Molecular Dynamics (MD) on GPUs and RELION too

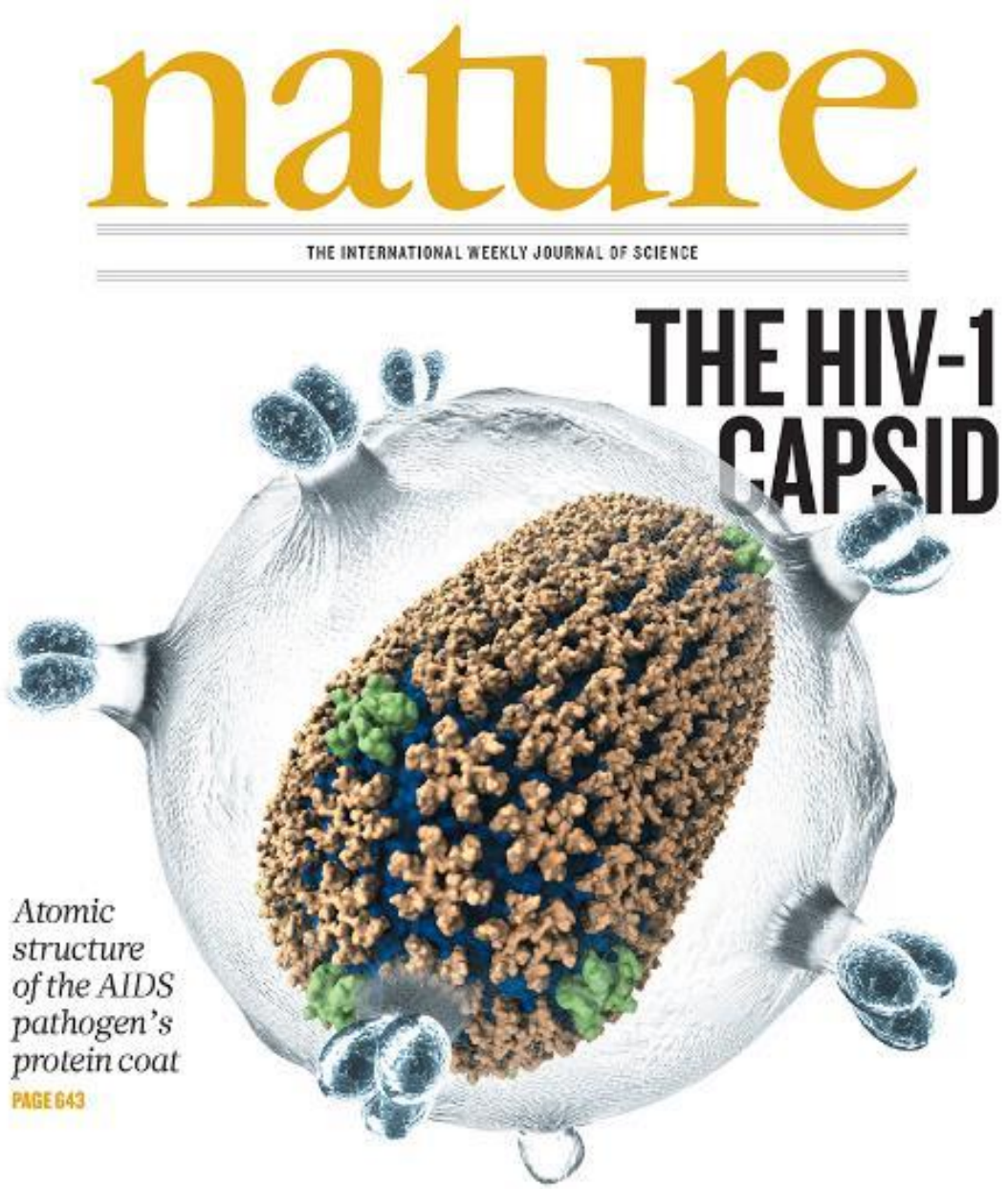
October 2017

NVIDIA

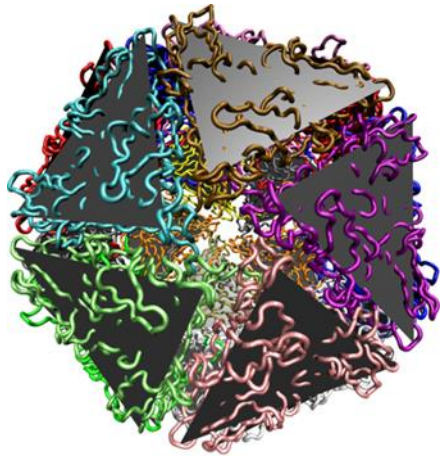
Accelerating Discoveries

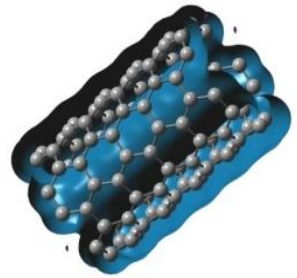
Using a supercomputer powered by the Tesla Platform with over 3,000 Tesla accelerators, University of Illinois scientists performed the first all-atom simulation of the HIV virus and discovered the chemical structure of its capsid — “the perfect target for fighting the infection.”

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*, mdcore, MELD, miniMD, NAMD, OpenMM, PolyFTS, 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

“Classical” Molecular Dynamics	Quantum Chemistry (MO, PW, DFT, Semi-Emp)
Simulates positions of atoms over time; chemical-biological or chemical-material behaviors	Calculates electronic properties; ground state, excited states, spectral properties, making/breaking bonds, physical properties
Forces calculated from simple empirical formulas (bond rearrangement generally forbidden)	Forces derived from electron wave function (bond rearrangement OK, e.g., bond energies)
Up to millions of atoms	Up to a few thousand atoms
Solvent included without difficulty	Generally in a vacuum but if needed, solvent treated classically (QM/MM) or using implicit methods
Single precision dominated	Double precision is important
Uses cuFFT, CUDA	Uses cuBLAS, cuFFT, OpenACC, Eigen / Tensor Solvers
GeForce (Workstations), Tesla (Servers)	Tesla recommended
ECC off	ECC on

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

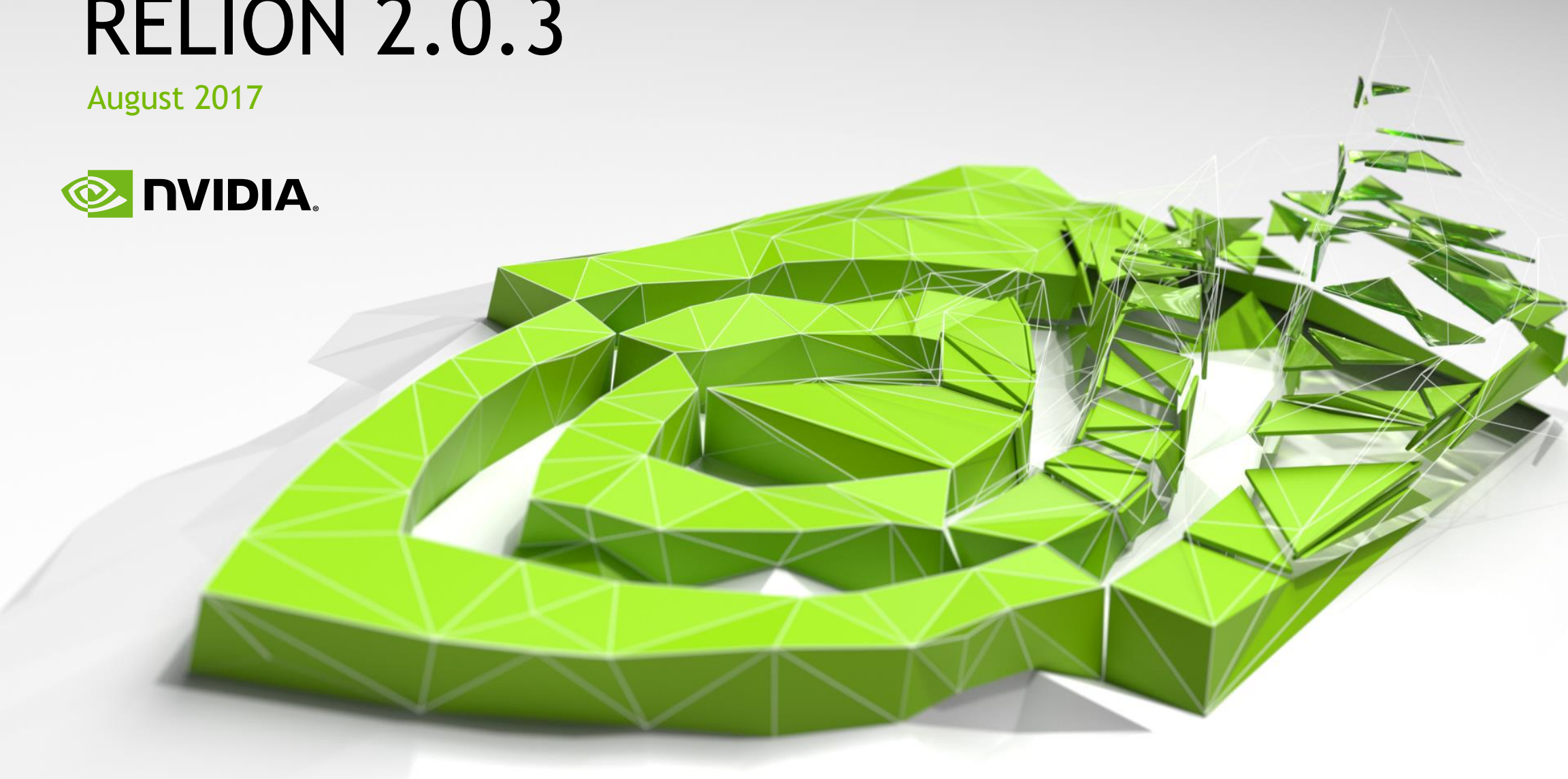
Why wouldn't you want to turbocharge your research?

- 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

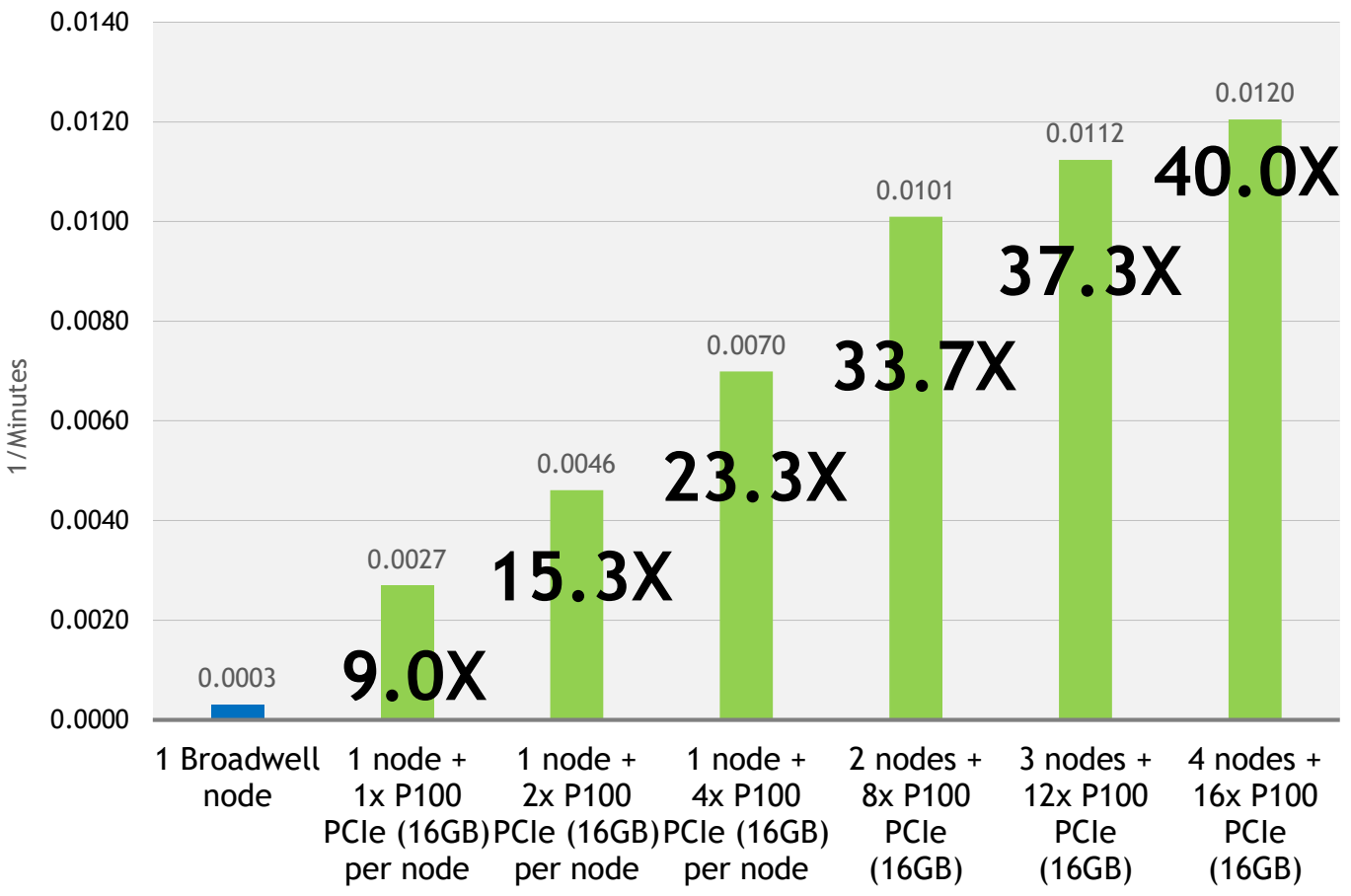
Try GPU accelerated MD apps for free – www.nvidia.com/GPUTestDrive

RELION 2.0.3

August 2017



RELION: Plasmodium ribosome on P100s PCIe



Running RELION version 2.0.3

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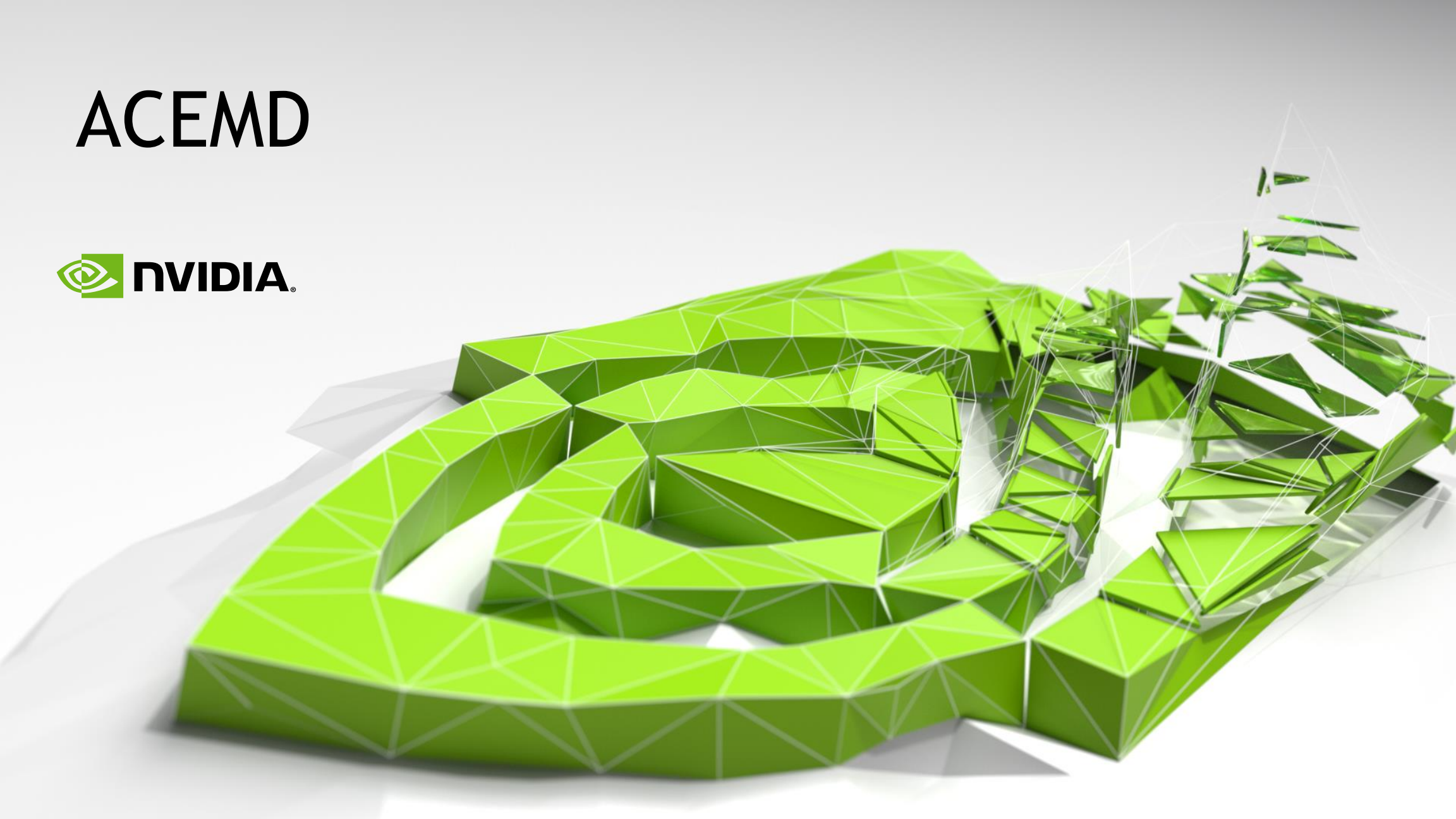
Data Citation:
http://en.community.dell.com/techcenter/high-performance-computing/b/general_hpc/archive/2017/03/14/application-performance-on-p100-pcie-gpus

ACEMD



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ACEMD molecular simulations : Extremely efficient and robust MD software built on GPUs

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

M. Harvey, G. Giupponi and G. de Fabritiis, *ACEMD: Accelerated molecular dynamics simulations in the microseconds timescale*, J. Chem. Theory and Comput. 5, 1632 (2009)

ACEMD
molecular simulations

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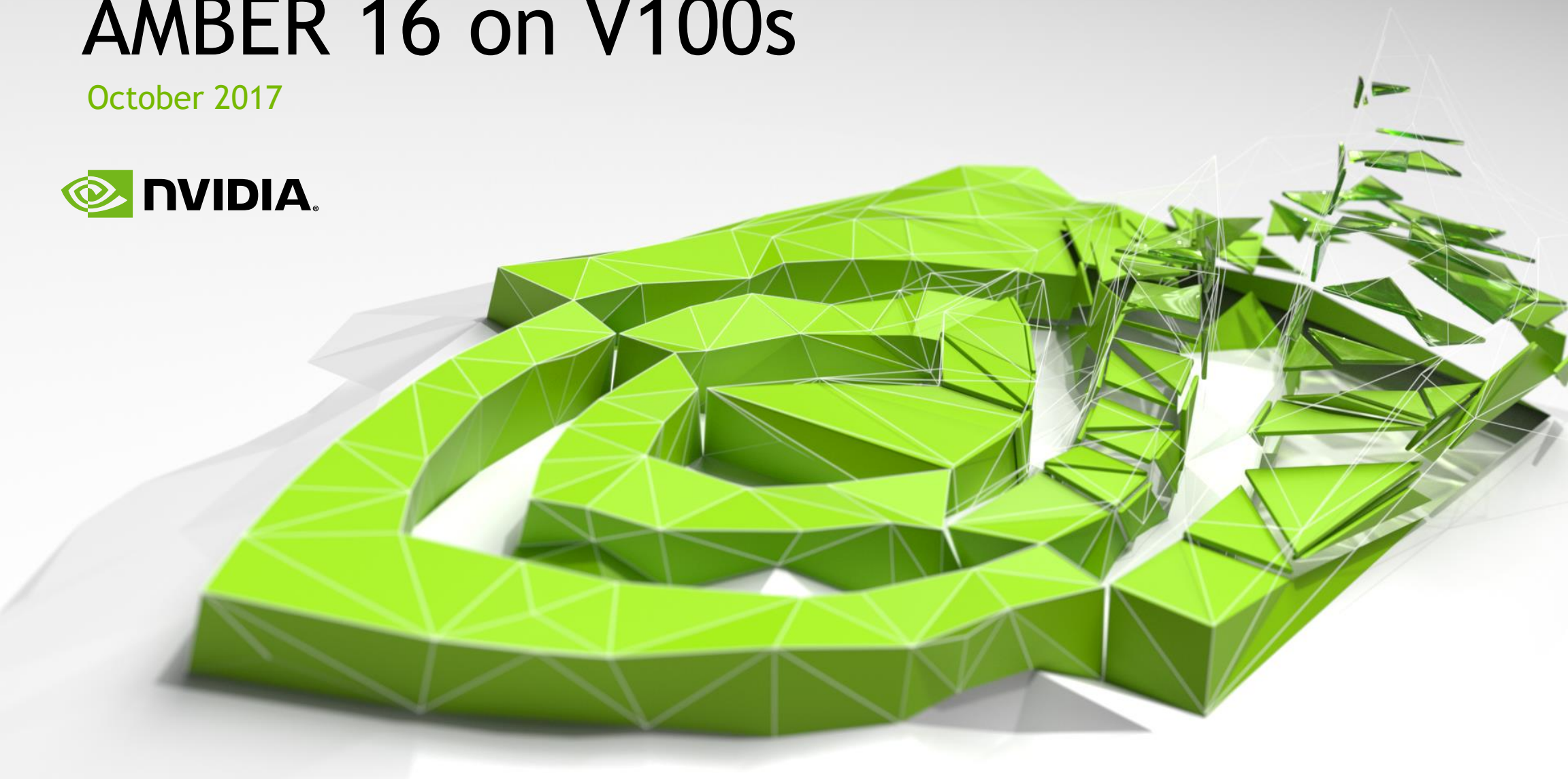
- **Standardised and easy to use**: ACEMD reads CHARMM/NAMD and AMBER input files and uses similar syntax to other MD software.
- **Fully featured**: NVT, NPT, PME, TCL, PLUMED.[1]
- **Robust**: ACEMD is a proven computational engine and is used in one of the largest distributed projects Worldwide: GPUGRID.
- **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]

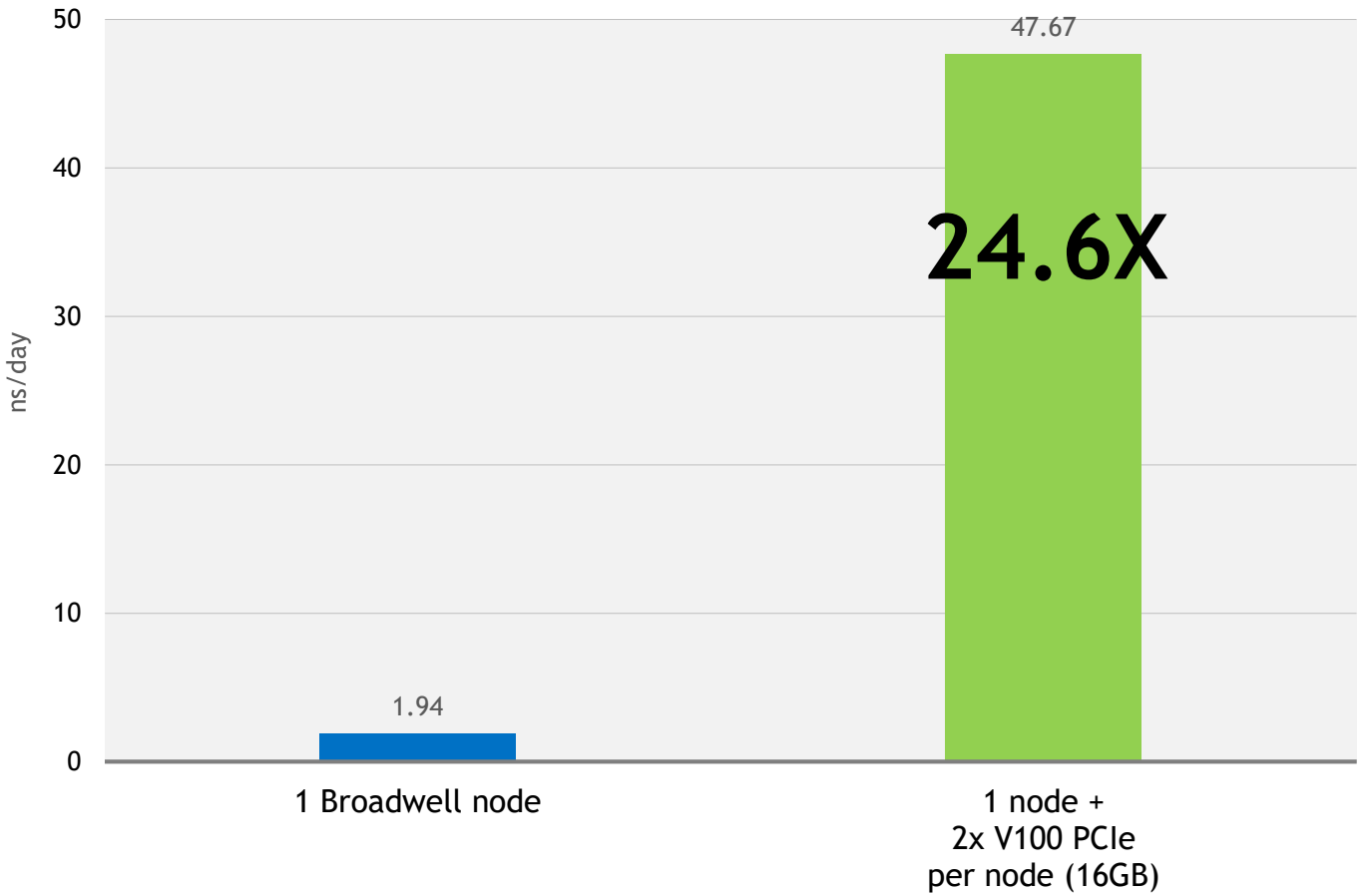
1. M. J. Harvey, and G. de Fabritiis, *An implementation of the smooth particle-mesh Ewald (PME) method on GPU hardware*, J. Chem. Theory Comput., 5, 2371-2377 (2009)
2. For a list of selected references see http://www.acellera.com/science

AMBER 16 on V100s

October 2017



PME-Cellulose_NPT on V100s PCIe



(Untuned on Volta)
Running AMBER version 16.8

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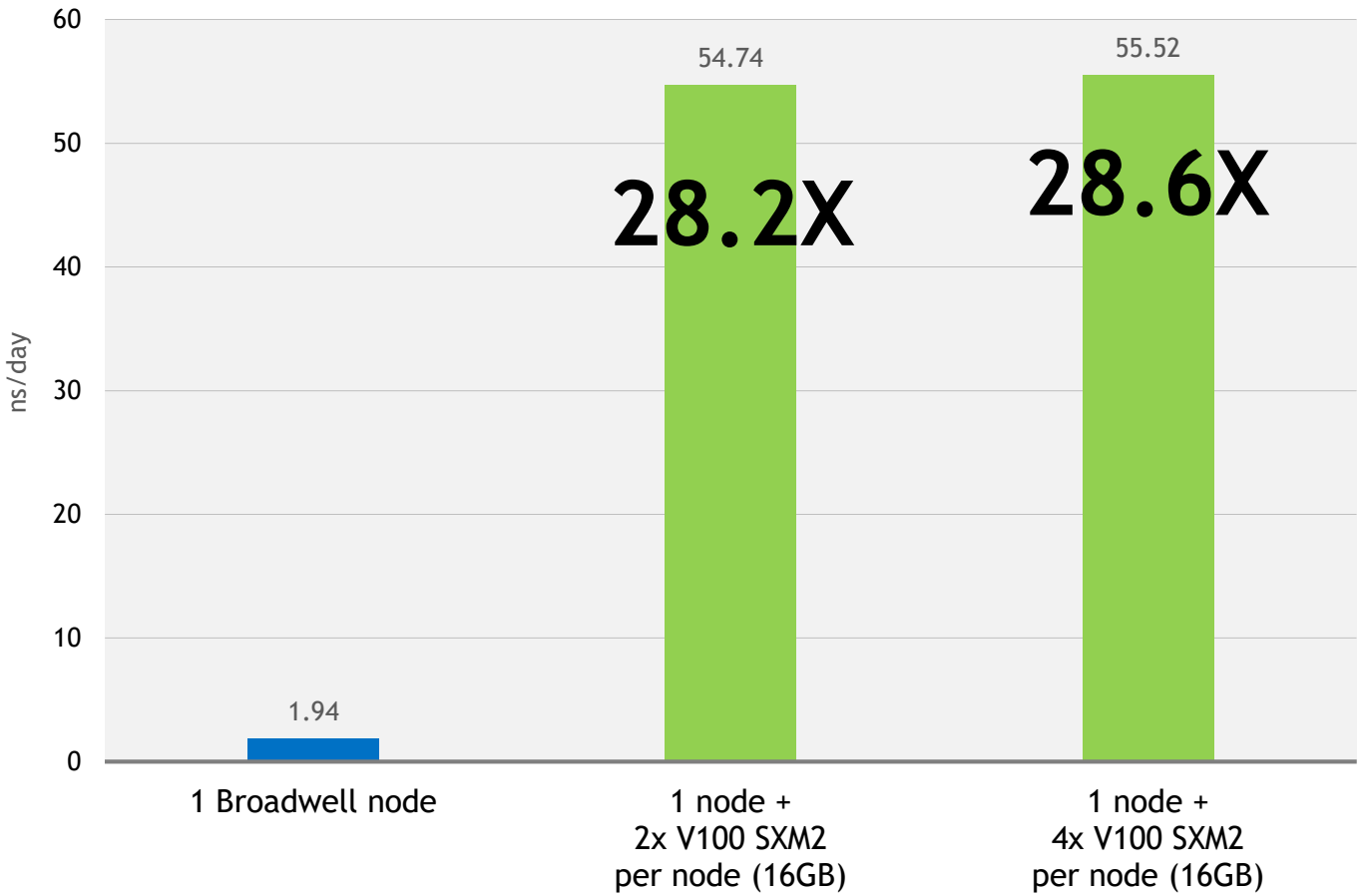
PME-Cellulose_NPT on V100s SXM2



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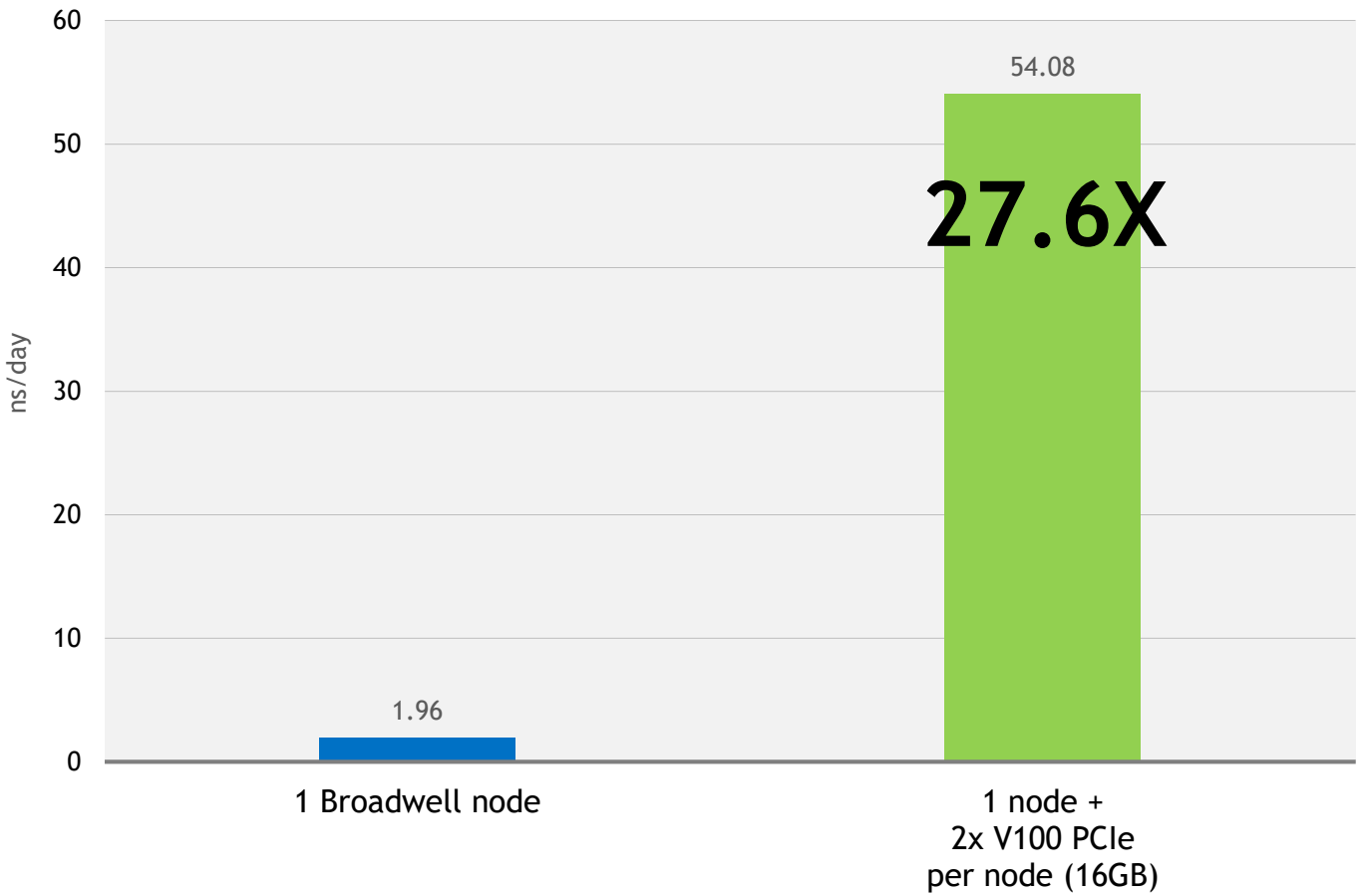

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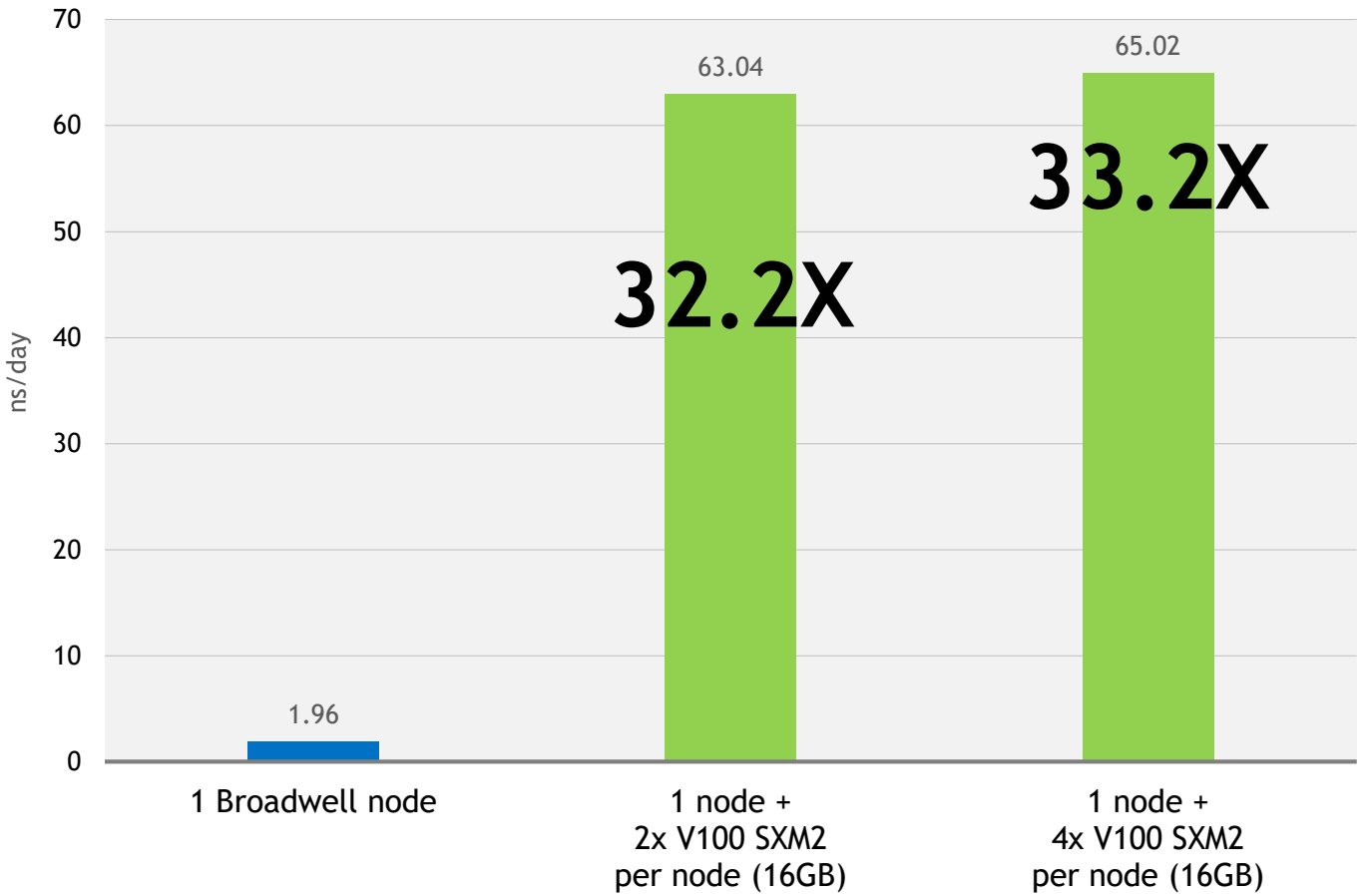

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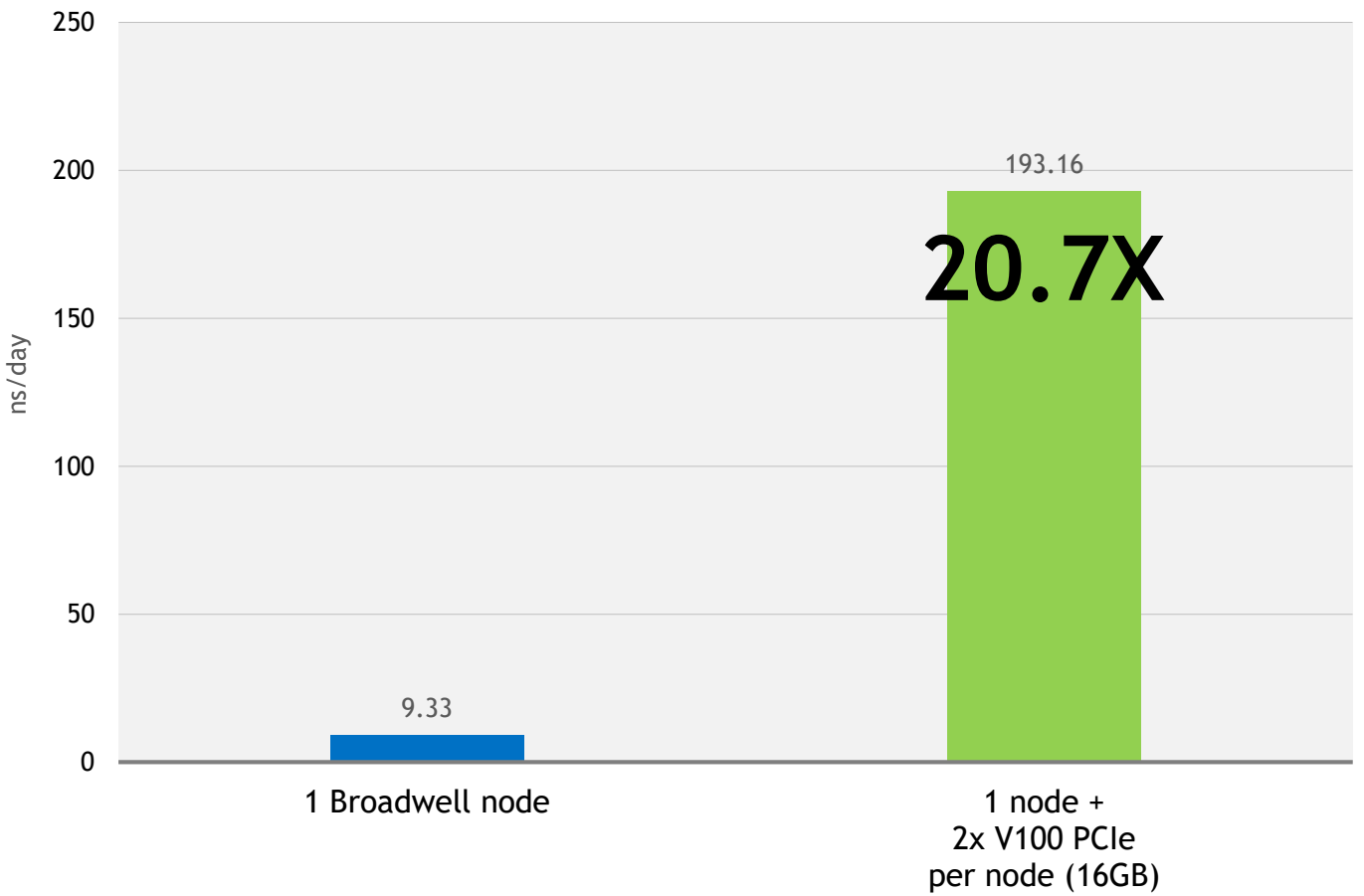
PME-FactorIX_NPT on V100s PCIe



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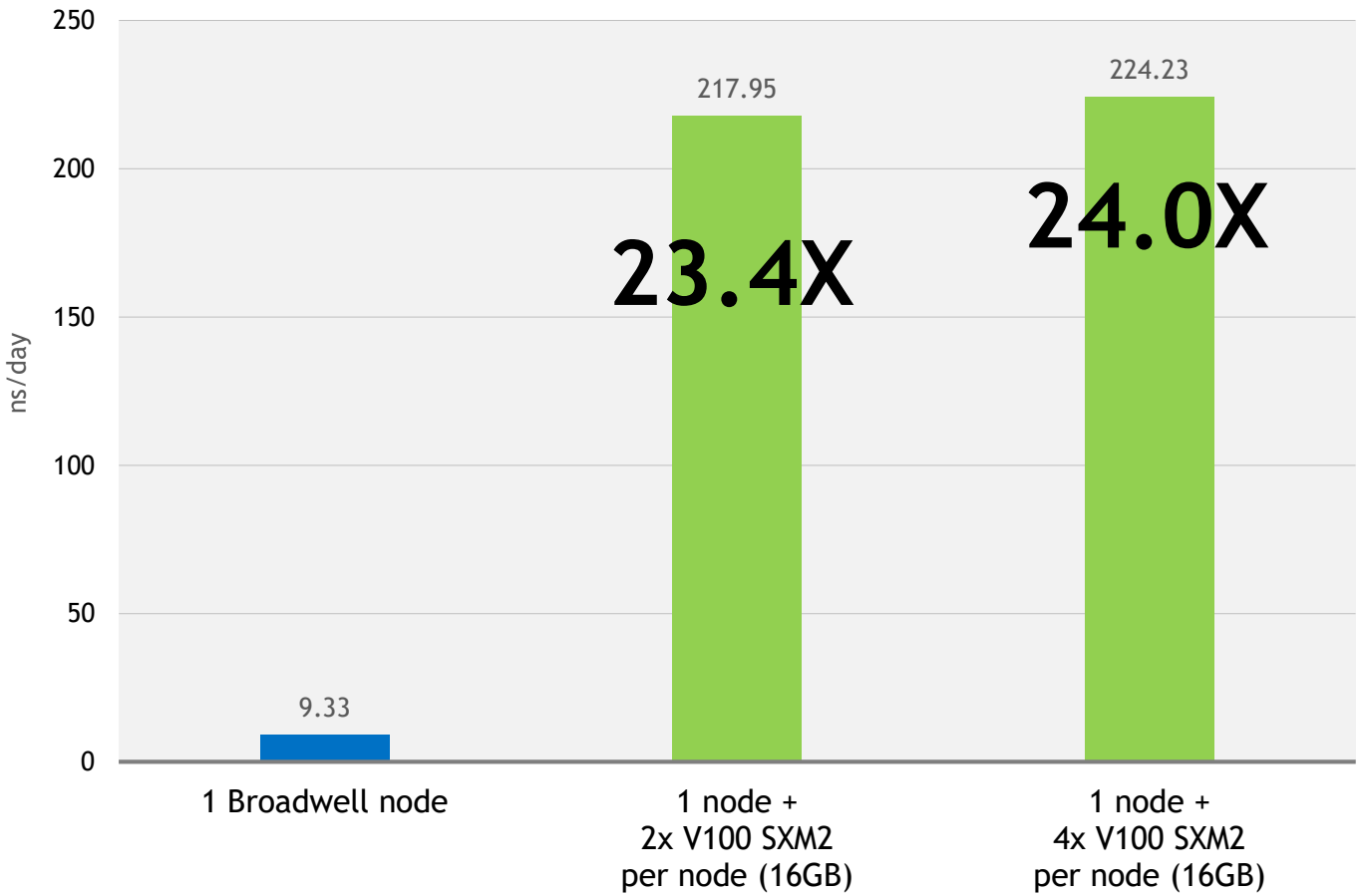

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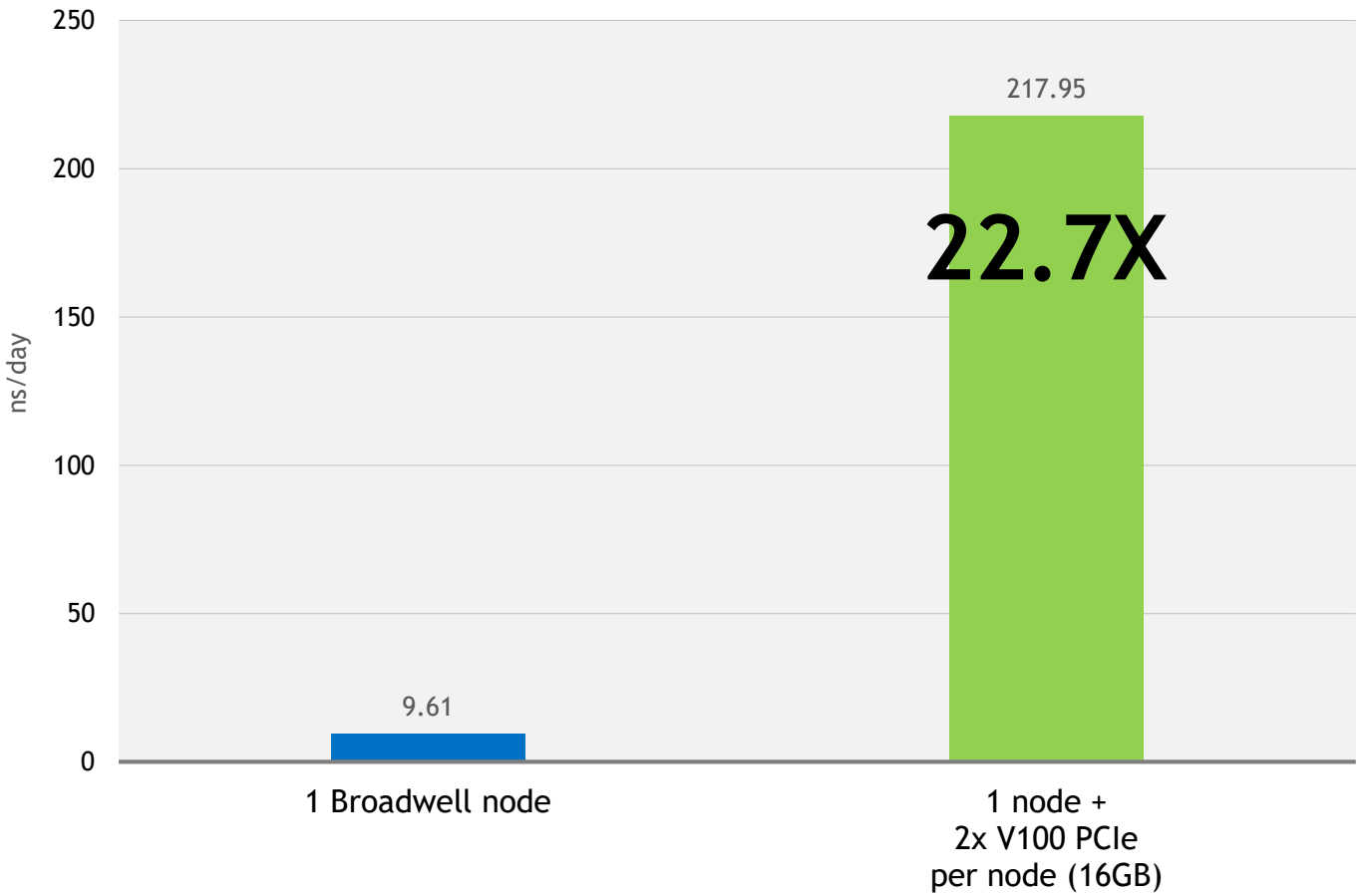

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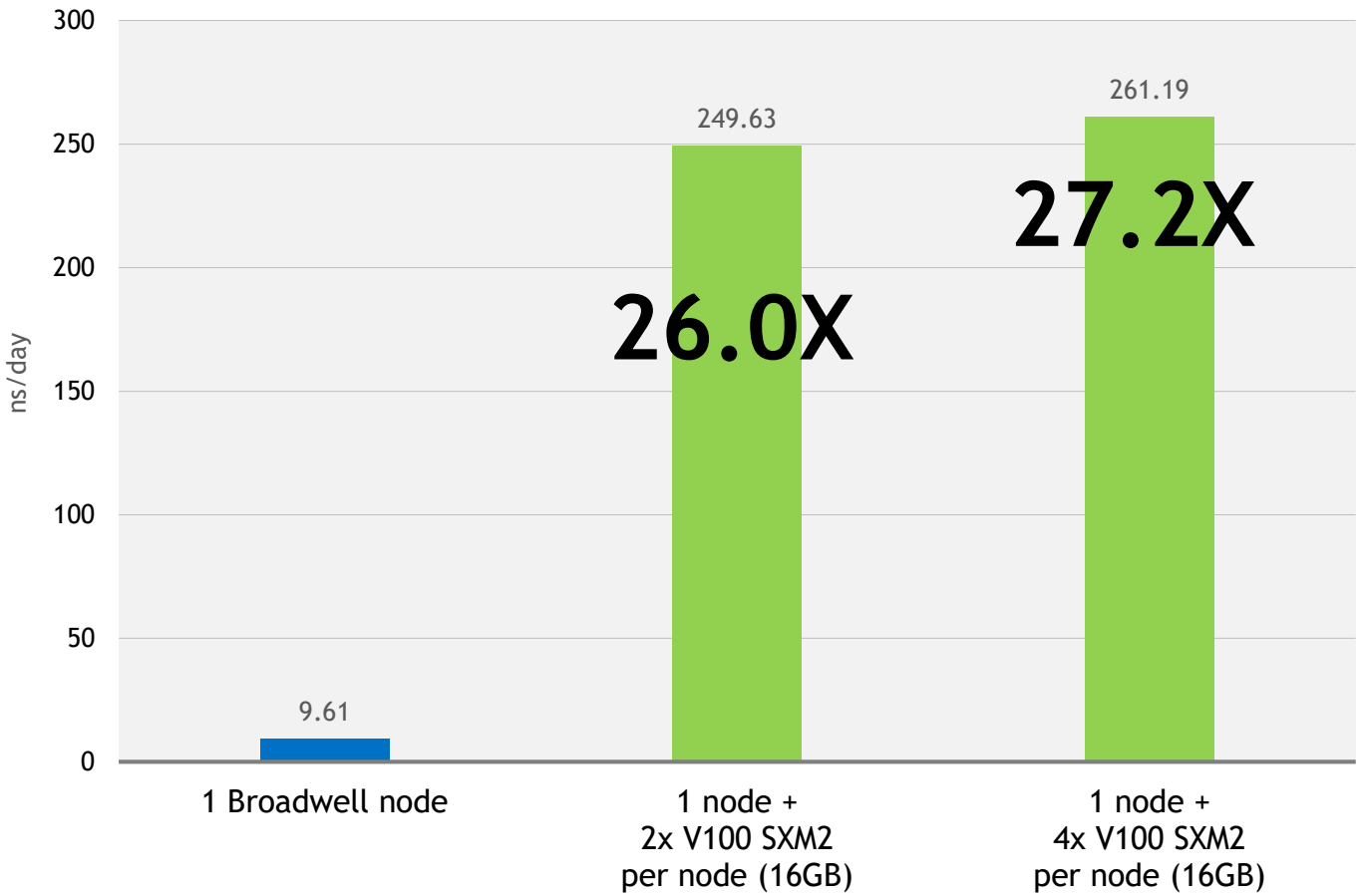

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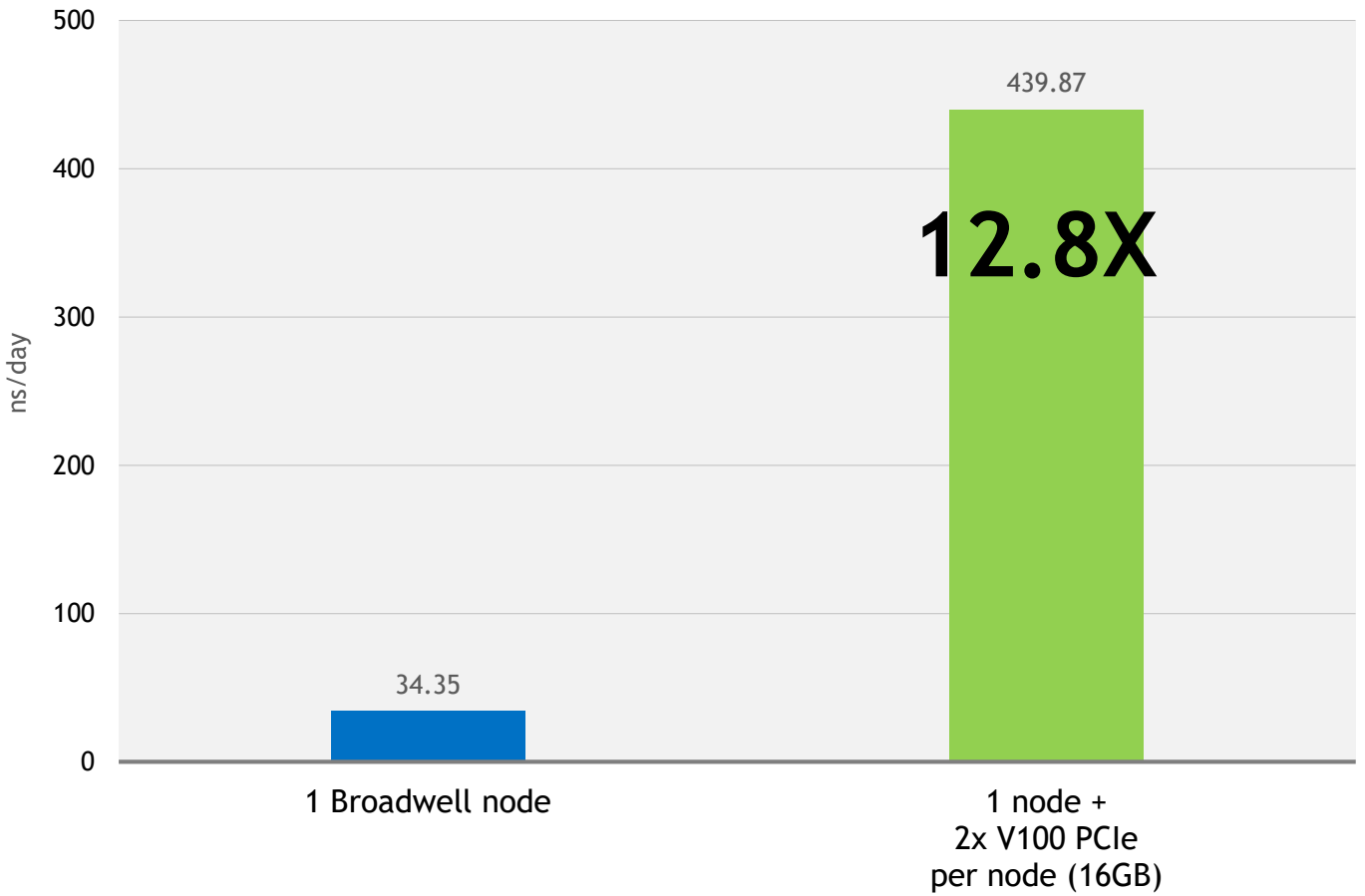
PME-JAC_NPT on V100s PCIe



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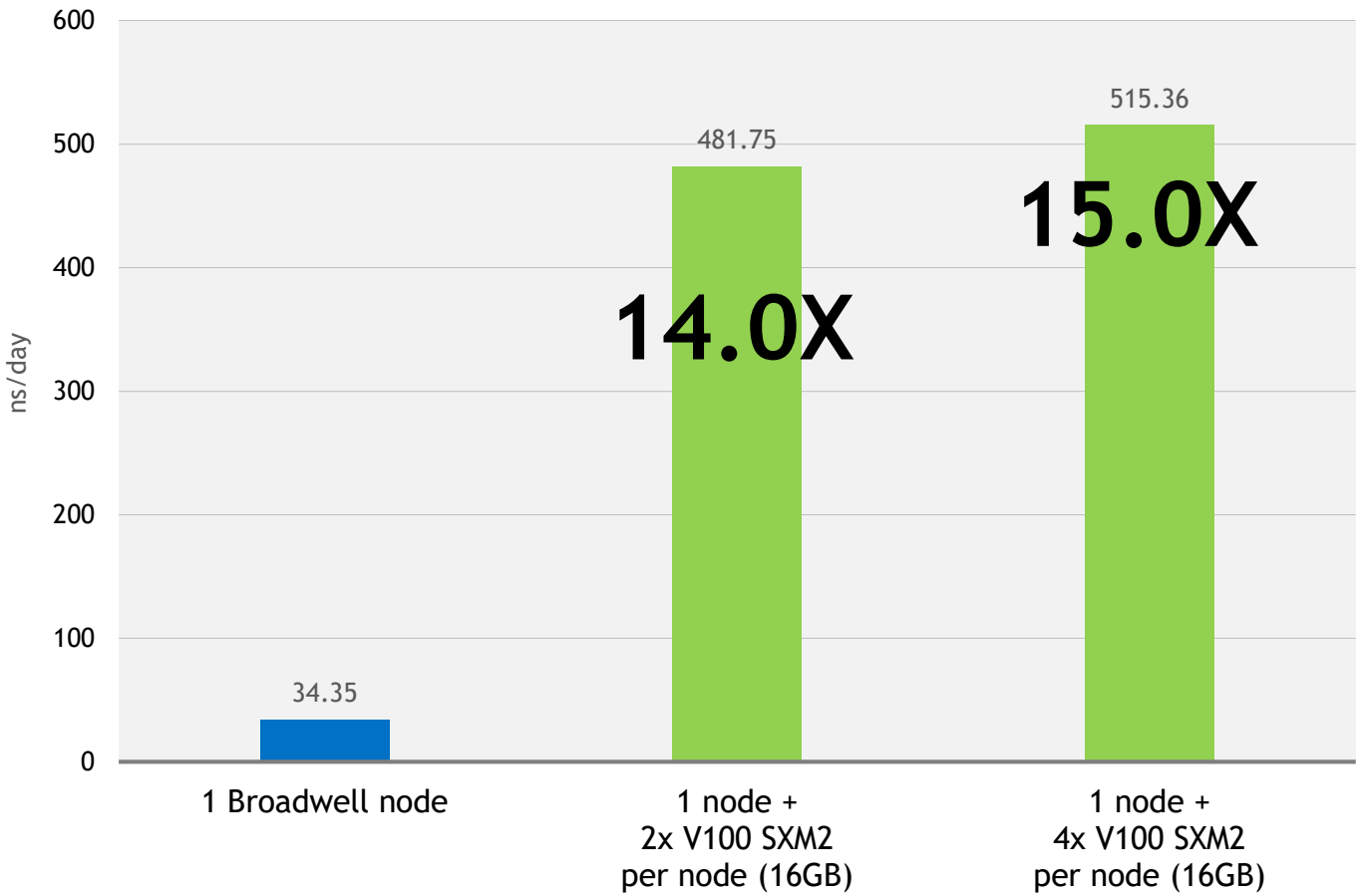

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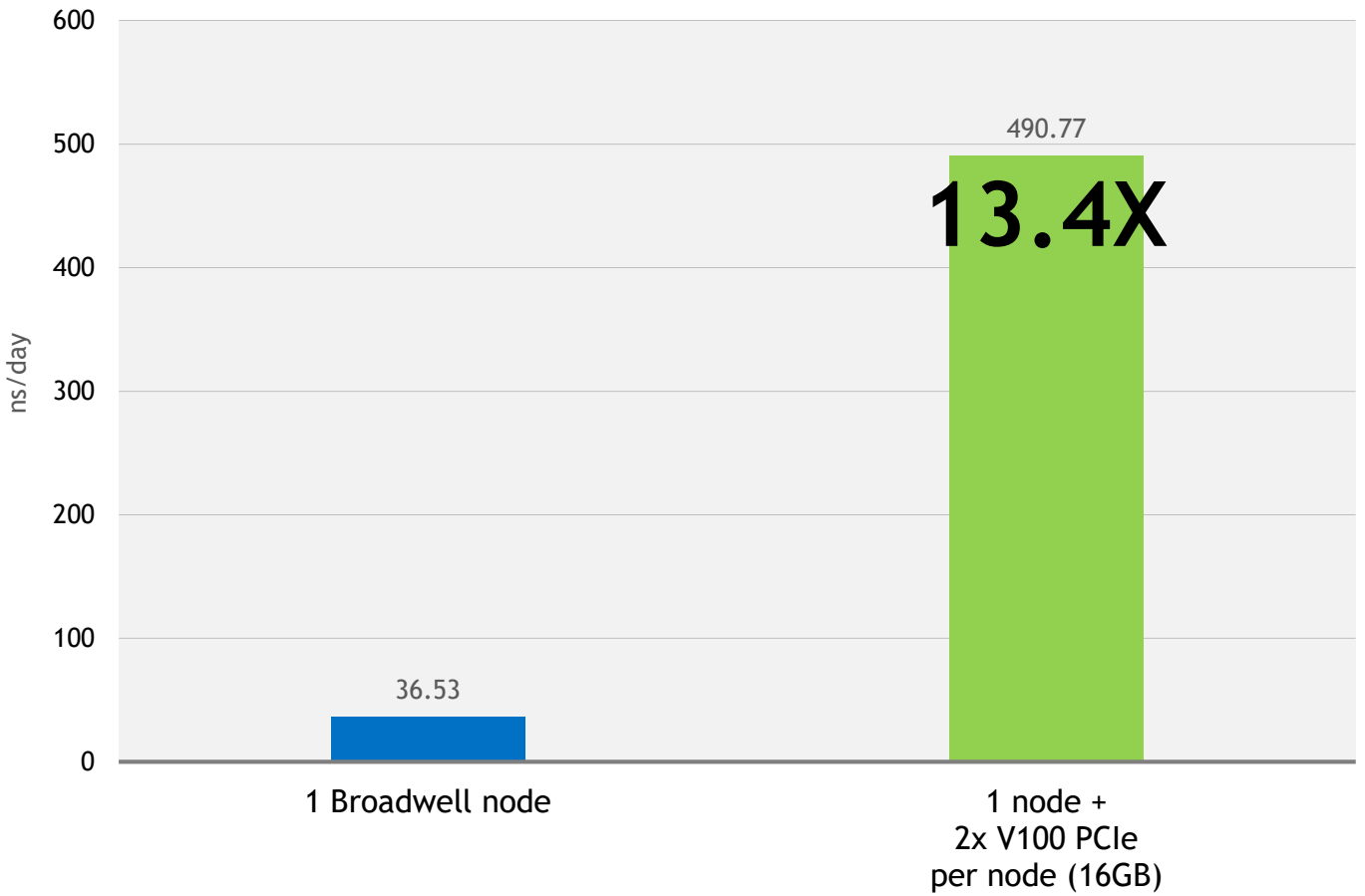

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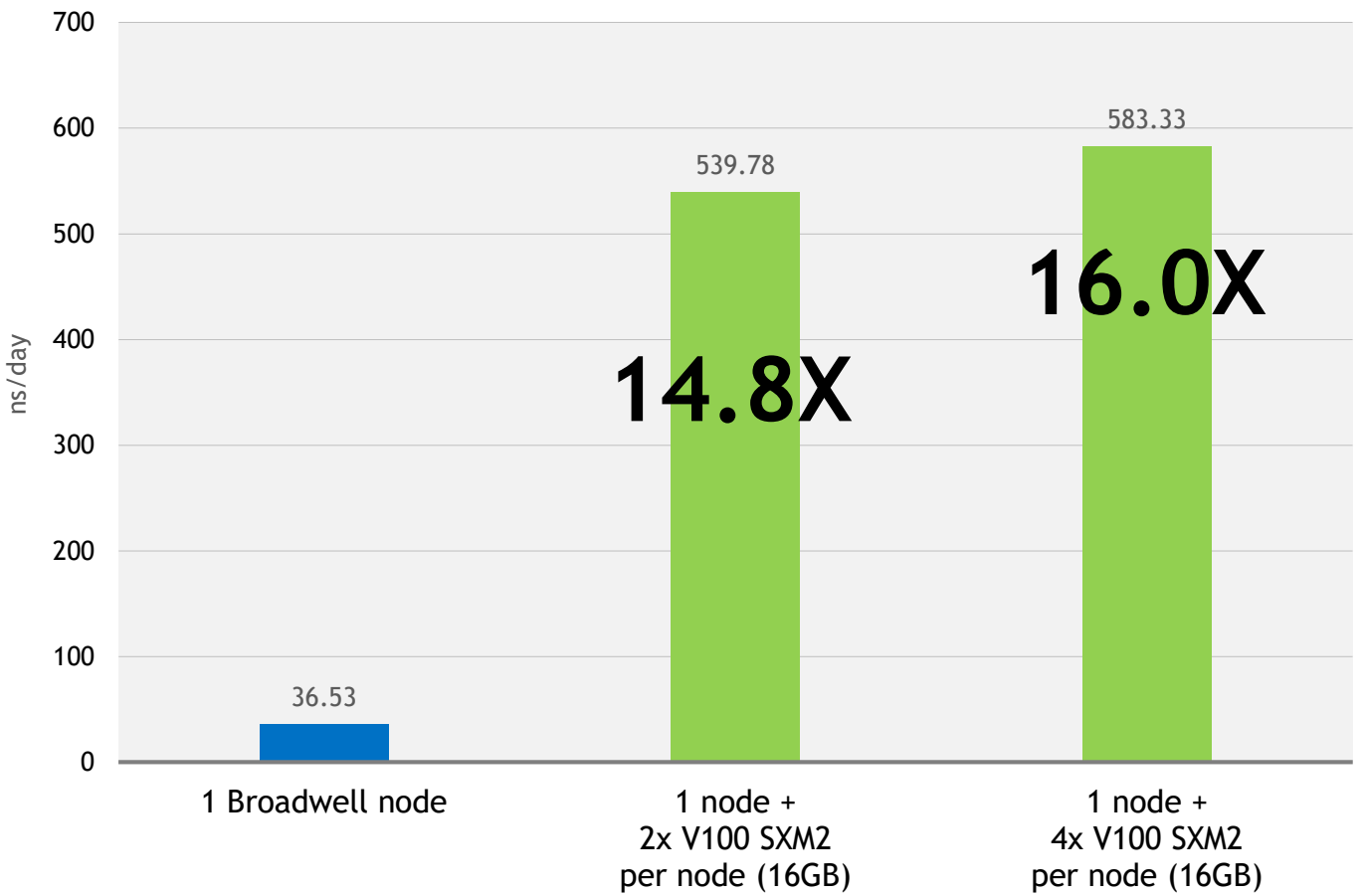

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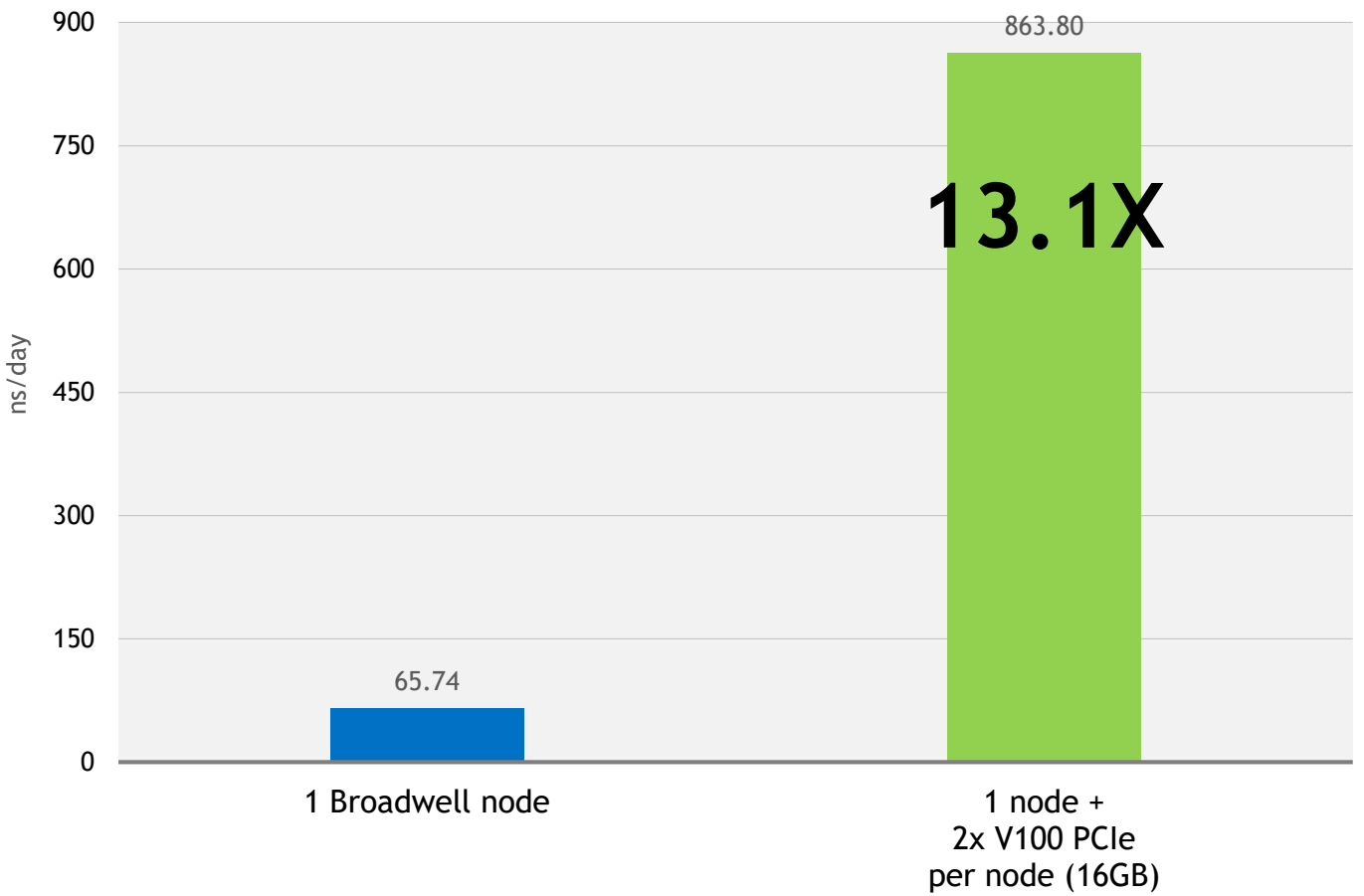
PME-JAC_NPT_4fs on V100s PCIe



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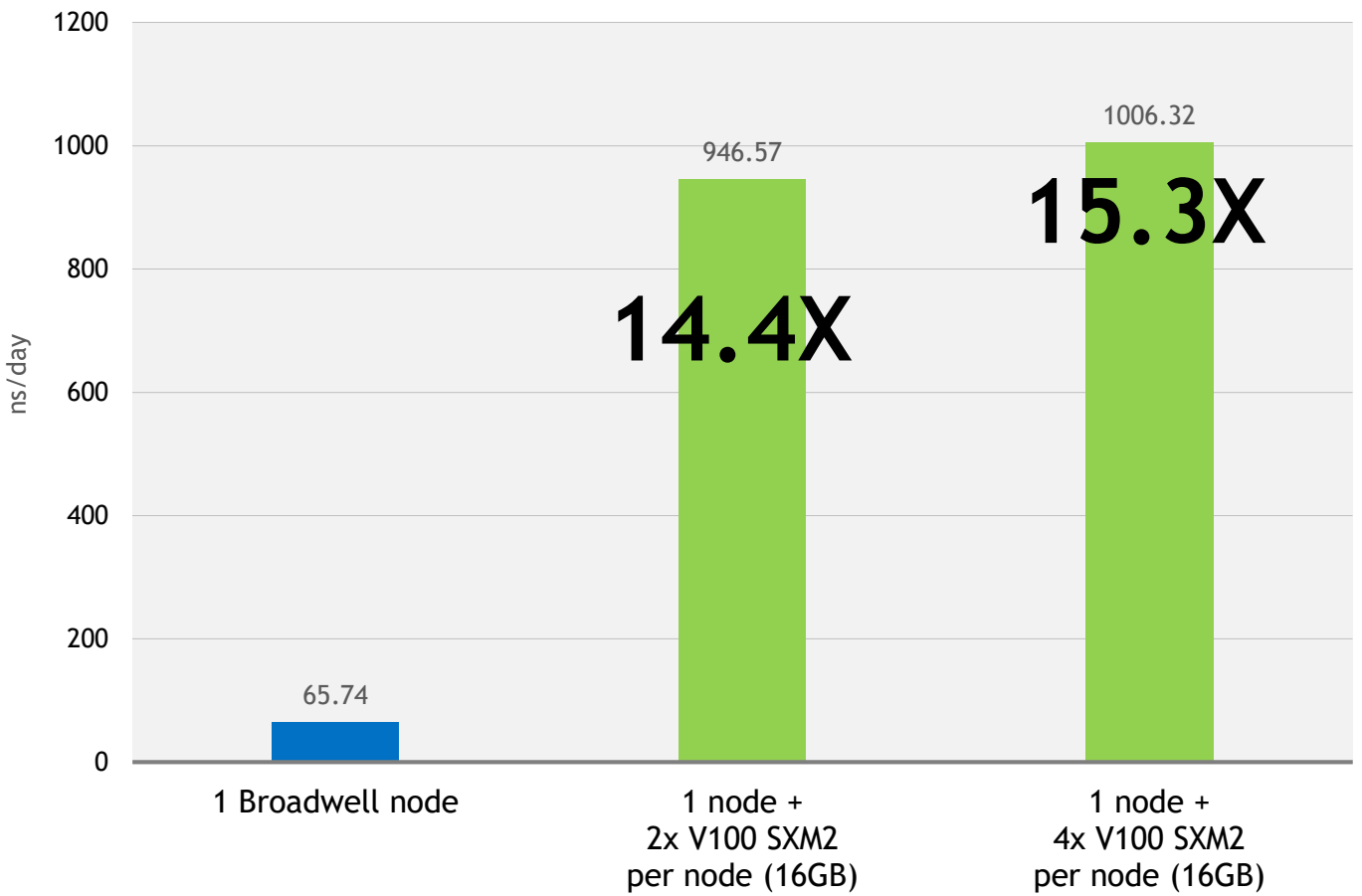

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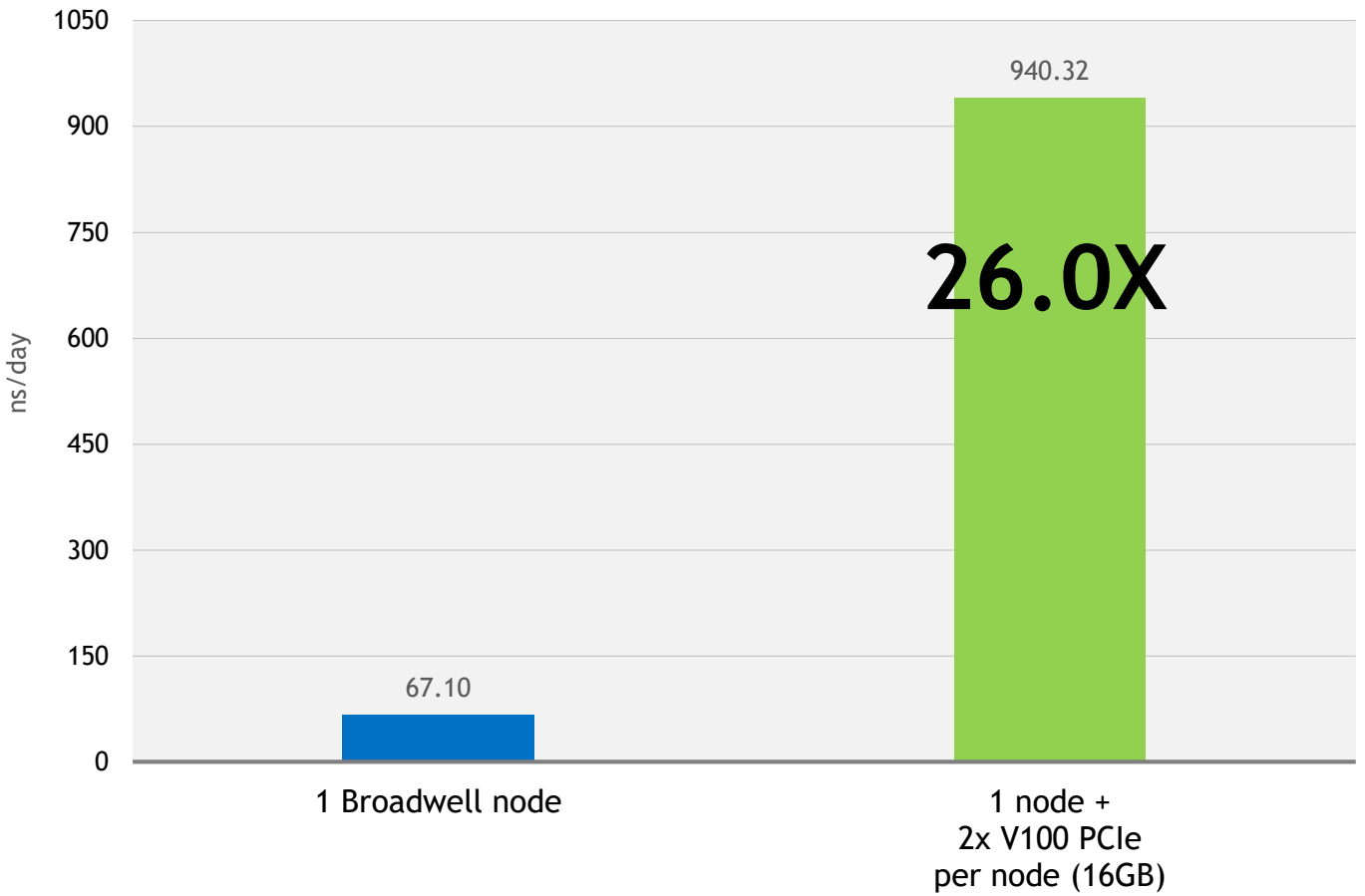

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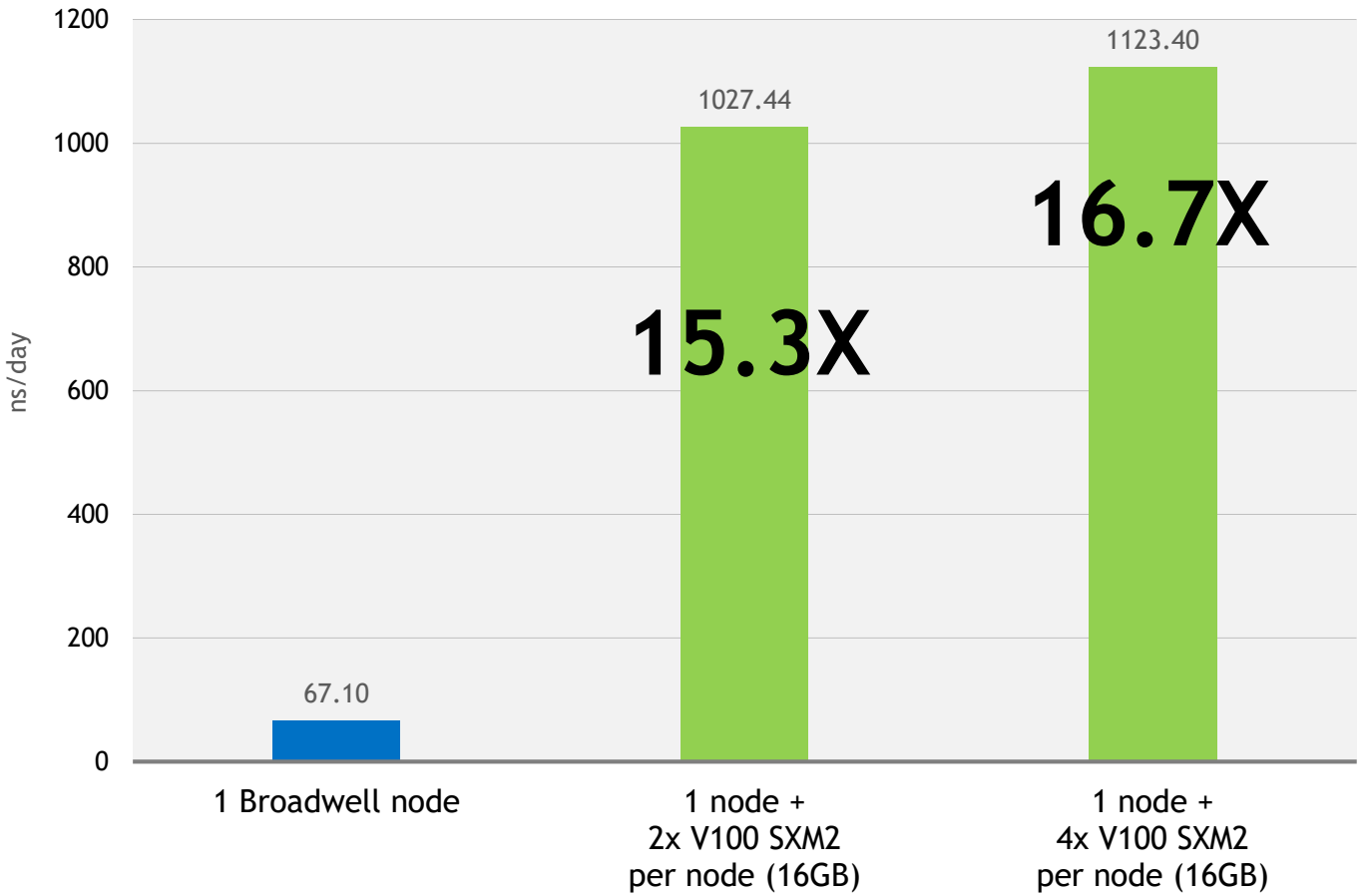

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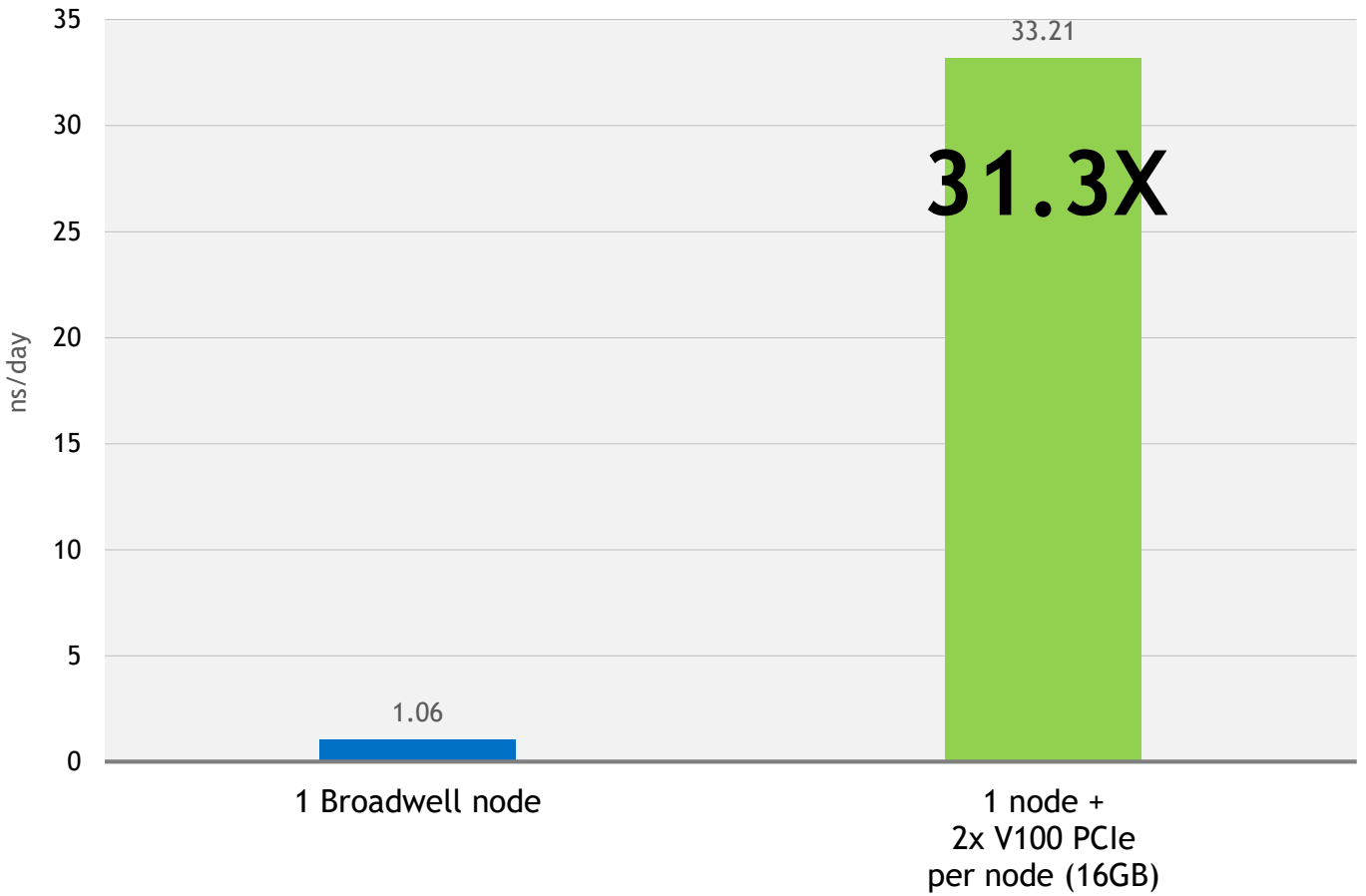
PME-STMV_NPT_4fs on V100s PCIe



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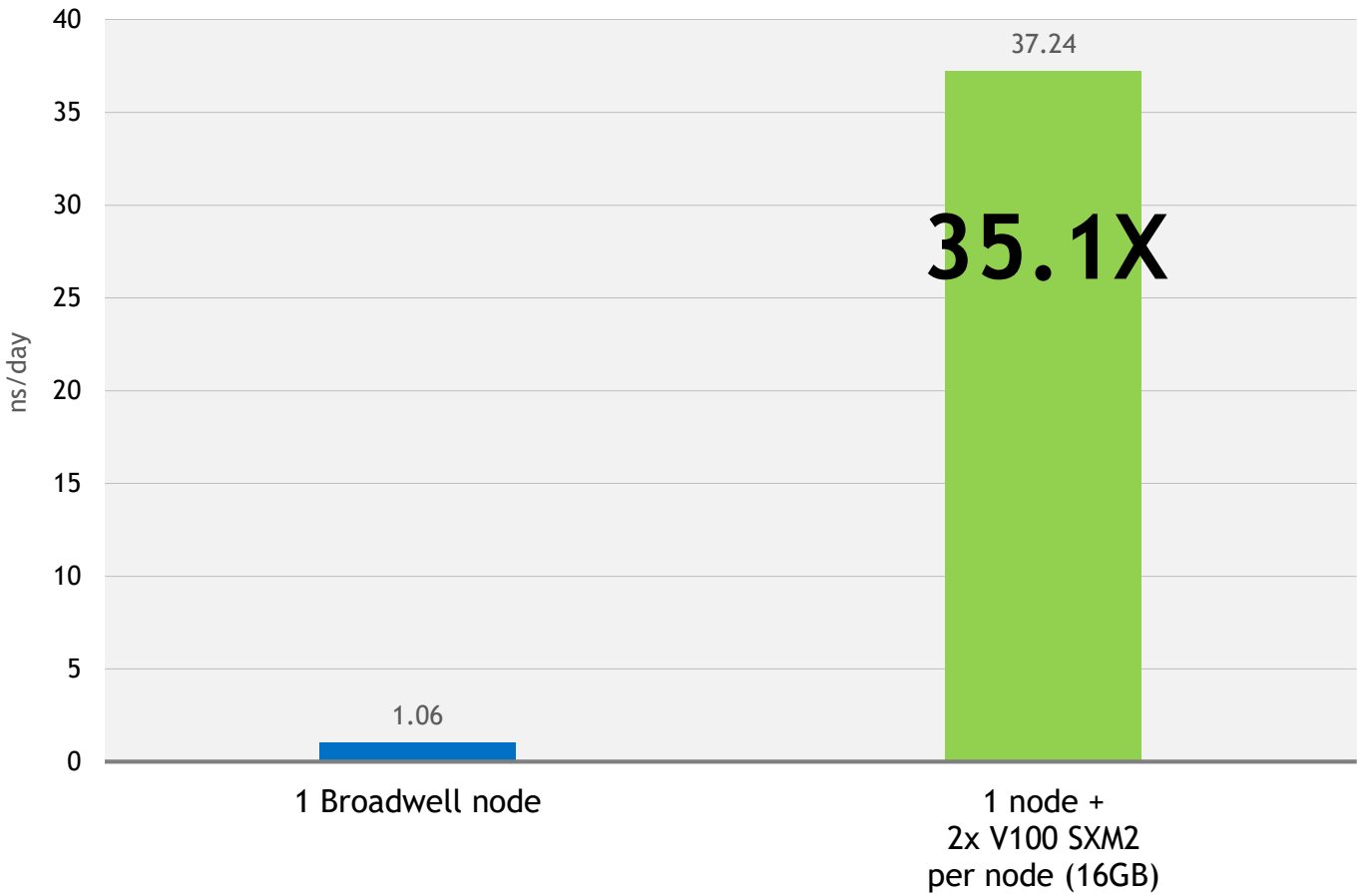

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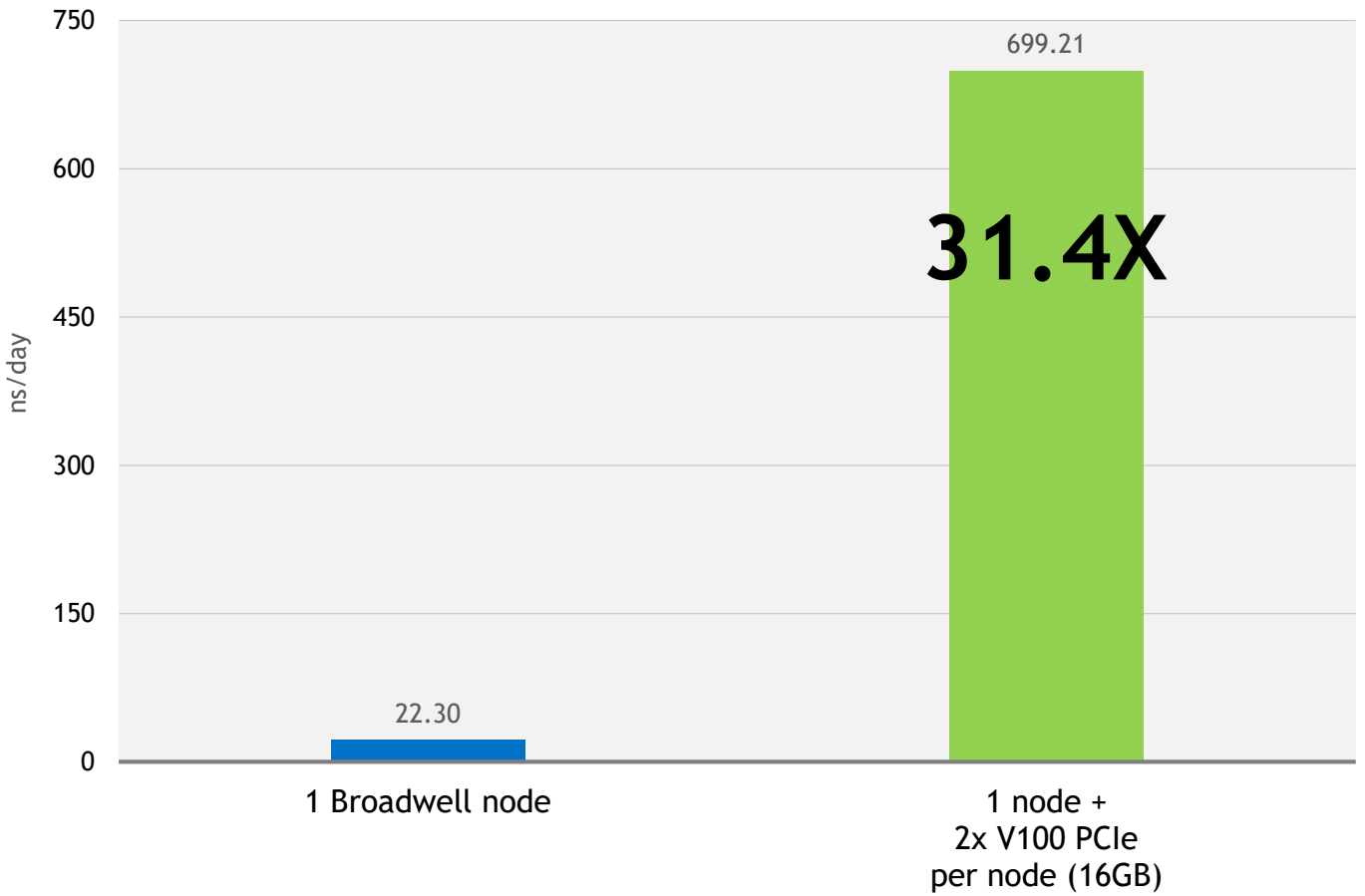
GB-Myoglobin on V100s PCIe



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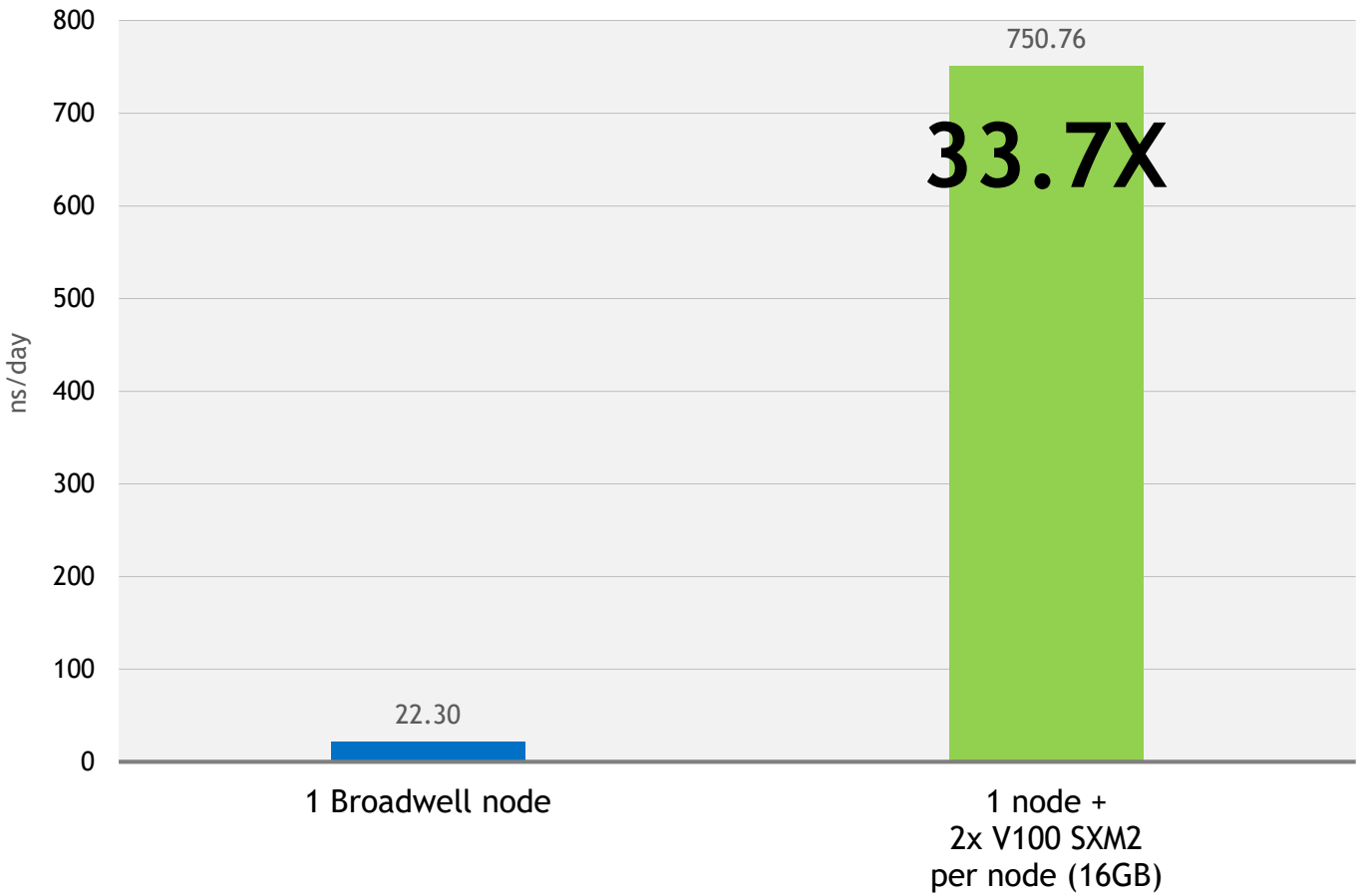

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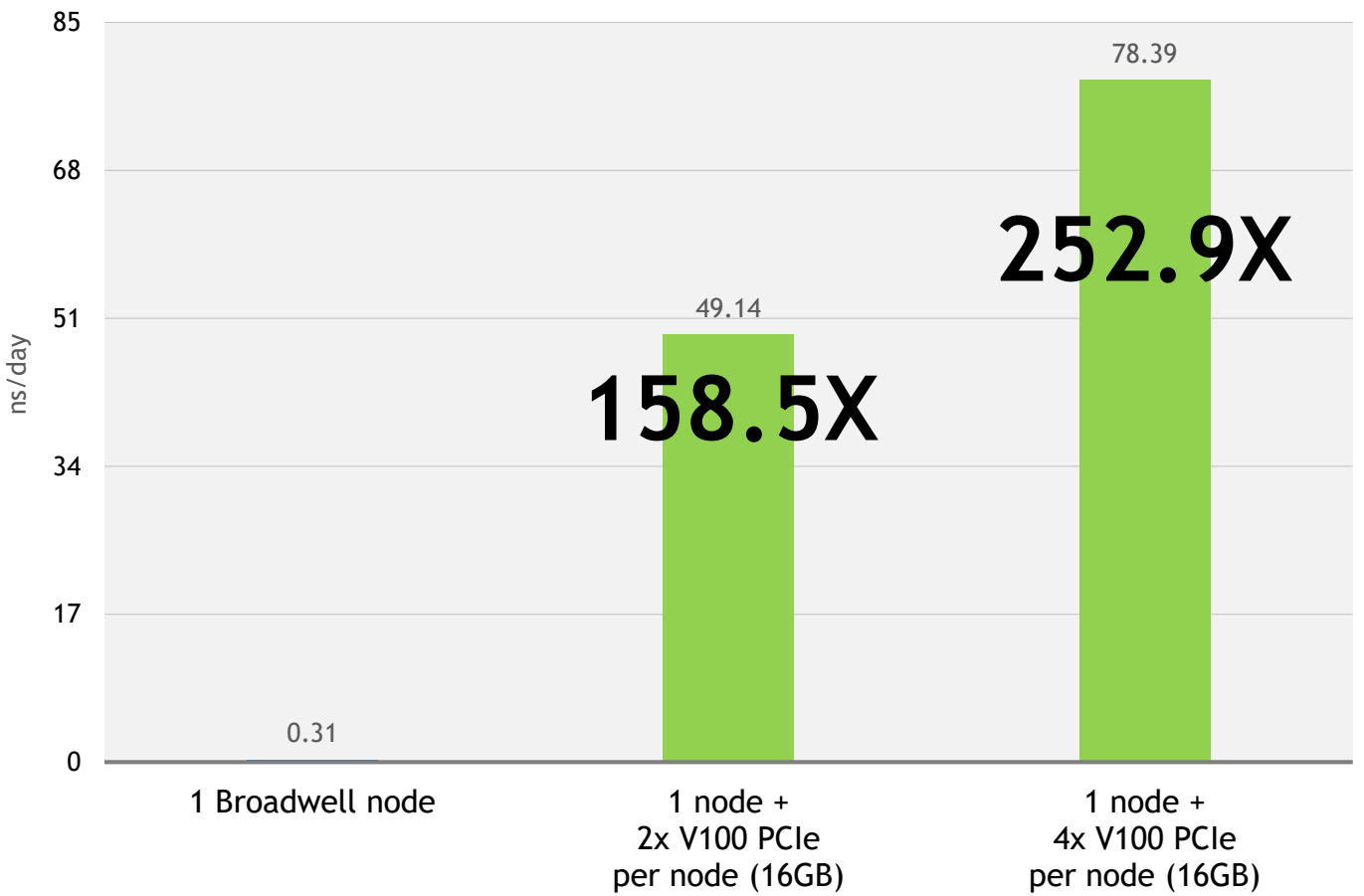
GB-Nucleosome on V100s PCIe



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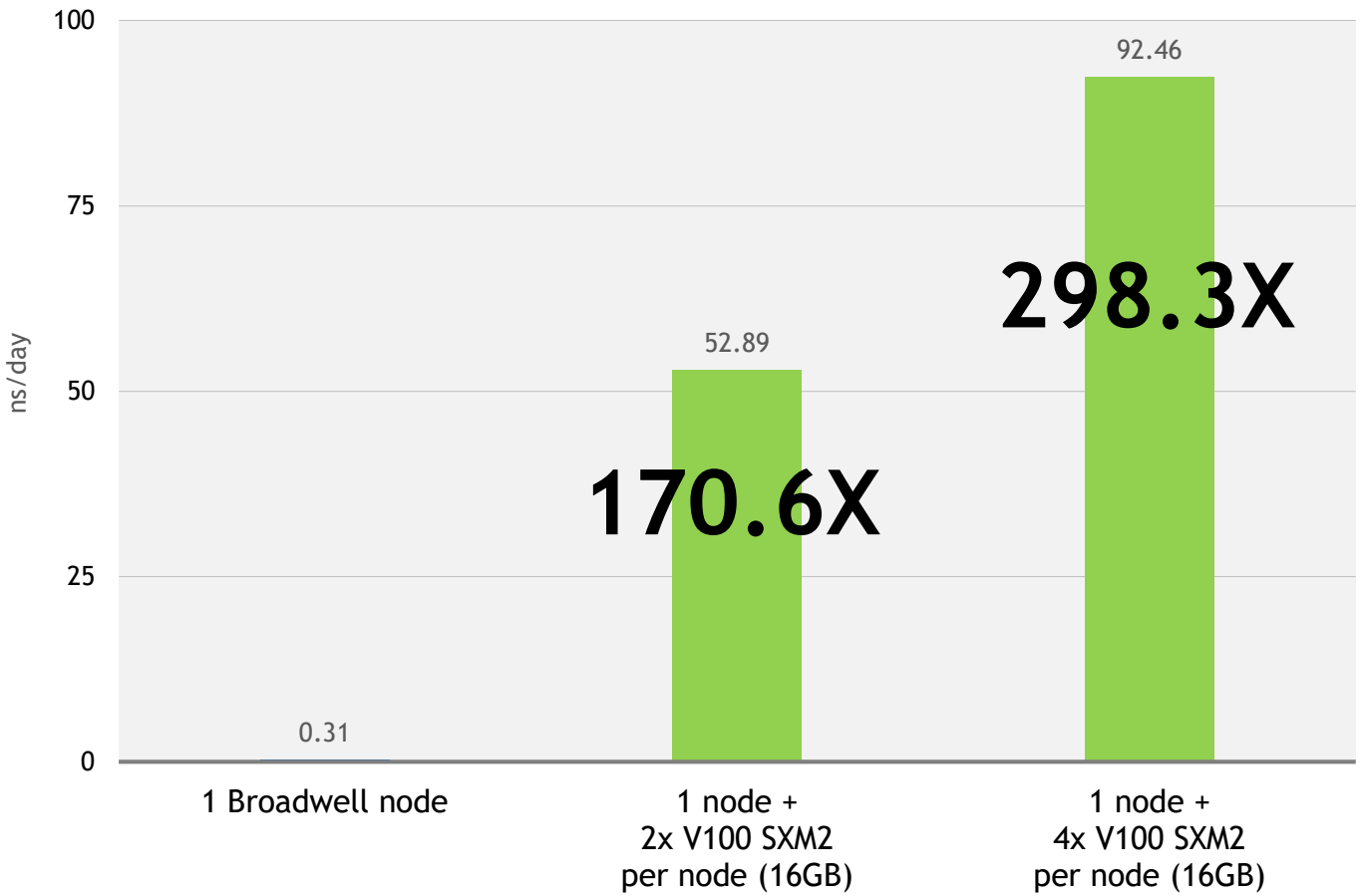

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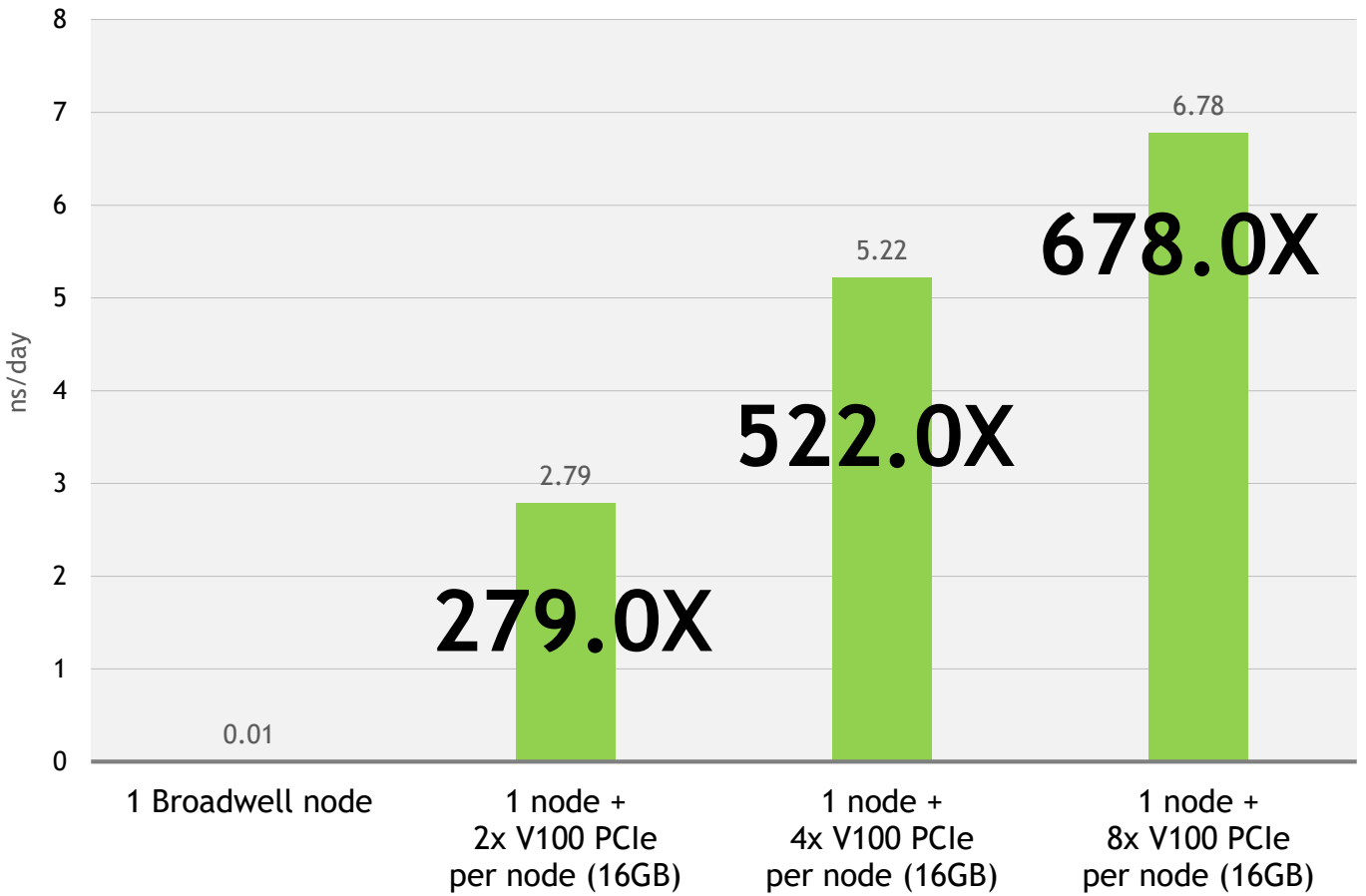
Rubisco on V100s PCIe



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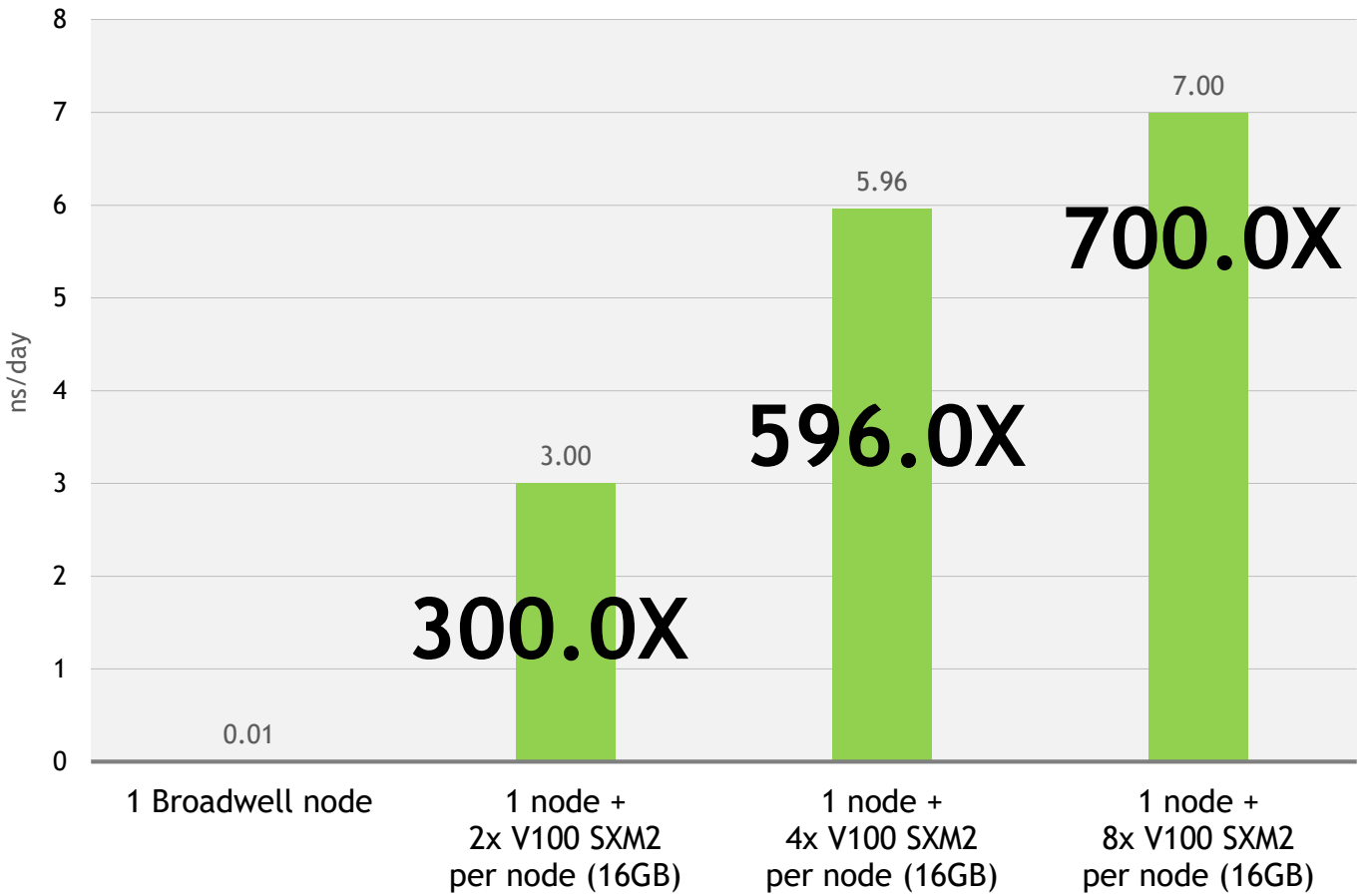
Rubisco on V100s SXM2



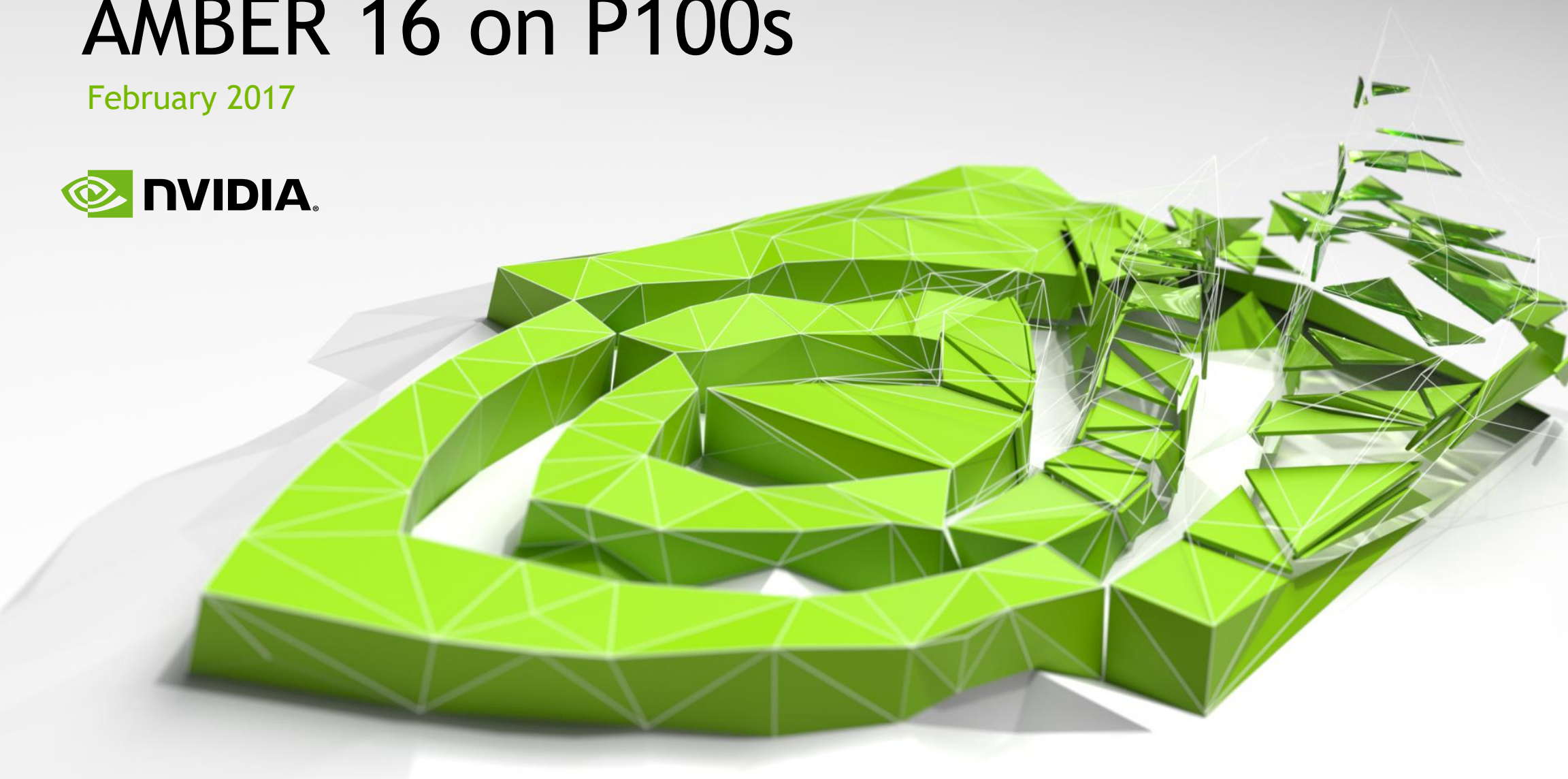
(Untuned on Volta)
Running AMBER version 16.8

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

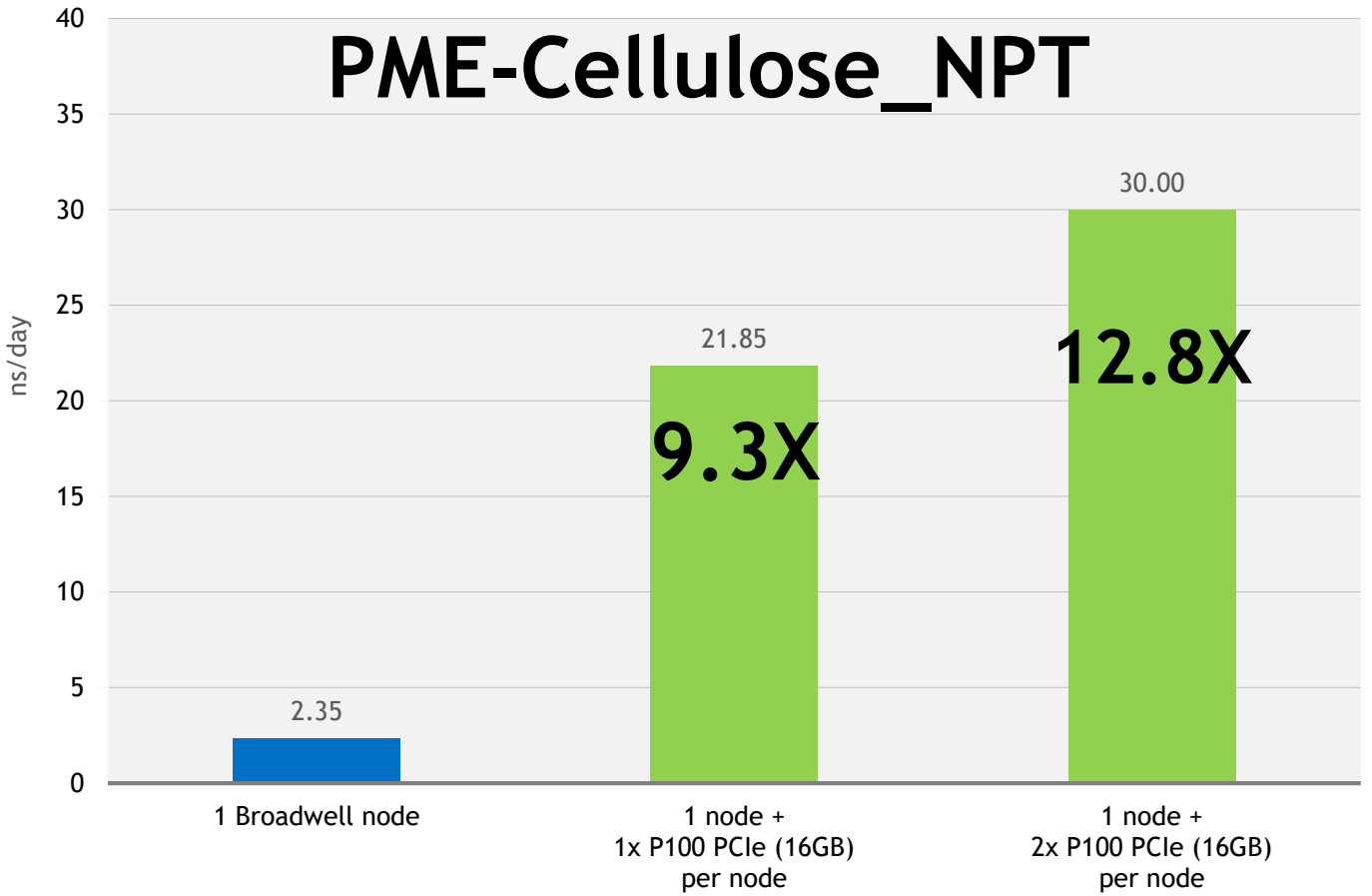
The green nodes contain Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla V100 SXM2 (16GB) GPUs

AMBER 16 on P100s

February 2017



PME-Cellulose_NPT on P100s PCIe



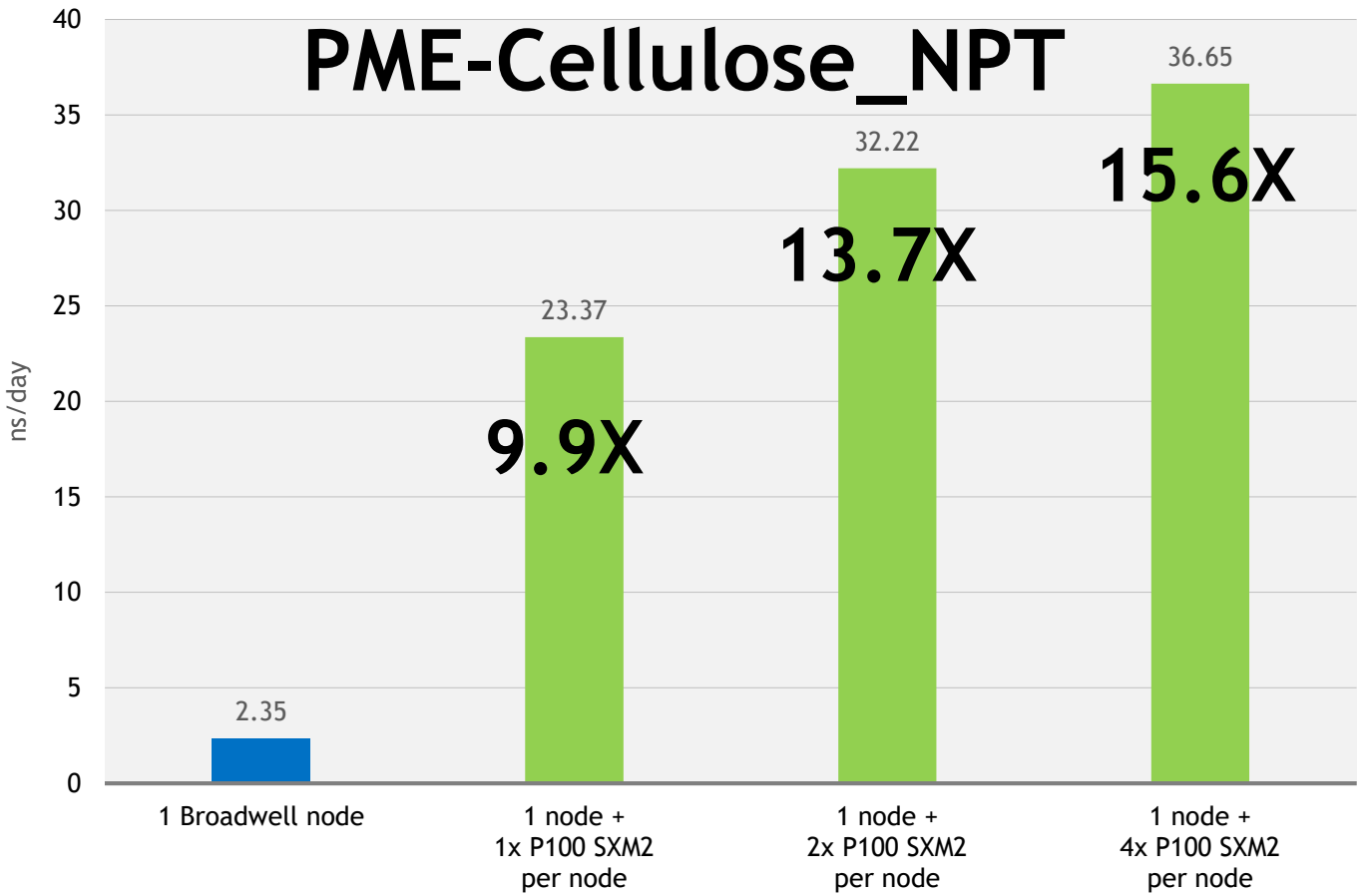
Running AMBER version 16.3

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)

PME-Cellulose_NPT on P100s SXM2



Running AMBER version 16.3

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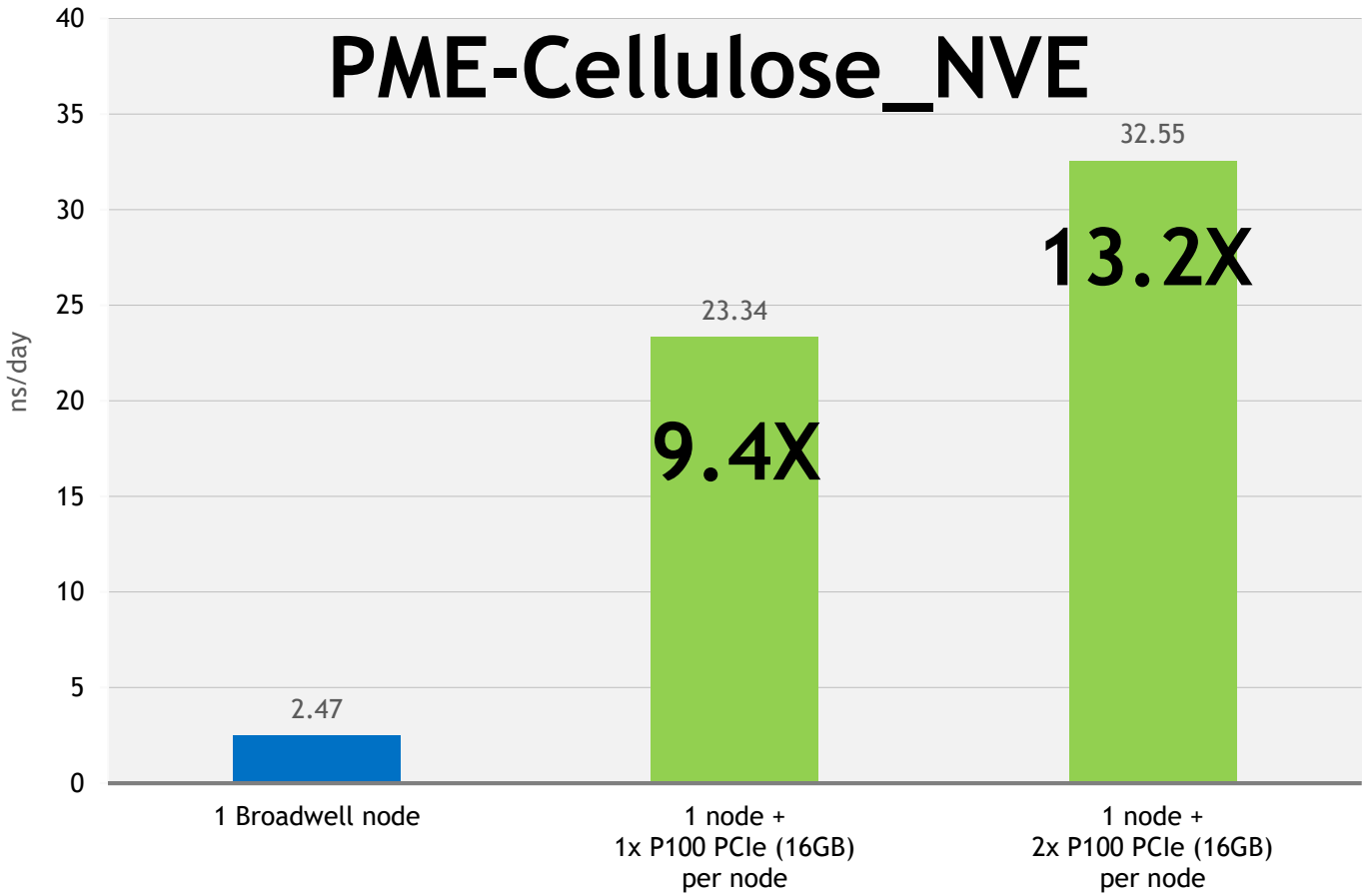
- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

PME-Cellulose_NVE on P100s PCIe



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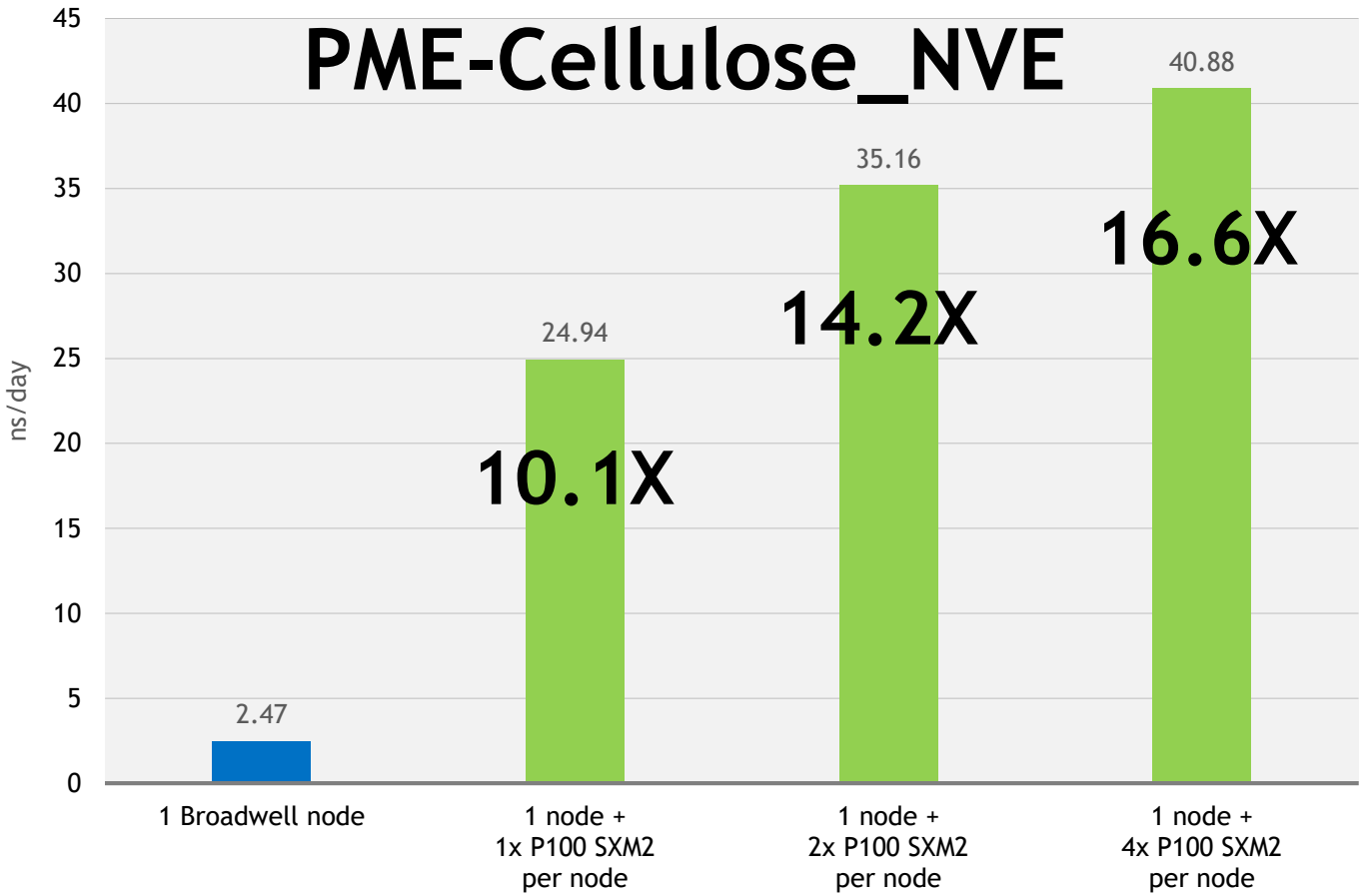
PME-Cellulose_NVE on P100s SXM2



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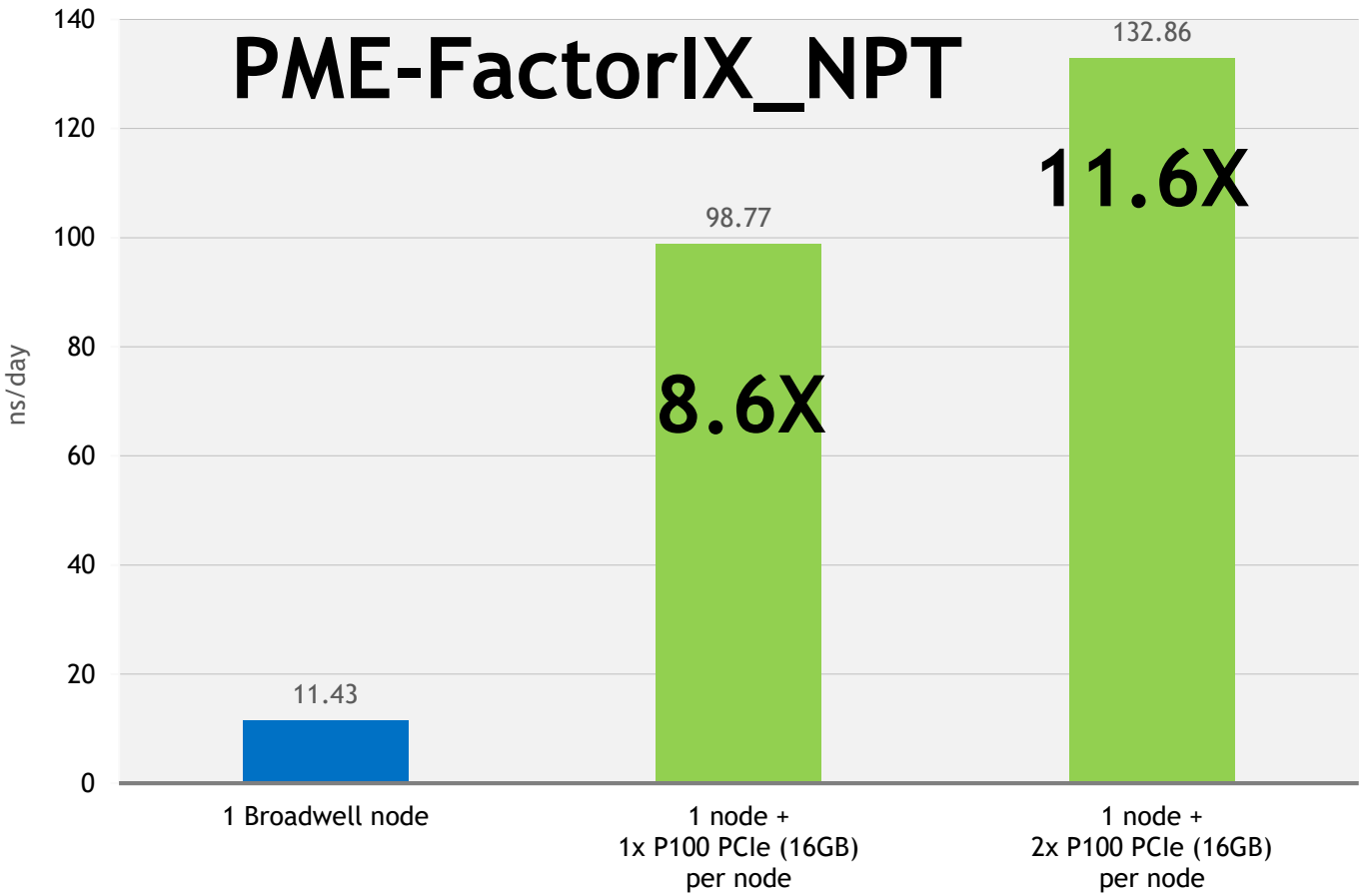
PME-FactorIX_NPT on P100s PCIe



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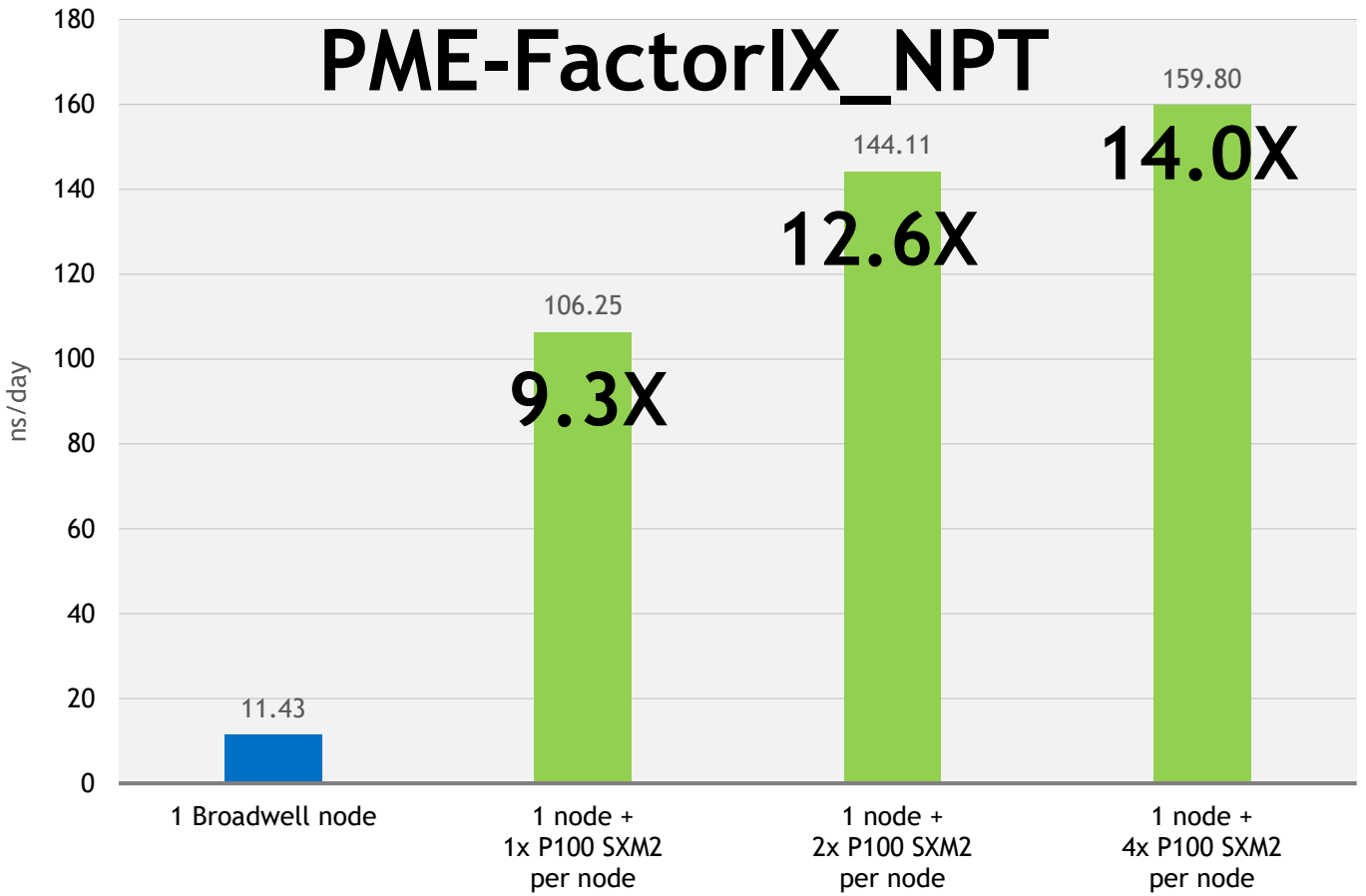
PME-FactorIX_NPT on P100s SXM2



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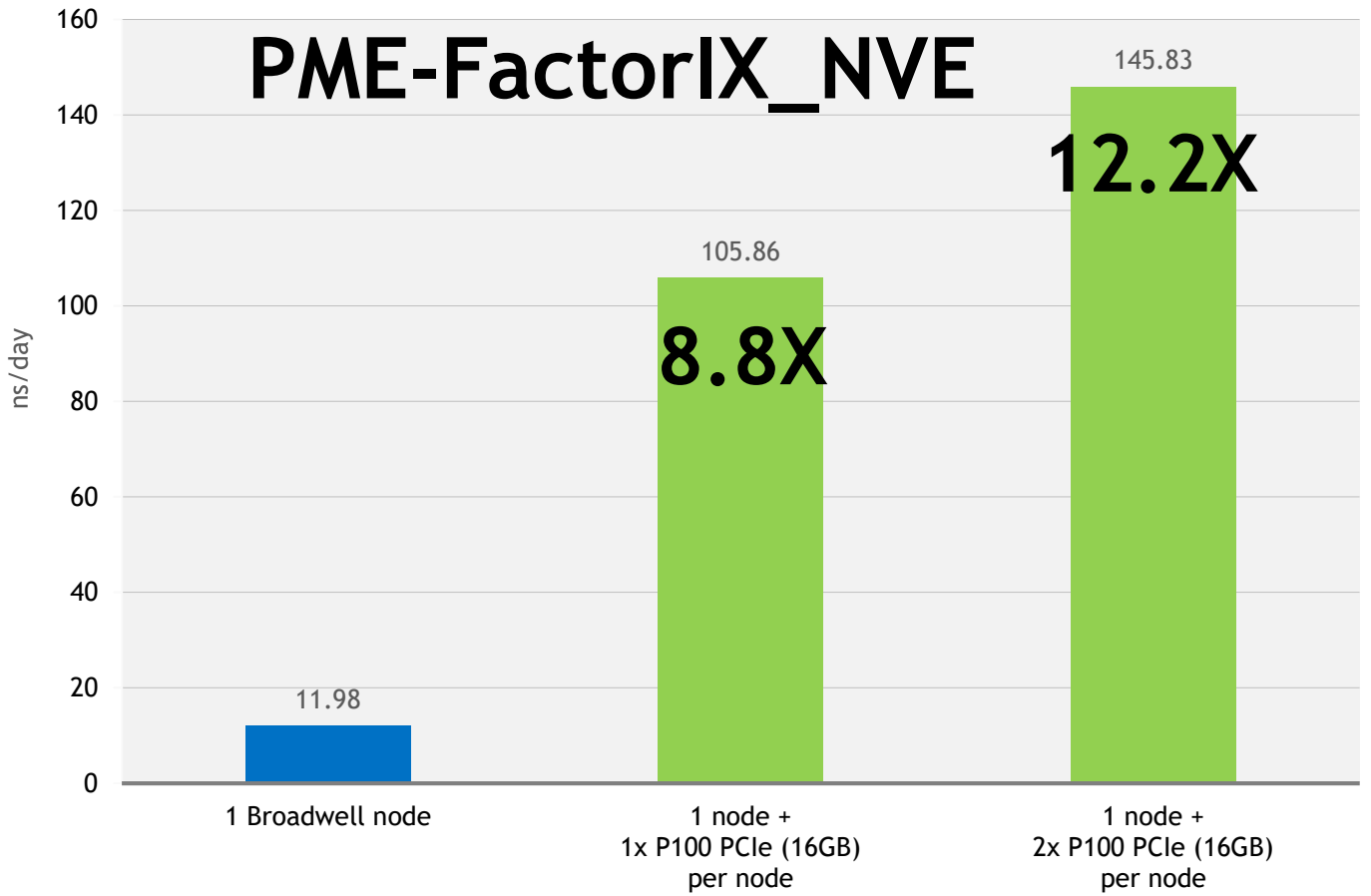

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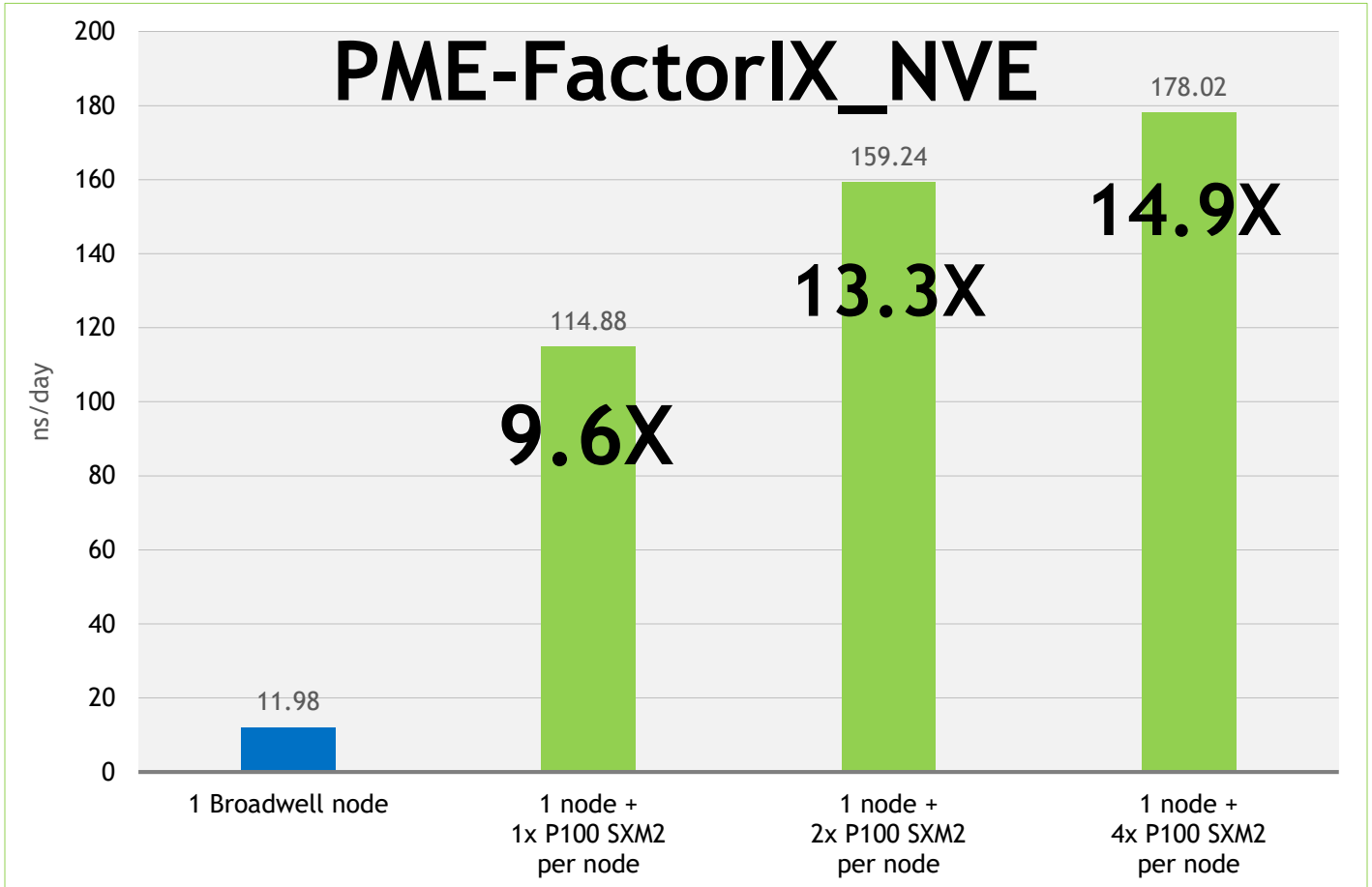
PME-FactorIX_NVE on P100s SXM2



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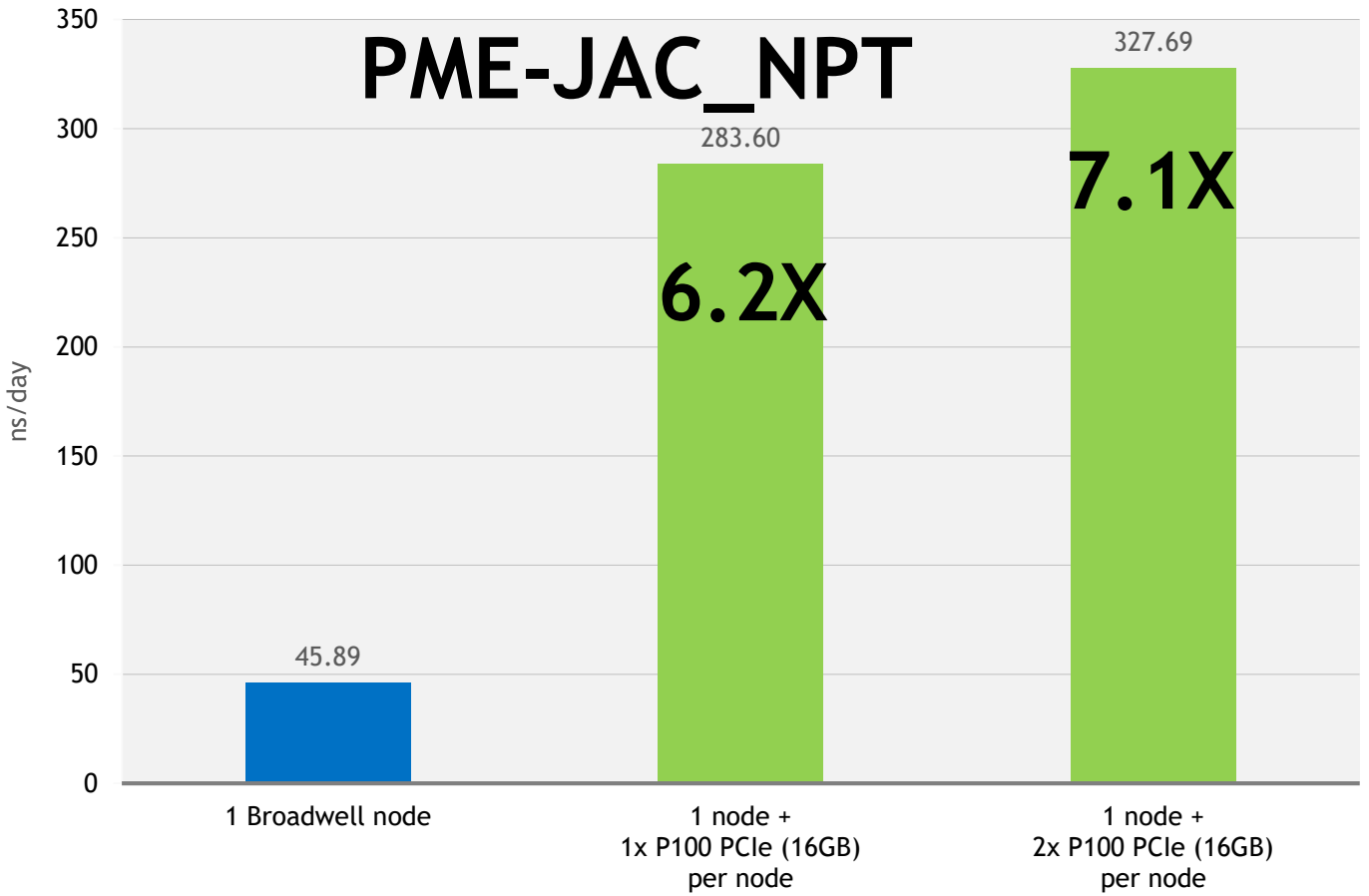
PME-JAC_NPT on P100s PCIe



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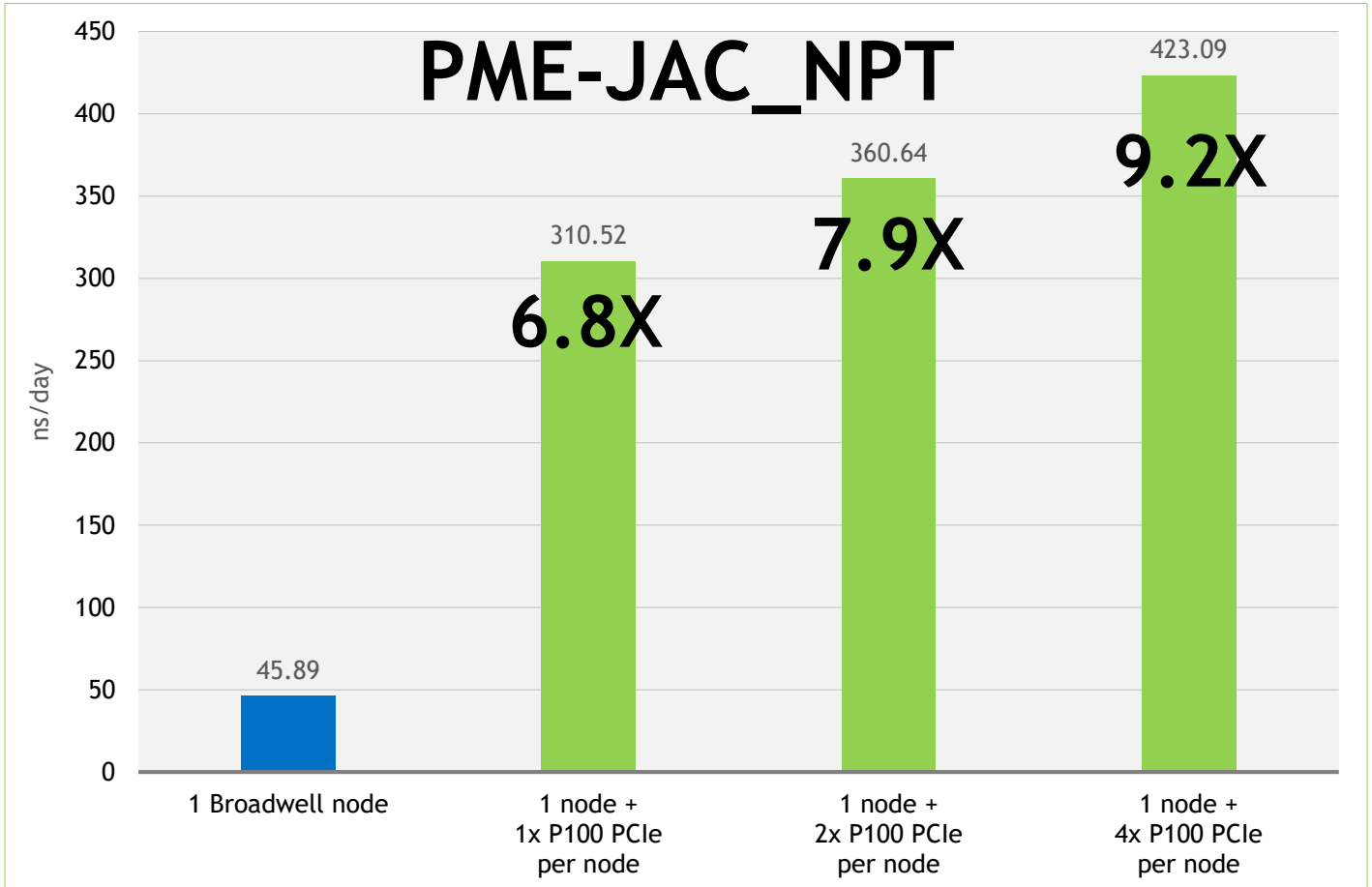
PME-JAC_NPT on P100s SXM2



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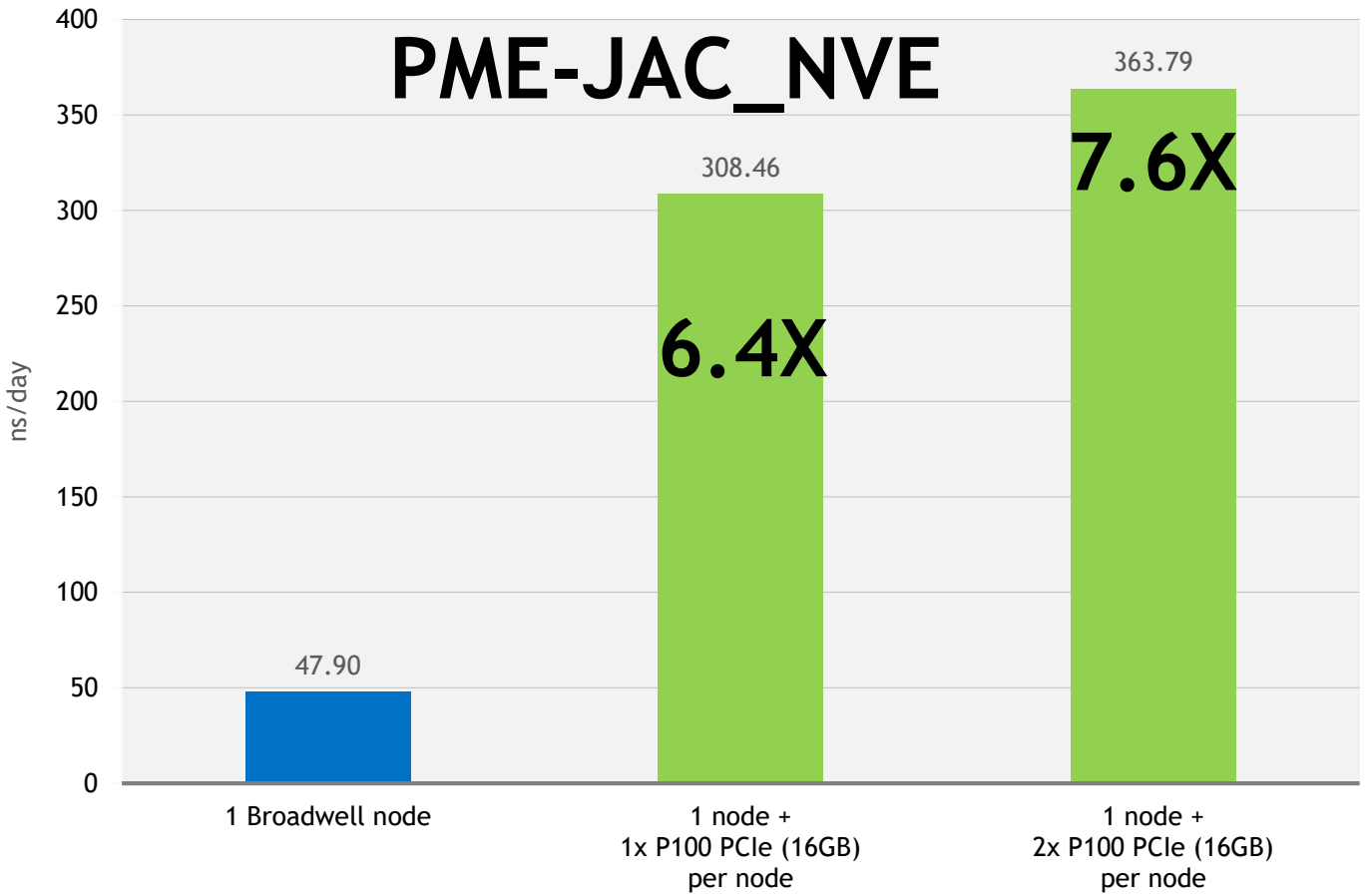
PME-JAC_NVE on P100s PCIe



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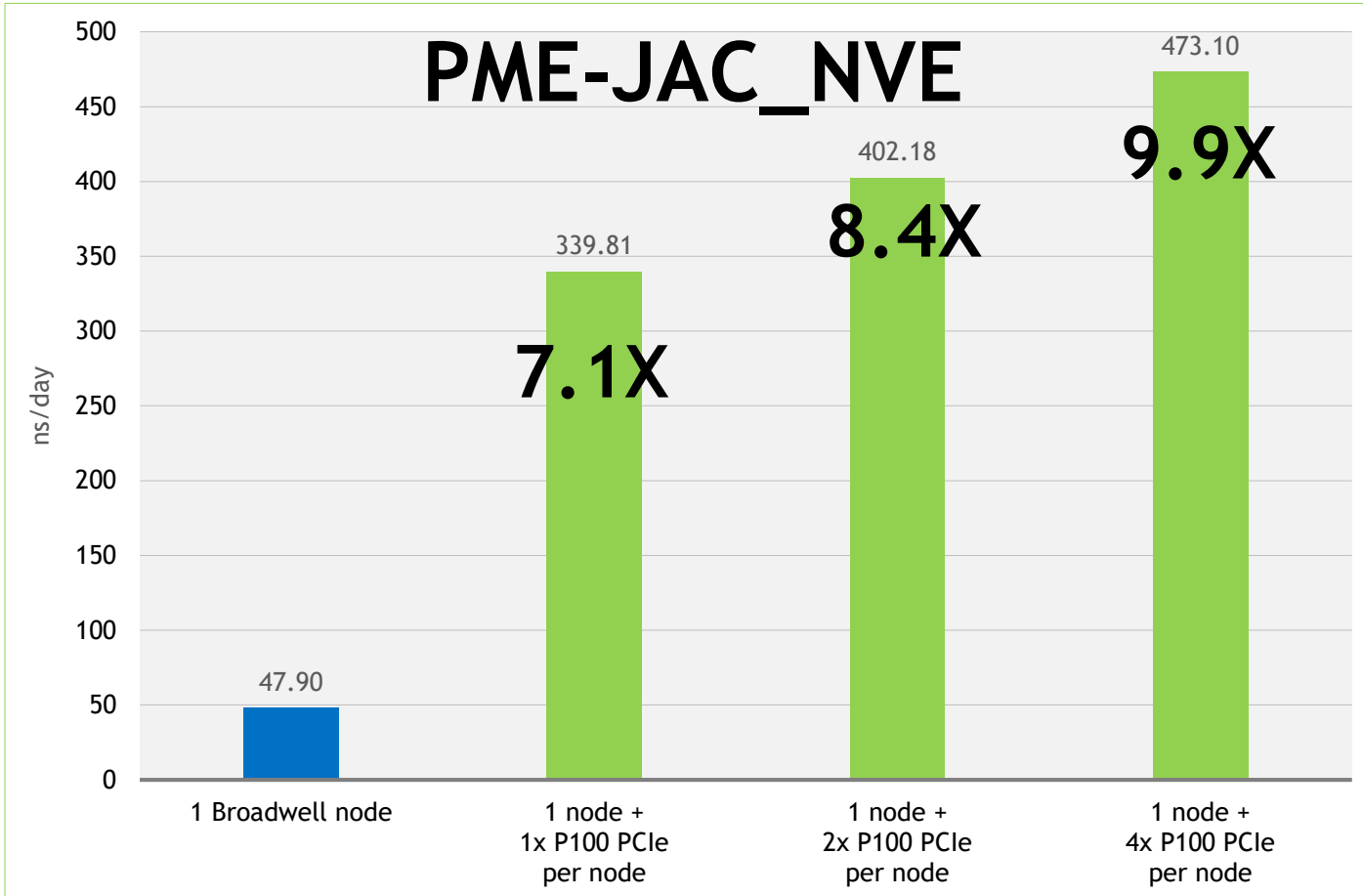
PME-JAC_NVE on P100s SXM2



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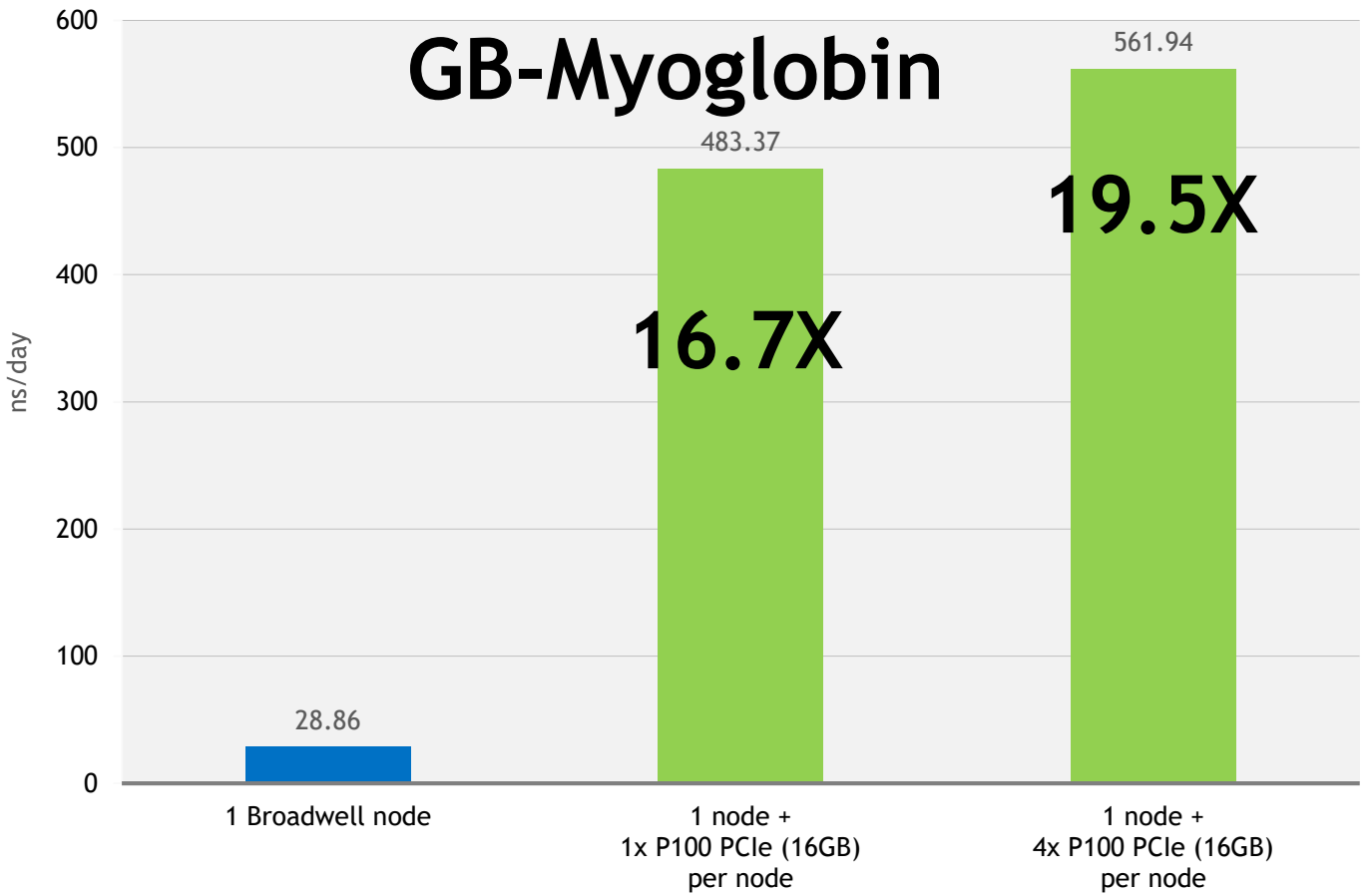
GB-Myoglobin on P100s PCIe



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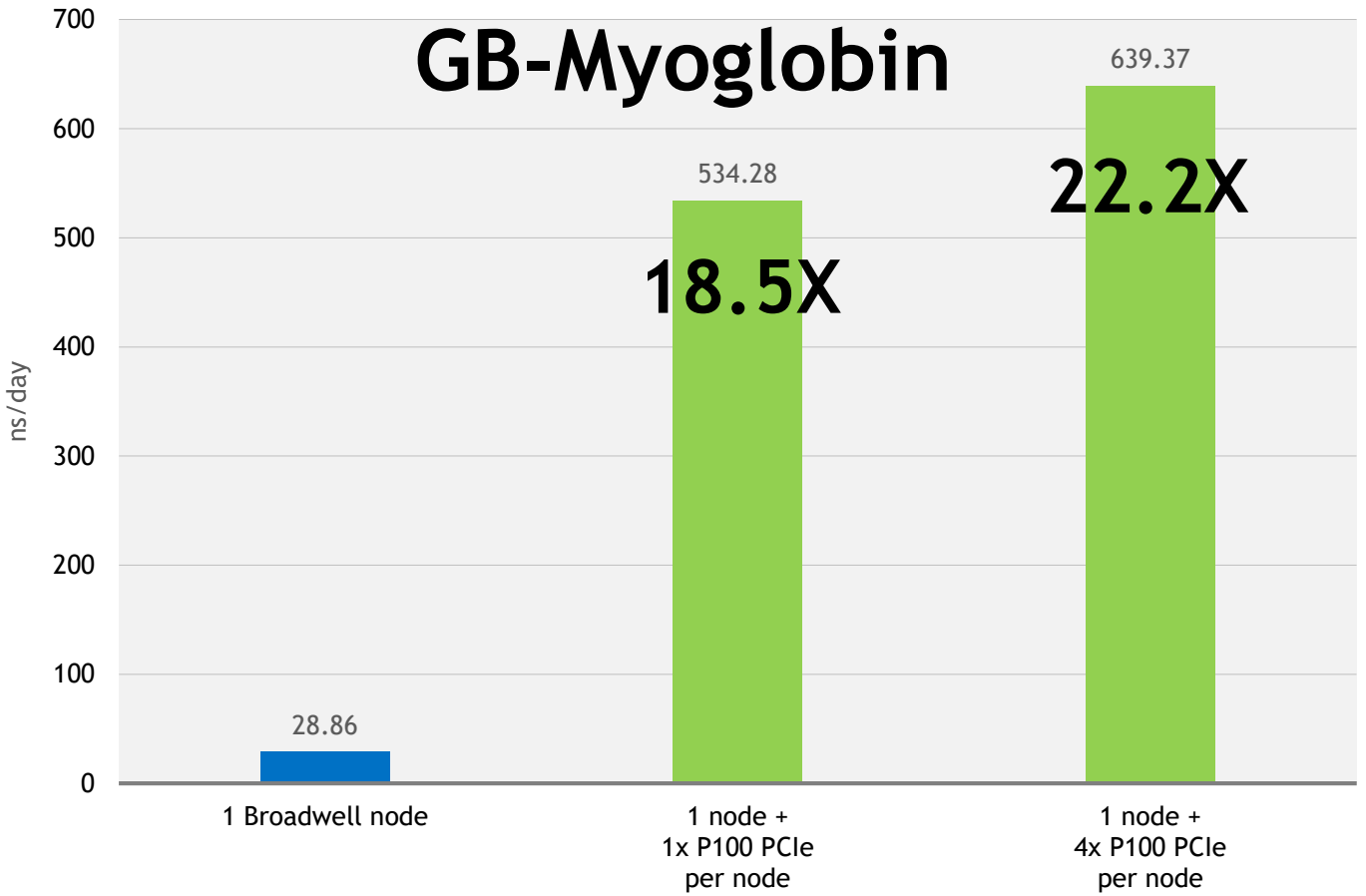
GB-Myoglobin on P100s SXM2



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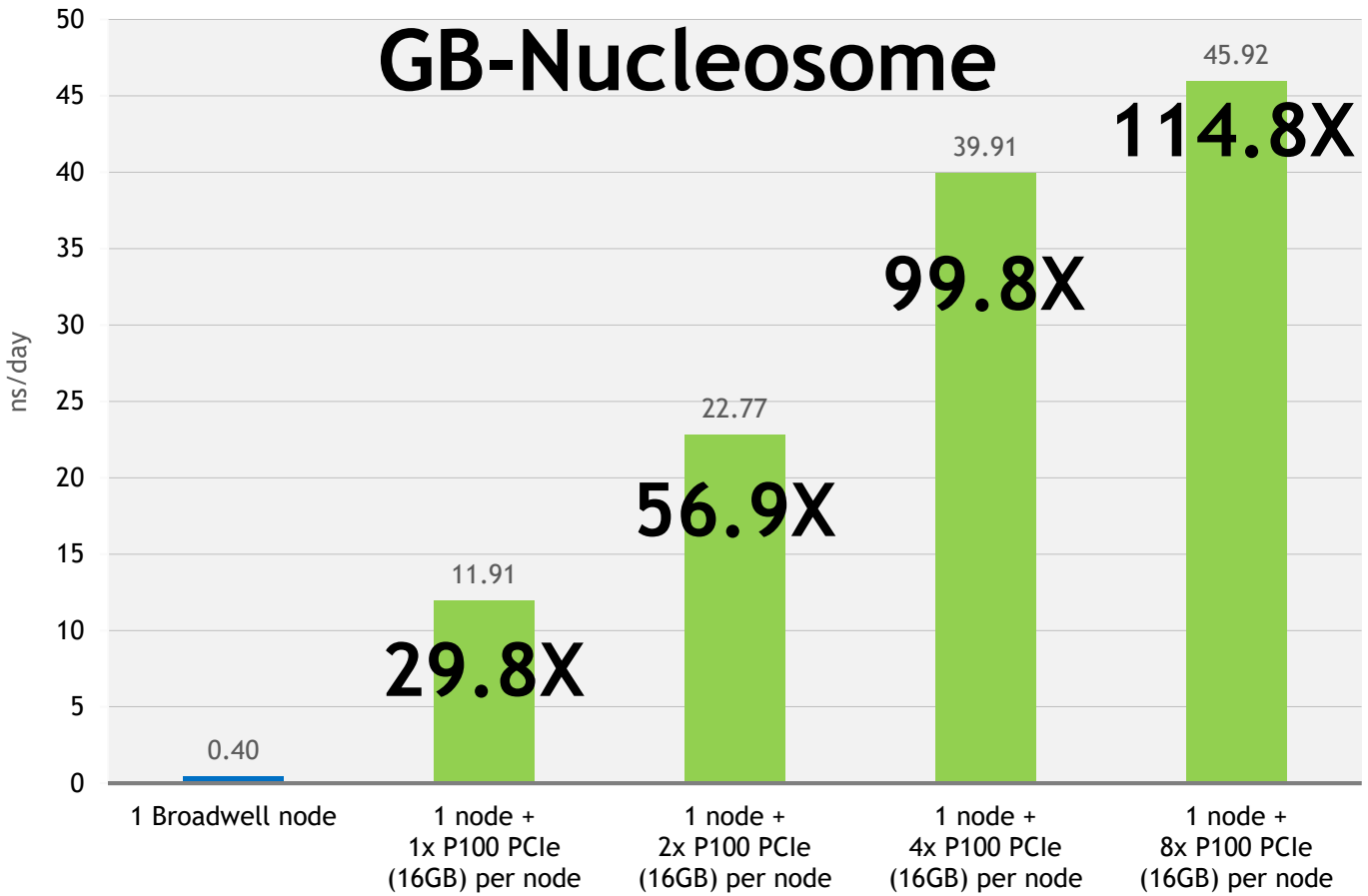
GB-Nucleosome on P100s PCIe



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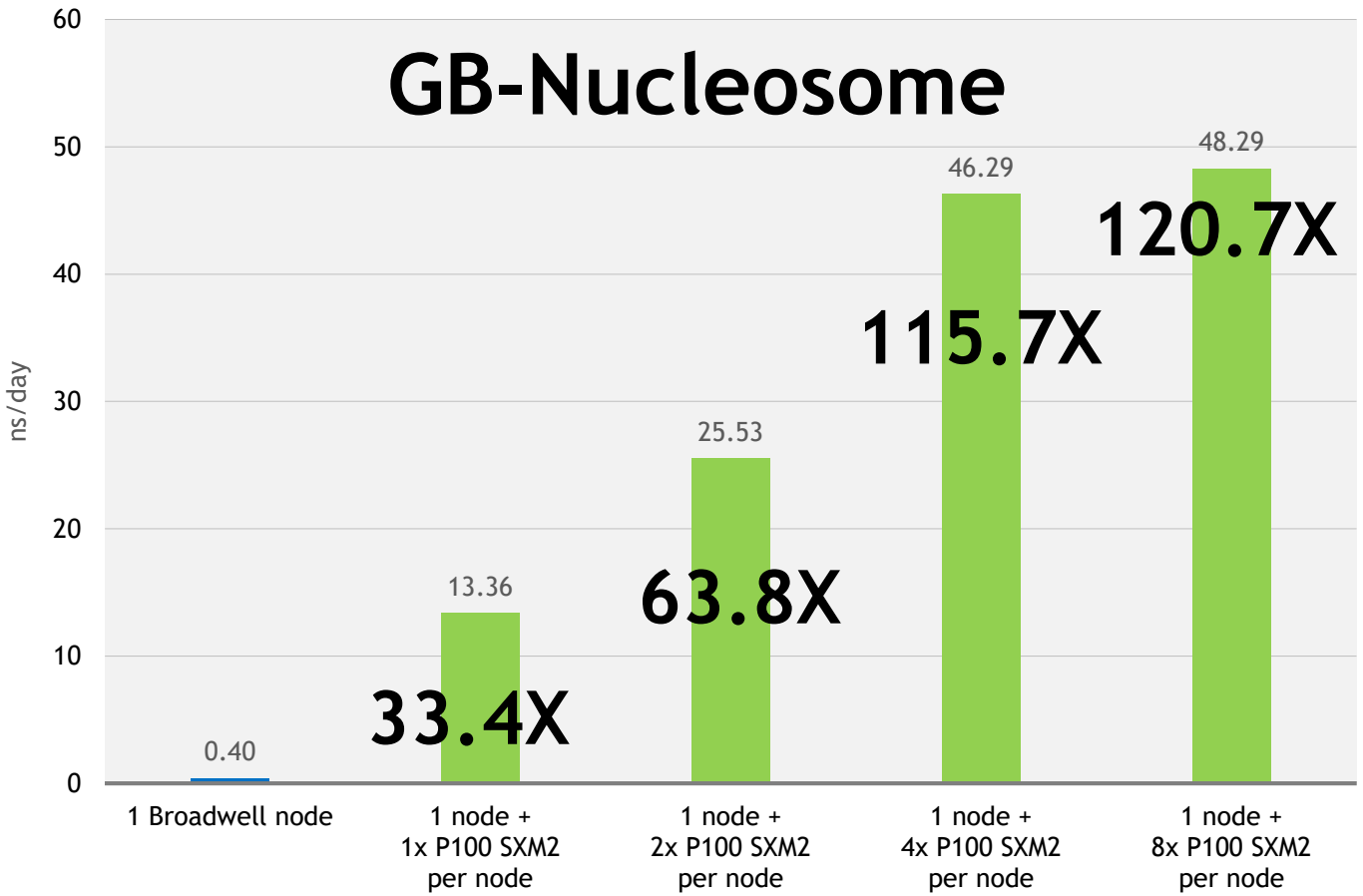
- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

GB-Nucleosome on P100s SXM2



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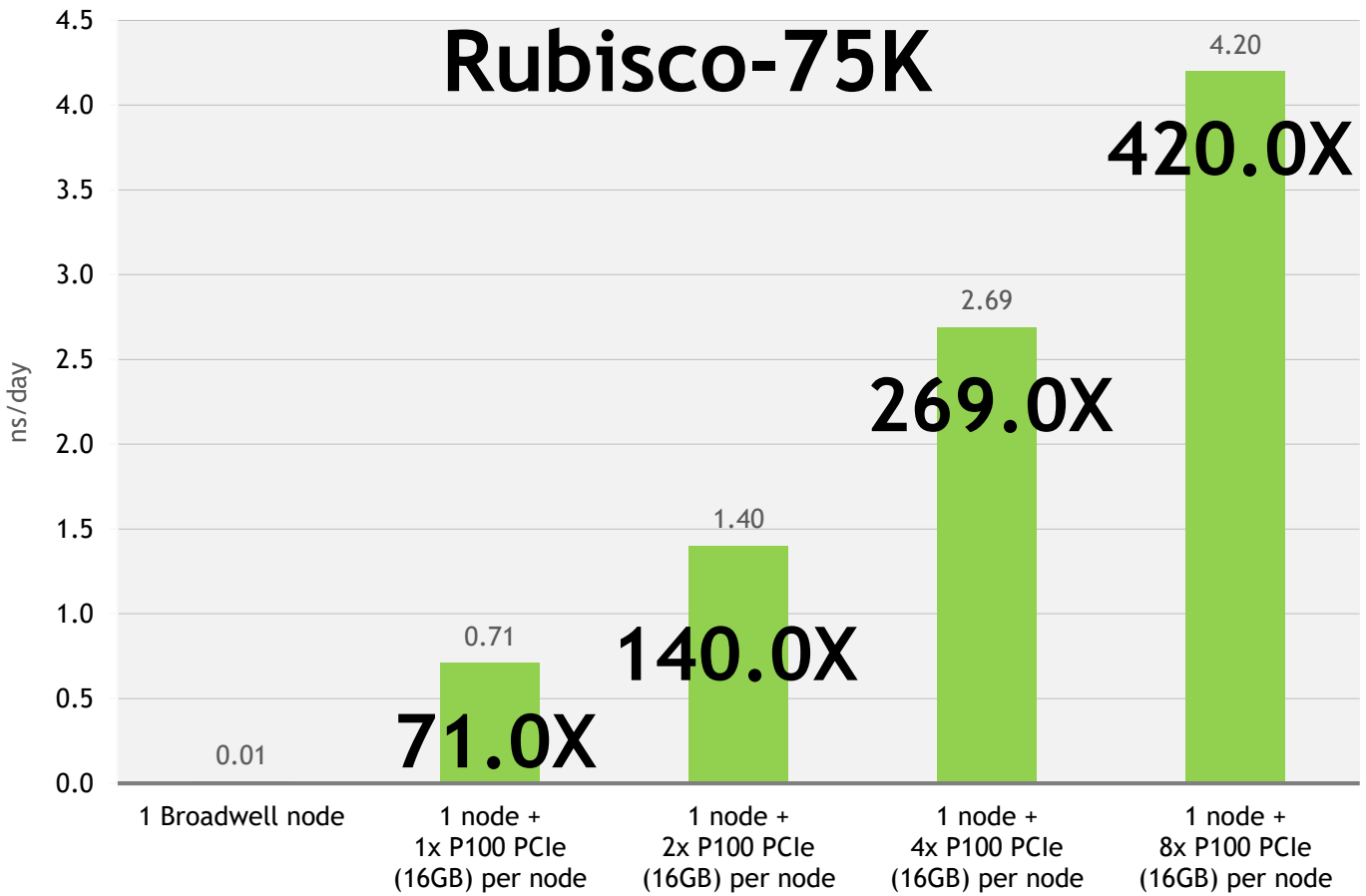
- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

Rubisco-75K on P100s PCIe



Running AMBER version 16.3

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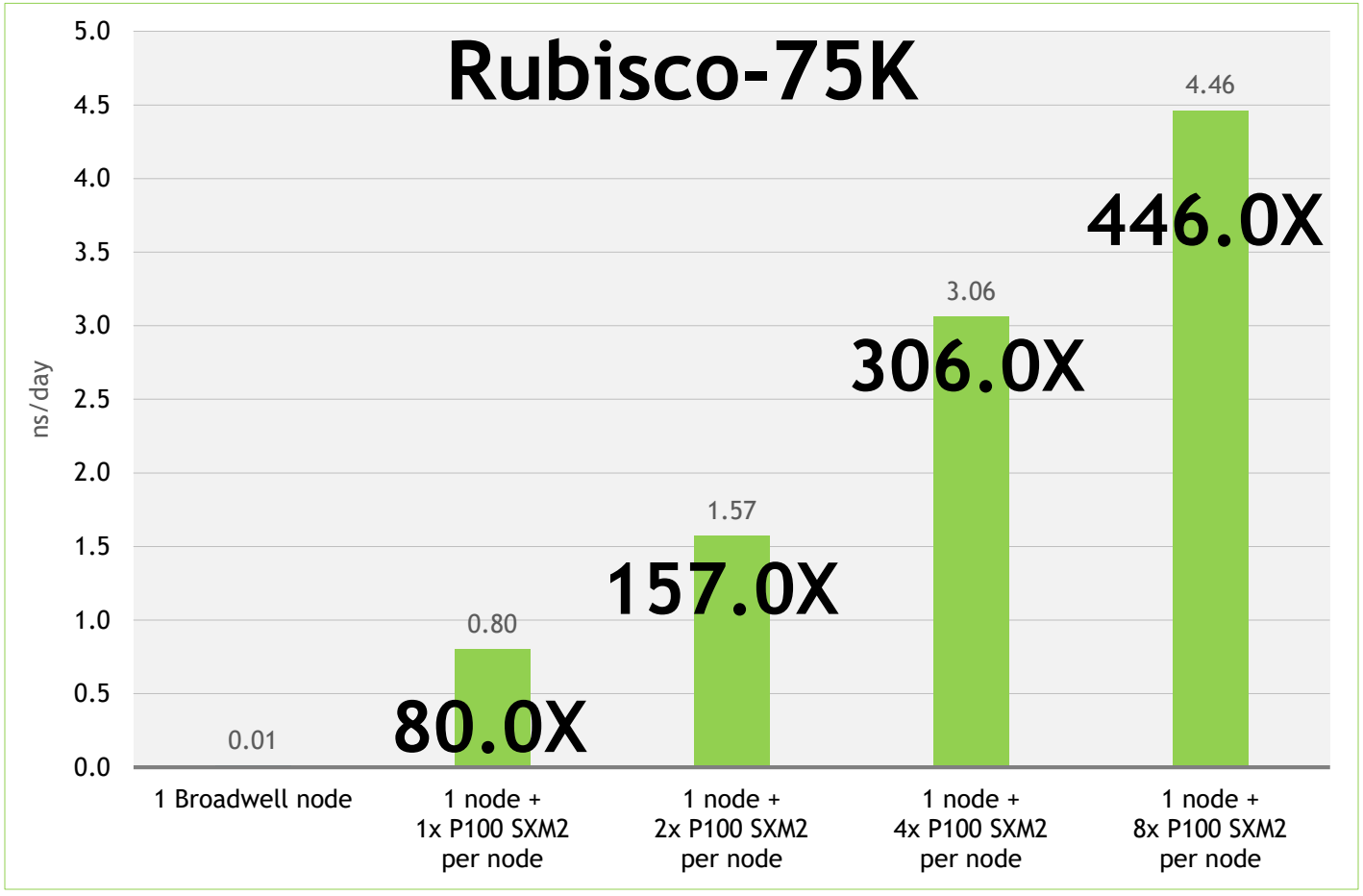
- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

Rubisco-75K on P100s SXM2



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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

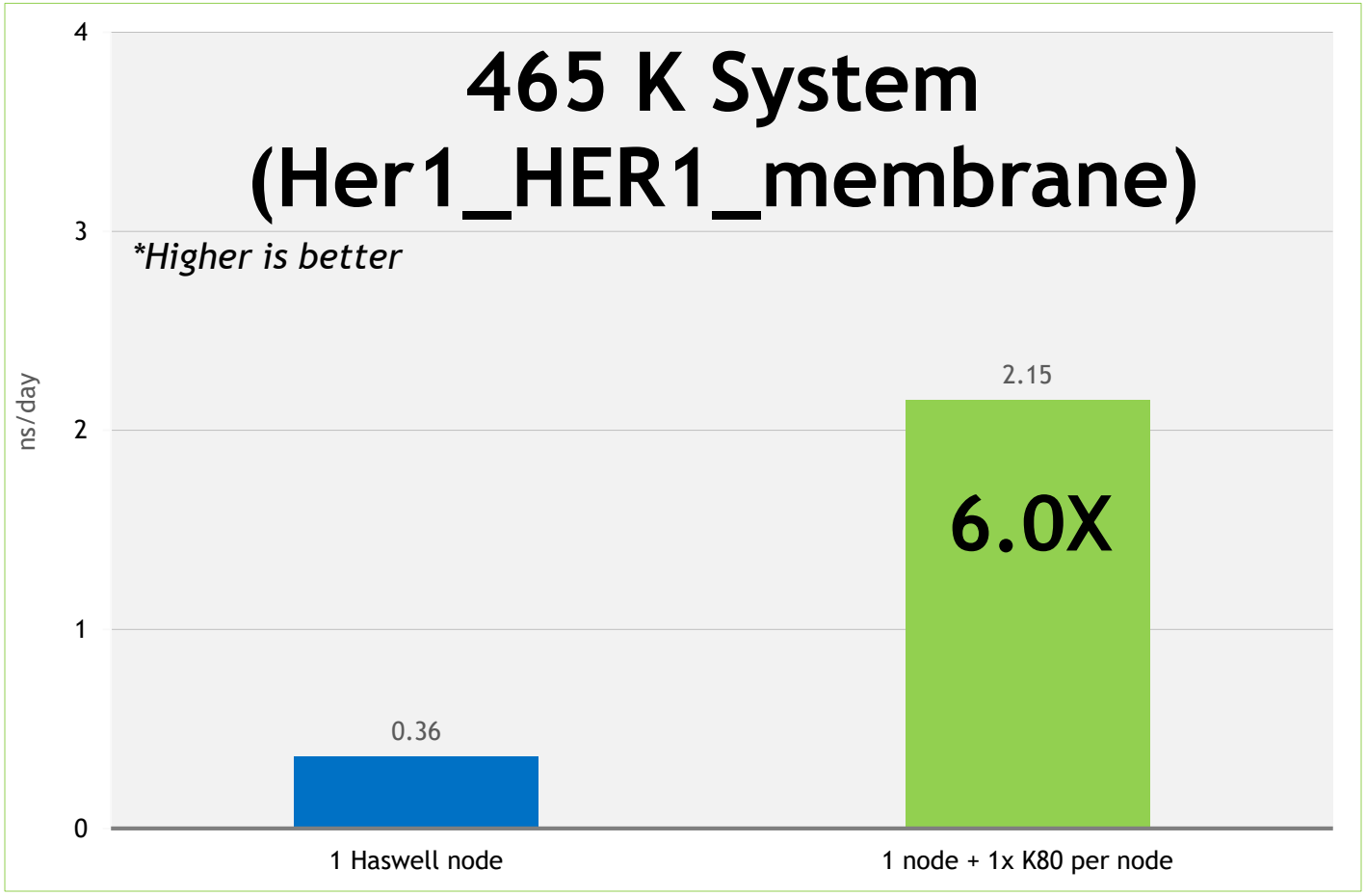
Workstation or Single Node Configuration	
# of CPU sockets	2
Cores per CPU socket	6+ (1 CPU core drives 1 GPU)
CPU speed (Ghz)	2.66+
System memory per node (GB)	16
GPUs	P100, V100
# of GPUs per CPU socket	1-4
GPU memory preference (GB)	6
GPU to CPU connection	PCIe 3.0 16x or higher
Server storage	2 TB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

Scale to multiple nodes with same single node configuration

CHARMM DOMDEC-GUI

July 2016

CHARMM DOMDEC-GUI 465 K System Benchmark



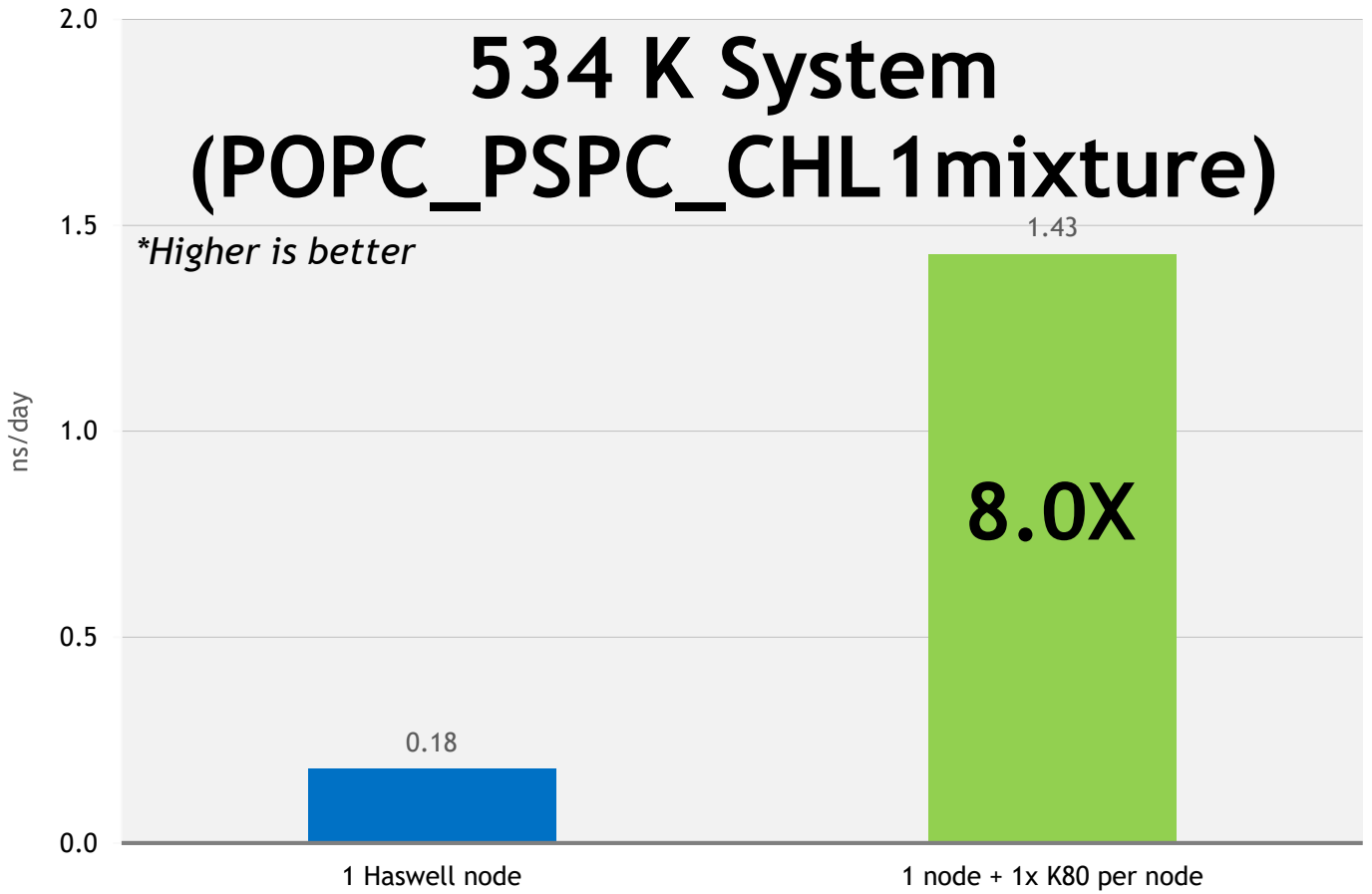
Running CHARMM version c40a1

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.

CHARMM DOMDEC-GUI 534 K System Benchmark



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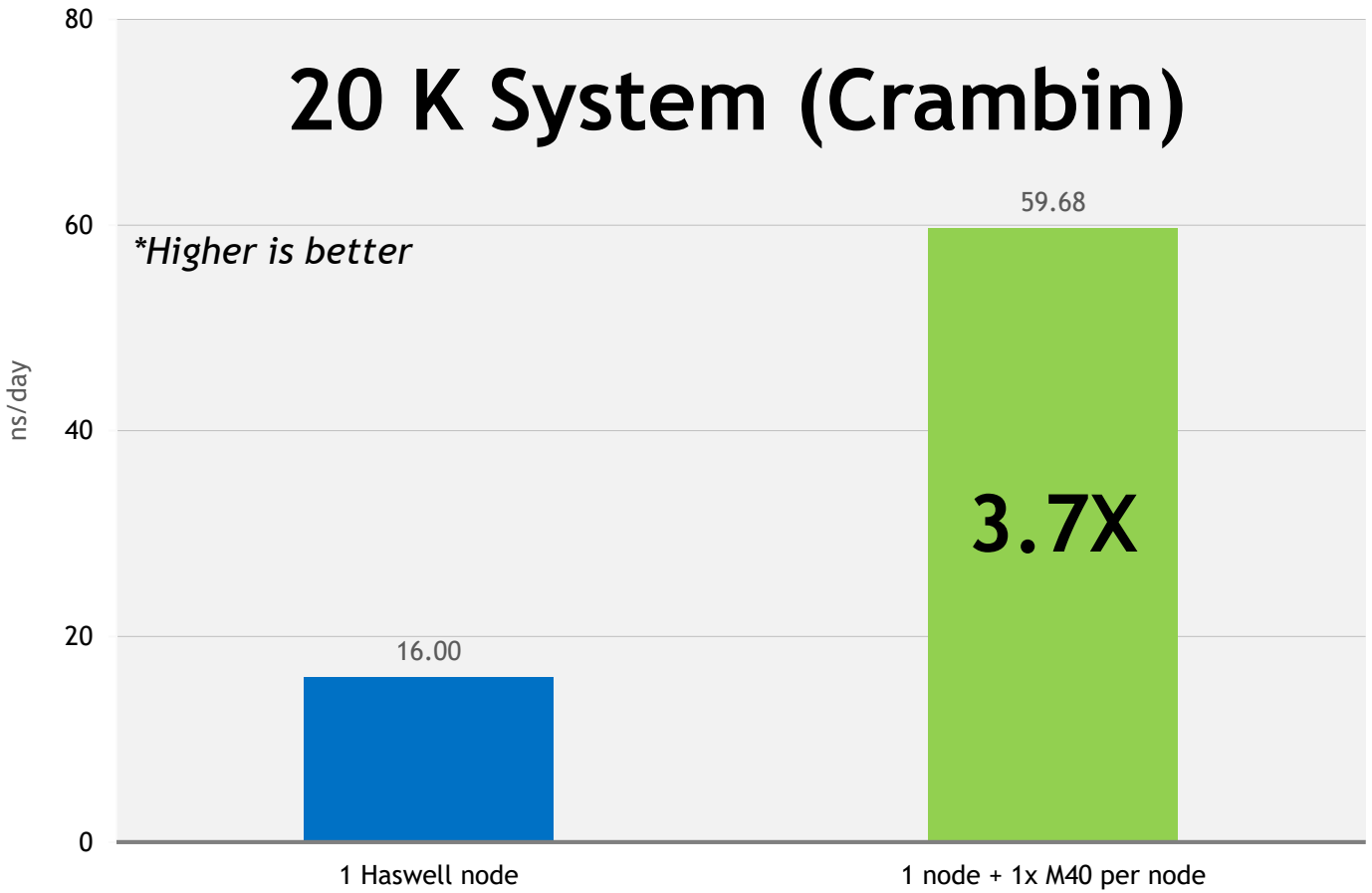
CHARMM DOMDEC-GUI 20 K System Benchmark



Running CHARMM version c40a1

The blue node contains Dual Intel Xeon E5-2698 v3@2.30 GHz (Haswell) CPUs

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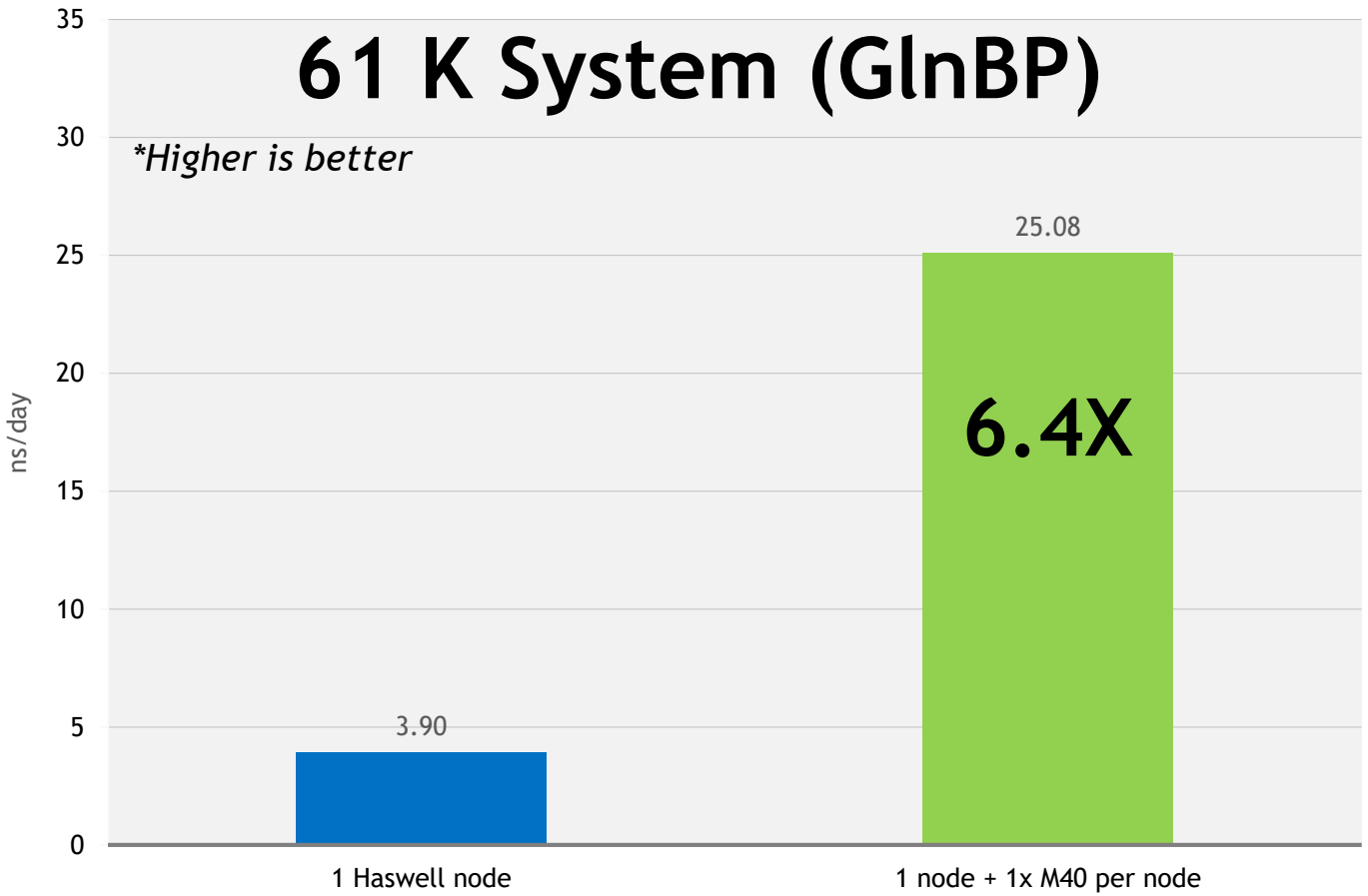
CHARMM DOMDEC-GUI 61 K System Benchmark



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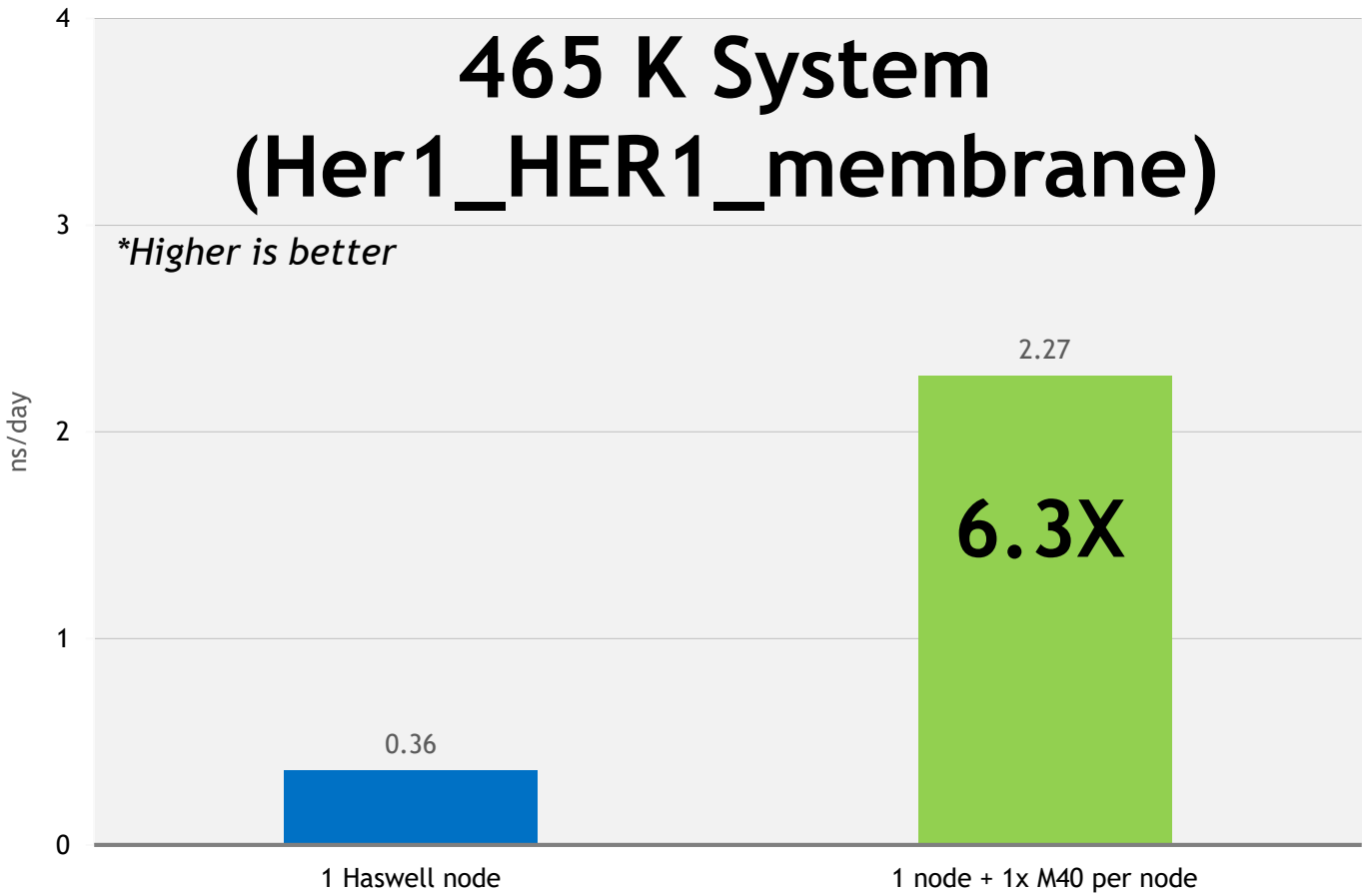
CHARMM DOMDEC-GUI 465 K System Benchmark



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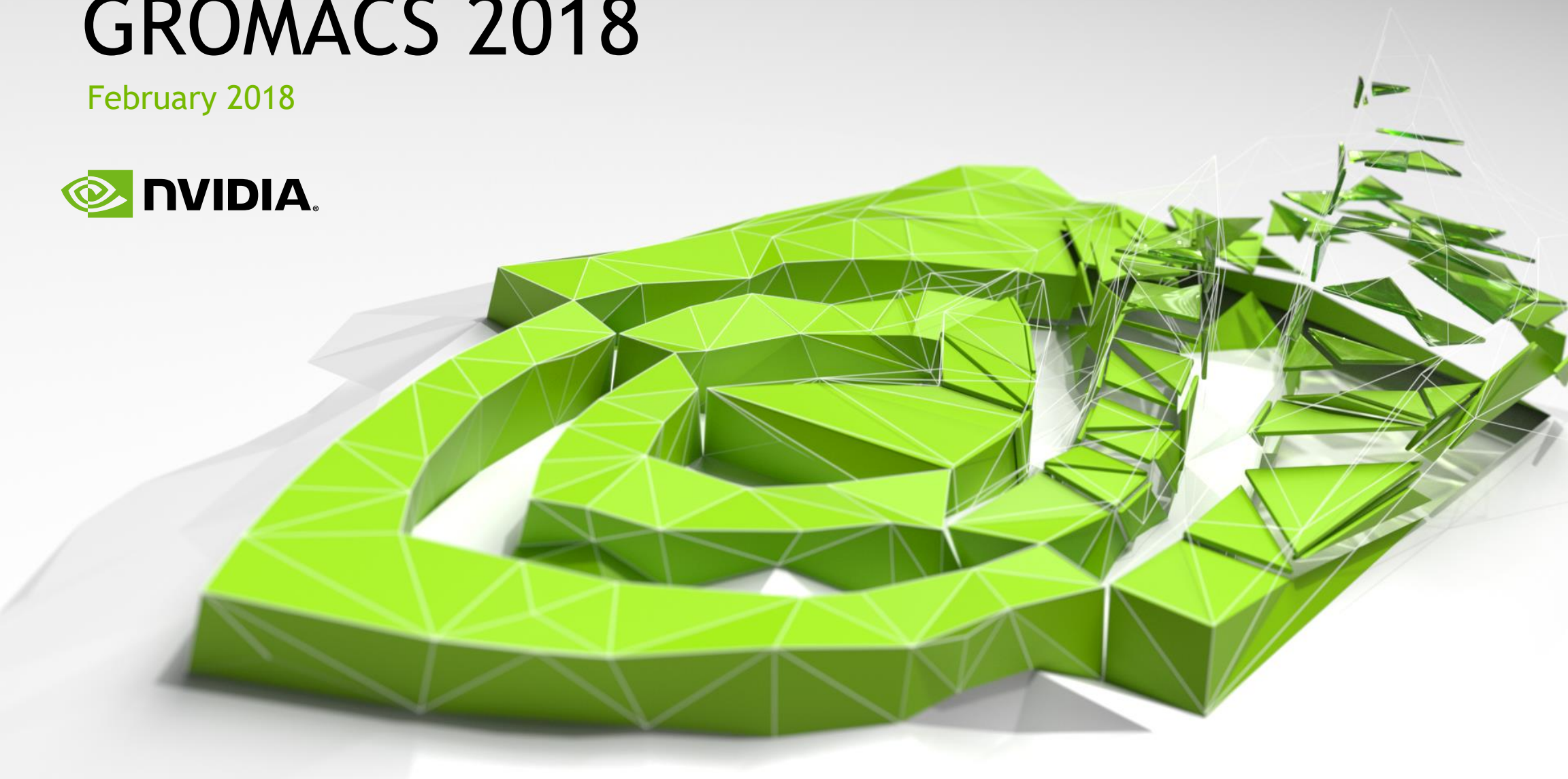
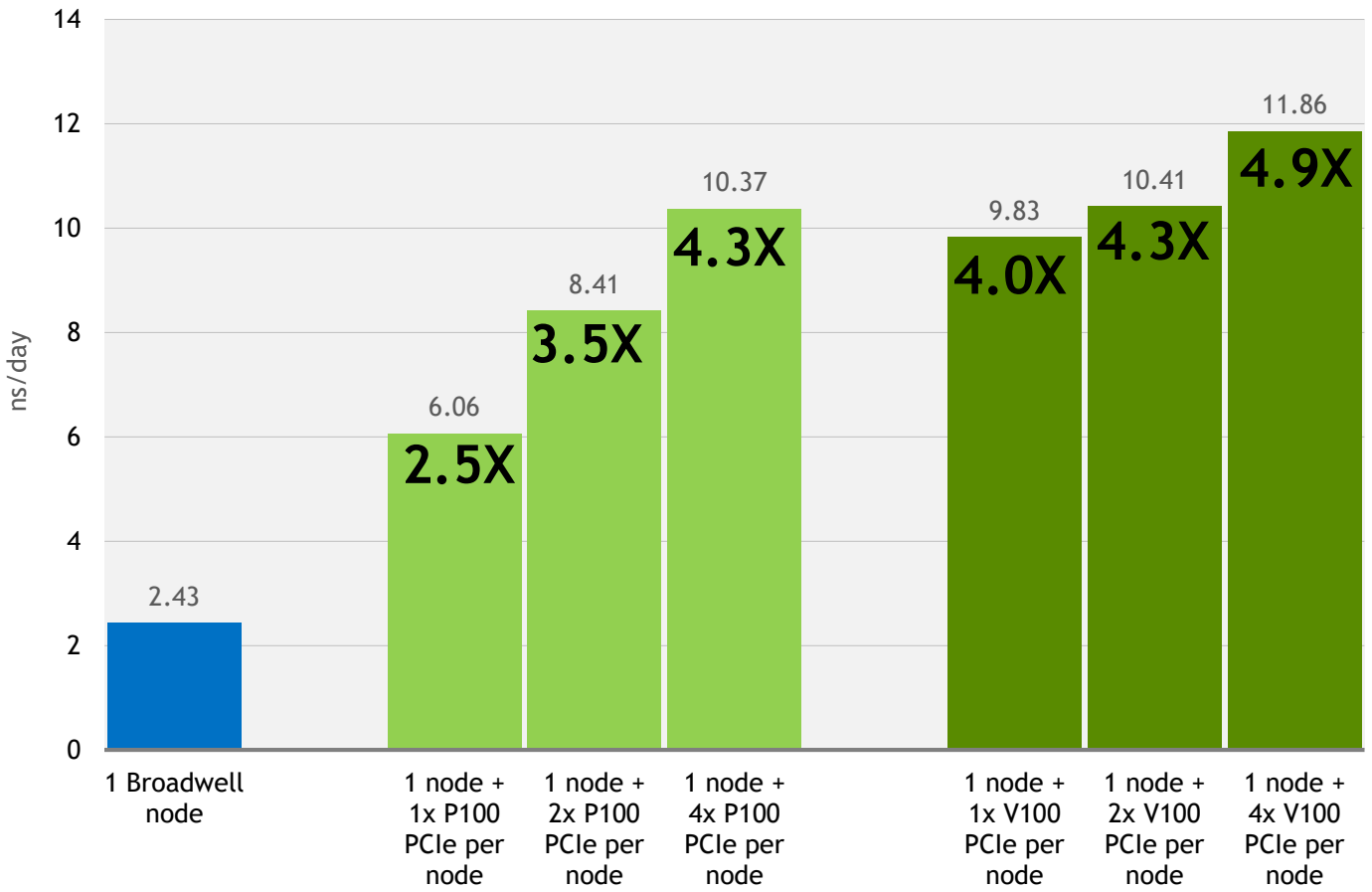
GROMACS 2018

February 2018



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



(Untuned on Volta)
Running GROMACS version 2018

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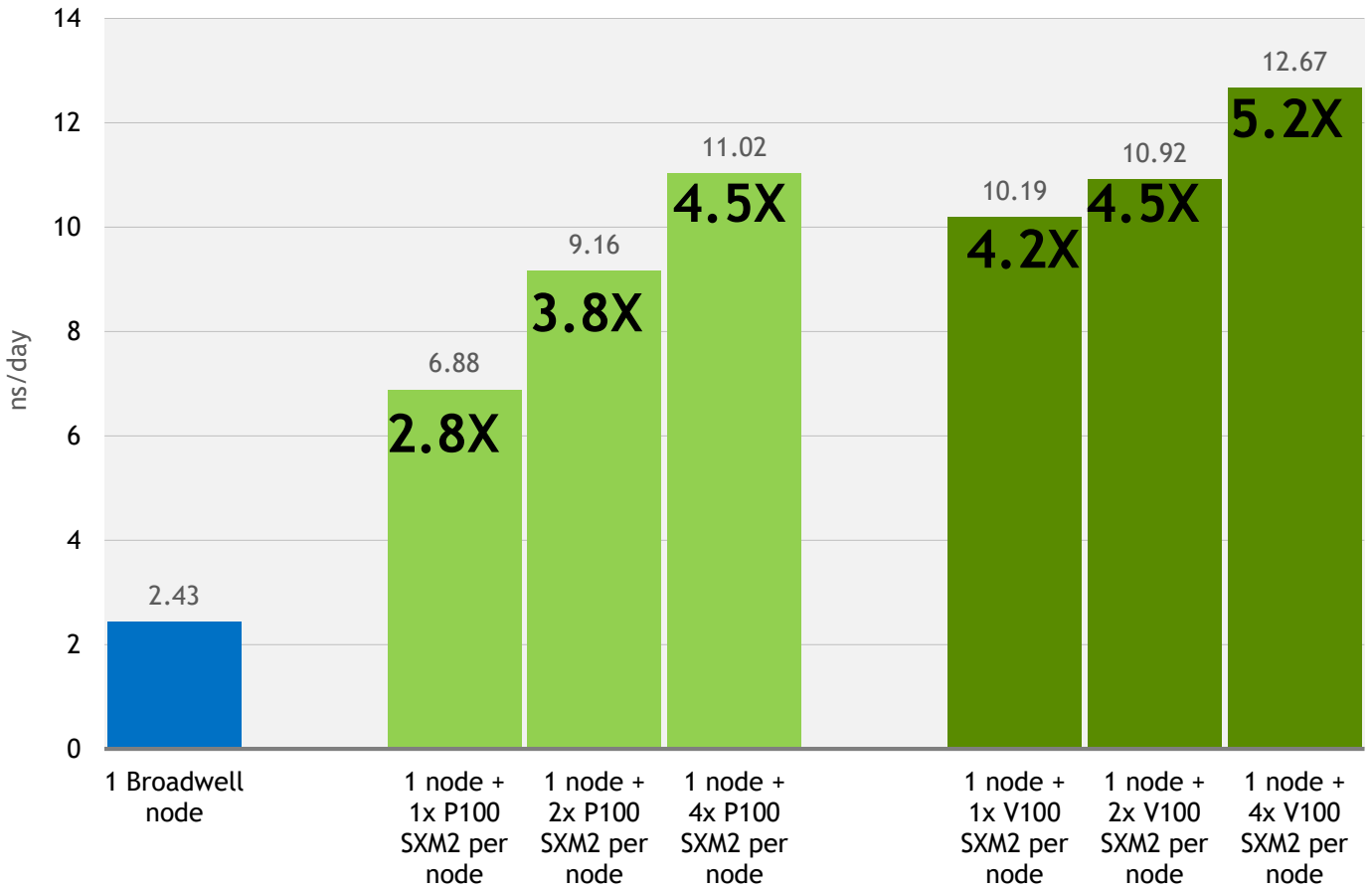
The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe (16GB) or V100 PCIe (16GB) GPUs

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



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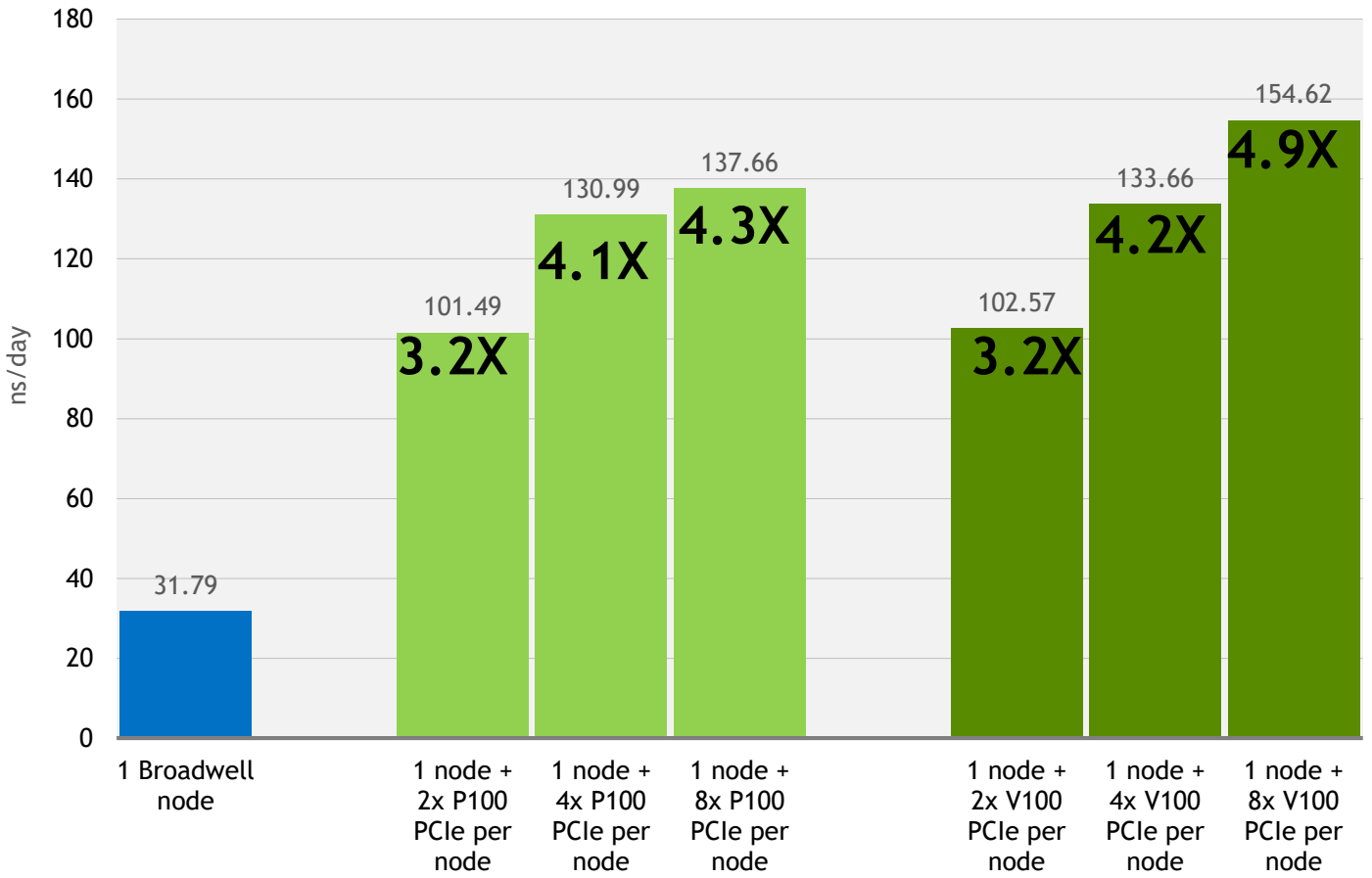
GROMACS ADH Dodec
on V100 vs P100 (PCIe 16GB)



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GROMACS ADH Dodec
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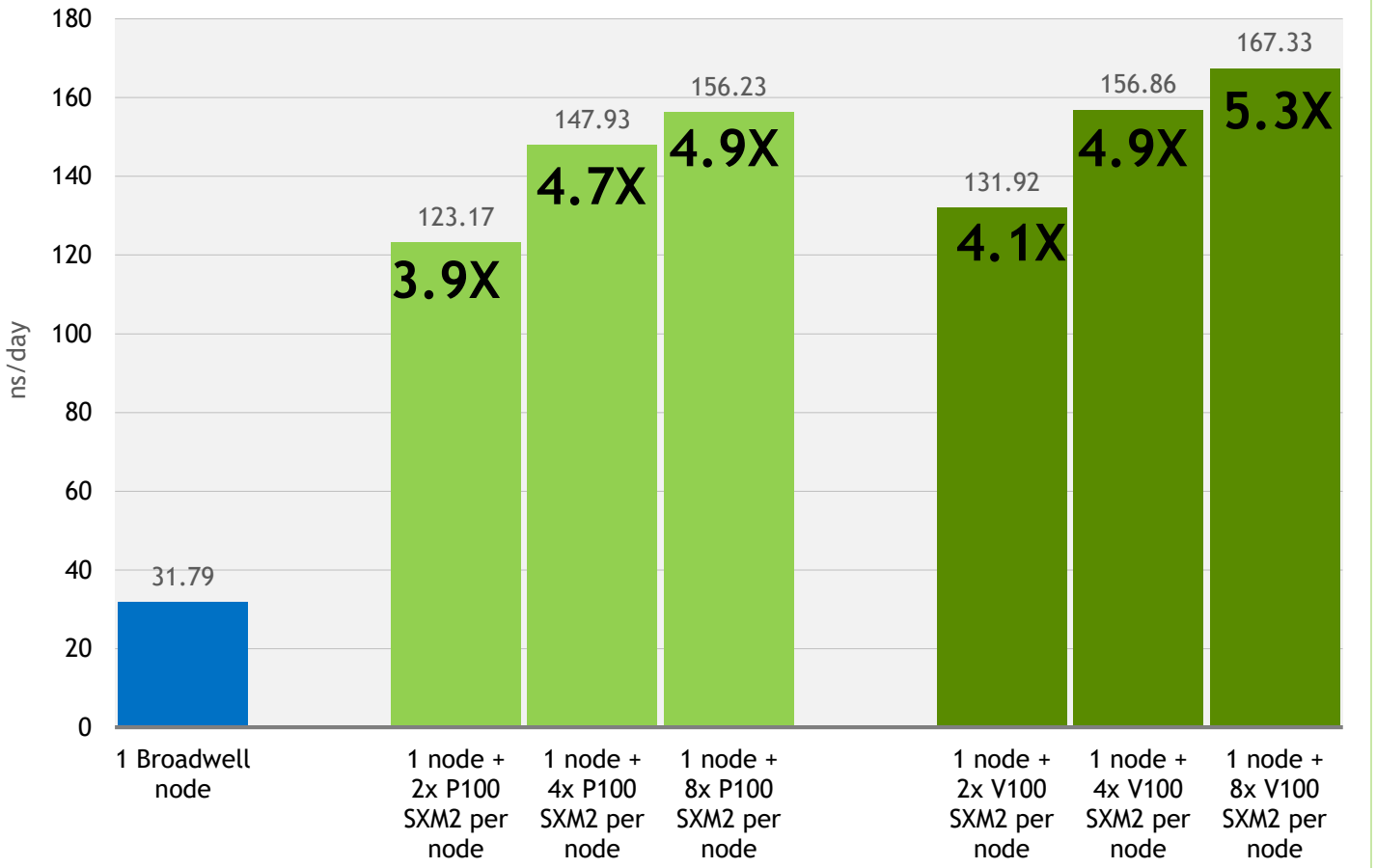

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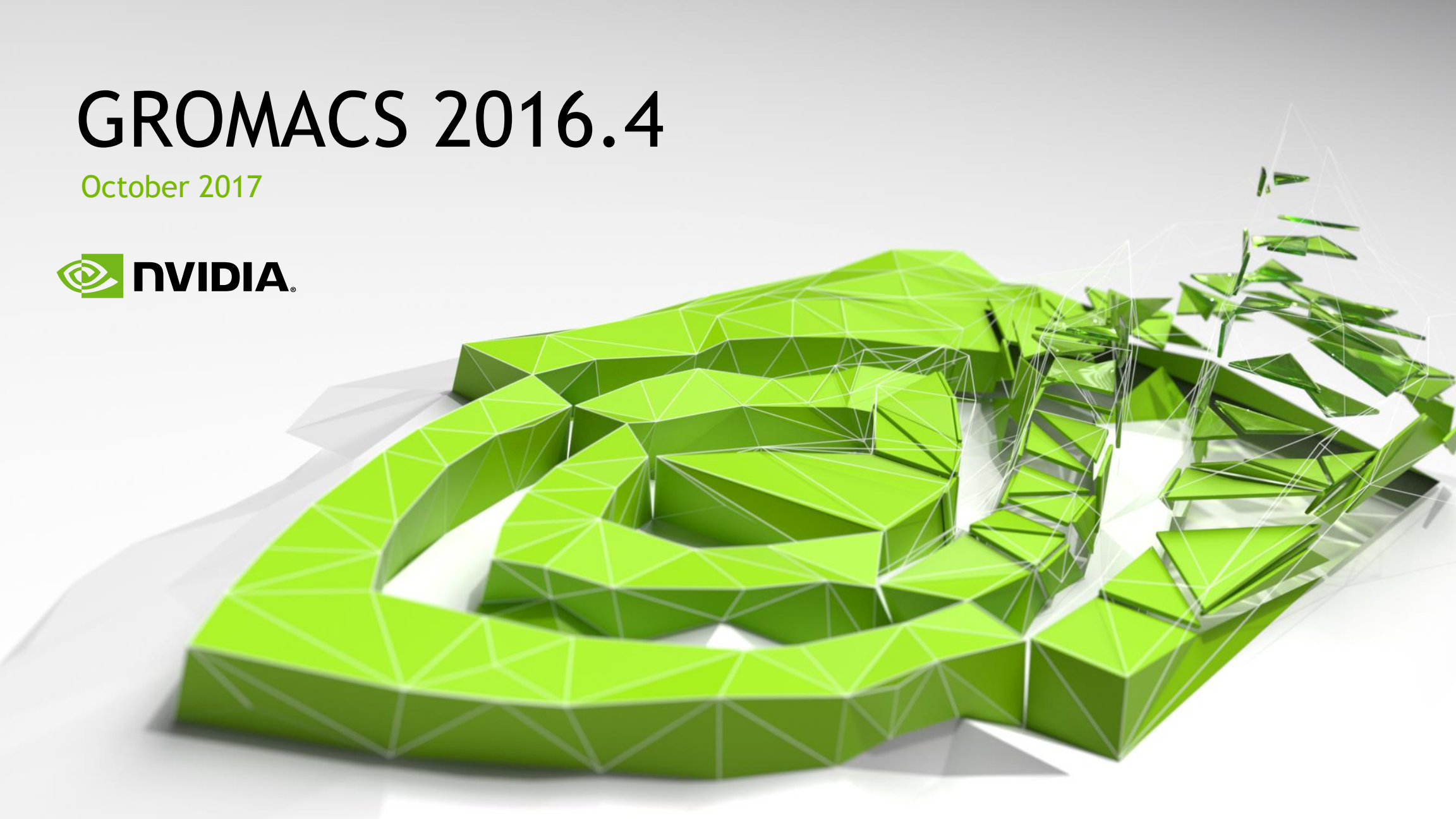
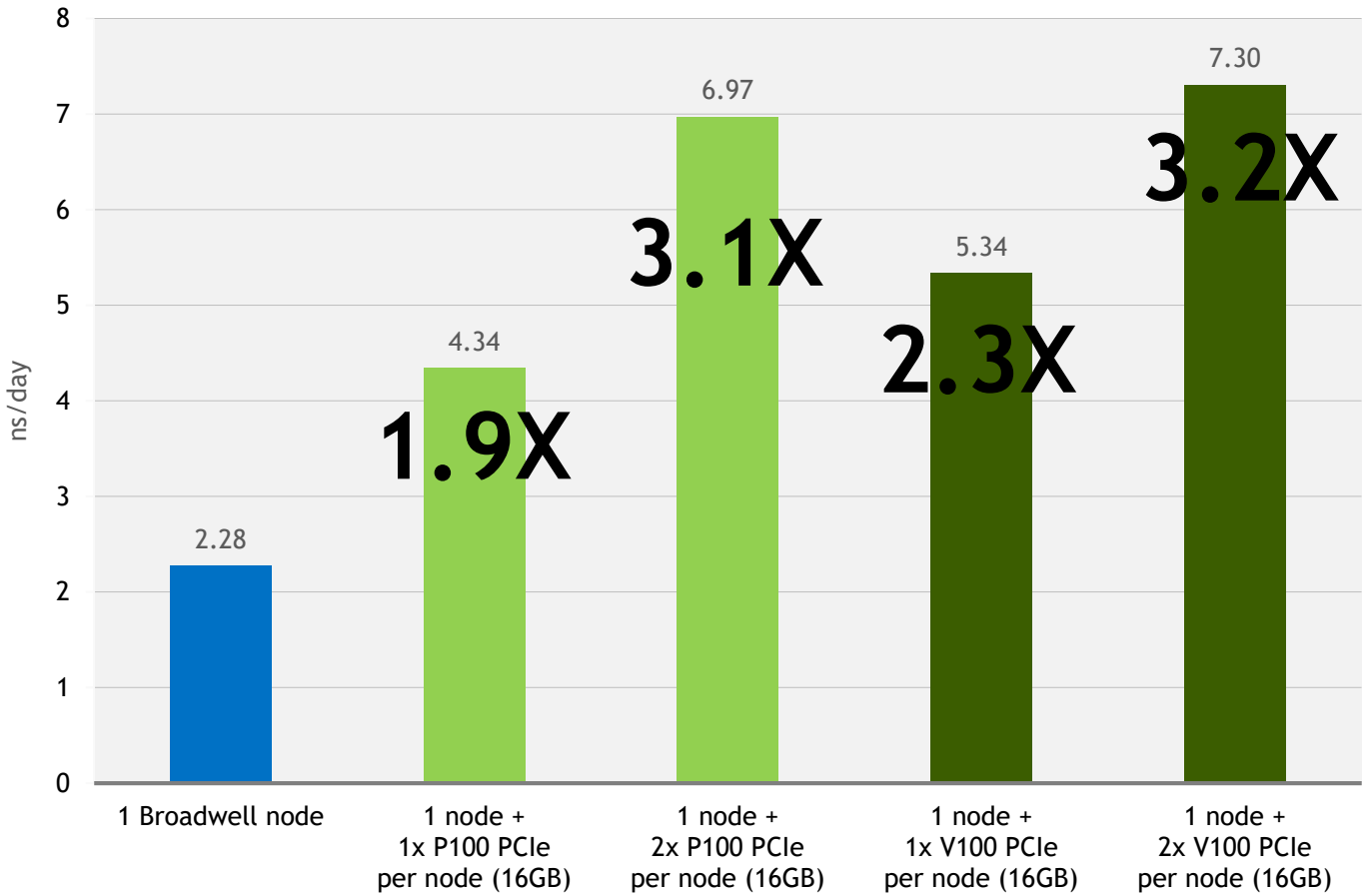
GROMACS 2016.4

October 2017



Water 1.5M on V100 vs P100 (PCIe)

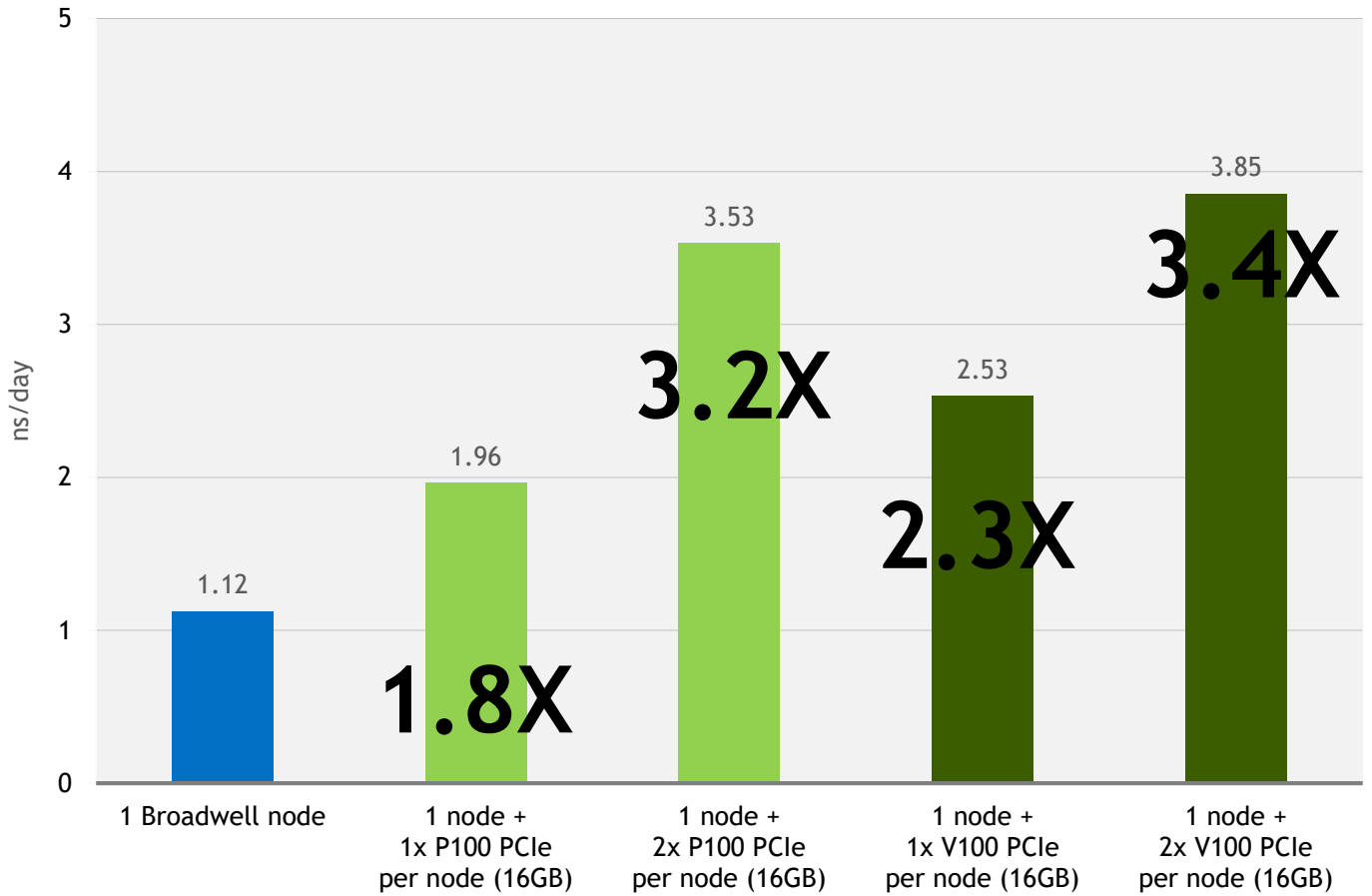


(Untuned on Volta)
Running GROMACS version 2016.4

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)



(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

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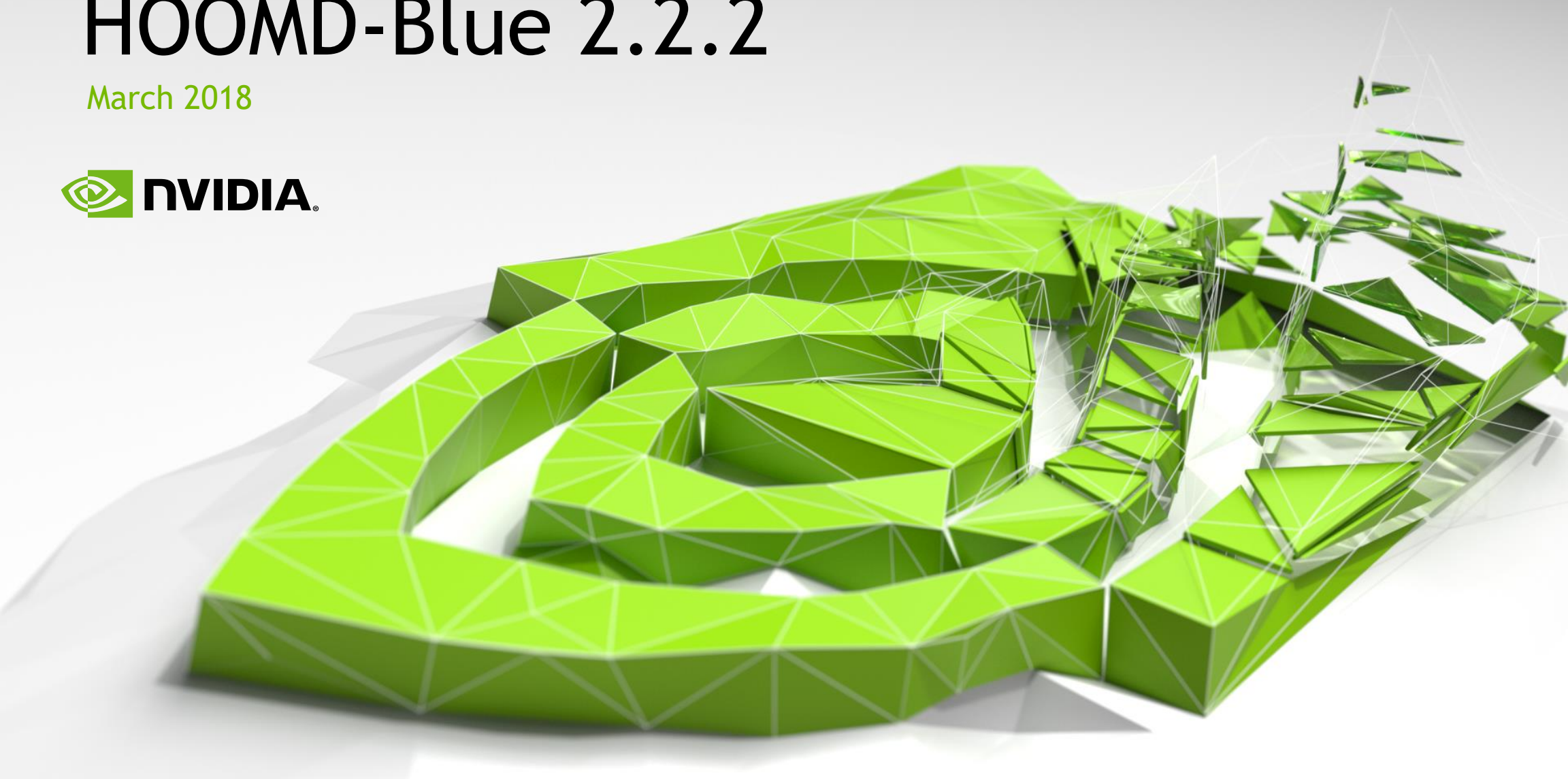
Recommended GPU Node Configuration for GROMACS Computational Chemistry

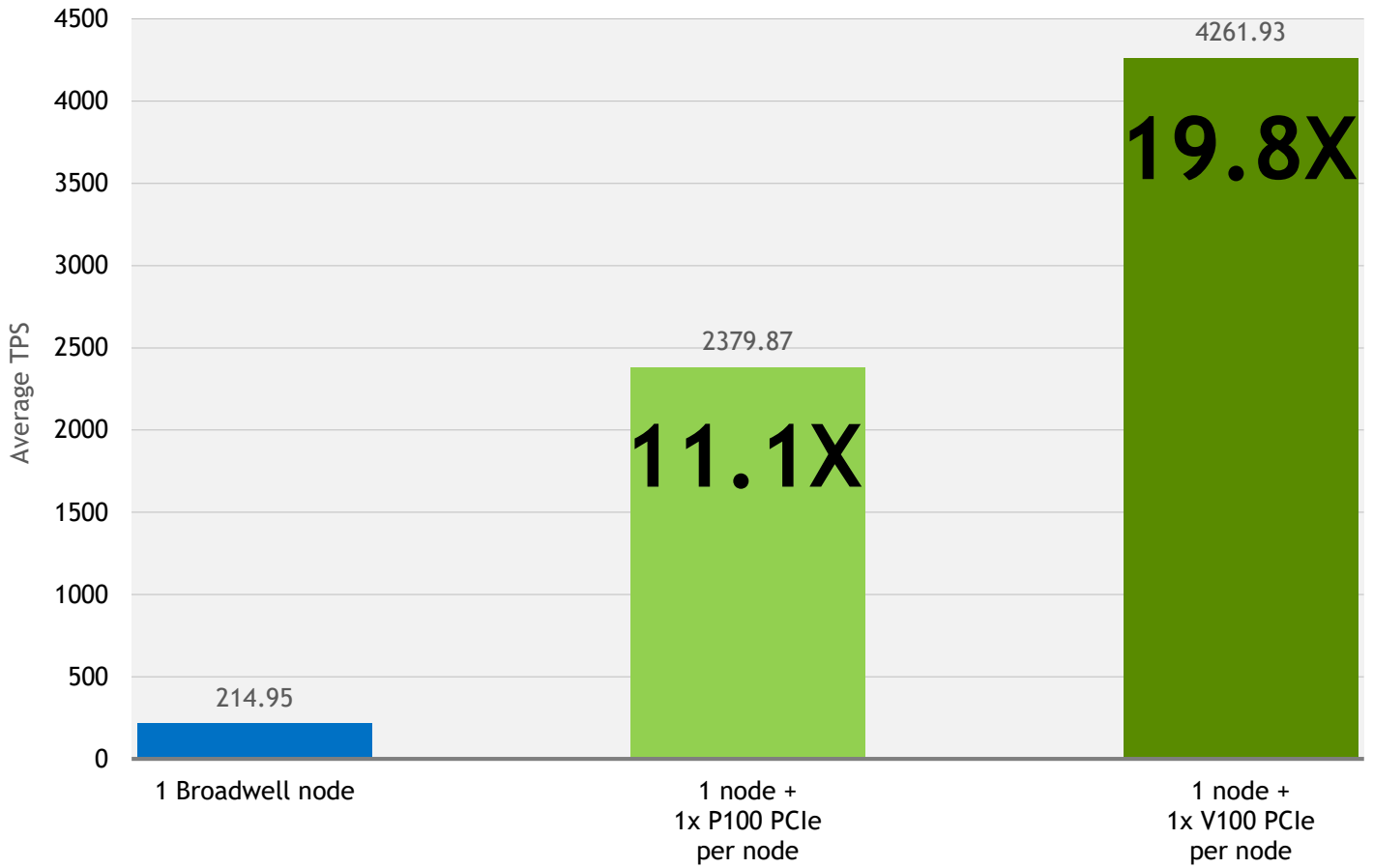
Workstation or Single Node Configuration	
# of CPU sockets	2
Cores per CPU socket	6+
CPU speed (Ghz)	2.66+
System memory per socket (GB)	32
GPUs	Tesla P100, V100
# of GPUs per CPU socket	2x Volta GPUs: need fast Skylake or Broadwell
GPU memory preference (GB)	6
GPU to CPU connection	PCIe 3.0 or higher
Server storage	500 GB or higher
Network configuration	Gemini, InfiniBand

HOOMD-Blue 2.2.2

March 2018



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



Running HOOMD-Blue version 2.2.2

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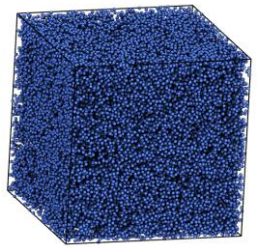
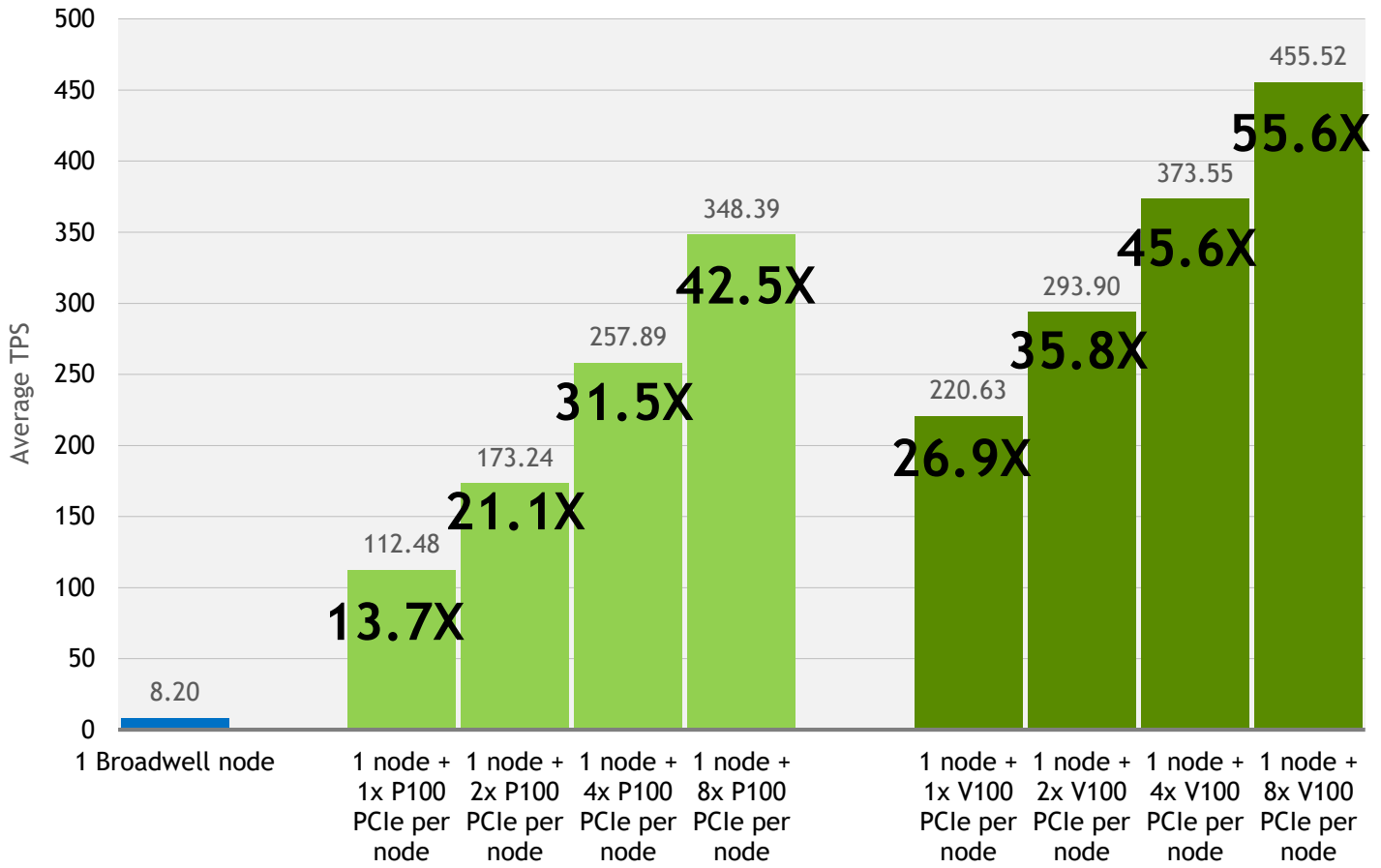
The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe (16GB) or V100 PCIe (16GB) GPUs

64,000 particles
Force field/method: Lennard-Jones MD
This is a synthetic benchmark for historical reasons and for making direct comparisons with LAMMPS



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

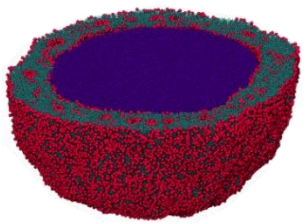


Running HOOMD-Blue version 2.2.2

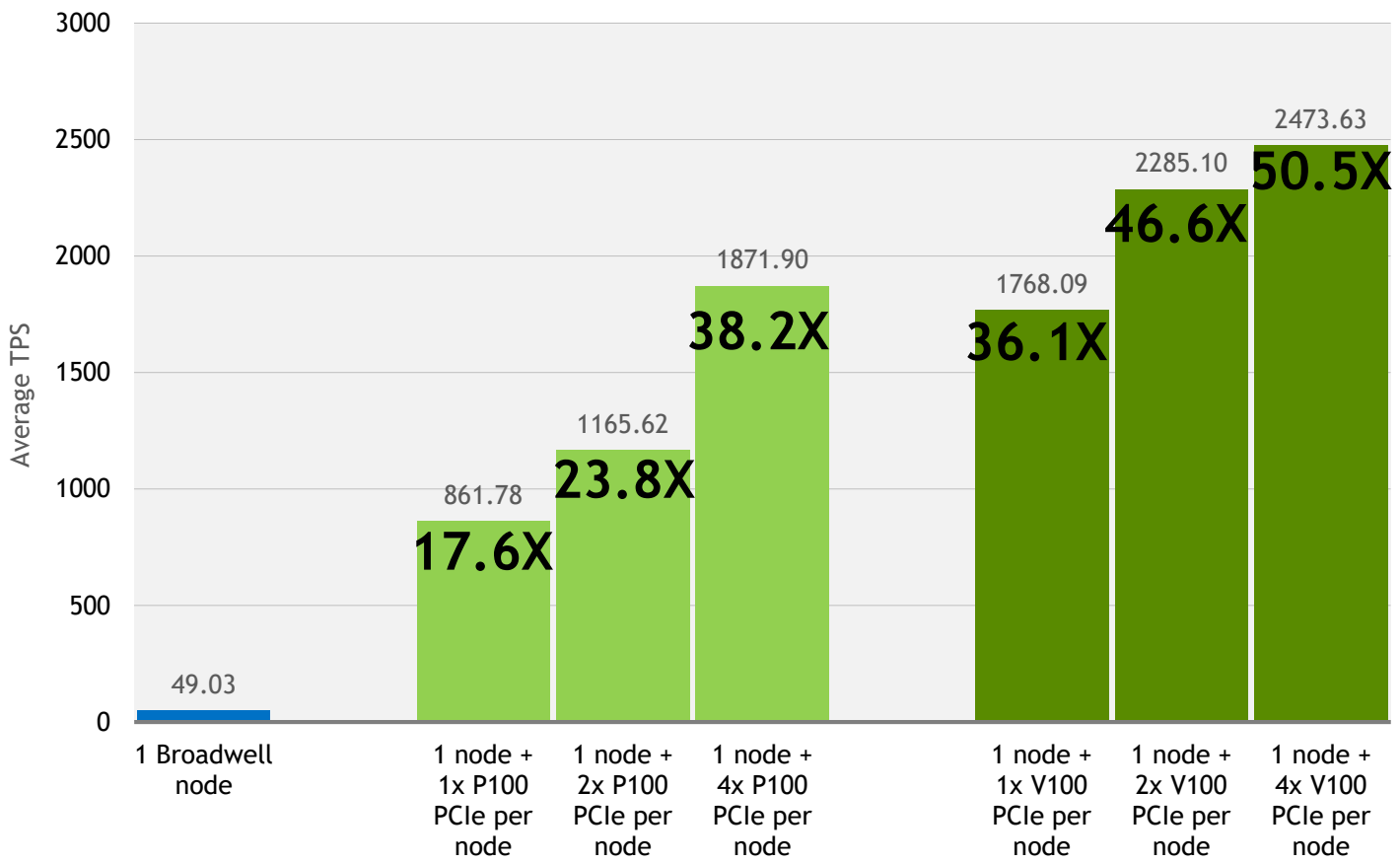
The blue node contains Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs

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 polymbers via dissipative particle dynamics
Results published in:
http://dx.doi.org/10.1002/adma.201501329



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



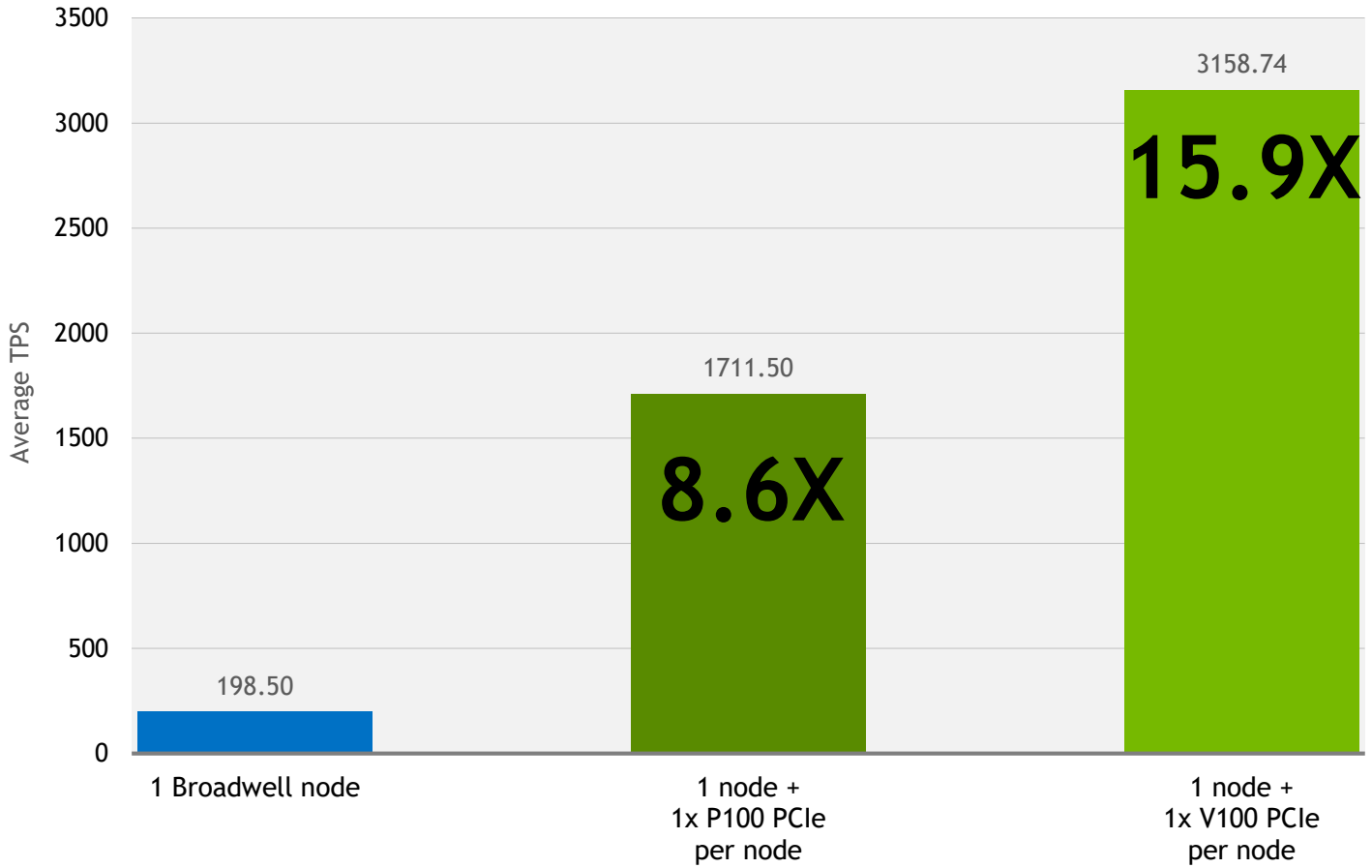
Running HOOMD-Blue version 2.2.2

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

HOOMD-Blue triblock-copolymer
on V100 vs P100 (PCIe 16GB)



Running HOOMD-Blue version 2.2.2

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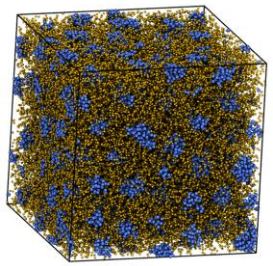
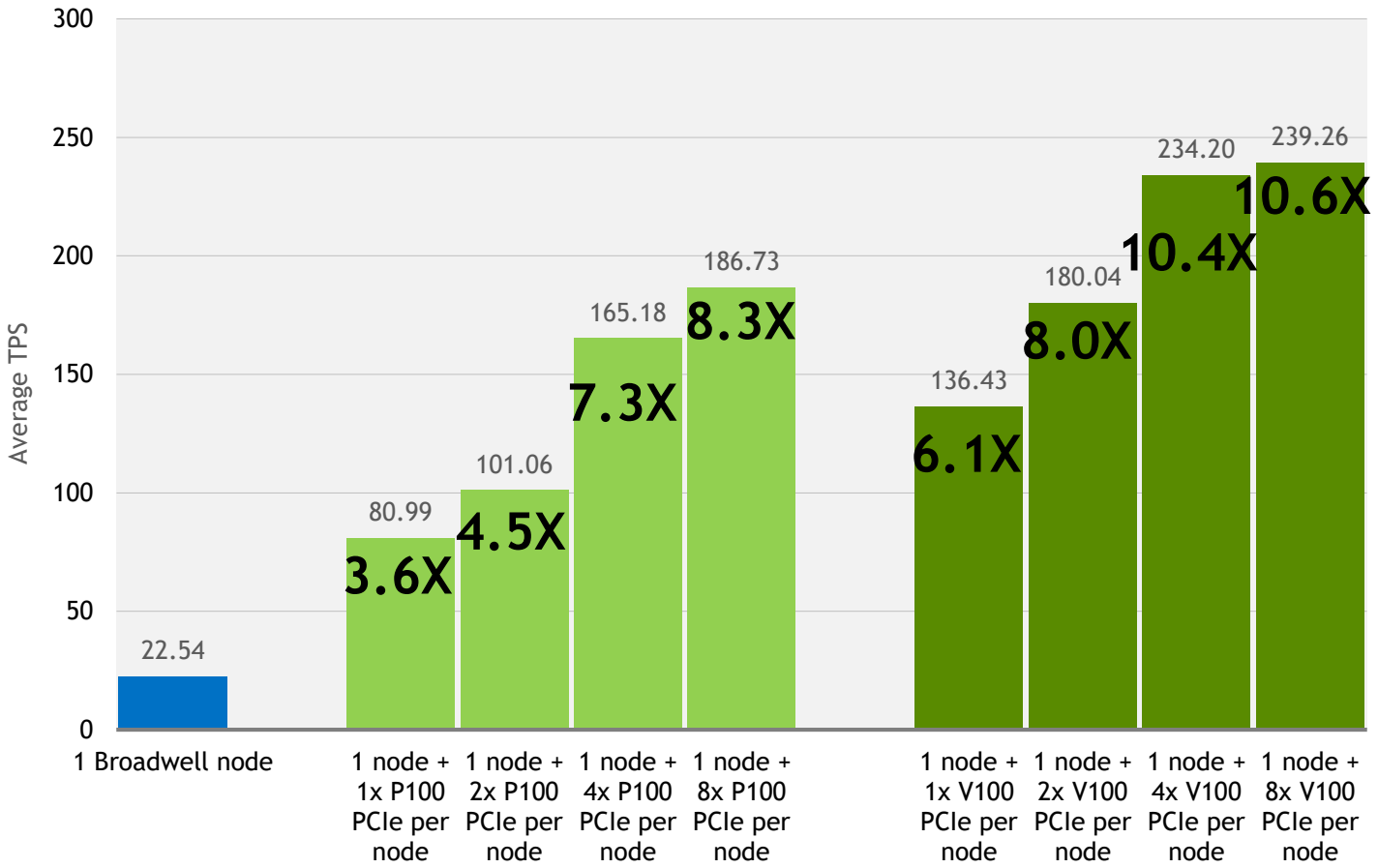
The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe (16GB) or V100 PCIe (16GB) GPUs

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)

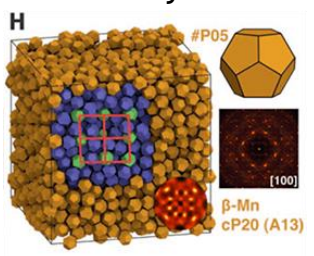


Running HOOMD-Blue version 2.2.2

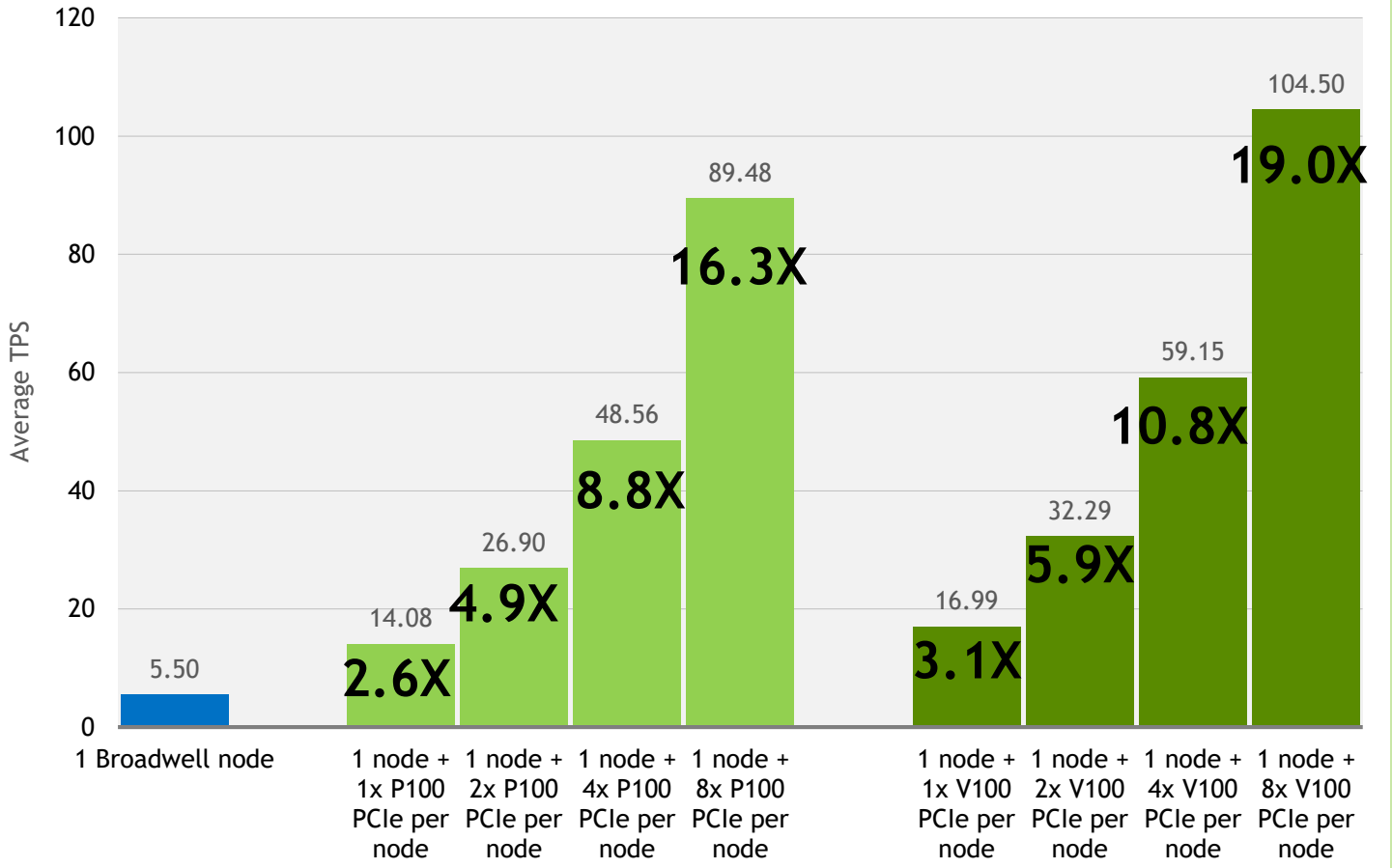
The blue node contains Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs

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 synethic 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

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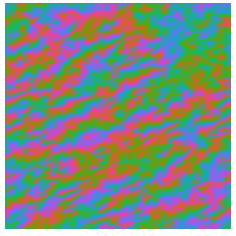
The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe (16GB) or V100 PCIe (16GB) GPUs

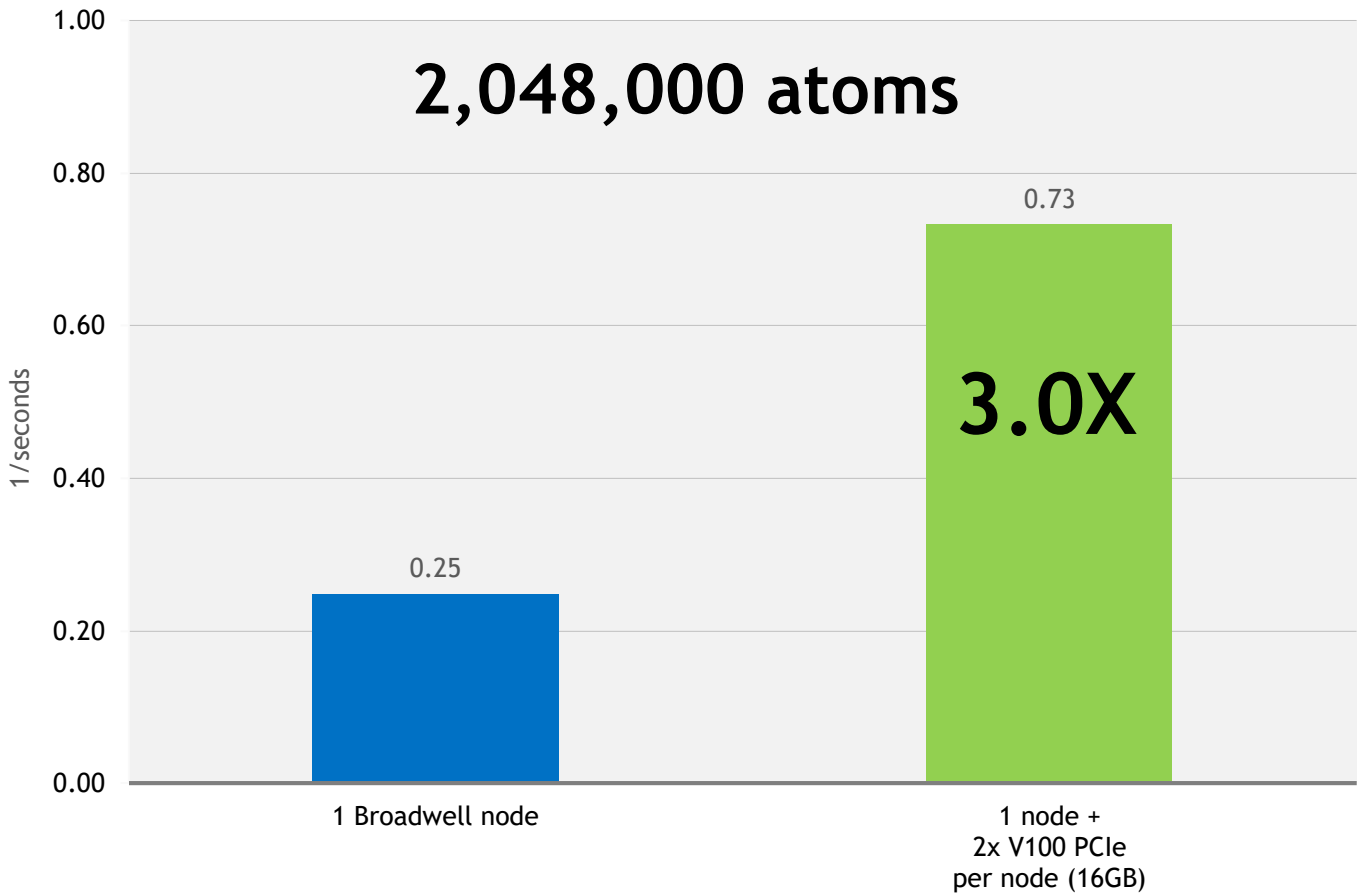
1,048,576 particles
Force field/method: Hard hexagons (via MC simulation)
Results published in:
http://dx.doi.org/10.1103/PhysRevX.7.021001



LAMMPS 2017

October 2017

Atomic-Fluid Lennard-Jones 2.5 Cutoff on V100s PCIe



(Untuned on Volta)
Running LAMMPS version 2017

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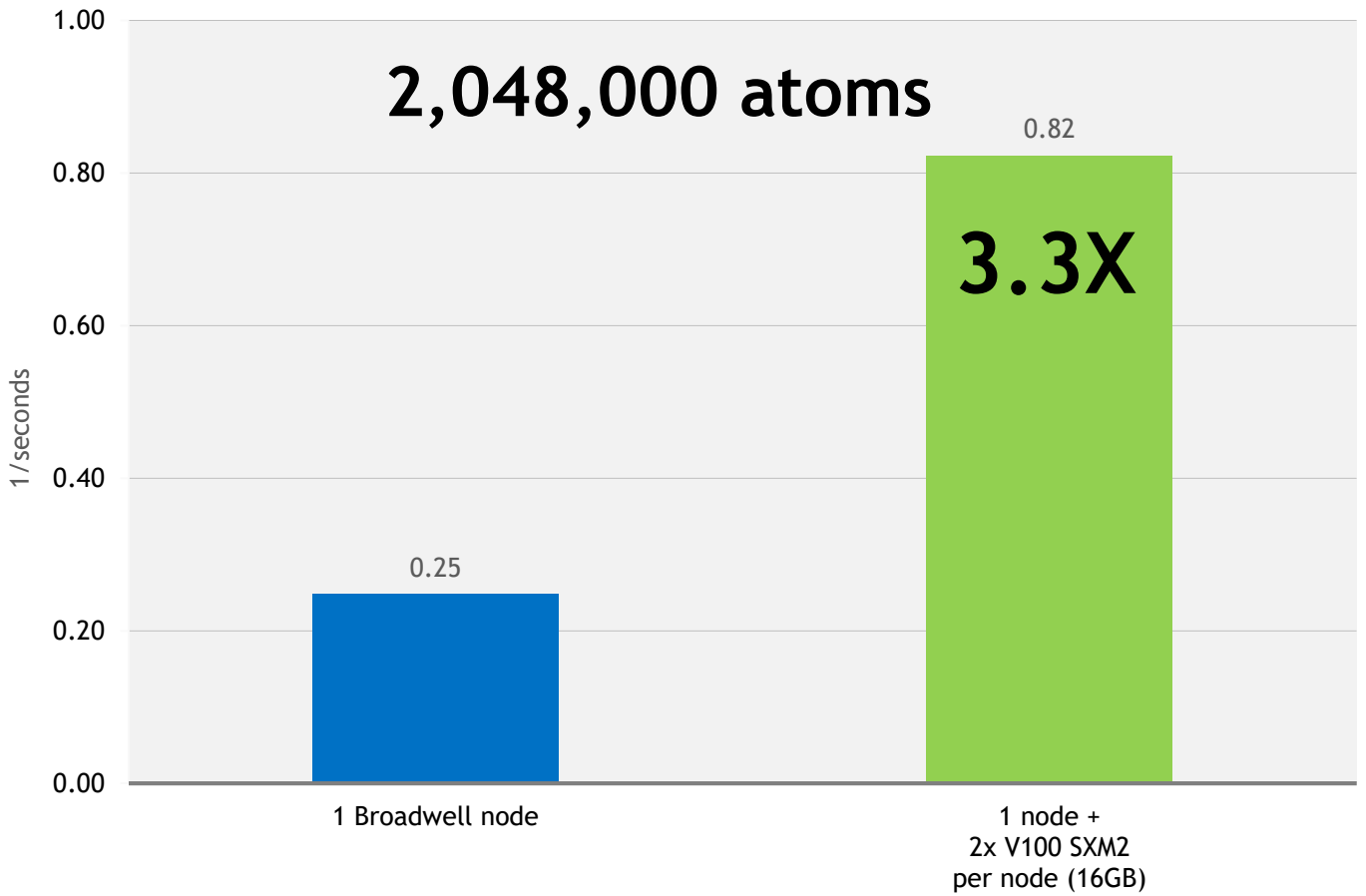
Atomic-Fluid Lennard-Jones 2.5 Cutoff on V100s SXM2



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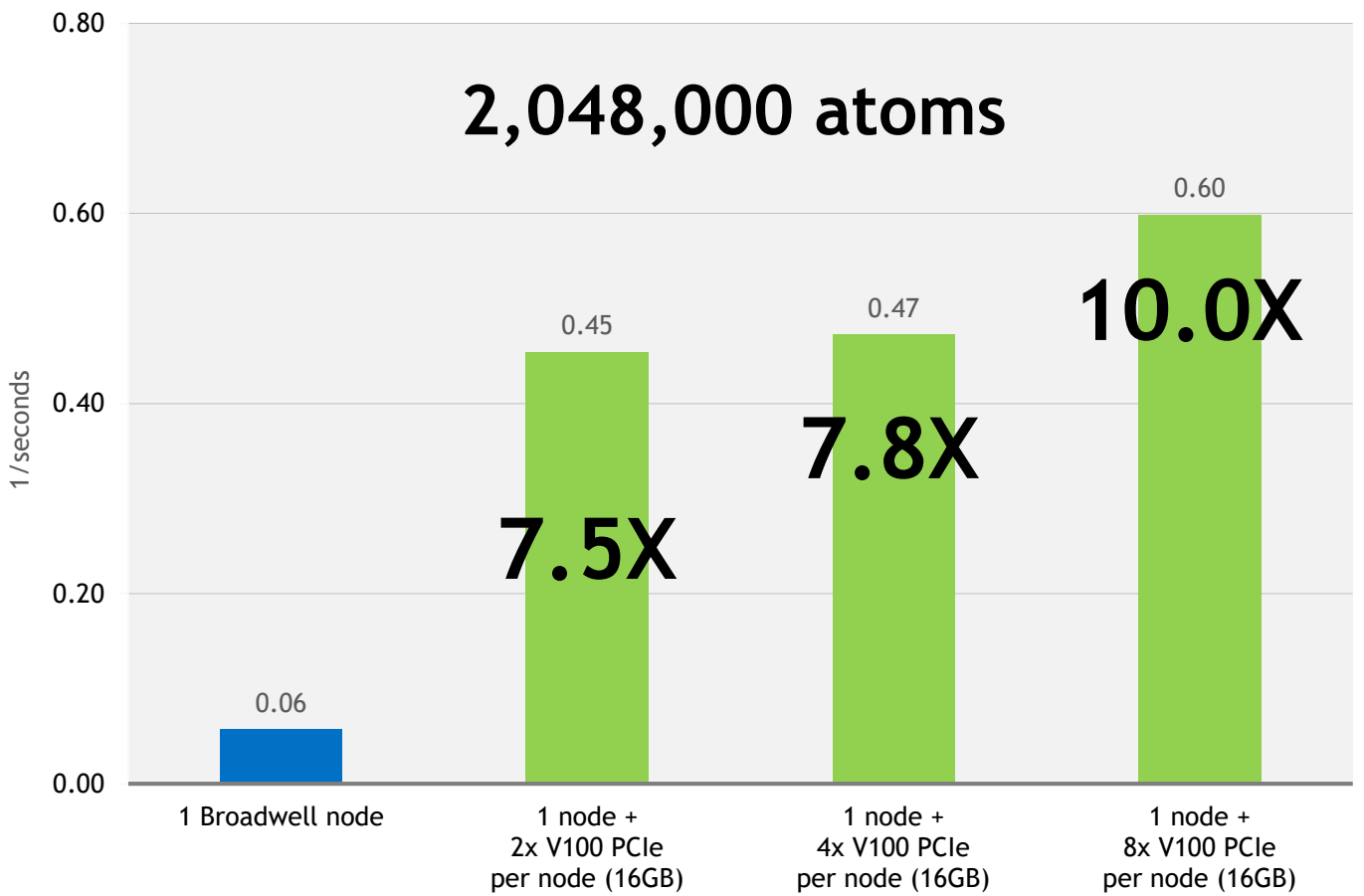
Atomic-Fluid Lennard-Jones 5.0 Cutoff on V100s PCIe



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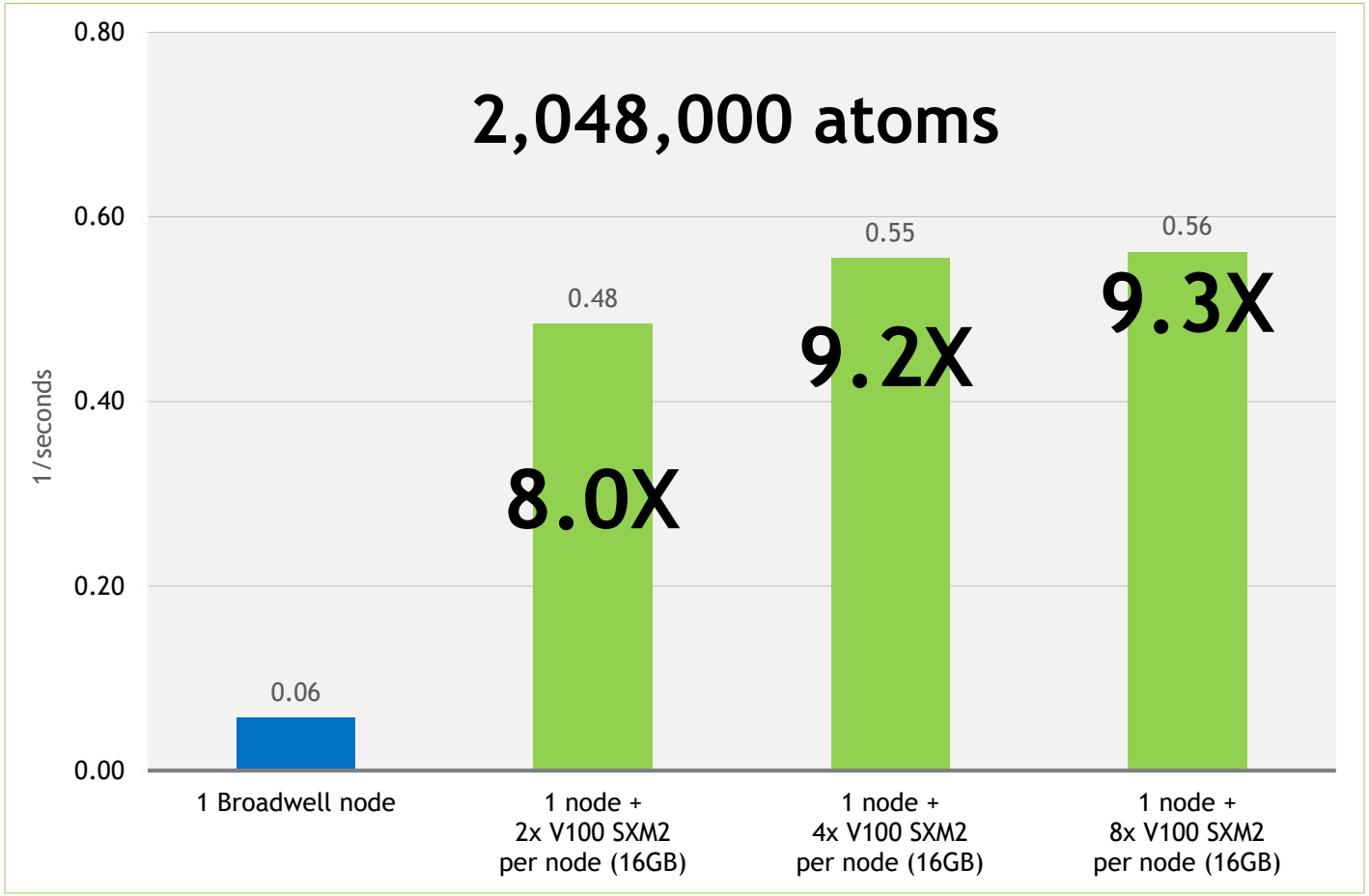
Atomic-Fluid Lennard-Jones 5.0 Cutoff on V100s SXM2



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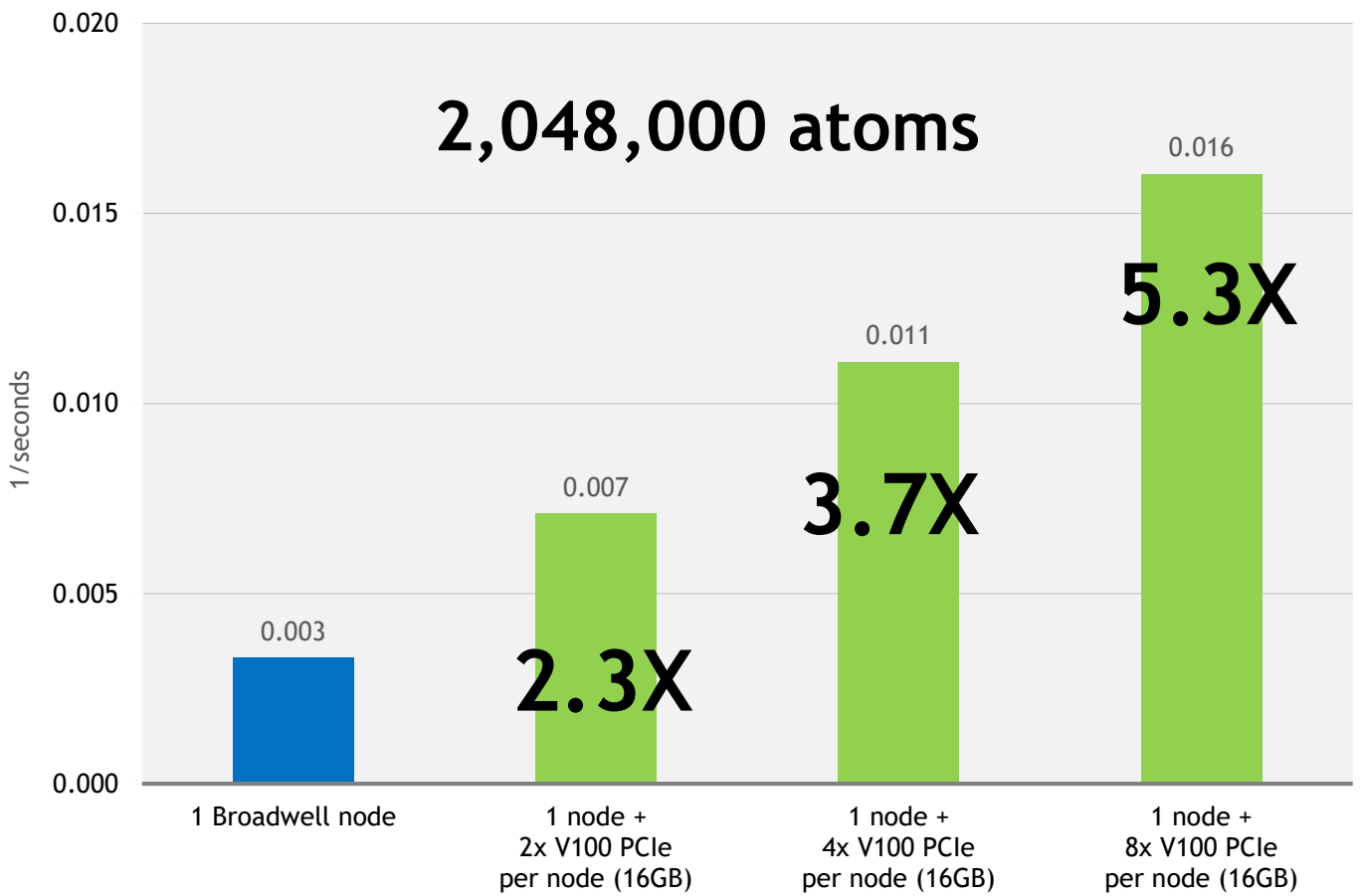
Course-grain Water on V100s PCIe



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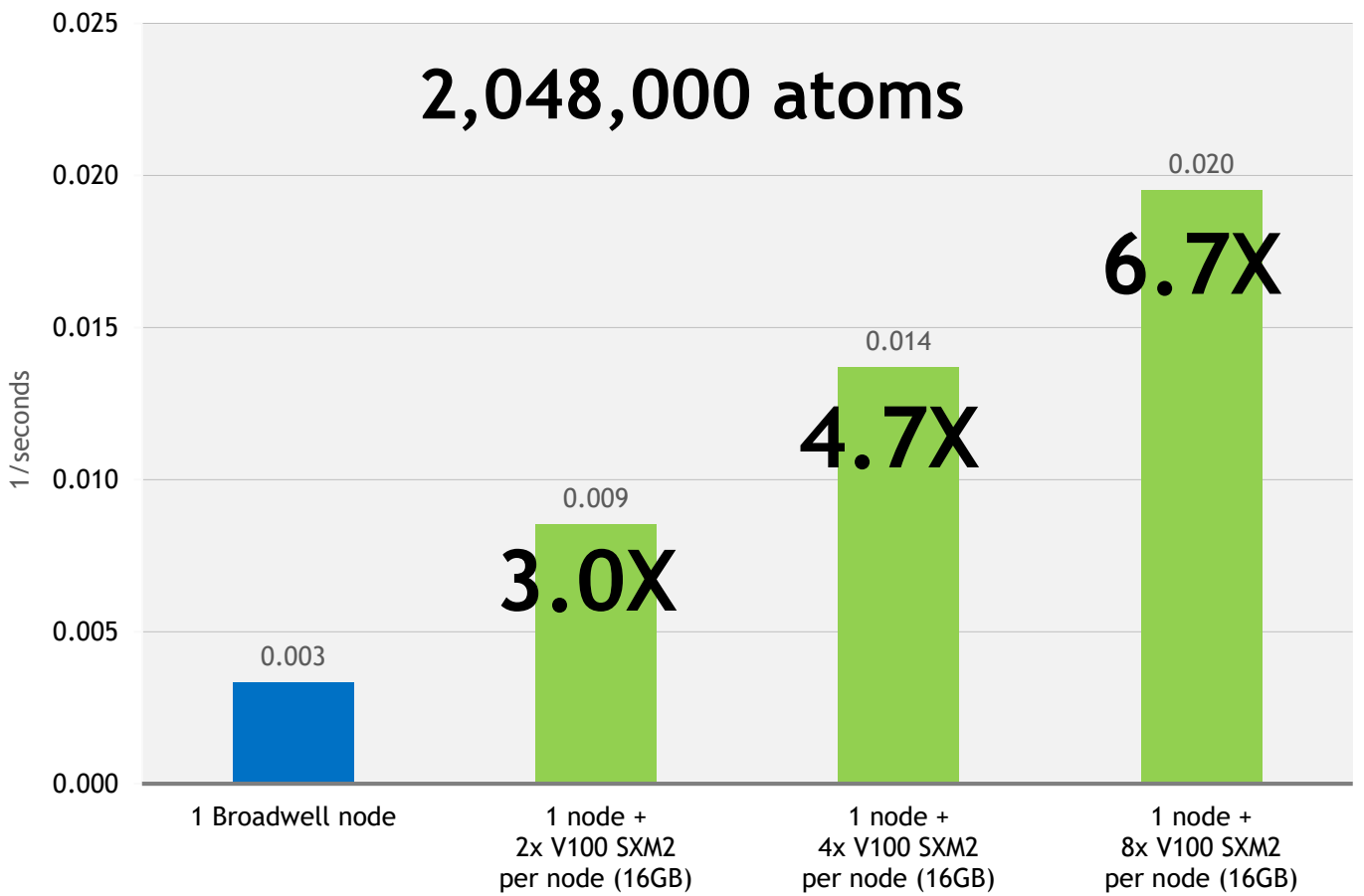
Course-grain Water on V100s SXM2



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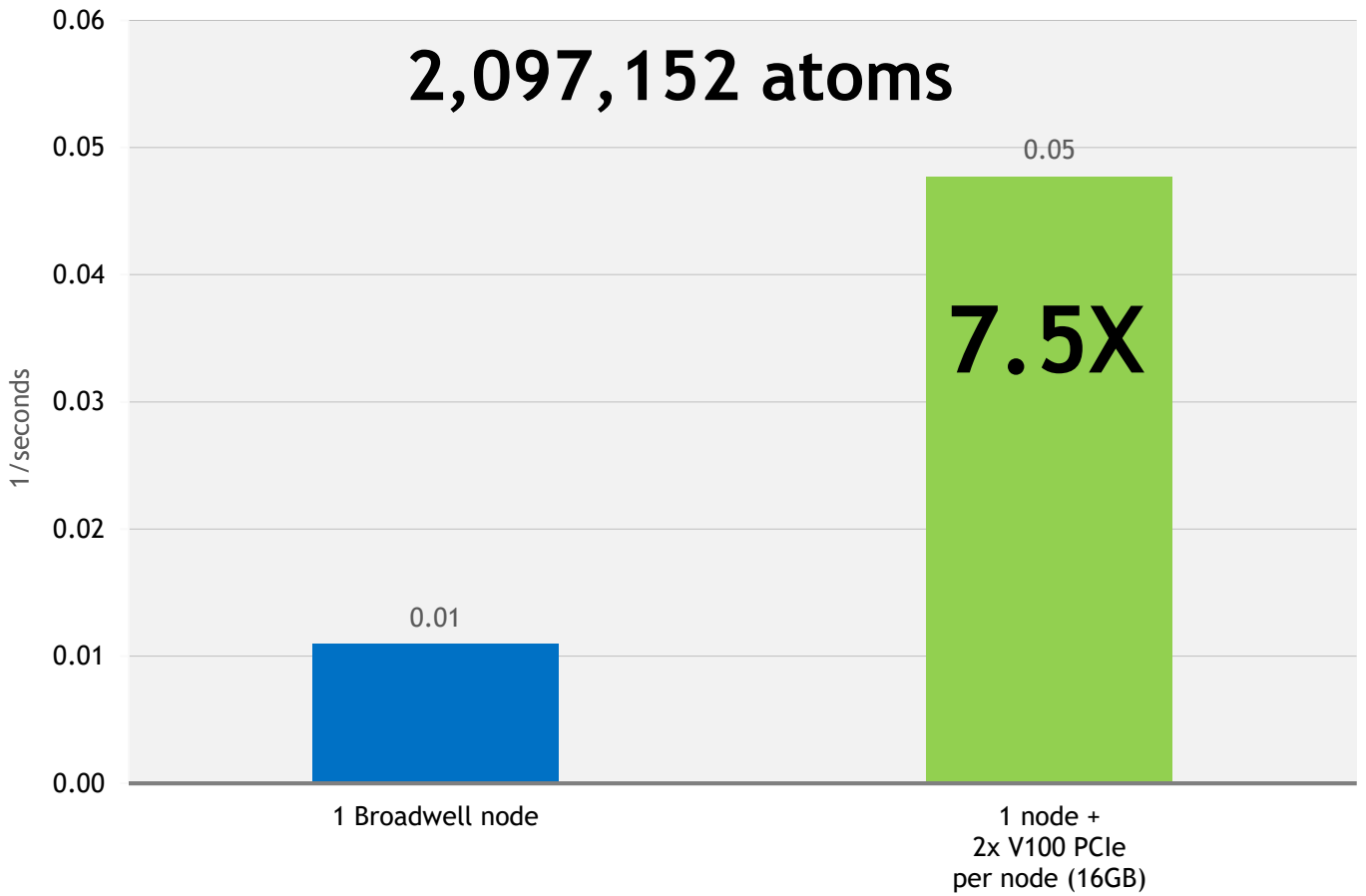
Gay-Berne on V100s PCIe



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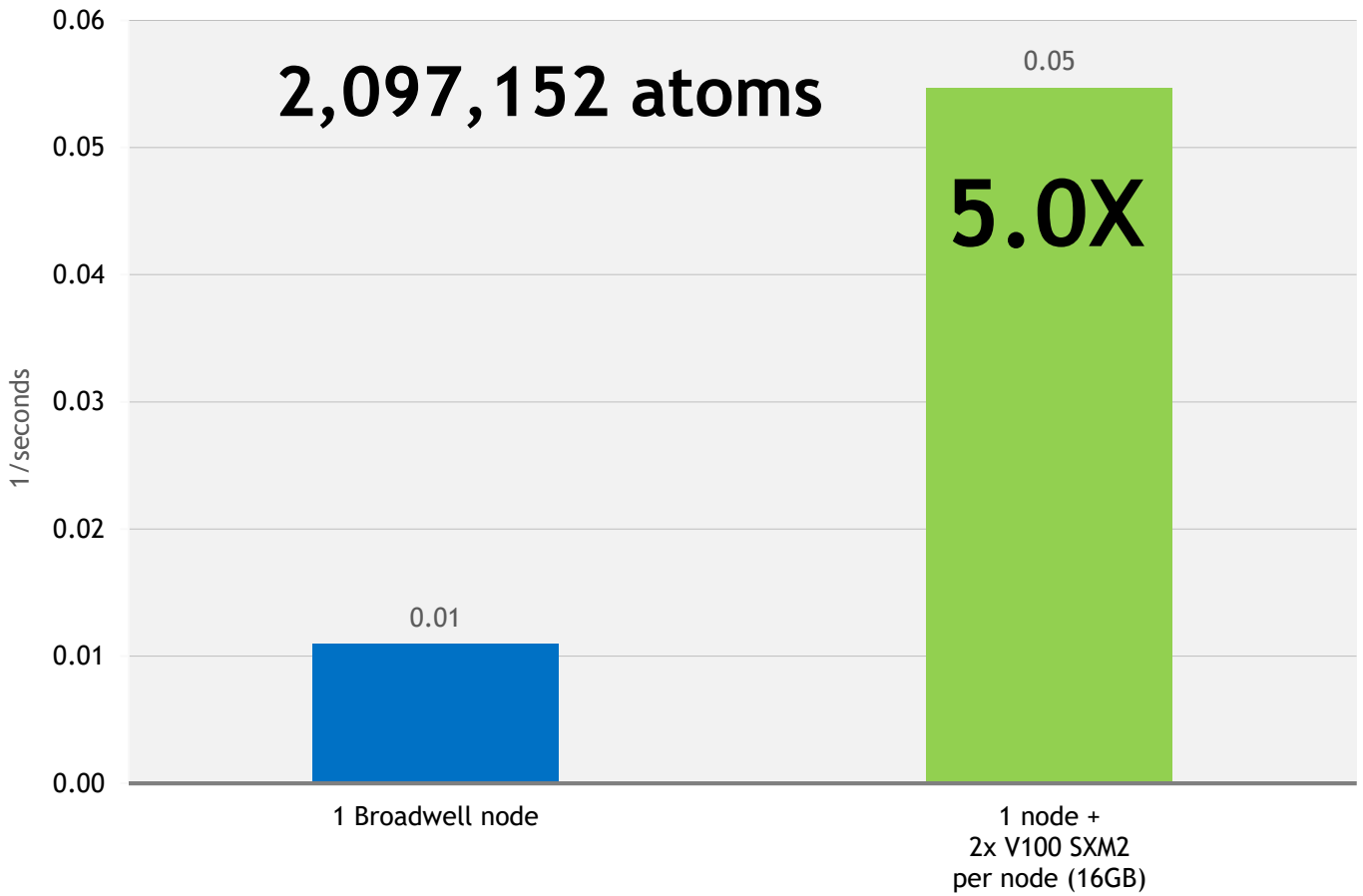
Gay-Berne on V100s SXM2



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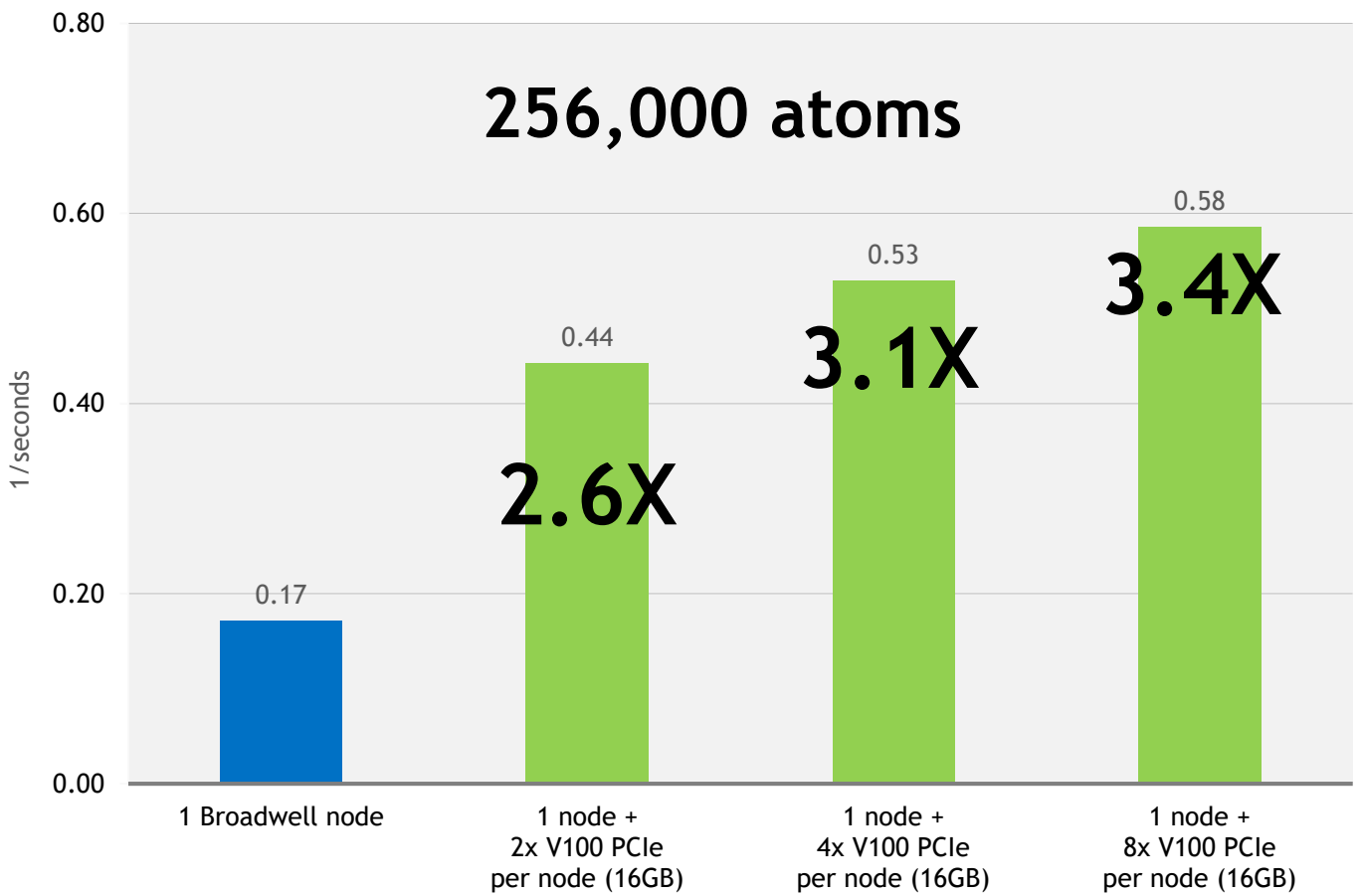
Rhodopsin on V100s PCIe



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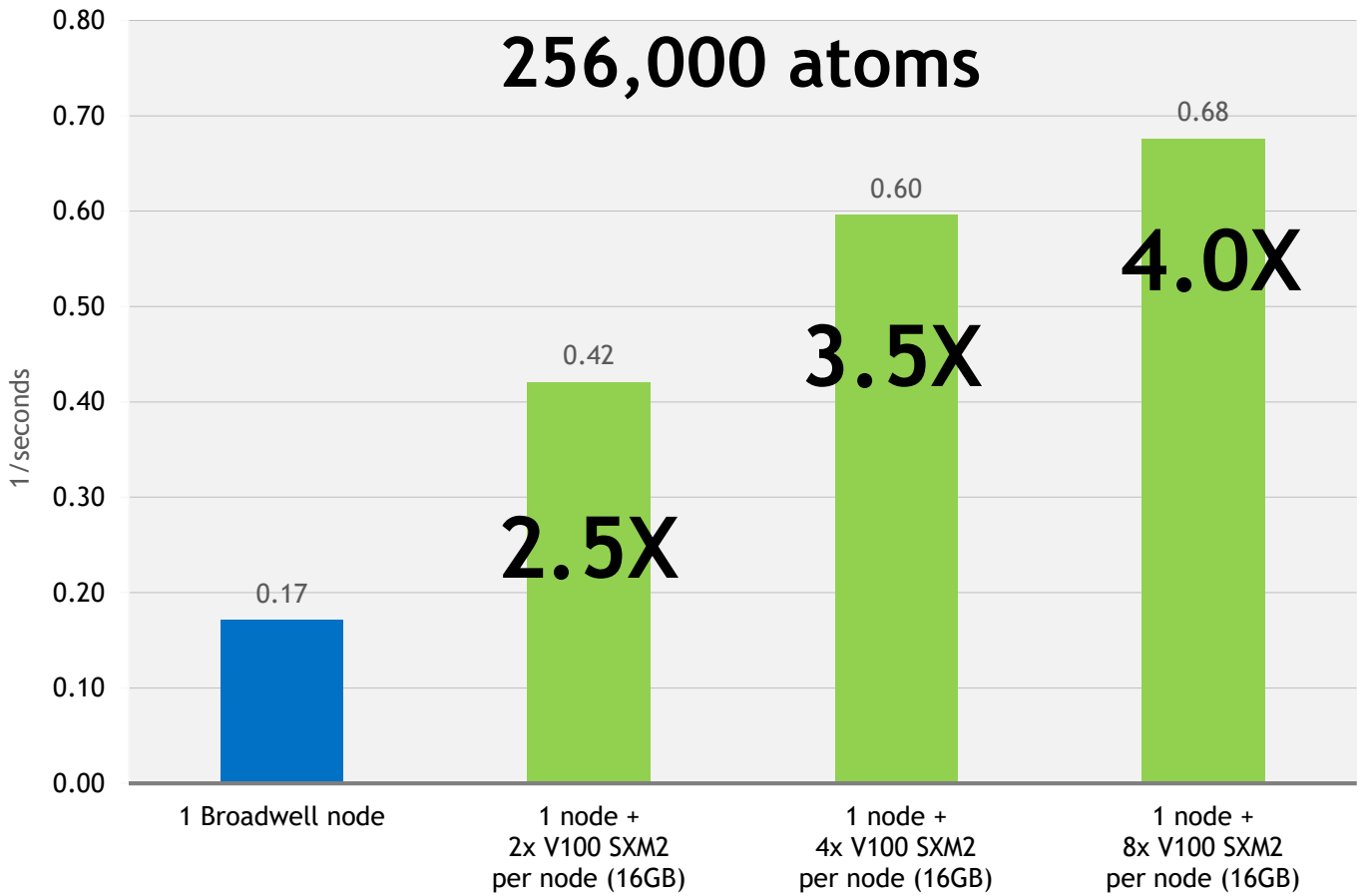
Rhodopsin on V100s SXM2



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Recommended GPU Node Configuration for LAMMPS Computational Chemistry

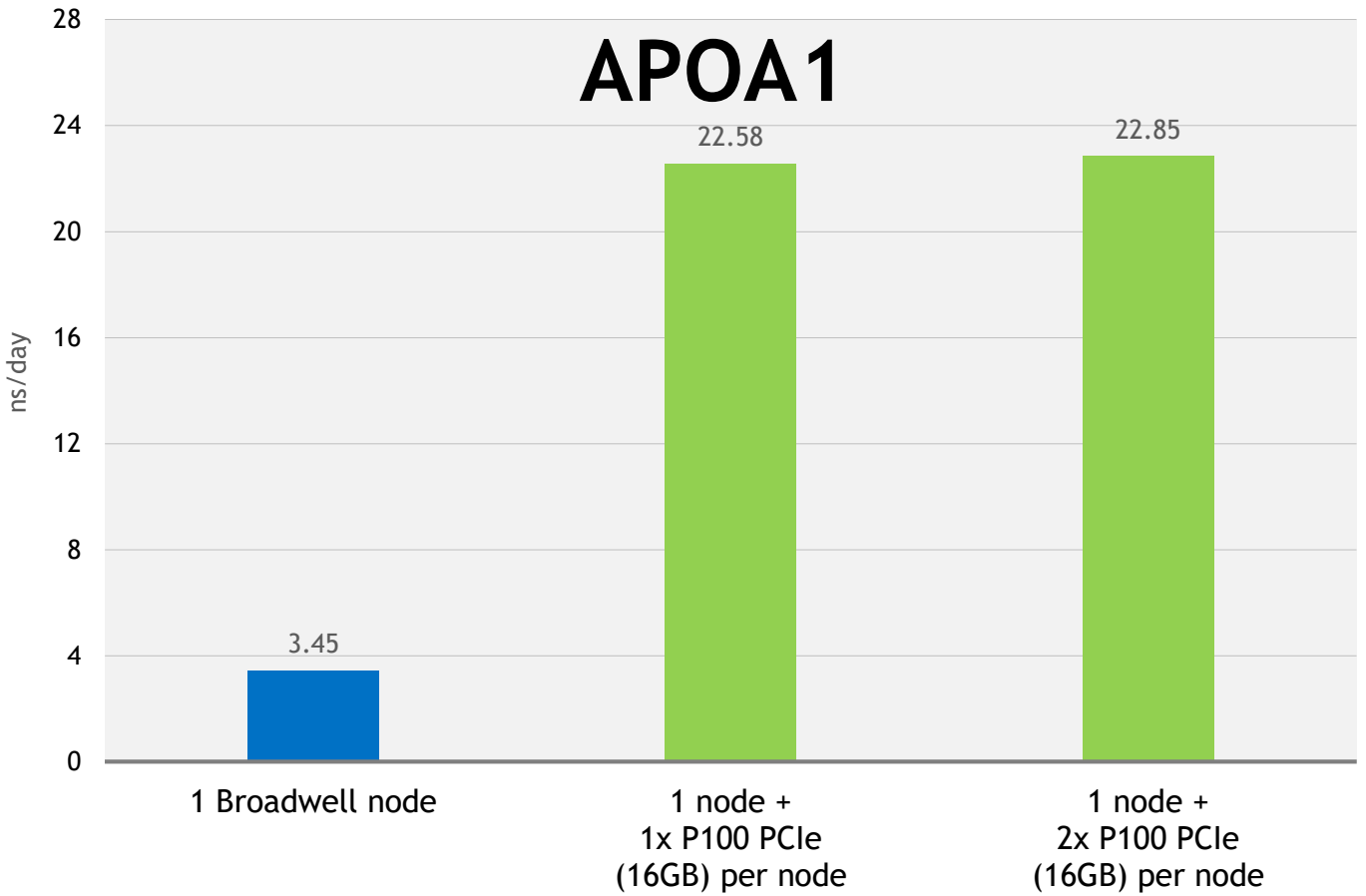
Workstation or Single Node Configuration	
# of CPU sockets	2
Cores per CPU socket	6+
CPU speed (Ghz)	2.66+
System memory per socket (GB)	32
GPUs	GTX Titan X, Tesla P100, V100
# of GPUs per CPU socket	1-2
GPU memory preference (GB)	6+
GPU to CPU connection	PCIe 3.0 or higher
Server storage	500 GB or higher
Network configuration	Gemini, InfiniBand

Scale to thousands of nodes with same single node configuration

NAMD 2.12

July 2017

APOA1 on P100s PCIe



Running NAMD version 2.12

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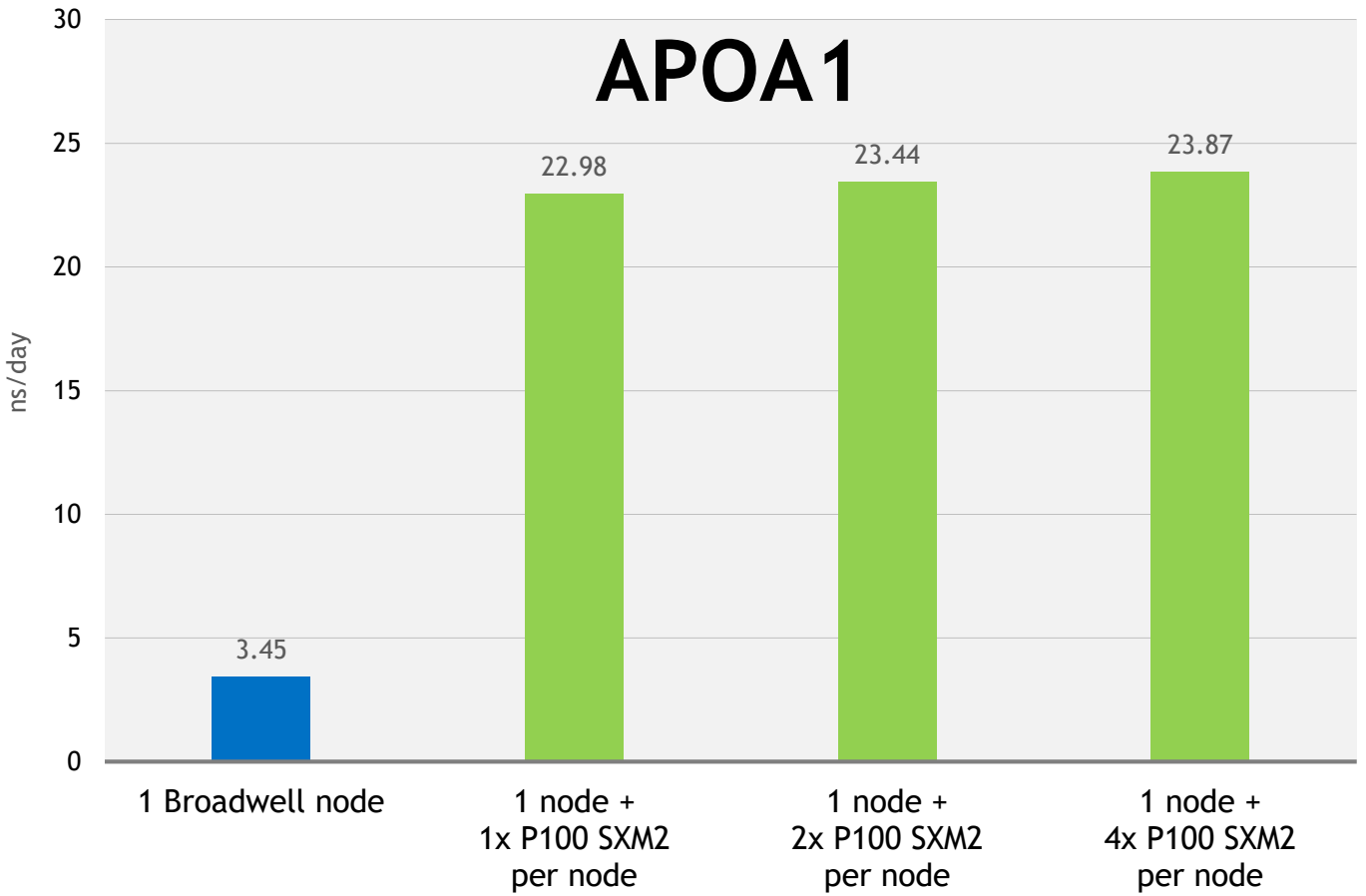
APOA1 on P100s SXM2



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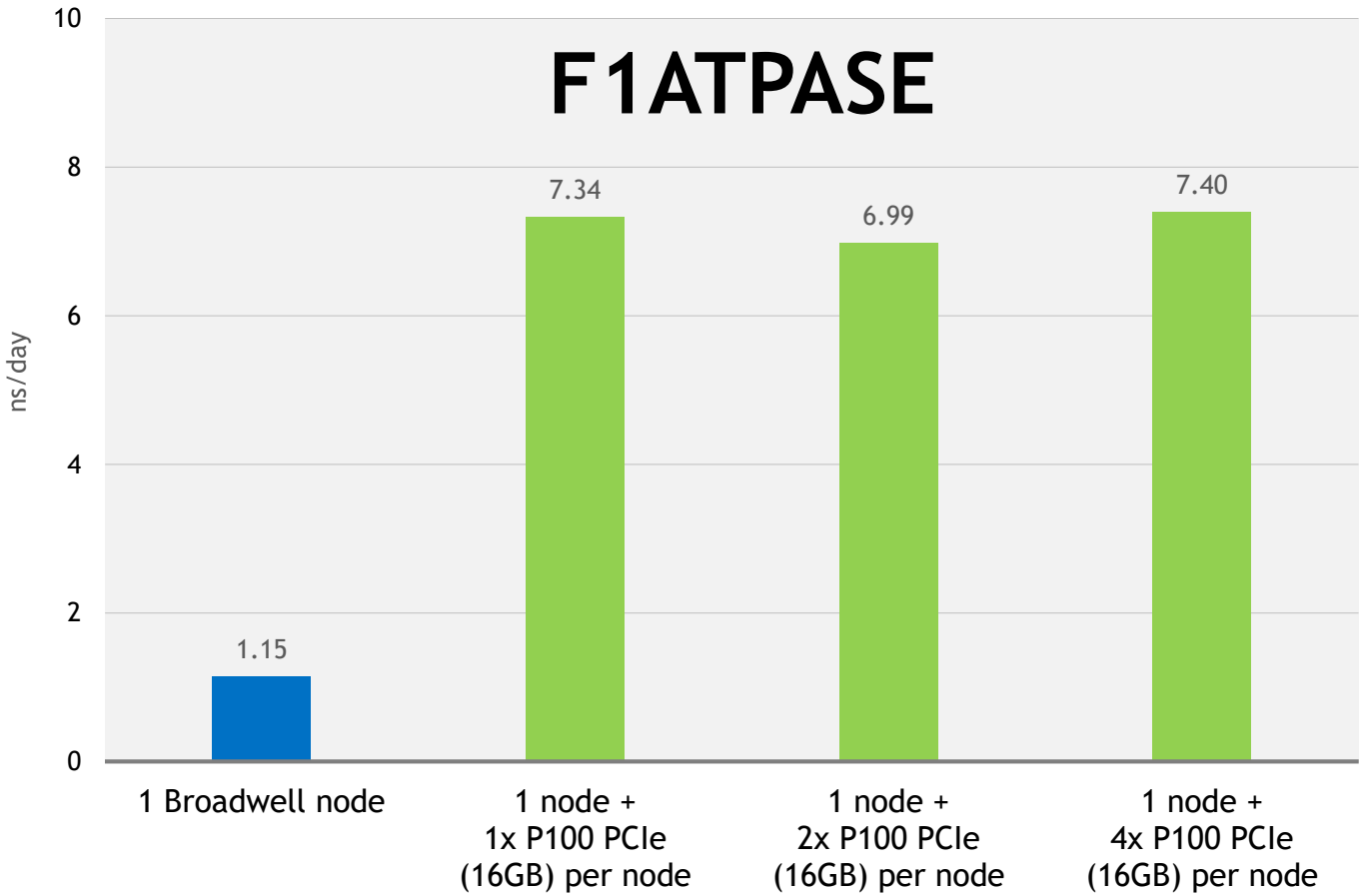
F1ATPASE on P100s PCIe



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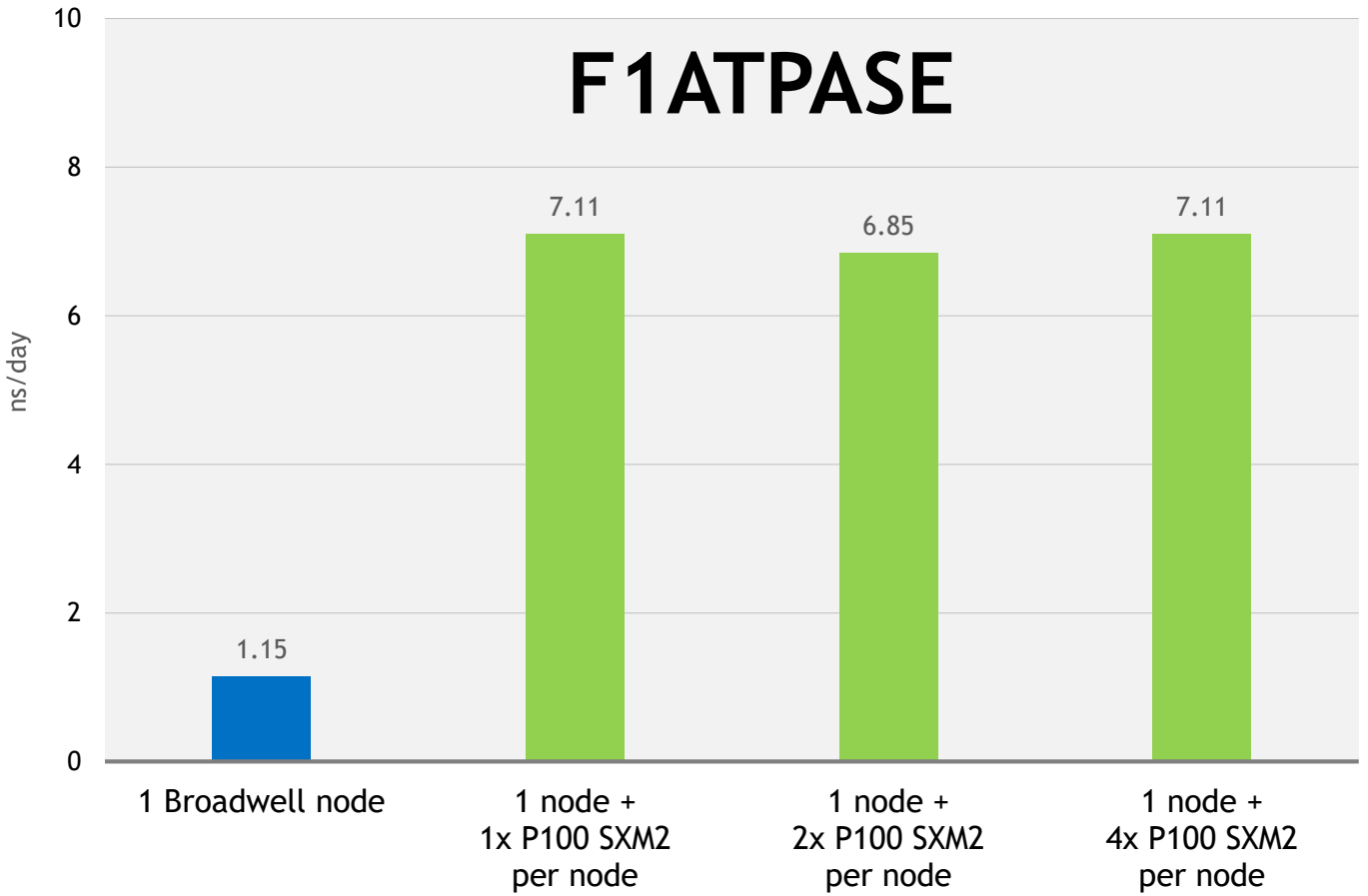
F1ATPASE on P100s SXM2



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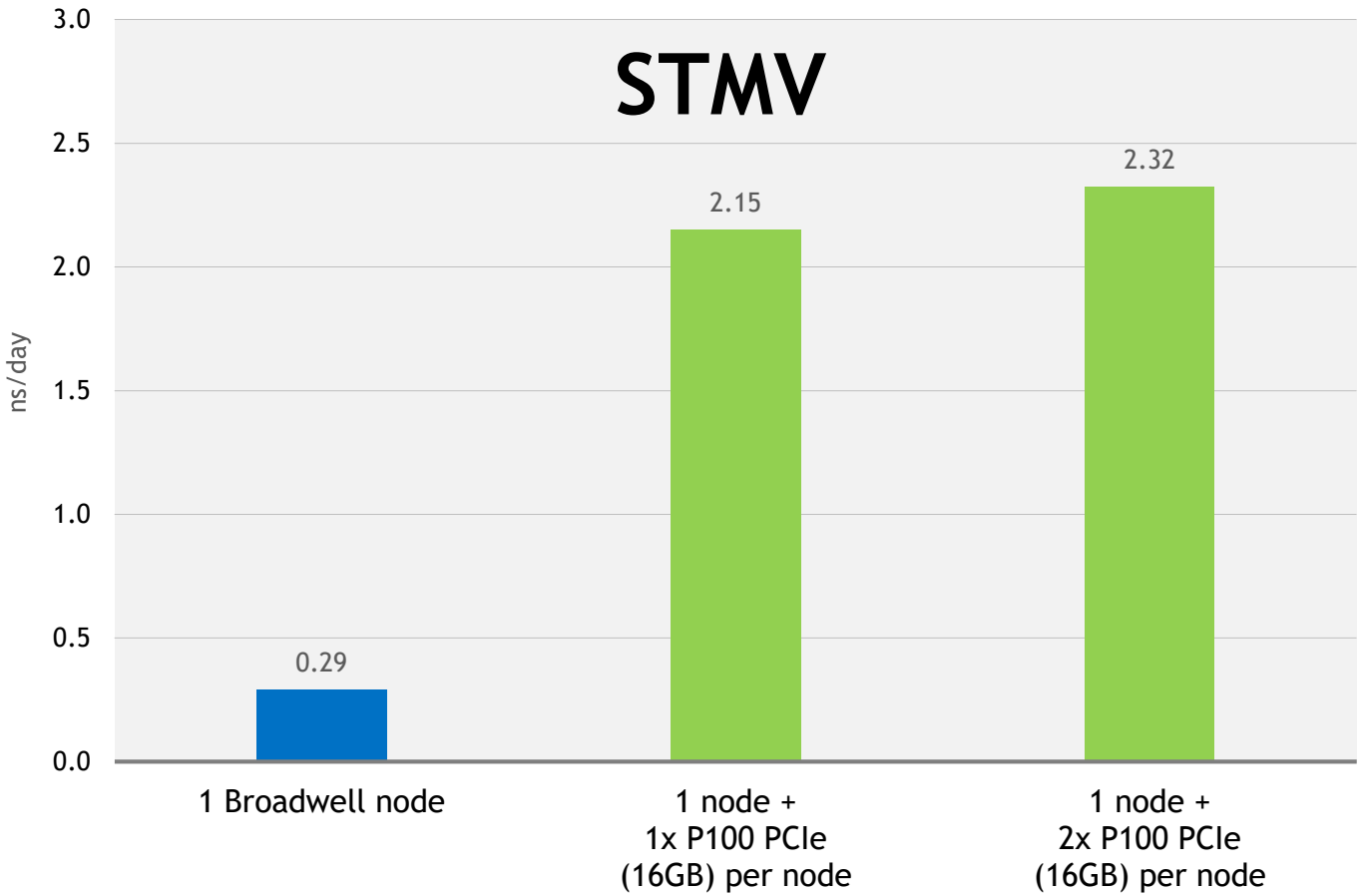
STMV on P100s PCIe



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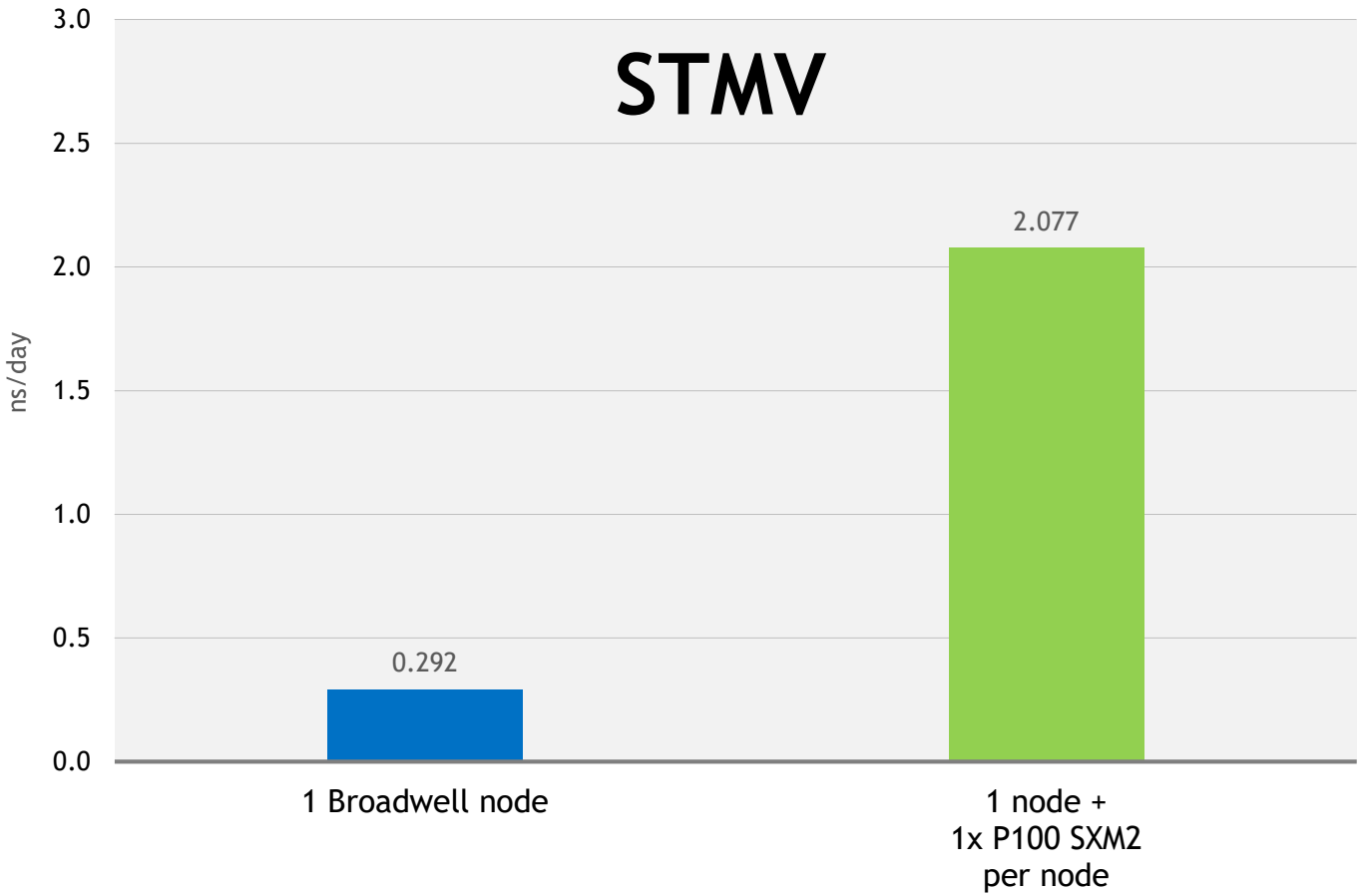
STMV on P100s SXM2



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Benefits of MD GPU-Accelerated Computing

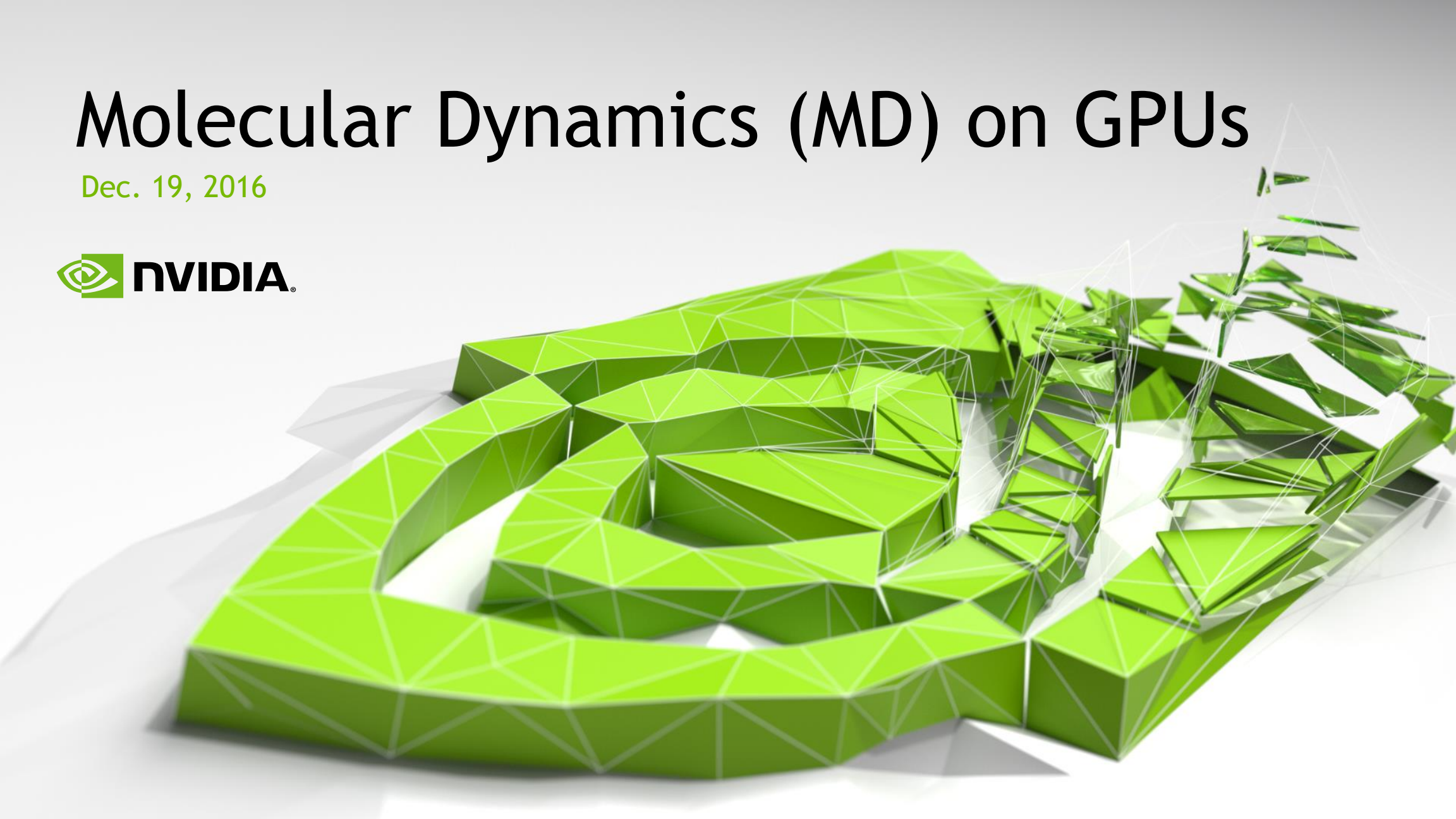
Why wouldn't you want to turbocharge your research?

- 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
- K80 GPU is our fastest and lowest power high performance GPU yet

Try GPU accelerated MD apps for free – www.nvidia.com/GPUTestDrive

Molecular Dynamics (MD) on GPUs

Dec. 19, 2016



GPU-Accelerated Quantum Chemistry Apps

Green Lettering Indicates Performance Slides Included

- Abinit
- ACES III
- ADF
- BigDFT
- CP2K
- GAMESS-US
- Gaussian
- GPAW
- LATTE
- LSDalton
- MOLCAS
- Mopac2012
- NWChem
- Octopus
- ONETEP
- Petot
- Q-Chem
- QMCPACK
- Quantum Espresso
- Quantum SuperCharger Library
- RMG
- TeraChem
- UNM
- VASP
- WL-LSMS

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