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)
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)
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 (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>Performance (ns/day)</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>2.47</td>
<td></td>
</tr>
<tr>
<td>1 node + 1x P100 PCIe (16GB) per node</td>
<td>9.4X</td>
<td></td>
</tr>
<tr>
<td>1 node + 2x P100 PCIe (16GB) per node</td>
<td>13.2X</td>
<td></td>
</tr>
<tr>
<td>1 Broadwell node</td>
<td>32.55</td>
<td></td>
</tr>
</tbody>
</table>
PME-Cellulose_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)

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<table>
<thead>
<tr>
<th>Configuration</th>
<th>PME-Cellulose_NVE ns/day</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>2.47</td>
</tr>
<tr>
<td>1 node + 1x P100 SXM2 per node</td>
<td>10.1X</td>
</tr>
<tr>
<td>1 node + 2x P100 SXM2 per node</td>
<td>14.2X</td>
</tr>
<tr>
<td>1 node + 4x P100 SXM2 per node</td>
<td>16.6X</td>
</tr>
<tr>
<td>1 node + 4x P100 SXM2 per node</td>
<td>40.88</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

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Performance (ns/day)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>11.43</td>
</tr>
<tr>
<td>1 node + 1x P100 SXM2 per node</td>
<td>106.25</td>
</tr>
<tr>
<td>1 node + 2x P100 SXM2 per node</td>
<td>144.11</td>
</tr>
<tr>
<td>1 node + 4x P100 SXM2 per node</td>
<td>159.80</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_NVE on P100s PCIe

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PME-FactorIX_NVE on P100s SXM2

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- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 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 (16GB) GPUs

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

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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

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)
GB-Myoglobin on P100s SXM2

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- 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)
GB-Nucleosome on P100s SXM2

Running AMBER version 16.3

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- 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>GB-Nucleosome</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Broadwell node</td>
<td>0.40</td>
<td></td>
</tr>
<tr>
<td>1 node + 1x P100 SXM2 per node</td>
<td>13.36</td>
<td>33.4X</td>
</tr>
<tr>
<td>1 node + 2x P100 SXM2 per node</td>
<td>25.53</td>
<td>63.8X</td>
</tr>
<tr>
<td>1 node + 4x P100 SXM2 per node</td>
<td>46.29</td>
<td>115.7X</td>
</tr>
<tr>
<td>1 node + 8x P100 SXM2 per node</td>
<td>48.29</td>
<td>120.7X</td>
</tr>
</tbody>
</table>
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

## 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+ (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.