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

1.94

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

47.67

24.6X
PME-Cellulose_NPT 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

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<table>
<thead>
<tr>
<th>Configuration</th>
<th>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</td>
</tr>
<tr>
<td>1 node + 4x V100 SXM2 per node (16GB)</td>
<td>55.52</td>
</tr>
</tbody>
</table>

**Performance Comparison:**

- 28.2X
- 28.6X
PME-Cellulose_NVE on V100s PCIe

(Untuned on Volta)
Running AMBER version 16.8

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1 node + 2x V100 SXM2 per node (16GB) = 32.2X
1 node + 4x V100 SXM2 per node (16GB) = 33.2X
1 Broadwell node = 1.96

63.04
65.02
PME-FactorIX_NPT on V100s PCIe

(UNTUNED on Volta)
Running AMBER version 16.8

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PME-FactorIX_NPT on V100s SXM2

Running AMBER version 16.8

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PME-FactorIX_NVE on V100s PCIe

(UNTUNED ON VOLTA)
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PME-FactorIX_NVE on V100s SXM2

( Untuned on Volta)
Running AMBER version 16.8

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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
PME-JAC_NPT on V100s SXM2

- **1 Broadwell node**: 34.35 ns/day
- **1 node + 2x V100 SXM2 per node (16GB)**: 481.75 ns/day **14.0X**
- **1 node + 4x V100 SXM2 per node (16GB)**: 515.36 ns/day **15.0X**

(Untuned on Volta)
Running AMBER version 16.8

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PME-JAC_NVE on V100s PCIe

1 Broadwell node

\[
\text{ns/day} = 490.77
\]

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

\[
\text{ns/day} = 36.53 \times 13.4X
\]

(Untuned on Volta)
Running AMBER version 16.8

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PME-JAC_NVE on V100s SXM2

(Untuned on Volta)
Running AMBER version 16.8

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PME-JAC_NPT_4fs on V100s PCIe

(Untuned on Volta)
Running AMBER version 16.8

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PME-JAC_NPT_4fs on V100s SXM2

(Untuned on Volta)
Running AMBER version 16.8

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(Untuned on Volta)
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1 Broadwell node

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

26.0X
PME-JAC_NVE_4fs on V100s SXM2

(Untuned on Volta)
Running AMBER version 16.8

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PME-STMV_NPT_4fs on V100s PCIe

31.3X

(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-STMV_NPT_4fs on V100s SXM2

1 Broadwell node

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

35.1X

(Untuned on Volta)
Running AMBER version 16.8

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**GB-Myoglobin on V100s PCIe**

(Untuned on Volta)
Running AMBER version 16.8

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GB-Myoglobin on V100s SXM2

(Untuned on Volta)
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GB-Nucleosome on V100s PCIe

(Untuned on Volta)
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GB-Nucleosome on V100s SXM2

( Untuned on Volta )
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<thead>
<tr>
<th>Configuration</th>
<th>ns/day</th>
<th>Increase</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>0.31</td>
<td>1</td>
</tr>
<tr>
<td>1 node + 2x V100 SXM2 per node (16GB)</td>
<td>52.89</td>
<td>170.6X</td>
</tr>
<tr>
<td>1 node + 4x V100 SXM2 per node (16GB)</td>
<td>92.46</td>
<td>298.3X</td>
</tr>
</tbody>
</table>
Rubisco on V100s PCIe

(Untuned on Volta)
Running AMBER version 16.8

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Rubisco on V100s SXM2

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# Recommended GPU Node Configuration for AMBER Computational Chemistry

## Workstation or Single Node Configuration

<table>
<thead>
<tr>
<th>Specification</th>
<th>Specification Details</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>P100, V100</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