon Structure</th>
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<tbody>
<tr>
<td>Quark-Gluon Plasma</td>
<td>Beyond Standard Model (New Physics)</td>
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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, computationally intensive algorithms (QOP)

http://www.usqcd.org/usqcd-software/
MILC code has been modified to use this code

For a tutorial and simple examples
Wilson Dslash with QOP/QOP

Continuum: \[ \mathcal{D}\psi(x) = \gamma_\mu (\partial^\mu - igA_\mu(x))\psi(x) \]

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:

```c
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
Performance

The graph shows the performance (MFlop/s-core) against the score. The x-axis represents the MFlop/s-core values ranging from 200 to 600, and the y-axis represents the frequency or number of occurrences. The bars indicate the distribution of data points with peaks at certain MFlop/s-core values.
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:
- Design 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