BSMBench: A HPC Benchmark for Beyond the Standard Model Lattice Physics

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Abstract: Beyond the Standard Model (BSM) Lattice Physics is a growing area of computational theoretical physics encompassing extensions to or modifications of lattice QCD, which requires increasingly powerful machines. Depending on the theory under investigation, it can place greater demands on either the communications or the compute performance of a multi-node environment, relative to lattice QCD. Lattice QCD has been used to benchmark machines for many years. To allow for more accurate analysis of machines’ suitability for a particular theory, as well as a more general analysis of machine’s performance than a QCD benchmark would give, we present a new tool to benchmark the performance of all BSM theories, using a method close to that of Lüscher (2002), but based on the HiRep code of Pica et al. (2009, 2011). Three regimes are probed, one QCD-like regime balancing demands on communications and compute power, and two emphasising each of those over the other. Some initial benchmark statistics are included for clusters, Blue Gene/P, and Blue Gene/Q machines.

What is Lattice QCD?
- Quantum Chromodynamics (QCD) being a Quantum Field Theory (QFT) of the strong interaction, which binds atomic nuclei together
- It cannot be solved analytically
- A numerical solution is possible after discretising spacetime onto a four-dimensional lattice of discrete points.

What is BSM?
- Beyond the Standard Model physics seeks to generalise QCD to explain new physics
- Fundamental variables are:
  - an $SU(N)$ matrix on each link [QCD Exps $N = 3$]
  - a vector (spinor field) comprising either 4 (or 4$^{N-1}$) values on each site; QCD has the former

Lattice Computations
- Lattice volume (number of sites $V$)
  - Parallelisation splits lattice into parts, one per process
  - High-availability is the Dirac operator, a large, sparse matrix acting on all spinor variables
  - Main computations involve inverting this matrix on selected vectors

Why is HPC necessary?
- Smallest lattices fit on a desktop (44 lattice)
- Current research looks at 1284 lattices (and beyond) – on a desktop this would require ~1500G RAM, ~10 years per data point
- BSM code can require more power again
- This is using state-of-the-art numerical techniques to minimise the amount of compute power necessary

Benchmarks
- QCD is already used to benchmark supercomputers [1]
- QCD codes place roughly equal demands on communications and compute speed
- BSM codes vary this
- BSM-derived benchmark allows more flexible testing of a machine’s characteristics
  - Testing of machine’s suitability for a given theory
  - More general comparisons/compare comparisons

HiRep
- Chroma (described in [2]), the most commonly-avoidable lattice code, only deals with QCD-like theories
- HiRep (described in [3], [4]) has been developed to be more flexible
  - Allows varying of $N$, type of spinor field
  - Forms a complete, state-of-the-art suite for lattice BSM

Results
- Square norm test demands less of inter-node communications; shows approximate scaling on all machines
- Dirac operator application is more physically demonstrative; drop in performance on non-infiniband cluster highlights higher demands placed on intra-node communications
- Rack-to-rack comparison between 128x644 lattice on Blue Gene/Q and equivalent data from a 64x324 lattice on Blue Gene/P
- Blue Gene/Q supports four hardware threads per core, with 16 cores per node. Multithreading gives no benefit to the comm or balanced theories, but does give a small benefit to the compute theory

Benchmark Strategy
- Based on that of Lüscher (described in [5])
  - Consistency check of arithmetic
  - Not used for performance analysis
  - Omitted for small machines
  - Three operations tested for a given period of time
    - Spinor field square norm (square)
    - Spinor field multiply-add (mad) (not shown)
    - Direct operator application (Dphi)
  - FLOPs counted, performance reported
  - Three regimes tested:
    - "Comms" - communications-intensive ST(2) theory, 2 adjoint fermions
    - "Balance" - QCD-like ST(2) theory, 2 fundamental fermions
    - "Compute" - computationally-intensive ST(2) theory, 2 fundamental fermions
  - Single lattice size of 64x32 used to allow direct comparison between machine sizes
  - Based on the HiRep code

Architectures
- Three different machines were tested
  - Blue Gene/P:
    - 4 cores/node, 1 thread/core, 32-bit PowerPC CPU at 830MHz, 1 MPI process per core
    - Nodes connected by high-speed 3D torus
    - 4GB RAM, 512 L2, 4MB L3 cache per node
    - IBM XL C compiler 9.0 for Blue Gene
  - Blue Gene/Q:
    - 16 compute cores/node, 4 threads/core, 64-bit PowerPC CPU at 1.6GHz, 1 MPI process per core
    - Nodes connected by high-speed 5D torus
    - 16GB RAM, 32MB L2 cache per node
    - IBM XL C compiler 12.0 for Blue Gene Q
    - 64-bit cluster
      - 16 cores/node, 1 thread/core, 2 x Opteron 6128 CPU/node, 1 MPI process per core
      - Nodes connected by 1GigE (no Infiniband)
      - 96GB RAM, 8MB L2, 24MB L3 cache per node
      - GCC 4.1.2

Conclusions
- Three machines tested: Blue Gene/P, Blue Gene/Q, and an x86 cluster without Infiniband
- Square norm less demanding of communications; speed scales well beyond node size on cluster
- Dphi test is communications-intensive:
  - Speed scales well on Blue Gene
  - Speed drops off once exceeding node size of non-Infiniband cluster
- 8GB 4-5 times faster than 8GB per rack
- Multithreading cores can have modest benefit to some theories

References