Accelerating Discoveries

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.
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, ESPResso, Folding@Home, GPUgrid.net, GROMACS, HALMD, HOOMD-Blue*, LAMMPS, Lattice Microbes*, mdccore, MELD, miniMD, NAMD, OpenMM, PolyFTS, SOP-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</td>
<td>Double precision is important</td>
</tr>
<tr>
<td>Uses cuBLAS, cuFFT, CUDA</td>
<td>Uses cuBLAS, cuFFT, 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>
GPU-Accelerated Molecular Dynamics Apps
Green Lettering Indicates Performance Slides Included

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

GPU Perf compared against dual multi-core x86 CPU socket.
Benefits of MD GPU-Accelerated Computing

Why wouldn’t you want to turbocharge your research?

- 3x-8x Faster than CPU only systems in all tests (on average)
- Most major compute intensive aspects of classical MD ported
- Large performance boost with marginal price increase
- Energy usage cut by more than half
- GPUs scale well within a node and/or over multiple nodes
- K80 GPU is our fastest and lowest power high performance GPU yet

Try GPU accelerated MD apps for free – www.nvidia.com/GPUTestDrive
ACEMD: Extremely efficient and robust MD software built on GPUs

470 ns/day on 1 GPU for L-Iduronic acid (1362 atoms)
116 ns/day on 1 GPU for DHFR (23K atoms)

ACEMD

- **Standardised and easy to use:** ACEMD reads CHARMM/NAMD and AMBER input files and uses similar syntax to other MD software.

- **Fully featured:** NVT, NPT, PME, TCL, PLUMED, CAMSHIFT

- **Robust:** ACEMD is a proven computational engine and is used in one of the largest distributed computing projects worldwide: GPUGRID.

- **Compatible:** ACEMD works with CUDA and OpenCL, the new standard framework for parallel and high-performance computing.

- **Validated:** ACEMD is used in reputable academic and industrial institutions. Results describing its applications have appeared in peer-reviewed journals of high impact such as PNAS, PLoS and JACS.

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2 For a list of selected references see http://www.acellera.com/acemd/publications
PME-Cellulose_NPT on K80s

Running AMBER version 16.3

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla K80 (autoboost) GPUs

- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
PME-Cellulose_NPT on P100s SXM2

Running AMBER version 16.3

The blue node contains Dual Intel Xeon E5-2699 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 P100 SXM2 GPUs

- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

- 9.9X
- 13.7X
- 15.6X
PME-Cellulose_NVE on K80s

Running AMBER version 16.3

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla K80 (autoboost) GPUs

- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

![Graph showing performance comparison](image_url)
PME-Cellulose_NVE on P100s PCIe

Running AMBER version 16.3

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

<table>
<thead>
<tr>
<th></th>
<th>1 Broadwell node</th>
<th>1 node + 1x P100 PCIe per node</th>
<th>1 node + 2x P100 PCIe per node</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time (ns/day)</td>
<td>2.47</td>
<td>9.4X</td>
<td>13.2X</td>
</tr>
<tr>
<td>Speed-up</td>
<td></td>
<td>9.4X</td>
<td>13.2X</td>
</tr>
</tbody>
</table>

---
Running AMBER version 16.3

The blue node contains Dual Intel Xeon E5-2699 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 P100 SXM2 GPUs

- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
PME-FactorIX_NPT on K80s

Running AMBER version 16.3

- The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs
- The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla K80 (autoboost) GPUs
  - 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

<table>
<thead>
<tr>
<th>Configuration</th>
<th>ns/day</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>11.43</td>
</tr>
<tr>
<td>1 node + 1x K80 per node</td>
<td>48.54</td>
</tr>
<tr>
<td>1 node + 2x K80 per node</td>
<td>66.68</td>
</tr>
</tbody>
</table>

- 4.2X
- 5.8X
PME-FactorIX_NPT on P100s PCIe

Running AMBER version 16.3

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
PME-FactorIX_NPT on P100s SXM2

Running AMBER version 16.3

The **blue node** contains Dual Intel Xeon E5-2699 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 P100 SXM2 GPUs

- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Running AMBER version 16.3

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla K80 (autoboost) GPUs

- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
PME-FactorIX_NVE on P100s PCIe

Running AMBER version 16.3

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
PME-FactorIX_NVE on P100s SXM2

Running AMBER version 16.3

The **blue node** contains Dual Intel Xeon E5-2699 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 P100 SXM2 GPUs

- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
PME-JAC_NPT on K80s

Running AMBER version 16.3

The **blue node** contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The **green nodes** contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla K80 (autoboost) GPUs

- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
PME-JAC_NPT on P100s PCIe

Running AMBER version 16.3

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
PME-JAC_NPT on P100s SXM2

Running AMBER version 16.3

The blue node contains Dual Intel Xeon E5-2699 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 P100 SXM2 GPUs

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PME-JAC_NVE on P100s PCIe

Running AMBER version 16.3

The **blue node** contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

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- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
GB-Myoglobin on K80s

Running AMBER version 16.3

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla K80 (autoboost) GPUs

- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
GB-Myoglobin on P100s PCIe

Running AMBER version 16.3

The **blue node** contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The **green nodes** contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

<table>
<thead>
<tr>
<th>Configuration</th>
<th>ns/day</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>28.86</td>
</tr>
<tr>
<td>1 node + 1x P100 PCIe per node</td>
<td>483.37</td>
</tr>
<tr>
<td>1 node + 4x P100 PCIe per node</td>
<td>561.94</td>
</tr>
</tbody>
</table>

16.7X vs 19.5X
GB-Myoglobin on P100s SXM2

Running AMBER version 16.3

The blue node contains Dual Intel Xeon E5-2699 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 P100 SXM2 GPUs

- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
GB-Nucleosome on K80s

Running AMBER version 16.3

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla K80 (autoboost) GPUs

- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
GB-Nucleosome on P100s PCIe

Running AMBER version 16.3

The **blue node** contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The **green nodes** contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
GB-Nucleosome on P100s SXM2

Running AMBER version 16.3

The blue node contains Dual Intel Xeon E5-2699 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 P100 SXM2 GPUs

- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Rubisco-75K on K80s

Running AMBER version 16.3

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla K80 (autoboost) GPUs

- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Rubisco-75K on P100s PCIe

Running AMBER version 16.3

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Rubisco-75K on P100s SXM2

Running AMBER version 16.3

The blue node contains Dual Intel Xeon E5-2699 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 P100 SXM2 GPUs

- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
AMBER 14 vs. AMBER 12

AMBER 14 Performance Improvement

[Chart showing performance improvement for JAC NVE, Factor IX NVE, and Cellulose NVE]

Courtesy of Scott Le Grand From GTC 2014 presentation
AMBER 14; large P2P and small Boost Clocks impacts

AMBER 14 (ns/day) on 4x K40; P2P and Boost Clocks Impact
DHFR NVE PME, 2fs Benchmark (CUDA 6.0, ECC off)

<table>
<thead>
<tr>
<th>Configuration</th>
<th>AMBER 14 (ns/day)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 x Xeon E5-2690 <a href="mailto:v2@3.00GHz">v2@3.00GHz</a> + 4 x Tesla K40@745MHz (no P2P)</td>
<td>125.77</td>
</tr>
<tr>
<td>2 x Xeon E5-2690 <a href="mailto:v2@3.00GHz">v2@3.00GHz</a> + 4 x Tesla K40@875MHz (no P2P)</td>
<td>132.97</td>
</tr>
<tr>
<td>2 x Xeon E5-2690 <a href="mailto:v2@3.00GHz">v2@3.00GHz</a> + 4 x Tesla K40@745MHz (P2P)</td>
<td>196.68</td>
</tr>
<tr>
<td>2 x Xeon E5-2690 <a href="mailto:v2@3.00GHz">v2@3.00GHz</a> + 4 x Tesla K40@875MHz (P2P)</td>
<td>215.18</td>
</tr>
</tbody>
</table>
AMBER Performance Over Time

JAC NVE Performance

- CPU
- GPU

2008 2009 2010 2011 2012 2013 2014

Courtesy of Scott Le Grand From GTC 2014 presentation
Cellulose on K40s, K80s and M6000s

Running AMBER version 14

The blue node contains Dual Intel E5-2698 v3@2.3GHz, 3.6GHz Turbo CPUs

The green nodes contain Dual Intel E5-2698 v3@2.3GHz, 3.6GHz Turbo CPUs + either NVIDIA Tesla K40@875Mhz, Tesla K80@562Mhz (autoboost), or Quadro M6000@987Mhz GPUs
Factor IX on K40s, K80s and M6000s

Running AMBER version 14

The **blue node** contains Dual Intel E5-2698 v3@2.3GHz, 3.6GHz Turbo CPUs

The **green nodes** contain Dual Intel E5-2698 v3@2.3GHz, 3.6GHz Turbo CPUs + either NVIDIA Tesla K40@875Mhz, Tesla K80@562Mhz (autoboost), or Quadro M6000@987Mhz GPUs
JAC on K40s, K80s and M6000s

Running AMBER version 14

The blue node contains Dual Intel E5-2698 v3@2.3GHz, 3.6GHz Turbo CPUs

The green nodes contain Dual Intel E5-2698 v3@2.3GHz, 3.6GHz Turbo CPUs + either NVIDIA Tesla K40@875Mhz, Tesla K80@562Mhz (autoboost), or Quadro M6000@987Mhz GPUs
Cellulose on M40s

Running AMBER version 14

The blue node contain Single Intel Xeon E5-2698 v3@2.30GHz (Haswell) CPUs

The green nodes contain Single Intel Xeon E5-2697 v2@2.70GHz (IvyBridge) CPUs + Tesla M40 (autoboost) GPUs
Cellulose on M40s

Running AMBER version 14

The blue node contain Single Intel Xeon E5-2698 v3@2.30GHz (Haswell) CPUs

The green nodes contain Single Intel Xeon E5-2697 v2@2.70GHz (IvyBridge) CPUs + Tesla M40 (autoboost) GPUs
FactorIX on M40s

The blue node contain Single Intel Xeon E5-2698 v3@2.30GHz (Haswell) CPUs

The green nodes contain Single Intel Xeon E5-2697 v2@2.70GHz (IvyBridge) CPUs + Tesla M40 (autoboost) GPUs

Running AMBER version 14

Simulated Time (ns/Day)
FactorIX on M40s

Running AMBER version 14

The blue node contain Single Intel Xeon E5-2698 v3@2.30GHz (Haswell) CPUs

The green nodes contain Single Intel Xeon E5-2697 v2@2.70GHz (IvyBridge) CPUs + Tesla M40 (autoboost) GPUs
JAC on M40s

Running AMBER version 14

The blue node contain Single Intel Xeon E5-2698 v3@2.30GHz (Haswell) CPUs

The green nodes contain Single Intel Xeon E5-2697 v2@2.70GHz (IvyBridge) CPUs + Tesla M40 (autoboost) GPUs
JAC on M40s

Running AMBER version 14

The blue node contain Single Intel Xeon E5-2698 v3@2.30GHz (Haswell) CPUs

The green nodes contain Single Intel Xeon E5-2697 v2@2.70GHz (IvyBridge) CPUs + Tesla M40 (autoboost) GPUs
Myoglobin on M40s

Running AMBER version 14

The blue node contain Single Intel Xeon E5-2698 v3@2.30GHz (Haswell) CPUs

The green nodes contain Single Intel Xeon E5-2697 v2@2.70GHz (IvyBridge) CPUs + Tesla M40 (autoboost) GPUs
Nucleosome on M40s

Running **AMBER** version 14

The **blue node** contain Single Intel Xeon E5-2698 v3@2.30GHz (Haswell) CPUs

The **green nodes** contain Single Intel Xeon E5-2697 v2@2.70GHz (IvyBridge) CPUs + Tesla M40 (autoboost) GPUs
TrpCage on M40s

Running AMBER version 14

The blue node contain Single Intel Xeon E5-2698 v3@2.30GHz (Haswell) CPUs

The green nodes contain Single Intel Xeon E5-2697 v2@2.70GHz (IvyBridge) CPUs + Tesla M40 (autoboost) GPUs
# Recommended GPU Node Configuration for AMBER Computational Chemistry

**Workstation or Single Node Configuration**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td># of CPU sockets</td>
<td>2</td>
</tr>
<tr>
<td>Cores per CPU socket</td>
<td>6+ (1 CPU core drives 1 GPU)</td>
</tr>
<tr>
<td>CPU speed (Ghz)</td>
<td>2.66+</td>
</tr>
<tr>
<td>System memory per node (GB)</td>
<td>16</td>
</tr>
<tr>
<td>GPUs</td>
<td>Kepler K20, K40, K80, P100</td>
</tr>
<tr>
<td># of GPUs per CPU socket</td>
<td>1-4</td>
</tr>
<tr>
<td>GPU memory preference (GB)</td>
<td>6</td>
</tr>
<tr>
<td>GPU to CPU connection</td>
<td>PCIe 3.0 16x or higher</td>
</tr>
<tr>
<td>Server storage</td>
<td>2 TB</td>
</tr>
<tr>
<td>Network configuration</td>
<td>Infiniband QDR or better</td>
</tr>
</tbody>
</table>

Scale to multiple nodes with same single node configuration
CHARMM DOMDEC-GUI 465 K System Benchmark

465 K System (Her1_HER1_membrane)

Running CHARMM version c40a1

The blue node contains Dual Intel Xeon E5-2698 v3@2.30 GHz (Haswell) CPUs

The green nodes contain Dual Intel Xeon E5-2698 v3@2.30 GHz (Haswell) CPUs + Tesla K80 (autoboost) GPUs

Benchmarks were done based on the STANDARD CHARMM c40a1 version by the Yang group (FSU), who is responsible for possible benchmarking error.
CHARMM DOMDEC-GUI 534 K System Benchmark

534 K System (POPC_PSPC_CHL1mixture)

*Higher is better

Running CHARMM version c40a1

The blue node contains Dual Intel Xeon E5-2698 v3@2.30 GHz (Haswell) CPUs

The green nodes contain Dual Intel Xeon E5-2698 v3@2.30 GHz (Haswell) CPUs + Tesla K80 (autoboost) GPUs

Benchmarks were done based on the STANDARD CHARMM c40a1 version by the Yang group (FSU), who is responsible for possible benchmarking error.
CHARMM DOMDEC-GUI 20 K System Benchmark

20 K System (Crambin)

Running CHARMM version c40a1

The blue node contains Dual Intel Xeon E5-2698 v3@2.30 GHz (Haswell) CPUs

The green nodes contain Dual Intel Xeon E5-2698 v3@2.30 GHz (Haswell) CPUs + Tesla M40 GPUs

Benchmarks were done based on the STANDARD CHARMM c40a1 version by the Yang group (FSU), who is responsible for possible benchmarking error.
CHARMM DOMDEC-GUI 61 K System Benchmark

**Running CHARMM version c40a1**

The blue node contains Dual Intel Xeon E5-2698 v3@2.30 GHz (Haswell) CPUs

The green nodes contain Dual Intel Xeon E5-2698 v3@2.30 GHz (Haswell) CPUs + Tesla M40 GPUs

Benchmarks were done based on the STANDARD CHARMM c40a1 version by the Yang group (FSU), who is responsible for possible benchmarking error.
CHARMM DOMDEC-GUI 465 K System Benchmark

465 K System
(Her1_HER1_membrane)

*Higher is better

Running CHARMM version c40a1

The blue node contains Dual Intel Xeon E5-2698 v3@2.30 GHz (Haswell) CPUs

The green nodes contain Dual Intel Xeon E5-2698 v3@2.30 GHz (Haswell) CPUs + Tesla M40 GPUs

Benchmarks were done based on the STANDARD CHARMM c40a1 version by the Yang group (FSU), who is responsible for possible benchmarking error.
GROMACS 2016
October 2016
Erik Lindahl (GROMACS developer) video
Water 1.5M on K80s

Running GROMACS version 2016

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 K80 (autoboost) GPUs
Water 3M on K80s

Running GROMACS version 2016

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 K80 (autoboost) GPUs
Water 1.5M on M40s

Running GROMACS version 2016

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 M40 (autoboost) GPUs
Water 3M on M40s

Running GROMACS version 2016

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 M40 (autoboost) GPUs

NVIDIA CONFIDENTIAL. DO NOT DISTRIBUTE.
Water 1.5M on P40s

Running GROMACS version 2016

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 P40 GPUs

NVIDIA CONFIDENTIAL. DO NOT DISTRIBUTE.
Running GROMACS version 2016

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 P40 GPUs

### Water 3M on P40s

<table>
<thead>
<tr>
<th>Configuration</th>
<th>ns/day</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>1.32</td>
</tr>
<tr>
<td>1 node + 2x P40 per node</td>
<td>2.5X</td>
</tr>
<tr>
<td>1 node + 4x P40 per node</td>
<td>3.2X</td>
</tr>
</tbody>
</table>

**Graph:**
- **Y-axis**: ns/day
- **X-axis**: 1 Broadwell node, 1 node + 2x P40 per node, 1 node + 4x P40 per node
Water 1.5M on P100 PCIs

Running GROMACS version 2016

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 P100 PCIe GPUs
Water 3M on P100 PCIs

Running GROMACS version 2016

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 P100 PCIe GPUs

NVIDIA CONFIDENTIAL. DO NOT DISTRIBUTE.
Water 1.5M on K80s

Running GROMACS version 5.1.2

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla K80 (autoboost) GPUs

- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Water 1.5M on P100s PCIe

Running GROMACS version 5.1.2

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
**Water 1.5M on P100s SXM2**

Running GROMACS version 5.1.2

The blue node contains Dual Intel Xeon E5-2699 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 P100 SXM2 GPUs

- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

---

**Water 1.5M**

<table>
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<tr>
<th>Configuration</th>
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<tr>
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<tr>
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<td>1.4X</td>
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<tr>
<td>1 node + 2x 100 SXM2 per node</td>
<td>6.70</td>
<td>2.2X</td>
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<tr>
<td>1 node + 4x P100 SXM2 per node</td>
<td>7.18</td>
<td>2.4X</td>
</tr>
<tr>
<td>1 node + 8x P100 SXM2 per node</td>
<td>7.88</td>
<td>2.6X</td>
</tr>
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</table>
Water 3M on K80s

Running GROMACS version 5.1.2

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla K80 (autoboost) GPUs

- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Water 3M on P100s PCIe

Running GROMACS version 5.1.2

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Water 3M on P100s SXM2

Running GROMACS version 5.1.2

The blue node contains Dual Intel Xeon E5-2699 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 P100 SXM2 GPUs

- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
# Recommended GPU Node Configuration for GROMACS Computational Chemistry

## Workstation or Single Node Configuration

<table>
<thead>
<tr>
<th>Feature</th>
<th>Specification</th>
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<tbody>
<tr>
<td># of CPU sockets</td>
<td>2</td>
</tr>
<tr>
<td>Cores per CPU socket</td>
<td>6+</td>
</tr>
<tr>
<td>CPU speed (Ghz)</td>
<td>2.66+</td>
</tr>
<tr>
<td>System memory per socket (GB)</td>
<td>32</td>
</tr>
<tr>
<td>GPUs</td>
<td>Kepler K20, K40, K80</td>
</tr>
<tr>
<td># of GPUs per CPU socket</td>
<td>1x</td>
</tr>
<tr>
<td>Kepler GPUs: need fast Sandy Bridge</td>
<td>or Ivy Bridge, or high-end AMD Opterons</td>
</tr>
<tr>
<td>GPU memory preference (GB)</td>
<td>6</td>
</tr>
<tr>
<td>GPU to CPU connection</td>
<td>PCIe 3.0 or higher</td>
</tr>
<tr>
<td>Server storage</td>
<td>500 GB or higher</td>
</tr>
<tr>
<td>Network configuration</td>
<td>Gemini, InfiniBand</td>
</tr>
</tbody>
</table>
HOOMD-Blue 1.3.3
February 2017
lj-liquid on K80s

Running HOOMD-Blue version 1.3.3

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla K80 (autoboost) GPUs

- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
lj-liquid on P100s PCIe

Running HOOMD-Blue version 1.3.3

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
lj-liquid on P100s SXM2

Running HOOMD-Blue version 1.3.3

The blue node contains Dual Intel Xeon E5-2699 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 P100 SXM2 GPUs

- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
lj_liquid_512k on K80s

Running HOOMD-Blue version 1.3.3

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

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lj_liquid_512k on P100s PCIe

Running HOOMD-Blue version 1.3.3

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- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

<table>
<thead>
<tr>
<th>Configuration</th>
<th>avg timesteps/sec</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>43.43</td>
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<tr>
<td>1 node + 1x P100 PCIe per node</td>
<td>398.12</td>
</tr>
<tr>
<td>1 node + 2x P100 PCIe per node</td>
<td>534.54</td>
</tr>
<tr>
<td>1 node + 4x P100 PCIe per node</td>
<td>770.18</td>
</tr>
<tr>
<td>1 node + 8x P100 PCIe per node</td>
<td>1045.50</td>
</tr>
</tbody>
</table>

lj_liquid_512k
lj_liquid_512k on P100s SXM2

Running HOOMD-Blue version 1.3.3

The blue node contains Dual Intel Xeon E5-2699 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 P100 SXM2 GPUs

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The **blue node** contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

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- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
lj_liquid_1m on P100s PCIe

Running HOOMD-Blue version 1.3.3

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
lj_liquid_1m on P100s SXM2

Running HOOMD-Blue version 1.3.3

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- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Microsphere on K80s

Running HOOMD-Blue version 1.3.3

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla K80 (autoboost) GPUs

- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Running HOOMD-Blue version 1.3.3

The **blue node** contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The **green nodes** contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Microsphere on P100s SXM2

Running HOOMD-Blue version 1.3.3

The blue node contains Dual Intel Xeon E5-2699 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 P100 SXM2 GPUs

- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Polymer on K80s

Running HOOMD-Blue version 1.3.3

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla K80 (autoboost) GPUs

- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Polymer on P100s PCIe

Running HOOMD-Blue version 1.3.3

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Polymer on P100s SXM2

Running HOOMD-Blue version 1.3.3

The **blue node** contains Dual Intel Xeon E5-2699 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 P100 SXM2 GPUs

- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Quasicrystal on K80s

Running HOOMD-Blue version 1.3.3

The **blue node** contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The **green nodes** contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla K80 (autoboost) GPUs

- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Quasicrystal on P100s PCIe

Running HOOMD-Blue version 1.3.3

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Avg Timesteps/sec</th>
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<tbody>
<tr>
<td>1 Broadwell node</td>
<td>78.32</td>
</tr>
<tr>
<td>1 node + 1x P100 PCIe per node</td>
<td>851.29</td>
</tr>
<tr>
<td>1 node + 2x P100 PCIe per node</td>
<td>1199.64</td>
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<td>1 node + 4x P100 PCIe per node</td>
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<td>1 node + 8x P100 PCIe per node</td>
<td>2261.72</td>
</tr>
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</table>

10.9X  15.3X  22.9X  28.9X
Running HOOMD-Blue version 1.3.3

The **blue node** contains Dual Intel Xeon E5-2699 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 P100 SXM2 GPUs

- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Triblock-copolymer on K80s

Running HOOMD-Blue version 1.3.3

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla K80 (autoboost) GPUs

- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Avg Timesteps/sec</th>
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<tbody>
<tr>
<td>1 Broadwell node</td>
<td>361.42</td>
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<tr>
<td>1 node + 1x K80 per node</td>
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<tr>
<td>1 node + 2x K80 per node</td>
<td>1170.47</td>
</tr>
<tr>
<td>1 node + 4x K80 per node</td>
<td>1492.01</td>
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- 2.6X
- 3.2X
- 4.1X
Running HOOMD-Blue version 1.3.3

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Triblock-copolymer on P100s SXM2

Running HOOMD-Blue version 1.3.3

The **blue node** contains Dual Intel Xeon E5-2699 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 P100 SXM2 GPUs

- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
LAMMPS 2016
February 2017
Atomic-Fluid Lennard-Jones 2.5 Cutoff on K80s

Running LAMMPS version 2016

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

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Atomic-Fluid Lennard-Jones 2.5 Cutoff on P100s PCIe

Running LAMMPS version 2016

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe (autoboost) GPUs
Atomic-Fluid Lennard-Jones 2.5 Cutoff on P100s SXM2

Running LAMMPS version 2016

The blue node contains Dual Intel Xeon E5-2699 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 P100 SXM2 (autoboost) GPUs
Atomic-Fluid Lennard-Jones 5.0 Cutoff on K80s

Running LAMMPS version 2016

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla K80 (autoboost) GPUs

- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

<table>
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<tr>
<th>Configuration</th>
<th>Cutoff Speed</th>
<th>Speedup</th>
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<td>1 Broadwell node</td>
<td>0.10</td>
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</tr>
<tr>
<td>1 node + 1x K80 per node</td>
<td>0.14</td>
<td>1.4X</td>
</tr>
<tr>
<td>1 node + 2x K80 per node</td>
<td>0.26</td>
<td>2.6X</td>
</tr>
<tr>
<td>1 node + 4x K80 per node</td>
<td>0.36</td>
<td>3.6X</td>
</tr>
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</table>
Running LAMMPS version 2016

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Atomic-Fluid Lennard-Jones 5.0 Cutoff on P100s SXM2

Running LAMMPS version 2016

The **blue node** contains Dual Intel Xeon E5-2699 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 P100 SXM2 GPUs

- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Course-grain Water on K80s

Running LAMMPS version 2016

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

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Course-grain Water on P100s PCIe

Running LAMMPS version 2016

The **blue node** contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

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Course-grain Water on P100s SXM2

Running LAMMPS version 2016

The blue node contains Dual Intel Xeon E5-2699 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 P100 SXM2 GPUs
EAM on K80s

Running LAMMPS version 2016

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla K80 (autoboost) GPUs

- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Running LAMMPS version 2016

The **blue node** contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The **green nodes** contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Running LAMMPS version 2016

The **blue node** contains Dual Intel Xeon E5-2699 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 P100 SXM2 GPUs

- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Gay-Berne on K80s

Running LAMMPS version 2016

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla K80 (autoboost) GPUs

- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Gay-Berne on P100s PCIe

Running LAMMPS version 2016

The **blue node** contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The **green nodes** contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

---

### Gay-Berne

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Time (1/seconds)</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>0.01</td>
<td></td>
</tr>
<tr>
<td>1 node + 1x P100 PCIe per node</td>
<td>0.02</td>
<td>2.0X</td>
</tr>
<tr>
<td>1 node + 2x P100 PCIe per node</td>
<td>0.04</td>
<td>4.0X</td>
</tr>
<tr>
<td>1 node + 4x P100 PCIe per node</td>
<td>0.05</td>
<td>5.0X</td>
</tr>
</tbody>
</table>
Gay-Berne on P100s SXM2

Running LAMMPS version 2016

The blue node contains Dual Intel Xeon E5-2699 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 P100 SXM2 GPUs

- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
Rhodopsin on K80s

Running LAMMPS version 2016

The **blue node** contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The **green nodes** contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla K80 (autoboost) GPUs

- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

### Performance Comparison

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Time (seconds)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>0.22</td>
</tr>
<tr>
<td>1 node + 1x K80 per node</td>
<td>0.22</td>
</tr>
<tr>
<td>1 node + 2x K80 per node</td>
<td>0.31</td>
</tr>
<tr>
<td>1 node + 4x K80 per node</td>
<td>0.38</td>
</tr>
</tbody>
</table>

1.4X

1.7X
Rhodopsin on P100s PCIe

<table>
<thead>
<tr>
<th>Configuration</th>
<th>1/seconds</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>0.22</td>
</tr>
<tr>
<td>1 node + 1x P100 PCIe per node</td>
<td>0.29</td>
</tr>
<tr>
<td>1 node + 2x P100 PCIe per node</td>
<td>0.33</td>
</tr>
<tr>
<td>1 node + 4x P100 PCIe per node</td>
<td>0.48</td>
</tr>
<tr>
<td>1 node + 8x P100 PCIe per node</td>
<td>0.52</td>
</tr>
</tbody>
</table>

Running LAMMPS version 2016

The **blue node** contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The **green nodes** contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

1.3X
1.5X
2.2X
2.4X
Rhodopsin on P100s SXM2

Running LAMMPS version 2016

The blue node contains Dual Intel Xeon E5-2699 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 P100 SXM2 GPUs

- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
# Recommended GPU Node Configuration for LAMMPS Computational Chemistry

<table>
<thead>
<tr>
<th>Workstation or Single Node Configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td># of CPU sockets</td>
</tr>
<tr>
<td>Cores per CPU socket</td>
</tr>
<tr>
<td>CPU speed (Ghz)</td>
</tr>
<tr>
<td>System memory per socket (GB)</td>
</tr>
</tbody>
</table>

- **GPUs**
  - GTX Titan X, Kepler K20, K40, K80, M40

- # of GPUs per CPU socket: 1-2
- GPU memory preference (GB): 6+
- GPU to CPU connection: PCIe 3.0 or higher
- Server storage: 500 GB or higher
- Network configuration: Gemini, InfiniBand

*Scale to thousands of nodes with same single node configuration*
NAMD 2.11 - Up to 2X Faster
New GPU features in NAMD 2.11

Selected Text from the NAMD website

- GPU-accelerated simulations up to twice as fast as NAMD 2.10
- Pressure calculation with fixed atoms on GPU works as on CPU
- Improved scaling for GPU-accelerated particle-mesh Ewald calculation
  - CPU-side operations overlap better and are parallelized across cores.
- Improved scaling for GPU-accelerated simulations
  - Nonbonded force calculation results are streamed from the GPU for better overlap.
- NVIDIA CUDA GPU-acceleration binaries for Mac OS X
NAMD 2.11 is up to 2x faster

APoA1 (92,224 atoms)

NAMD 2.10 & NAMD 2.11 contain Dual Intel E5-2697 v2@2.7GHz (IvyBridge) CPUs + 2 Tesla K80 (autoboost) GPUs
NAMD 2.11 APoA1 on 1 and 2 nodes

Running NAMD version 2.11

The blue nodes contain Dual Intel E5-2698 v3@2.3GHz (Haswell) CPUs

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

Simulated Time (ns/day)

APoA1 (92,224 atoms)
NAMD 2.11 APoA1 on 4 and 8 nodes

Running NAMD version 2.11

The **blue nodes** contain Dual Intel E5-2698 v3@2.3GHz (Haswell) CPUs

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

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Simulated Time (ns/day)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 Nodes</td>
<td>10.27</td>
</tr>
<tr>
<td>4 Nodes + 1x K80</td>
<td>20.64</td>
</tr>
<tr>
<td>4 Nodes + 2x K80</td>
<td>23.52</td>
</tr>
<tr>
<td>8 Nodes</td>
<td>16.85</td>
</tr>
<tr>
<td>8 Nodes + 1x K80</td>
<td>27.83</td>
</tr>
<tr>
<td>8 Nodes + 2x K80</td>
<td>27.74</td>
</tr>
</tbody>
</table>

**APoA1** (92,224 atoms)
NAMD 2.11 is up to 1.8x faster

F1-ATPase (327,506 atoms)

NAMD 2.10 & NAMD 2.11 contain Dual Intel E5-2697 v2@2.7GHz (IvyBridge) CPUs + 2 Tesla K80 (autoboost) GPUs
NAMD 2.11 F1-ATPase on 1 and 2 nodes

Running NAMD version 2.11

The **blue nodes** contain Dual Intel E5-2698 v3@2.3GHz (Haswell) CPUs

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

F1-ATPase (327,506 atoms)

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Simulated Time (ns/day)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Node</td>
<td>0.94</td>
</tr>
<tr>
<td>1 Node + 1x K80</td>
<td>3.87</td>
</tr>
<tr>
<td>1 Node + 2x K80</td>
<td>6.11</td>
</tr>
<tr>
<td>2 Nodes</td>
<td>1.86</td>
</tr>
<tr>
<td>2 Nodes + 1x K80</td>
<td>7.23</td>
</tr>
<tr>
<td>2 Nodes + 2x K80</td>
<td>10.58</td>
</tr>
<tr>
<td>2 Nodes + 1x K80</td>
<td>5.7X</td>
</tr>
<tr>
<td>2 Nodes + 2x K80</td>
<td>4.1X</td>
</tr>
<tr>
<td>2 Nodes + 2x K80</td>
<td>6.5X</td>
</tr>
</tbody>
</table>
NAMD 2.11 F1-ATPase on 4 and 8 nodes

Running NAMD version 2.11

The blue nodes contain Dual Intel E5-2698 v3@2.3GHz (Haswell) CPUs

The green nodes contain Dual Intel E5-2698 v3@2.3GHz (Haswell) CPUs + Tesla K80 (autoboost) GPUs
NAMD 2.11 is up to 1.5x faster

STMV (1,066,628 atoms)

NAMD 2.10 & NAMD 2.11 contain Dual Intel E5-2697 v2@2.7GHz (IvyBridge) CPUs + 2 Tesla K80 (autoboost) GPUs
NAMD 2.11 STMV on 1 and 2 nodes

Running NAMD version 2.11

The **blue nodes** contain Dual Intel E5-2698 v3@2.3GHz (Haswell) CPUs

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NAMD 2.11 STMV on 4 and 8 nodes

Running NAMD version 2.11

The **blue nodes** contain Dual Intel E5-2698 v3@2.3GHz (Haswell) CPUs

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

STMV
(1,066,628 atoms)

<table>
<thead>
<tr>
<th>Nodes</th>
<th>Simulated Time (ns/day)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>0.90</td>
</tr>
<tr>
<td>4 + 1x K80</td>
<td>3.61</td>
</tr>
<tr>
<td>4 + 2x K80</td>
<td>4.54</td>
</tr>
<tr>
<td>8</td>
<td>1.74</td>
</tr>
<tr>
<td>8 + 1x K80</td>
<td>5.86</td>
</tr>
<tr>
<td>8 + 2x K80</td>
<td>6.24</td>
</tr>
</tbody>
</table>

STMV (1,066,628 atoms)
APOA1 on K80s

Running NAMD version 2.11

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- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
APOA1 on P100s PCIe

Running NAMD version 2.11

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- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
F1ATPASE on K80s

Running NAMD version 2.11

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STMV on P100s PCIe

Running NAMD version 2.11

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The **green nodes** contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
# Recommended GPU Node Configuration for NAMD Computational Chemistry

## Workstation or Single Node Configuration

<table>
<thead>
<tr>
<th>Specification</th>
<th>Requirement</th>
</tr>
</thead>
<tbody>
<tr>
<td># of CPU sockets</td>
<td>2</td>
</tr>
<tr>
<td>Cores per CPU socket</td>
<td>6+</td>
</tr>
<tr>
<td>CPU speed (Ghz)</td>
<td>2.66+</td>
</tr>
<tr>
<td>System memory per socket (GB)</td>
<td>32</td>
</tr>
<tr>
<td>GPUs</td>
<td>Kepler K20, K40, K80</td>
</tr>
<tr>
<td># of GPUs per CPU socket</td>
<td>1-2</td>
</tr>
<tr>
<td>GPU memory preference (GB)</td>
<td>6-12</td>
</tr>
<tr>
<td>GPU to CPU connection</td>
<td>PCIe 3.0 or higher</td>
</tr>
<tr>
<td>Server storage</td>
<td>500 GB or higher</td>
</tr>
<tr>
<td>Network configuration</td>
<td>Gemini, InfiniBand</td>
</tr>
</tbody>
</table>

Scale to thousands of nodes with same single node configuration
Benefits of **MD GPU-Accelerated Computing**

Why wouldn’t you want to turbocharge your research?

- 3x-8x Faster than CPU only systems in all tests (on average)
- Most major compute intensive aspects of classical MD ported
- Large performance boost with marginal price increase
- Energy usage cut by more than half
- GPUs scale well within a node and/or over multiple nodes
- K80 GPU is our fastest and lowest power high performance GPU yet

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Molecular Dynamics (MD) on GPUs

Dec. 19, 2016