Quantum Mechanical Material Simulations on Blue Gene/Q

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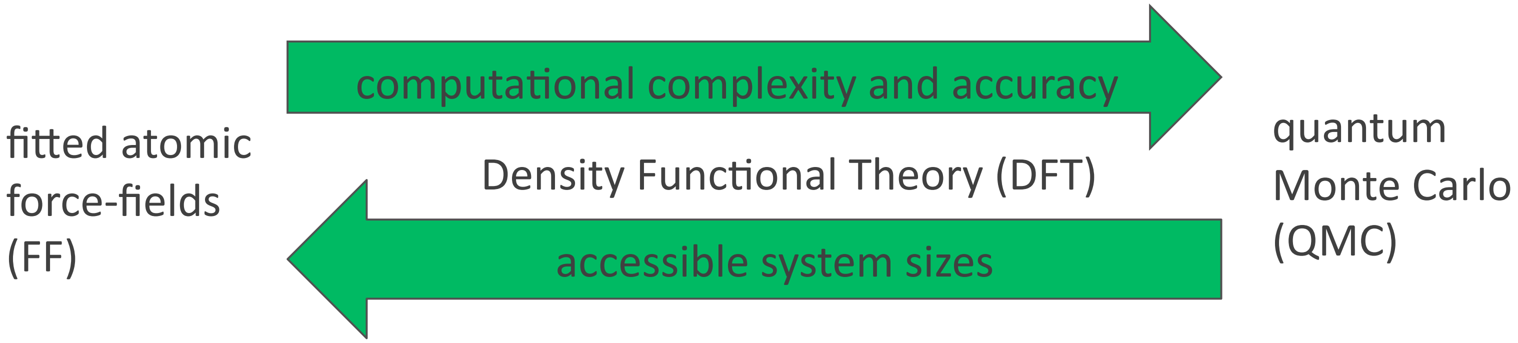
Atomic simulations methods in a nutshell

Primarily for ground-state simulations in material science, chemistry, and condensed matter physics



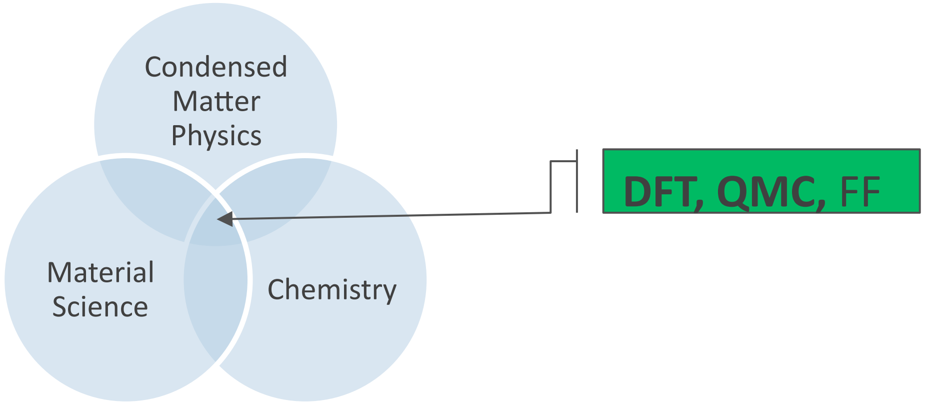
computational complexity and accuracy

fitted atomic force-fields (FF)

Density Functional Theory (DFT)

quantum Monte Carlo (QMC)

accessible system sizes



Condensed Matter Physics

Material Science

Chemistry

DFT, QMC, FF

Motifs in Quantum Mechanical Simulation

- Type 1A: Capability due to high accuracy in the level of theory
  - QMC $\mathcal{O}(N^{3\text{-}4})$
  - Hybrid DFT $\mathcal{O}(N^4)$
  - quantum chemistry $\mathcal{O}(N^{5\text{-}7})$
- Type 1S: Capability due to problem size (mostly pure DFT $\mathcal{O}(N^3)$)
  - Canonical DFT has a number issues, especially with non-local representations of Ψ
    - Dense diagonalization exhibits poor performance (see http://arxiv.org/pdf/1205.2107v1)
    - Instabilities in SCF algorithms (see Phys. Rev. B 64, 121101(R) (2001))
    - $O(N^3)$ “wall”
  - Reduced-scaling methods are needed in quantum mechanical approaches (mostly in DFT, but also many-body methods)
    - Fragment-type methods (GAMESS, LS3DF) or localization methods (CONQUEST, MADNESS, SIESTA, and many others)
    - Lots of progress, but also many remaining challenges (metals vs. insulators, precision, etc.)

Motifs in Quantum Mechanical Simulation (cont'd)

- Type 2: Loosely coupled, but not too loosely coupled
  - Might be doable in the cloud or on the grid, but communication between "images" needs to occur in a "lockstep" fashion
  - Nudge-elastic band calculations, Phonon spectrum, replica-exchange calculation, etc.
  - Even some aspects of quantum Monte Carlo
- Type 3: Capacity due to large parameter sweeps (i.e. High-throughput computing)
  - No control or data dependencies among calculations
  - Still not suitable for SETI@Home since each calculation may require many MPI tasks or lots of memory
  - Managing jobs with very different wall-clock times
  - Analysis of large data sets

What will you get out of this talk?

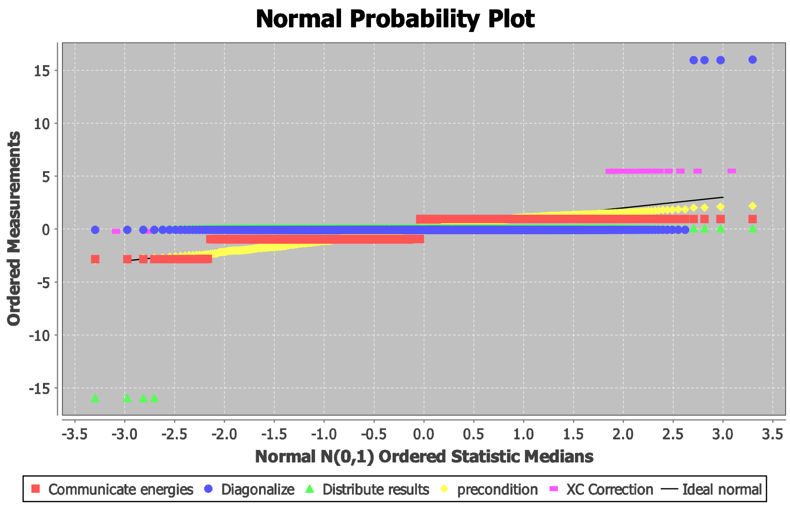
- It won’t answer:
  - Should I buy a Blue Gene/Q for my institution?
- It will begin to answer:
  - Is my electronic structure calculation well-suited for Blue Gene/Q?
- It will probably answer:
  - What types of electronic structure calculations are running well now?
  - What is involved in getting your code running on Blue Gene/Q?
    - Porting is easy
    - Using all the processing elements is easy
  - What is involved in getting your code optimized on Blue Gene/Q?
    - Getting good performance will require extra work
    - ALCF has a really excellent performance team (shameless self-promotion)

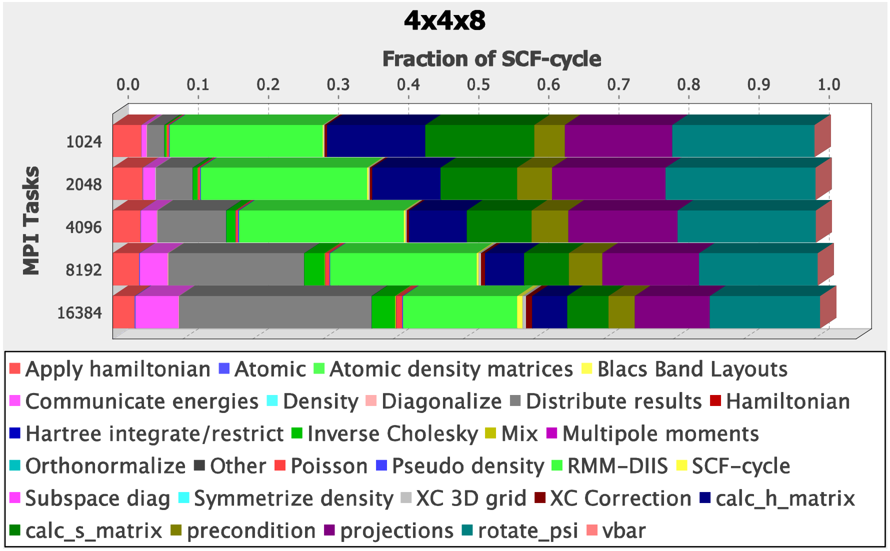
Quick code overview

- GPAW
  - Mira acceptance test code
  - Mainly used for Type 1S on Intrepid; largest calculations were 8 - 32-racks on 10,000 – 14,000 valence electrons
  - Consumed ~100 million core hours over the lifetime of Intrepid (includes INCITE/ALCC/ Discretionary)
  - Porting time on Blue Gene/Q ~ 1 day
- CPMD
  - INCITE/ALCC code
  - Used for Type 2, some Type 1S on Intrepid; largest Type 2 calculations were 8 - 32-racks
  - Will be used for Type 1A (hybrid DFT) on Mira
- QMCPACK
  - Early Science Program code
  - Not used on Intrepid for any scientific calculations due to insufficient memory per node
  - Will be used for Type 1A (QMC) on Mira
  - Porting time to Blue Gene/Q ~ 1 day, early issues with XL compiler, but resolved now

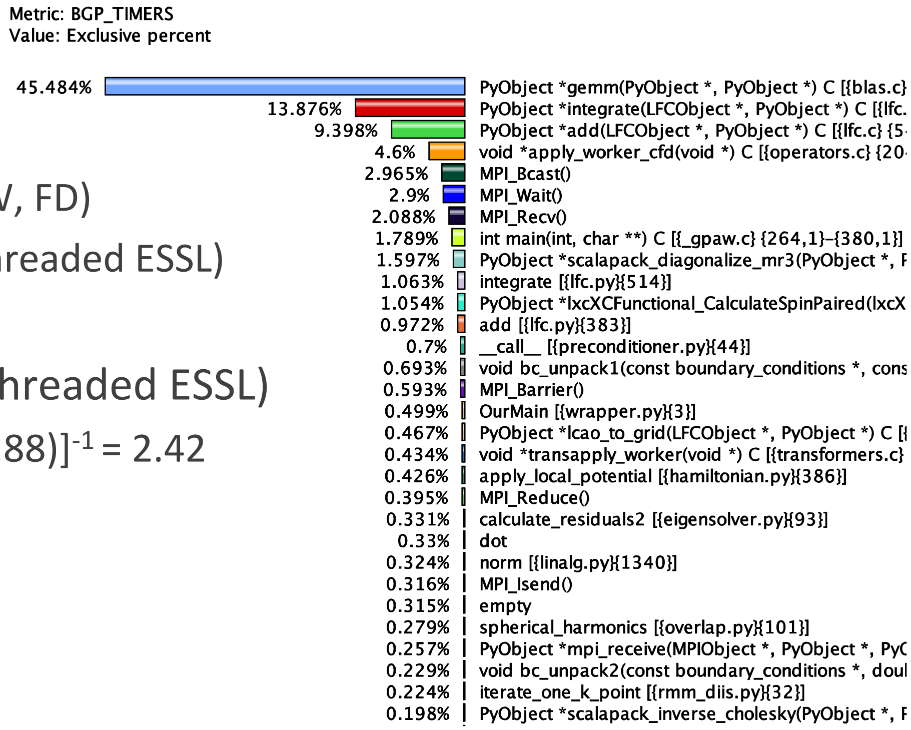
GPAW - performance on Blue Gene/P

- Density functional theory
  - Projector Augmented Wave (PAW) using finite-difference (FD) stencils on uniform real-space grid
  - MPI parallelism only, written in Python and C
- Algorithmic issues for Type 1S (> 10,000 electrons)
  - Large number of SCF cycles (>200) to obtain convergence (not shown).
  - Poor performance of dense diagonalization (inferred from dark grey on right figure)





GPAW - performance on Blue Gene/Q



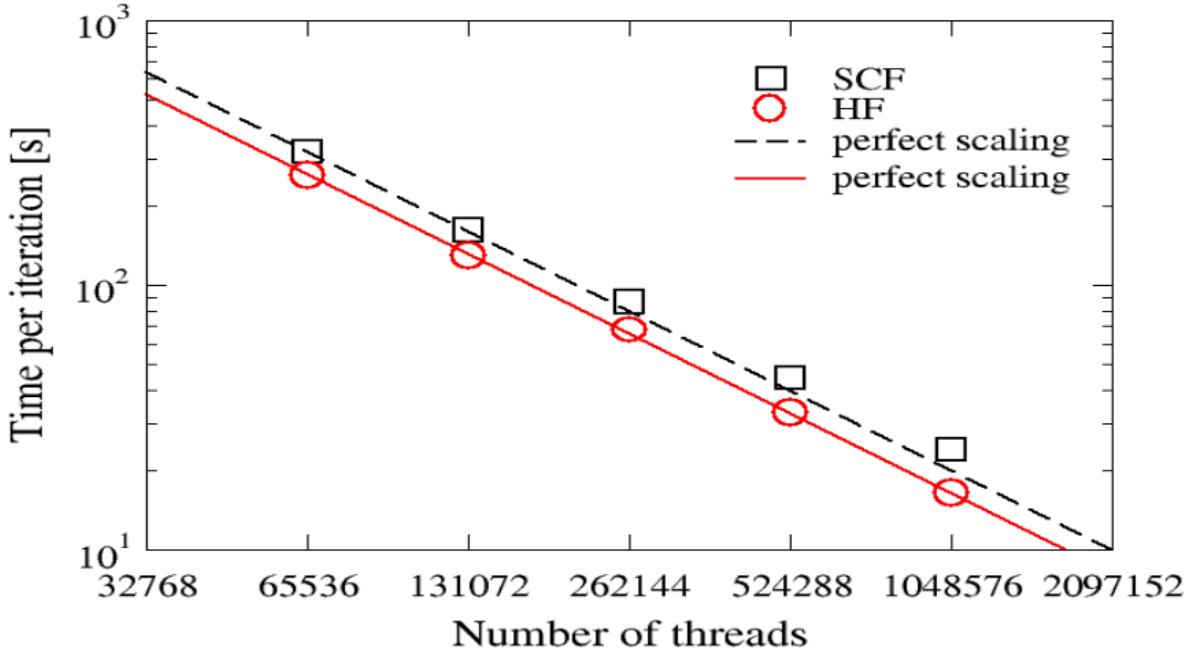
- Performance characteristics:
  - Simple flat profile
  - Representative of other DFT codes (PW, FD)
  - TAU profile from BG/P (4 rpn, single-threaded ESSL)
  - 45% DGEMM and 55% other stuff
- Core-to-core speed-up (16 rpn, multi-threaded ESSL)
  - Theoretical: $[(0.45/2.0/1.88) + (0.55/1.88)]^{-1} = 2.42$
    - Factor of 2.0 from quad-FPU
    - Factor of 1.88 from clock-rate
  - Actual: 1.57
  - Reason?
    - ESSL's DGEMM requires some tuning
      - 45% of peak on BG/P at 4 rpn single-threaded
      - 18% of peak on BG/Q at 16 and 32 rpn multi-threaded
    - Factor of 1.88 is not free:
      - Most applications do not get ideal instruction mix. GPAW gets 18% FPU / 82% FXU.
      - Two instruction streams per core required, one instruction stream per hardware thread

GPAW - moving forward

- Status on Blue Gene/Q
  - Possible to get 2X core-to-core speed-up with 16 rpn on some cases
    - Operate on very large chunk of matrix increases peak performance (40%) of ESSL's multi-threaded DGEMM
    - Leads to large messages size in parallel matrix multiply but network seems to keep up
  - Working with IBM to improve DGEMM
  - Core-to-core speed-up:
    - Speculation/potential : $[(0.45/2.0/1.88*2.0) + (0.55/1.88)]^{-1} = 2.88$
    - Assumptions:
      - >80% of peak for DGEMM on BG/Q,
      - Three remaining kernels can be threaded and have ideal instruction mix
  - Scalable to 8-racks but still suffers from the aforementioned algorithmic issues.
- Challenges ahead:
  - Reduced-scaling DFT code needed for Type 1S calculations
  - LCF staff (Jeff Hammond, Alvaro Vazquez) are working on MADNESS for the Type 1S calculations.

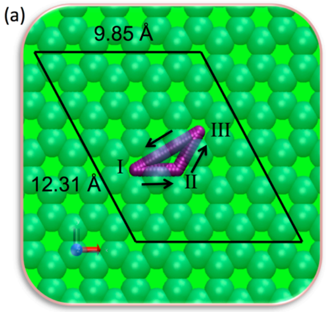
CPMD - performance on Blue Gene/Q

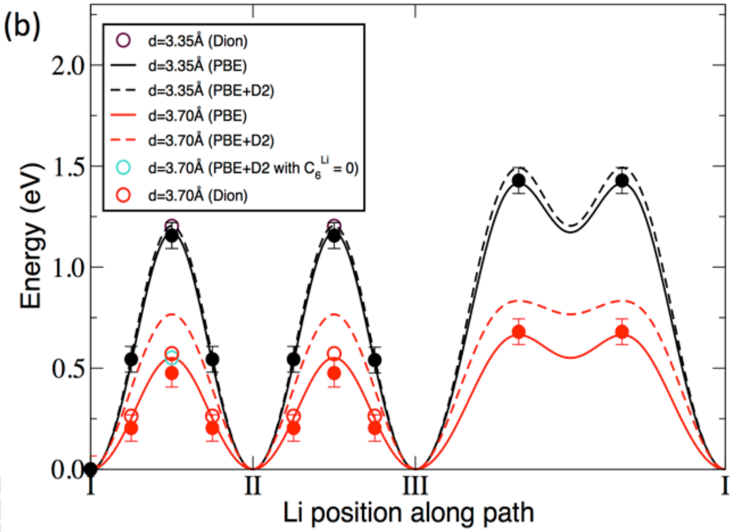
- Type 1A calculation (data from Curioni (IBM Zurich)):
  - hybrid DFT (PBE0) in a PW basis
  - Precondition conjugate gradient for minimization of wave function
  - 1000 atoms



QMCPACK - scientific motivation

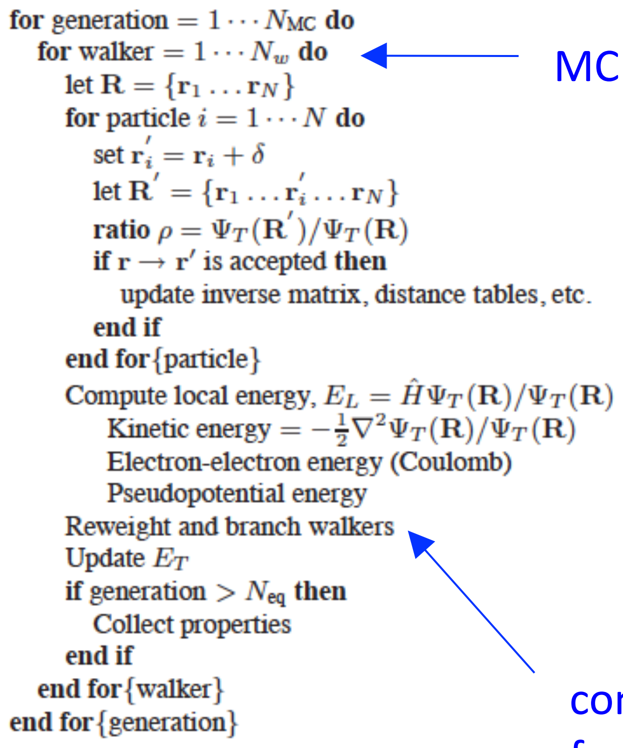
- quantum Monte Carlo (QMC)
  - Variational Monte Carlo (VMC) and Diffusion Monte Carlo (DMC).
    - Supports many basis: PW, B-splines, LCAO
    - Supports many boundary conditions
  - MPI and OpenMP parallelism, written in C++ and C.
  - Mainly used for Type 1A calculations, especially where DFT is problematic
    - vdW systems
    - Strong-correlated systems
- Li-ion diffusion and binding in graphitic battery anodes, by Ganesh, Kent, Reboredo & Kim





QMCPACK - performance on Blue Gene/P

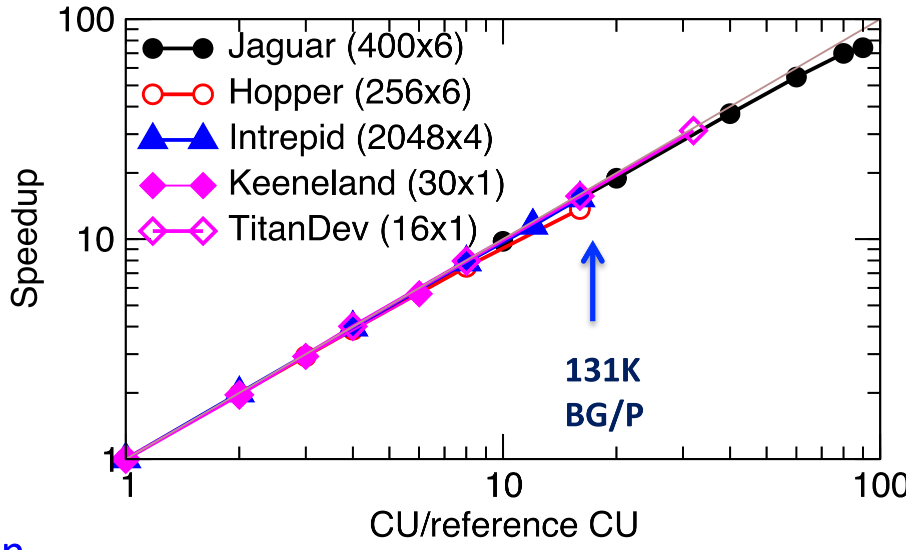
- Performance characteristics
  - Little communication, scales nearly perfectly
  - Easier to talk about node-to-node speed-up and thus realize full potential of BG/Q



```
for generation $= 1 \cdots N_{\mathrm{MC}}$ do
  for walker $= 1 \cdots N_w$ do
    let $\mathbf{R} = \{\mathbf{r}_1 \ldots \mathbf{r}_N\}$
    for particle $i = 1 \cdots N$ do
      set $\mathbf{r}_i^{'} = \mathbf{r}_i + \delta$
      let $\mathbf{R}^{'} = \{\mathbf{r}_1 \ldots \mathbf{r}_i^{'} \ldots \mathbf{r}_N\}$
      ratio $\rho = \Psi_T(\mathbf{R}^{'})/\Psi_T(\mathbf{R})$
      if $\mathbf{r} \rightarrow \mathbf{r}'$ is accepted then
        update inverse matrix, distance tables, etc.
      end if
    end for{particle}
    Compute local energy, $E_L = \hat{H}\Psi_T(\mathbf{R})/\Psi_T(\mathbf{R})$
       Kinetic energy $= -\frac{1}{2}\nabla^2\Psi_T(\mathbf{R})/\Psi_T(\mathbf{R})$
       Electron-electron energy (Coulomb)
       Pseudopotential energy
    Reweight and branch walkers
    Update $E_T$
    if generation $> N_{\mathrm{eq}}$ then
      Collect properties
    end if
  end for{walker}
end for{generation}
```

MC Walker is basic unit of parallelism

communication for DMC



131K BG/P

QMCPACK - performance on Blue Gene/Q

Eval_Z: Evaluation of spline

Eval_Z_VGH: Evaluation of spline derivatives

Symmetric_DTD: Distance table

- Original Esler Algorithm:

  4 nested loops (x,y,z,spline)

  No optimization of operations
- Killough Algorithm:

  2 nested loops (spline, x)

  2 unrolled loops (y,z)

  Optimization of operations
- Morozov Algorithm:

  4 nested loops (x,y,z,spline)

  Unrolling loops (4 times less iterations)
- Best Algorithms (GNU)

  - Eval_z: Morozov Algo.

  - Eval_z_vgh: Killough Algo.
- Best Algorithms (XL)

  - Eval_z: Morozov Algo.

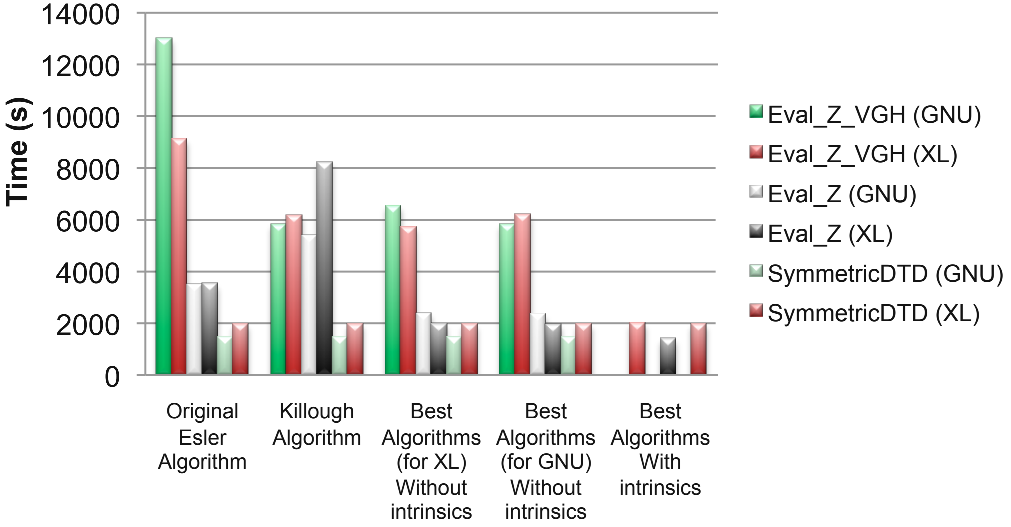
  - Eval_z_vgh: Benali Algo (Based on Morozov).
- Intrinsics (XL QPX)

  - Eval_z: Morozov Algo (with intrinsics).

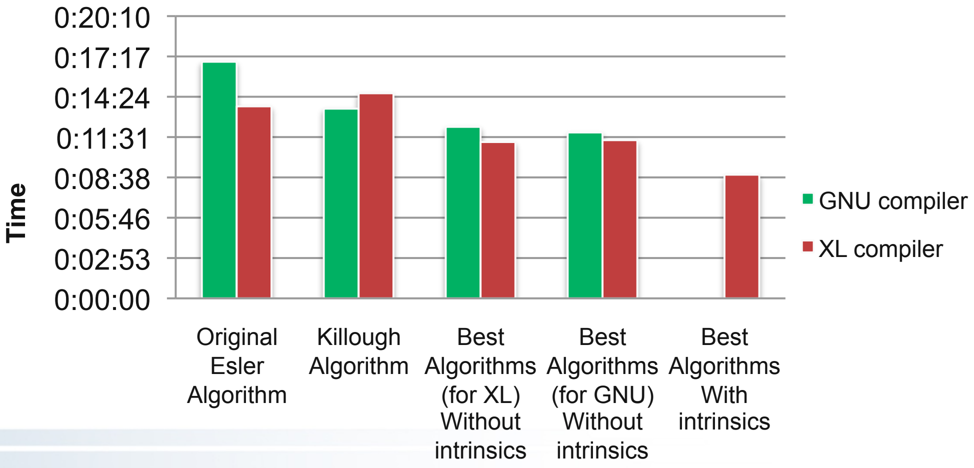
  - Eval_z_vgh: Benali Algo (Unrolling two loops

and adding intrinsics).

Kernels timing



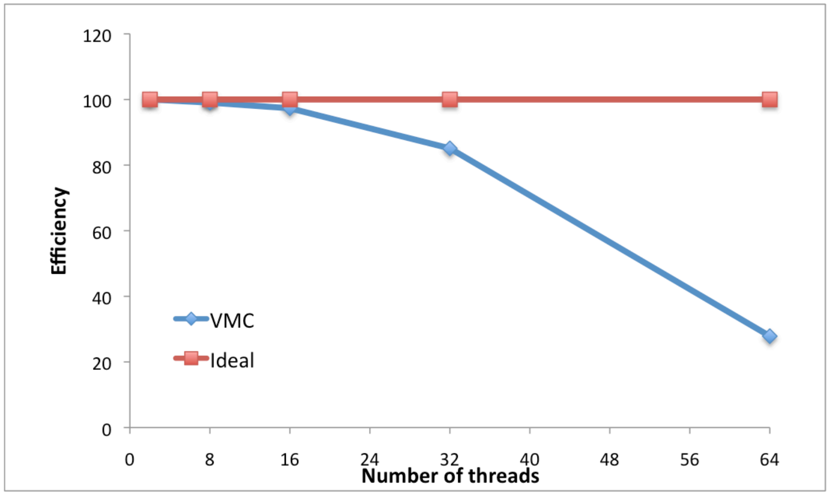
Total Application times



QMCPACK - performance on Blue Gene/Q (cont'd)

- Node-to-node speed-up (4 tpn on BG/P, 64 tpn on BG/Q):
  - Theoretical: 2.0*7.52 = 15.04
    - Factor of 2.0 from quad-FPU
    - Factor of 1.88 from clock-rate AND hardware threads
    - Factor of 4 from higher density of cores
  - Actual: 12.38
    - QPX speed-up of EVAL_Z_VGH by a factor of 3
    - 9.8 speed-up from OpenMP parallelism at 64 tpn compared to 4 tpn
    - Backward-port Blue Gene/P reference number based on best algorithm

Round-robin assignment of OpenMP threads to cores



QMCPACK - moving forward

- Status on Blue Gene/Q:
  - Science runs will begin soon.
  - Working on single precision version of Einspline
    - Needed for time-to-solution to be competitive with GPU version
    - Will reduce memory requirements for storing wave function, allows simulation of larger systems
  - We will scale QMCPACK to all 48-racks of Mira as proof-of-principle in the near future
- Challenges:
  - Percentage of peak is very low ~ 3%
    - Many kernels bandwidth limited (i.e. QPX will not help)
  - Large QMC problems (> 1000 valence electrons) will require nested OpenMP parallelism
  - More compact representations of the wave function needed
    - LAPW (in progress)
    - Distribute/tessellate wave function without a performance hit
  - Trial wave function currently optimized with serial LAPACK (general non-symmetric EVP)

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