Quantum Chemistry (QC) on GPUs

March 2018
Overview of Life & Material Accelerated Apps

**MD:** All key codes are GPU-accelerated

- Great multi-GPU performance
- Focus on dense (up to 16) GPU nodes &/or large # of GPU nodes
- ACEMD*, AMBER (PMEMD)*, BAND, CHARMM, DESMOND, ESPReso, Folding@Home, GPUgrid.net, GROMACS, HALMD, HTMD, HOOMD-Blue*, LAMMPS, Lattice Microbes*, mdcore, MELD, miniMD, NAMD, OpenMM, PolyFTS, SOPO-GPU* & more

**QC:** All key codes are ported or optimizing

- Focus on using GPU-accelerated math libraries, OpenACC directives
- GPU-accelerated and available today:
  - ABINIT, ACES III, ADF, BigDFT, CP2K, GAMESS, GAMESS-UK, GPAW, LATTE, LSDalton, LSMS, MOLCAS, MOPAC2012, NWChem, OCTOPUS*, PETot, QUICK, Q-Chem, QMCPack, Quantum Espresso/PWscf, QUICK, TeraChem*
- Active GPU acceleration projects:
  - CASTEP, GAMESS, Gaussian, ONETEP, Quantum Supercharger Library*, VASP & more

`green*` = application where >90% of the workload is on GPU
# MD vs. QC on GPUs

<table>
<thead>
<tr>
<th>“Classical” Molecular Dynamics</th>
<th>Quantum Chemistry (MO, PW, DFT, Semi-Emp)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simulates positions of atoms over time; chemical-biological or chemical-material behaviors</td>
<td>Calculates electronic properties; ground state, excited states, spectral properties, making/breaking bonds, physical properties</td>
</tr>
<tr>
<td>Forces calculated from simple empirical formulas (bond rearrangement generally forbidden)</td>
<td>Forces derived from electron wave function (bond rearrangement OK, e.g., bond energies)</td>
</tr>
<tr>
<td>Up to millions of atoms</td>
<td>Up to a few thousand atoms</td>
</tr>
<tr>
<td>Solvent included without difficulty</td>
<td>Generally in a vacuum but if needed, solvent treated classically (QM/MM) or using implicit methods</td>
</tr>
<tr>
<td>Single precision dominated (FP32)</td>
<td>Double precision is important (FP64)</td>
</tr>
<tr>
<td>Uses cuFFT, CUDA</td>
<td>Uses cuBLAS, cuFFT, Tensor/Eigen Solvers, OpenACC</td>
</tr>
<tr>
<td>GeForce (Workstations), Tesla (Servers)</td>
<td>Tesla recommended</td>
</tr>
<tr>
<td>ECC off</td>
<td>ECC on</td>
</tr>
</tbody>
</table>
Using a supercomputer powered by the Tesla Platform with over 3,000 Tesla accelerators, University of Illinois scientists performed the first all-atom simulation of the HIV virus and discovered the chemical structure of its capsid — “the perfect target for fighting the infection.”

Without gpu, the supercomputer would need to be 5x larger for similar performance.
GPU-Accelerated Quantum Chemistry Apps
Green Lettering Indicates Performance Slides Included

- Abinit
- ACES III
- ADF
- BigDFT
- CP2K
- DIRAC
- GAMESS-US
- Gaussian
  - GPAW
  - FHI-AIMS
  - LATTE
  - LSDalton
  - MOLCAS
  - Mopac2012
  - NWChem
  - Octopus
  - ONETEP
  - Petot
  - Q-Chem
  - QMCPACK
  - Quantum Espresso
- Quantum SuperCharger Library
  - RMG
  - TeraChem
  - UNM
  - VASP
  - WL-LSMS

GPU Perf compared against dual multi-core x86 CPU socket.
ABINIT on GPUS

Speed in the parallel version:

- For ground-state calculations, GPUs can be used. This is based on CUDA+MAGMA.

- For ground-state calculations, the wavelet part of ABINIT (which is BigDFT) is also very well parallelized: MPI band parallelism, combined with GPUs.
BigDFT
Multiscale Modelling Methods for Applications in Materials Science  CECAM JÜLICH, GERMANY

Introduction to Electronic Structure Calculations with BigDFT

Thierry Deutsch, Damien Caliste, Luigi Genovese

L_Sim - CEA Grenoble

17 September 2013
BigDFT version 1.7: capabilities

- Free, surface and periodic boundary conditions
- Geometry optimizations (with constraints)
- Born-Oppenheimer Molecular Dynamics
- Saddle point searches (Nudged-Elastic Band Method)
- Vibrations
- External electric fields
- Unoccupied KS orbitals
- Collinear and Non-collinear magnetism
- All XC functionals of the ABINIT package
- Hybrid functionals
- Empirical van der Waals interactions (many flavors)
- Also available within the ABINIT package
BigDFT version 1.7: capabilities

http://bigdft.org

- Free, surface and periodic boundary conditions
- Geometry optimizations (with constraints)
- Born-Oppenheimer Molecular Dynamics
- Saddle point searches (Nudged-Elastic Band Method)
- Vibrations
- External electric fields
- Unoccupied KS orbitals
- Collinear and Non-collinear magnetism
- All XC functionals of the ABINIT package
- Hybrid functionals
- Empirical van der Waals interactions (many flavors)
- Also available within the ABINIT package
GPU-porting operations in BigDFT (double precision)

Convolutions (OpenCL rewritten)

GPU speedups between 10 and 20 can be obtained for different sections

Linear algebra (CUBLAS library)

The interfacing with CUBLAS is immediate, with considerable speedups
BigDFT code on Hybrid architectures

BigDFT code can run on hybrid CPU/GPU supercomputers
In multi-GPU environments, **double precision** calculations

---

**No Hot-spot operations**

Different code sections can be ported on GPU
up to 20x speedup for some operations,
7x for the full parallel code
Hands on

See


- First runs with BigDFT
- Basis-set convergence
- Acceleration example on different platforms:
  
  *Kohn-Sham DFT Operation with GPU acceleration*
**GAMESS valinomycin rimp2 energy on V100 vs P100 (PCIe 16GB)**

- **1 Broadwell node**
- **1 node + 1x P100 PCIe per node**
- **1 node + 2x P100 PCIe per node**
- **1 node + 4x P100 PCIe per node**
- **1 node + 1x V100 PCIe per node**
- **1 node + 2x V100 PCIe per node**
- **1 node + 4x V100 PCIe per node**

(Untuned on Volta)
Running **GAMESS**

The **blue node** contains Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs

The **green nodes** contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe (16GB) or V100 PCIe (16GB) GPUs
Gaussian 16
March 2018
Using OpenACC allowed us to continue development of our fundamental algorithms and software capabilities simultaneously with the GPU-related work. In the end, we could use the same code base for SMP, cluster/network and GPU parallelism. PGI’s compilers were essential to the success of our efforts.
Effects of using K80 boards
Haswell E5-2698 v3@2.3GHz

Number of K80 boards
- 0
- 1
- 2
- 4

Speed-up over run without GPUs

- rg-a25
- rg-a25td
- rg-on
- rg-ontd
- rg-val

- 7.4 hrs
- 6.4 hrs
- 5.8 hrs
- 5.1 hrs
- 27.9 hrs
- 25.8 hrs
- 22.6 hrs
- 20.1 hrs
- 2.5 hrs
- 2.1 hrs
- 1.7 hrs
- 1.5 hrs
- 55.4 hrs
- 43.6 hrs
- 33.7 hrs
- 26.8 hrs
- 229.0 hrs
- 168.4 hrs
- 141.7 hrs
- 101.5 hrs
GAUSSIAN 16 P100 PERFORMANCE

Dual-socket 28-core Broadwell vs 8x P100 GPUs
GPU-ACCELERATED GAUSSIAN 16 AVAILABLE
100% PGI OpenACC Port (no CUDA)

- Gaussian is a Top Ten HPC (Quantum Chemistry) Application.
- **80-85% of use cases are GPU-accelerated** (Hartree-Fock and DFT: energies, 1st derivatives (gradients) and 2nd derivatives for ground & excited states). More functionality to come.
- K40, K80, P100 support; B.01 release.
- **No pricing difference** between Gaussian CPU and GPU versions.
- Existing Gaussian 09 **customers under maintenance contract get (free) upgrade**.
- Existing non-maintenance customers required to pay upgrade fee.
- To get the bits or to ask about the upgrade fee, please contact Gaussian, Inc.’s Jim Hess, Operations Manager; jhess@gaussian.com.
rg-a25 on K80s

Running Gaussian version 16

The blue node contains Dual Intel Xeon E5-2698 v3@2.3GHz (Haswell) CPUs

The green nodes contain Dual Intel Xeon E5-2698 v3@2.3GHz (Haswell) CPUs + Tesla K80 (autoboost) GPUs

Alanine 25. Two steps: Force and Frequency. APFD 6-31G*  
nAtoms = 259, nBasis = 2195
rg-a25td on K80s

Running Gaussian version 16

The blue node contains Dual Intel Xeon E5-2698 v3@2.3GHz (Haswell) CPUs

The green nodes contain Dual Intel Xeon E5-2698 v3@2.3GHz (Haswell) CPUs + Tesla K80 (autoboost) GPUs

Alanine 25. Two Time-Dependent (TD) steps: Force and Frequency. APFD 6-31G* nAtoms = 259, nBasis = 2195

```
25.8 hrs
22.6 hrs
20.1 hrs
```

```
1 Haswell node
1 node + 1x K80 per node
1 node + 2x K80 per node
1 node + 4x K80 per node
```
rg-on on K80s

Running Gaussian version 16

The **blue node** contains Dual Intel Xeon E5-2698 v3@2.3GHz (Haswell) CPUs

The **green nodes** contain Dual Intel Xeon E5-2698 v3@2.3GHz (Haswell) CPUs + Tesla K80 (autoboost) GPUs

GFP ONIOM. Two steps: Force and Frequency. APFD/6-311+G(2d,p):amber=softfirst)=embed nAtoms = 3715 (48/3667), nBasis = 813
rg-ontd on K80s

Running **Gaussian** version 16

The **blue node** contains Dual Intel Xeon E5-2698 v3@2.3GHz (Haswell) CPUs

The **green nodes** contain Dual Intel Xeon E5-2698 v3@2.3GHz (Haswell) CPUs + Tesla K80 (autoboost) GPUs

GFP ONIOM. Two Time-Dependent (TD) steps: Force and Frequency. APFD/6-311+G(2d,p):amber=softfirst)=embed

nAtoms = 3715 (48/3667), nBasis = 813
**rg-val on K80s**

<table>
<thead>
<tr>
<th>Speed-up vs Dual Haswell</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5x</td>
</tr>
<tr>
<td>2.0x</td>
</tr>
<tr>
<td>1.5x</td>
</tr>
<tr>
<td>1.0x</td>
</tr>
<tr>
<td>0.5x</td>
</tr>
<tr>
<td>0.0x</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Haswell node</td>
<td>229.0 hrs</td>
</tr>
<tr>
<td>1 node + 1x K80 per node</td>
<td>168.4 hrs</td>
</tr>
<tr>
<td>1 node + 2x K80 per node</td>
<td>141.7 hrs</td>
</tr>
<tr>
<td>1 node + 4x K80 per node</td>
<td>101.5 hrs</td>
</tr>
</tbody>
</table>

Running **Gaussian** version 16

The **blue node** contains Dual Intel Xeon E5-2698 v3@2.3GHz (Haswell) CPUs

The **green nodes** contain Dual Intel Xeon E5-2698 v3@2.3GHz (Haswell) CPUs + Tesla K80 (autoboost) GPUs

Valinomycin. Two steps: Force and Frequency. APFD 6-311+G(2d,p)

\[ n_{\text{Atoms}} = 168, \ n_{\text{Basis}} = 2646 \]
Gaussian 16 Supported Platforms

- 4-way collaboration; Gaussian, Inc., NVIDIA (& PGI) and HPE
- HPE, NVIDIA and PGI is the development platform
- All released/certified x86_64 versions of Gaussian 16 use the PGI compilers
- Certified versions of Gaussian 16 use Intel only for Itanium, XLF for some IBM platforms, Fujitsu compilers for some SPARC-based machines and PGI for the rest (including some Apple products)
- GINC is collaborating with IBM, PGI (and NVIDIA) to release an OpenPower version of Gaussian that also uses the PGI compiler
- See Gaussian Supported Platforms for more details: http://gaussian.com/g16/g16_plat.pdf
CLOSING REMARKS

Significant Progress has been made in enabling Gaussian on GPUs with OpenACC

OpenACC is increasingly becoming more versatile

Significant work lies ahead to improve performance

Expand feature set:

  PBC, Solvation, MP2, triples-Corrections
ACKNOWLEDGEMENTS

Development is taking place with:

Hewlett-Packard (HP) Series SL2500 Servers (Intel® Xeon® E5-2680 v2 (2.8GHz/10-core/25MB/8.0GT-s QPI/115W, DDR3-1866))

NVIDIA® Tesla® GPUs (V100)

PGI Accelerator Compilers (18.x) with OpenACC (2.5 standard)
Increase Performance with Kepler

Running GPAW 10258

The **blue nodes** contain 1x E5-2687W CPU (8 Cores per CPU).

The **green nodes** contain 1x E5-2687W CPU (8 Cores per CPU) and 1x or 2x NVIDIA K20X for the GPU.
Increase Performance with Kepler

Running GPAW 10258

The **blue nodes** contain 1x E5-2687W CPU (8 Cores per CPU).

The **green nodes** contain 1x E5-2687W CPUs (8 Cores per CPU) and 2x NVIDIA K20 or K20X for the GPU.
Increase Performance with Kepler

Running **GPAW 10258**

The **blue nodes** contain 2x E5-2687W CPUs (8 Cores per CPU).

The **green nodes** contain 2x E5-2687W CPUs (8 Cores per CPU) and 2x NVIDIA K20 or K20X for the GPU.
Multi-GPU Accelerated Large Scale Electronic Structure Calculations

Samuli Hakala
COMP Centre of Excellence
Department of Applied Physics
Aalto University School of Science
Email: samuli.hakala@aalto.fi

GPU Technology Conference, March 2013
**GPAW**

- Density Functional Theory (DFT) program package for electronic structure calculations
- Time-Dependent Density Functional Theory (TDDFT) is implemented in the linear response and time propagation schemes
- Can use real-space grids, atom centered basis functions or plane waves
- Random Phase Approximation (RPA) also available
- Scales to thousands of cores and suitable for large scale calculations
- Open Source software licensed under GPL

*Ground state DFT calculation of 561 Au atom cluster on Blue Gene/P.
LibXC on GPUs

- A reusable library of >250 exchange-correlation functionals
- Used by 15 different codes (Abinit, GPAW, BigDFT, etc.)
- Can be a performance bottleneck for small systems
- Can “clone” existing functionals for GPU use with fairly minimal changes to existing LibXC code and parallelizes well over grid points
- More information:
  - [https://confluence.slac.stanford.edu/display/SUNCAT/libxc+on+GPUs](https://confluence.slac.stanford.edu/display/SUNCAT/libxc+on+GPUs)
- Work by Lin Li, Jun Yan, Christopher O’Grady (Stanford/SLAC)

<table>
<thead>
<tr>
<th>Functional</th>
<th>Type</th>
<th>Speedup ((GPU+CPU)/CPU)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PW, PW Mode, OB PW, PW RPA</td>
<td>LDA Correlation</td>
<td>23, 23, 23, 37</td>
</tr>
<tr>
<td>PBE, PBE sol, xPBE, PBE JRGX, RGE2, APBE</td>
<td>GGA Correlation</td>
<td>56, 58, 58, 58, 58, 58</td>
</tr>
<tr>
<td>RPBE</td>
<td>GGA Exchange</td>
<td>95</td>
</tr>
<tr>
<td>TPSS</td>
<td>MGGA Exchange</td>
<td>51</td>
</tr>
</tbody>
</table>
Ground State Performance

**Bulk Silicon**
- 95 atoms with periodic boundary conditions, 380 bands and 1 k-point. Grid size: 56x56x80.
- Time is in seconds per one SCF iteration.
- Intel Xeon X5650, NVIDIA Tesla M2070

<table>
<thead>
<tr>
<th>Si95</th>
<th>CPU</th>
<th>GPU</th>
<th>%</th>
<th>S-Up</th>
</tr>
</thead>
<tbody>
<tr>
<td>Poisson Solver</td>
<td>1.8</td>
<td>0.13</td>
<td>1%</td>
<td>14</td>
</tr>
<tr>
<td>Orthonormalization</td>
<td>23</td>
<td>3.0</td>
<td>23%</td>
<td>7.7</td>
</tr>
<tr>
<td>Precondition</td>
<td>9.4</td>
<td>0.77</td>
<td>6%</td>
<td>12</td>
</tr>
<tr>
<td>RMM-DIIS other</td>
<td>32</td>
<td>3.2</td>
<td>25%</td>
<td>10</td>
</tr>
<tr>
<td>Subspace Diag</td>
<td>23</td>
<td>2.1</td>
<td>16%</td>
<td>11</td>
</tr>
<tr>
<td>Other</td>
<td>2.7</td>
<td>2.7</td>
<td>21%</td>
<td>1.0</td>
</tr>
<tr>
<td><strong>Total (SCF-Iter)</strong></td>
<td><strong>93</strong></td>
<td><strong>13</strong></td>
<td><strong>9.7/7.7</strong></td>
<td></td>
</tr>
</tbody>
</table>

**Fullerene**
- C60 molecule with 240 valence electrons. Grid size: 84x84x84
- Intel Xeon X5650, NVIDIA Tesla M2070

<table>
<thead>
<tr>
<th>C60</th>
<th>CPU</th>
<th>GPU</th>
<th>%</th>
<th>S-Up</th>
</tr>
</thead>
<tbody>
<tr>
<td>Poisson Solver</td>
<td>13</td>
<td>0.64</td>
<td>7%</td>
<td>20</td>
</tr>
<tr>
<td>Orthonormalization</td>
<td>11</td>
<td>1.2</td>
<td>13%</td>
<td>9.2</td>
</tr>
<tr>
<td>Precondition</td>
<td>16</td>
<td>0.99</td>
<td>11%</td>
<td>16</td>
</tr>
<tr>
<td>RMM-DIIS other</td>
<td>8.1</td>
<td>0.6</td>
<td>7%</td>
<td>13</td>
</tr>
<tr>
<td>Subspace Diag</td>
<td>22</td>
<td>2.1</td>
<td>23%</td>
<td>10</td>
</tr>
<tr>
<td>Other</td>
<td>3.5</td>
<td>3.2</td>
<td>35%</td>
<td>1.1</td>
</tr>
<tr>
<td><strong>Total (SCF-Iter)</strong></td>
<td><strong>76</strong></td>
<td><strong>9.1</strong></td>
<td><strong>13/8.3</strong></td>
<td></td>
</tr>
</tbody>
</table>
Multi-GPU Parallelization

- Parallelization is done with MPI
- Multiple GPUs can be used by domain decomposition or parallelization over k-points or spins
- Domain decomposition for the stencil operations involves exchanging boundary regions between neighboring nodes
- Communications between nodes require data movement: device memory → host memory → destinations node host memory → destinations node device memory.
- Overlaps receives, sends and computations in the middle part of the grid, BUT this causes issues with small grids
  - Small grids: Synchronous transfers
  - Medium grids: Asynchronous transfers
  - Large grids: Overlap calculations and asynchronous transfers
  - Combine of several wave functions and boundary regions into few large transfers
Weak Scalability (Carbon)

- The size of a carbon nanotube and the number of MPI tasks are varied from 80 atoms (240 states) to 320 atoms (1280 states) and 1 task to 12 tasks.
- Comparison between equal number of GPUs and CPU cores.
- CPU: Intel Xeon X5650  GPU: NVIDIA Tesla M2070
- Calculations performed on Vuori cluster at CSC

<table>
<thead>
<tr>
<th># MPI tasks</th>
<th>1</th>
<th>2</th>
<th>4</th>
<th>6</th>
<th>8</th>
<th>10</th>
<th>12</th>
</tr>
</thead>
<tbody>
<tr>
<td>Speed-Up</td>
<td>8.8</td>
<td>8.7</td>
<td>10.5</td>
<td>10.2</td>
<td>11.5</td>
<td>11.3</td>
<td>11.9</td>
</tr>
</tbody>
</table>
Strong Scalability

- Bulk silicon with 1151 atoms with periodic boundary conditions, 4604 bands and 1 k-point in the Brillouin zone.
- The number of GPUs is increased from 64 to 256.
- Grid size: 164x164x108
- Speed-up comparison to 64 GPUs.
- NVIDIA Tesla M2090
- Calculations performed on CURIE cluster in France at GENCI/CEA
Weak Scalability (Silicon)

- The size of bulk silicon system and the number of MPI tasks are varied from 383 atoms (1532 bands) to 2046 atoms (8188 bands) and 8 task to 256 tasks with periodic boundary conditions.
- The largest system requires about 1.3TB of memory for calculations.
- CPU: Intel Xeon E5640 GPU: NVIDIA Tesla M2090
Random Phase Approximation

GPAW Random Phase Approximation (RPA) code:
- 6000 lines of python, 1000 lines of C/CUDA (and re-uses many GPAW functions)
- Better than DFT for correlated materials, but more computationally expensive
- Useful for oxides, Van der Waals systems, etc.

GPU Techniques:
- Use BLAS3 "zherk" instead of BLAS2 "zher"
- Batch FFTs
- GPU kernels parallelized over atoms/bands/projector-functions
- No thunking: all calculations on GPU

Preliminary ((GPU+CPU)/CPU) speedup for 202-electron $N_2$-on-Ru: 30x

Work by Jun Yan, Lin Li, Christopher O’Grady (Stanford/SLAC)
Summary

- We have accelerated the most numerically intensive parts of ground state DFT calculations.
- Overall speed-ups in our tests varied from 8.8 to 19 depending on system size.
- Our multi-GPU implementation scales well even on large hybrid clusters.
- Code is available at GPAW Subversion repository.
- Acknowledgements to CSC and PRACE for computing resources.

OpenACC makes GPU computing approachable for domain scientists. Initial OpenACC implementation required only minor effort, and more importantly, no modifications of our existing CPU implementation.

Janus Juul Eriksen, PhD Fellow
qLEAP Center for Theoretical Chemistry, Aarhus University

NWChem
NWChem 6.3 Release with GPU Acceleration

Addresses large complex and challenging molecular-scale scientific problems in the areas of catalysis, materials, geochemistry and biochemistry on highly scalable, parallel computing platforms to obtain the fastest time-to-solution.

Researchers can for the first time be able to perform large scale coupled cluster with perturbative triples calculations utilizing the NVIDIA GPU technology. A highly scalable multi-reference coupled cluster capability will also be available in NWChem 6.3.

The software, released under the Educational Community License 2.0, can be downloaded from the NWChem website at www.nwchem-sw.org
NWChem - Speedup of the non-iterative calculation for various configurations/tile sizes

System: cluster consisting of dual-socket nodes constructed from:

- 8-core AMD Interlagos processors
- 64 GB of memory
- Tesla M2090 (Fermi) GPUs

The nodes are connected using a high-performance QDR Infiniband interconnect

Courtesy of Kowolski, K., Bhaskaran-Nair, at al @ PNNL, JCTC (submitted)
Kepler, Faster Performance (NWChem)

Performance improves by **2x** with one GPU and by **3.1x** with 2 GPUs.
CUDA Fortran gives us the full performance potential of the CUDA programming model and NVIDIA GPUs. !$CUF KERNELS directives give us productivity and source code maintainability. It’s the best of both worlds.

Filippo Spiga
Head of Research Software Engineering
University of Cambridge

www.quantum-espresso.org
QUANTUM ESPRESSO PERFORMANCE

Benchmark Si63GE-vc-relax

System information:

KNL: Cineca System A2 nodes (Xeon Phi 7250 @ 1.4GHz, 68 cores, 16GB MCDRAM and 96GB DDR4 per node)
Broadwell: CSCS Piz Dora Cray XC50 nodes (2 Xeon E5-2695 V4 @ 2.1GHz, 36 cores and 128GB DDR4 per node)
P100: CSCS Piz Dora Cray XC50 nodes (1 Xeon E5-2695 V4 @ 2.1GHz, 18 cores, 64/128GB DDR4 and one Tesla P100 per node)
All timings for complete energy and gradient Calculations

K80 = 1 GPU on Board, not both

Slide courtesy of PetaChem LLC / Todd Martinez
TERACHEM 1.5K; TRIPCAGE ON TESLA K40S

TeraChem 1.5K; TripCage on Tesla K40s & IVB CPUs
(Total Processing Time in Seconds)
**TERACHEM 1.5K; TRIPCAGE ON TESLA K40S & HASWELL CPUS**

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Total Processing Time (Seconds)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 x Xeon E5-2698 <a href="mailto:v3@2.30GHz">v3@2.30GHz</a> + 1 x Tesla K40@875Mhz (1 node)</td>
<td>160</td>
</tr>
<tr>
<td>2 x Xeon E5-2698 <a href="mailto:v3@2.30GHz">v3@2.30GHz</a> + 2 x Tesla K40@875Mhz (1 node)</td>
<td>80</td>
</tr>
<tr>
<td>2 x Xeon E5-2698 <a href="mailto:v3@2.30GHz">v3@2.30GHz</a> + 4 x Tesla K40@875Mhz (1 node)</td>
<td>40</td>
</tr>
</tbody>
</table>
TERACHEM 1.5K; TRIPCAGE ON TESLA K80S & IVB CPUS

TeraChem 1.5K; TripCage on Tesla K80s & IVB CPUs
(Total Processing Time in Seconds)
TERACHEM 1.5K; TRIPCAGE ON TESLA K80S & HASWELL CPUS

TeraChem 1.5K; TripCage on Tesla K80s & Haswell CPUs
(Total Processing Time in Seconds)

- 2 x Xeon E5-2698 v3@2.30GHz + 1 x Tesla K80 board (1 node)
- 2 x Xeon E5-2698 v3@2.30GHz + 2 x Tesla K80 boards (1 node)
- 2 x Xeon E5-2698 v3@2.30GHz + 4 x Tesla K80 boards (1 node)
TERACHEM 1.5K; BPTI ON TESLA K40S & IVB CPUs

(Total Processing Time in Seconds)
TERACHEM 1.5K; BPTI ON TESLA K80S & IVB CPUS

TeraChem 1.5K; BPTI on Tesla K80s & IVB CPUs
(Total Processing Time in Seconds)

- 2 x Xeon E5-2697 v2@2.70GHz + 1 x Tesla K80 board (1 node)
- 2 x Xeon E5-2697 v2@2.70GHz + 2 x Tesla K80 boards (1 node)
- 2 x Xeon E5-2697 v2@2.70GHz + 4 x Tesla K80 boards (1 node)
TeraChem 1.5K; BPTI on Tesla K40s & Haswell CPUs
(Total Processing Time in Seconds)
TERACHEM 1.5K; BPTI ON TESLA K80S & HASWELL CPUS

TeraChem 1.5K; BPTI on Tesla K80s & Haswell CPUs
(Total Processing Time in Seconds)

- 2 x Xeon E5-2698 v3@2.30GHz + 1 x Tesla K80 board (1 node)
- 2 x Xeon E5-2698 v3@2.30GHz + 2 x Tesla K80 boards (1 node)
- 2 x Xeon E5-2698 v3@2.30GHz + 4 x Tesla K80 boards (1 node)
Beyond VASP 5.4.4 Development

March 2018
For VASP, OpenACC is the way forward for GPU acceleration. Performance is similar to CUDA, and OpenACC dramatically decreases GPU development and maintenance efforts. We’re excited to collaborate with NVIDIA and PGI as an early adopter of Unified Memory.
B.aP107 on V100s PCIe

(Untuned on Volta)
Running VASP version 5.4.4

The blue node contains Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla V100 PCIe (16GB) GPUs

107 Boron atoms (symmetry broken 107-atom $B'$ variant)
216 bands
110592 plane waves
Hybrid functional calculation (exact exchange) with blocked Davidson. No KPoint parallelization.
Hybrid Functional with blocked Davidson (ALGO=Normal) LHFCALC=.True. (Exact Exchange)
Silica IFPEN on V100s PCIe

(Untuned on Volta)
Running VASP version 5.4.4

The blue node contains Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla V100 PCIe (16GB) GPUs

240 ions, cristobalite (high) bulk
720 bands
? plane waves
ALGO = Very Fast (RMM-DIIS)
VASP Dev Version OpenACC Performance

silica IFPEN, RMM-DIIS on P100

Reasons for performance gain:

- OpenACC port covers more VASP routines
- OpenACC port planned top down, with complete analysis of the call tree
- OpenACC port leverages improvements in latest VASP Fortran source base
VASP with OpenACC is an ongoing project. The developers in Vienna are integrating some OpenACC into their code base and there are plans to continue porting in that direction. Given that there is ongoing work, chances are the next major release will contain some of the results of this work. But from NV’s side, we can neither comment on any release schedule for VASP in general, nor on any feature set for upcoming releases.
VASP 5.4.4
February 2018
VASP Silica IFPEN
on Gold 6140 vs V100 PCIe (32GB)

Running VASP version 5.4.4

The blue node contains Dual Intel Xeon Gold 6140@2.30GHz [2.301GHz Turbo] (Skylake) CPUs

The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla V100 PCIe (32GB) GPUs

240 ions, cristobalite (high) bulk
720 bands
? plane waves
ALGO = Very Fast (RMM-DIIS)
**VASP Silica IFPEN on Gold 6140 vs V100 SXM2 (32GB)**

(Untuned on Volta)
Running VASP version 5.4.4

The **blue node** contains Dual Intel Xeon Gold 6140@2.30GHz [2.301GHz Turbo] (Skylake) CPUs

The **green nodes** contain Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla V100 SXM2 (32GB) GPUs

240 ions, cristobalite (high) bulk
720 bands
? plane waves

ALGO = Very Fast (RMM-DIIS)
The blue node contains Dual Intel Xeon Platinum 8180@2.50GHz [2.501GHz Turbo] (Skylake) CPUs

The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla V100 PCIe (32GB) GPUs

240 ions, cristobalite (high) bulk, 720 bands, plane waves
ALGO = Very Fast (RMM-DIIS)
VASP Silica IFPEN
on Platinum 8180 vs V100 SXM2 (32GB)

Running VASP version 5.4.4

The blue node contains Dual Intel Xeon Platinum 8180@2.50GHz [2.501GHz Turbo] (Skylake) CPUs

The green nodes contain Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla V100 SXM2 (32GB) GPUs

240 ions, cristobalite (high) bulk
720 bands
? plane waves
ALGO = Very Fast (RMM-DIIS)
VASP Si-Huge on Gold 6140 vs V100 PCIe (32GB)

Running VASP version 5.4.4

The blue node contains Dual Intel Xeon Gold 6140@2.30GHz [2.301GHz Turbo] (Skylake) CPUs

The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla V100 PCIe (32GB) GPUs

512 Si atoms
1282 bands
864000 Plane Waves
Algo = Normal (blocked Davidson)
VASP Si-Huge
on Gold 6140 vs V100 SXM2 (32GB)

Running VASP version 5.4.4

The blue node contains Dual Intel Xeon Gold 6140@2.30GHz [2.301GHz Turbo] (Skylake) CPUs

The green nodes contain Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla V100 SXM2 (32GB) GPUs

512 Si atoms
1282 bands
864000 Plane Waves
Algo = Normal (blocked Davidson)
VASP Si-Huge on Platinum 8180 vs V100 PCIe (32GB)

The blue node contains Dual Intel Xeon Platinum 8180@2.50GHz [2.501GHz Turbo] (Skylake) CPUs

The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla V100 PCIe (32GB) GPUs

512 Si atoms
1282 bands
864000 Plane Waves
Algo = Normal (blocked Davidson)

(Untuned on Volta)
Running VASP version 5.4.4
**VASP Si-Huge on Platinum 8180 vs V100 SXM2 (32GB)**

Running VASP version 5.4.4

The blue node contains Dual Intel Xeon Platinum 8180@2.50GHz [2.501GHz Turbo] (Skylake) CPUs

The green nodes contain Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla V100 SXM2 (32GB) GPUs

512 Si atoms

1282 bands

864000 Plane Waves

Algo = Normal (blocked Davidson)
### VASP B.hR105 on Gold 6140 vs V100 PCIe (32GB)

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Performance (1/seconds)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Skylake node</td>
<td>0.0015</td>
</tr>
<tr>
<td>1 node + 1x V100 PCIe per node</td>
<td>0.0047</td>
</tr>
<tr>
<td>1 node + 2x V100 PCIe per node</td>
<td>0.0067</td>
</tr>
<tr>
<td>1 node + 4x V100 PCIe per node</td>
<td>0.0112</td>
</tr>
<tr>
<td>1 node + 8x V100 PCIe per node</td>
<td>0.0120</td>
</tr>
</tbody>
</table>

(Untuned on Volta)
Running VASP version 5.4.4

The **blue node** contains Dual Intel Xeon Gold 6140@2.30GHz [2.301GHz Turbo] (Skylake) CPUs

The **green nodes** contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla V100 PCIe (32GB) GPUs

105 Boron atoms (B-rhombohedral structure)
216 bands
110592 plane waves
Hybrid Functional with blocked Davicson (ALGO=Normal)
LHFCALC=.True. (Exact Exchange)
VASP B.hR105 on Gold 6140 vs V100 SXM2 (32GB)

Running VASP version 5.4.4

The blue node contains Dual Intel Xeon Gold 6140@2.30GHz [2.301GHz Turbo] (Skylake) CPUs

The green nodes contain Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla V100 SXM2 (32GB) GPUs

105 Boron atoms (B-rhombohedral structure)
216 bands
110592 plane waves
Hybrid Functional with blocked Davicson (ALGO=Normal)
LHFCALC=.True. (Exact Exchange)
VASP B.hR105 on Platinum 8180 vs V100 PCIe (32GB)

The blue node contains Dual Intel Xeon Platinum 8180@2.50GHz [2.501GHz Turbo] (Skylake) CPUs

The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla V100 PCIe (32GB) GPUs

105 Boron atoms (B-rhombohedral structure)  
216 bands  
110592 plane waves  
Hybrid Functional with blocked Davicson (ALGO=Normal)  
LHFCALC=.True. (Exact Exchange)
VASP B.hR105 on Platinum 8180 vs V100 SXM2 (32GB)

The blue node contains Dual Intel Xeon Platinum 8180@2.50GHz [2.501GHz Turbo] (Skylake) CPUs

The green nodes contain Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla V100 SXM2 (32GB) GPUs

105 Boron atoms (B-rhombohedral structure)
216 bands
110592 plane waves
Hybrid Functional with blocked Davicson (ALGO=Normal)
LHFCALC=.True. (Exact Exchange)

Running VASP version 5.4.4

(Untuned on Volta)
VASP 5.4.4
October 2017
Silica IFPEN on V100s PCIe

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Performance</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>0.00210</td>
</tr>
<tr>
<td>1 node + 2x V100 PCIe per node</td>
<td>0.00418</td>
</tr>
<tr>
<td>1 node + 4x V100 PCIe per node</td>
<td>0.00537 (2.6X)</td>
</tr>
<tr>
<td>1 node + 8x V100 PCIe per node</td>
<td>0.00628 (3.0X)</td>
</tr>
</tbody>
</table>

(Untuned on Volta)
Running VASP version 5.4.4

The **blue node** contains Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs

The **green nodes** contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla V100 PCIe (16GB) GPUs

- 240 ions, cristobalite (high) bulk
- 720 bands
- ? plane waves
- ALGO = Very Fast (RMM-DIIS)
Silica IFPEN on V100s SXM2

(Untuned on Volta)
Running VASP version 5.4.4

The blue node contains Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla V100 SXM2 (16GB) GPUs

240 ions, cristobalite (high) bulk
720 bands
? plane waves
ALGO = Very Fast (RMM-DIIS)
Si-Huge on V100s PCIe

(Untuned on Volta)
Running VASP version 5.4.4

The blue node contains Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla V100 PCIe (16GB) GPUs

512 Si atoms
1282 bands
864000 Plane Waves
Algo = Normal (blocked Davidson)
## Si-Huge on V100s SXM2

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Time (seconds)</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>0.00017</td>
<td></td>
</tr>
<tr>
<td>1 node + 2x V100 SXM2 per node (16GB)</td>
<td>0.00044</td>
<td>2.6X</td>
</tr>
<tr>
<td>1 node + 4x V100 SXM2 per node (16GB)</td>
<td>0.00056</td>
<td>3.3X</td>
</tr>
<tr>
<td>1 node + 8x V100 SXM2 per node (16GB)</td>
<td>0.00067</td>
<td>4.0X</td>
</tr>
</tbody>
</table>

**Graph:**
- **Y-axis:** Time (seconds)
- **X-axis:** Configuration

**Legend:**
- **Blue node:** Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs
- **Green nodes:** Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla V100 SXM2 (16GB) GPUs

**Details:**
- **Running VASP version 5.4.4**
- **512 Si atoms**
- **1282 bands**
- **864000 Plane Waves**
- **Algo = Normal (blocked Davidson)**
- **(Untuned on Volta)**
Supported Systems on V100s PCIe

(Untuned on Volta)
Running VASP version 5.4.4

The blue node contains Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla V100 PCIe (16GB) GPUs

267 ions
788 bands
762048 plane waves
ALGO = Fast (Davidson + RMM-DIIS)
Supported Systems on V100s SXM2

(Untuned on Volta)
Running VASP version 5.4.4

The blue node contains Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla V100 SXM2 (16GB) GPUs

267 ions
788 bands
762048 plane waves
ALGO = Fast (Davidson + RMM-DIIS)
NiAl-MD on V100s PCIe

(Untuned on Volta)
Running VASP version 5.4.4

The blue node contains Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla V100 PCIe (16GB) GPUs

500 ions
3200 bands
729000 plane waves
ALGO = Fast (Davidson + RMM-DIIS)
NiAl-MD on V100s SXM2

(Untuned on Volta)  
Running VASP version 5.4.4

The blue node contains Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla V100 SXM2 (16GB) GPUs

500 ions  
3200 bands  
729000 plane waves  
ALGO = Fast (Davidson + RMM-DIIS)
B.hR105 on V100s PCIe

(UNTUNED ON VOLTA)

RUNNING VASP VERSION 5.4.4

THE BLUE NODE CONTAINS DUAL INTEL XEON E5-2690 V4@2.6GHz [3.5GHz Turbo] (BROADWELL) CPUs

THE GREEN NODES CONTAIN DUAL INTEL XEON E5-2690 V4@2.6GHz [3.5GHz Turbo] (BROADWELL) CPUs + TESLA V100 PCIe (16GB)GPUS

105 BORON ATOMS (B-RHOMBOHEDRAL STRUCTURE)

216 BANDS

110592 PLANE WAVES

HYBRID FUNCTIONAL WITH BLOCKED DAVICSON (ALGO=Normal)

LHFCALC.=.True. (EXACT EXCHANGE)
B.hR105 on V100s SXM2

<table>
<thead>
<tr>
<th></th>
<th>1 Broadwell node</th>
<th>1 node + 2x V100 SXM2 per node (16GB)</th>
<th>1 node + 4x V100 SXM2 per node (16GB)</th>
<th>1 node + 8x V100 SXM2 per node (16GB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time (seconds)</td>
<td>0.0008</td>
<td>0.0079</td>
<td>0.0116</td>
<td>0.0128</td>
</tr>
<tr>
<td>Speedup</td>
<td>9.9X</td>
<td>14.5X</td>
<td>16.0X</td>
<td></td>
</tr>
</tbody>
</table>

(Untuned on Volta)
Running VASP version 5.4.4

The **blue node** contains Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The **green nodes** contain Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla V100 SXM2 (16GB) GPUs

105 Boron atoms (B-rhombohedral structure)
216 bands
110592 plane waves
Hybrid Functional with blocked Davicson (ALGO=Normal)
LHFCALC=.True. (Exact Exchange)
B.aP107 on V100s PCIe

(Untuned on Volta)
Running VASP version 5.4.4

The blue node contains Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs
The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla V100 PCIe (16GB) GPUs

107 Boron atoms (symmetry broken 107-atom B' variant)
216 bands
110592 plane waves
Hybrid functional calculation (exact exchange) with blocked Davidson. No KPoint parallelization.
Hybrid Functional with blocked Davidson (ALGO=Normal) LHFCALC=.True. (Exact Exchange)
B. aP107 on V100s SXM2

(Untuned on Volta)  
Running VASP version 5.4.4

The blue node contains Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs
The green nodes contain Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla V100 SXM2 (16GB) GPUs

107 Boron atoms (symmetry broken 107-atom $\beta'$ variant)  
216 bands  
110592 plane waves  
Hybrid functional calculation (exact exchange) with blocked Davidson. No KPoint parallelization.  
Hybrid Functional with blocked Davidson (ALGO=Normal)  
LHFCALC=.True. (Exact Exchange)
Quantum Chemistry (QC) on GPUs
March 2018
GPU-Accelerated Molecular Dynamics Apps

Green Lettering Indicates Performance Slides Included

- ACEMD
- AMBER
- CHARMM
- DESMOND
- ESPResSO
- Folding@Home
- GENESIS
- GPUGrid.net
- GROMACS
- HALMD
- HOOMD-Blue
- HTMD
- LAMMPS
- mdcore
- MELD
- NAMD
- OpenMM
- PolyFTS

GPU Perf compared against dual multi-core x86 CPU socket.