Performance Evaluation of NWChem Ab-Initio Molecular Dynamics (AIMD) Simulations on the Intel® Xeon Phi™ Processor

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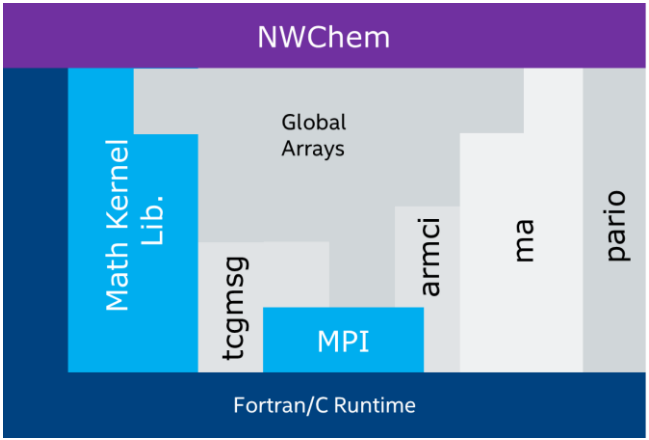
Notice revision #20110804

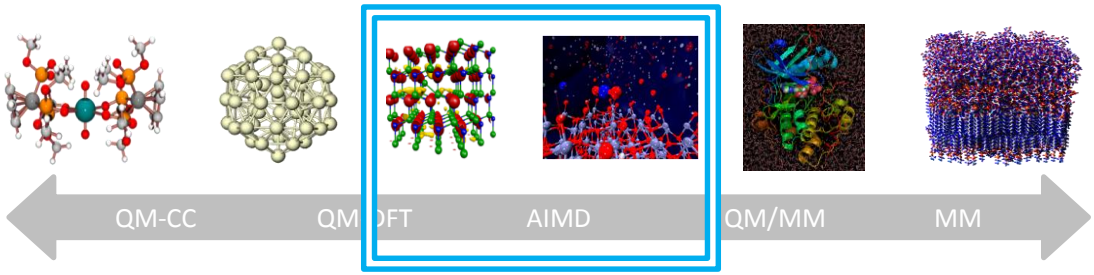
NWChem Fun Facts

- URL: www.nwchem-sw.org



Language	# files	LOC
Fortran 77	17147	4823003
C	857	242622
Bourne Shell	39	164184
HTML	182	55168
make	398	44373
TeX	115	39884
C/C++ Header	377	31217
Fortran 90	58	30525
Python	95	22571
m4	126	21894
C++	67	13489
Java	66	12311

Introduction: Plane Wave Methods



- 100-1000 atoms, uses plane wave basis
- Many FFTs and DGEMM operations
- “Meaty”: Lots of FLOPs, but also bandwidth sensitive

$$(-1/2)\nabla^2\Psi + V_{ext}\Psi + V_H\Psi + V_{xc}\Psi + V_{x,exact}\Psi = E\Psi$$

$$\langle \Psi_i | \Psi_j \rangle = \delta_{ij}$$

N_eN_g

$(N_aN_g + N_gLogN_g + N_eN_g) + N_aN_eN_g$

$N_eN_gLogN_g+N_eN_g+2N_gLogN_g+N_g+N_eN_g$

$N_eN_gLogN_g + N_eN_g$

$N_e(N_e+1)N_g\ LogN_g$

$N_e^2N_g + N_e^3$

N_a - number of atoms
N_e - number of electrons
N_g – size of FFT grid

Strong Scaling is Key

- 20 psec of simulation time ≈ 200,000 steps
  - 1 sec/step = 2-3 days simulation time
  - 10 sec/step = 23 days simulation time
  - 13 sec/step = 70 days simulation time
- Mesoscale phenomena at longer time scales
  - Assume 1 sec/step
  - 100 psec = 10-15 days simulation time
  - 1 nsec = 100 - 150 days simulation time
- Strong scaling required to reduce time per time step as much as possible
  - At least below 1sec/step

Plane Wave Discretization

$$H\psi_i(r) = -\tfrac{1}{2}\nabla^2 + V_L(r) + (1-\alpha)V_X[\rho](r) + V_C[\rho](r)$$
$$+ V_{NL} + V_H[\rho](r) - \alpha\sum_j K_{ij}(r)\psi_i(r)$$

Matrix multiplication in reciprocal space, SUMMA

$$\nabla^2 V_{H,X,C}(r) = -4\pi\rho(r) \qquad \nabla^2 K_{ij}(r) = -4\pi\psi_i(r)\psi_j(r)$$

N_e 3D-FFT Poisson $(N_e+1)N_e$ 3D-FFT

$$\rho(r) = \sum_{i=1}^{N}|\psi_i(r)|^2 \qquad \int_W \psi_i(r)\psi_j(r)dr = \delta_{ij}$$

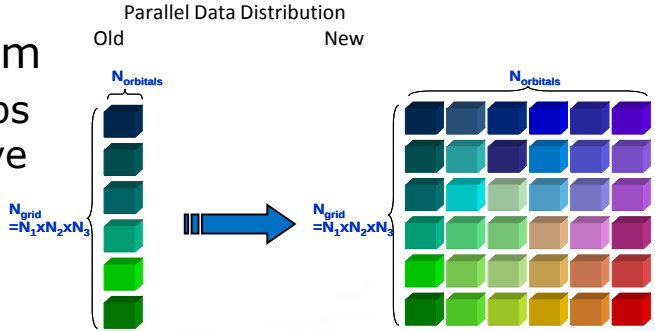
Density Orthogonality (matrix multiplication, SUMMA)

Plane Wave AIMD Computational Hotspots

- Three major hotspots with different performance behavior
- Applying V_H and V_{xc}, involving calculation of $2N_e$ 3D FFTs
- Non-local Pseudopotentials, V_{NL} with matrix multiplications of tall-and-skinny matrices
- Enforcing Orthogonality, with matrix multiplications of tall-and-skinny matrices

Plane Wave Data Distribution

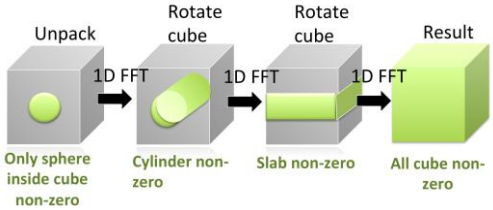
- Smart data distribution and communication algorithms enable DFT and hybrid-DFT to scale to large numbers of processors
- Multiple levels of parallelism
  - k-points through subgroups (fewer of them as we move to larger systems)
  - Parallel distribution of grid points and orbitals



Gygi et al. Supercomputing '06

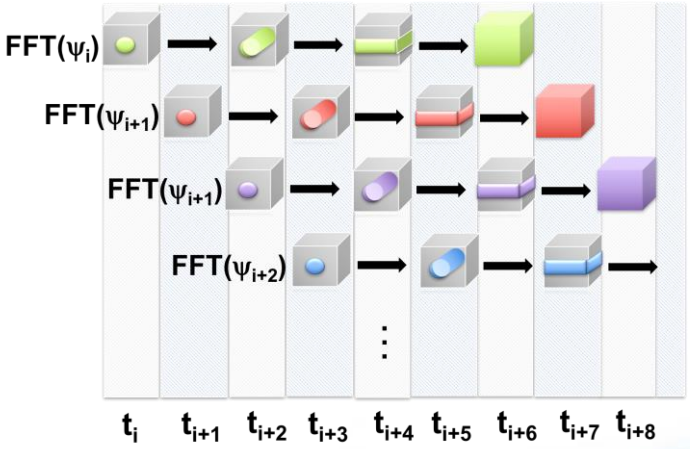
3D FFTs

- Performed at each step
  - 2 N_e 3D FFTs for DFT
  - Plus (N_e+1)*N_e 3D FFTs for hybrid DFT
- In reciprocal space, sphere of radius E_{cut} is stored
- Forward FFTs:
  1. Unpack sphere into a 3D cube (z,x,y)
  2. Perform $n_x \times n_y$ 1D FFTs along the z-dimension
  3. Rotate the cube ($z; x; y$) → ($y; z; x$)
  4. Perform $n_z \times n_x$ 1D FFTs along the y-dimension
  5. Rotate the cube ($y; z; x$) → ($x; y; z$)
  6. Perform $n_y \times n_z$ 1D FFTs along the x-dimension
- Backward FFTs: reverse above steps



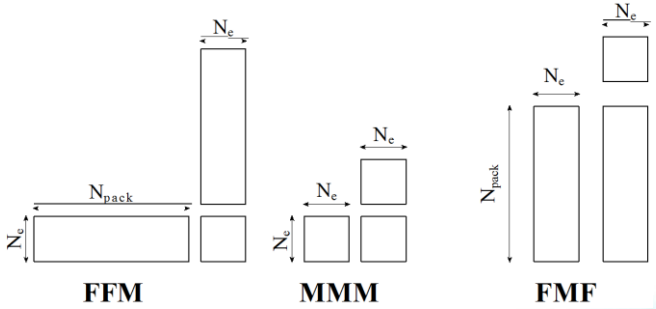
3D FFTs – Pipelined Implementation

- Performed at each step
  - 2 N_e 3D FFTs for DFT
  - Plus $(N_e+1)*N_e$ 3D FFTs for hybrid DFT
- In reciprocal space, sphere of radius E_{cut} is stored
- 3D FFTs are pipelined
  - Overlap communication and computation
  - Latency reduction
  - N^2 1D FFTs per stage execute in parallel

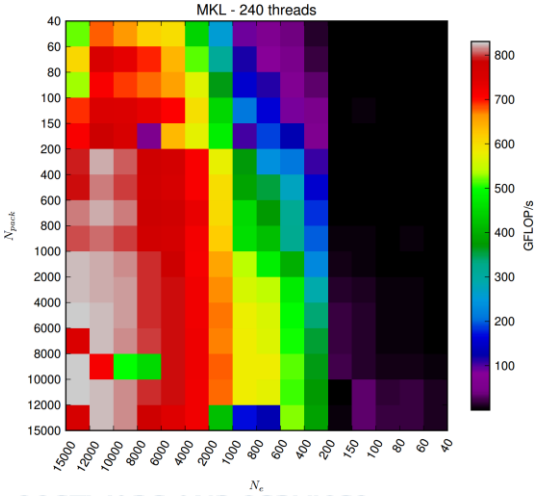


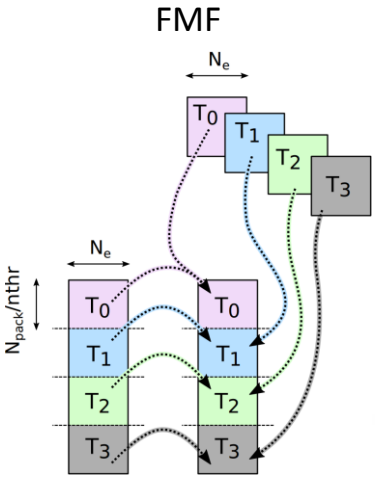
Lagrange Multiplier

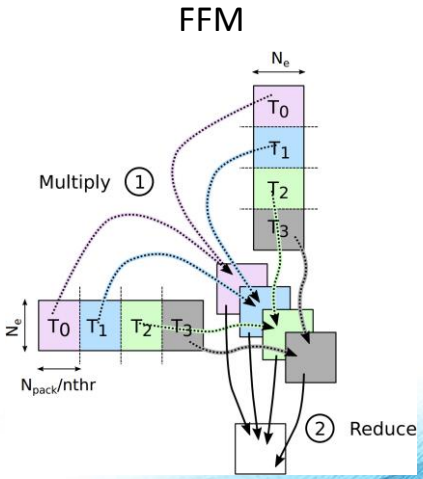
- Sequence of matrix products of shape F or M
  - F: N_{pack} x N_e or N_e x N_{pack} matrix (tall & skinny)
  - M: N_e x N_e matrix
  - In general: N_{pack} >> N_e



Lagrange Multiplier – Parallelization







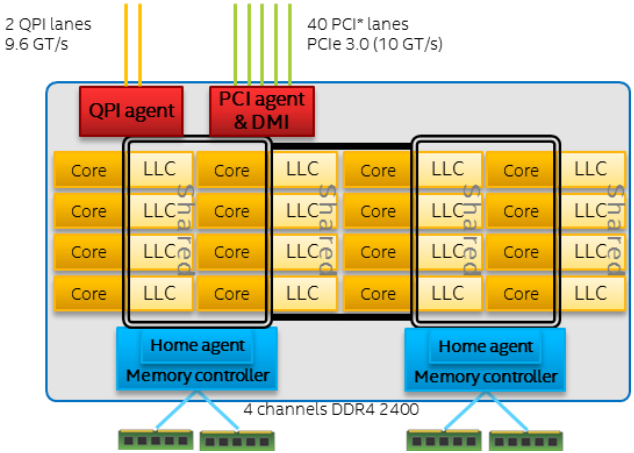
SOFTWARE AND SERVICES

Experimental Setup – NERSC Cori

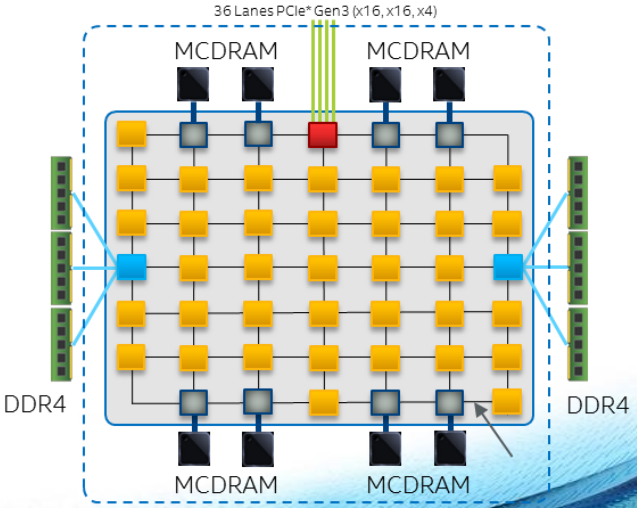
- "Haswell", HSW
  - Cray* XC40
  - 2S Intel® Xeon® E5-2698v3 processors
  - 32 cores, no Hyper-Threading
  - 2.3 GHz clock frequency
  - 128 GB of DDR4 at 2133 MHz
  - Cray* Aries* w/ Dragonfly
- "Knights Landing", KNL
  - Cray* XC40
  - Intel® Xeon Phi™ 7250 processors
  - 68 cores w/ 4 hardware threads
  - 1.4 GHz clock frequency
  - 96 GB of DDR4 at 2400 MHz
  - Cache mode
  - Quadrant cluster mode
  - Cray* Aries* w/ Dragonfly

Experimental Setup – Processor Architectures

- Intel® Xeon® E5-2697v3



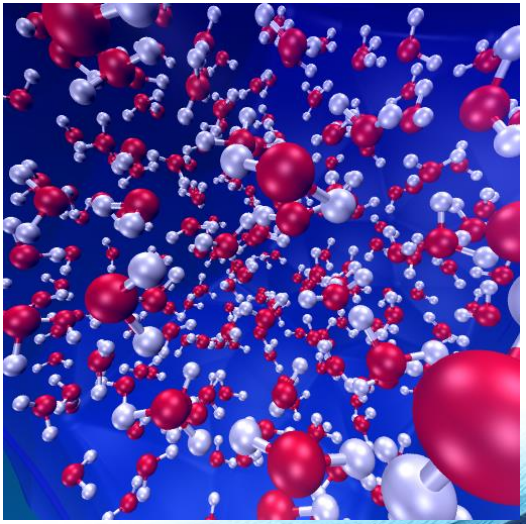
- Intel® Xeon Phi™ 7250



SOFTWARE AND SERVICES

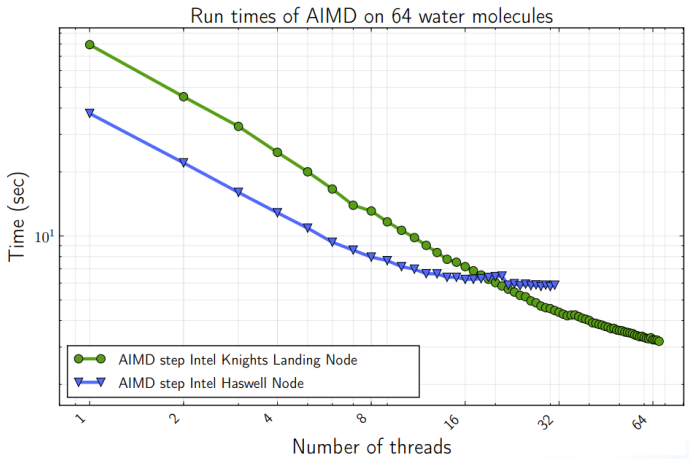
Experimental Setup – Benchmarks

- water64:
  - 64 water molecules in a box
  - test intra-node strong scaling
- water256:
  - 256 water molecules
  - test cluster strong scaling
  - N_e=2056
  - N_g=5,832,000 (180^3)
  - N_{pack}=437,000



Intra-node Performance

- Insight into performance without fabric effects
- Xeon node saturates at about 16 cores, reaching memory bandwidth limits
- Xeon Phi node keeps strong scaling due to the on-package cache memory
- 1.8x speed-up of KNL over HSW node



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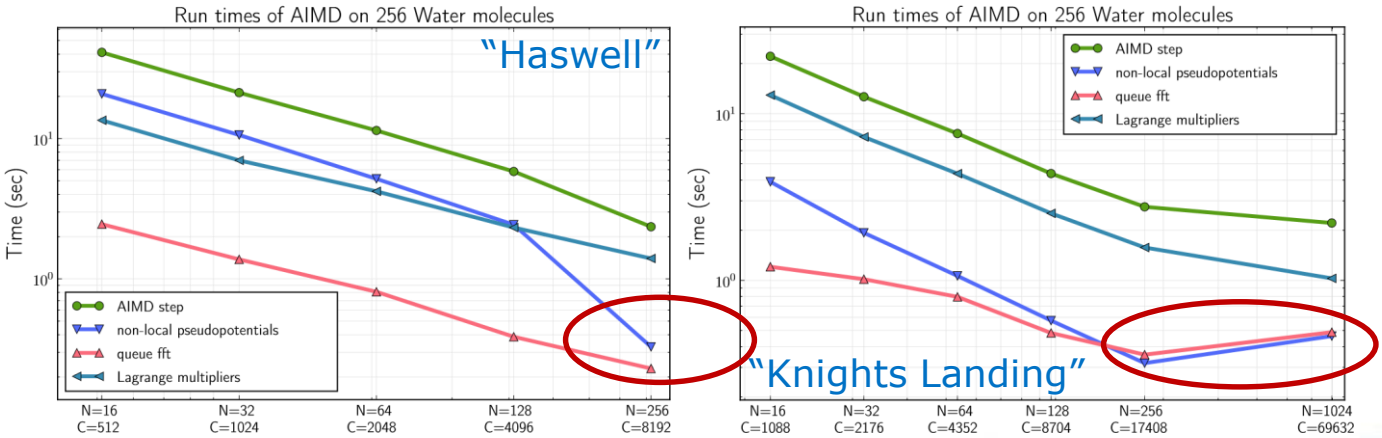
Performance



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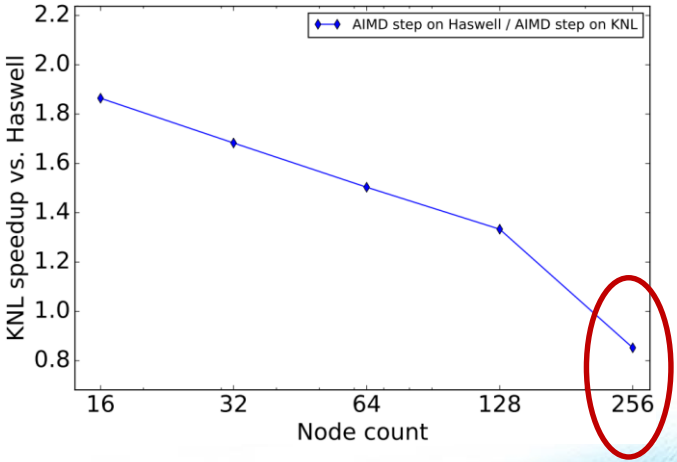
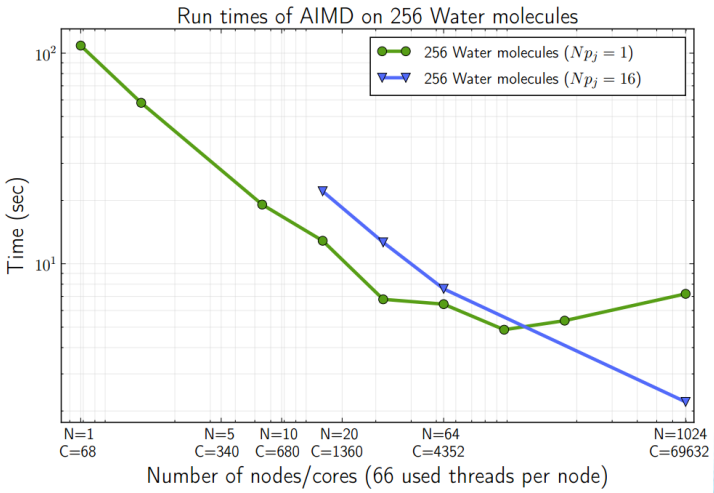
Relative Performance – HSW vs KNL

- Strong scaling regime
- Interconnect latency becomes visible
- Less occupancy of the network
- KNL seems to suffer from this more than HSW does



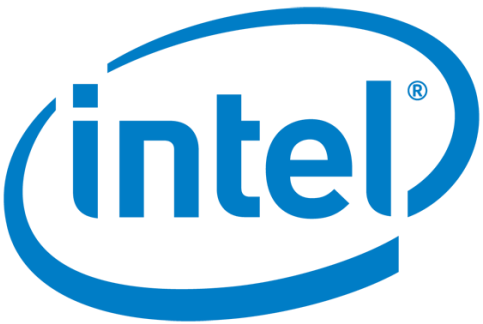
Performance – Effect of the Processor Grid

- Processor grid is a tradeoff
- 2D processor grid: $N_p = N_{pi} * N_{pj}$
- Large N_{pj} favors FFTs and non-local pseudopotentials
- Lagrange multiplier suffers from large N_{pi}
- Balancing N_{pi} and N_{pj} is required
  - problem size
  - number of ranks



The Last Slide…

- Hybridization of NWChem's AIMD code with MPI/OpenMP
- Plain library approaches were not good enough due to special requirements of the AIMD kernels
- Experiments show that AIMD can scale to O(1k) KNL nodes
- Future Work:
  - Re-use ideas of this work for hybrid DFTs and band-structure code
  - Investigate relationship between N_{pi} and N_{pj}
  - Apply all this to a "real" scientific problem ☺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