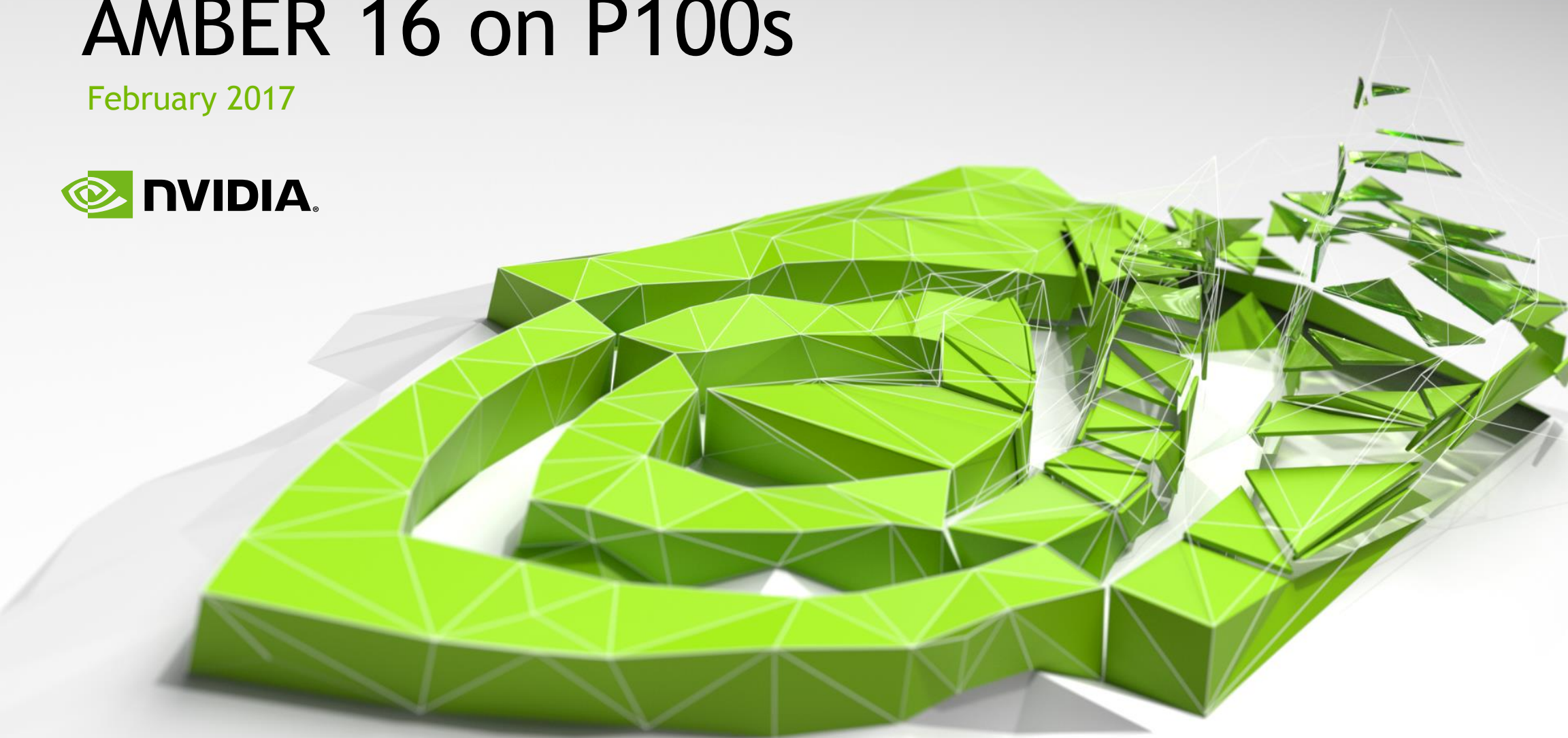
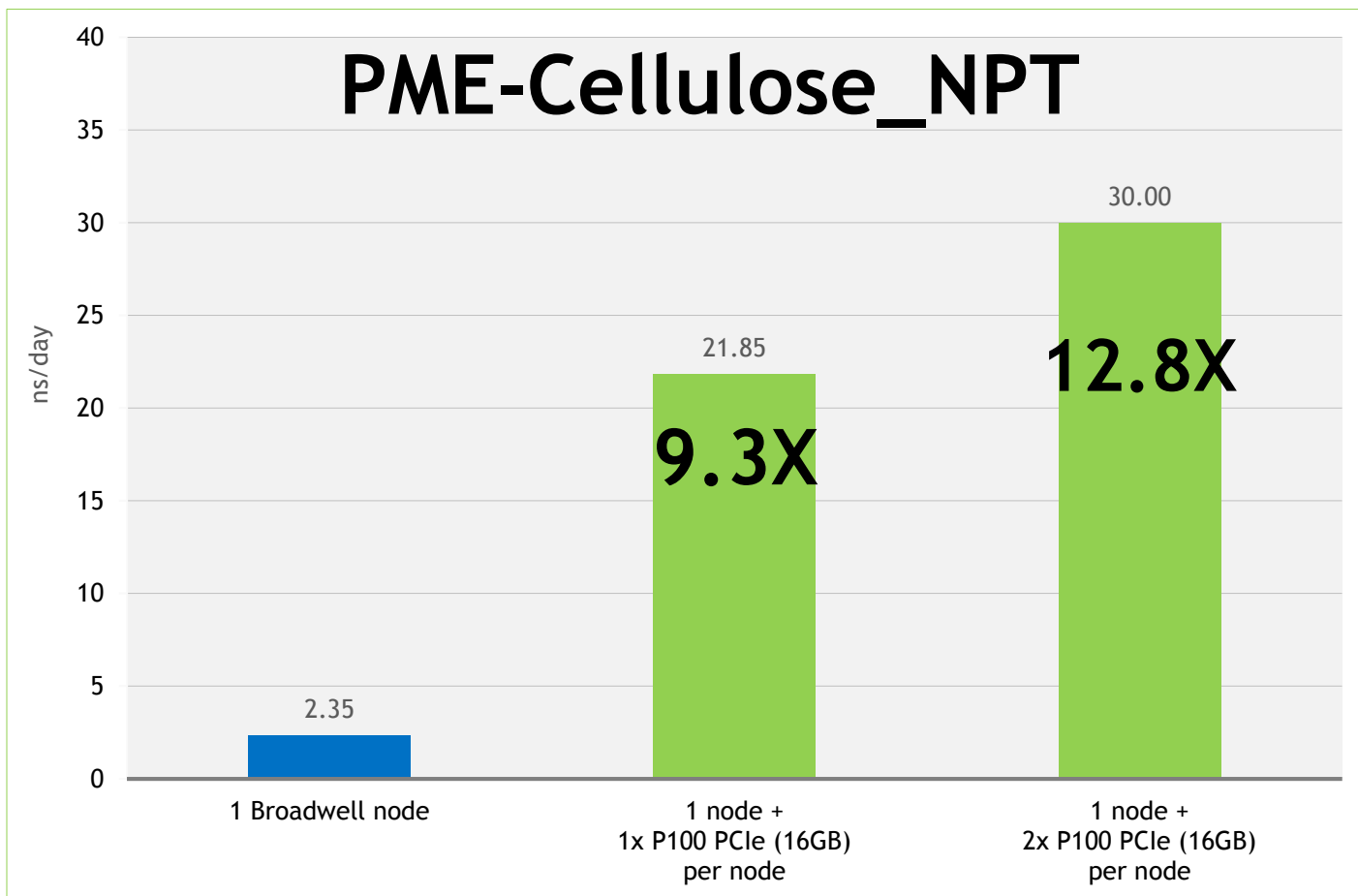


AMBER 16 on P100s

February 2017



PME-Cellulose_NPT on P100s PCIe



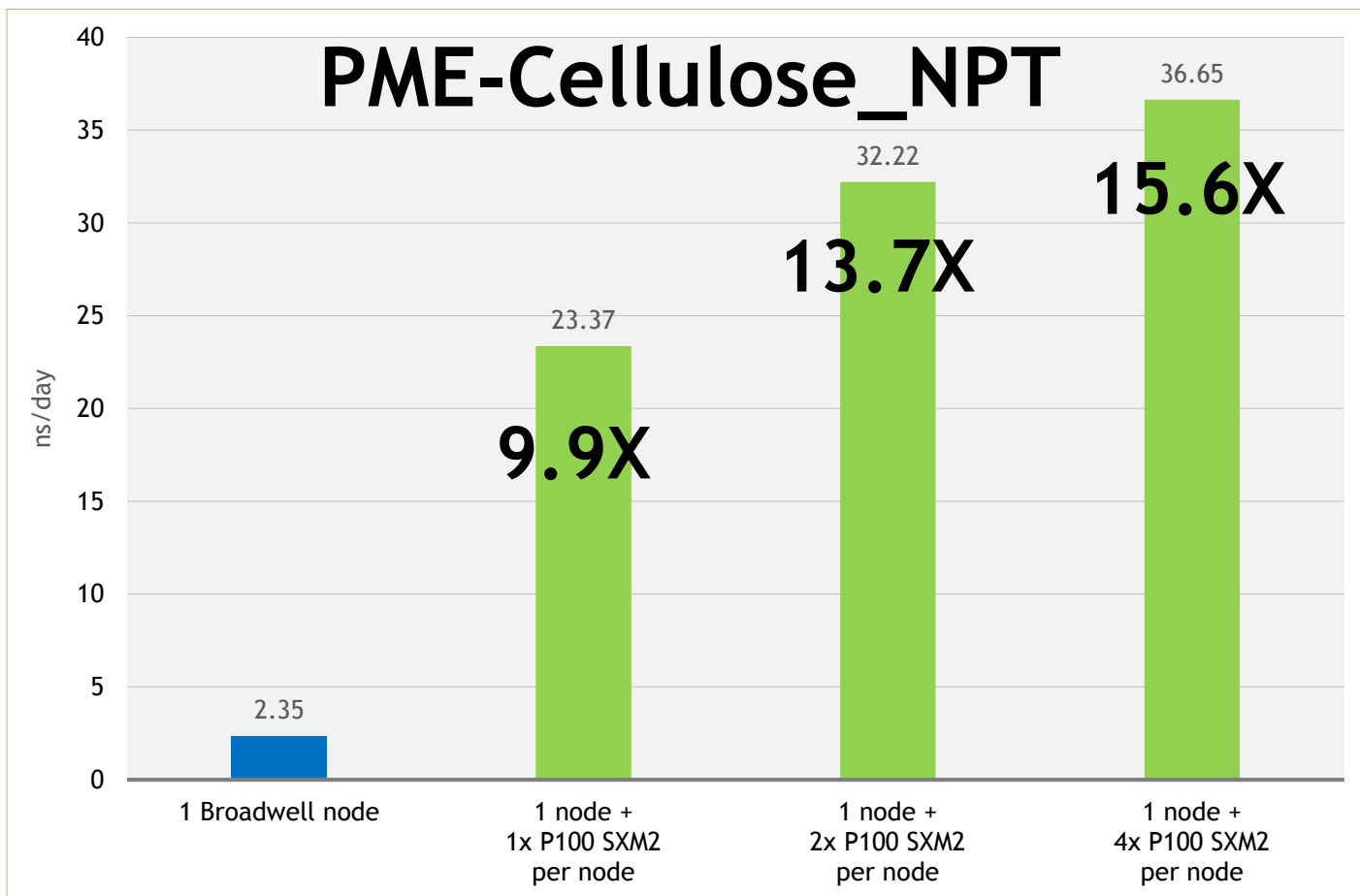
Running **AMBER** version 16.3

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



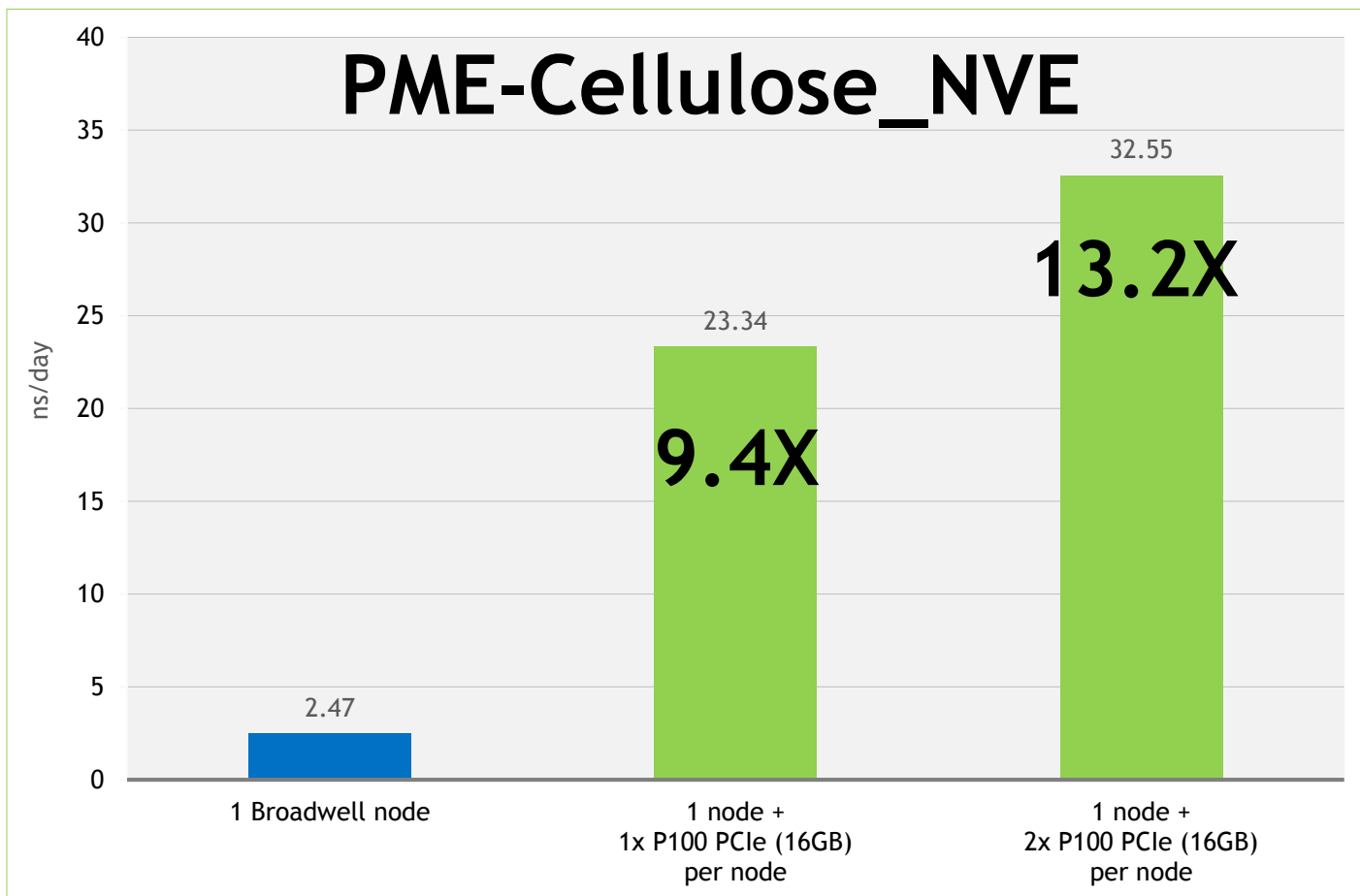
Running **AMBER** version 16.3

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



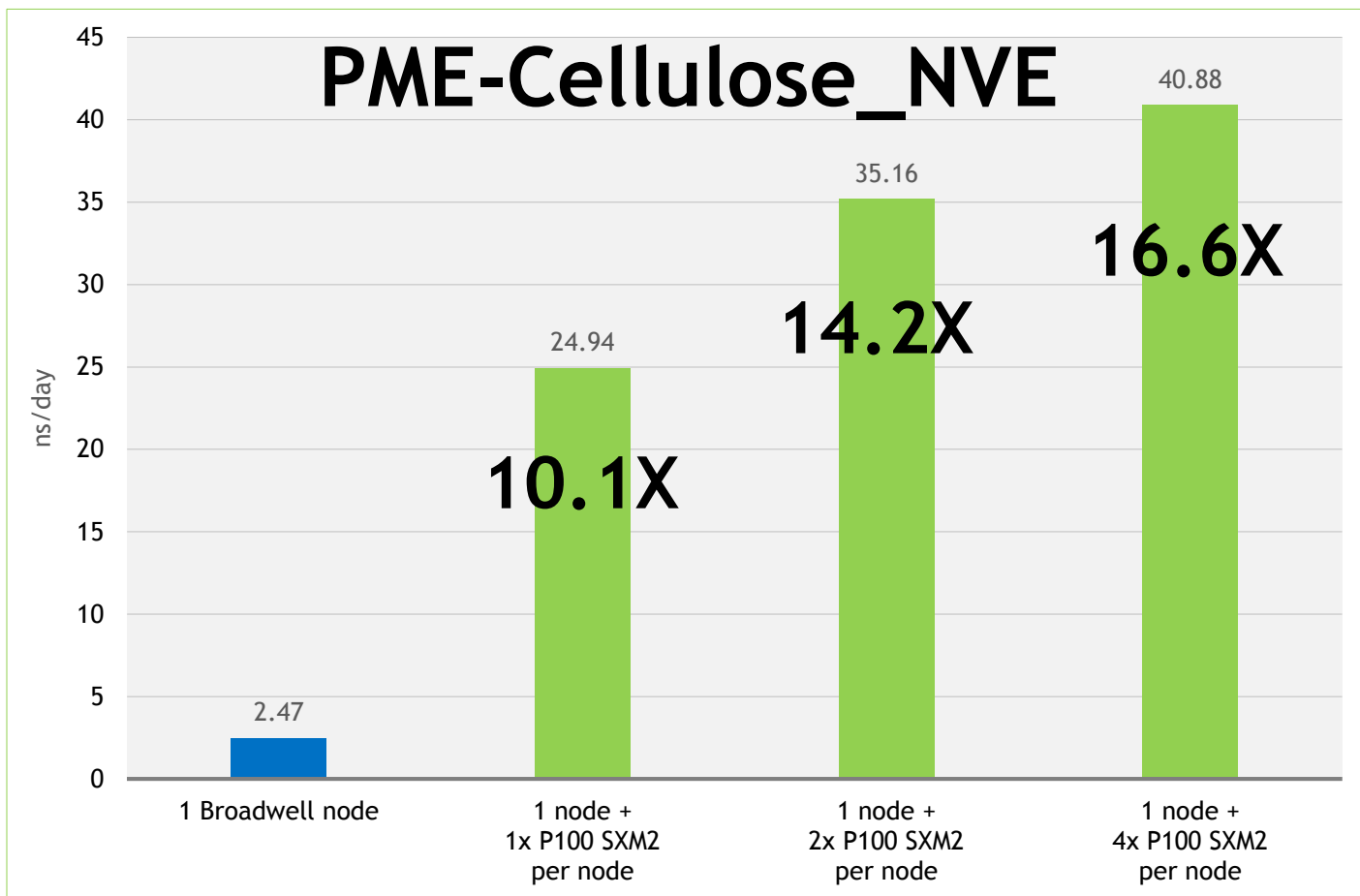
Running **AMBER** version 16.3

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)

PME-Cellulose_NVE on P100s SXM2



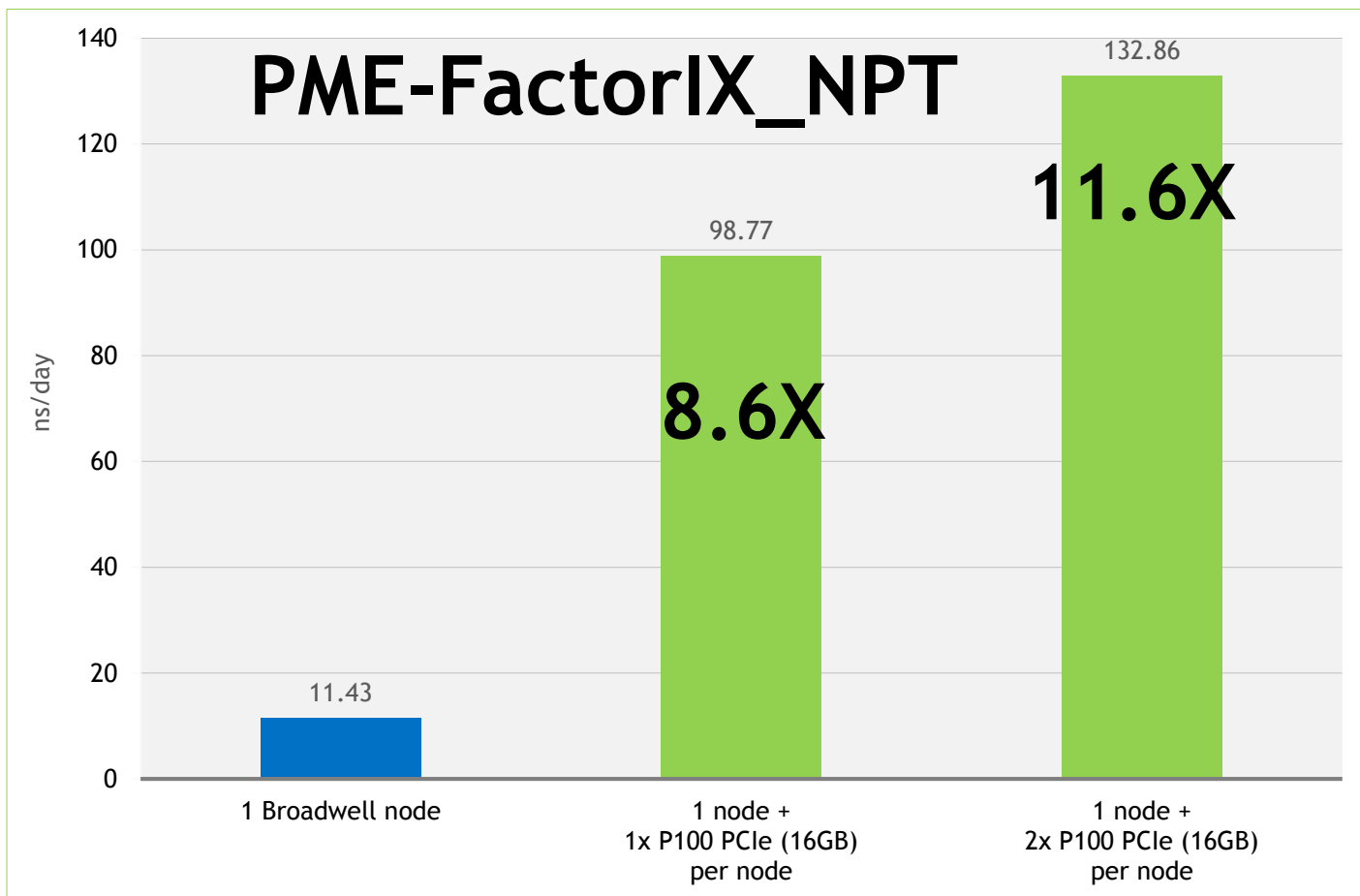
Running **AMBER** version 16.3

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)

PME-FactorIX_NPT on P100s PCIe



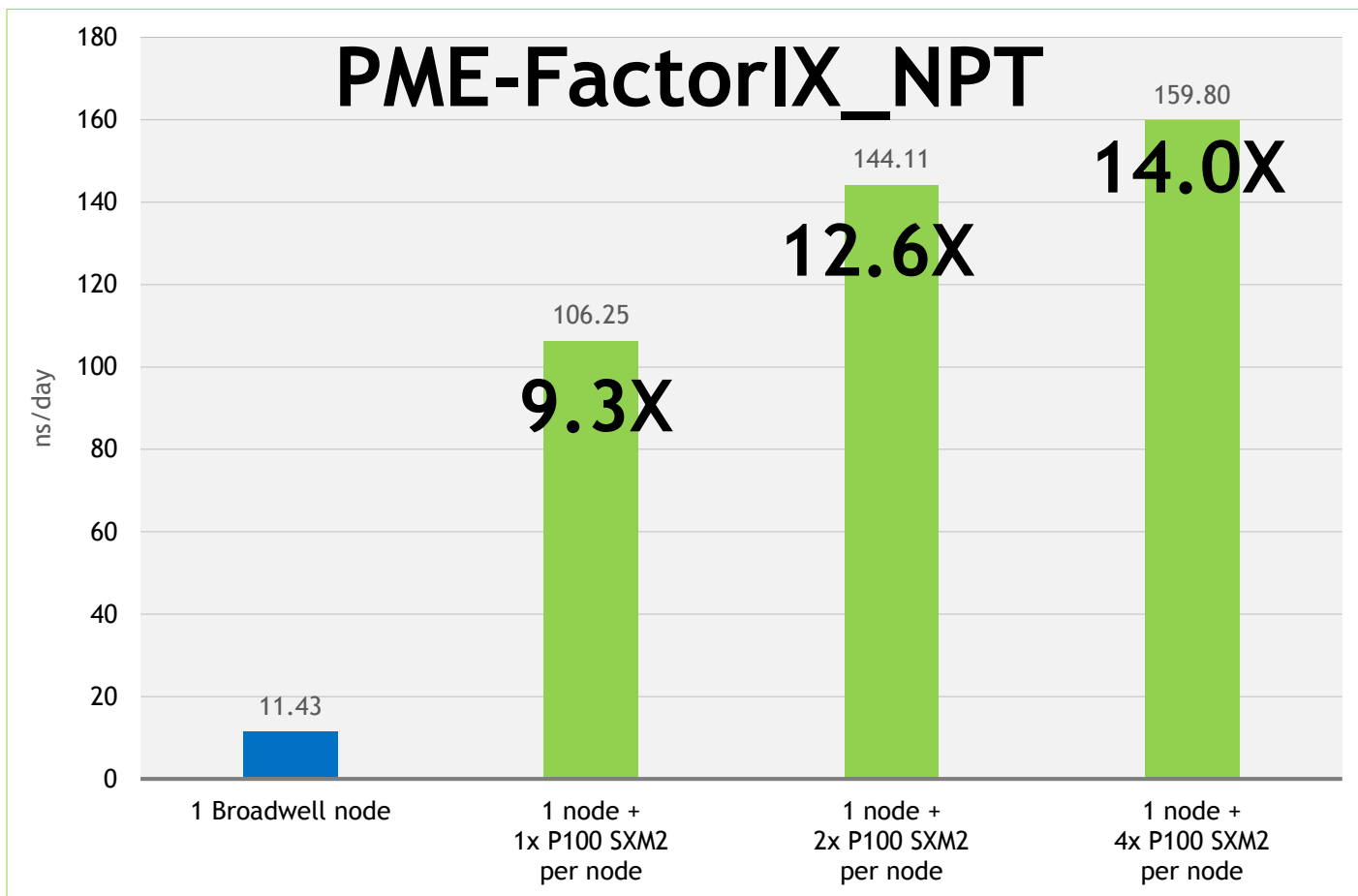
Running **AMBER** version 16.3

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



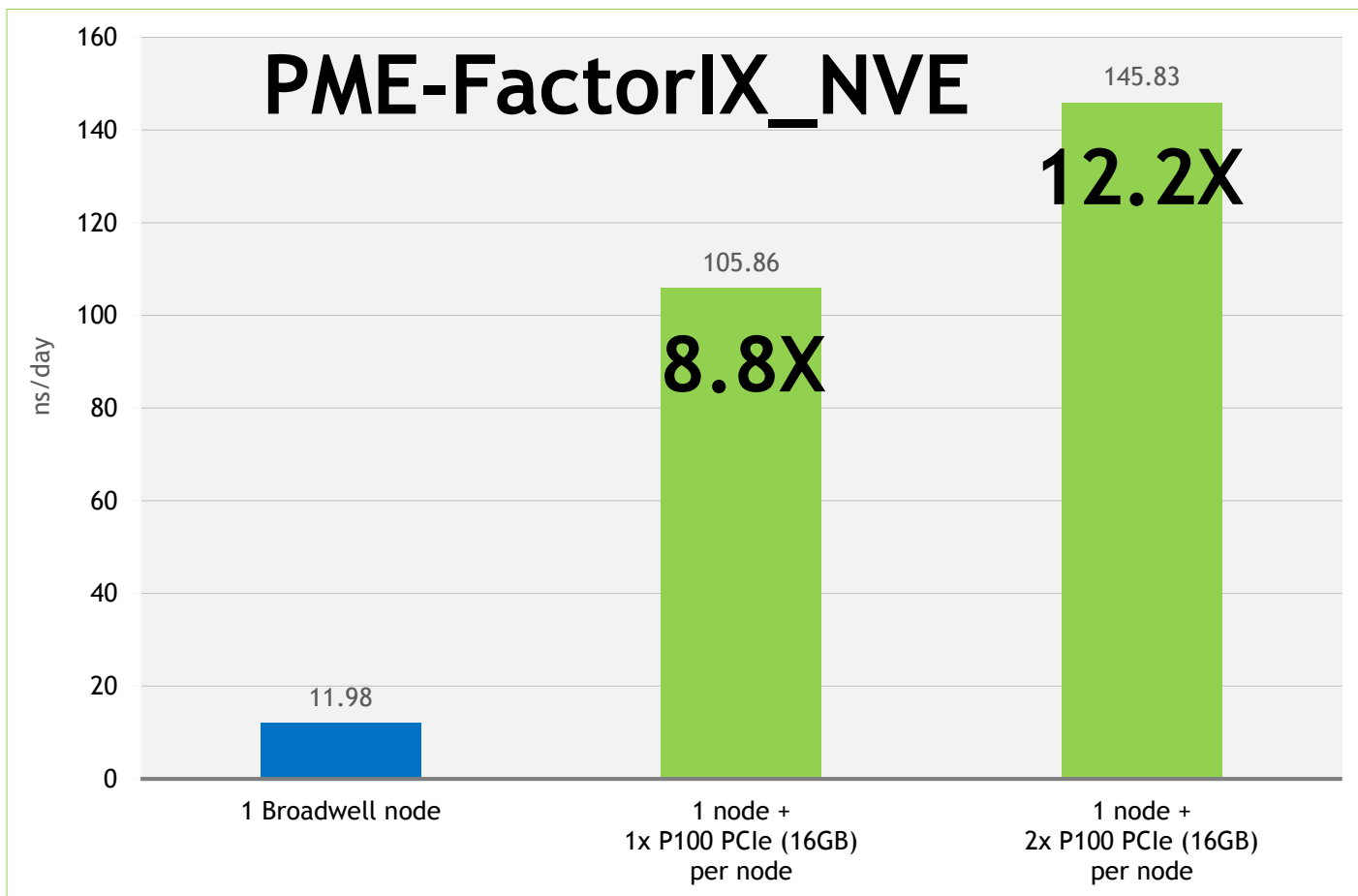
Running **AMBER** version 16.3

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



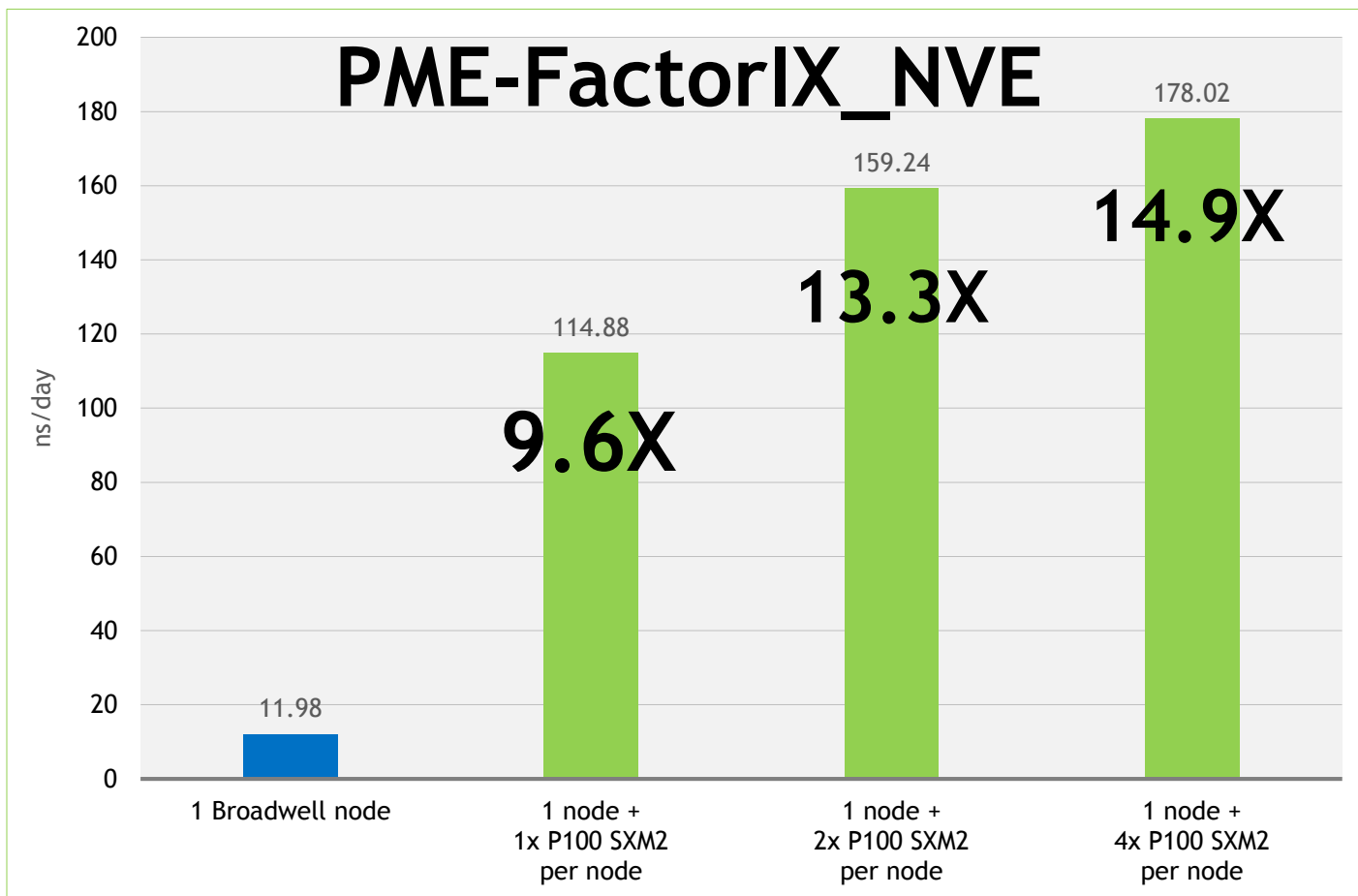
Running **AMBER** version 16.3

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_NVE on P100s SXM2



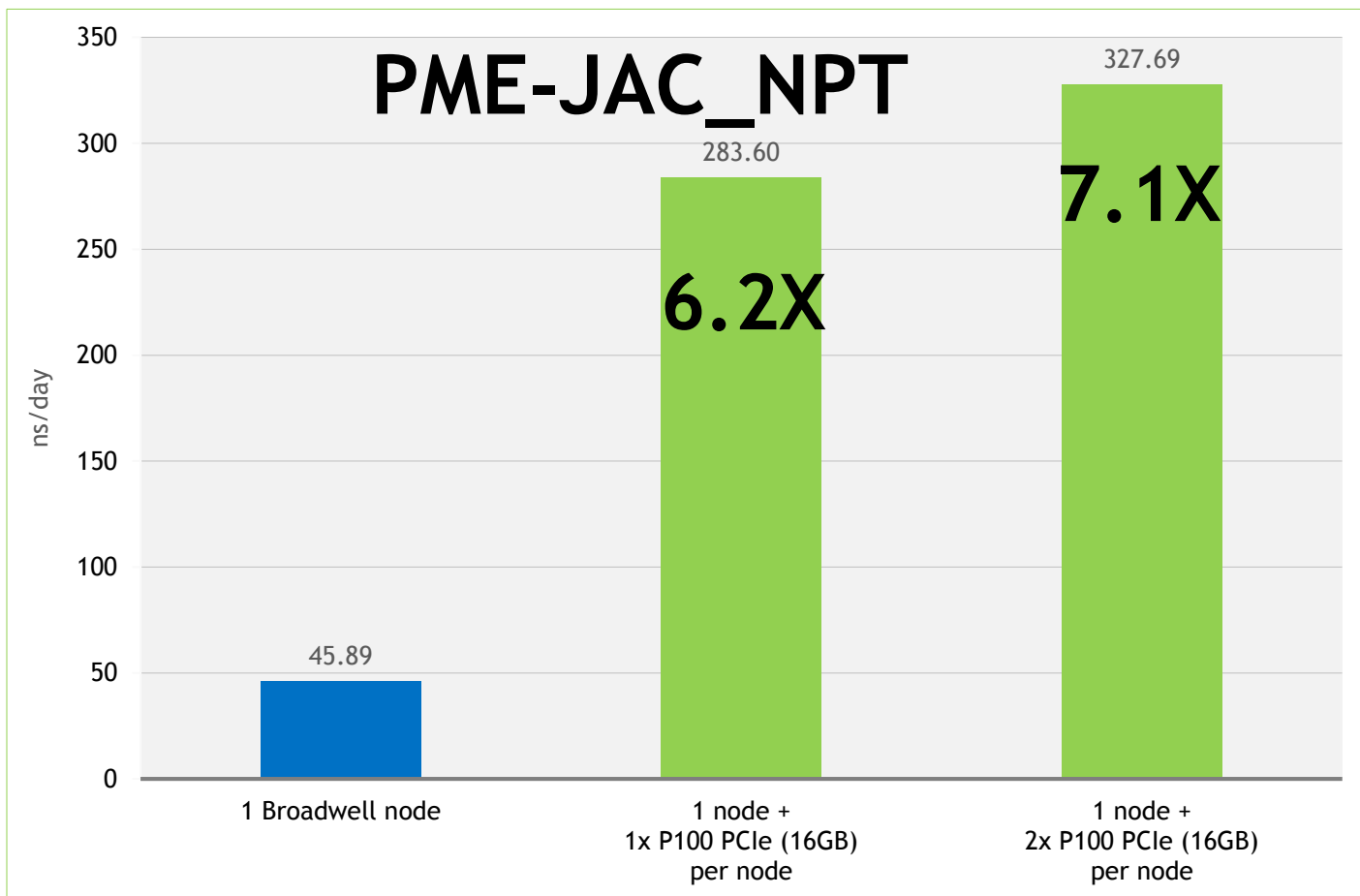
Running **AMBER** version 16.3

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 P100s PCIe



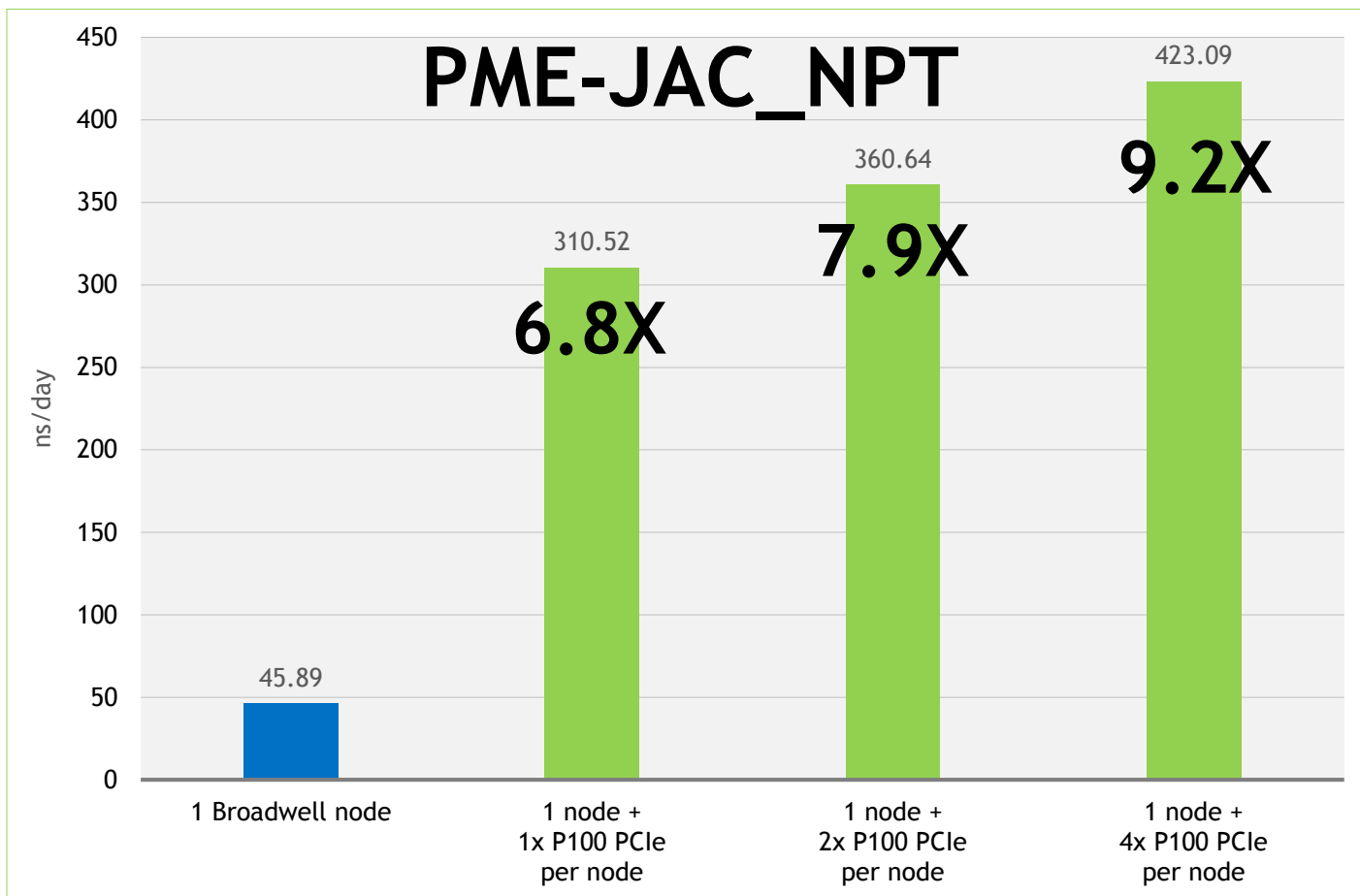
Running **AMBER** version 16.3

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-JAC_NPT on P100s SXM2



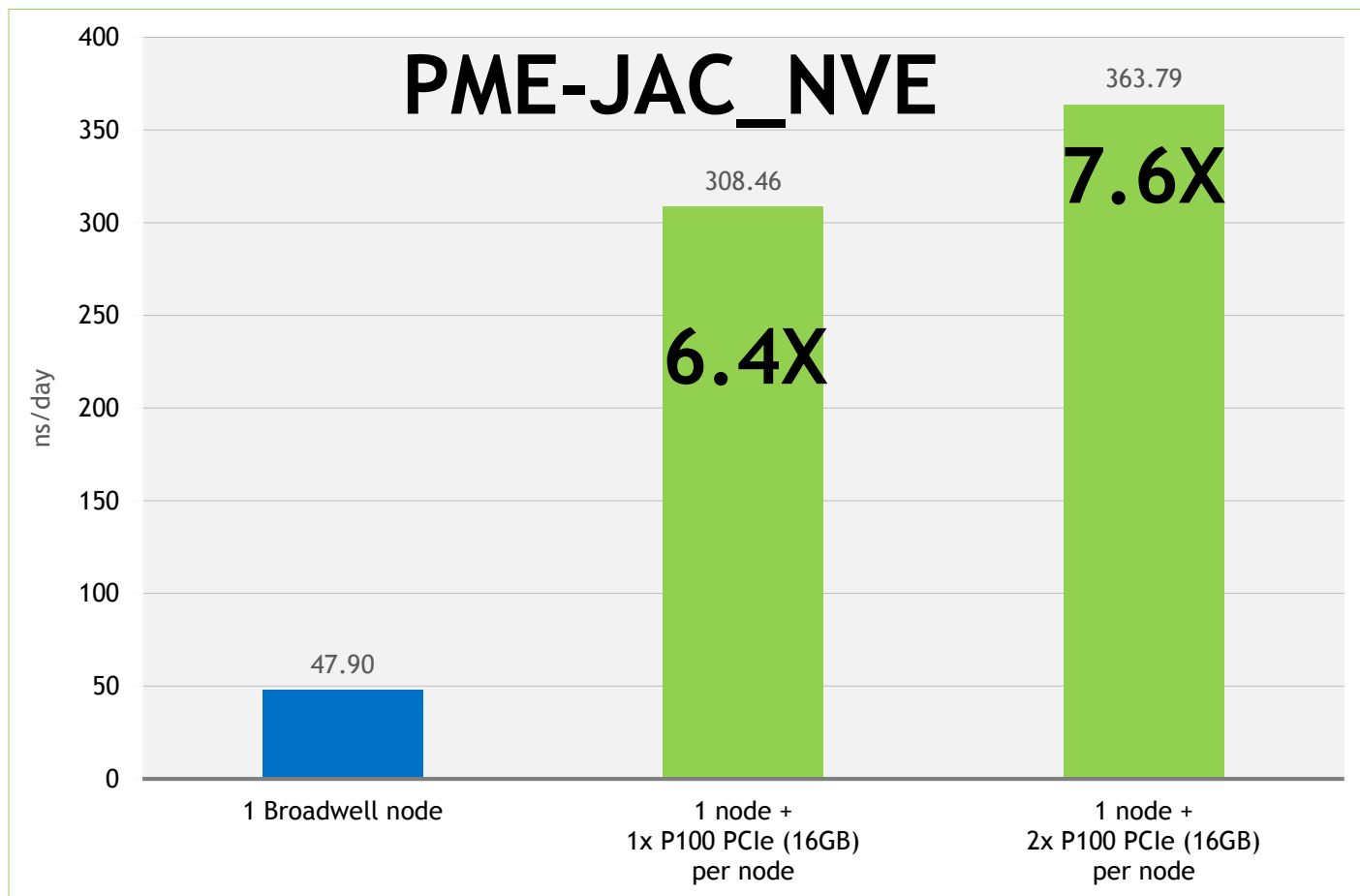
Running **AMBER** version 16.3

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

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

PME-JAC_NVE on P100s PCIe



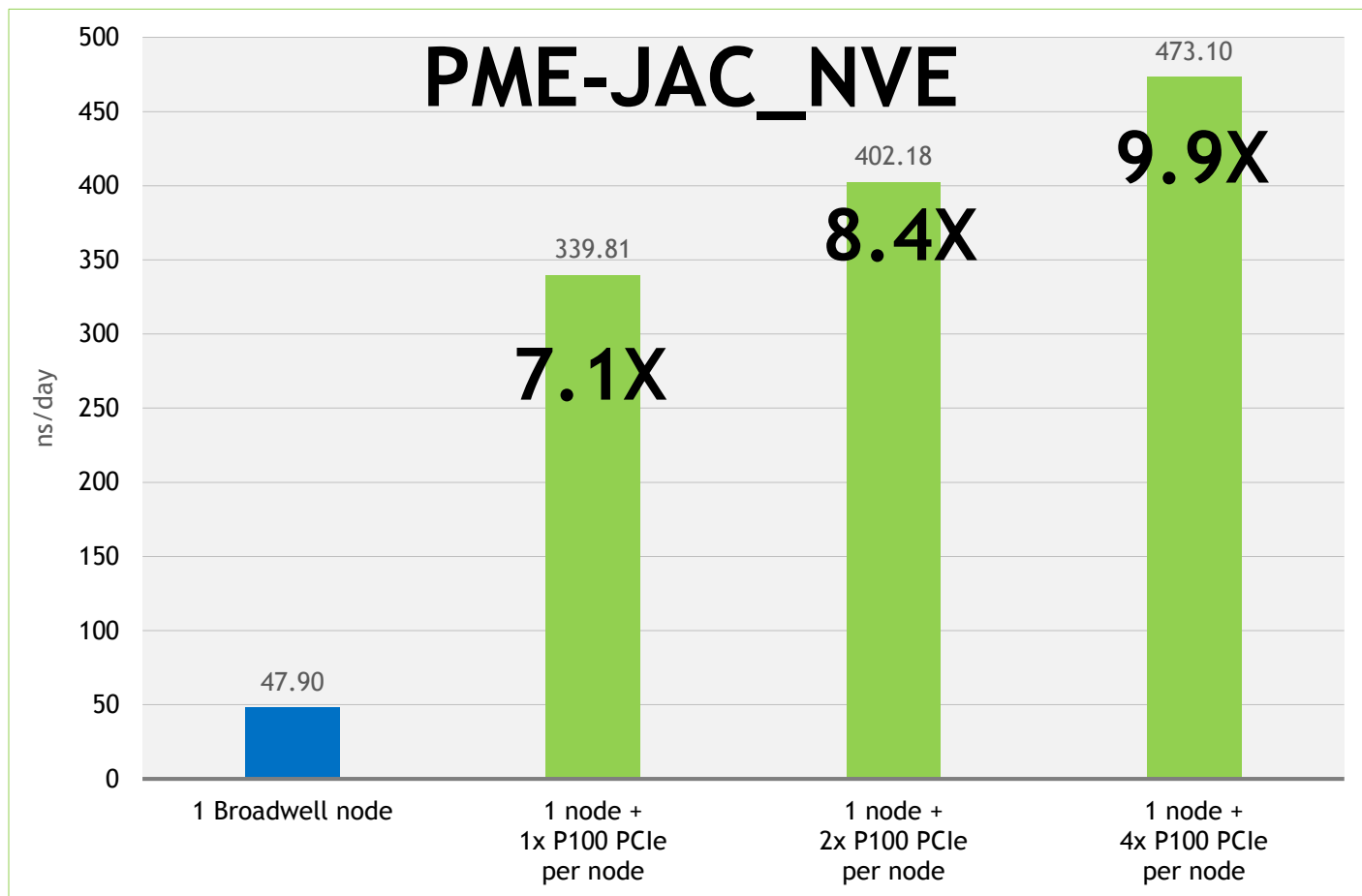
Running **AMBER** version 16.3

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

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-JAC_NVE on P100s SXM2



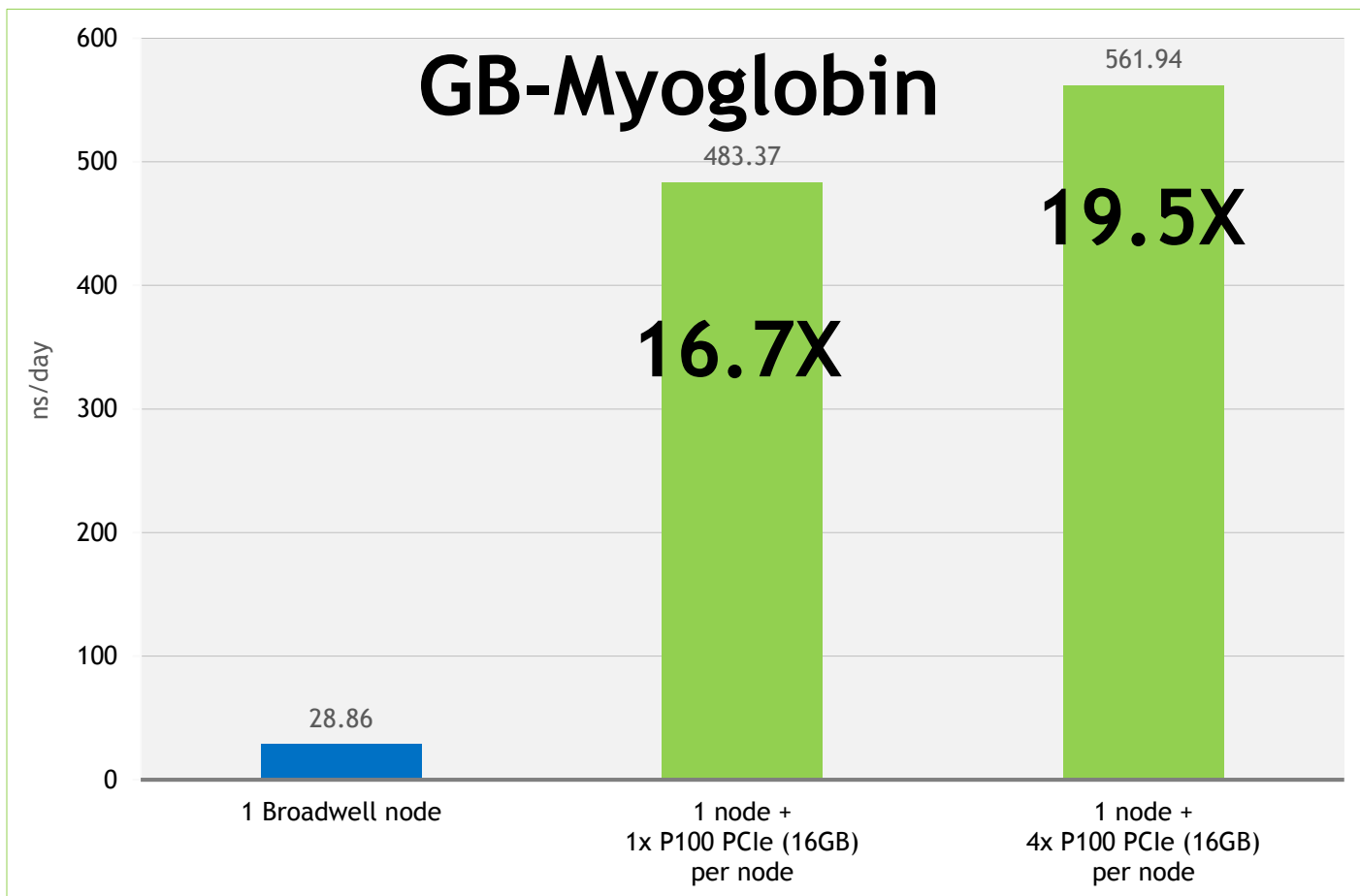
Running **AMBER** version 16.3

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)

GB-Myoglobin on P100s PCIe



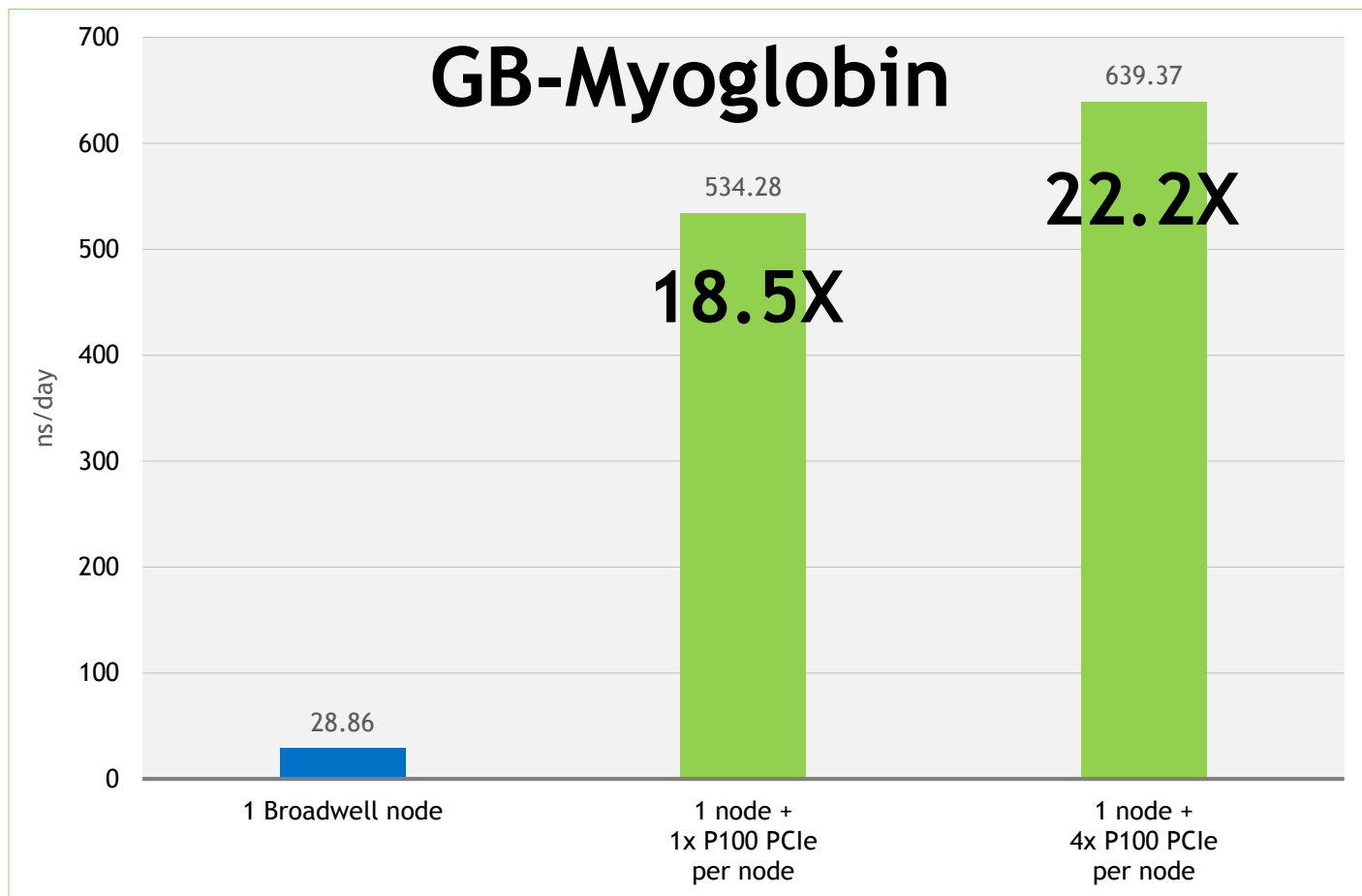
Running **AMBER** version 16.3

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



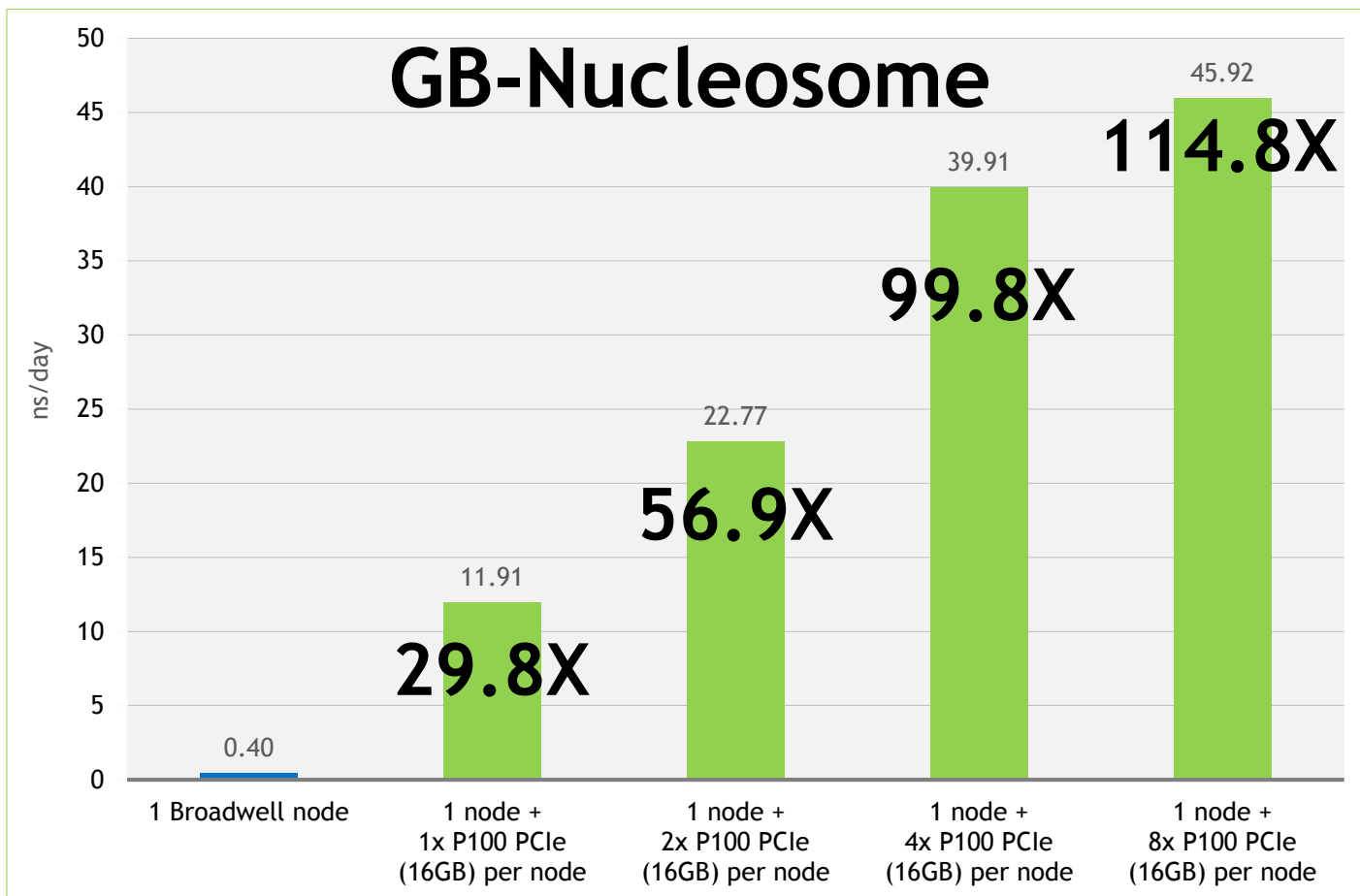
Running **AMBER** version 16.3

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 P100s PCIe



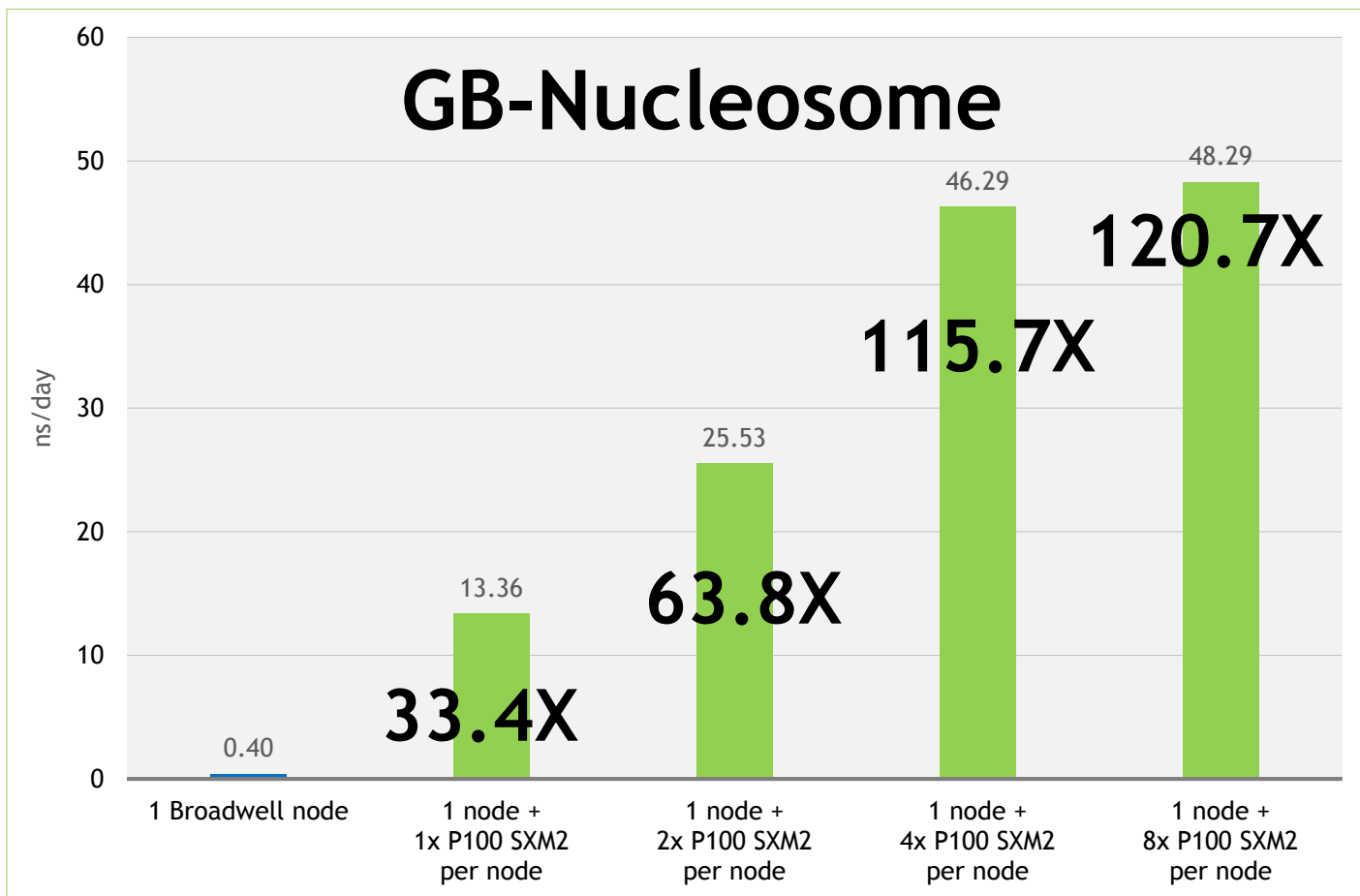
Running **AMBER** version 16.3

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



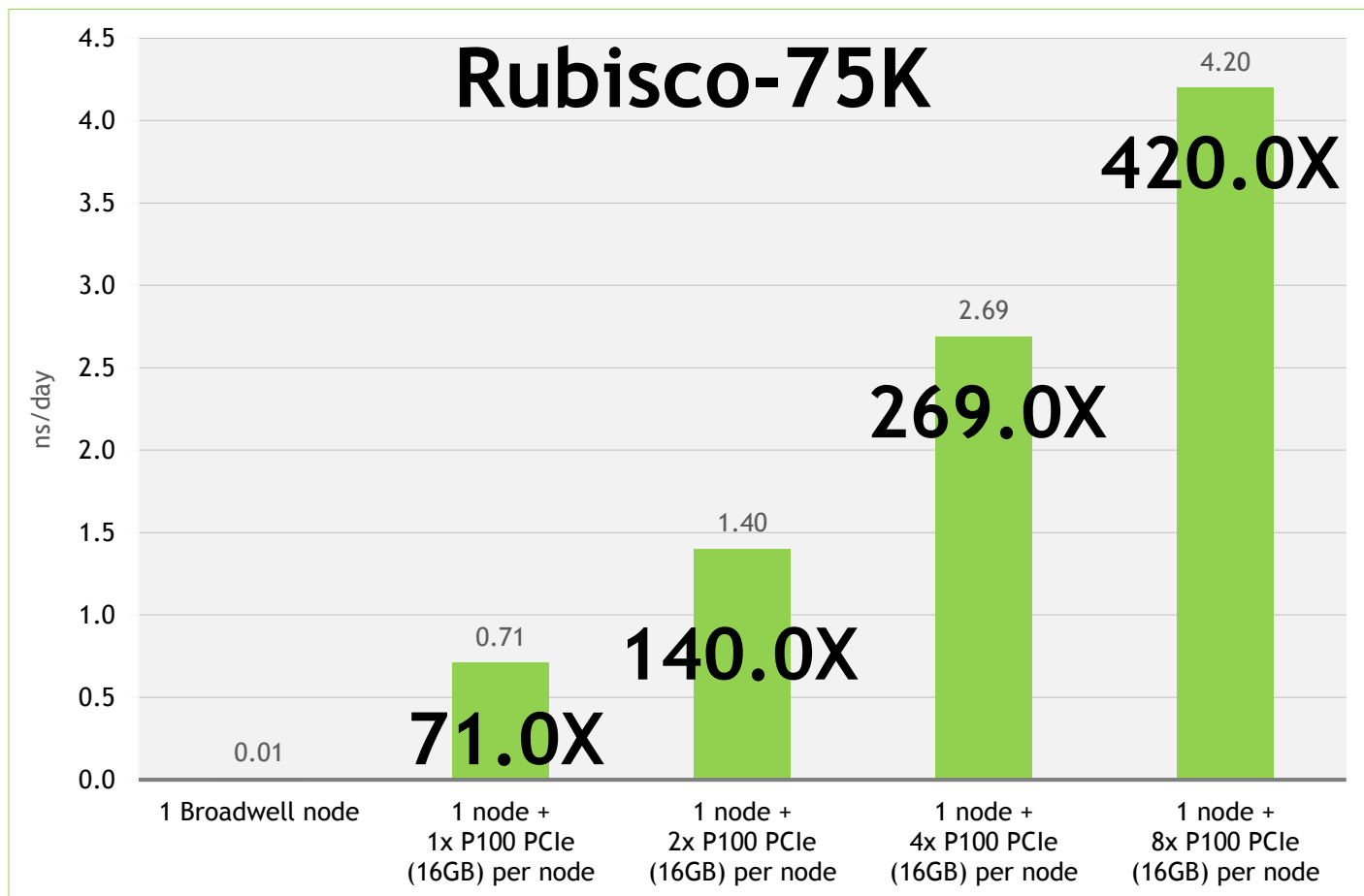
Running **AMBER** version 16.3

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



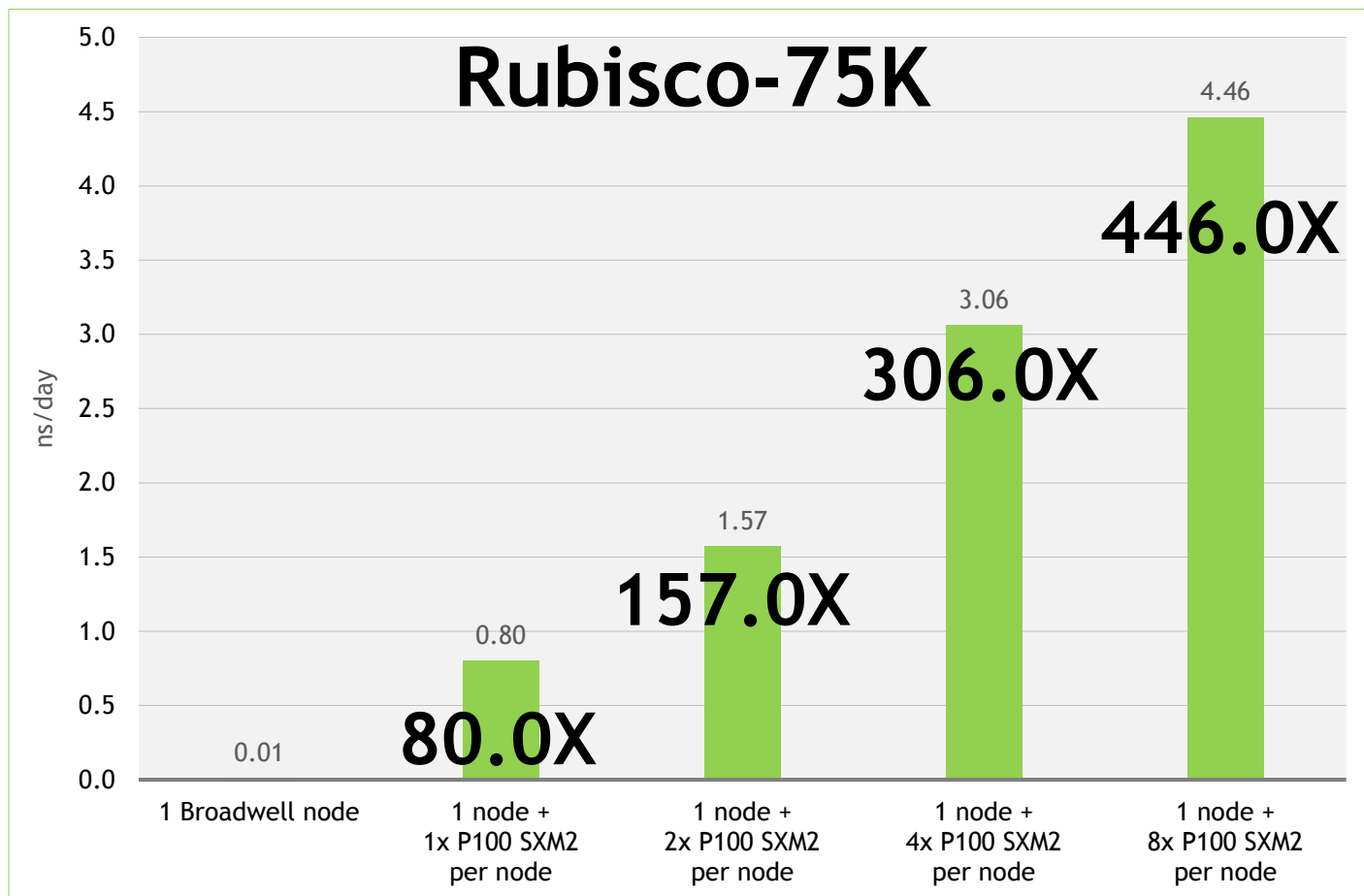
Running **AMBER** version 16.3

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

Workstation or Single Node Configuration

# of CPU sockets	2
Cores per CPU socket	6+ (1 CPU core drives 1 GPU)
CPU speed (Ghz)	2.66+
System memory per node (GB)	16
GPUs	P100, V100
# of GPUs per CPU socket	1-4
GPU memory preference (GB)	6
GPU to CPU connection	PCIe 3.0 16x or higher
Server storage	2 TB
Network configuration	Infiniband QDR or better

Scale to multiple nodes with same single node configuration