Molecular Dynamics (MD) on GPUs and RELION too
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*, mdcare, MELD, miniMD, NAMD, OpenMM, PolyFTrs, 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><strong>“Classical” Molecular Dynamics</strong></th>
<th><strong>Quantum Chemistry (MO, PW, DFT, Semi-Emp)</strong></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 cuFFT, CUDA</td>
<td>Uses cuBLAS, cuFFT, OpenACC, Eigen / Tensor Solvers</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
- GENESIS
- GPUGrid.net
- GROMACS
- HALMD
- HOOMD-Blue
- HTMD
- 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 and save “Big Money” on CPUs, networks
• Energy usage cut by more than half
• GPUs scale well within a node and/or over multiple nodes
• P100 GPU is our fastest and lowest power high performance GPU yet

Try GPU accelerated MD apps for free – www.nvidia.com/GPUTestDrive
RELION: Plasmodium ribosome on P100s PCIe

Data Citation:
ACEMD
ACEMD: Extremely efficient and robust MD software built on GPUs

610 ns/day on 1 GPU for DHFR (23K atoms)

• **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.¹

• **Robust**: ACEMD is a proven computational engine and is used in one of the largest distributed 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 Nature Chemistry, PNAS, Scientific Reports, PLoS and JACS.²


2. For a list of selected references see http://www.acellera.com/science
AMBER 16 on V100s

October 2017
PME-Cellulose_NPT on V100s PCIe

(Untuned on Volta)  
Running AMBER version 16.8

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

The graph shows a performance improvement of 24.6X with 1 node + 2x V100 PCIe per node (16GB) compared to 1 Broadwell node.
PME-Cellulose_NPT on V100s SXM2

(Unluted on Volta)
Running AMBER version 16.8

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

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<table>
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<tr>
<th>Configuration</th>
<th>Performance (ns/day)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>1.94</td>
</tr>
<tr>
<td>1 node + 2x V100 SXM2 per node (16GB)</td>
<td>54.74 28.2X</td>
</tr>
<tr>
<td>1 node + 4x V100 SXM2 per node (16GB)</td>
<td>55.52 28.6X</td>
</tr>
</tbody>
</table>
PME-Cellulose_NVE on V100s PCIe

(UNTUNED on Volta)
Running AMBER version 16.8

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

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PME-FactorIX_NPT on V100s PCIe

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PME-JAC_NPT on V100s PCIe

(Untuned on Volta)
Running AMBER version 16.8

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

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Running AMBER version 16.8

(Untuned on Volta)

1 Broadwell node
1 node + 2x V100 SXM2 per node (16GB)
1 node + 4x V100 SXM2 per node (16GB)

34.35
481.75
515.36

14.0X
15.0X
PME-JAC_NVE on V100s PCIe

(1 Broadwell node)

13.4X

(1 node + 2x V100 PCIe per node (16GB))

(Untuned on Volta)

Running AMBER version 16.8

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
PME-JAC_NVE on V100s SXM2

<table>
<thead>
<tr>
<th>Configuration</th>
<th>ns/day</th>
<th>Improvement</th>
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</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>36.53</td>
<td></td>
</tr>
<tr>
<td>1 node + 2x V100 SXM2 per node (16GB)</td>
<td>539.78</td>
<td>14.8X</td>
</tr>
<tr>
<td>1 node + 4x V100 SXM2 per node (16GB)</td>
<td>583.33</td>
<td>16.0X</td>
</tr>
</tbody>
</table>

(Untuned on Volta)
Running AMBER version 16.8

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
PME-JAC_NPT_4fs on V100s PCIe

(Untuned on Volta)
Running AMBER version 16.8

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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.

Running AMBER version 16.8
PME-JAC_NVE_4fs on V100s PCIe

(Untuned on Volta)
Running AMBER version 16.8

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

26.0X

ns/day

1 node + 2x V100 PCIe per node (16GB)

1 Broadwell node

67.10

940.32
PME-JAC_NVE_4fs on V100s SXM2

<table>
<thead>
<tr>
<th>Configuration</th>
<th>ns/day</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>67.10</td>
<td></td>
</tr>
<tr>
<td>1 node + 2x V100 SXM2 per node (16GB)</td>
<td>1027.44</td>
<td>15.3X</td>
</tr>
<tr>
<td>1 node + 4x V100 SXM2 per node (16GB)</td>
<td>1123.40</td>
<td>16.7X</td>
</tr>
</tbody>
</table>

(Untuned on Volta)
Running AMBER version 16.8

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
PME-STMV_NPT_4fs on V100s PCIe

Untuned on Volta
Running AMBER version 16.8

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
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GB-Myoglobin on V100s PCIe

(Untuned on Volta)
Running AMBER version 16.8

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GB-Nucleosome on V100s PCIe

(Untuned on Volta)
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GB-Nucleosome on V100s SXM2

(Untuned on Volta)  
Running AMBER version 16.8

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<tr>
<th>Configuration</th>
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</tr>
</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>0.31</td>
</tr>
<tr>
<td>1 node + 2x V100 SXM2 per node (16GB)</td>
<td>52.89</td>
</tr>
<tr>
<td>1 node + 4x V100 SXM2 per node (16GB)</td>
<td>92.46</td>
</tr>
</tbody>
</table>

- 170.6X
- 298.3X
Rubisco on V100s PCIe

(Untuned on Volta)
Running AMBER version 16.8

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
Rubisco on V100s SXM2

(Untuned on Volta)
Running AMBER version 16.8

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
AMBER 16 on P100s
February 2017
PME-Cellulose_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 (16GB) GPUs

- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 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

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- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)
PME-Cellulose_NVE on P100s PCIe

Running AMBER version 16.3

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The green nodes contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe (16GB) 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>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>2.47 ns/day</td>
</tr>
<tr>
<td>1 node + 1x P100 PCIe (16GB) per node</td>
<td>9.4X</td>
</tr>
<tr>
<td>1 node + 2x P100 PCIe (16GB) per node</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)

<table>
<thead>
<tr>
<th>Configuration</th>
<th>ns/day</th>
<th>Performance</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>2.47</td>
<td>1x</td>
</tr>
<tr>
<td>1 node + 1x P100 SXM2 per node</td>
<td>24.94</td>
<td>10.1X</td>
</tr>
<tr>
<td>1 node + 2x P100 SXM2 per node</td>
<td>35.16</td>
<td>14.2X</td>
</tr>
<tr>
<td>1 node + 4x P100 SXM2 per node</td>
<td>40.88</td>
<td>16.6X</td>
</tr>
</tbody>
</table>
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 (16GB) 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

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

---

![Graph showing performance comparison](image-url)

<table>
<thead>
<tr>
<th>Configuration</th>
<th>ns/day</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>47.90</td>
</tr>
<tr>
<td>1 node + 1x P100 PCIe (16GB) per node</td>
<td>308.46</td>
</tr>
<tr>
<td>1 node + 2x P100 PCIe (16GB) per node</td>
<td>363.79</td>
</tr>
</tbody>
</table>

- 1 node + 1x P100 PCIe (16GB) is 6.4X faster than 1 Broadwell node
- 1 node + 2x P100 PCIe (16GB) is 7.6X faster than 1 Broadwell node

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**Table:**

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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 P100s PCIe

Running AMBER version 16.3

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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 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 (16GB) 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>0.40</td>
</tr>
<tr>
<td>1 node + 1x P100 PCIe (16GB) per node</td>
<td>11.91</td>
</tr>
<tr>
<td>1 node + 2x P100 PCIe (16GB) per node</td>
<td>22.77</td>
</tr>
<tr>
<td>1 node + 4x P100 PCIe (16GB) per node</td>
<td>39.91</td>
</tr>
<tr>
<td>1 node + 8x P100 PCIe (16GB) per node</td>
<td>45.92</td>
</tr>
</tbody>
</table>

- 114.8X improvement compared to 1 Broadwell node
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 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 (16GB) 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)
### Recommended GPU Node Configuration for AMBER Computational Chemistry

<table>
<thead>
<tr>
<th>Workstation or Single Node Configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong># of CPU sockets</strong></td>
</tr>
<tr>
<td><strong>Cores per CPU socket</strong></td>
</tr>
<tr>
<td><strong>CPU speed (Ghz)</strong></td>
</tr>
<tr>
<td><strong>System memory per node (GB)</strong></td>
</tr>
<tr>
<td><strong>GPUs</strong></td>
</tr>
<tr>
<td><strong># of GPUs per CPU socket</strong></td>
</tr>
<tr>
<td><strong>GPU memory preference (GB)</strong></td>
</tr>
<tr>
<td><strong>GPU to CPU connection</strong></td>
</tr>
<tr>
<td><strong>Server storage</strong></td>
</tr>
<tr>
<td><strong>Network configuration</strong></td>
</tr>
</tbody>
</table>

Scale to multiple nodes with same single node configuration
CHARMM DOMDEC-GUI

July 2016
CHARMM DOMDEC-GUI 465 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 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.

465 K System (Her1_HER1_membrane)

*Higher is better

0.36  2.15

1 Haswell node  1 node + 1x K80 per node

6.0X
CHARMM DOMDEC-GUI 534 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 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

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.

![Bar Chart](image-url)

- **61 K System (GlnBP)**
- *Higher is better*

<table>
<thead>
<tr>
<th></th>
<th>1 Haswell node</th>
<th>1 node + 1x M40 per node</th>
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</thead>
<tbody>
<tr>
<td>ns/day</td>
<td>3.90</td>
<td>25.08</td>
</tr>
</tbody>
</table>

6.4X
CHARMM DOMDEC-GUI 465 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.
GROMACS 2018
February 2018
GROMACS Water 1.5M on V100 vs P100 (PCIe 16GB)

(Untuned on Volta)
Running GROMACS version 2018

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
GROMACS Water 1.5M on V100 vs P100 (SXM2 16GB)

(Untuned on Volta)
Running GROMACS version 2018

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

The green nodes contain Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 SXM2 (16GB) or V100 SXM2 (16GB) GPUs

<table>
<thead>
<tr>
<th>Configuration</th>
<th>ns/day</th>
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</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>2.43</td>
</tr>
<tr>
<td>1 node + 1x P100 SXM2 per node</td>
<td>6.88</td>
</tr>
<tr>
<td>1 node + 2x P100 SXM2 per node</td>
<td>9.16</td>
</tr>
<tr>
<td>1 node + 4x P100 SXM2 per node</td>
<td>11.02</td>
</tr>
<tr>
<td>1 node + 1x V100 SXM2 per node</td>
<td>10.19</td>
</tr>
<tr>
<td>1 node + 2x V100 SXM2 per node</td>
<td>10.92</td>
</tr>
<tr>
<td>1 node + 4x V100 SXM2 per node</td>
<td>12.67</td>
</tr>
</tbody>
</table>

4.2X 2.8X 3.8X 4.5X 4.5X 5.2X
GROMACS ADH Dodec on V100 vs P100 (PCIe 16GB)

Running GROMACS version 2018

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

(Untuned on Volta)
GROMACS ADH Dodec on V100 vs P100 (SXM2 16GB)

Running GROMACS version 2018

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

The green nodes contain Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 SXM2 (16GB) or V100 SXM2 (16GB) GPUs
Water 1.5M on V100 vs P100 (PCIe)

(Untuned on Volta)
Running GROMACS version 2016.4

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 P100 PCIe (16GB) or V100 PCIe (16GB) GPUs
**Water 3M on V100 vs P100 (PCIe)**

1.12

1.8X

1 Broadwell node

1.96

1 node + 1x P100 PCIe per node (16GB)

3.53

3.2X

1 node + 2x P100 PCIe per node (16GB)

2.53

2.3X

1 node + 1x V100 PCIe per node (16GB)

3.85

3.4X

1 node + 2x V100 PCIe per node (16GB)

(Untuned on Volta)

Running **GROMACS** version 2016.4

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 P100 PCIe (16GB) or V100 PCIe (16GB) GPUs
# Recommended GPU Node Configuration for GROMACS Computational Chemistry

## Workstation or Single Node Configuration

<table>
<thead>
<tr>
<th>Specification</th>
<th>Details</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><strong>GPUs</strong></td>
<td>Tesla P100, V100</td>
</tr>
<tr>
<td># of GPUs per CPU socket</td>
<td>2x</td>
</tr>
<tr>
<td><strong>Volta GPUs:</strong> need fast Skylake or Broadwell</td>
<td></td>
</tr>
<tr>
<td><strong>GPU memory preference (GB)</strong></td>
<td>6</td>
</tr>
<tr>
<td><strong>GPU to CPU connection</strong></td>
<td>PCIe 3.0 or higher</td>
</tr>
<tr>
<td><strong>Server storage</strong></td>
<td>500 GB or higher</td>
</tr>
<tr>
<td><strong>Network configuration</strong></td>
<td>Gemini, InfiniBand</td>
</tr>
</tbody>
</table>
HOOMD-Blue 2.2.2

March 2018
HOOMD-Blue lj-liquid on V100 vs P100 (PCIe 16GB)

Running HOOMD-Blue version 2.2.2

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

64,000 particles

Force field/method: Lennard-Jones MD

This is a synthetic benchmark for historical reasons and for making direct comparisons with LAMMPS

Average TPS

1 Broadwell node

1 node + 1x P100 PCIe per node

1 node + 1x V100 PCIe per node

11.1X

19.8X

214.95

2379.87

4261.93
HOOMD-Blue microsphere on V100 vs P100 (PCIe 16GB)

Running HOOMD-Blue version 2.2.2

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

1,428,364 particles

Force field/method: Bead spring polymers via dissipative particle dynamics

Results published in:
http://dx.doi.org/10.1002/adma.201501329
HOOMD-Blue quasicrystal on V100 vs P100 (PCIe 16GB)

Running **HOOMD-Blue** version 2.2.2

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

**100,000 particles**

*Force field/method: Oscilating pair potential MD*

*Results published in:*

[http://dx.doi.org/10.1038/NMAT4152](http://dx.doi.org/10.1038/NMAT4152)
HOOMD-Blue triblock-copolymer on V100 vs P100 (PCIe 16GB)

Running HOOMD-Blue version 2.2.2

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

64,017 particles

Force field/method: Bead-spring polymer MD

Results published in:
http://dx.doi.org/10.1021/ma061120f
HOOMD-Blue dodecahedron on V100 vs P100 (PCIe 16GB)

Average TPS

<table>
<thead>
<tr>
<th>Configuration</th>
<th>1 node + 1x P100 PCIe per node</th>
<th>1 node + 2x P100 PCIe per node</th>
<th>1 node + 4x P100 PCIe per node</th>
<th>1 node + 8x P100 PCIe per node</th>
<th>1 node + 1x V100 PCIe per node</th>
<th>1 node + 2x V100 PCIe per node</th>
<th>1 node + 4x V100 PCIe per node</th>
<th>1 node + 8x V100 PCIe per node</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>22.54</td>
<td>80.99</td>
<td>165.18</td>
<td>186.73</td>
<td>136.43</td>
<td>180.04</td>
<td>234.20</td>
<td>239.26</td>
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<tr>
<td>1 node + 1x P100 PCIe per node</td>
<td>3.6X</td>
<td>4.5X</td>
<td>7.3X</td>
<td>8.3X</td>
<td>6.1X</td>
<td>8.0X</td>
<td>10.4X</td>
<td>10.6X</td>
</tr>
</tbody>
</table>

Running HOOMD-Blue version 2.2.2

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

131,072 particles

Force field/method: Hard dodecahedra (via MC simulation)

This is a synthetic benchmark to test scalability and is much larger than anyone would reasonably run.
HOOMD-Blue hexagon on V100 vs P100 (PCIe 16GB)

Running HOOMD-Blue version 2.2.2

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

1,048,576 particles
Force field/method: Hard hexagons (via MC simulation)
Results published in: http://dx.doi.org/10.1103/PhysRevX.7.021001
Atomic-Fluid Lennard-Jones 2.5 Cutoff on V100s PCIe

2,048,000 atoms

(Untuned on Volta)
Running LAMMPS version 2017

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
Atomic-Fluid Lennard-Jones 2.5 Cutoff on V100s SXM2

- 2,048,000 atoms
- 3.3X

(UNTUNED ON VOLTA)
Running LAMMPS version 2017

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
Atomic-Fluid Lennard-Jones 5.0 Cutoff on V100s PCIe

2,048,000 atoms

(Untuned on Volta)
Running LAMMPS version 2017

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
Atomic-Fluid Lennard-Jones 5.0 Cutoff on V100s SXM2

2,048,000 atoms

(Untuned on Volta)
Running LAMMPS version 2017

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
Course-grain Water on V100s PCIe

2,048,000 atoms

<table>
<thead>
<tr>
<th>Configuration</th>
<th>1/seconds</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>0.003</td>
</tr>
<tr>
<td>1 node + 2x V100 PCIe per node (16GB)</td>
<td>0.007</td>
</tr>
<tr>
<td>1 node + 4x V100 PCIe per node (16GB)</td>
<td>0.011</td>
</tr>
<tr>
<td>1 node + 8x V100 PCIe per node (16GB)</td>
<td>0.016</td>
</tr>
</tbody>
</table>

(Untuned on Volta)
Running LAMMPS version 2017

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
Course-grain Water on V100s SXM2

2,048,000 atoms

1 Broadwell node
1 node + 2x V100 SXM2 per node (16GB)
1 node + 4x V100 SXM2 per node (16GB)
1 node + 8x V100 SXM2 per node (16GB)

(Untuned on Volta)
Running LAMMPS version 2017

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
Gay-Berne on V100s PCIe

2,097,152 atoms

(Untuned on Volta)
Running LAMMPS version 2017

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

1 Broadwell node

1 node + 2x V100 PCIe per node (16GB)
Gay-Berne on V100s SXM2

- 2,097,152 atoms

- 5.0X

(Untuned on Volta)
Running LAMMPS version 2017

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
Rhodopsin on V100s PCIe

256,000 atoms

(Untuned on Volta)
Running LAMMPS version 2017

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
Rhodopsin on V100s SXM2

(Untuned on Volta)
Running LAMMPS version 2017

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
### Recommended GPU Node Configuration for LAMMPS Computational Chemistry

<table>
<thead>
<tr>
<th>Workstation or Single Node Configuration</th>
<th></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>
</tbody>
</table>

**GPUs**
- GTX Titan X,
- Tesla P100, V100

| # 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
Running **NAMD** version 2.12

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) GPUs

APOA1 on P100s PCIe

<table>
<thead>
<tr>
<th>Configuration</th>
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<tbody>
<tr>
<td>1 Broadwell node</td>
<td>3.45</td>
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<tr>
<td>1 node + 1x P100 PCIe (16GB) per node</td>
<td>22.58</td>
</tr>
<tr>
<td>1 node + 2x P100 PCIe (16GB) per node</td>
<td>22.85</td>
</tr>
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</table>
Running **NAMD** version 2.12

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 SXM2 GPUs
F1ATPASE on P100s PCIe

Running **NAMD** version 2.12

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) GPUs

<table>
<thead>
<tr>
<th>Configuration</th>
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<tbody>
<tr>
<td>1 Broadwell node</td>
<td>1.15</td>
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<tr>
<td>1 node + 1x P100 PCIe (16GB) per node</td>
<td>7.34</td>
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<tr>
<td>1 node + 2x P100 PCIe (16GB) per node</td>
<td>6.99</td>
</tr>
<tr>
<td>1 node + 4x P100 PCIe (16GB) per node</td>
<td>7.40</td>
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</tbody>
</table>
F1ATPASE on P100s SXM2

Running NAMD version 2.12

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 SXM2 GPUs
STMV on P100s PCIe

Running NAMD version 2.12

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) GPUs
STMV on P100s SXM2

Running NAMD version 2.12

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 SXM2 GPUs
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- TeraChem
- UNM
- VASP
- WL-LSMS

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