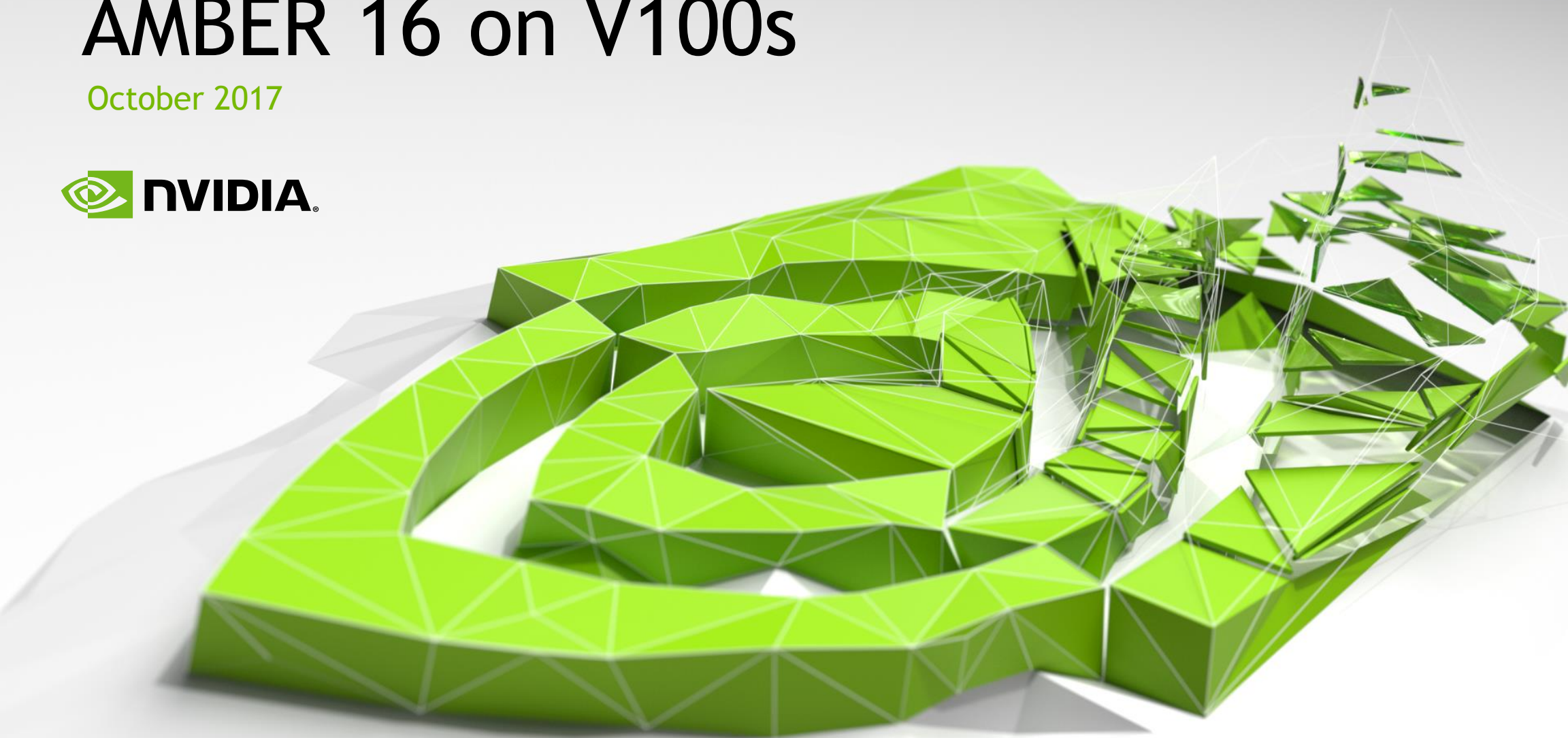
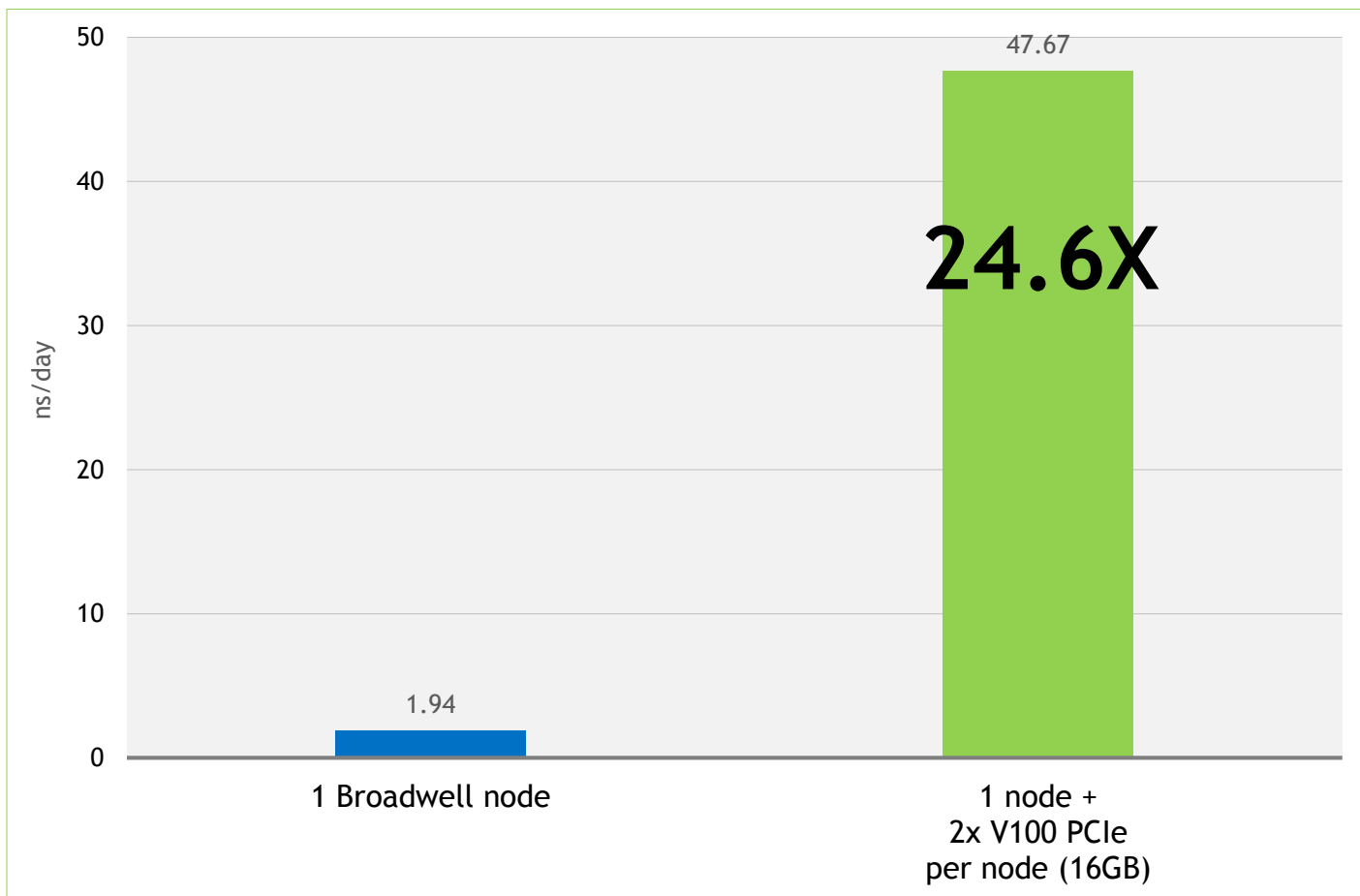


AMBER 16 on V100s

October 2017



PME-Cellulose_NPT on V100s PCIe

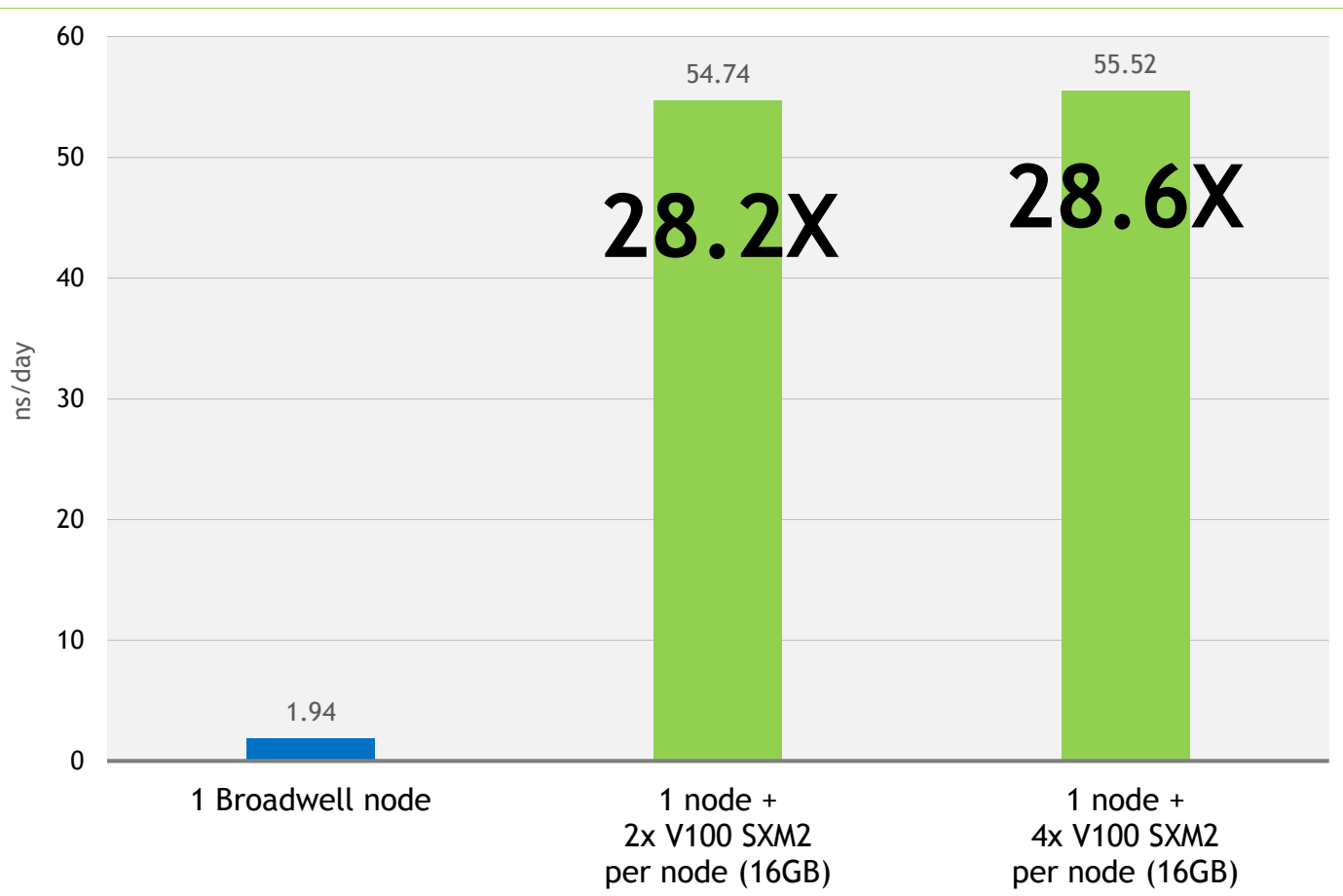


(Untuned on Volta)
Running **AMBER** version 16.8

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PME-Cellulose_NPT on V100s SXM2

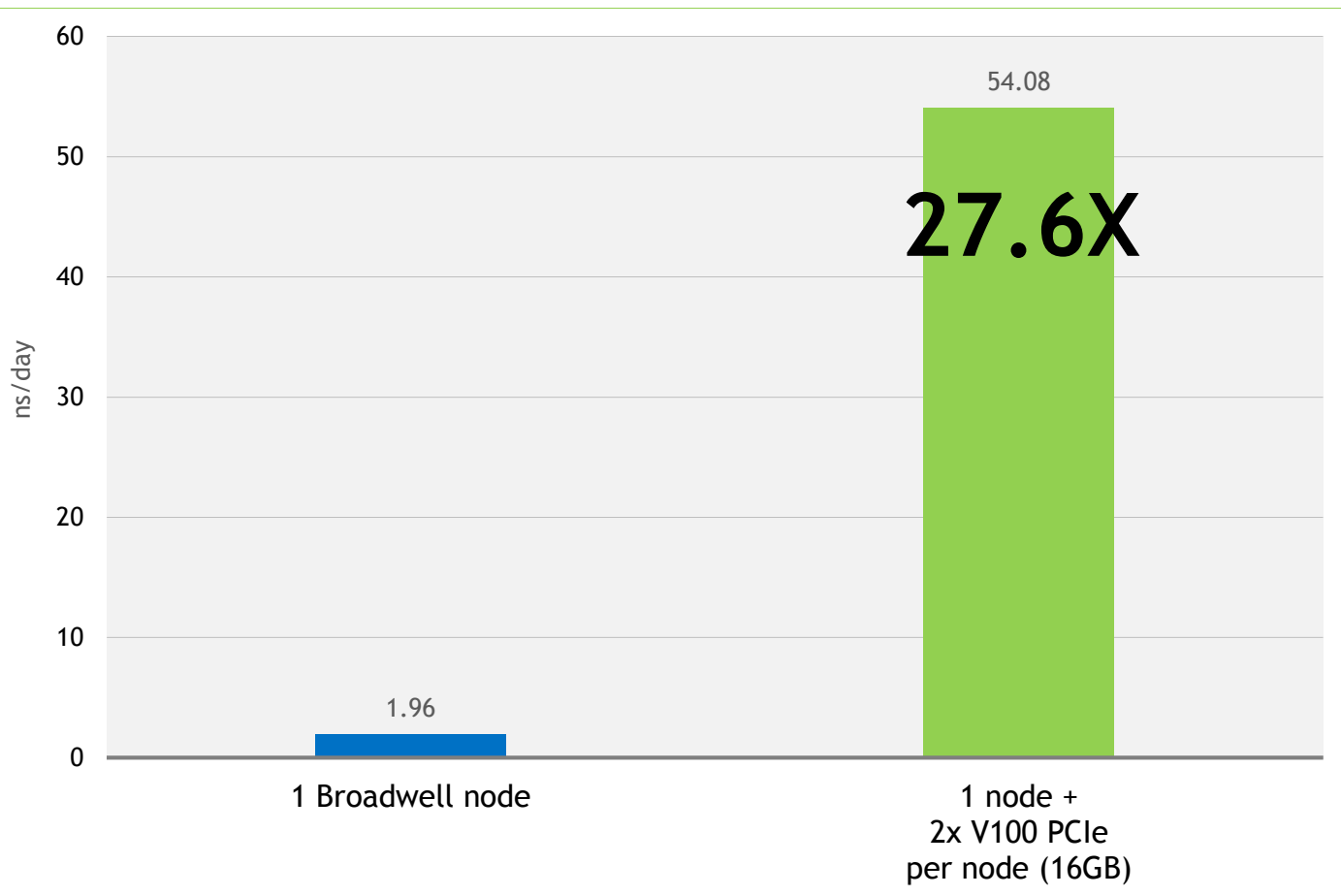


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PME-Cellulose_NVE on V100s PCIe

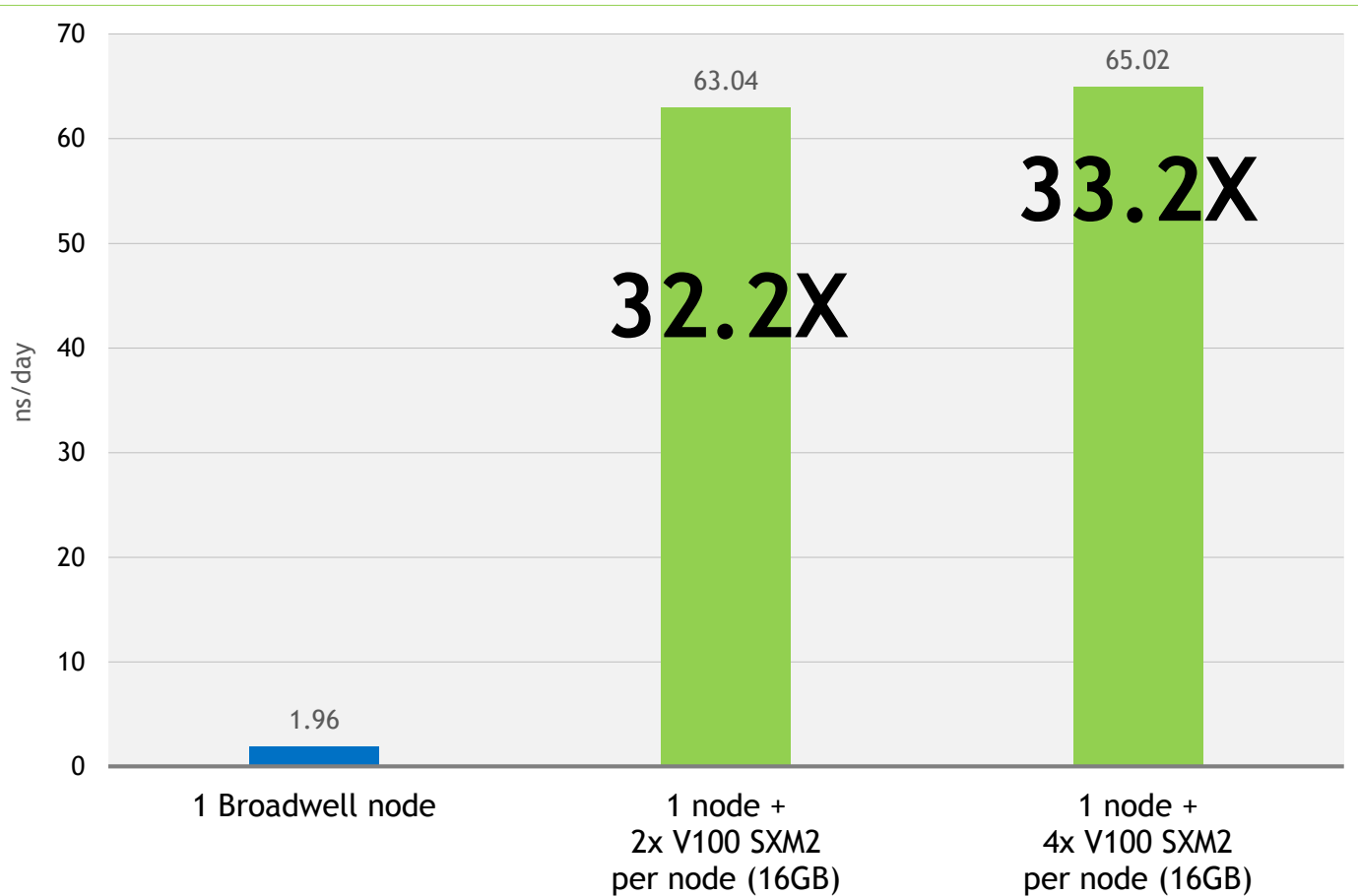


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PME-Cellulose_NVE on V100s SXM2

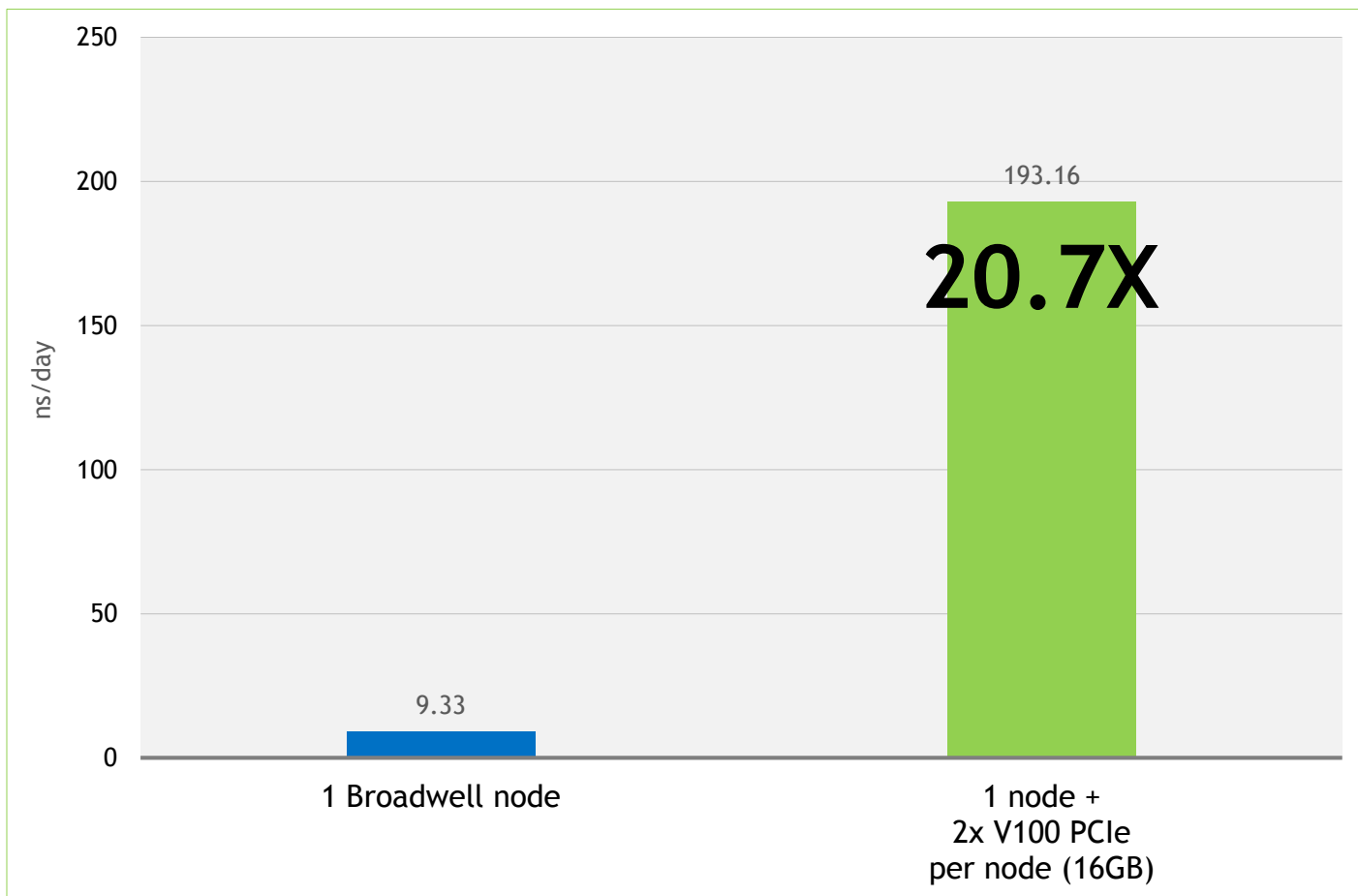


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PME-FactorIX_NPT on V100s PCIe

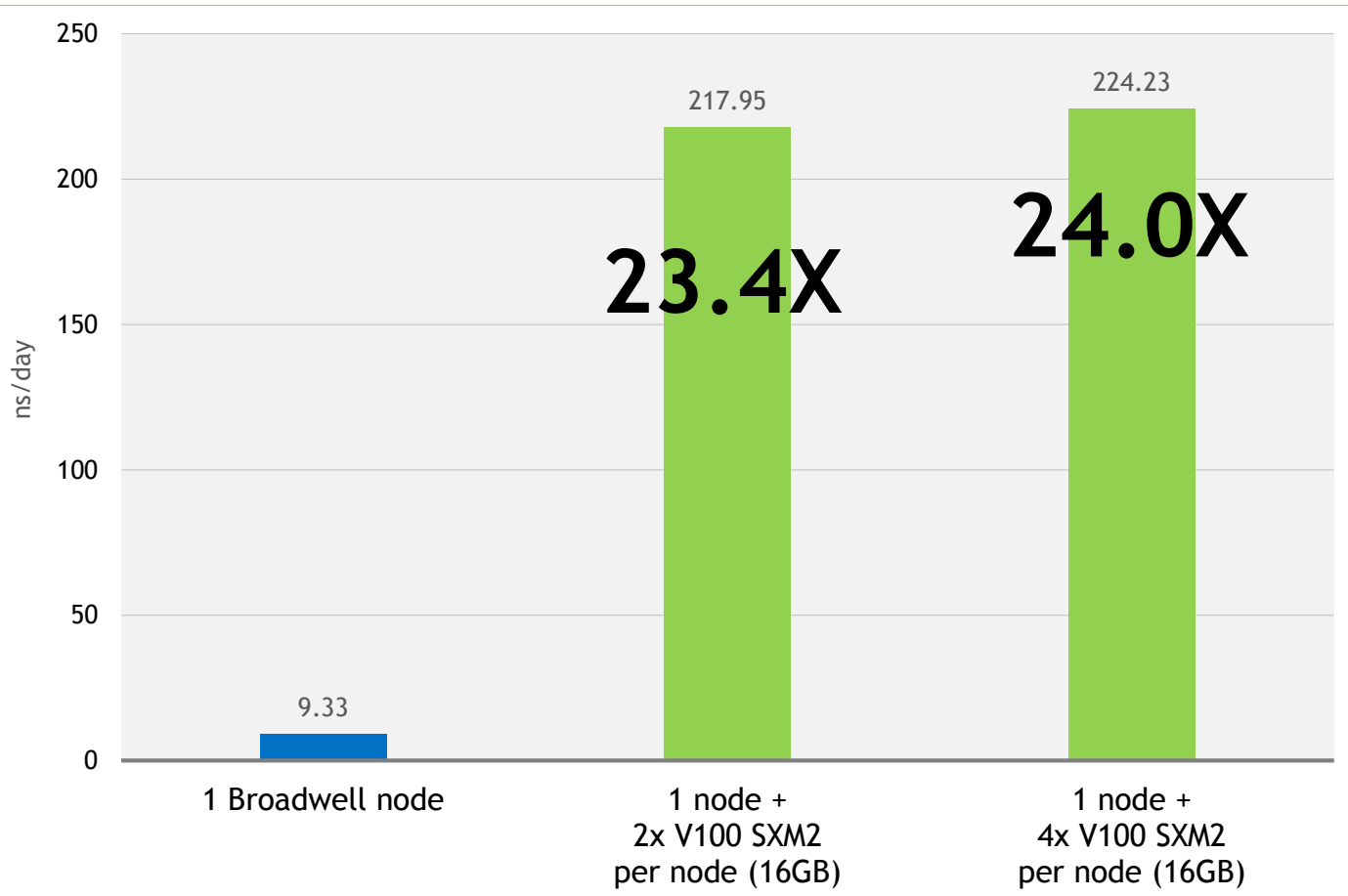


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PME-FactorIX_NPT on V100s SXM2

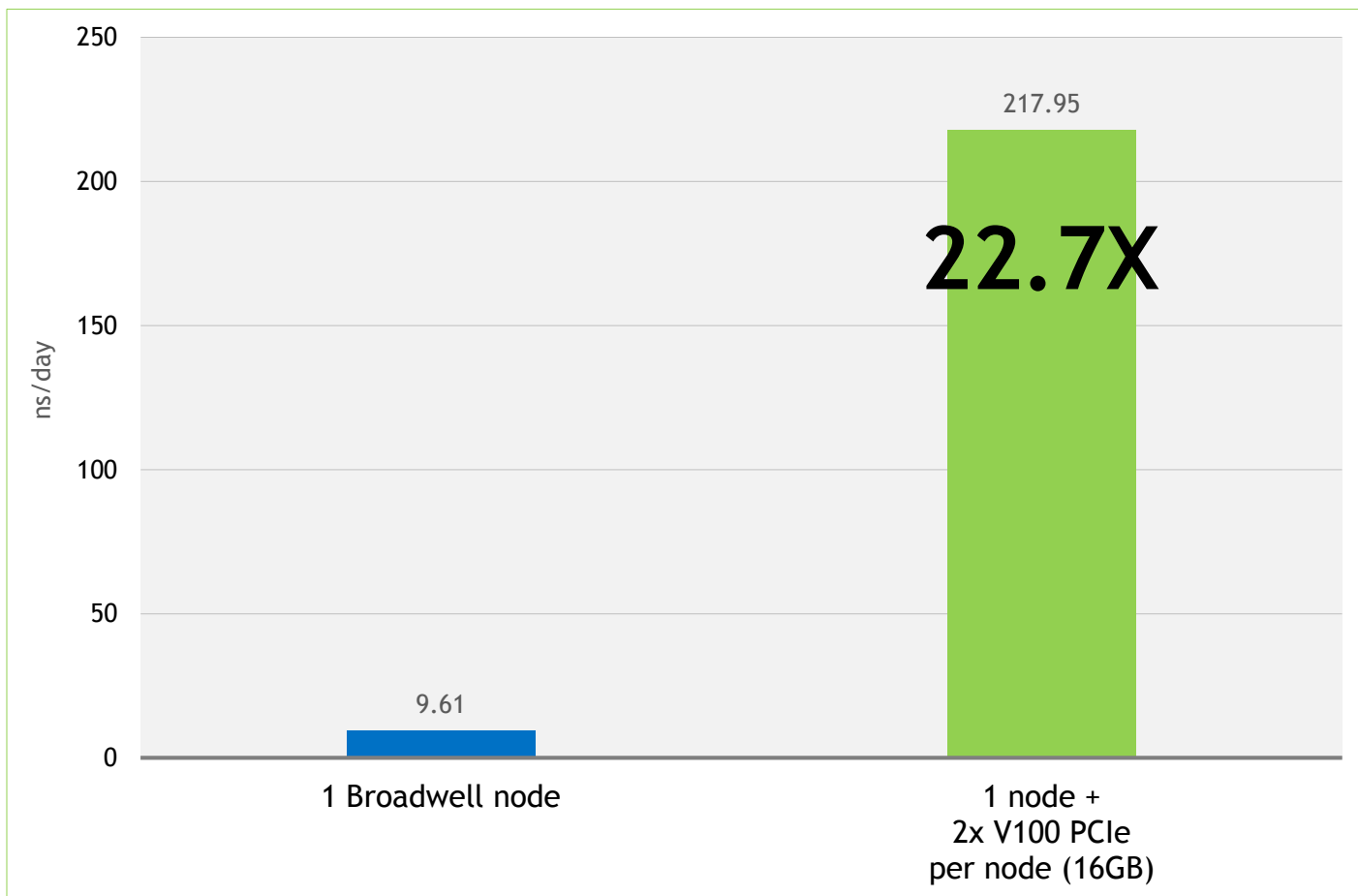


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PME-FactorIX_NVE on V100s PCIe

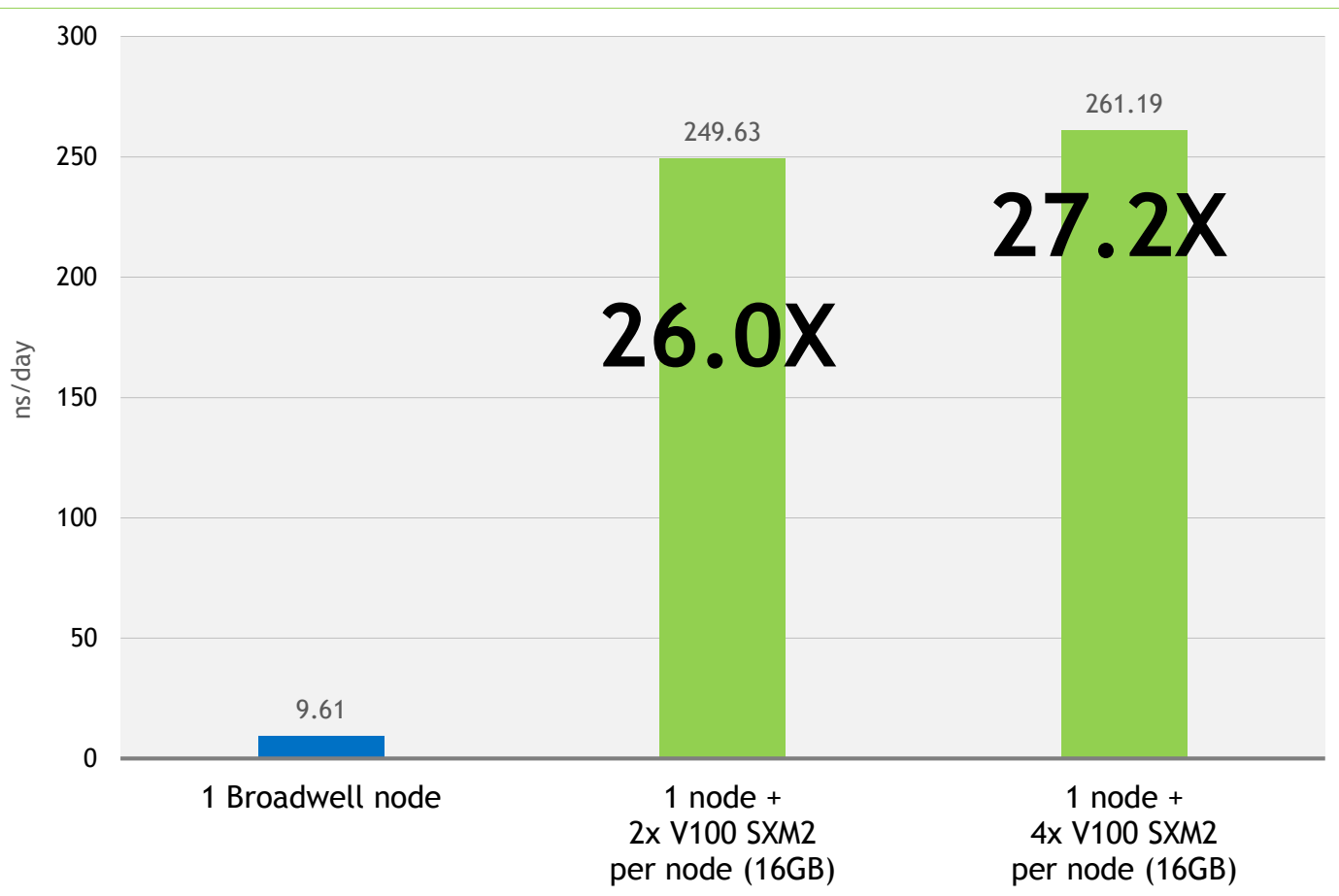


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PME-FactorIX_NVE on V100s SXM2

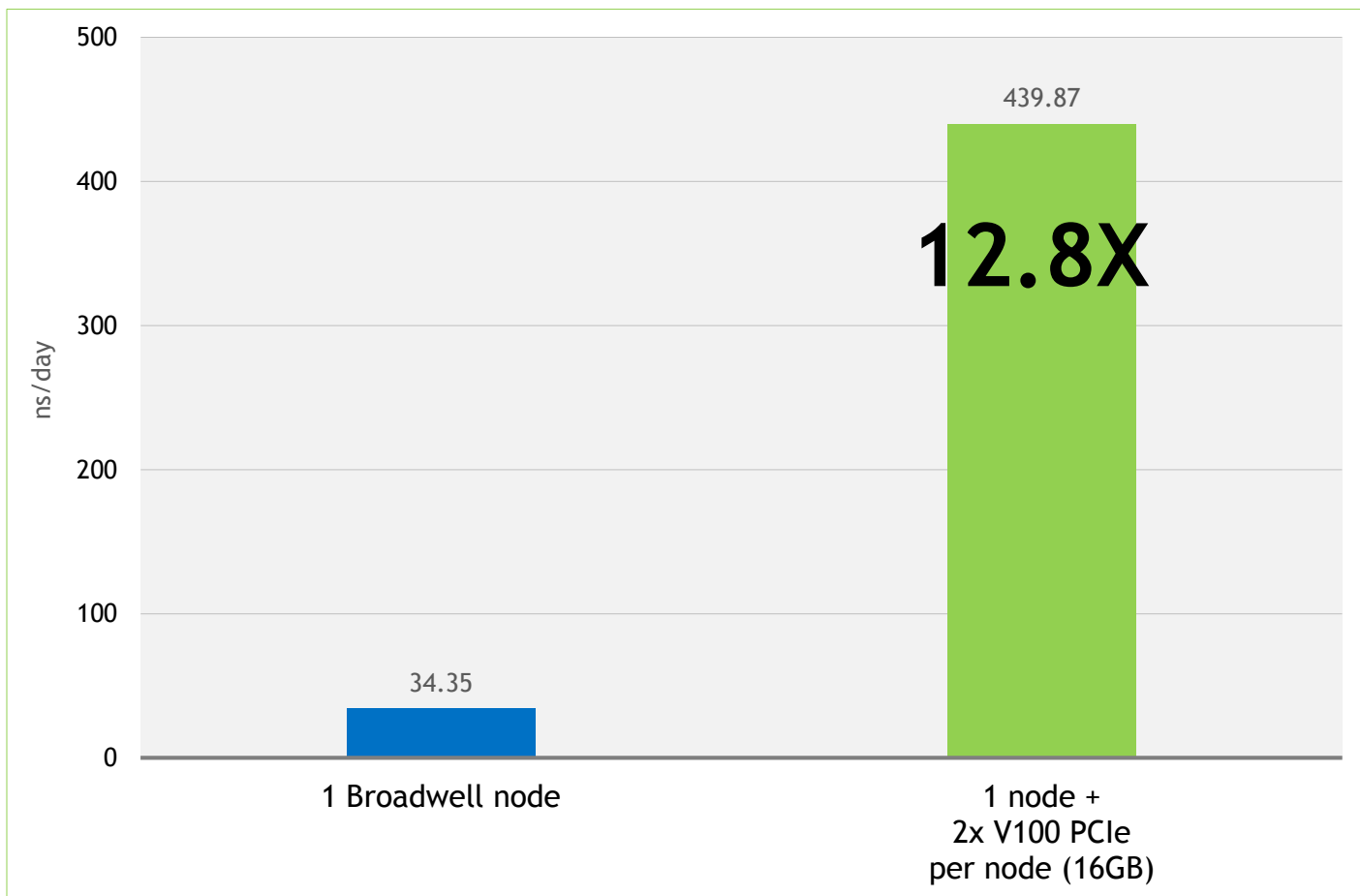


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PME-JAC_NPT on V100s PCIe

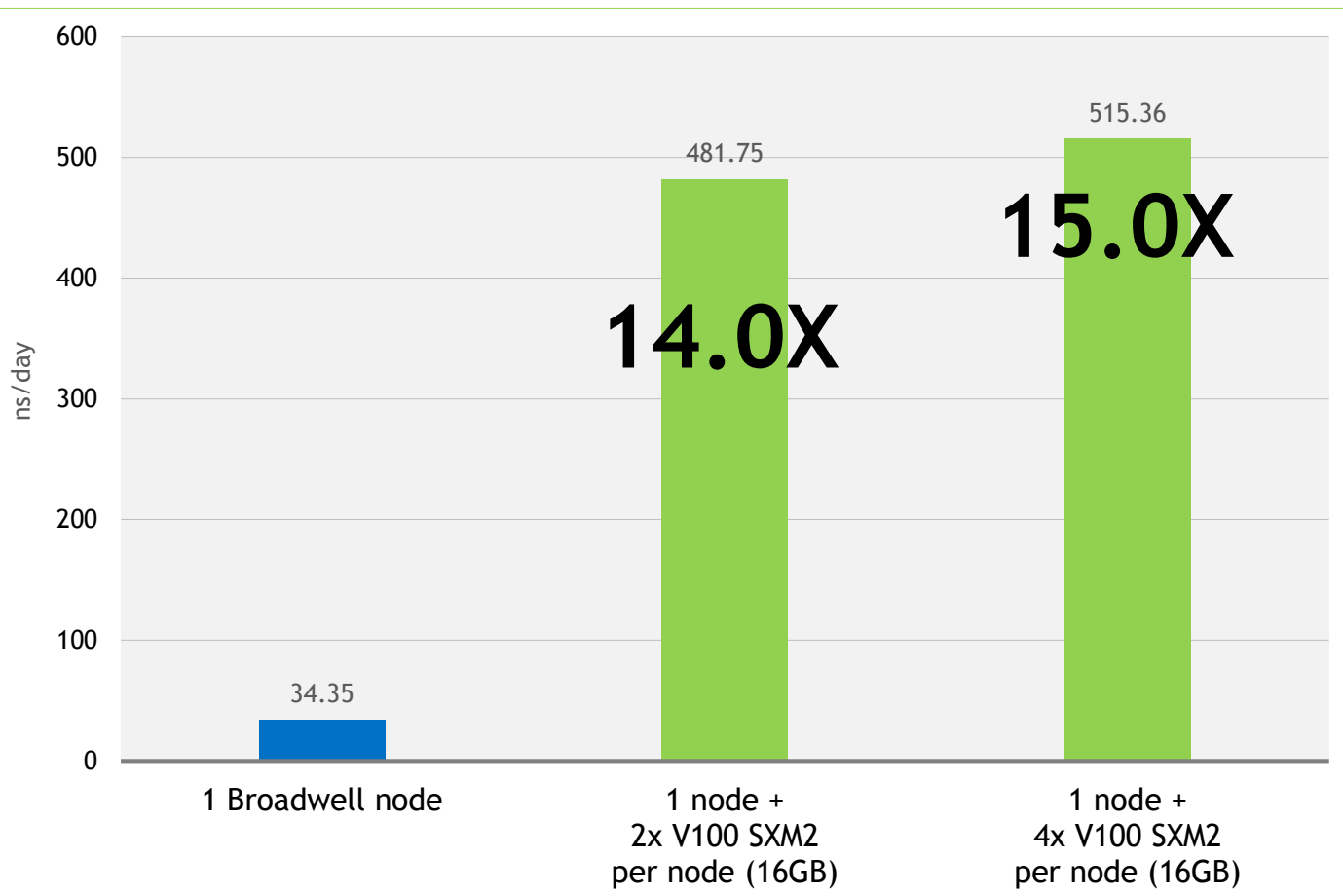


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PME-JAC_NPT on V100s SXM2

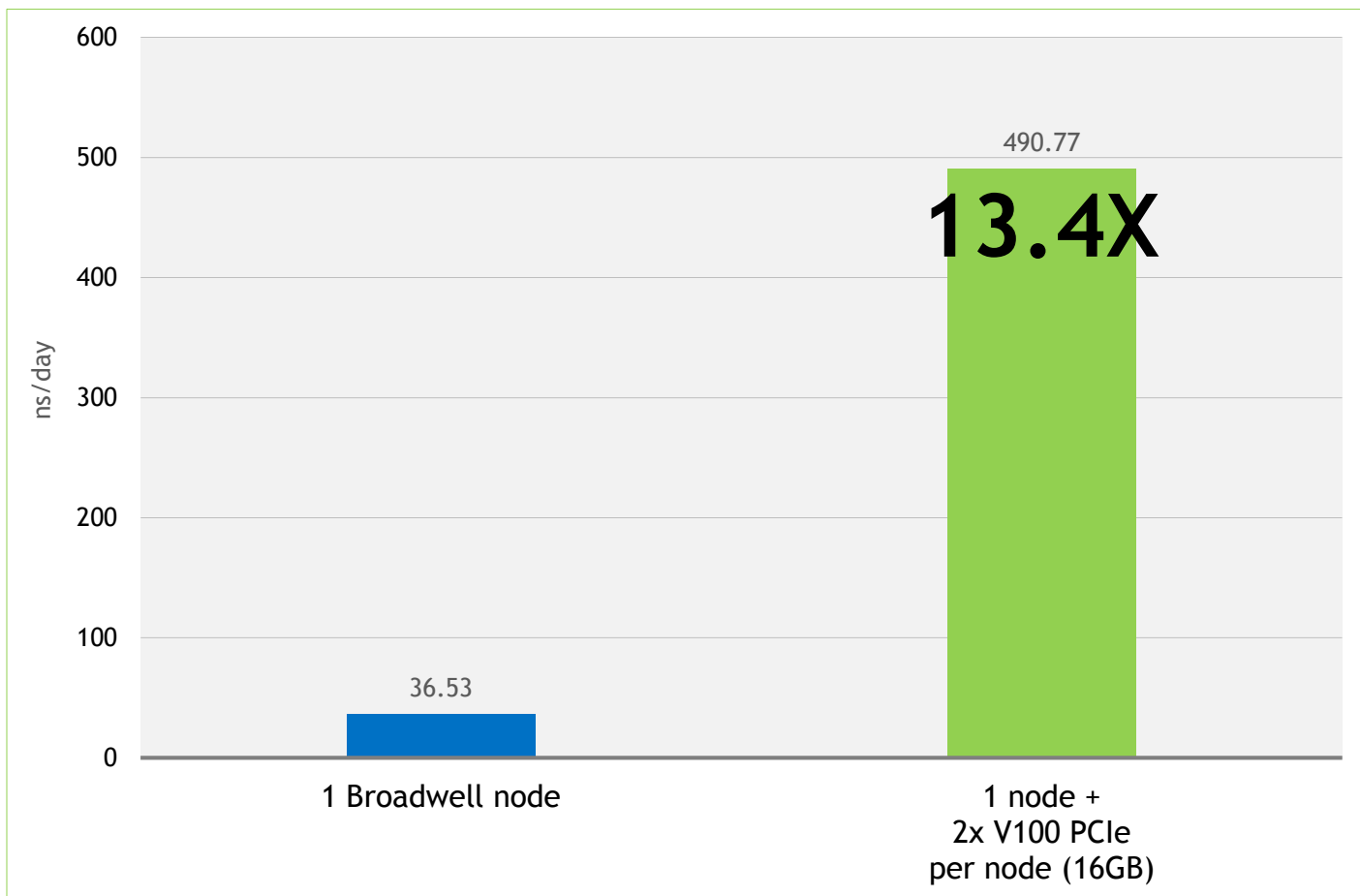


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PME-JAC_NVE on V100s PCIe

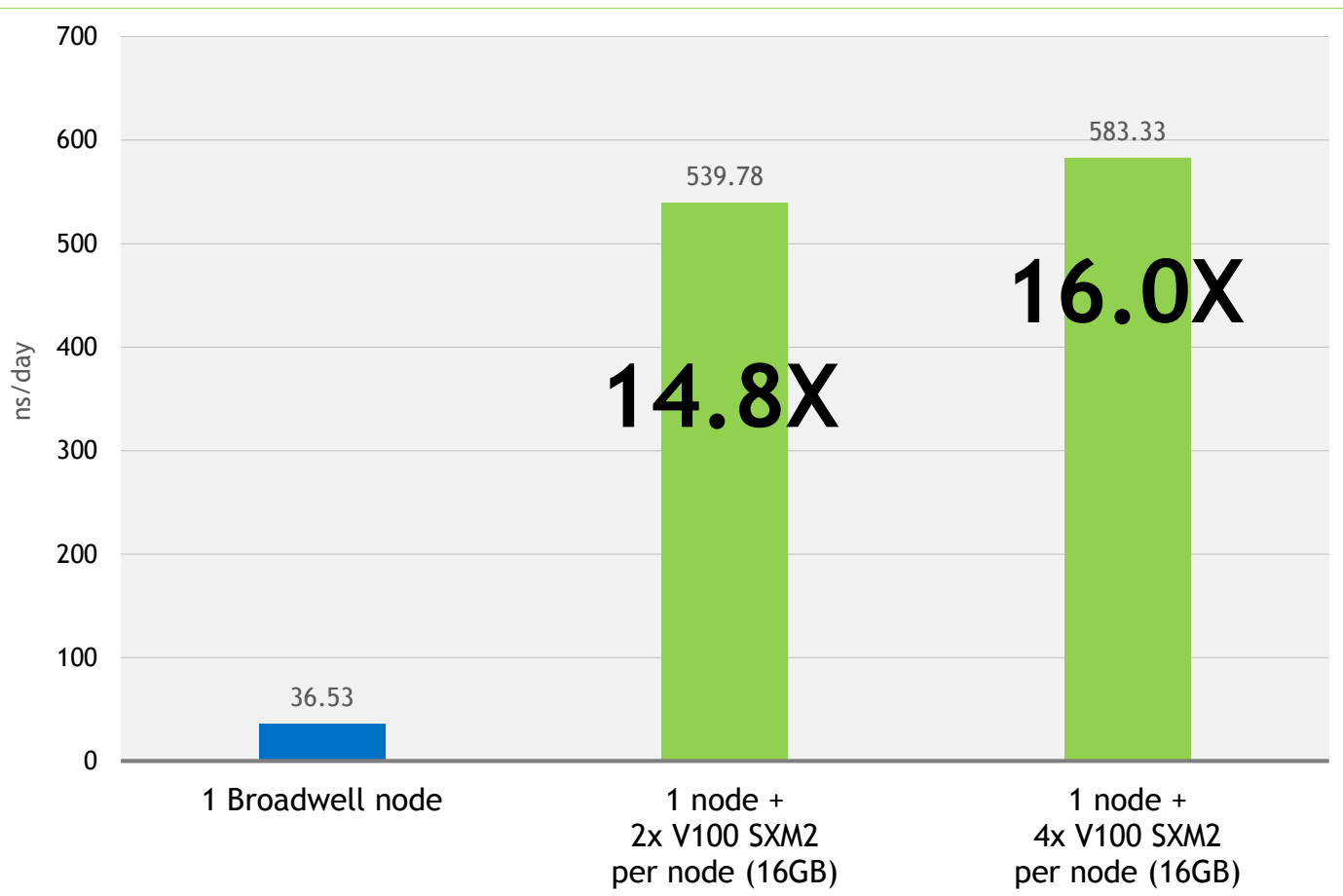


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PME-JAC_NVE on V100s SXM2

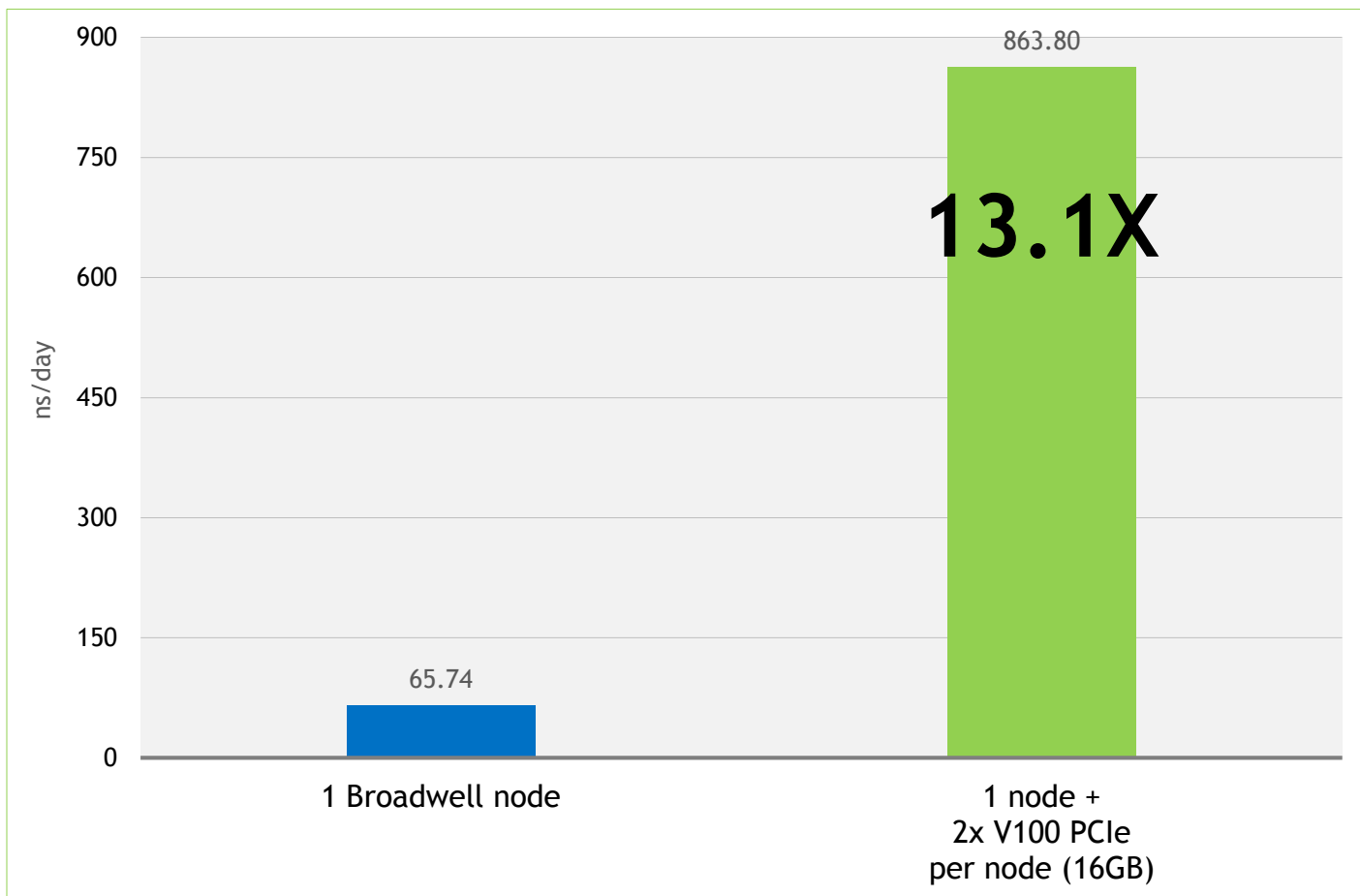


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PME-JAC_NPT_4fs on V100s PCIe

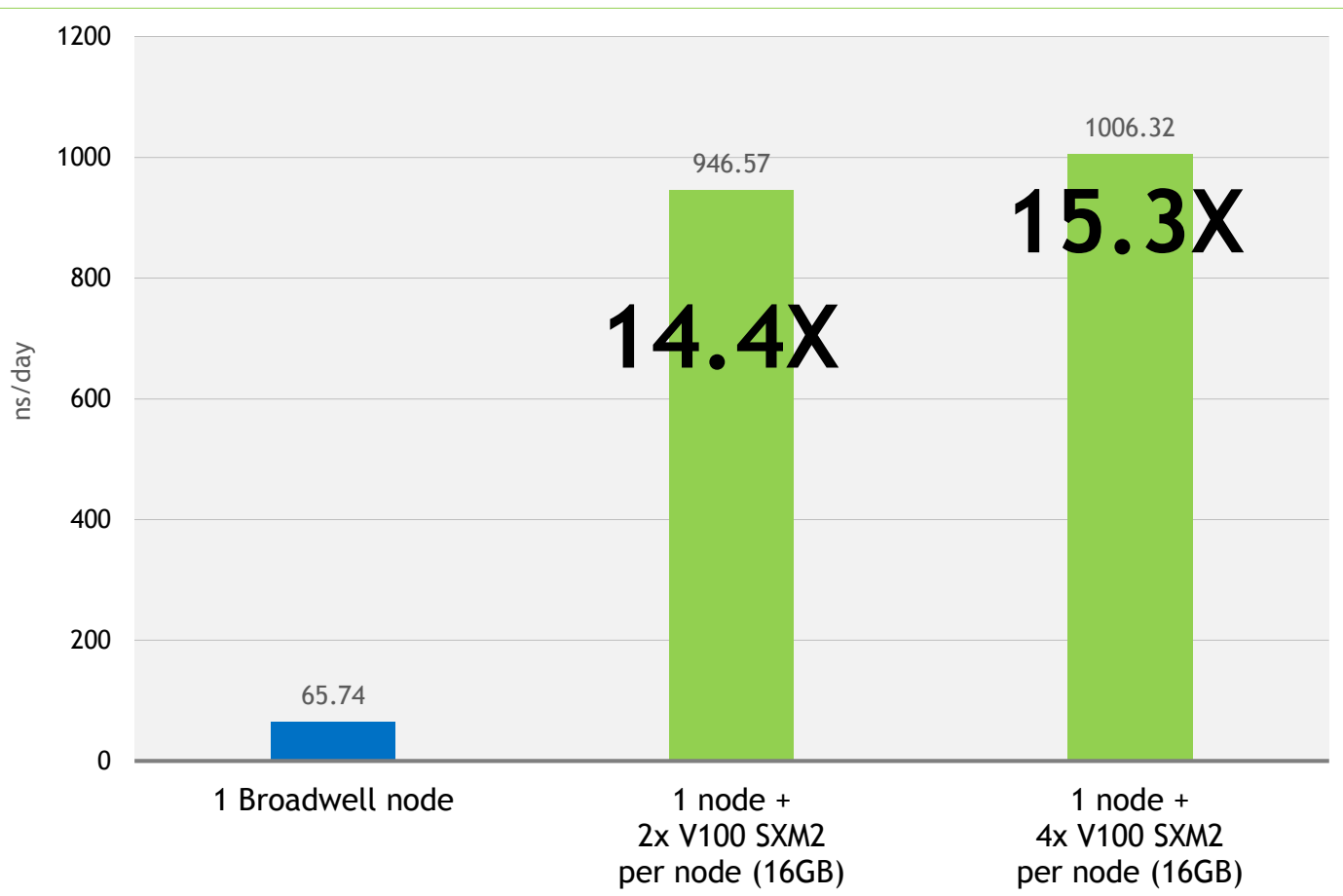


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PME-JAC_NPT_4fs on V100s SXM2

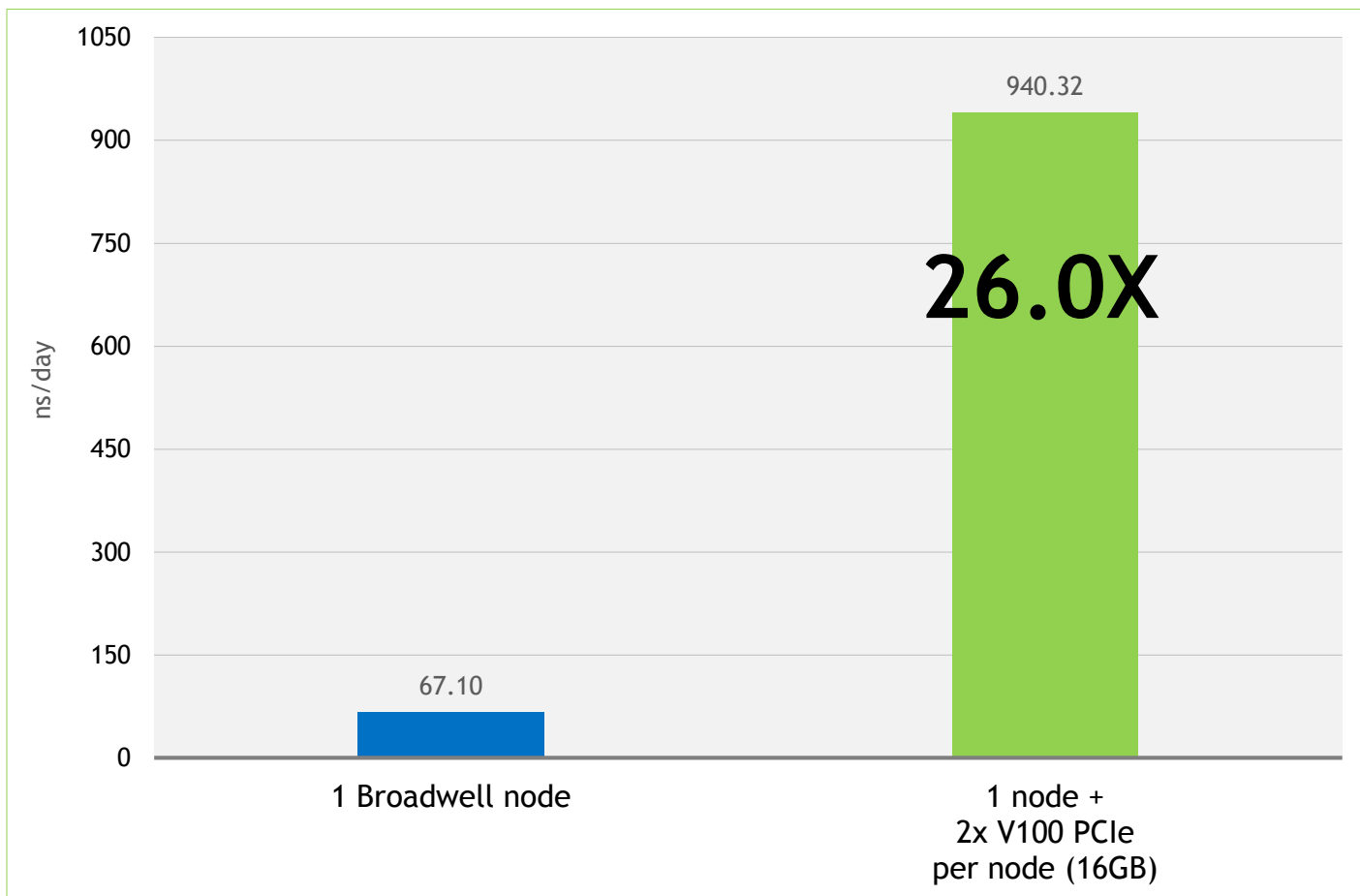


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PME-JAC_NVE_4fs on V100s PCIe

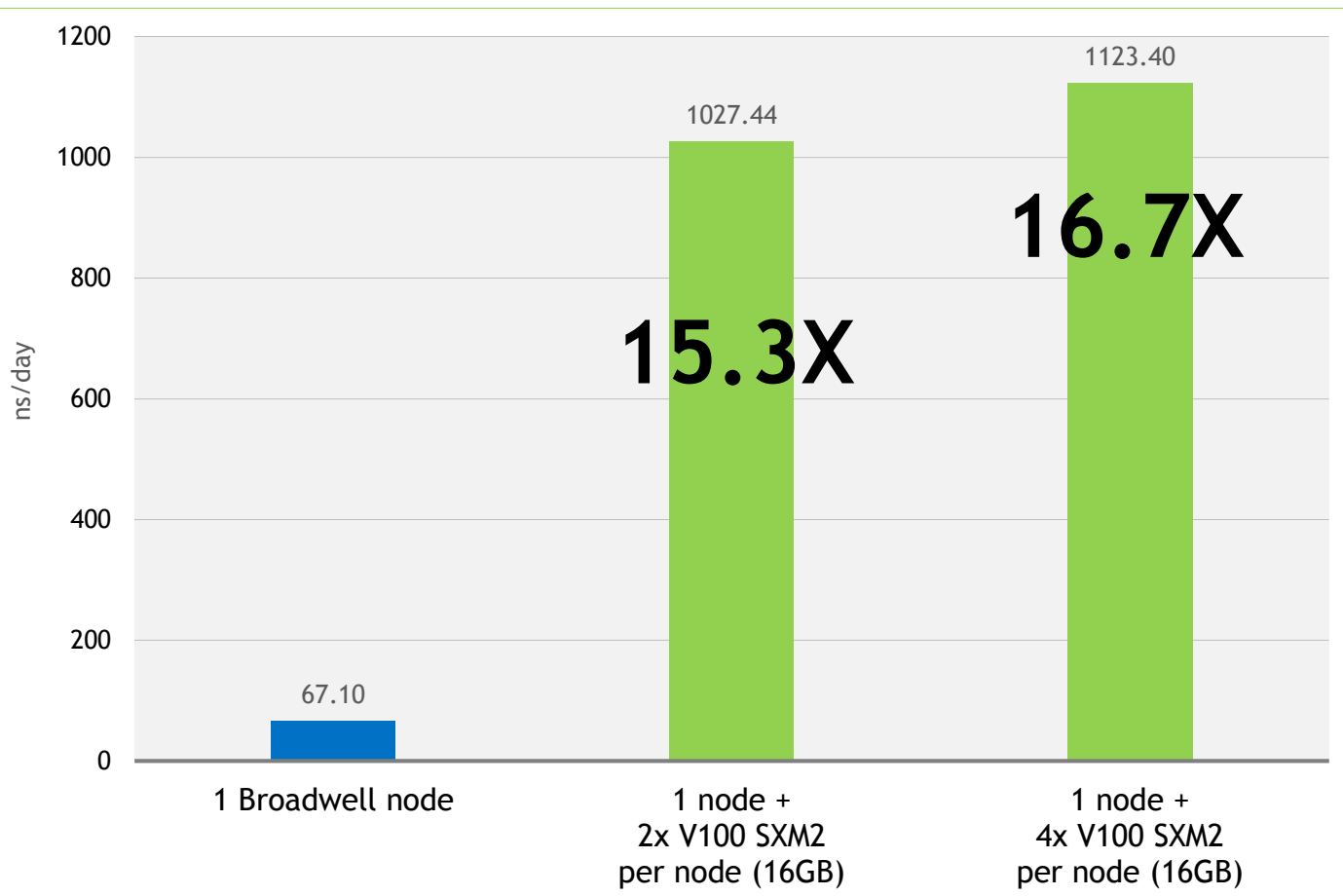


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PME-JAC_NVE_4fs on V100s SXM2

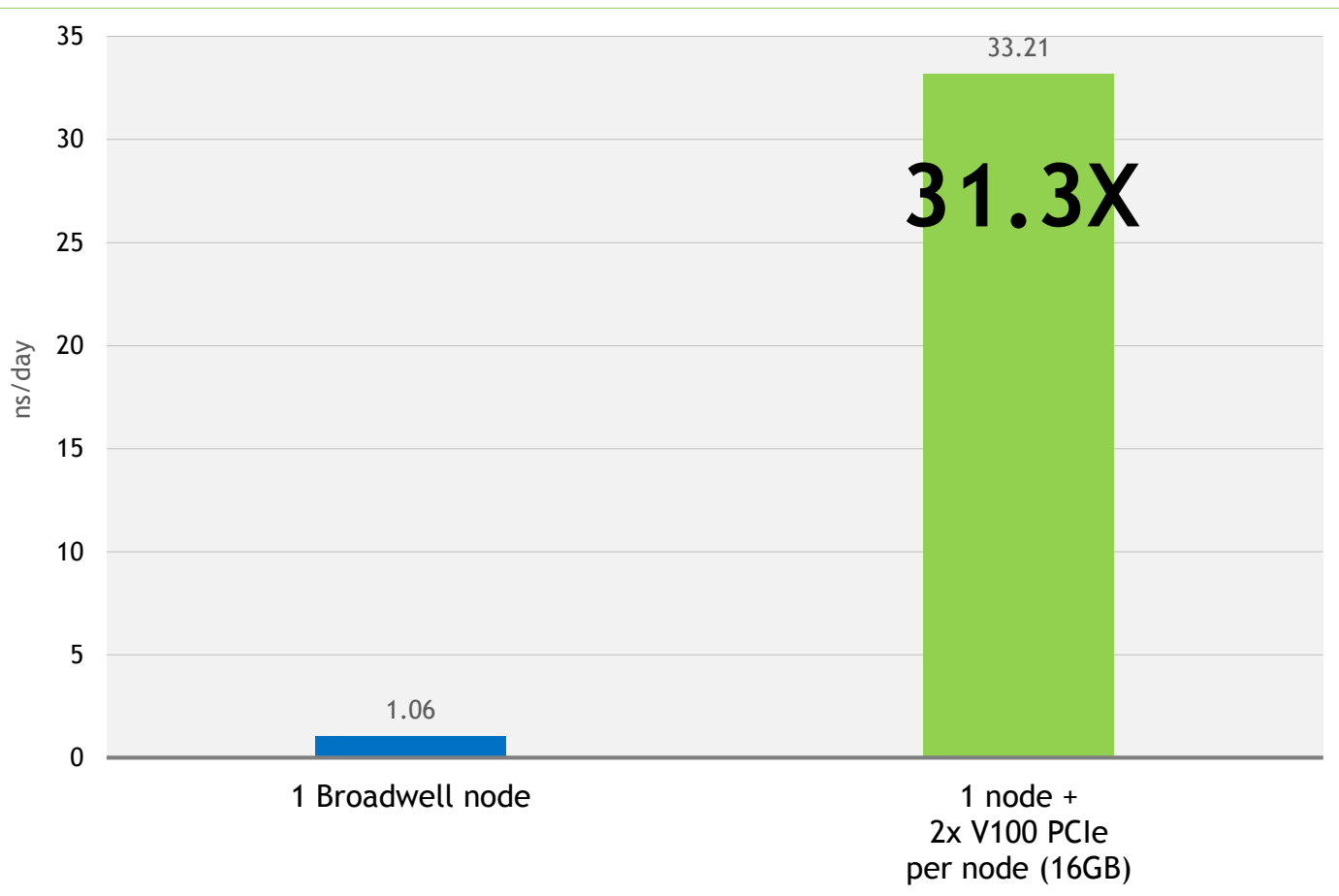


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PME-STMV_NPT_4fs on V100s PCIe

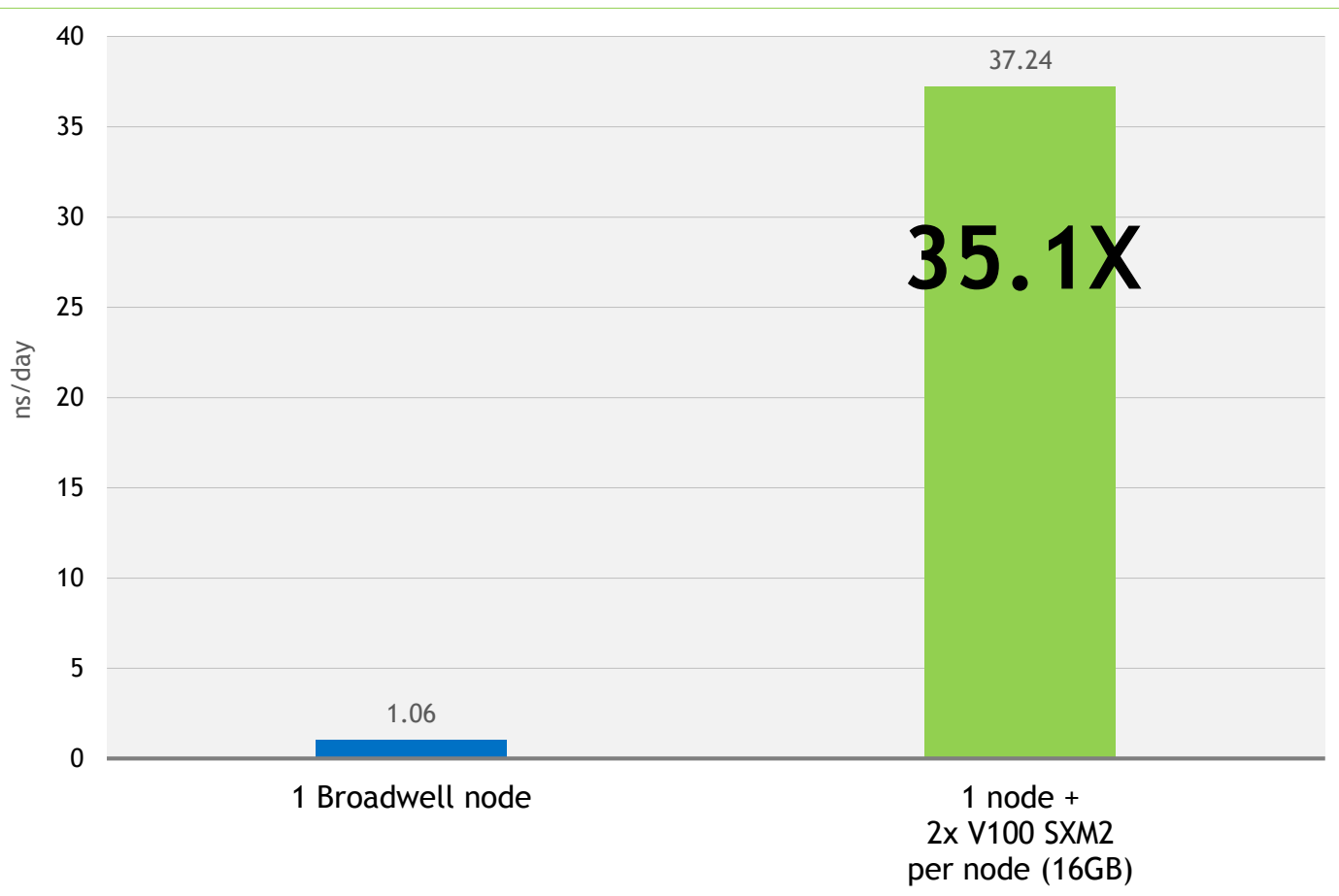


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PME-STMV_NPT_4fs on V100s SXM2

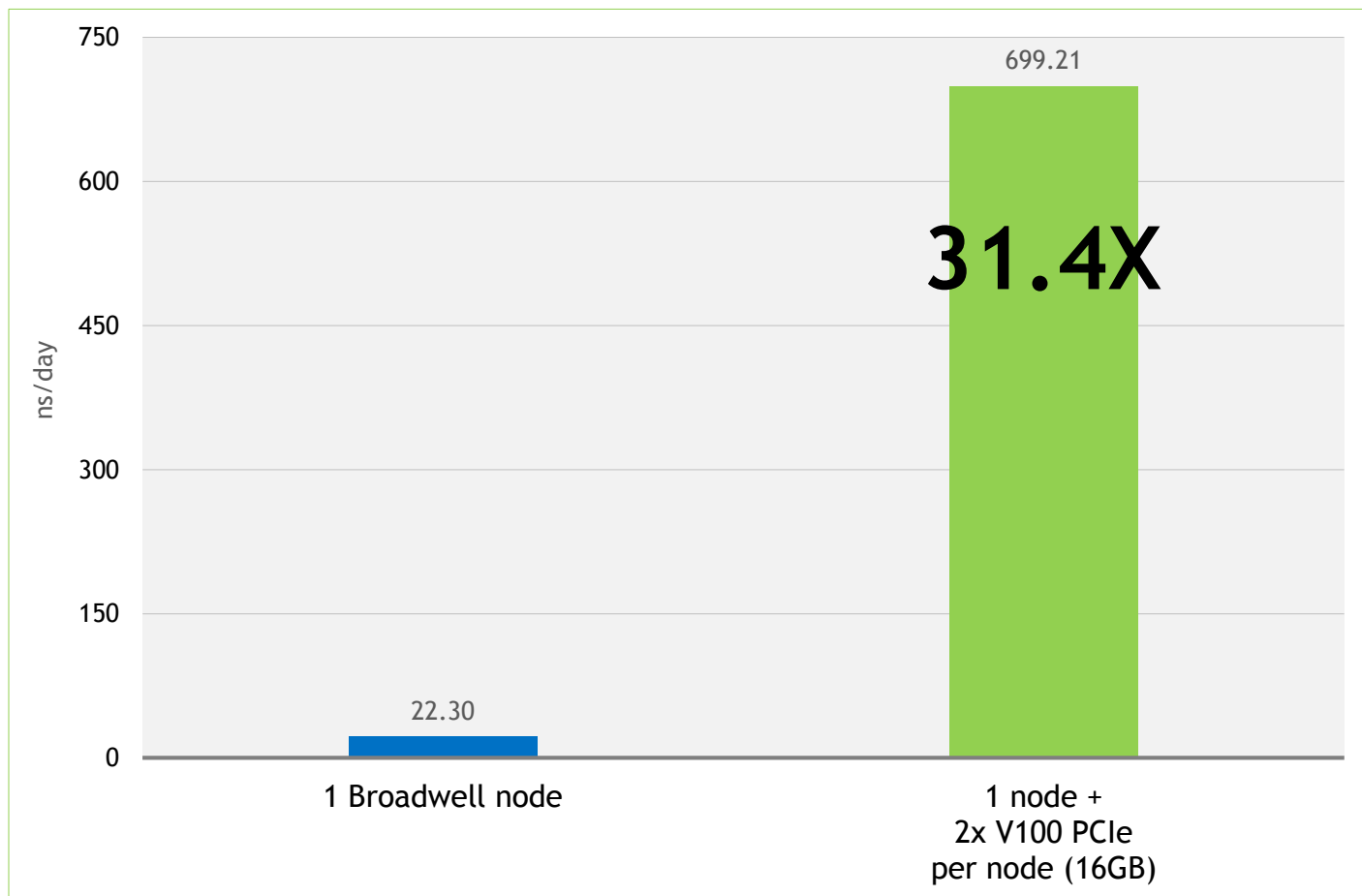


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GB-Myoglobin on V100s PCIe

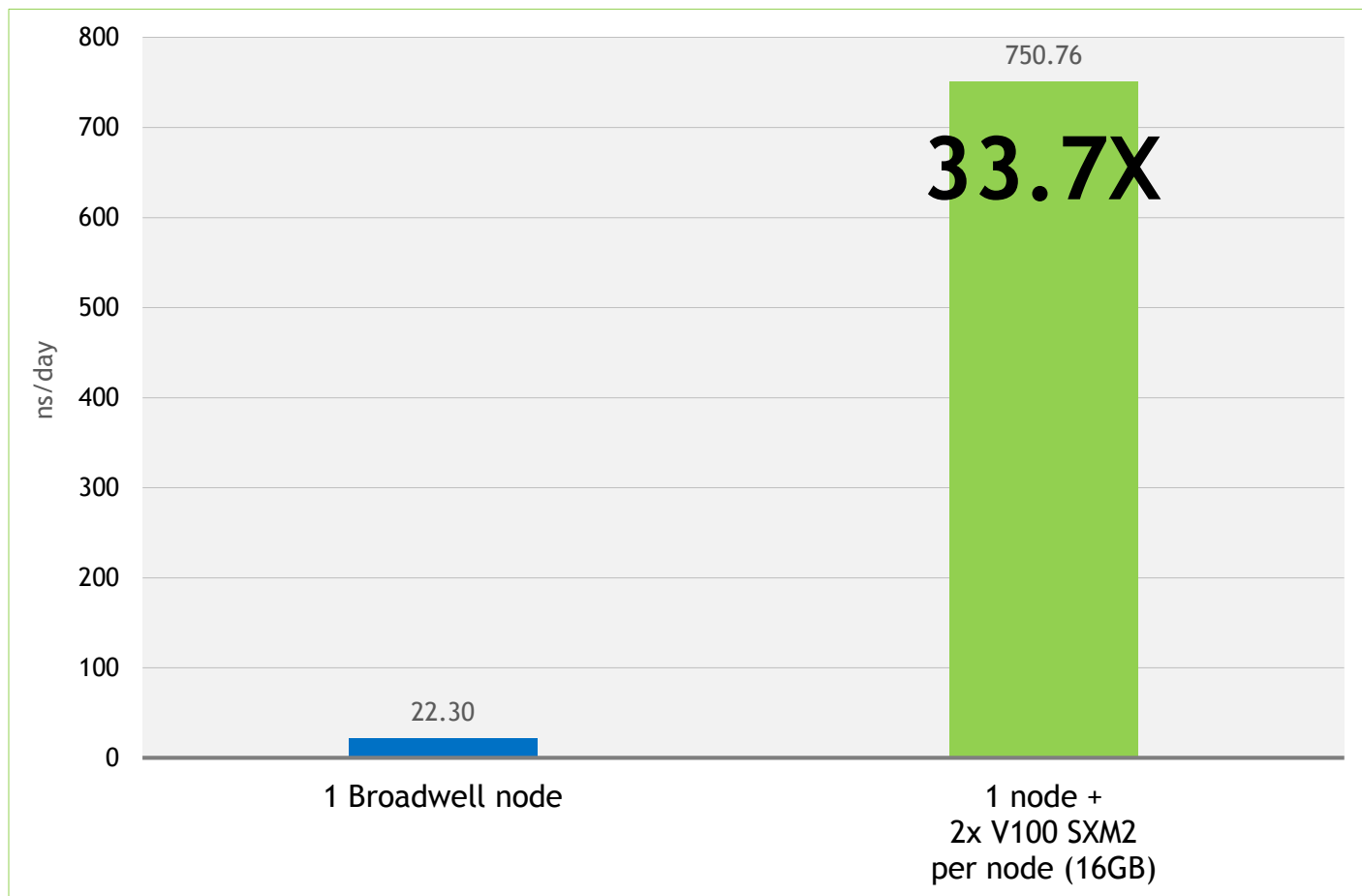


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GB-Myoglobin on V100s SXM2

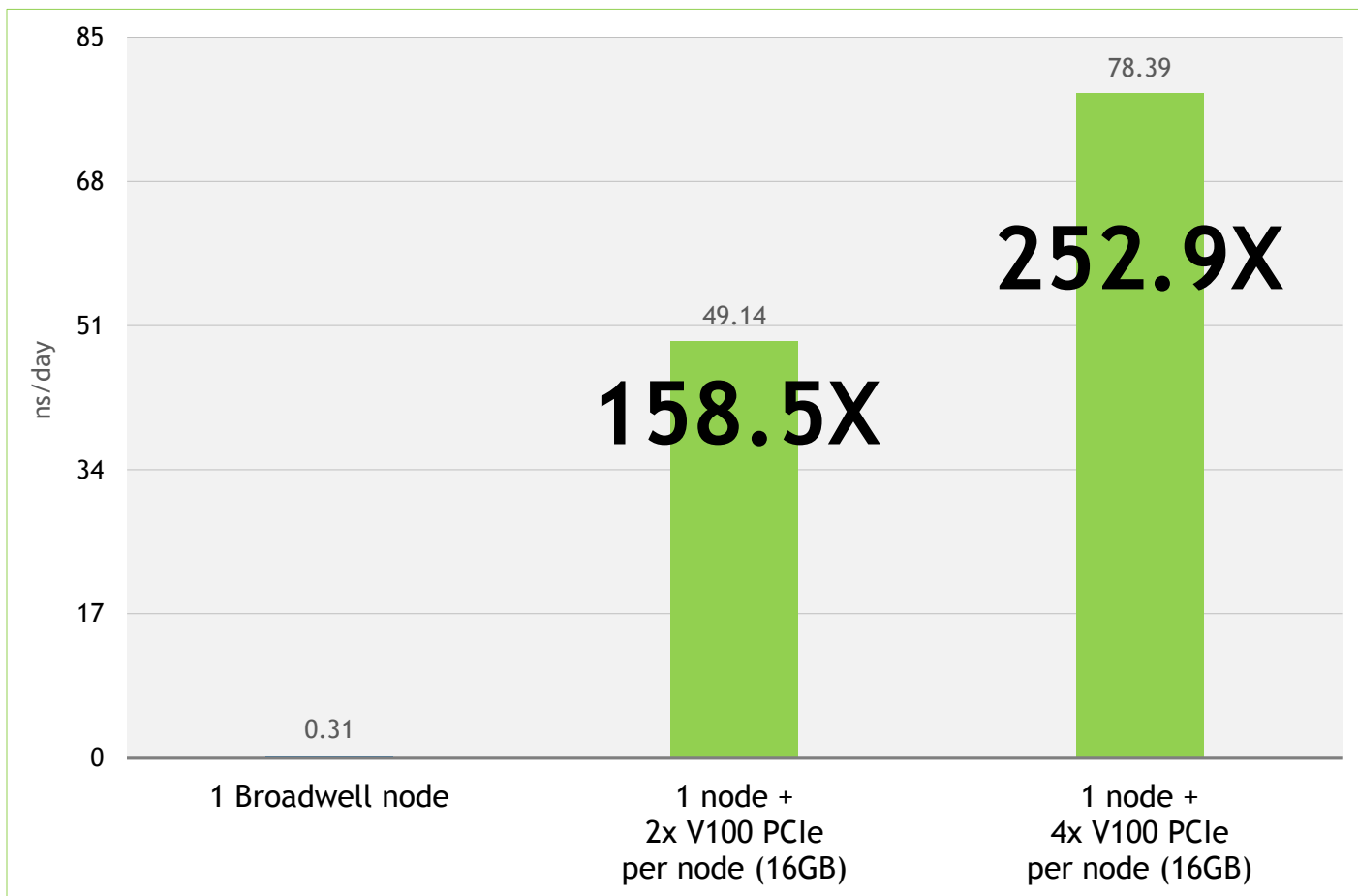


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GB-Nucleosome on V100s PCIe

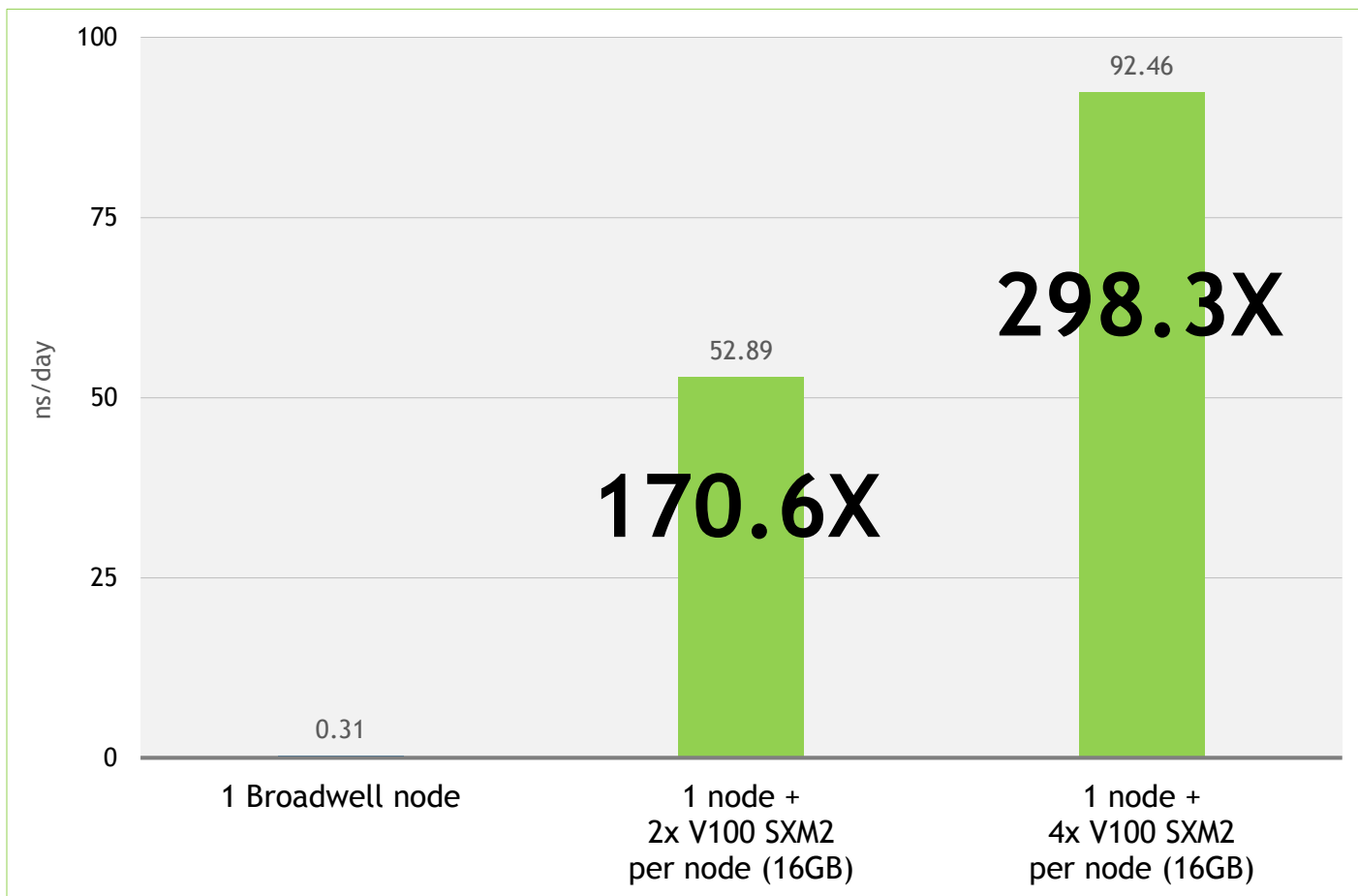


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GB-Nucleosome on V100s SXM2

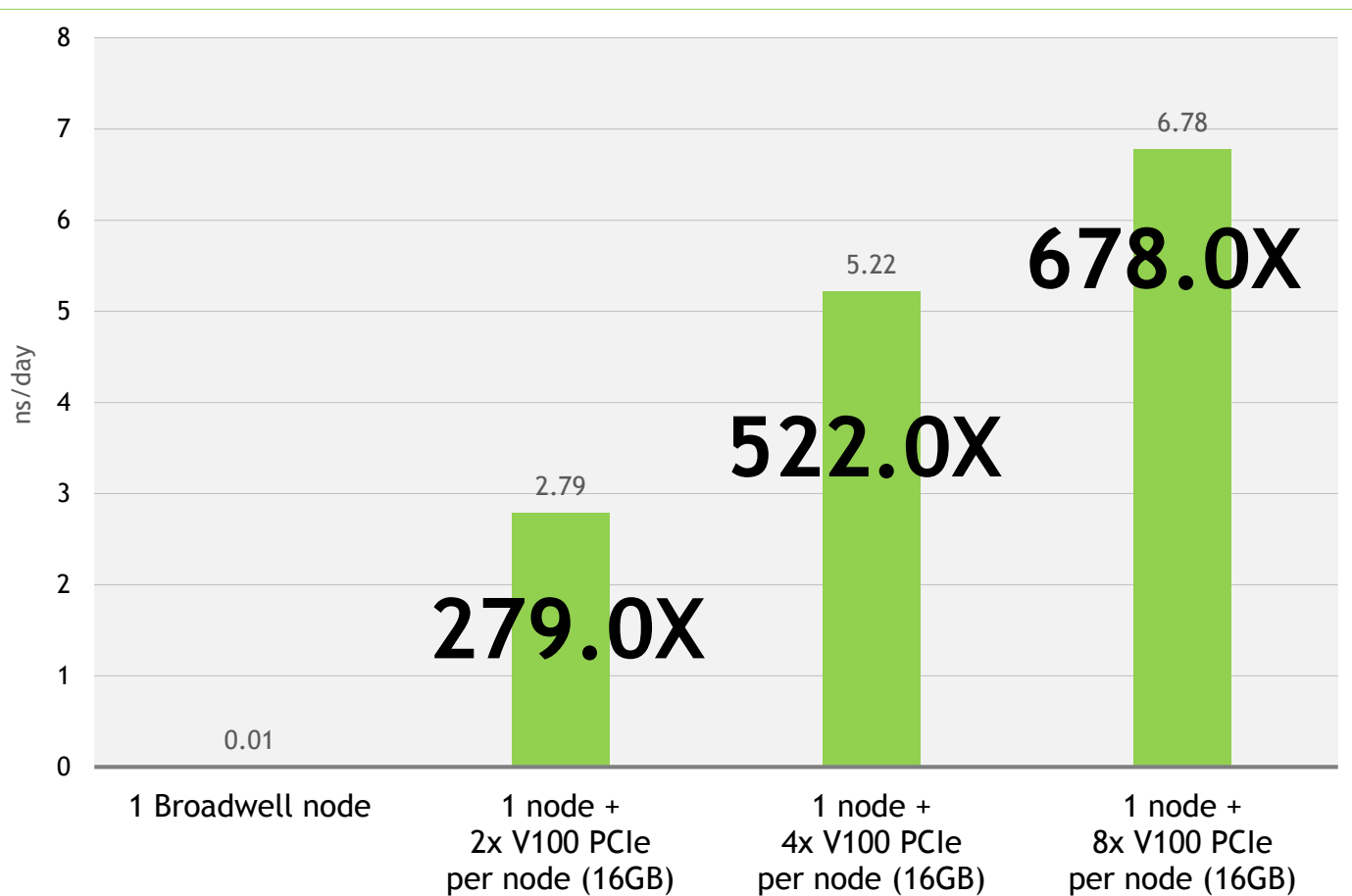


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Rubisco on V100s PCIe

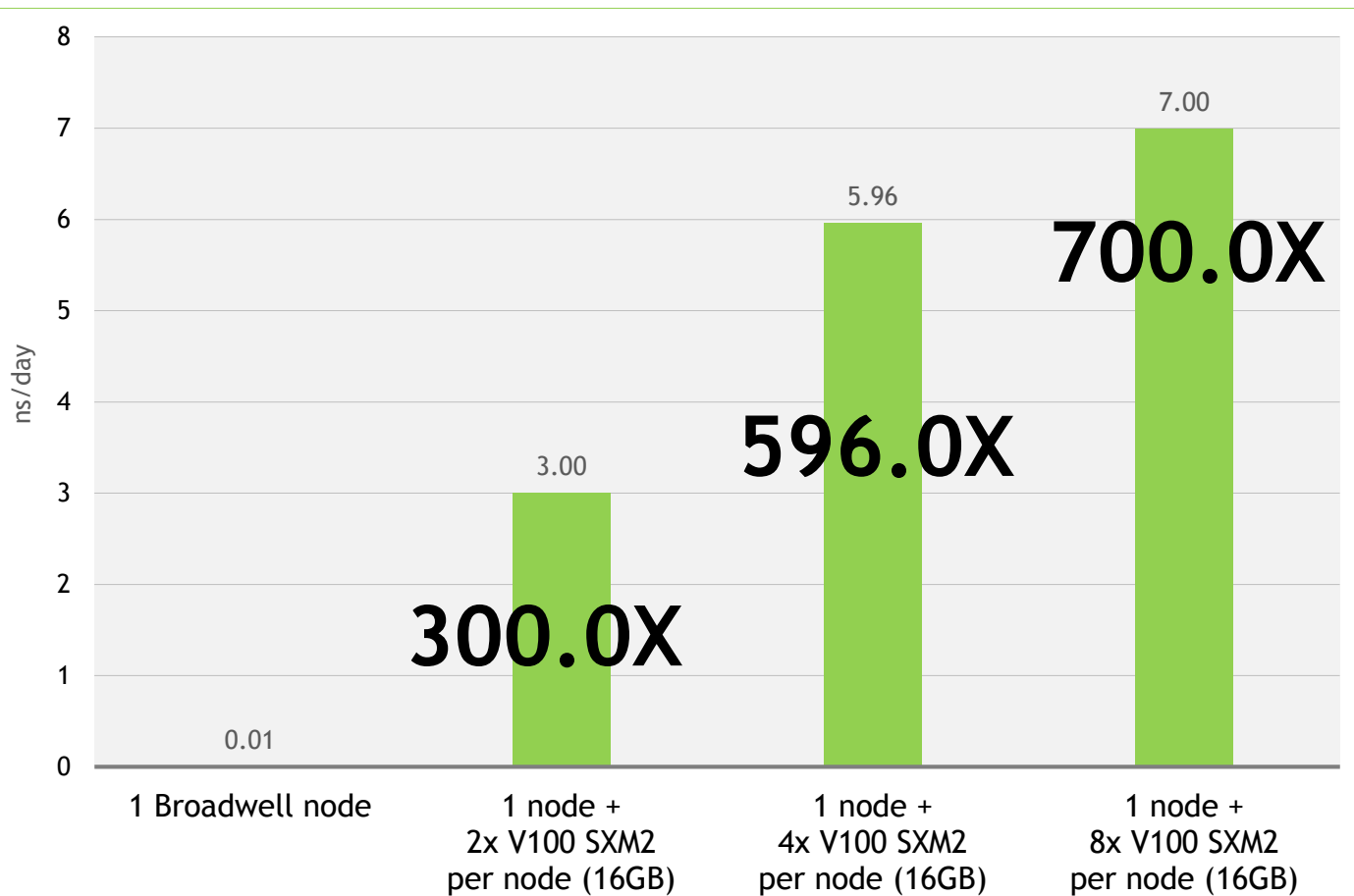


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Recommended GPU Node Configuration for AMBER Computational Chemistry

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