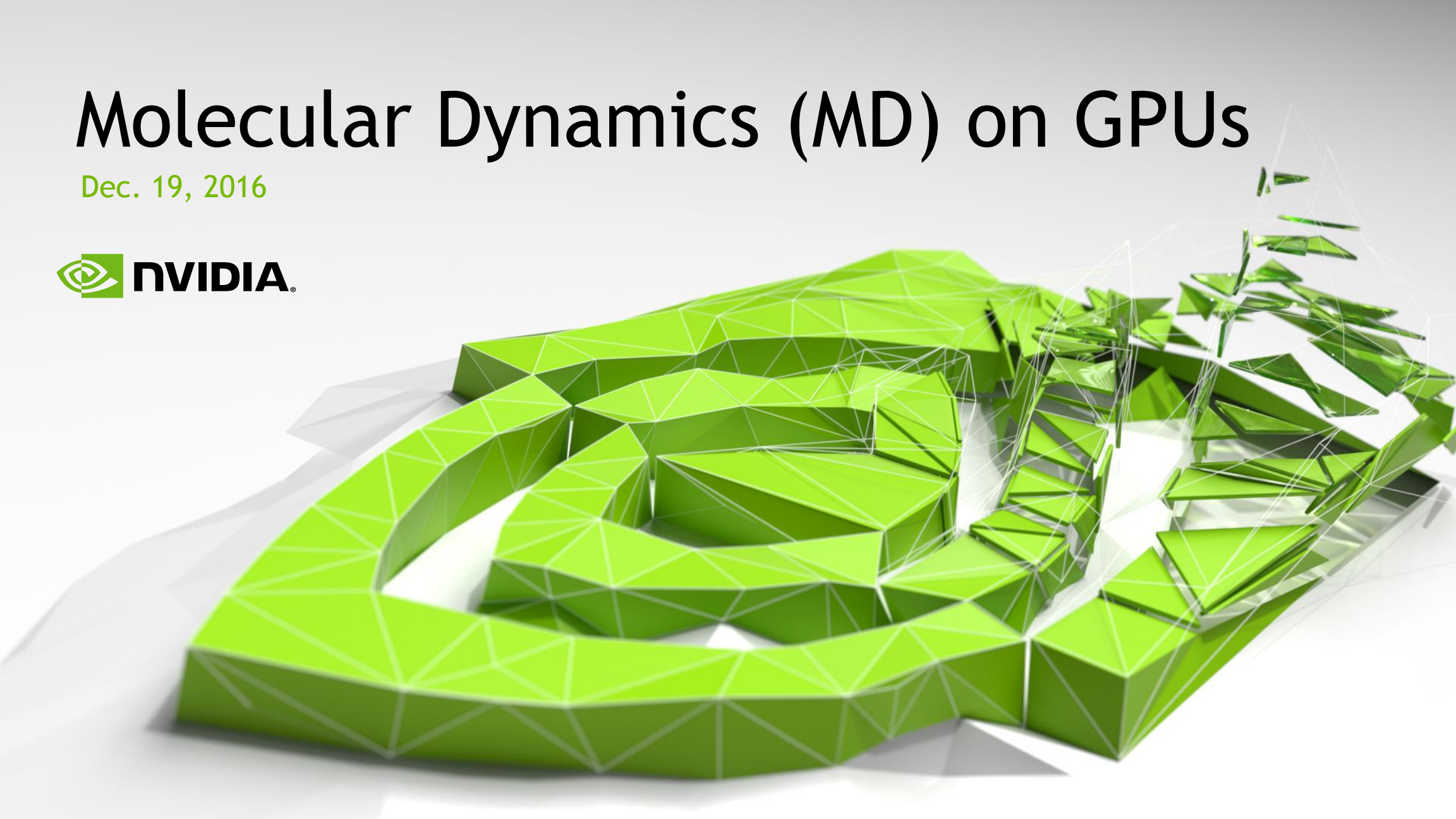
Molecular Dynamics (MD) on GPUs

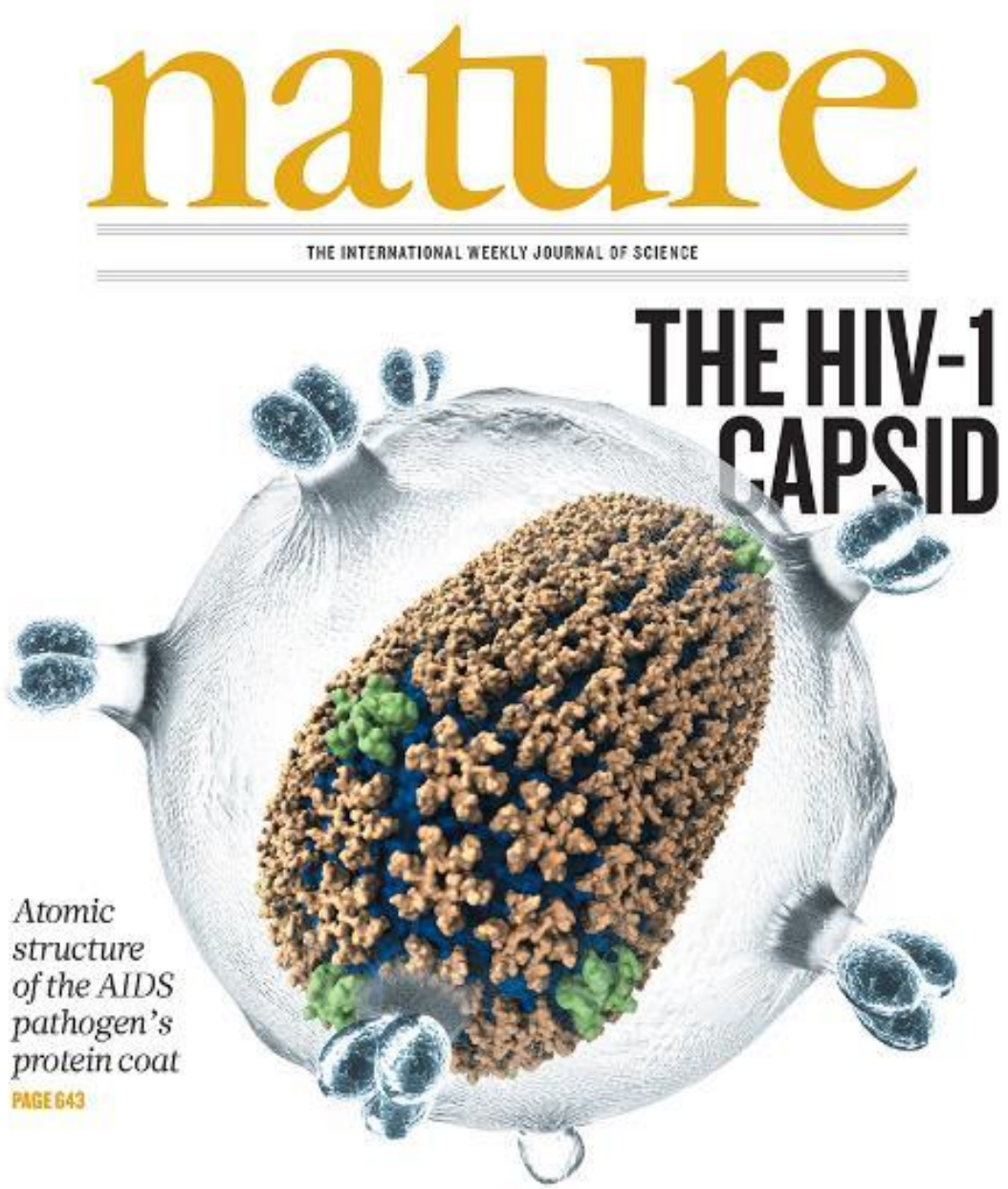
Dec. 19, 2016



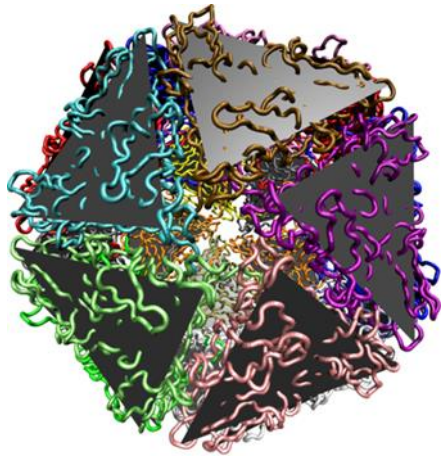
Accelerating Discoveries

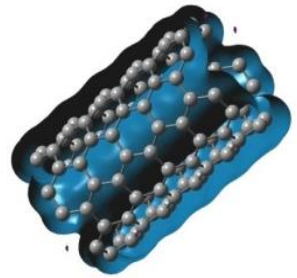
Using a supercomputer powered by the Tesla Platform with over 3,000 Tesla accelerators, University of Illinois scientists performed the first all-atom simulation of the HIV virus and discovered the chemical structure of its capsid — “the perfect target for fighting the infection.”

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 cuBLAS, cuFFT, CUDA	Uses cuBLAS, cuFFT, OpenACC
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
- GPUGrid.net
- GROMACS
- HALMD
- HOOMD-Blue
- LAMMPS
- mdcore
- MELD
- NAMD
- OpenMM
- PolyFTS

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

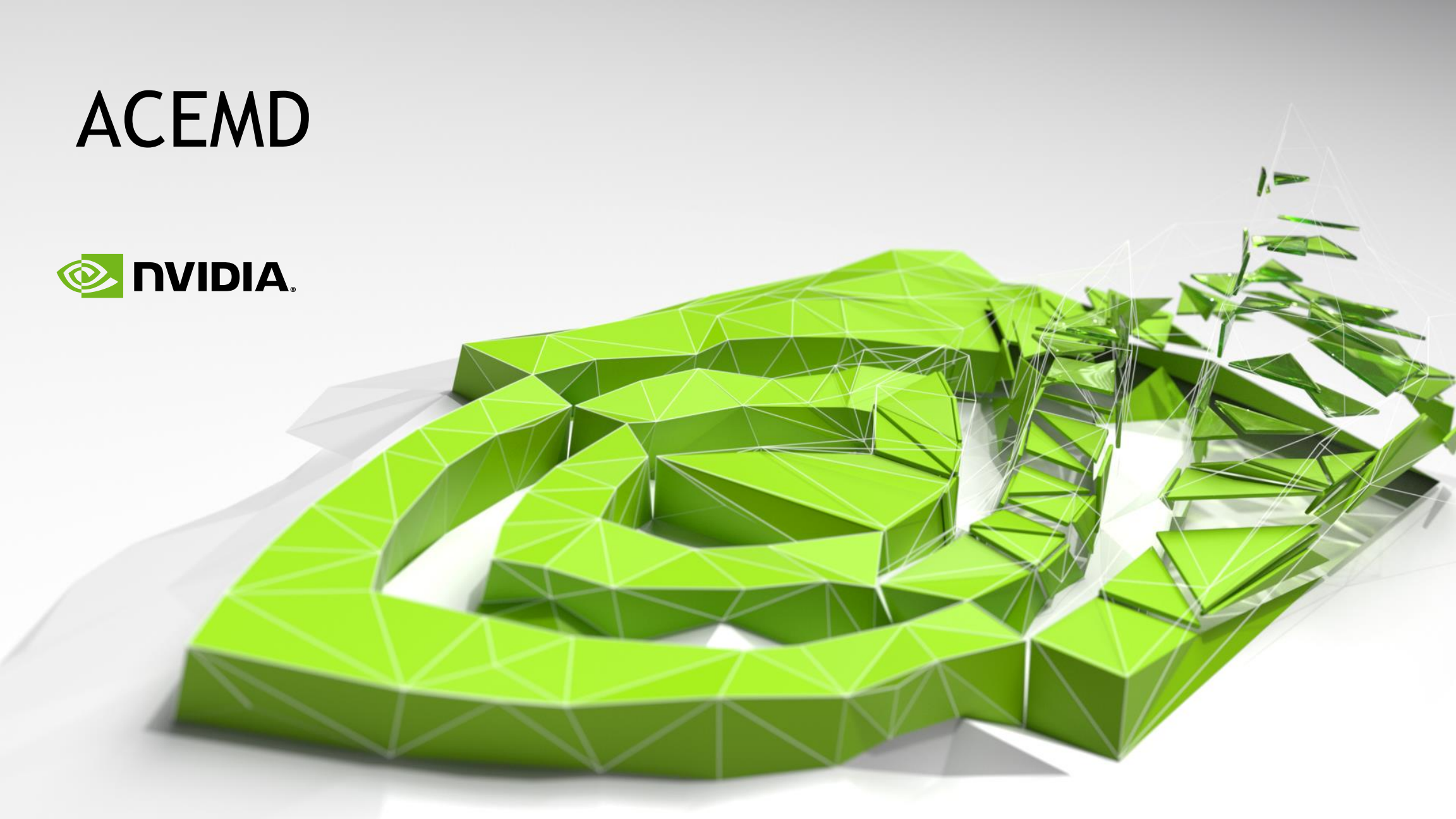
Benefits of MD GPU-Accelerated Computing

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 with marginal price increase
- 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

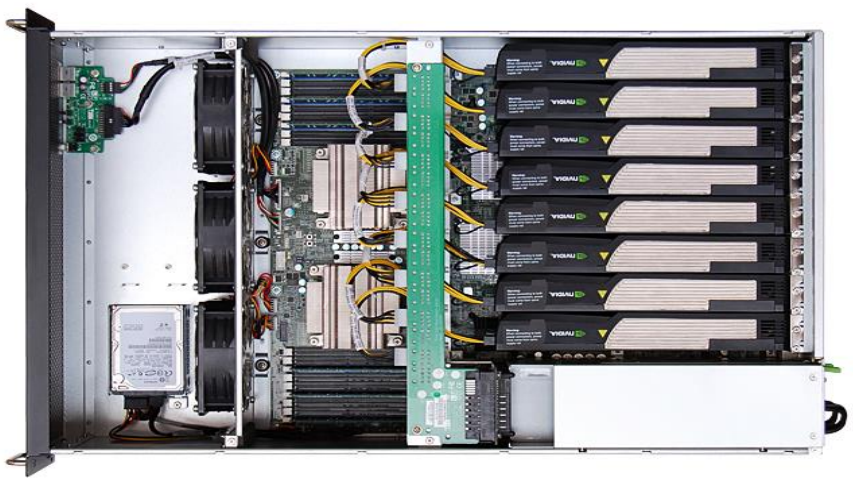
Try GPU accelerated MD apps for free – www.nvidia.com/GPUTestDrive

ACEMD



www.acellera.com

ACEMD: Extremely efficient and robust MD software built on GPUs



470 ns/day on 1 GPU for L-Iduronic acid (1362 atoms)

116 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)

www.acellera.com

ACEMD

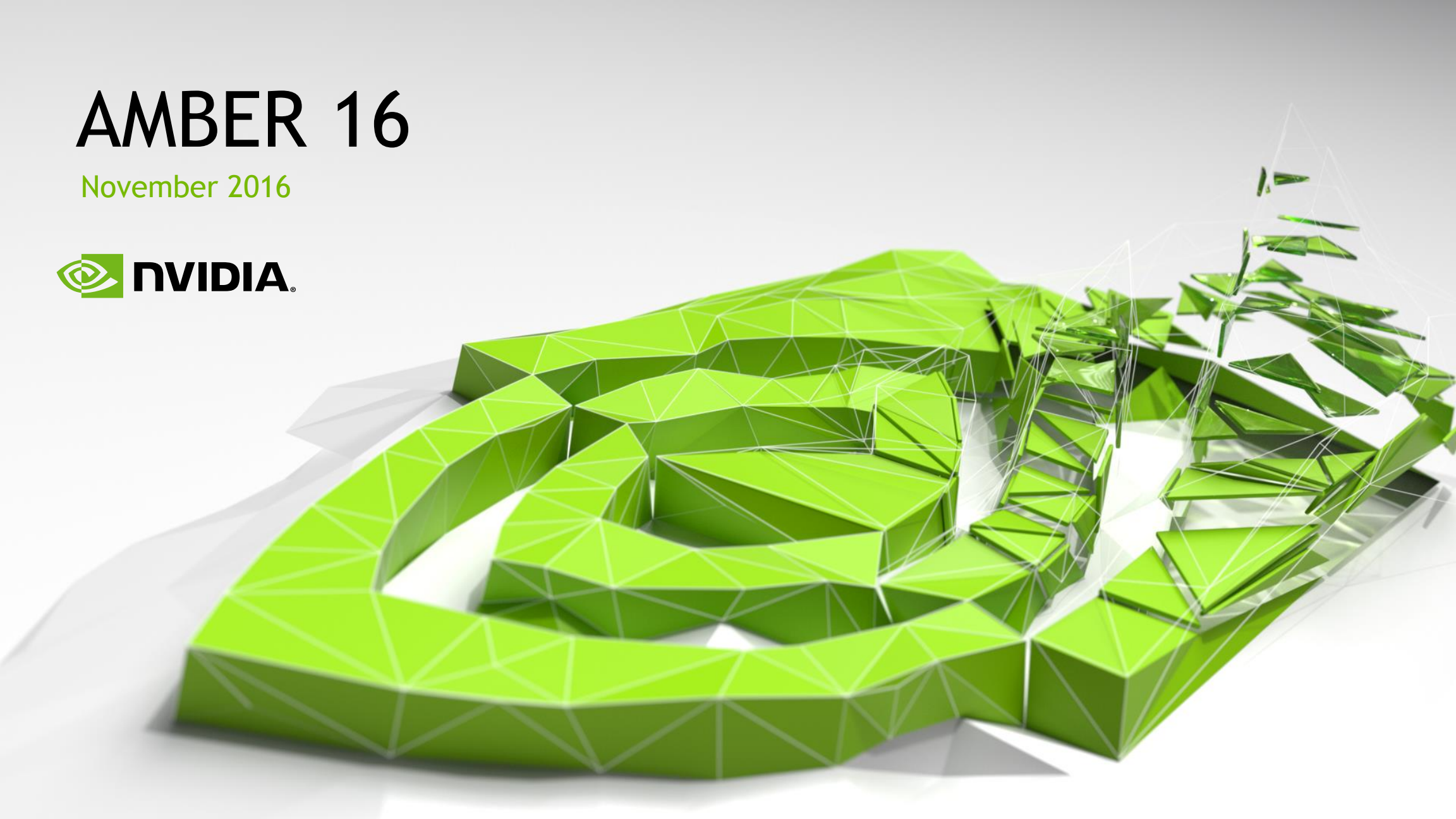
- **Standardised and easy to use**: ACEMD reads CHARMM/NAMD and AMBER input files and uses similar syntax to other MD software.
- **Fully featured:** NVT, NPT, PME, TCL, PLUMED, CAMSHIFT[1]
- **Robust**: ACEMD is a proven computational engine and is used in one of the largest distributed computing projects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

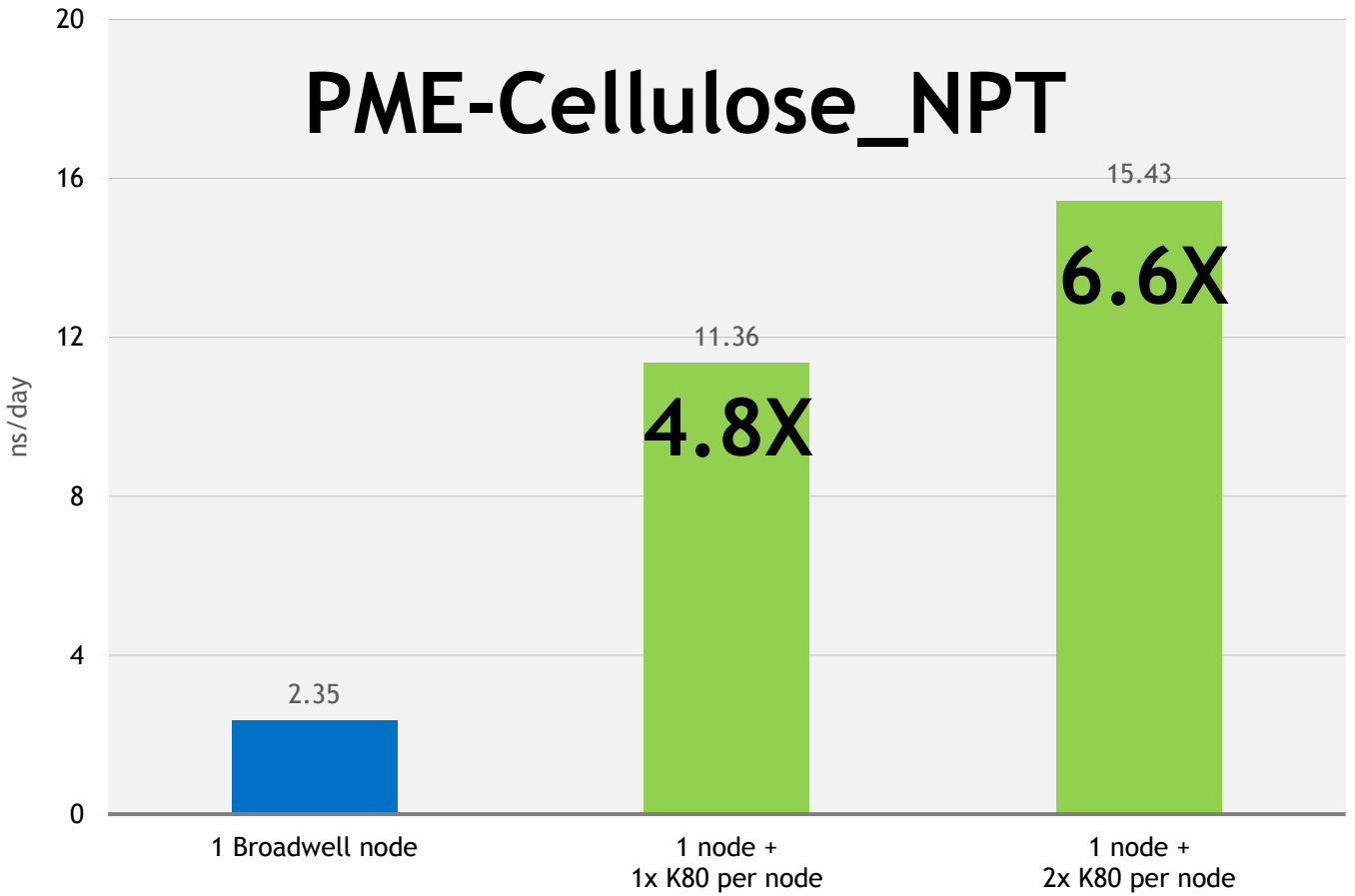
2 For a list of selected references see http://www.acellera.com/acemd/publications

AMBER 16

November 2016



PME-Cellulose_NPT on K80s



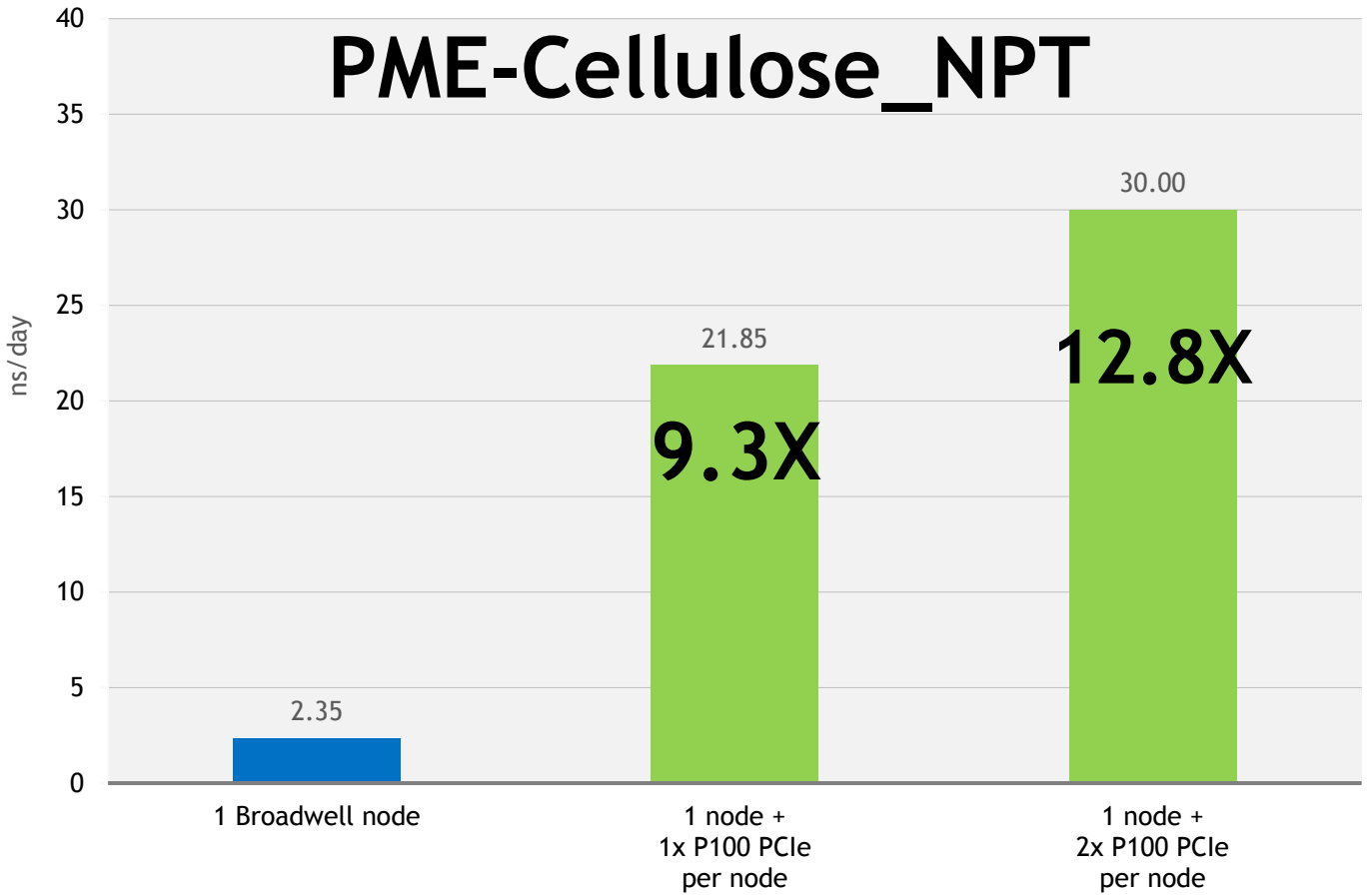
Running AMBER version 16.3

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 K80 (autoboost) GPUs

- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

PME-Cellulose_NPT on P100s PCIe



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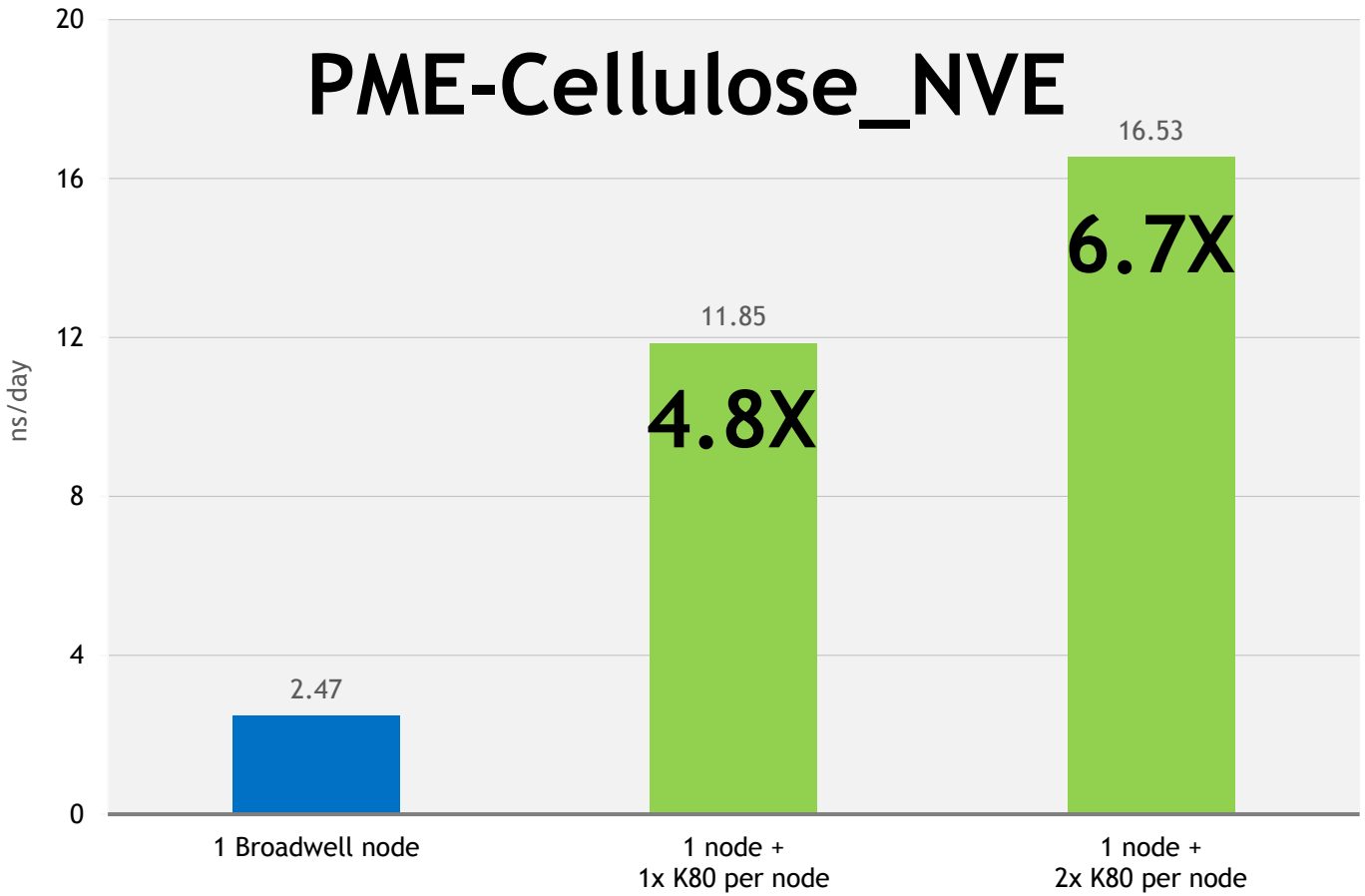
PME-Cellulose_NVE on K80s



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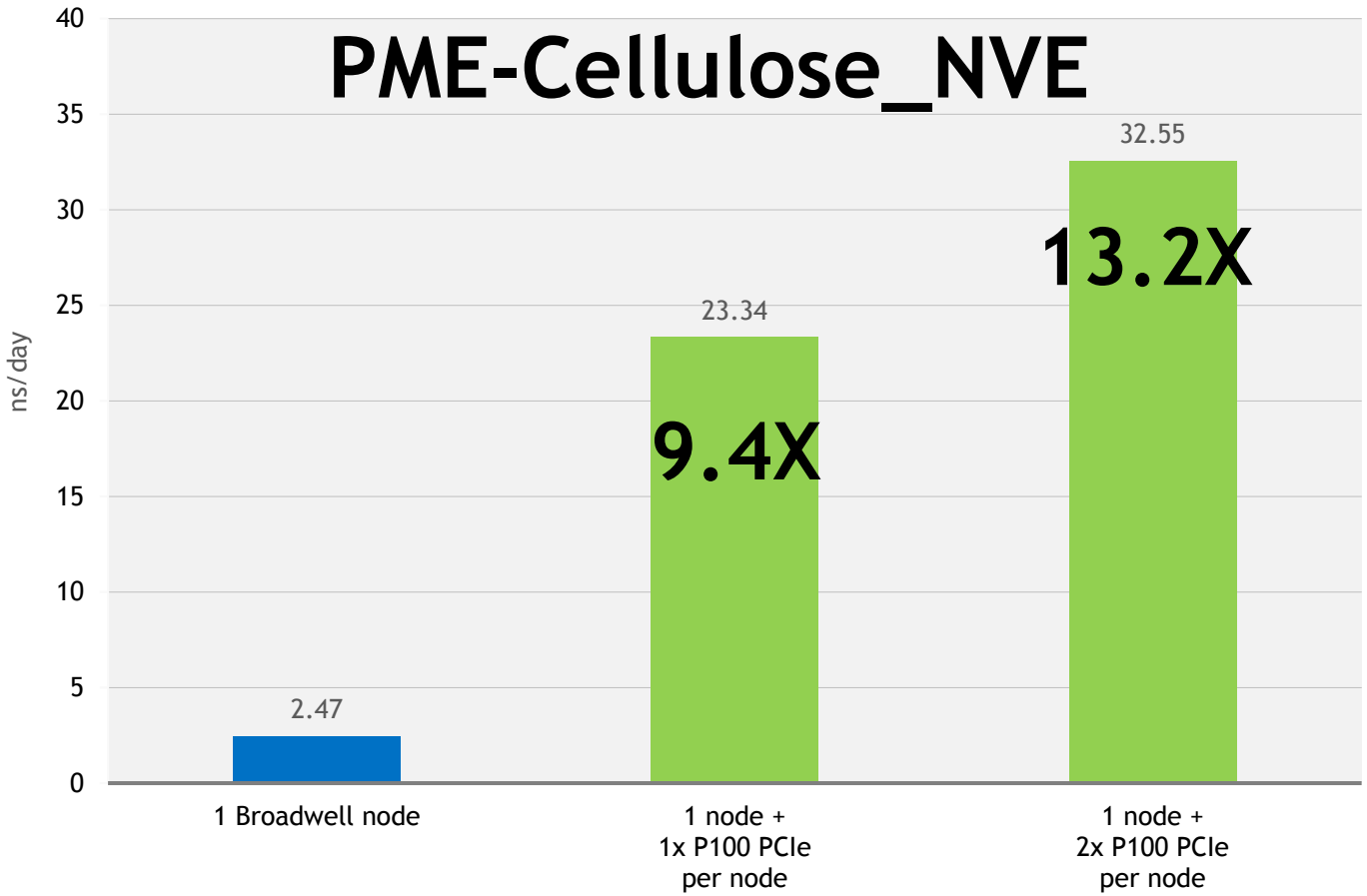

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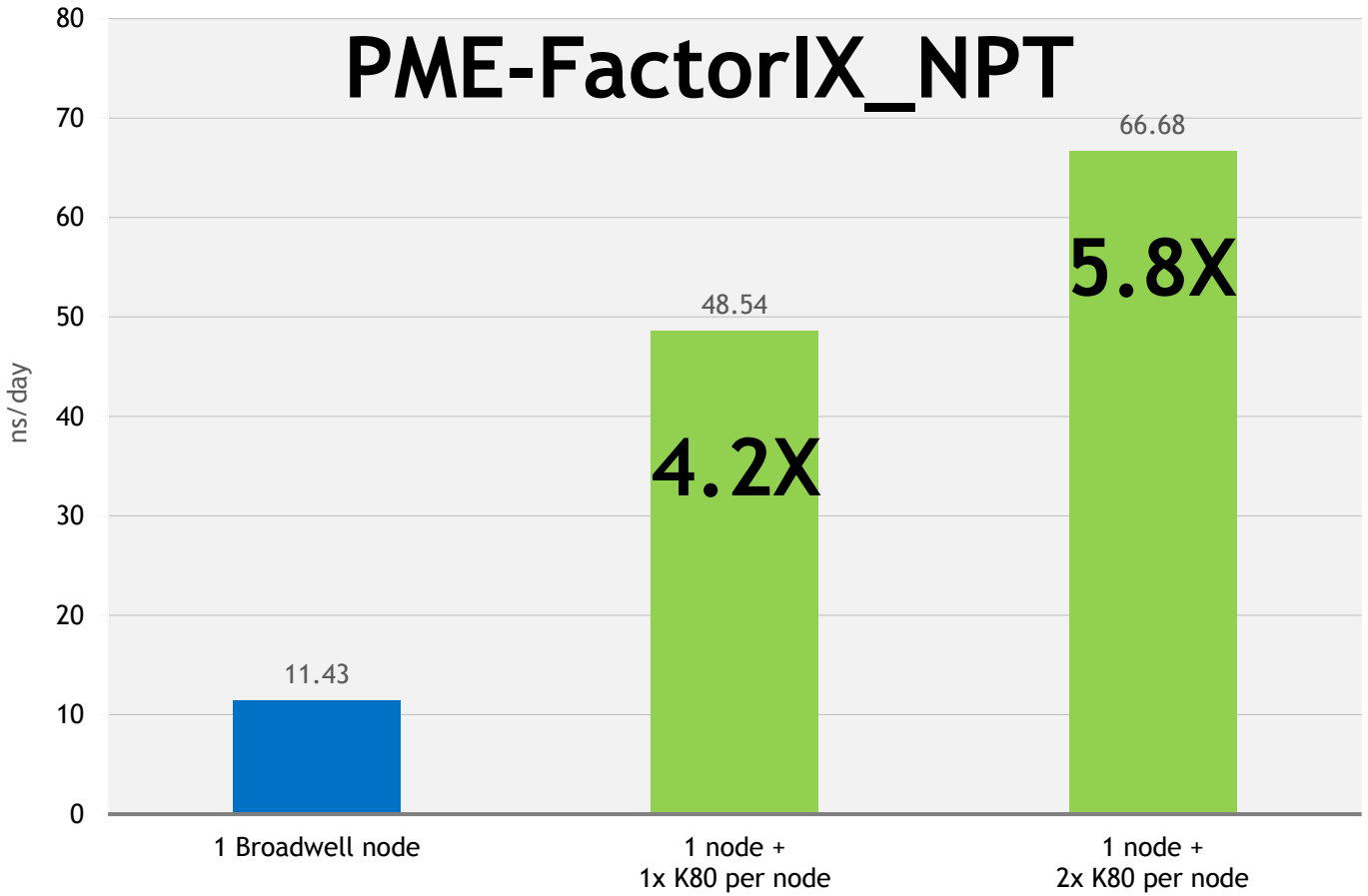
PME-FactorIX_NPT on K80s



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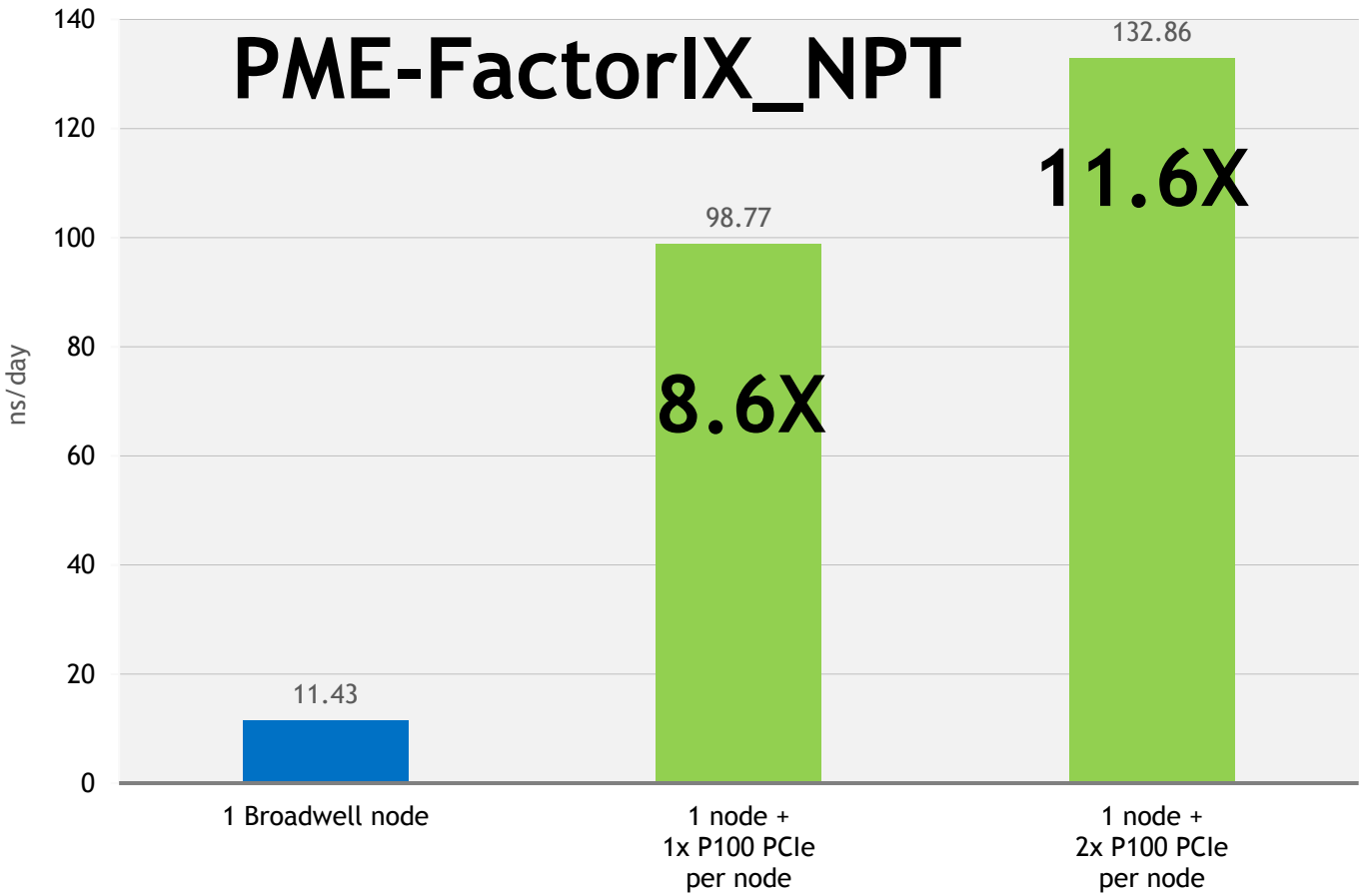

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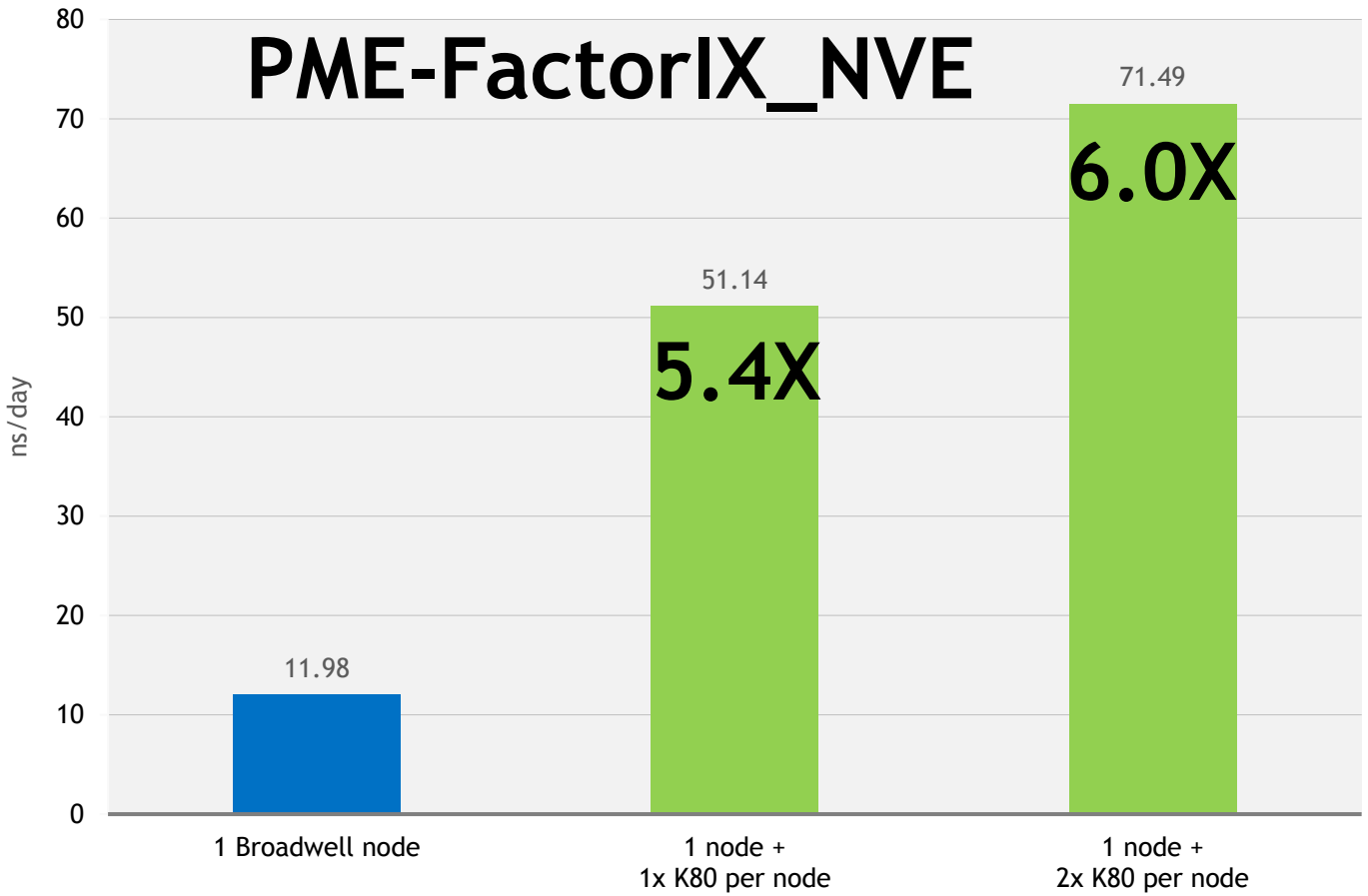

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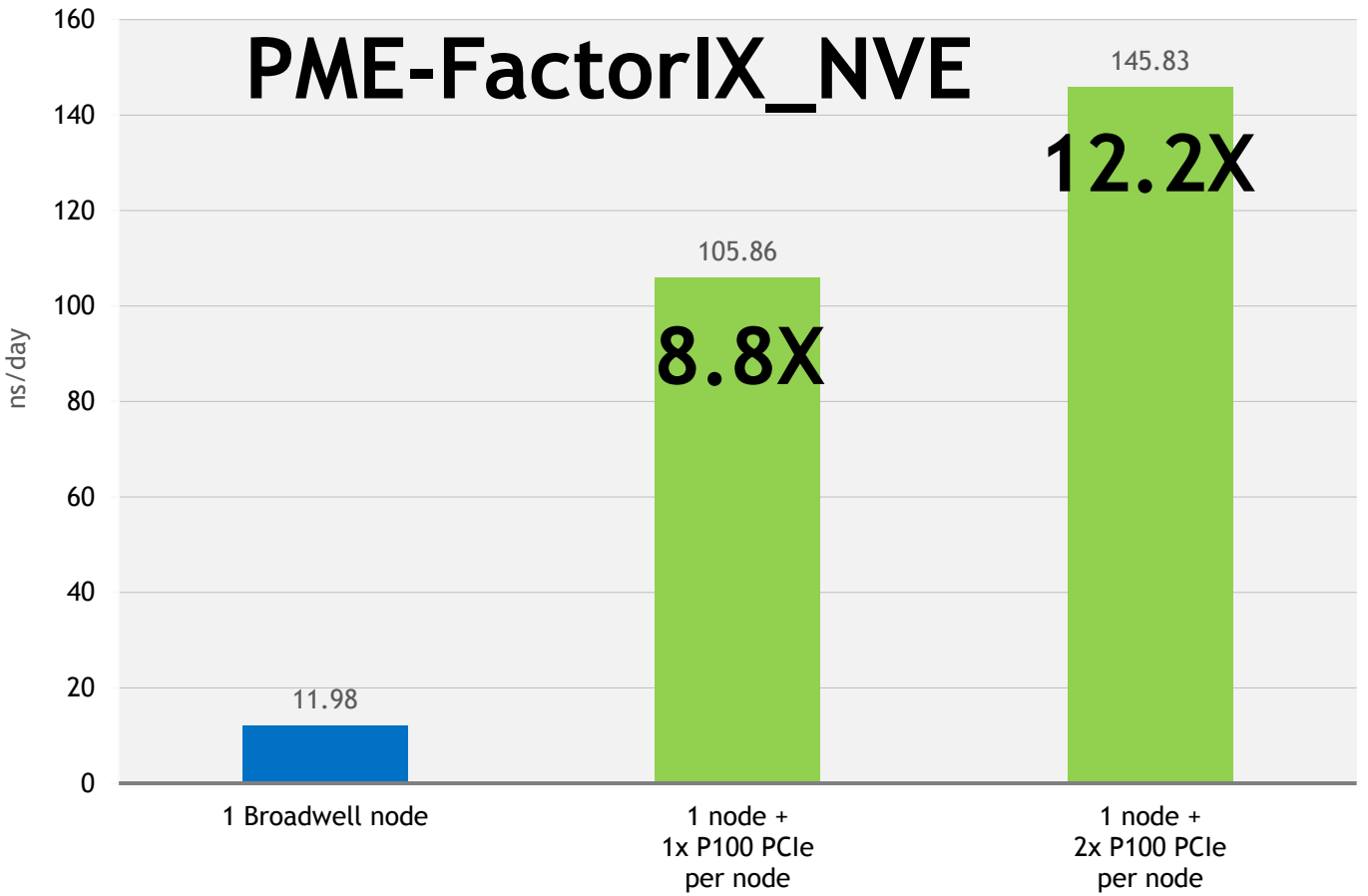

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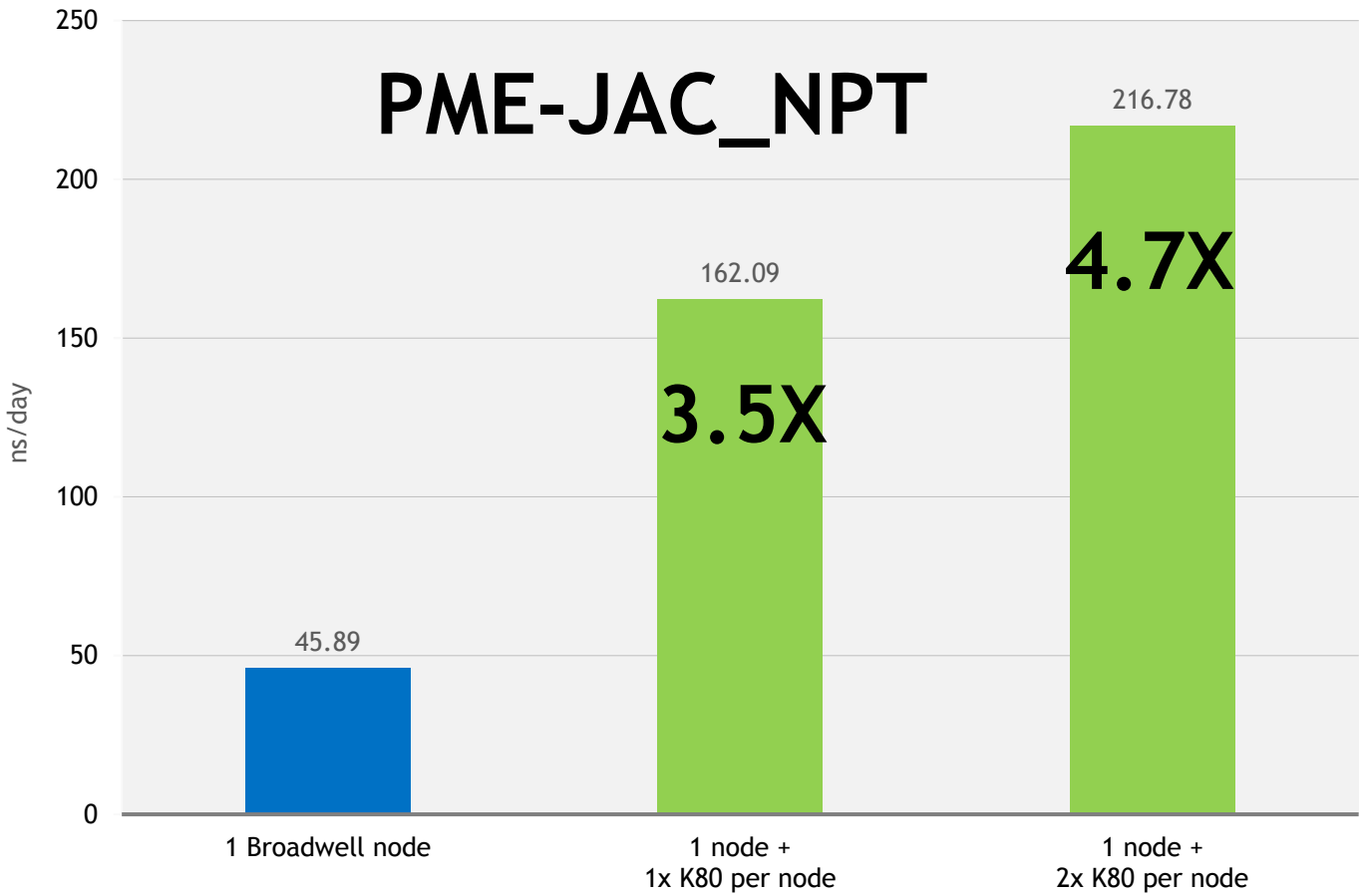
PME-JAC_NPT on K80s



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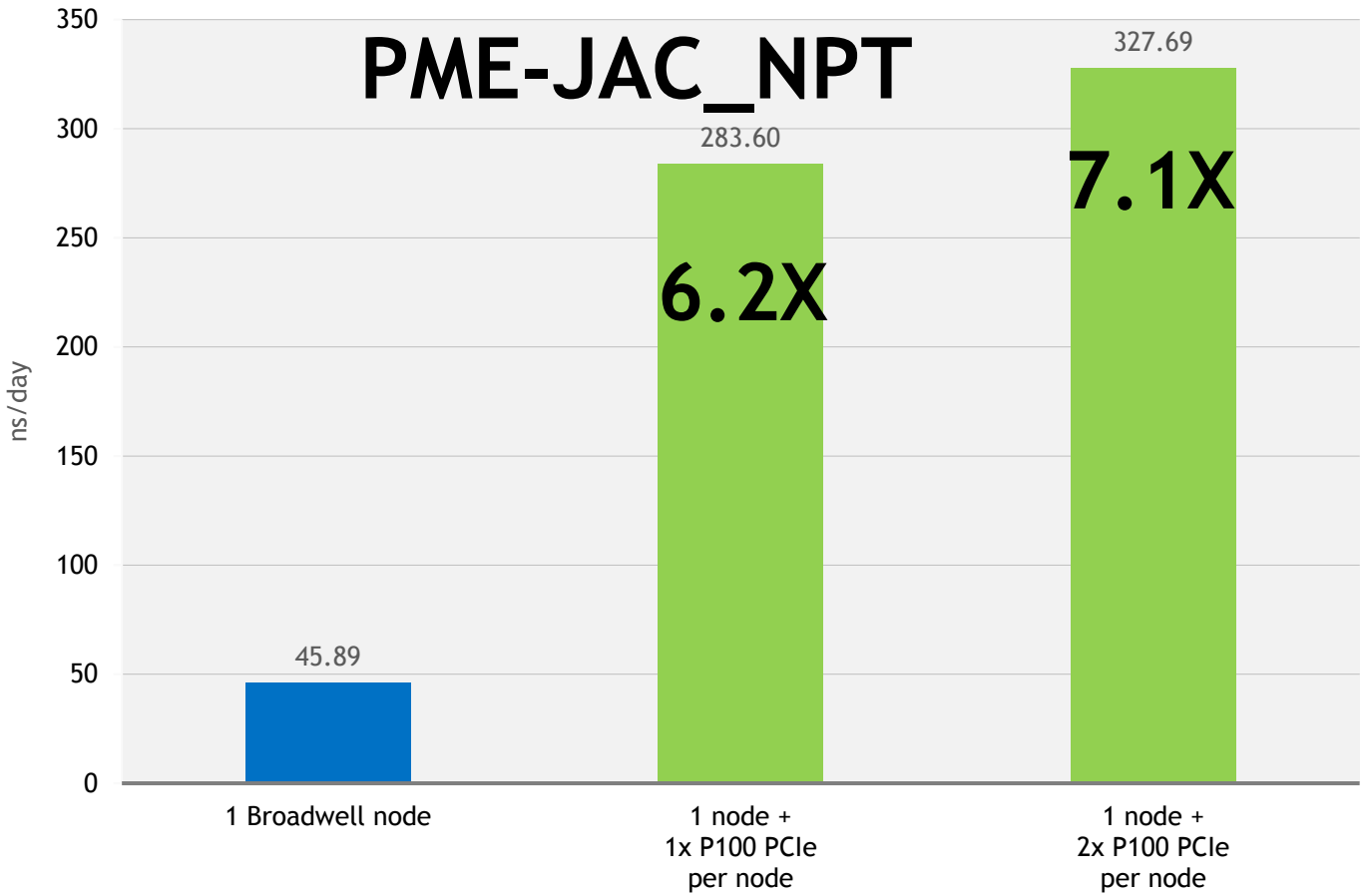

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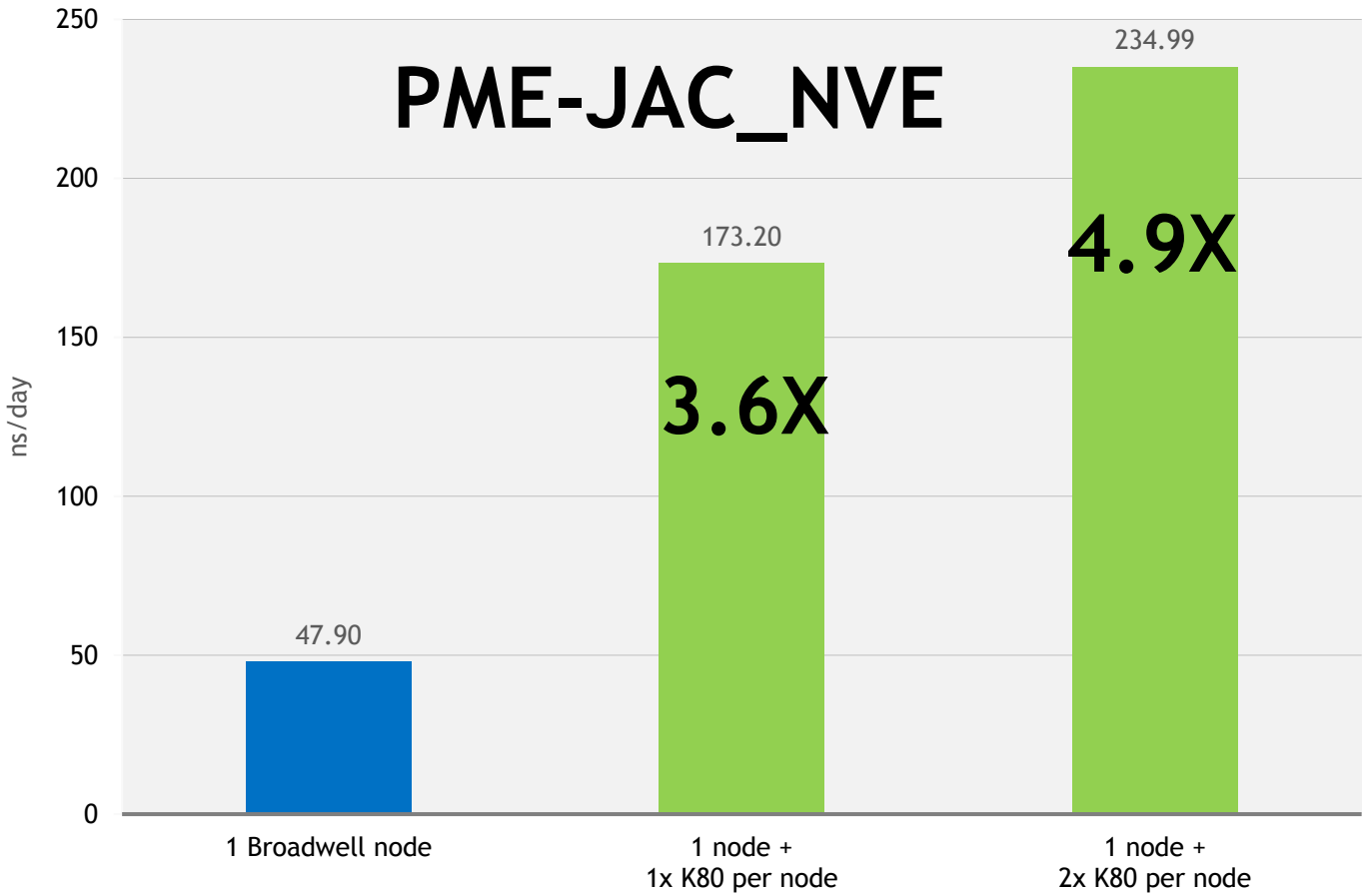

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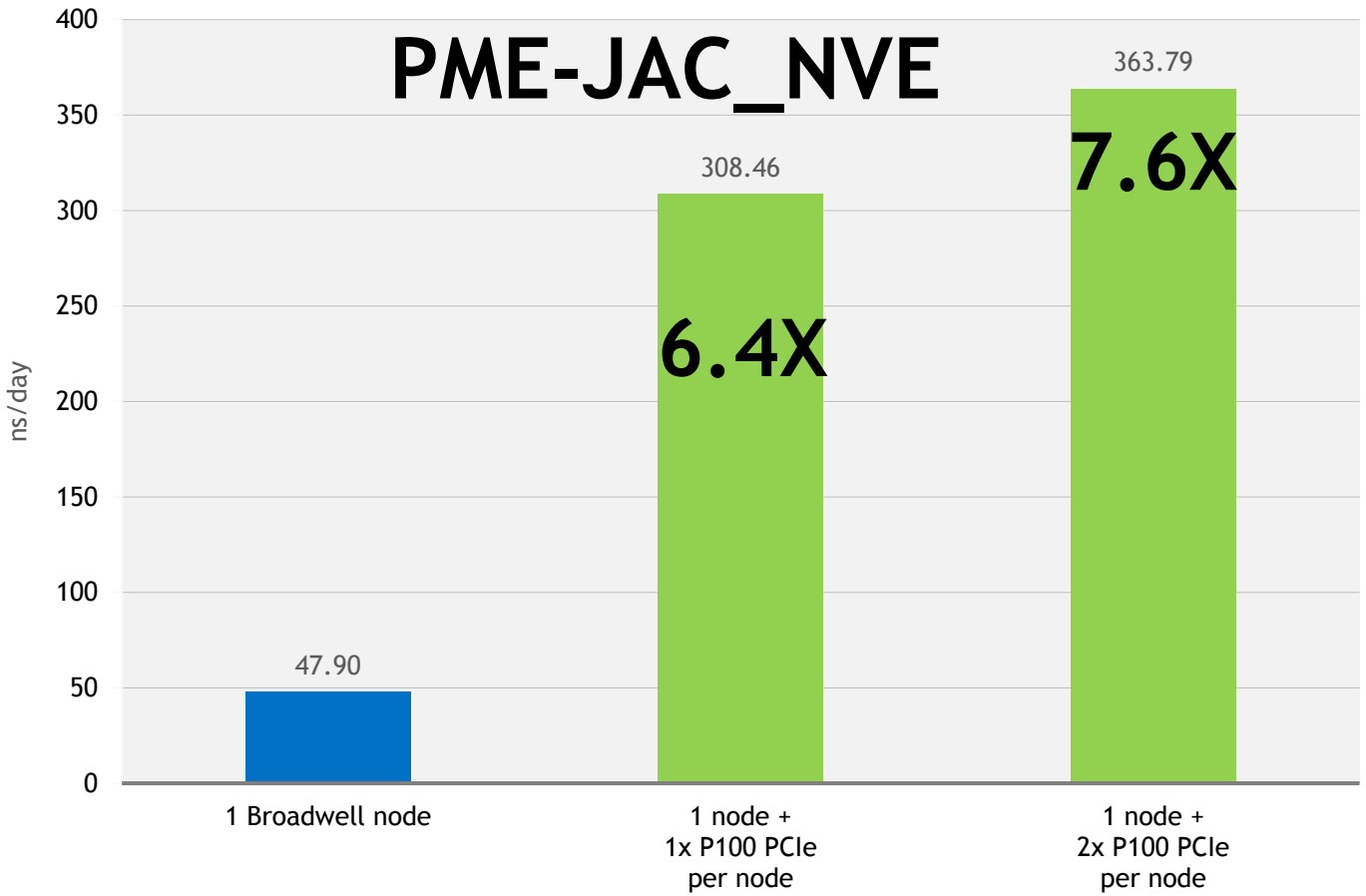

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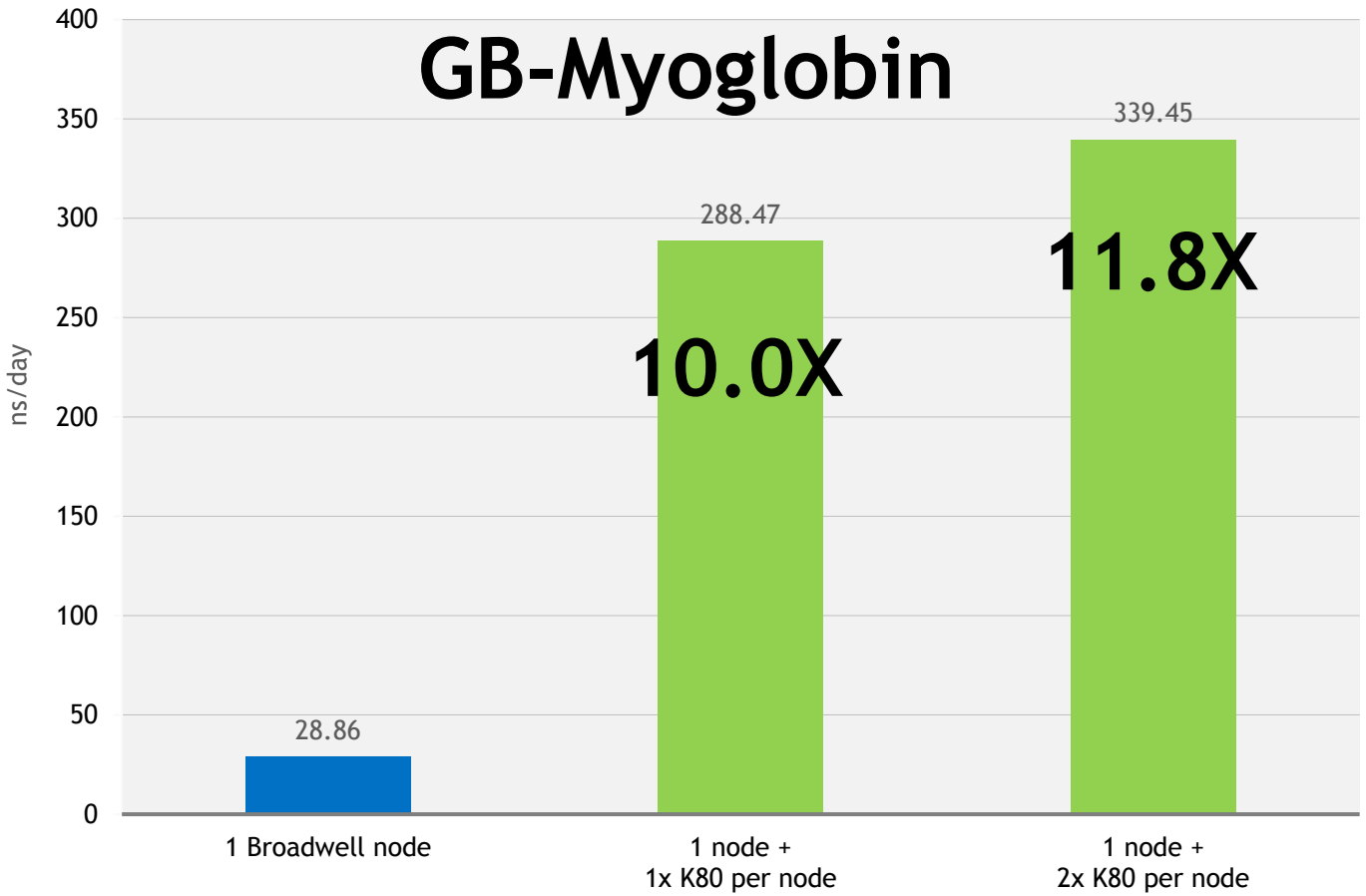
GB-Myoglobin on K80s



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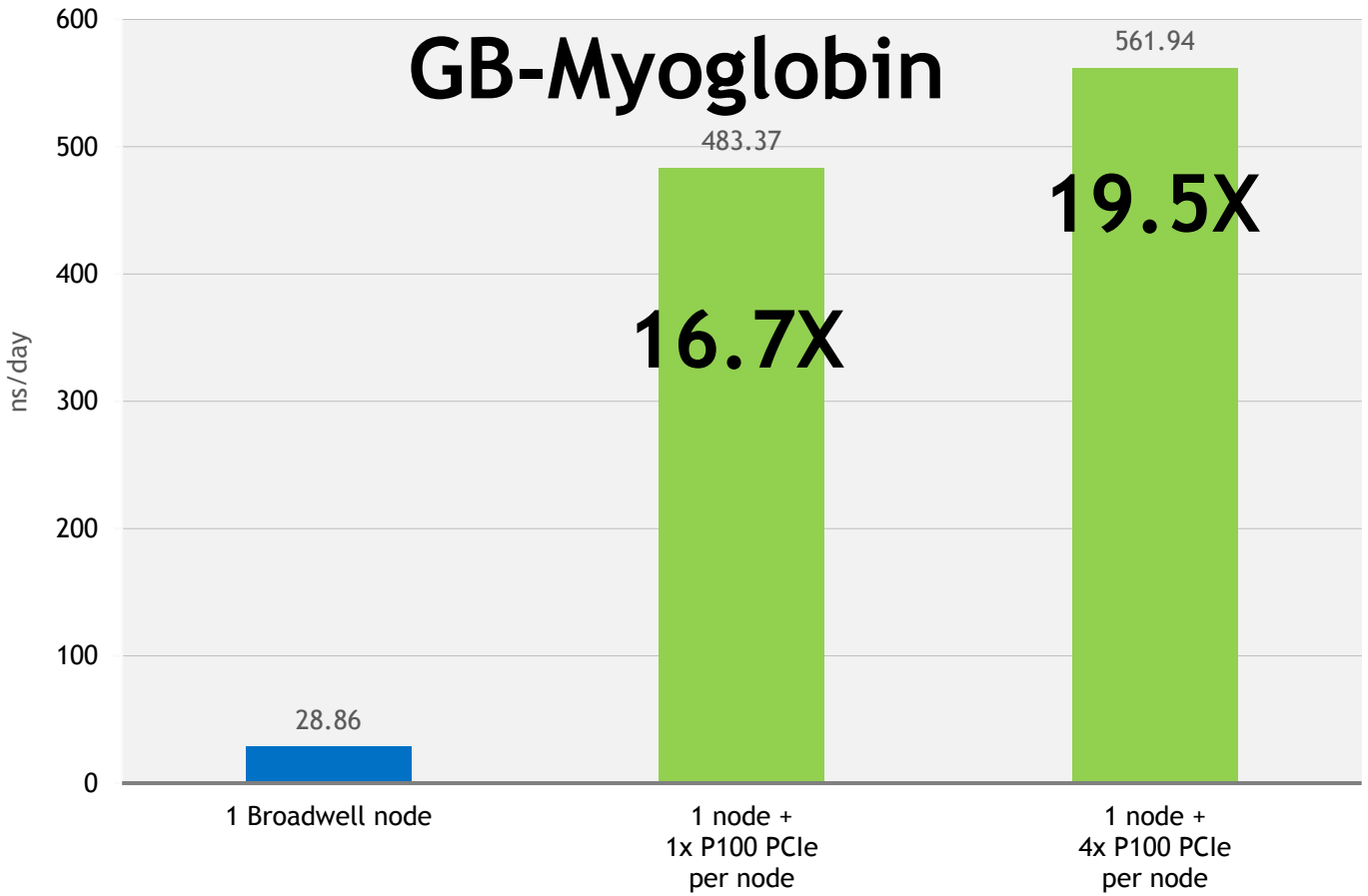
GB-Myoglobin on P100s PCIe



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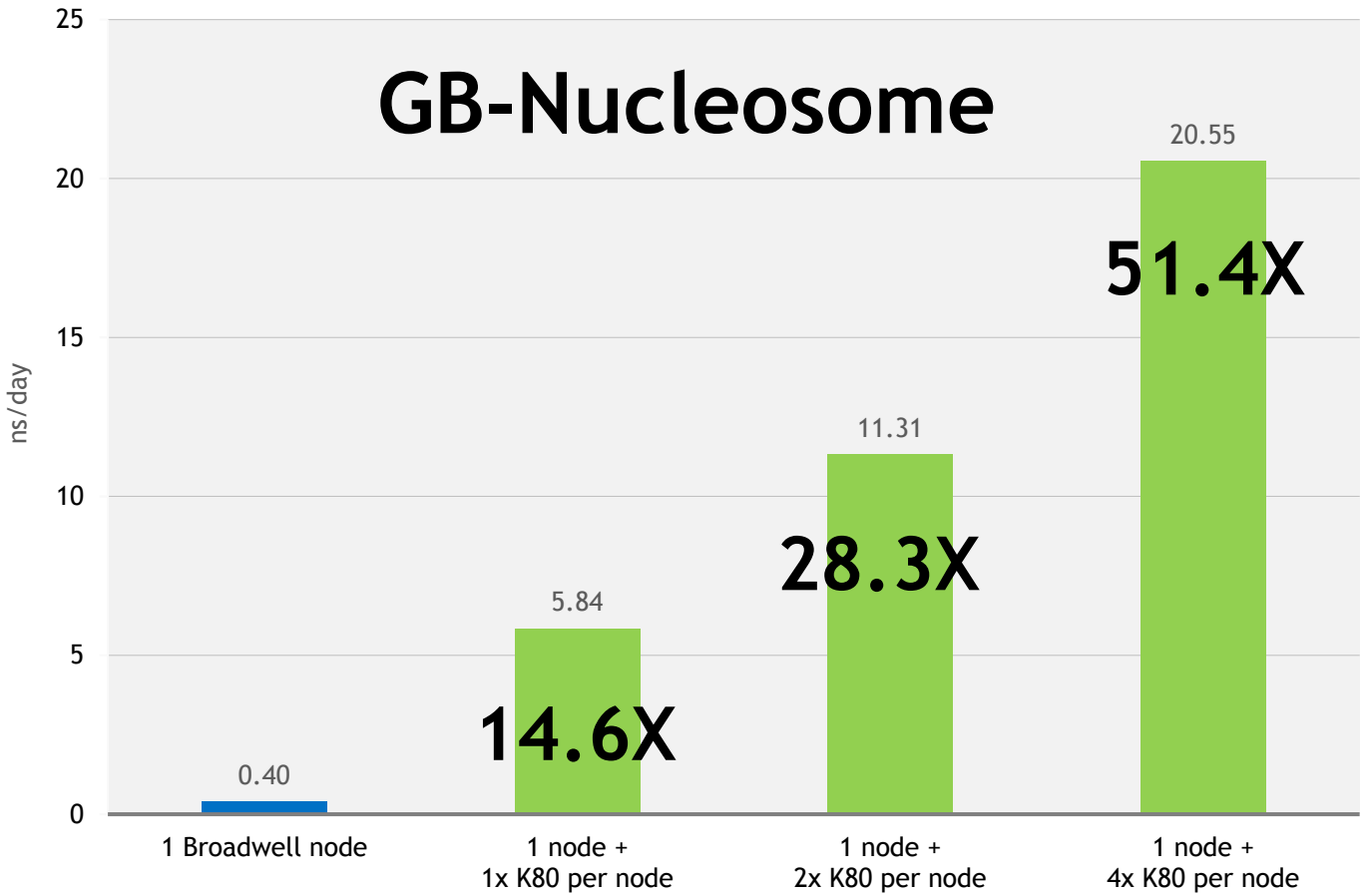
GB-Nucleosome on K80s



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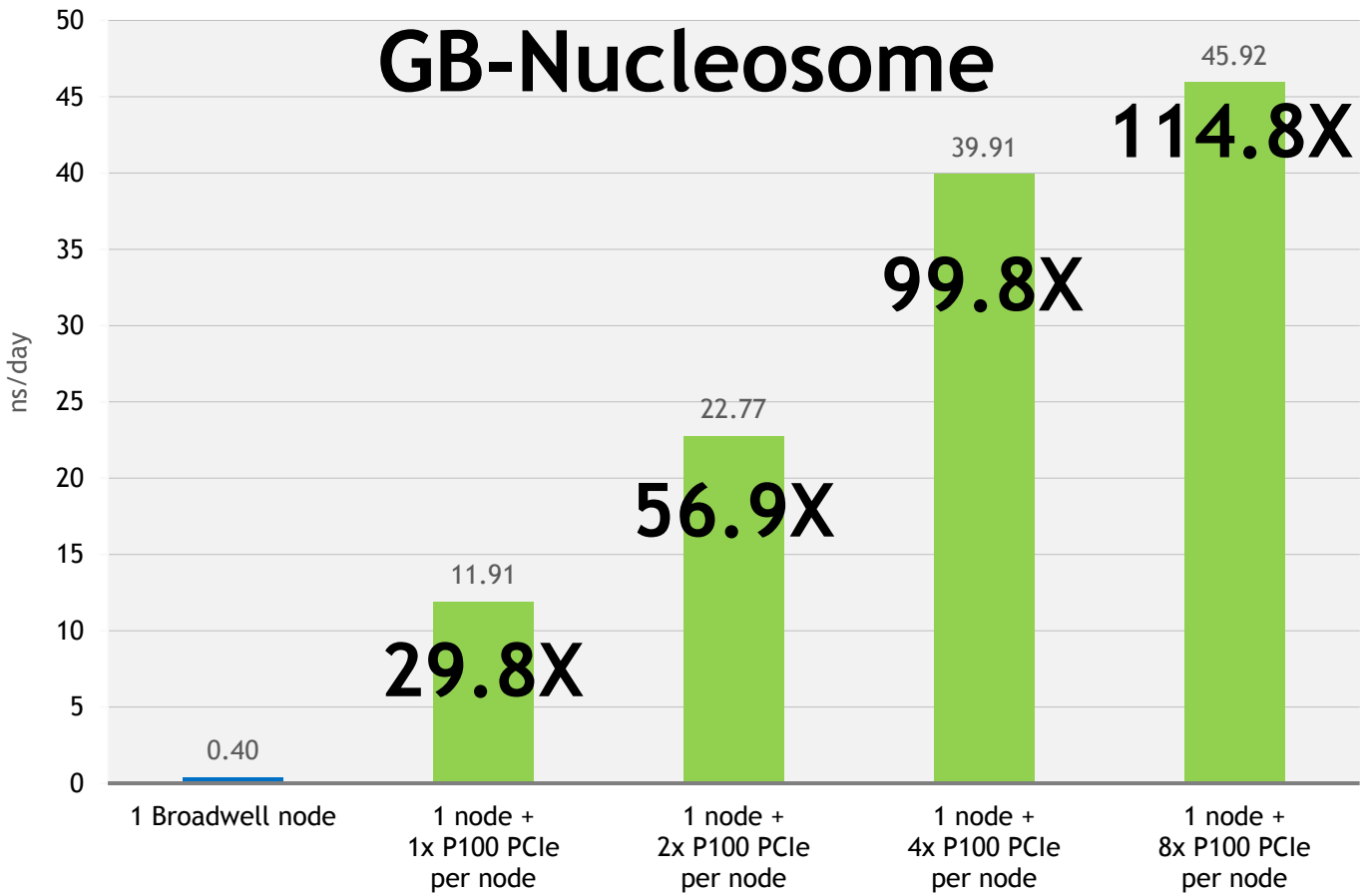
GB-Nucleosome on P100s PCIe



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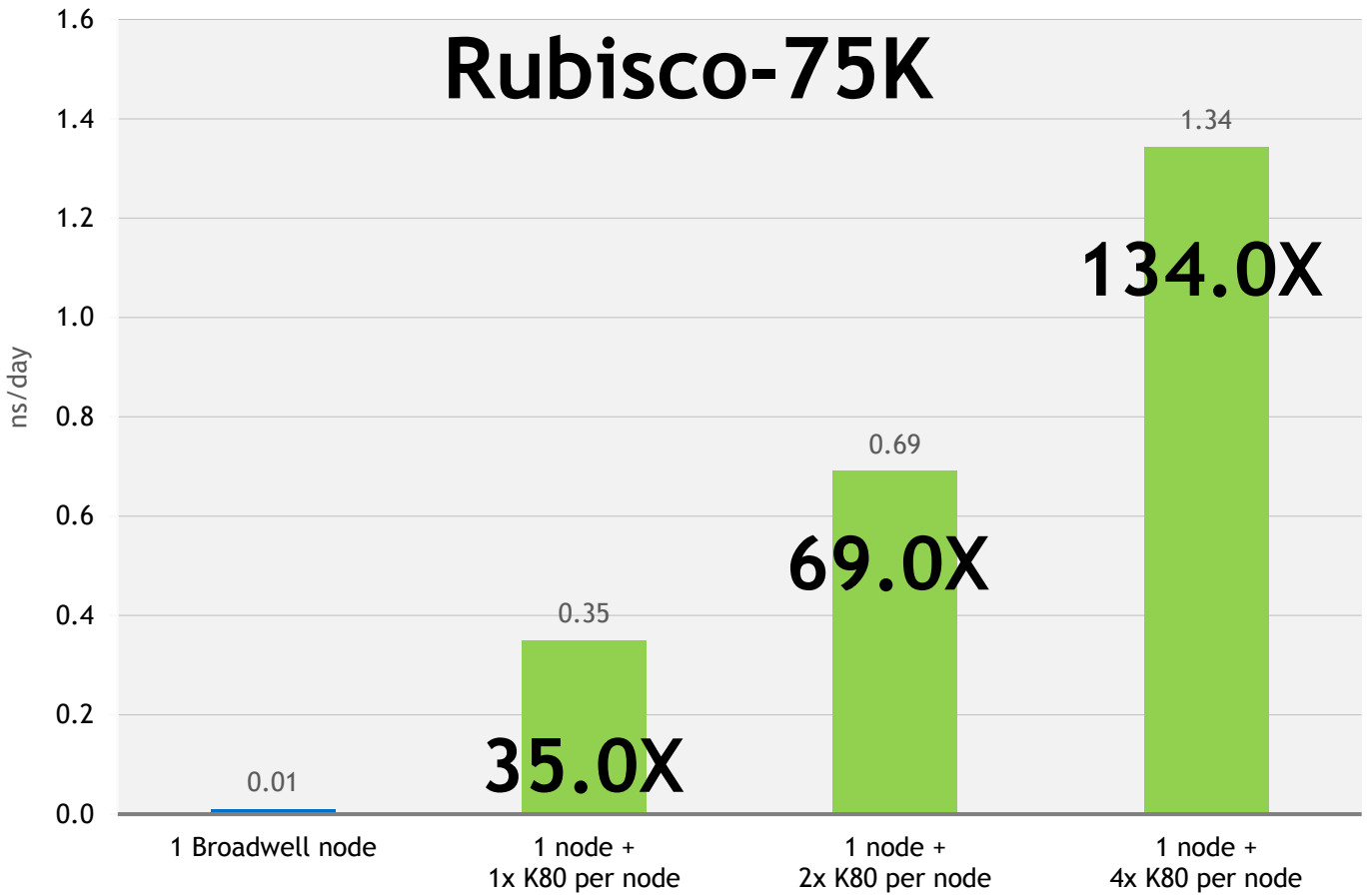
Rubisco-75K on K80s



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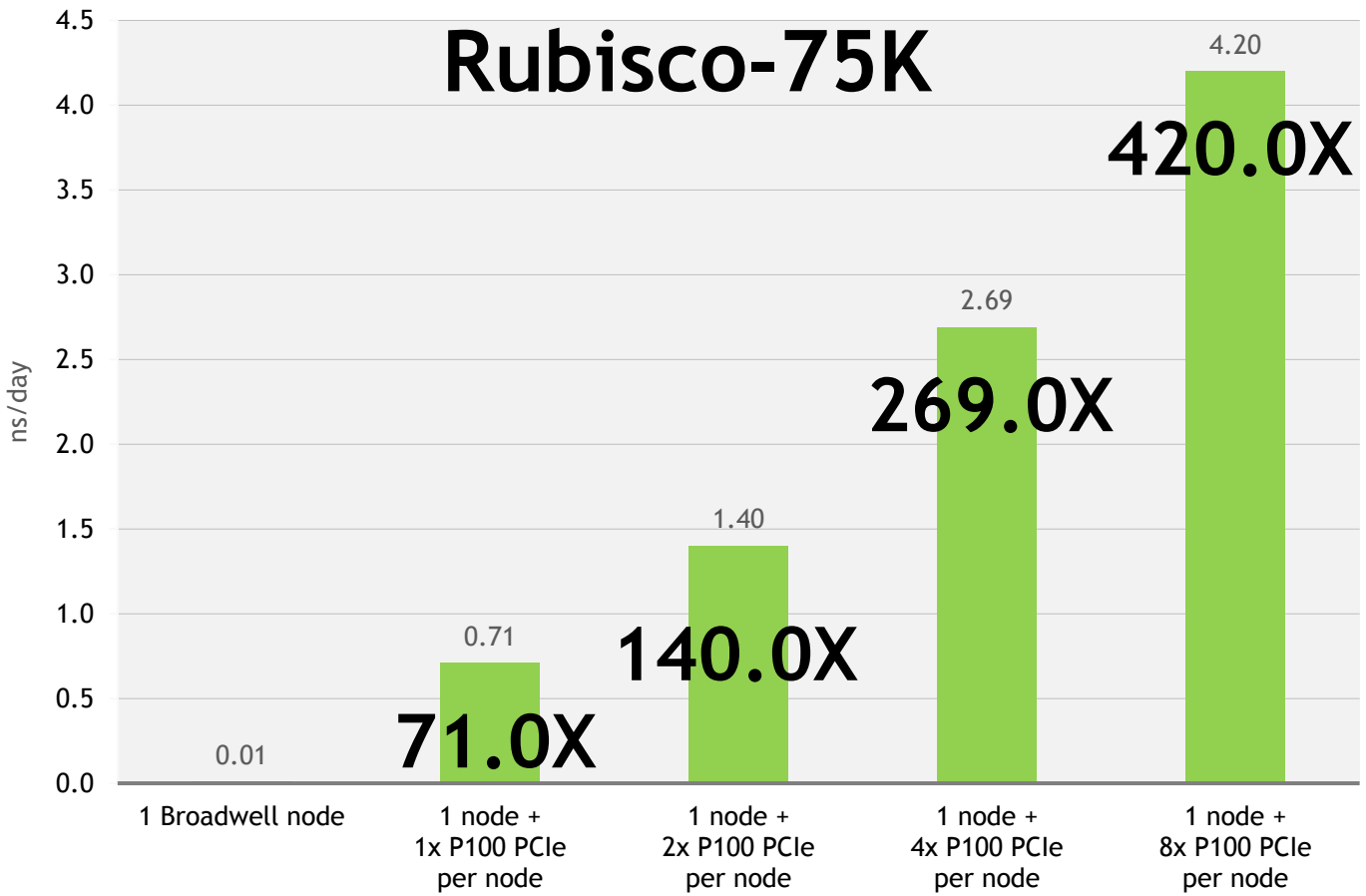
Rubisco-75K on P100s PCIe



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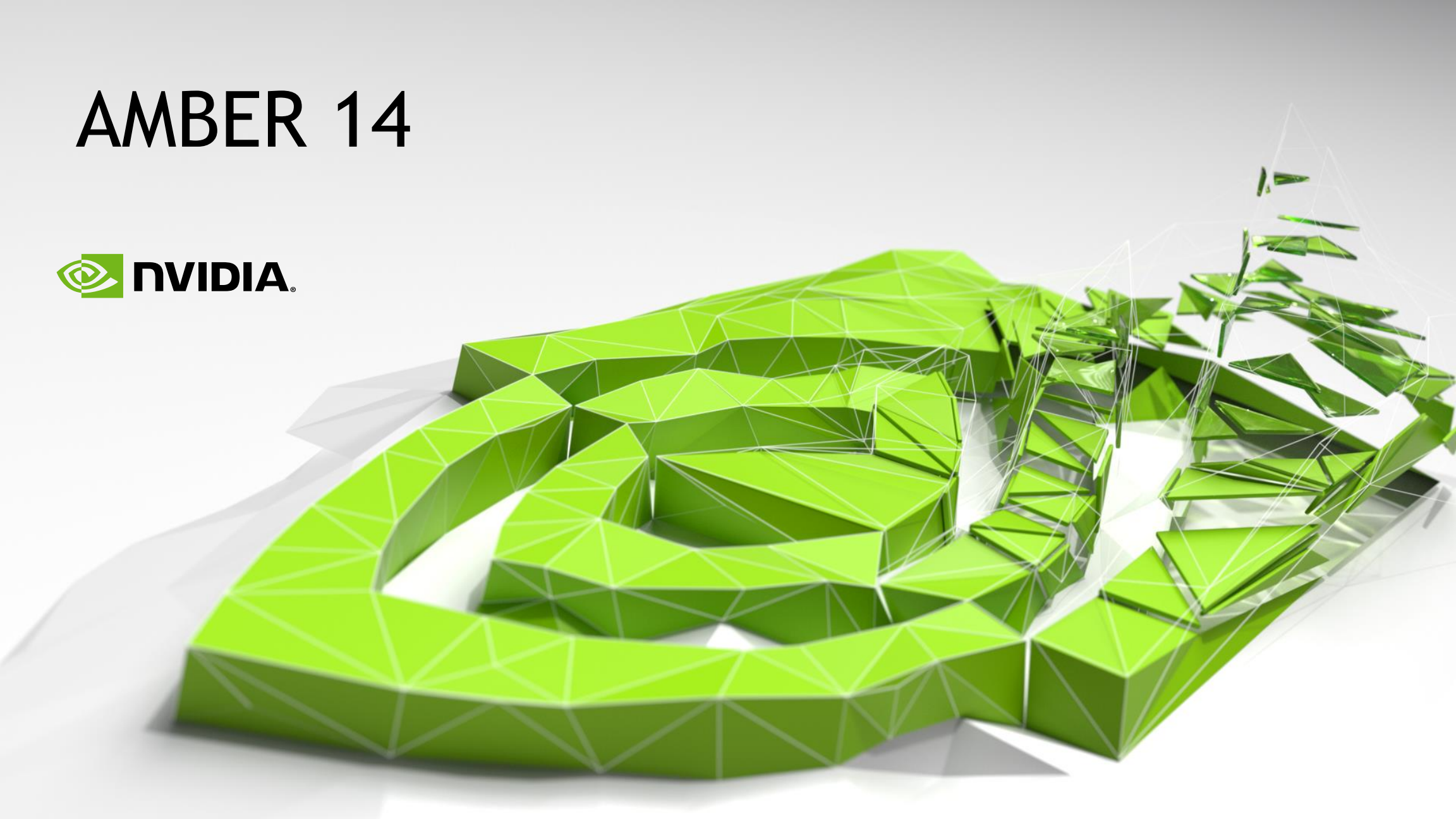
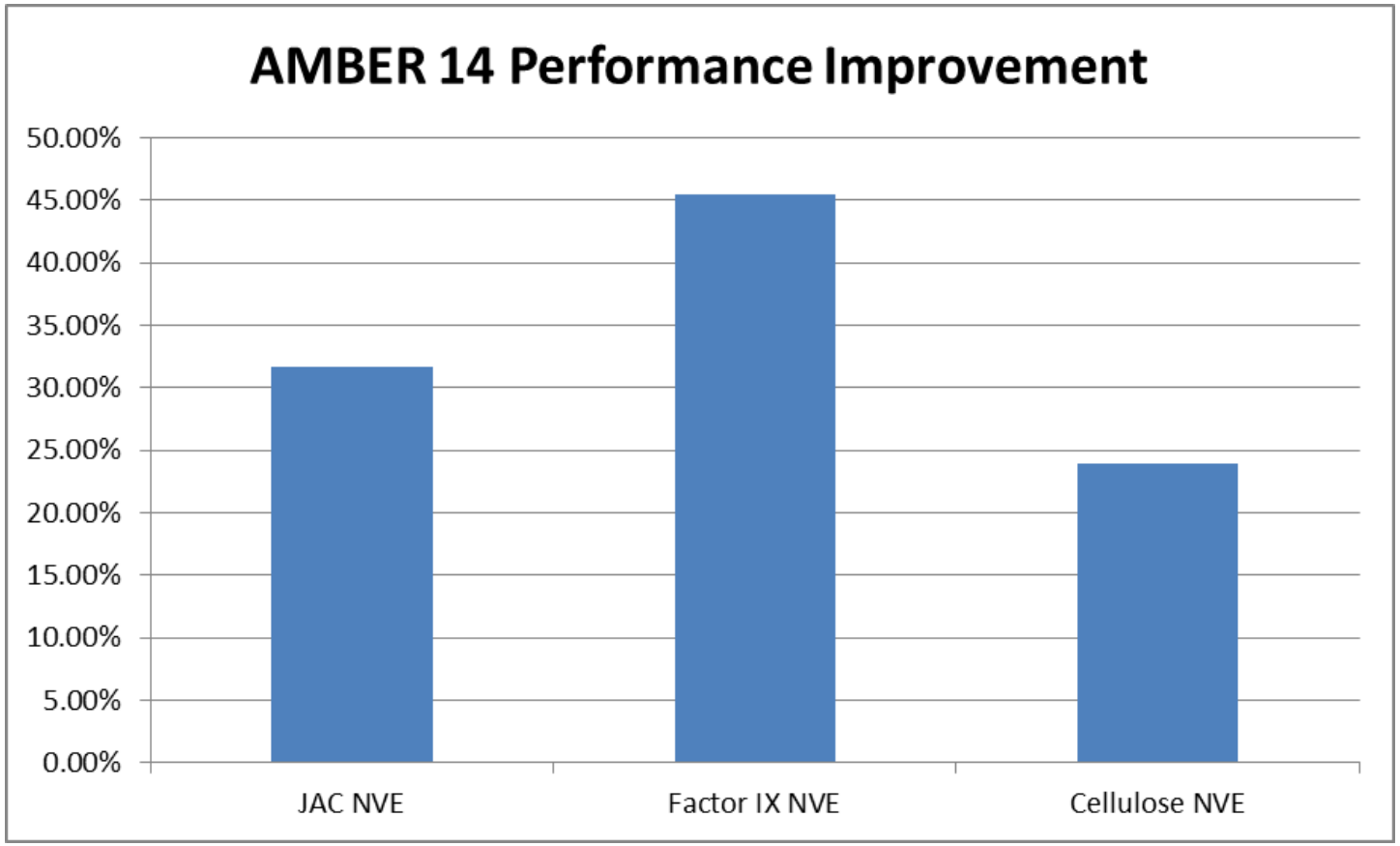
AMBER 14

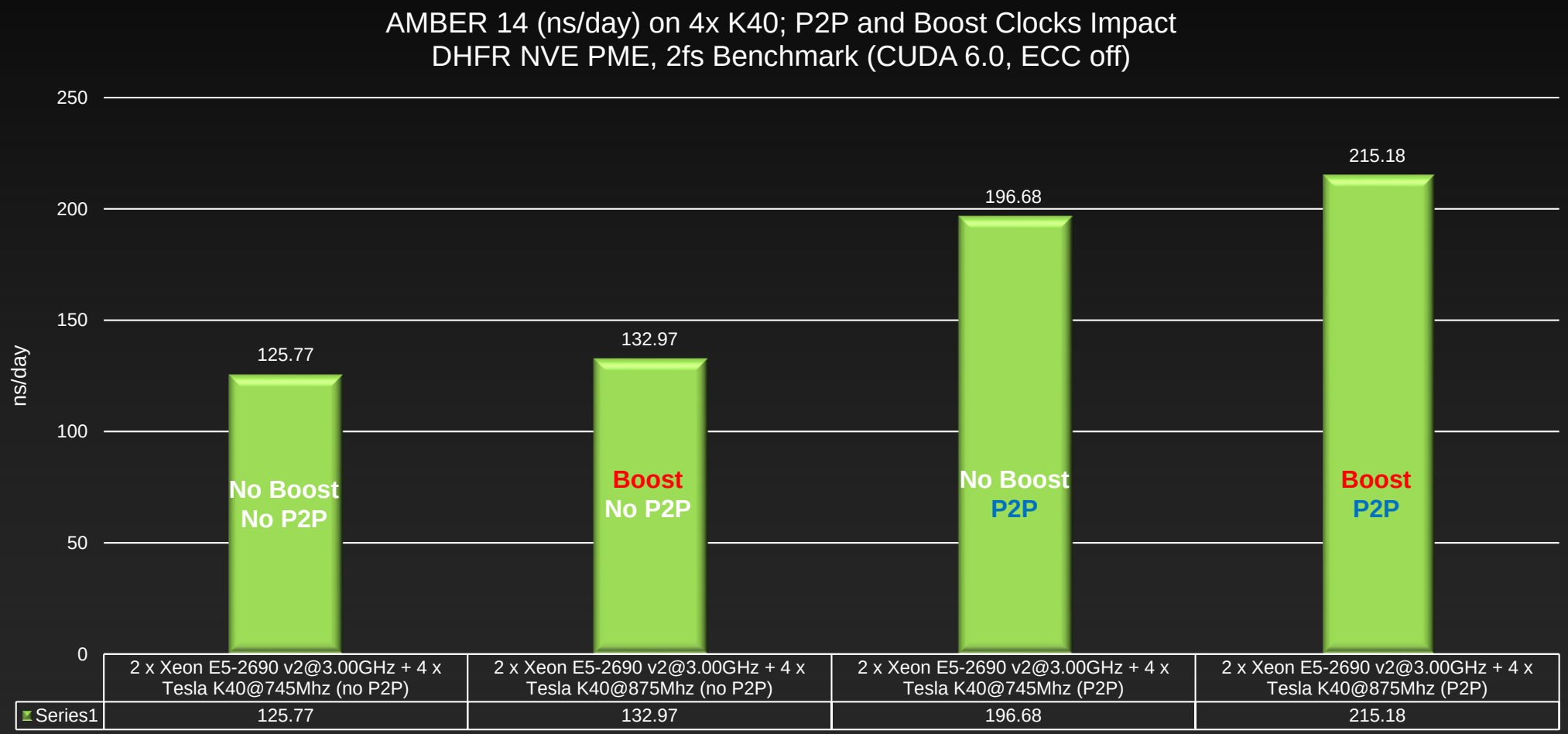


AMBER 14 vs. AMBER 12

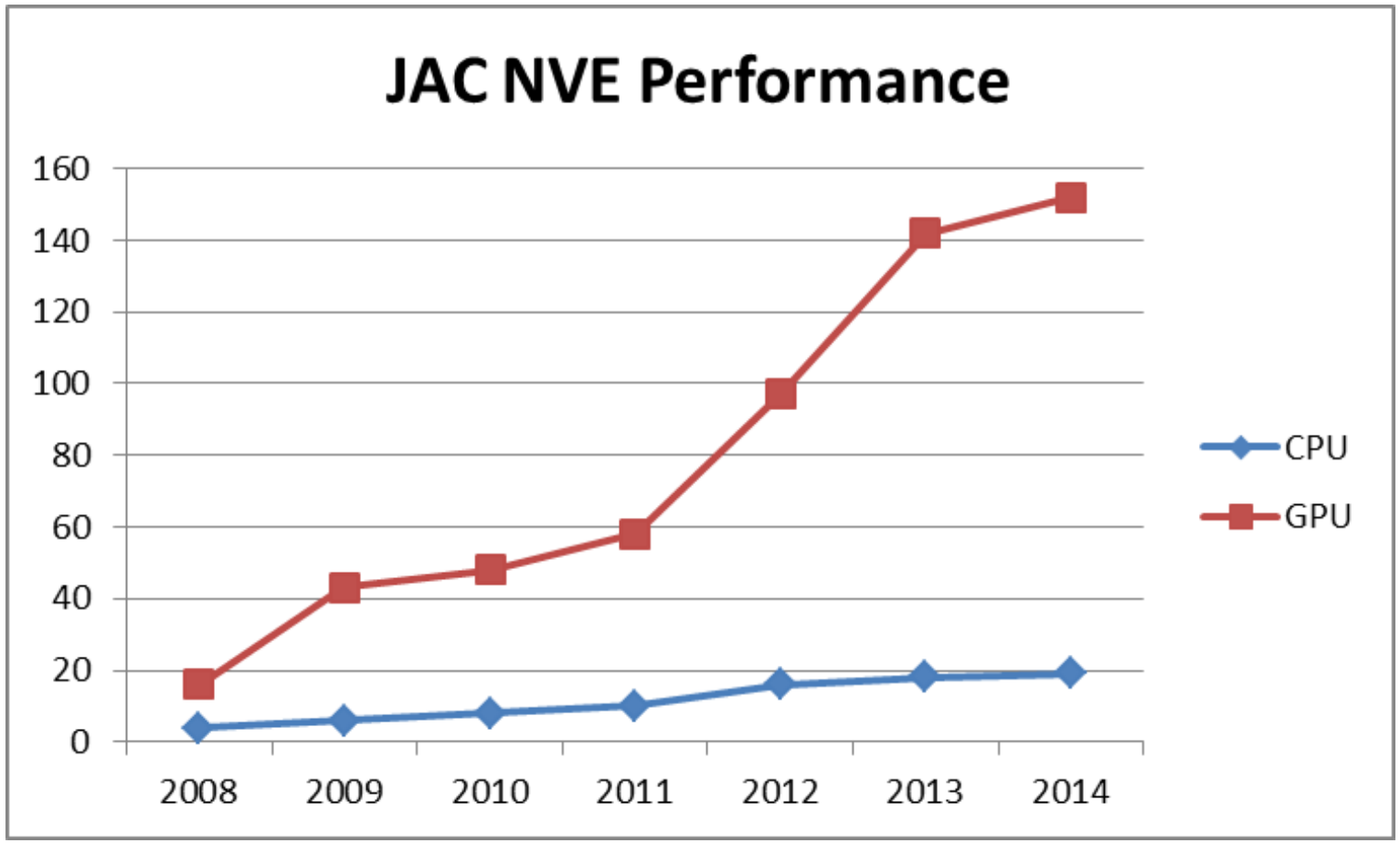


Courtesy of Scott Le Grand From GTC 2014 presentation

AMBER 14; large P2P and small Boost Clocks impacts

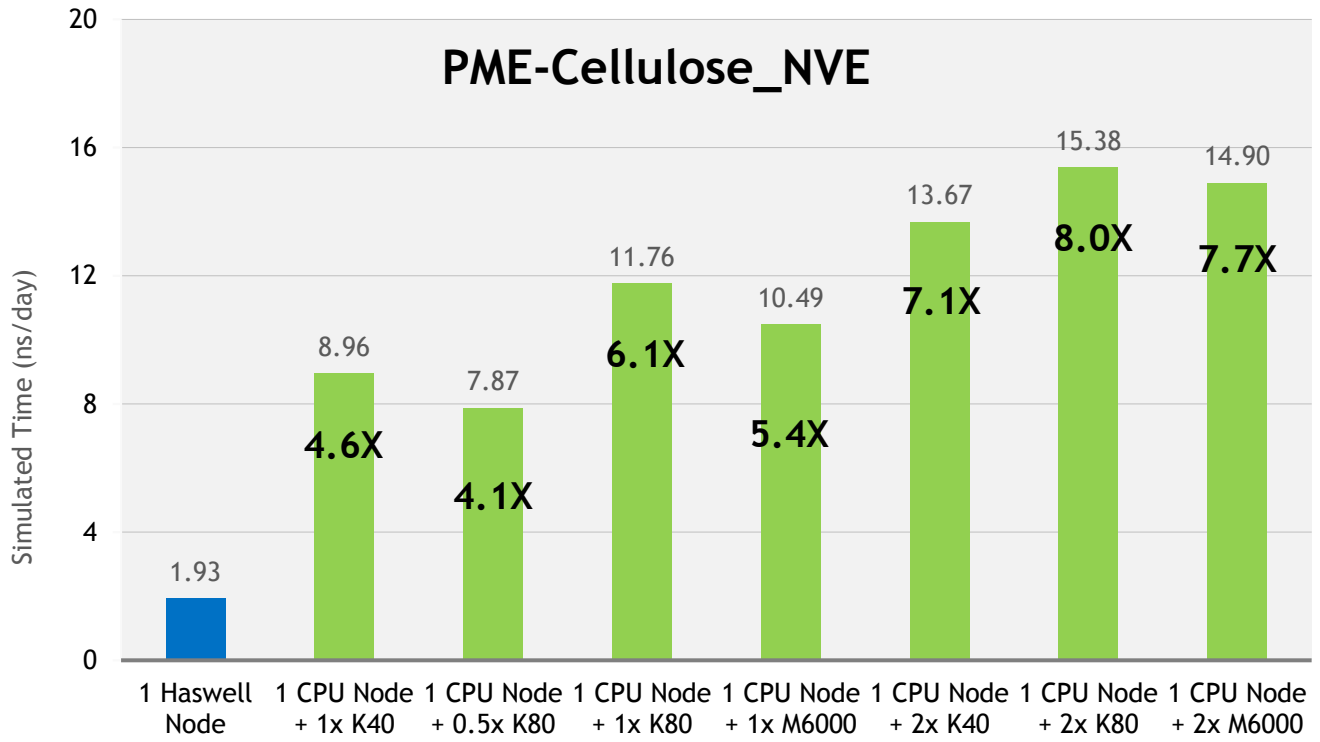


AMBER Performance Over Time



Courtesy of Scott Le Grand From GTC 2014 presentation

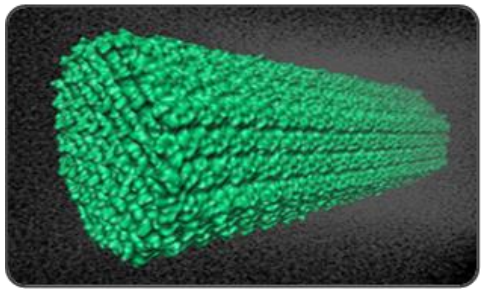
Cellulose on K40s, K80s and M6000s



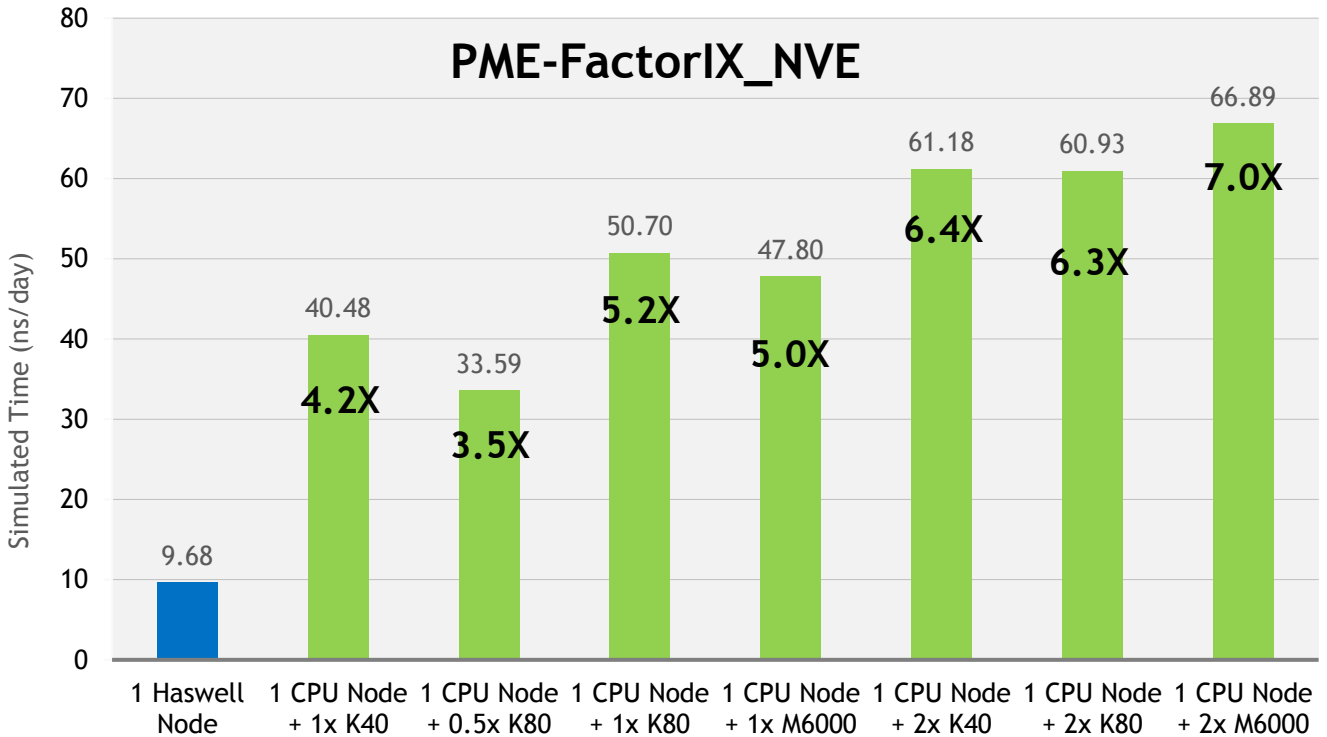
Running AMBER version 14

The blue node contains Dual Intel E5-2698 v3@2.3GHz, 3.6GHz Turbo CPUs

The green nodes contain Dual Intel E5-2698 v3@2.3GHz, 3.6GHz Turbo CPUs + either NVIDIA Tesla K40@875Mhz, Tesla K80@562Mhz (autoboost), or Quadro M6000@987Mhz GPUs



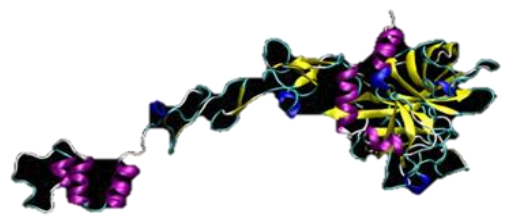
Factor IX on K40s, K80s and M6000s



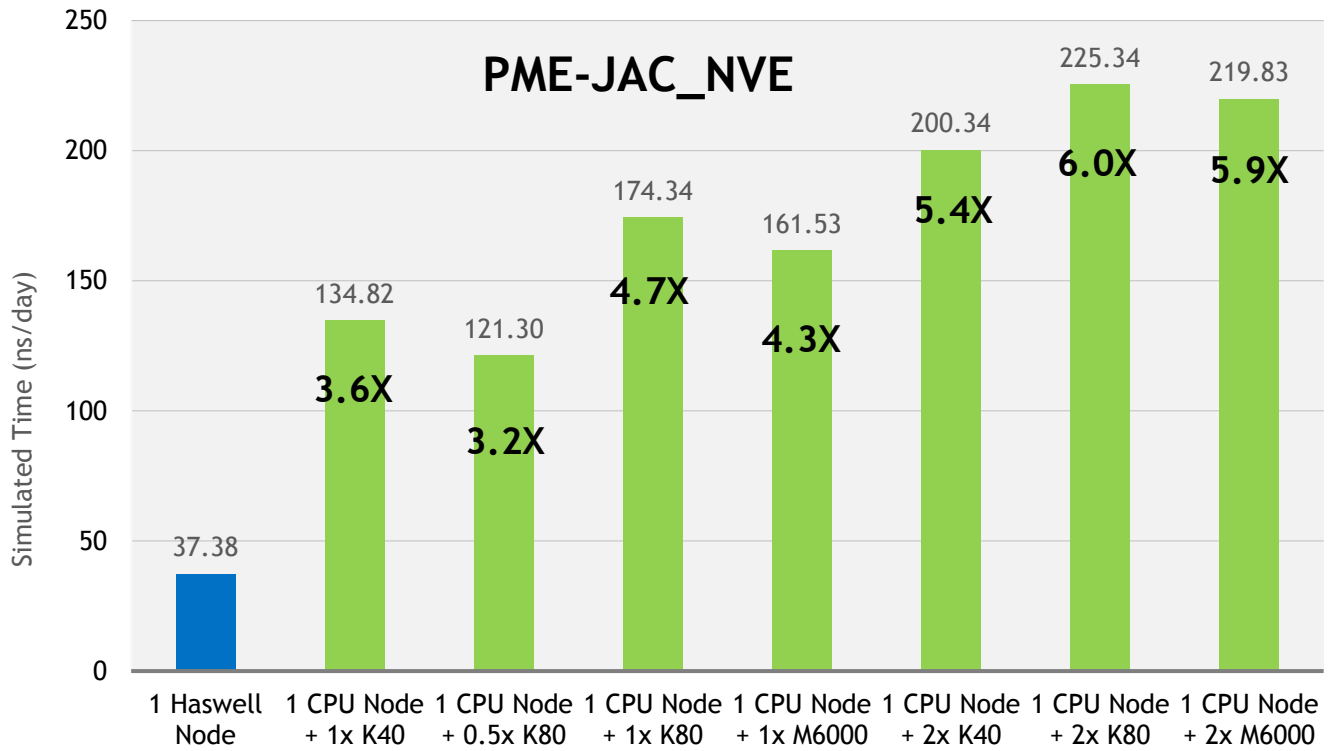
Running AMBER version 14

The blue node contains Dual Intel E5-2698 v3@2.3GHz, 3.6GHz Turbo CPUs

The green nodes contain Dual Intel E5-2698 v3@2.3GHz, 3.6GHz Turbo CPUs + either NVIDIA Tesla K40@875Mhz, Tesla K80@562Mhz (autoboost), or Quadro M6000@987Mhz GPUs



JAC on K40s, K80s and M6000s



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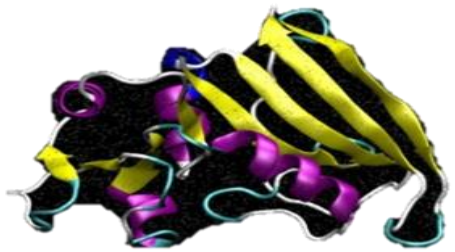
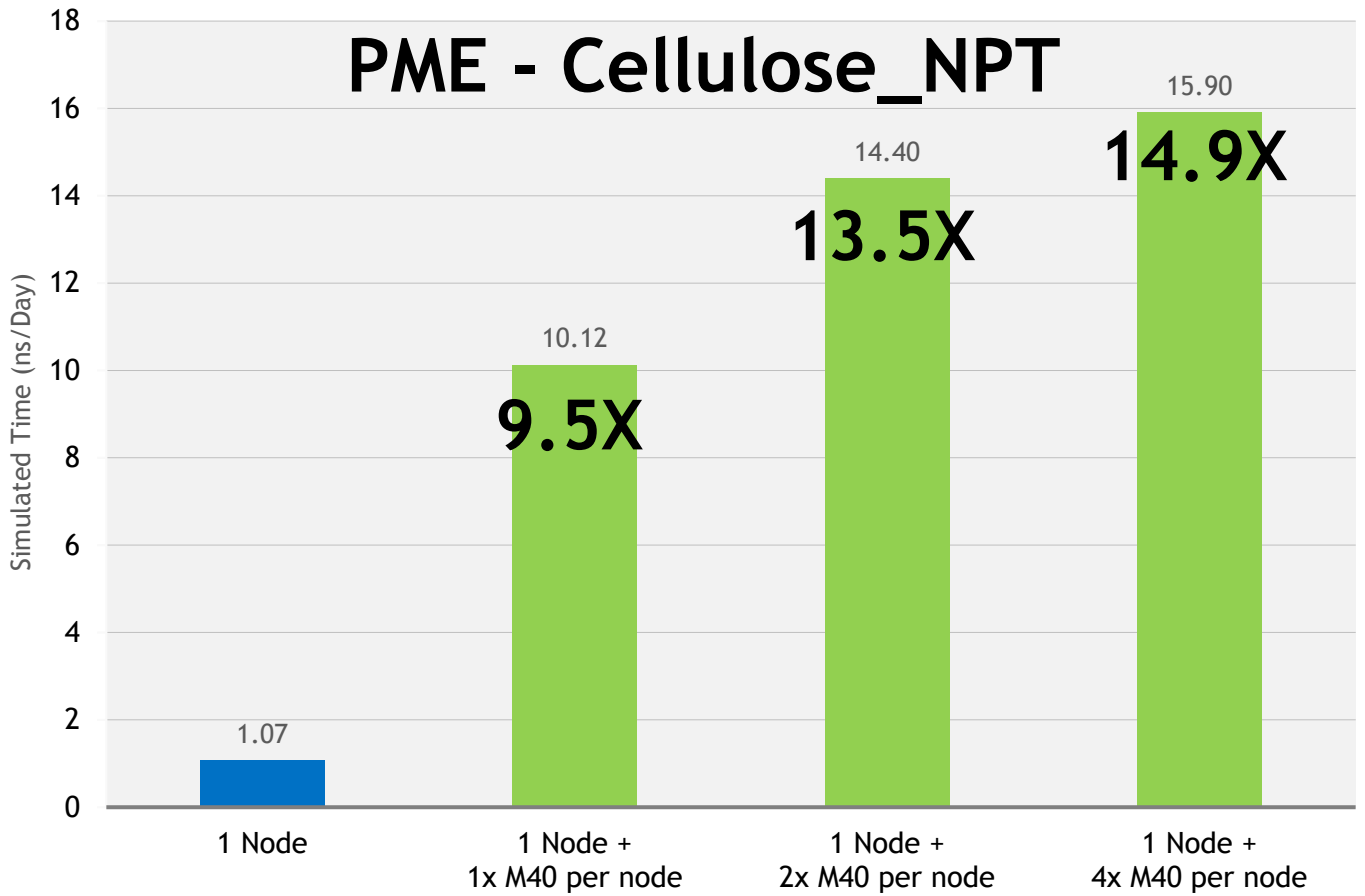


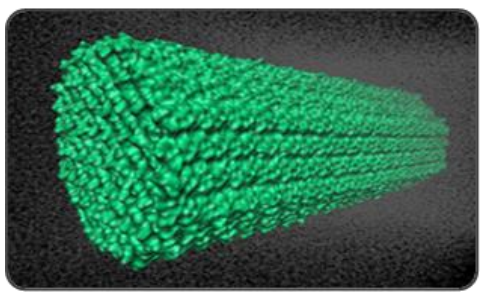
Cellulose on M40s



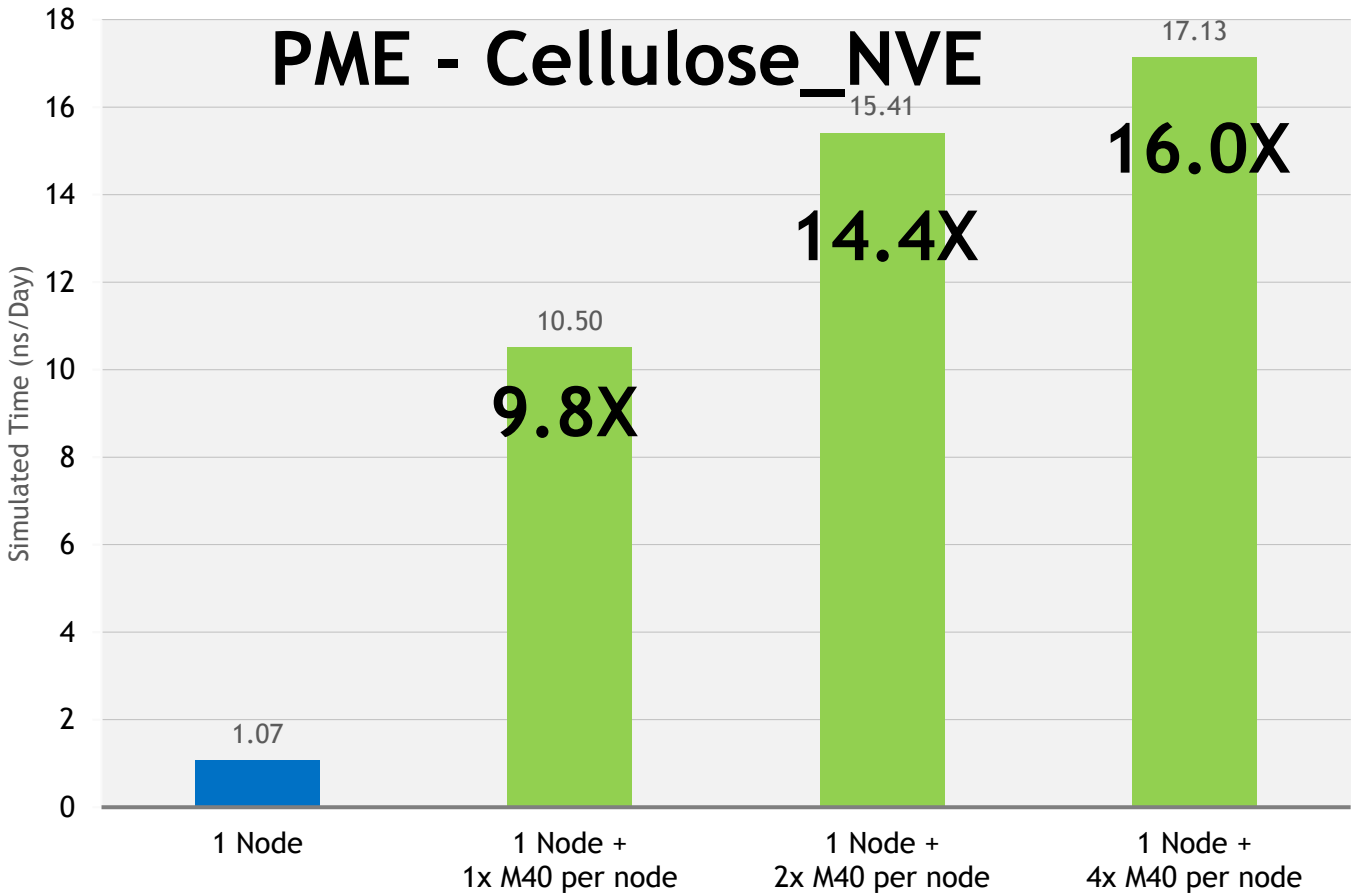
Running AMBER version 14

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

The green nodes contain Single Intel Xeon E5-2697 v2@2.70GHz (IvyBridge) CPUs + Tesla M40 (autoboost) GPUs



Cellulose on M40s



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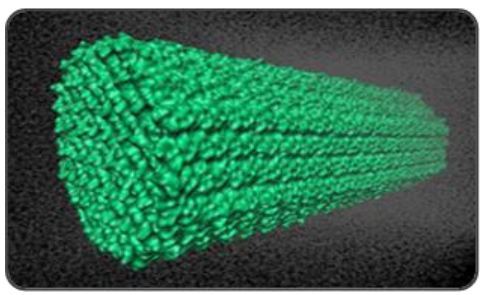
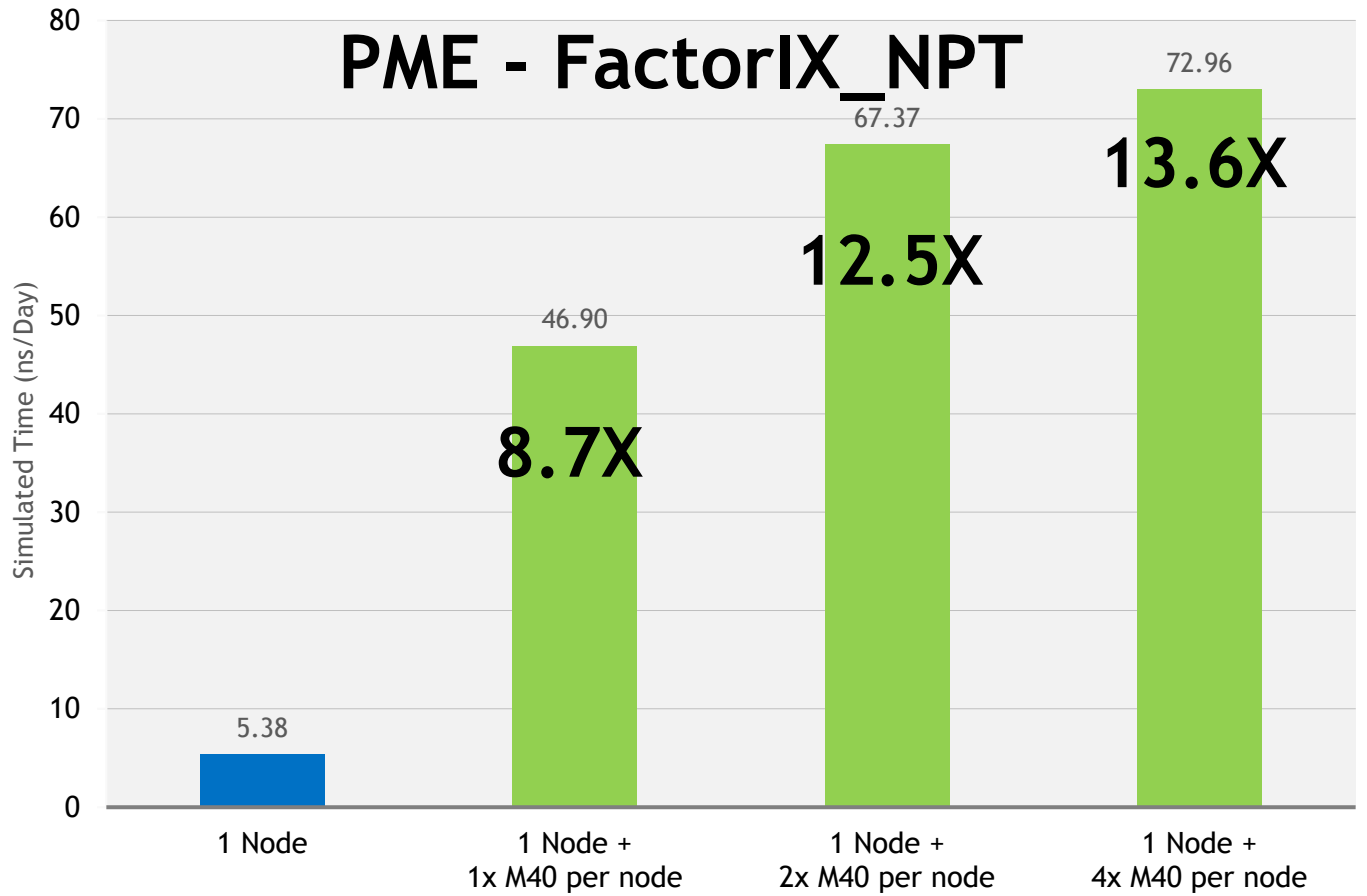


FactorIX on M40s



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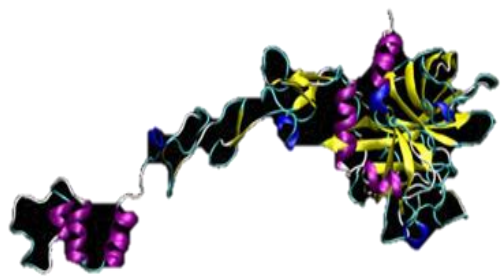
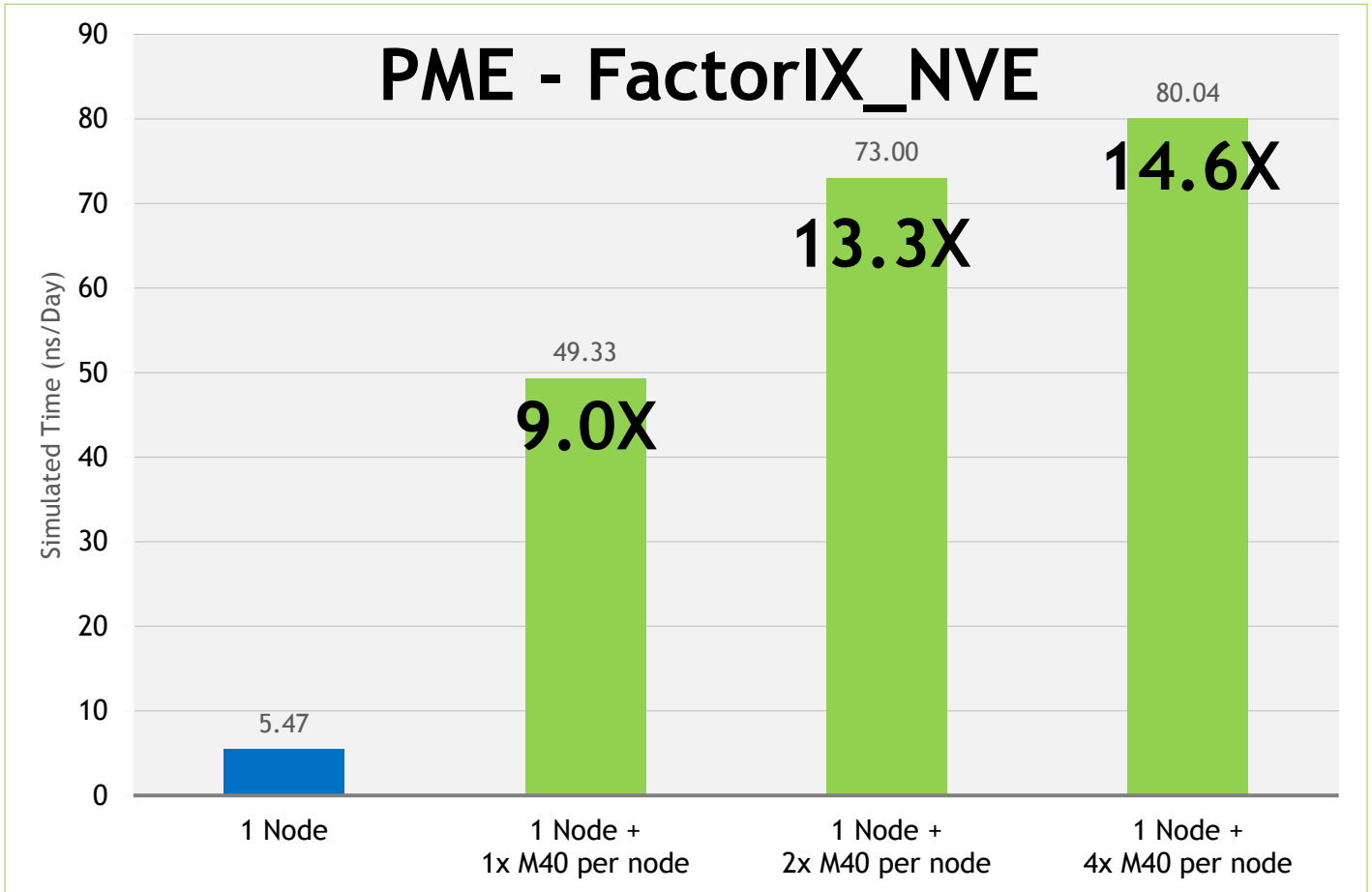


FactorIX on M40s



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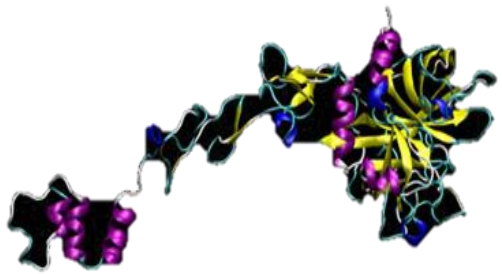
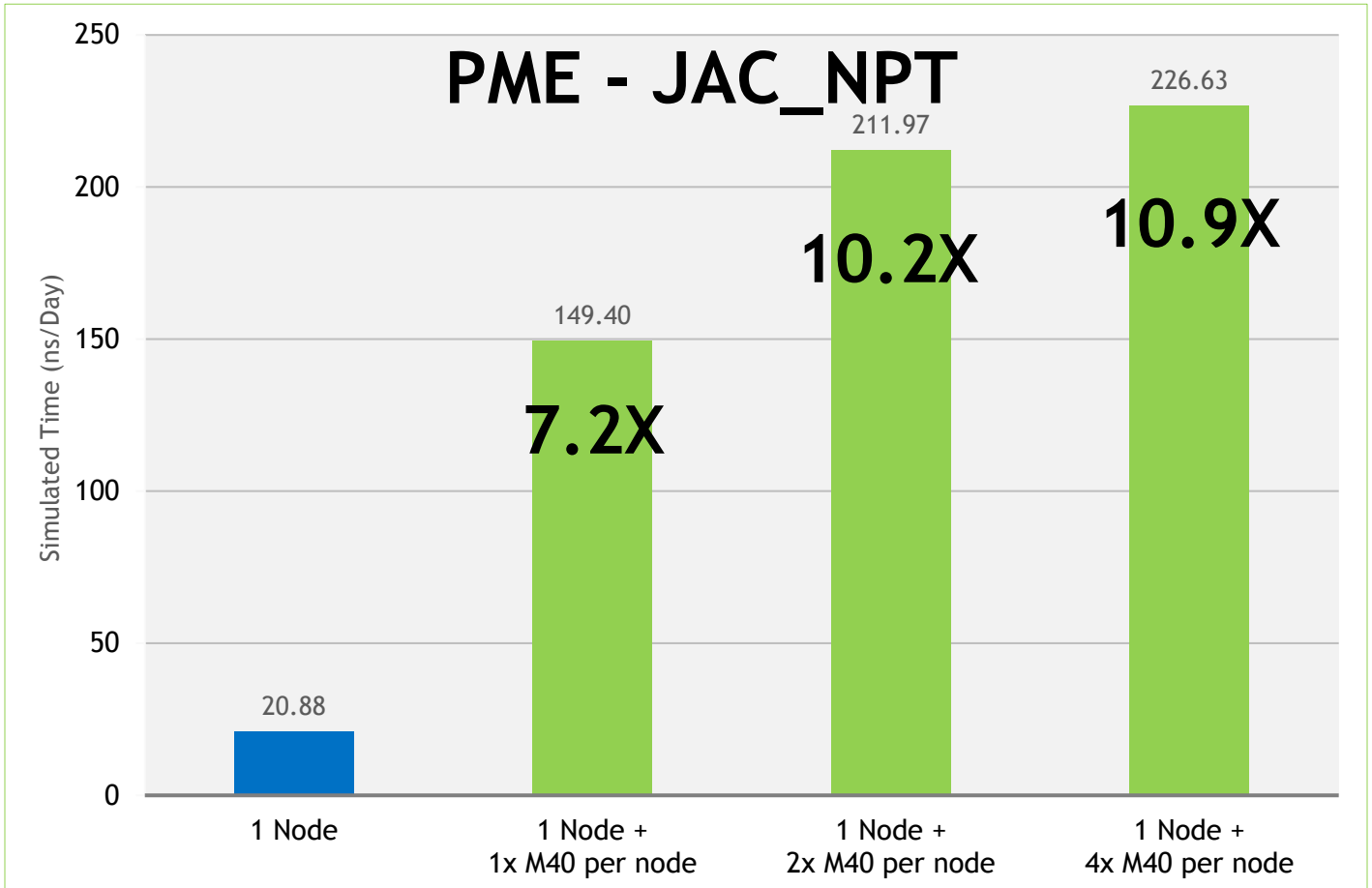


JAC on M40s



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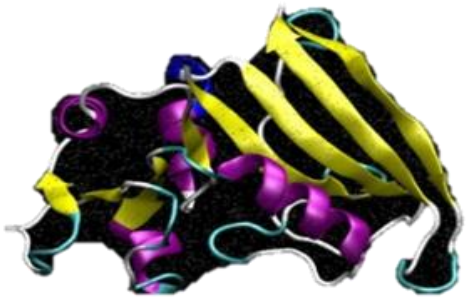
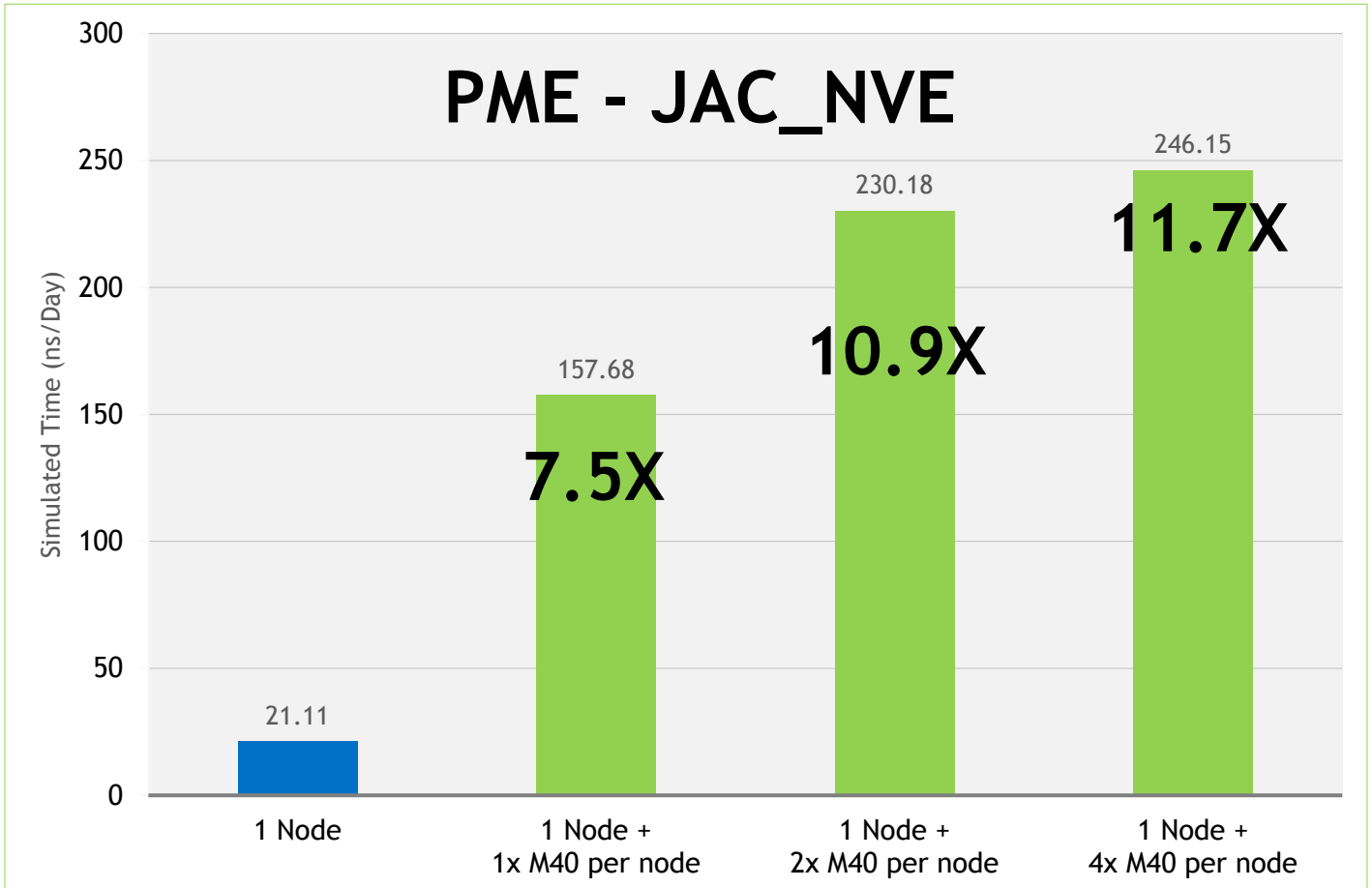


JAC on M40s



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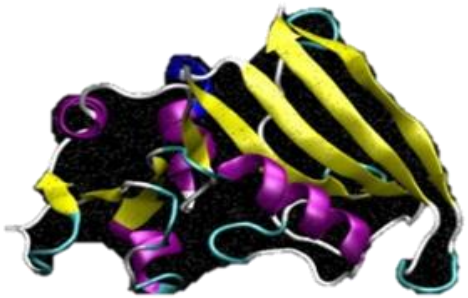
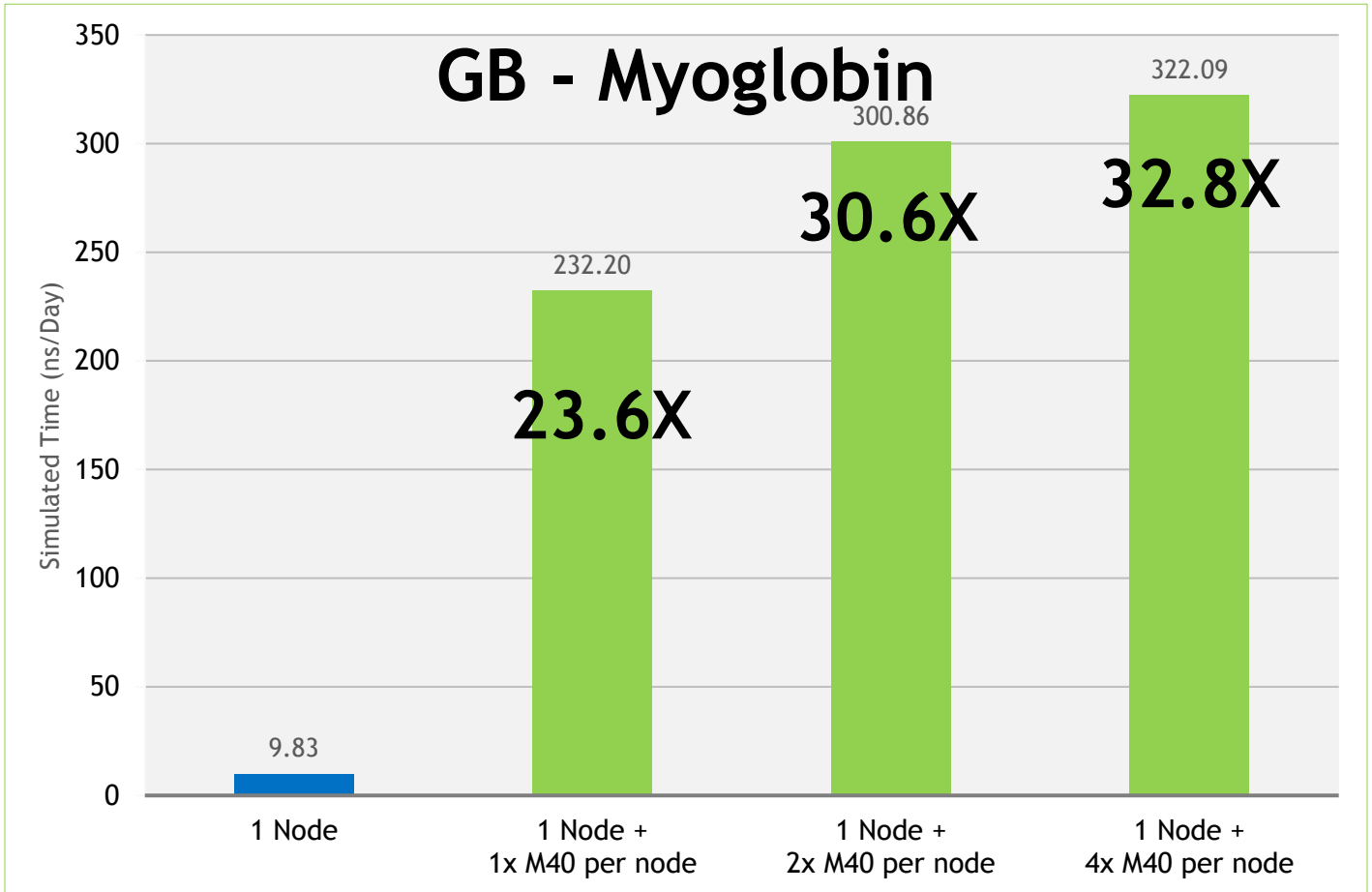


Myoglobin on M40s



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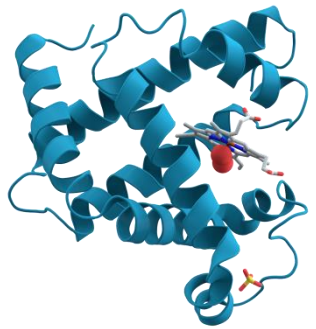
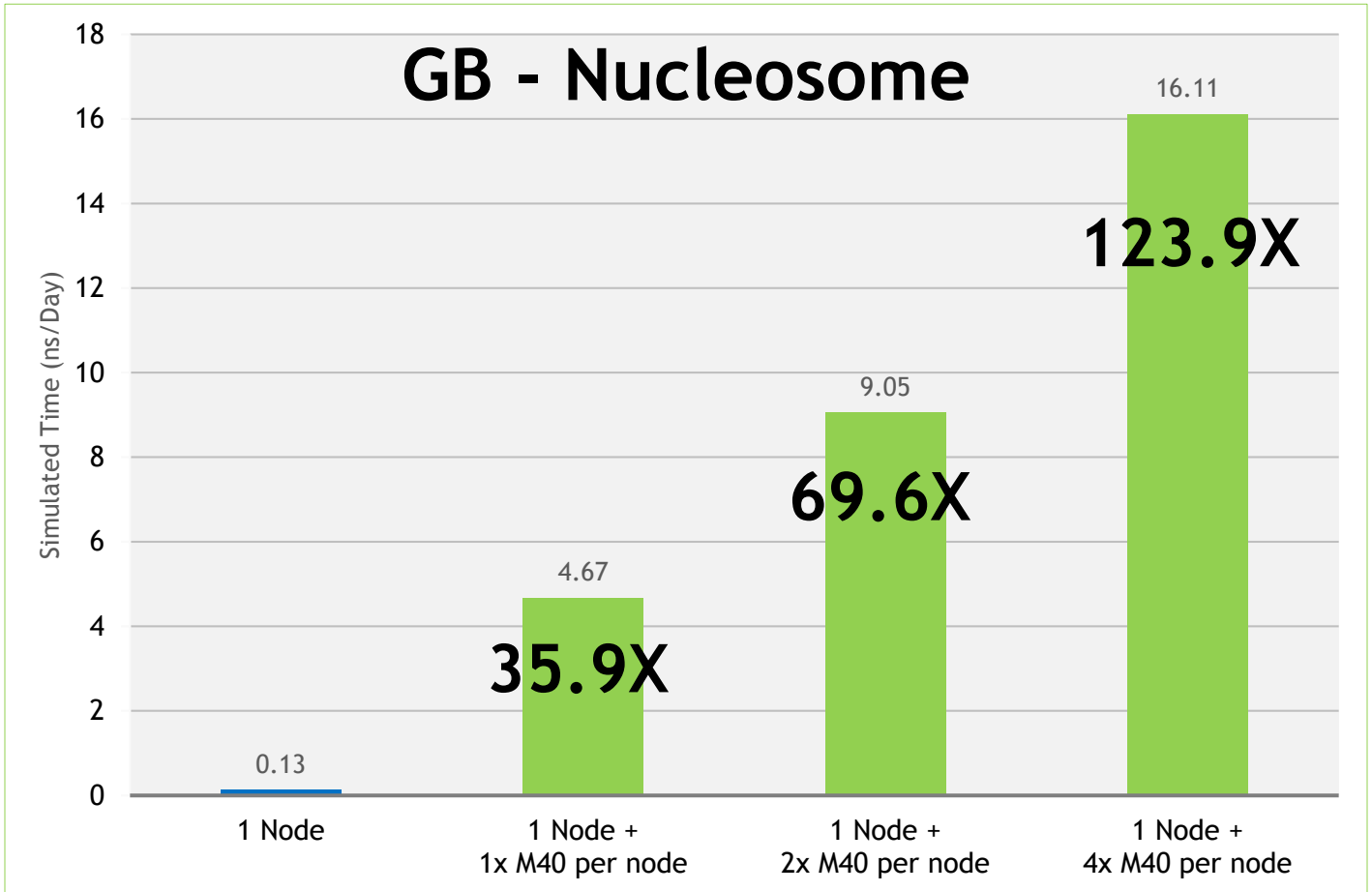


Nucleosome on M40s



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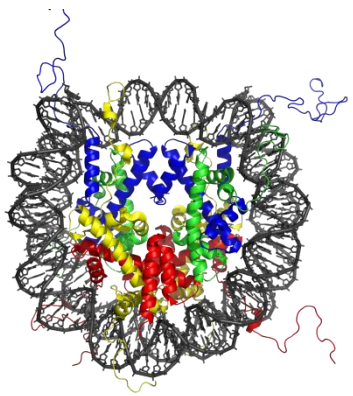
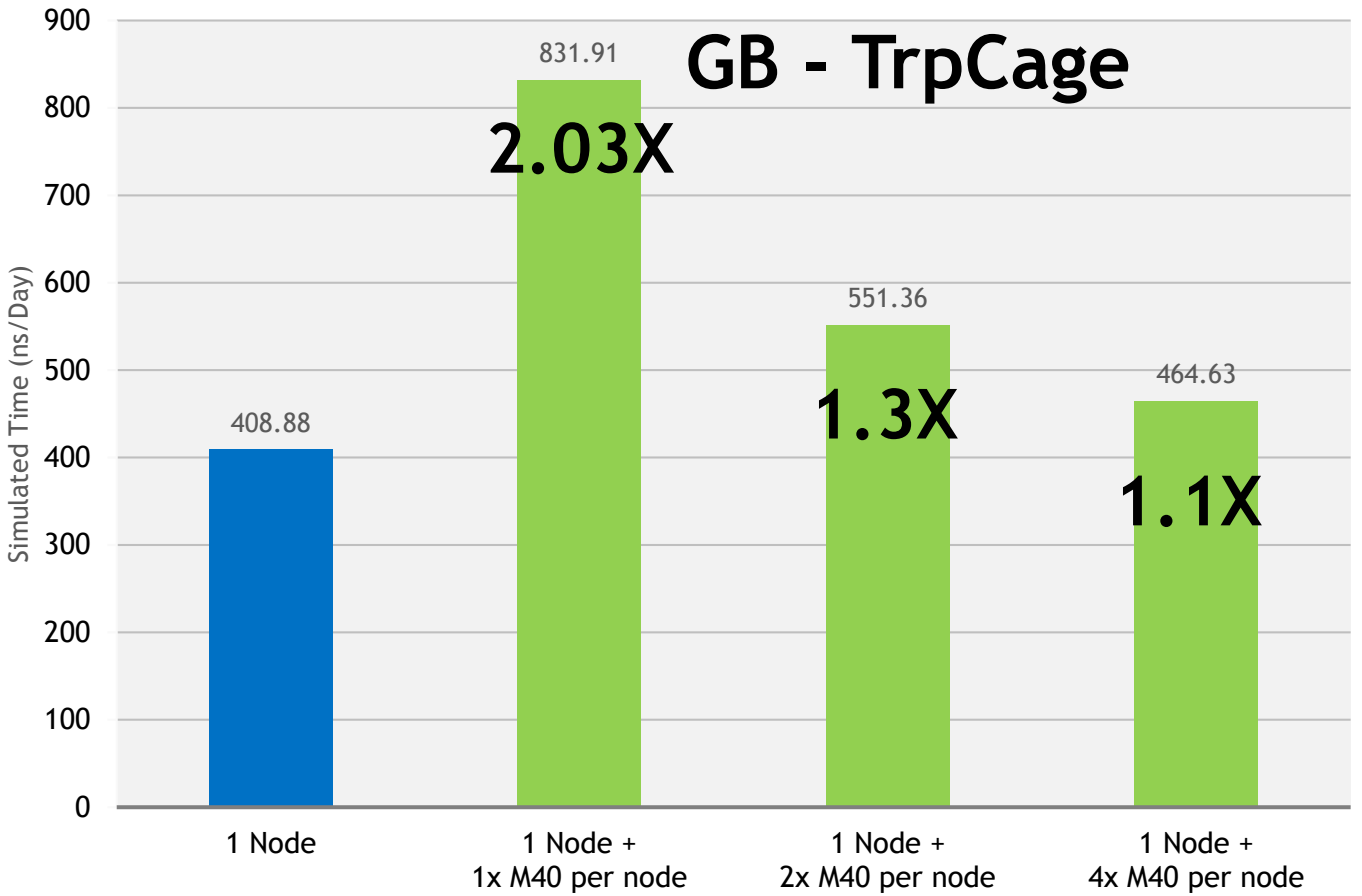


TrpCage on M40s



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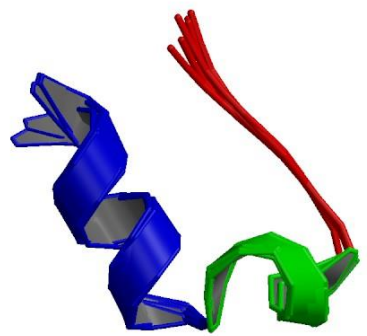


Recommended GPU Node Configuration for AMBER Computational Chemistry

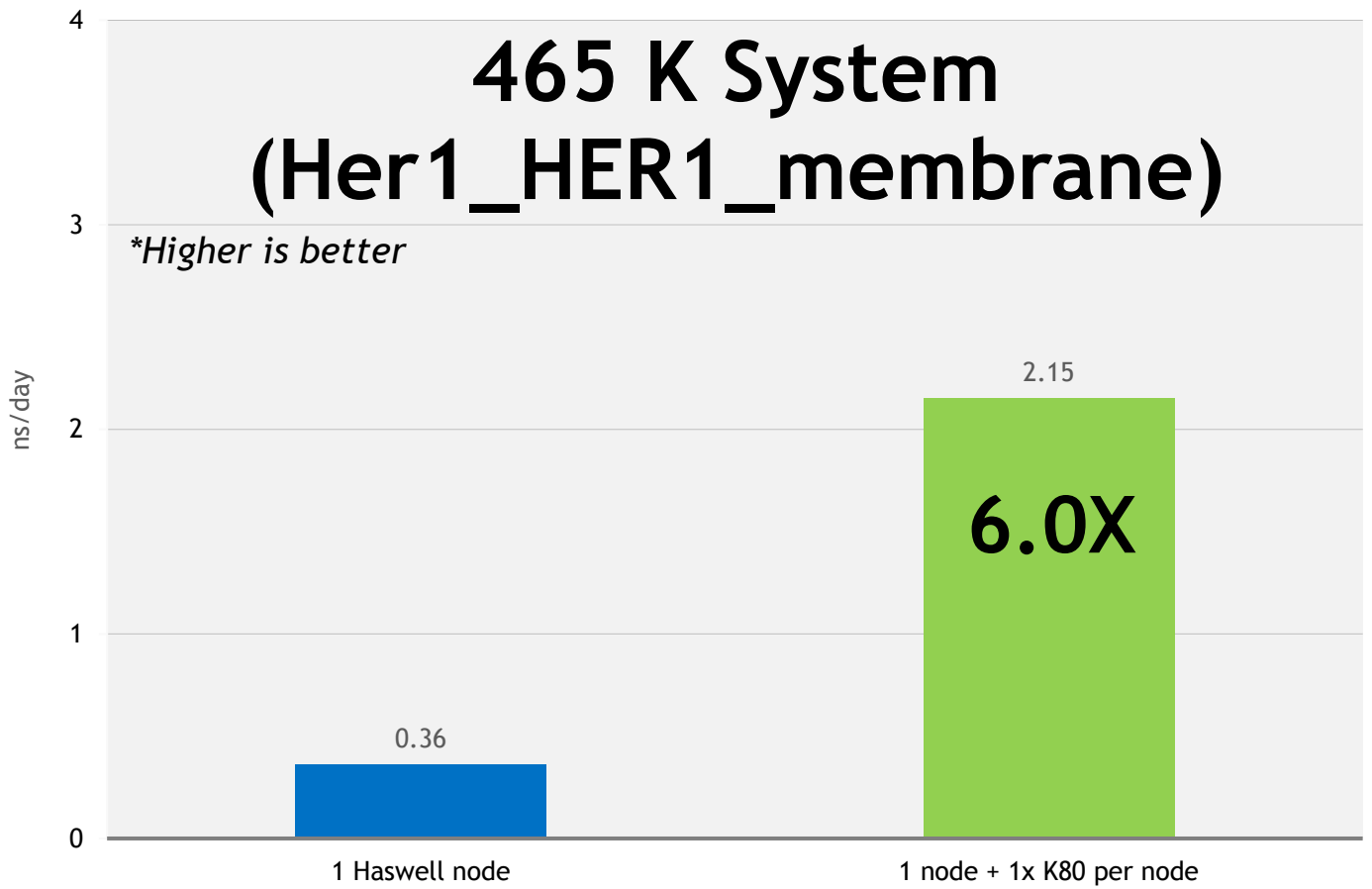
Workstation or Single Node Configuration	
# of CPU sockets	2
Cores per CPU socket	6+ (1 CPU core drives 1 GPU)
CPU speed (Ghz)	2.66+
System memory per node (GB)	16
GPUs	Kepler K20, K40, K80, P100
# of GPUs per CPU socket	1-4
GPU memory preference (GB)	6
GPU to CPU connection	PCIe 3.0 16x or higher
Server 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



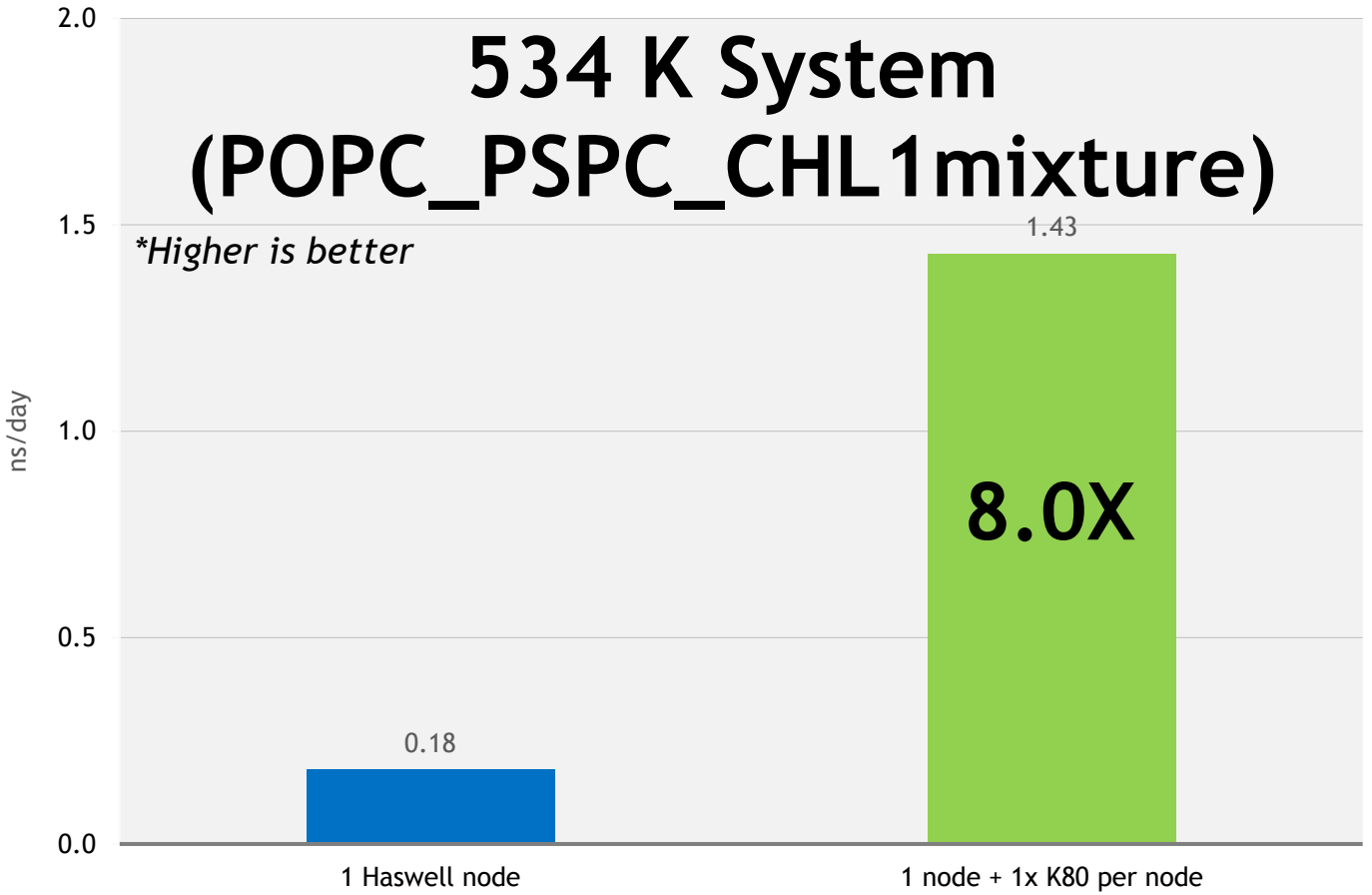
Running CHARMM version c40a1

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



Running CHARMM version c40a1

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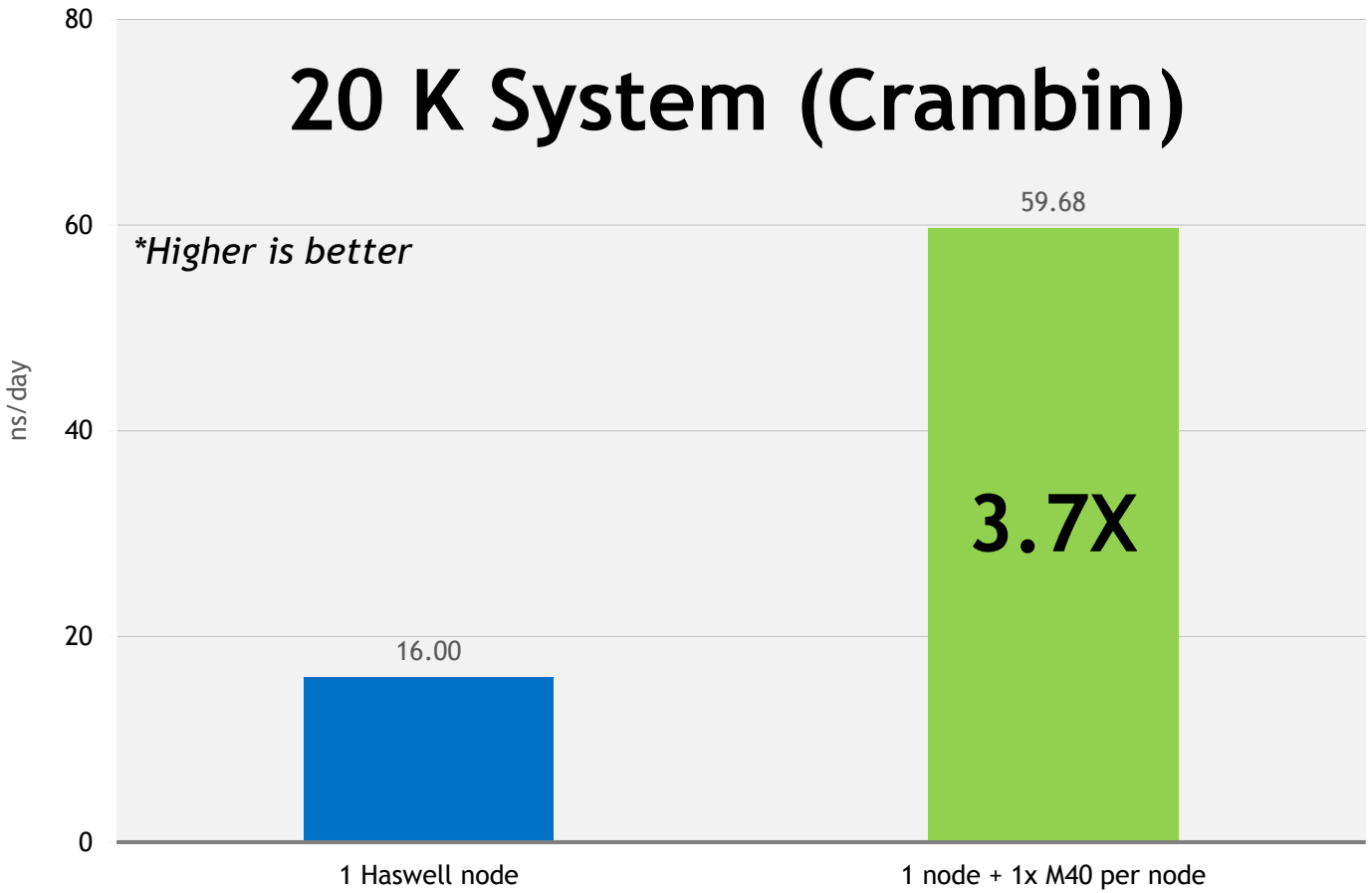
CHARMM DOMDEC-GUI 20 K System Benchmark



Running CHARMM version c40a1

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

The green nodes contain Dual Intel Xeon E5-2698 v3@2.30 GHz (Haswell) CPUs + Tesla M40 GPUs

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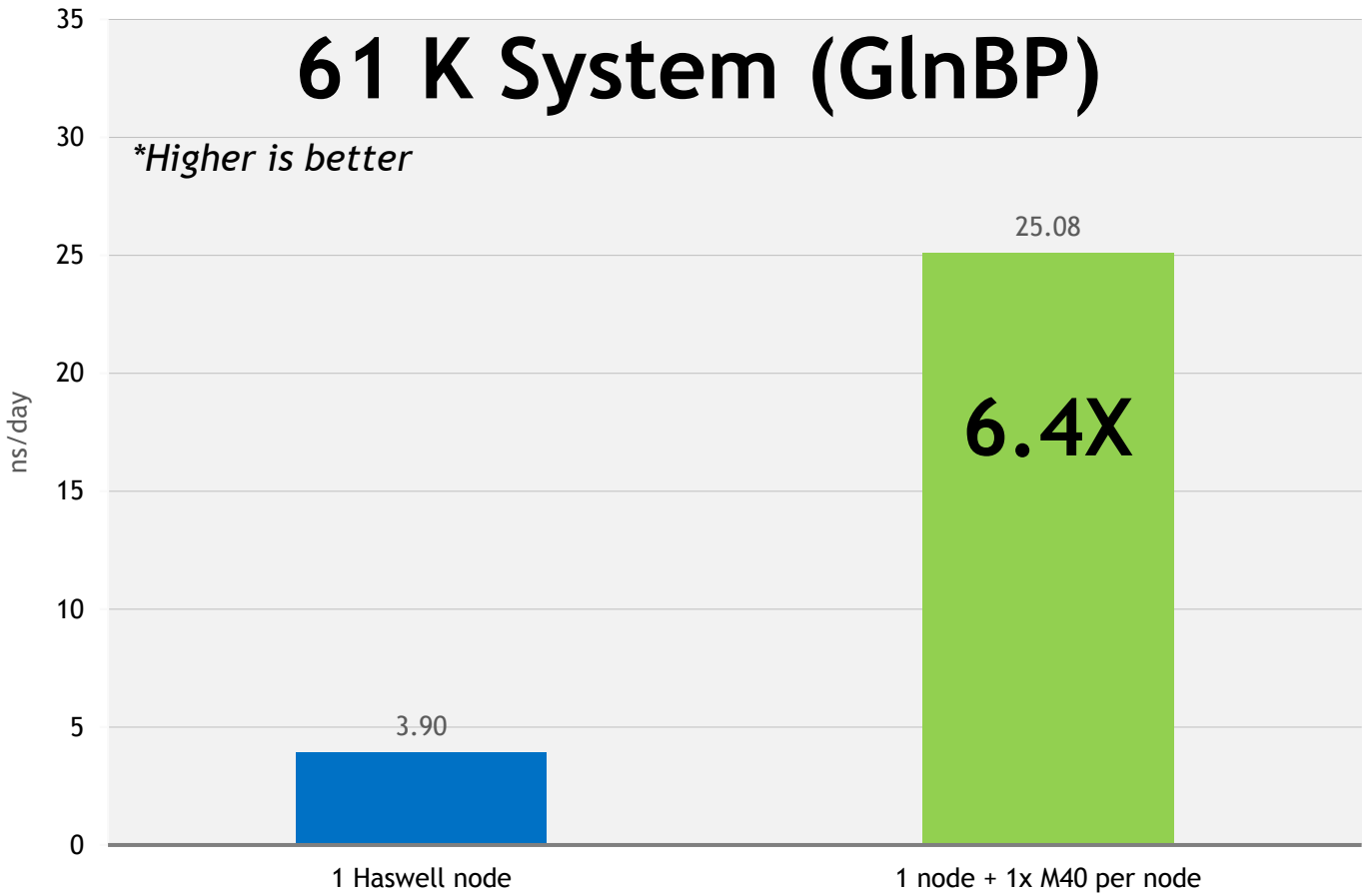
CHARMM DOMDEC-GUI 61 K System Benchmark



Running CHARMM version c40a1

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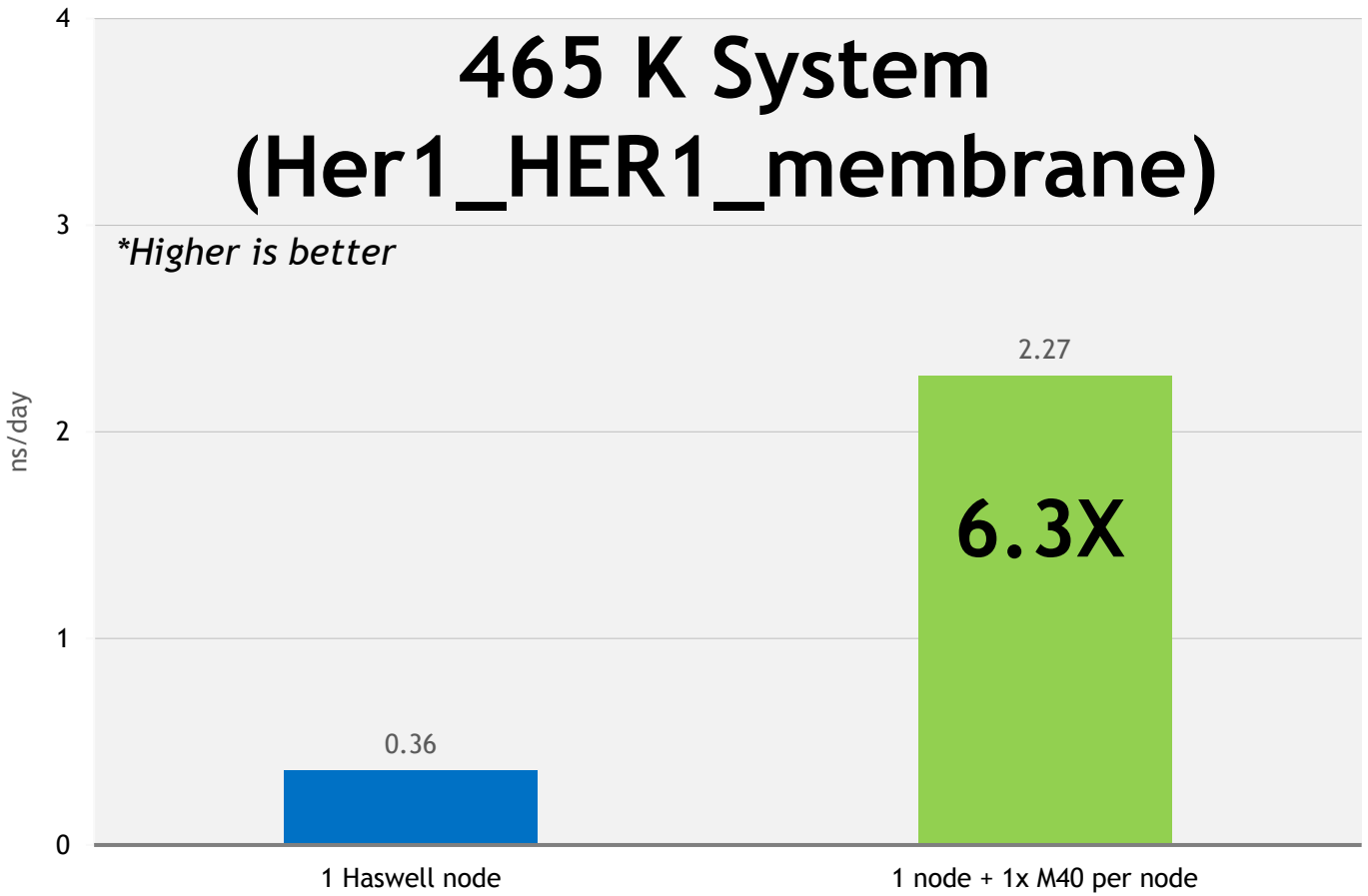
CHARMM DOMDEC-GUI 465 K System Benchmark



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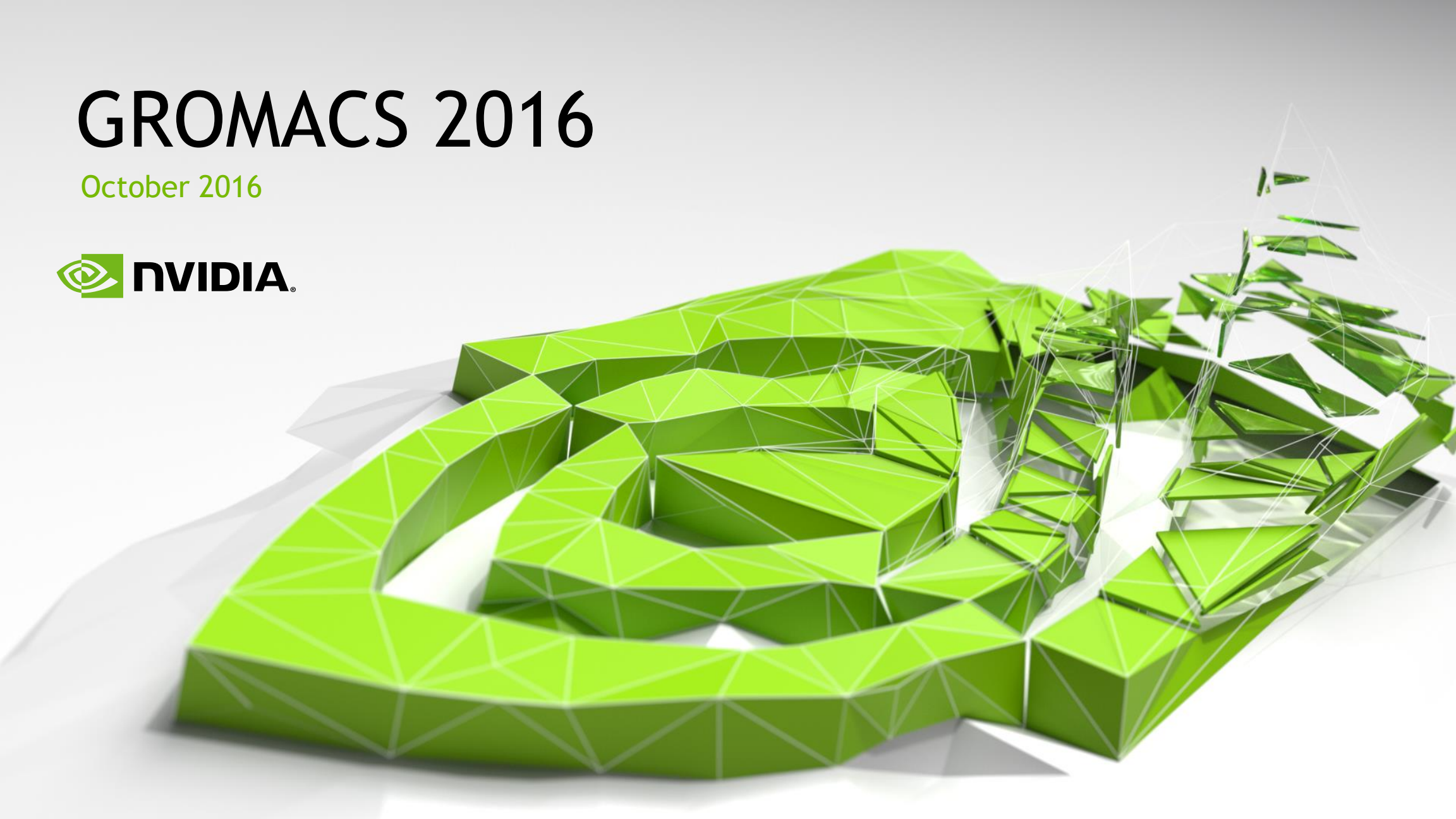
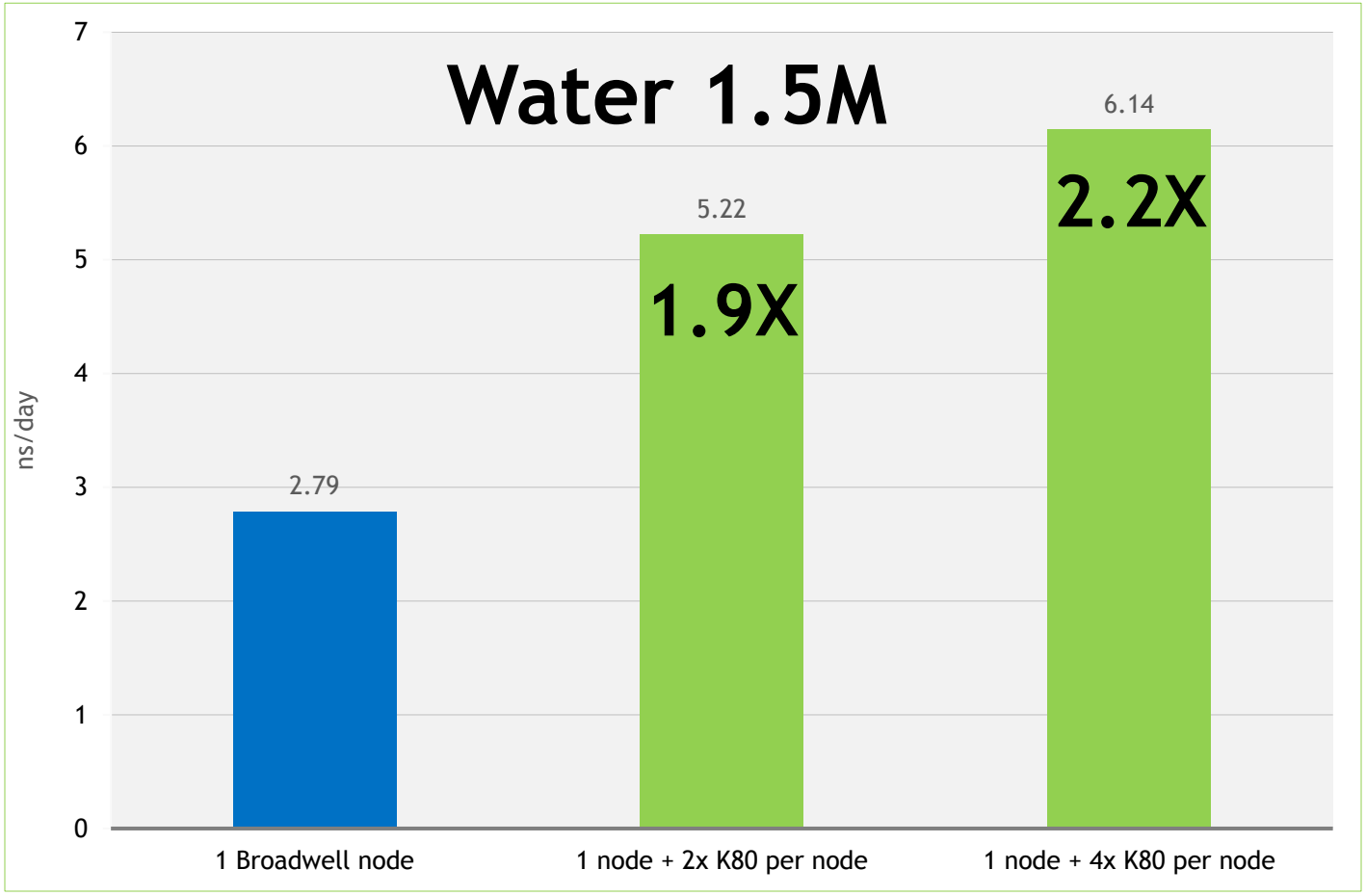
GROMACS 2016

October 2016



Erik Lindahl (GROMACS developer) video

Water 1.5M on K80s

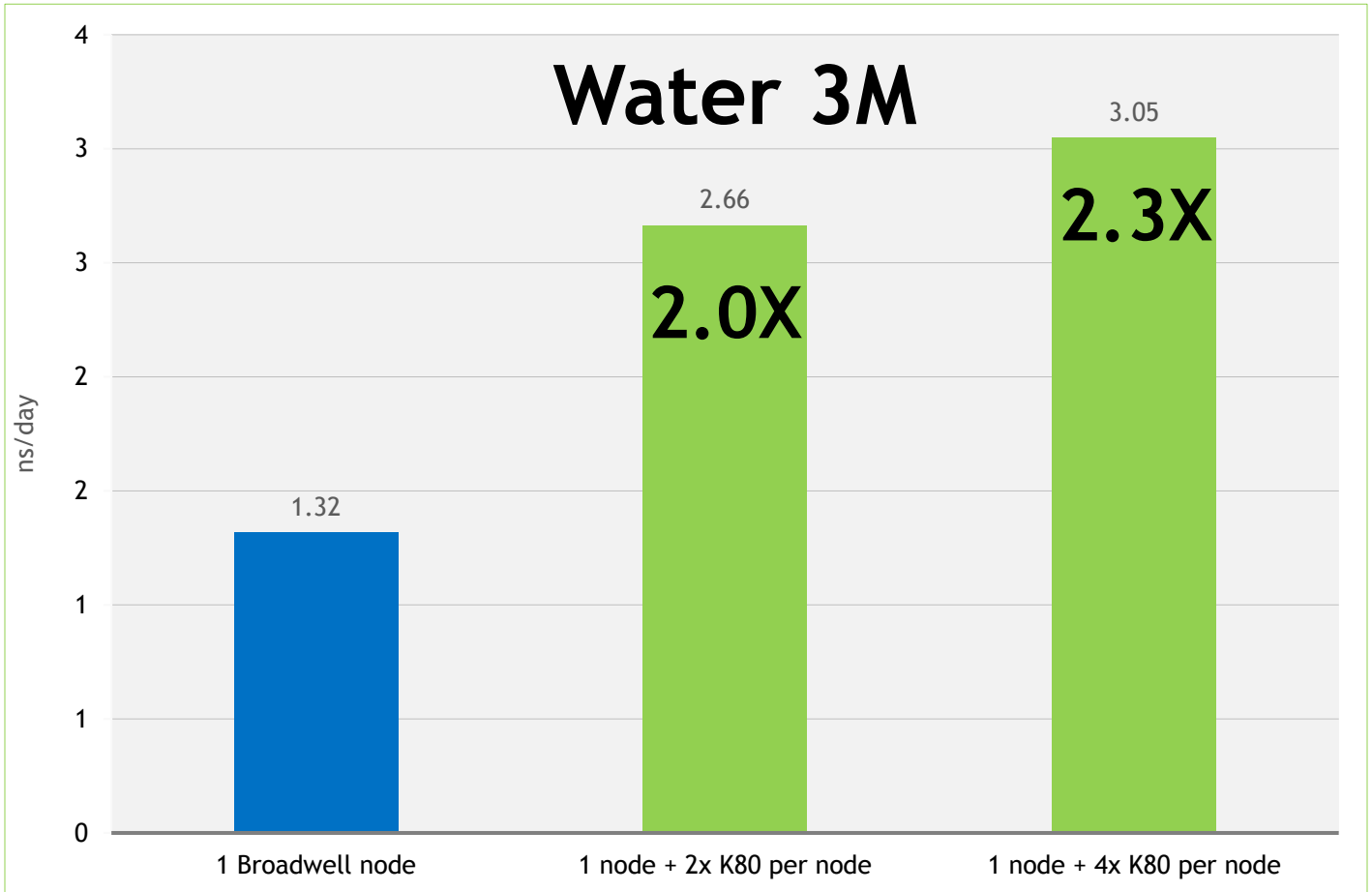


Running GROMACS version 2016

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 K80 (autoboost) GPUs

Water 3M on K80s



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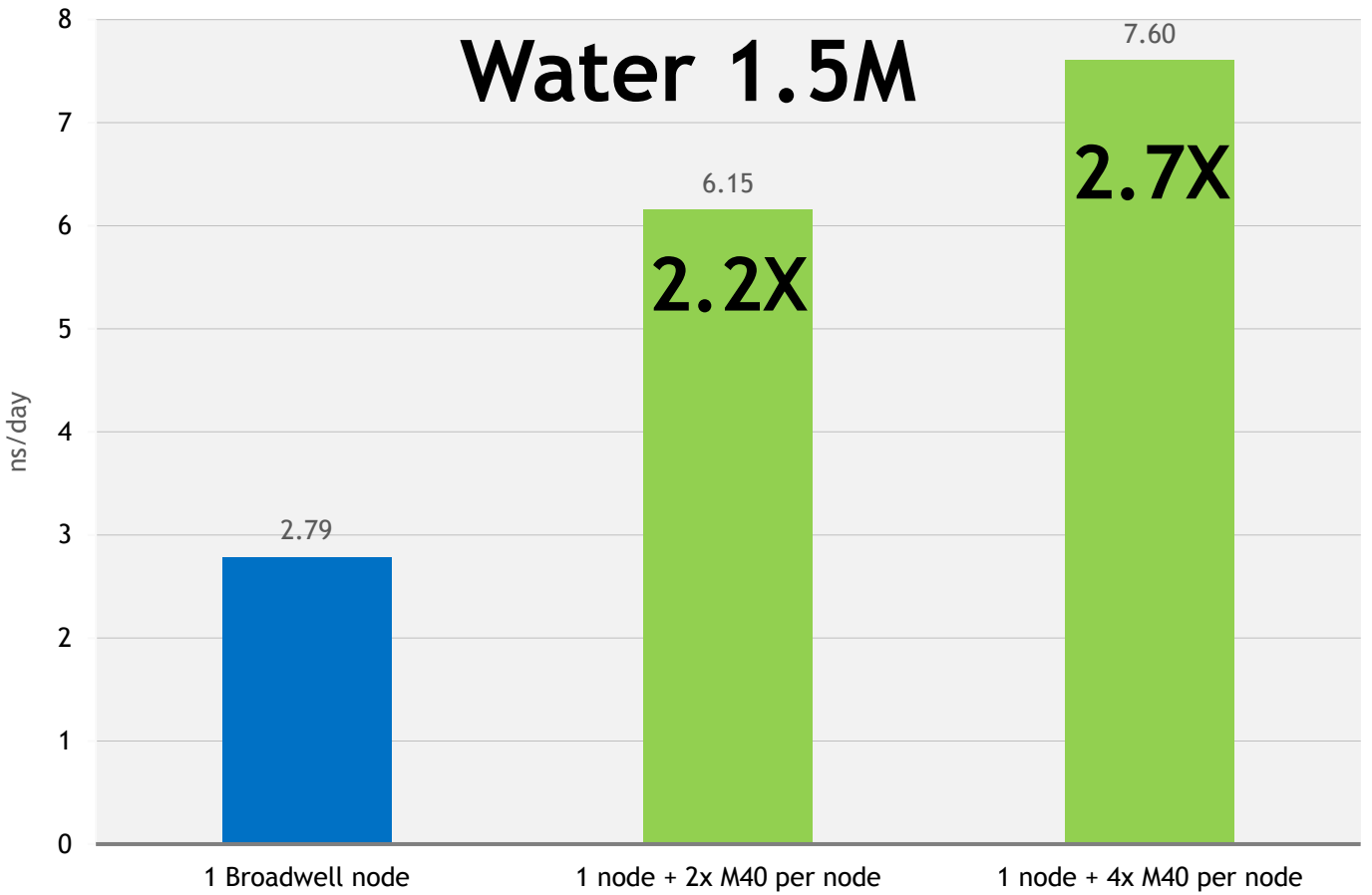
Water 1.5M on M40s



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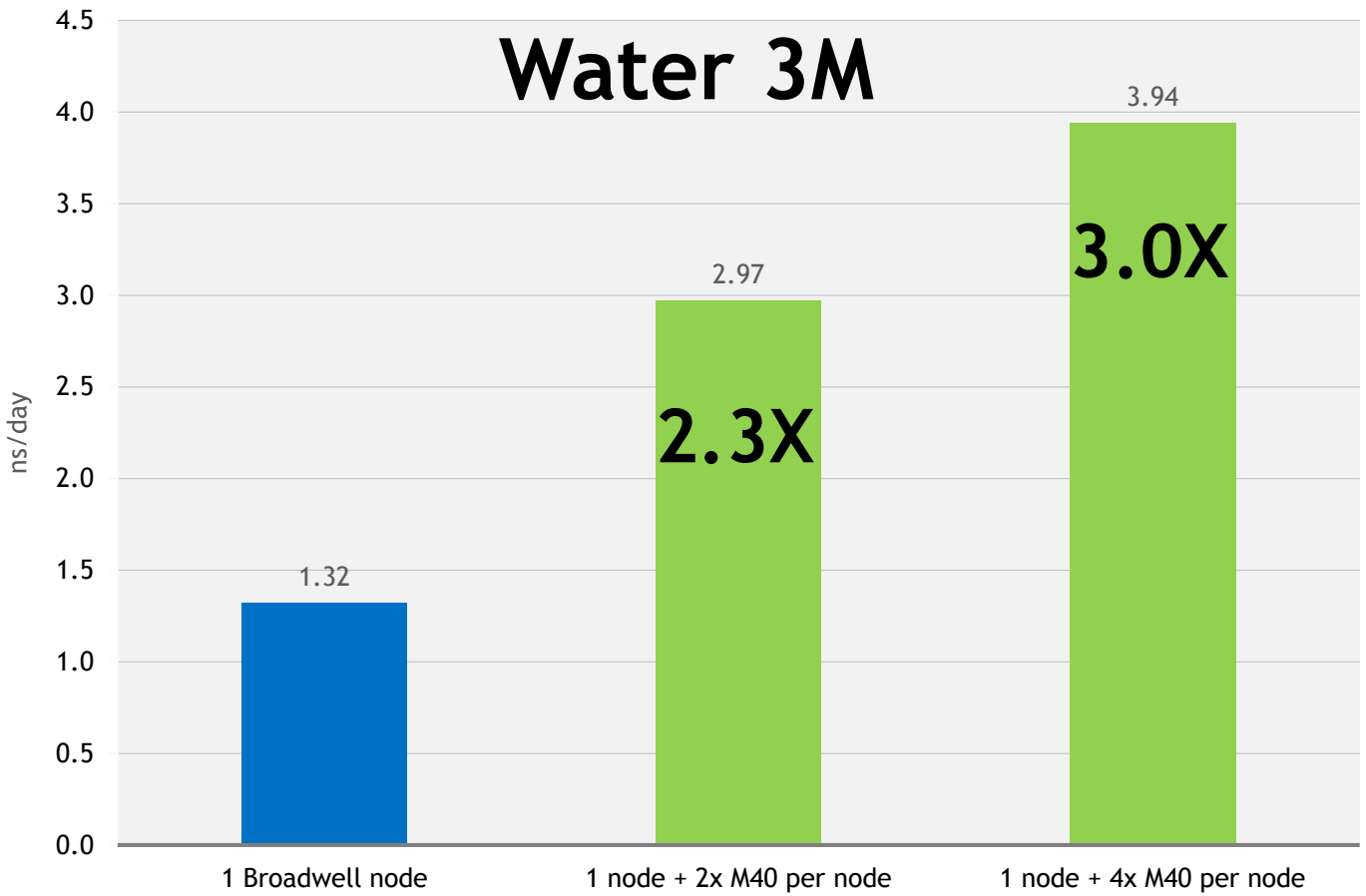
Water 3M on M40s



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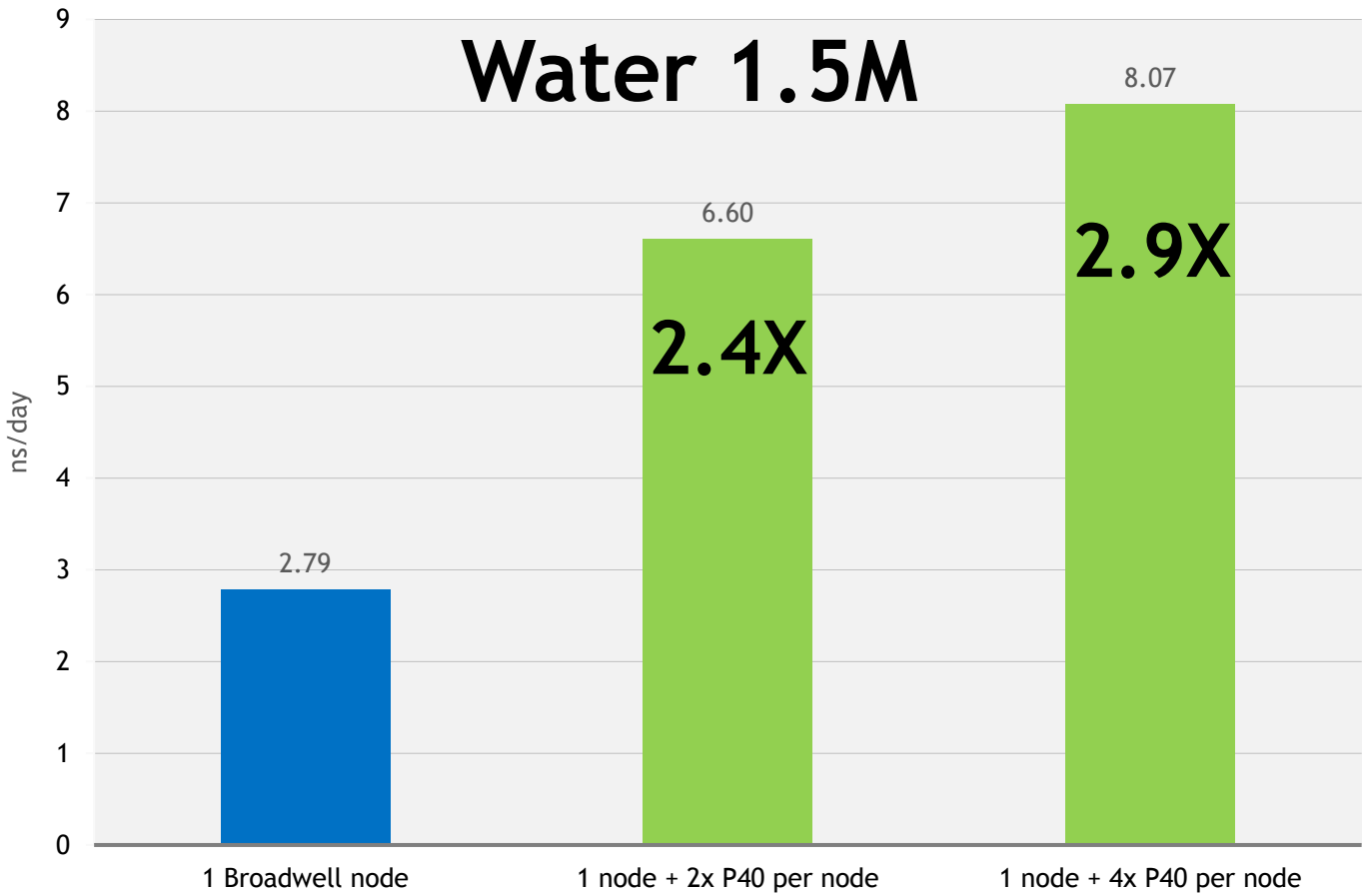
Water 1.5M on P40s



Running GROMACS version 2016

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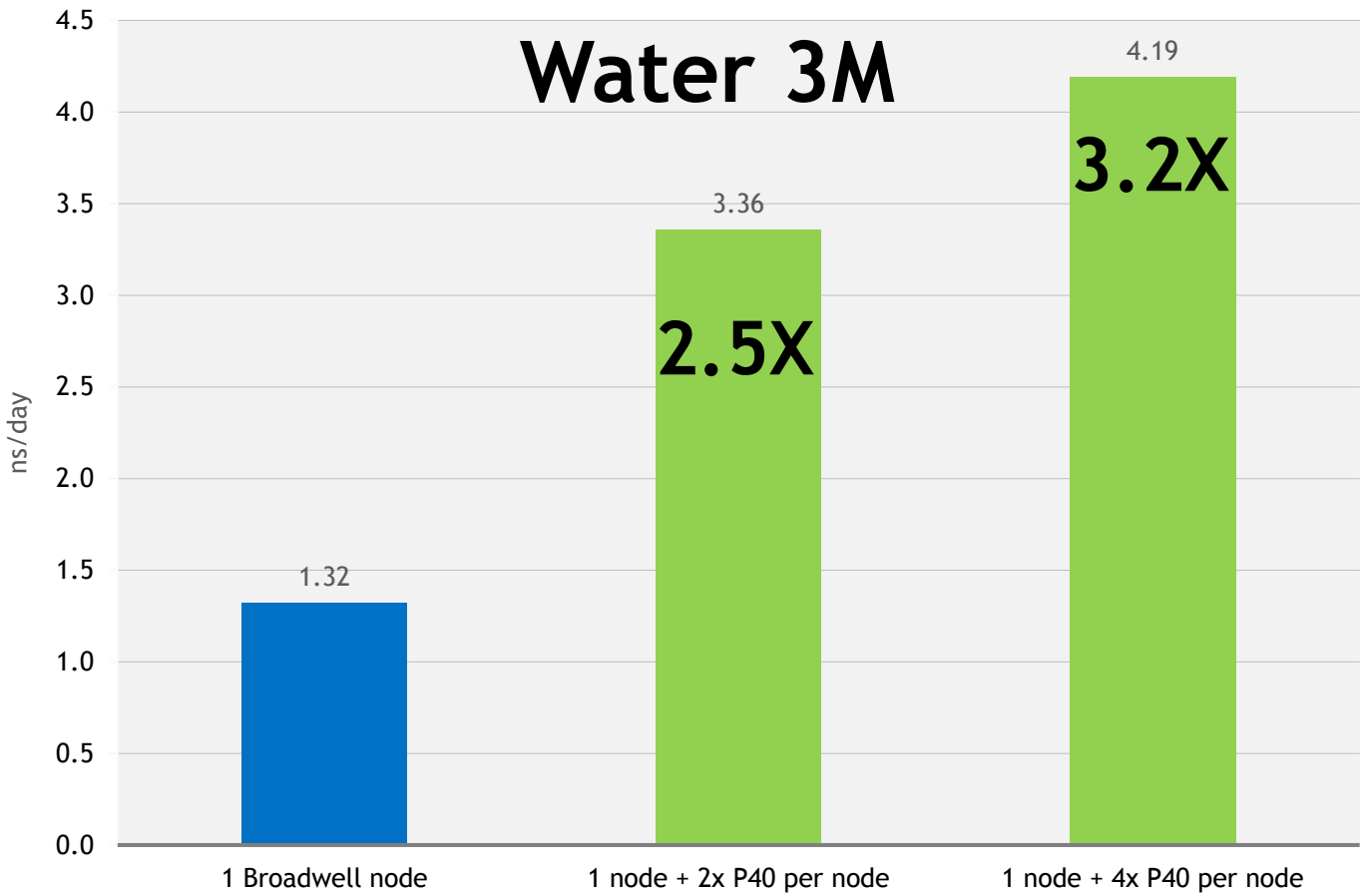
The green nodes contain Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P40 GPUs

Water 3M on P40s



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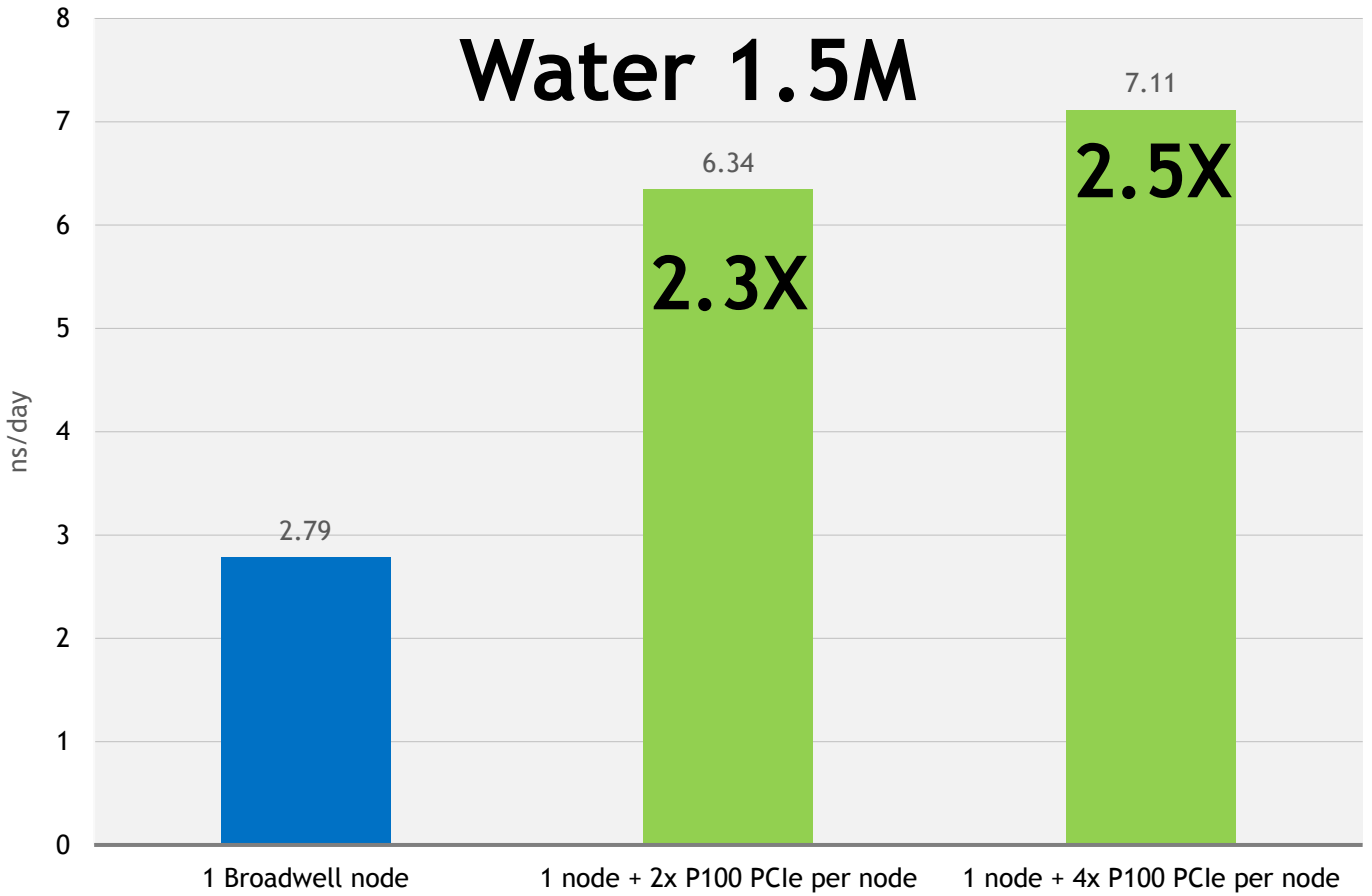
Water 1.5M on P100 PCIes



Running GROMACS version 2016

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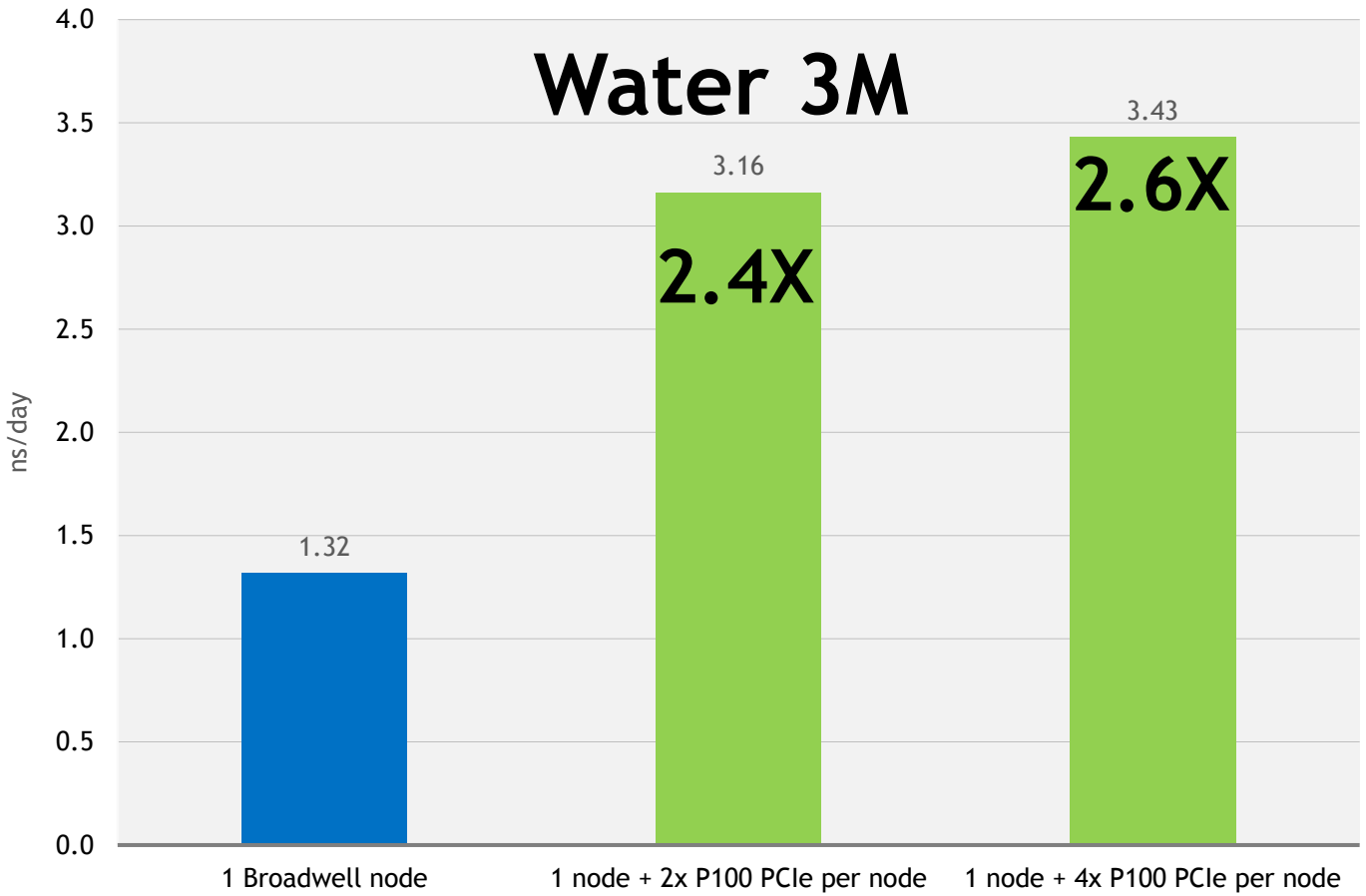
Water 3M on P100 PCIes



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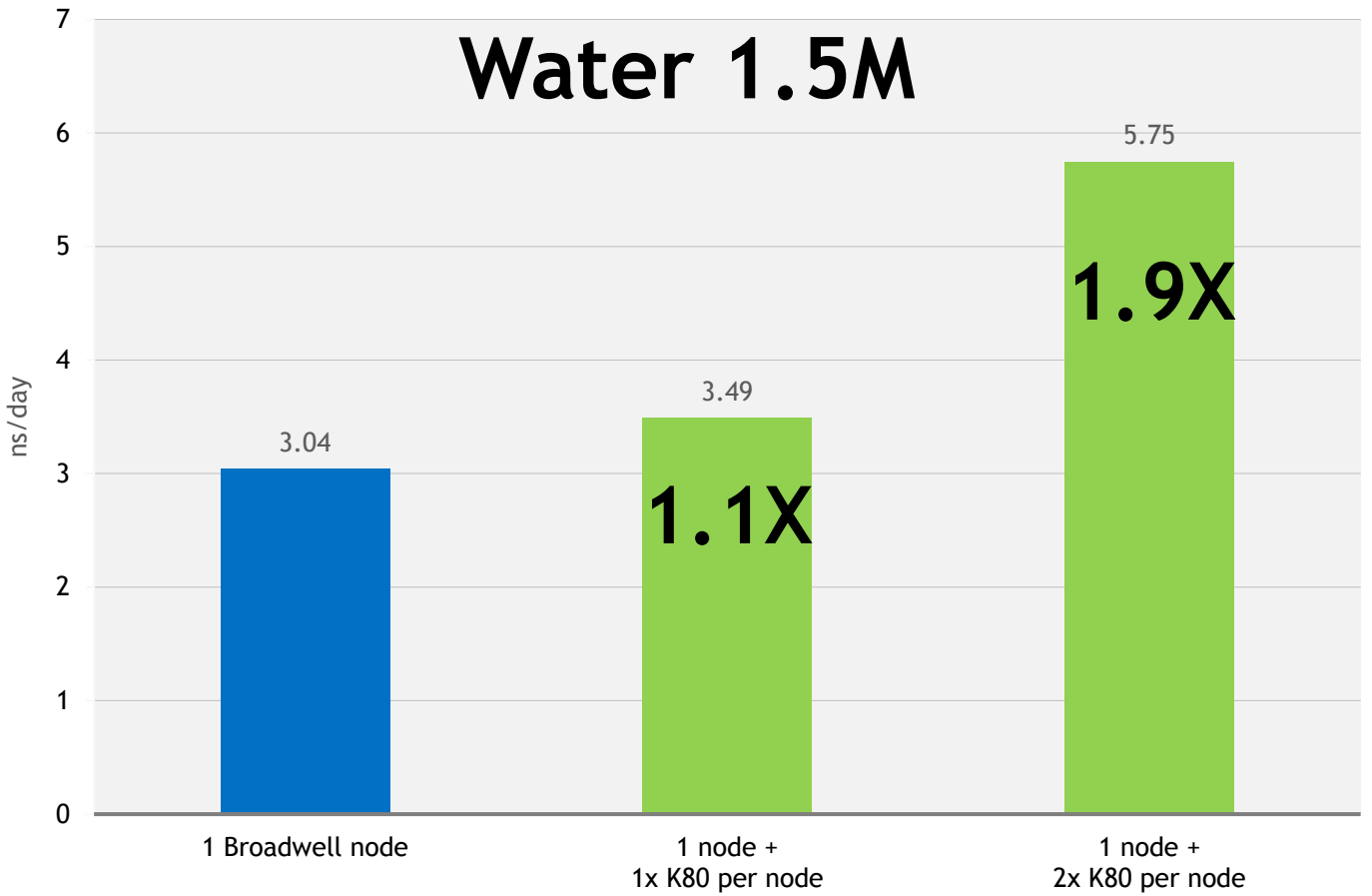
GROMACS 5.1.2

November 2016

Water 1.5M on K80s



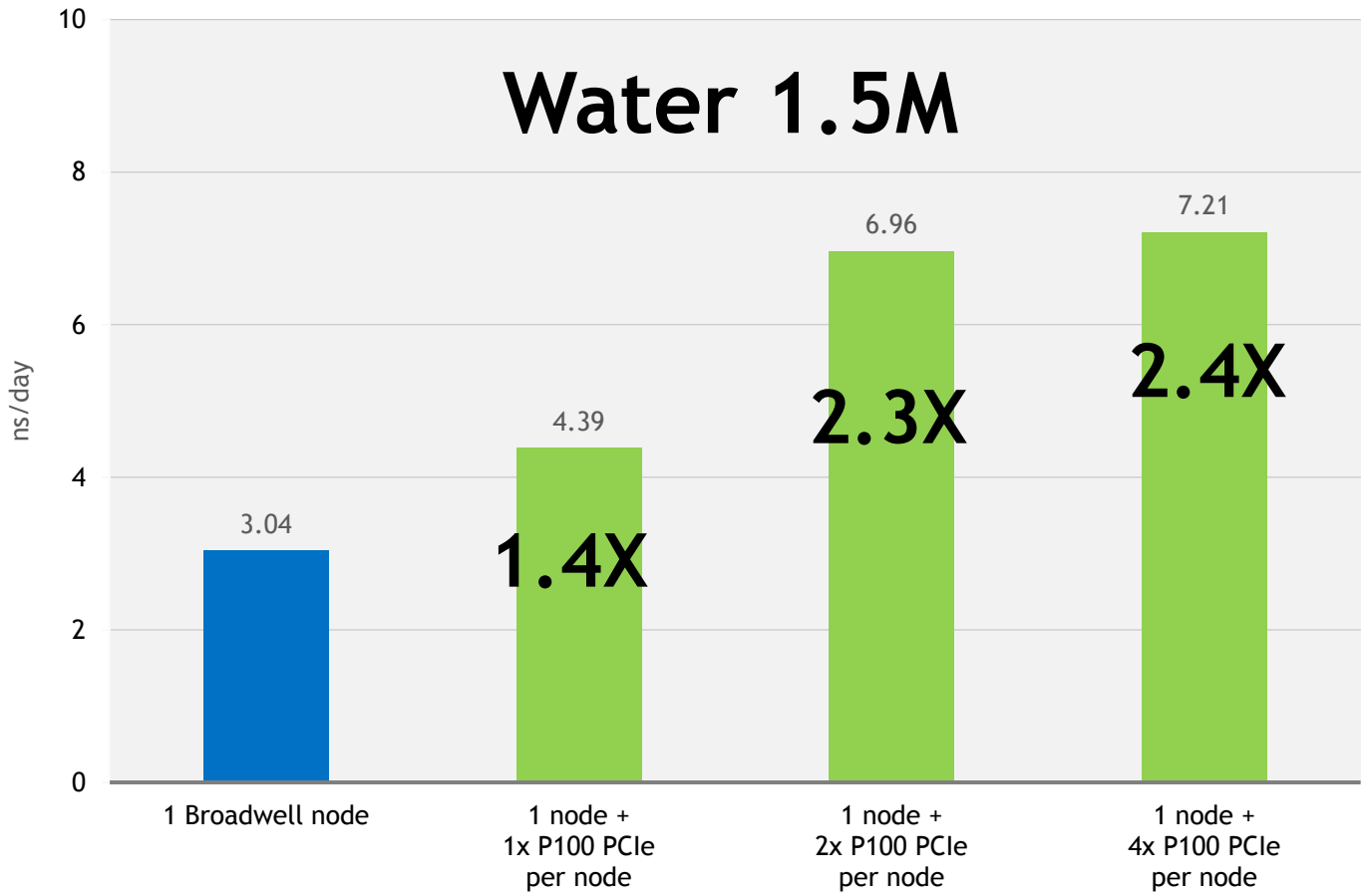
Running GROMACS version 5.1.2

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 K80 (autoboost) GPUs

- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

Water 1.5M on P100s PCIe



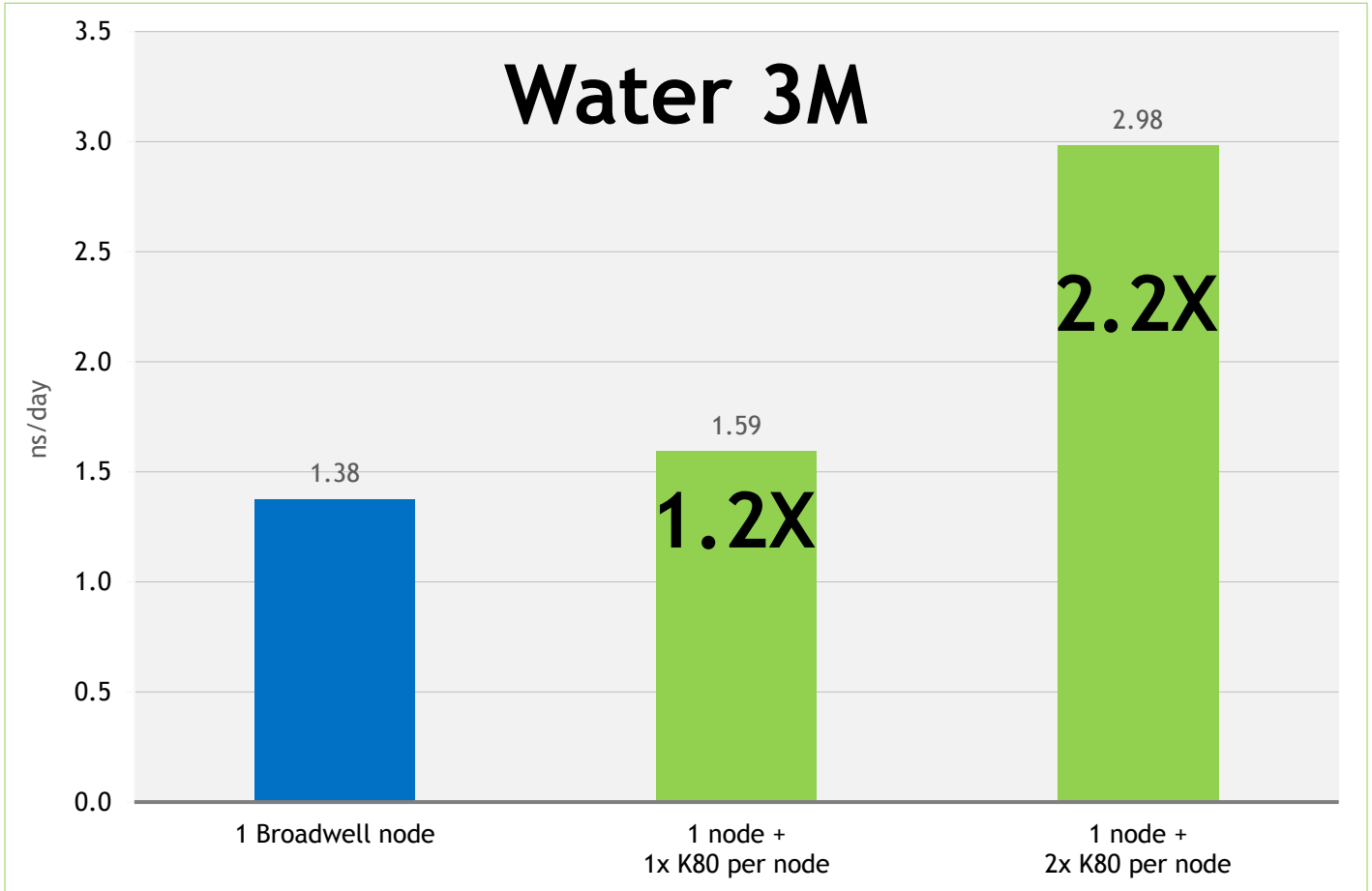
Running GROMACS version 5.1.2

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 GPUs

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

Water 3M on K80s



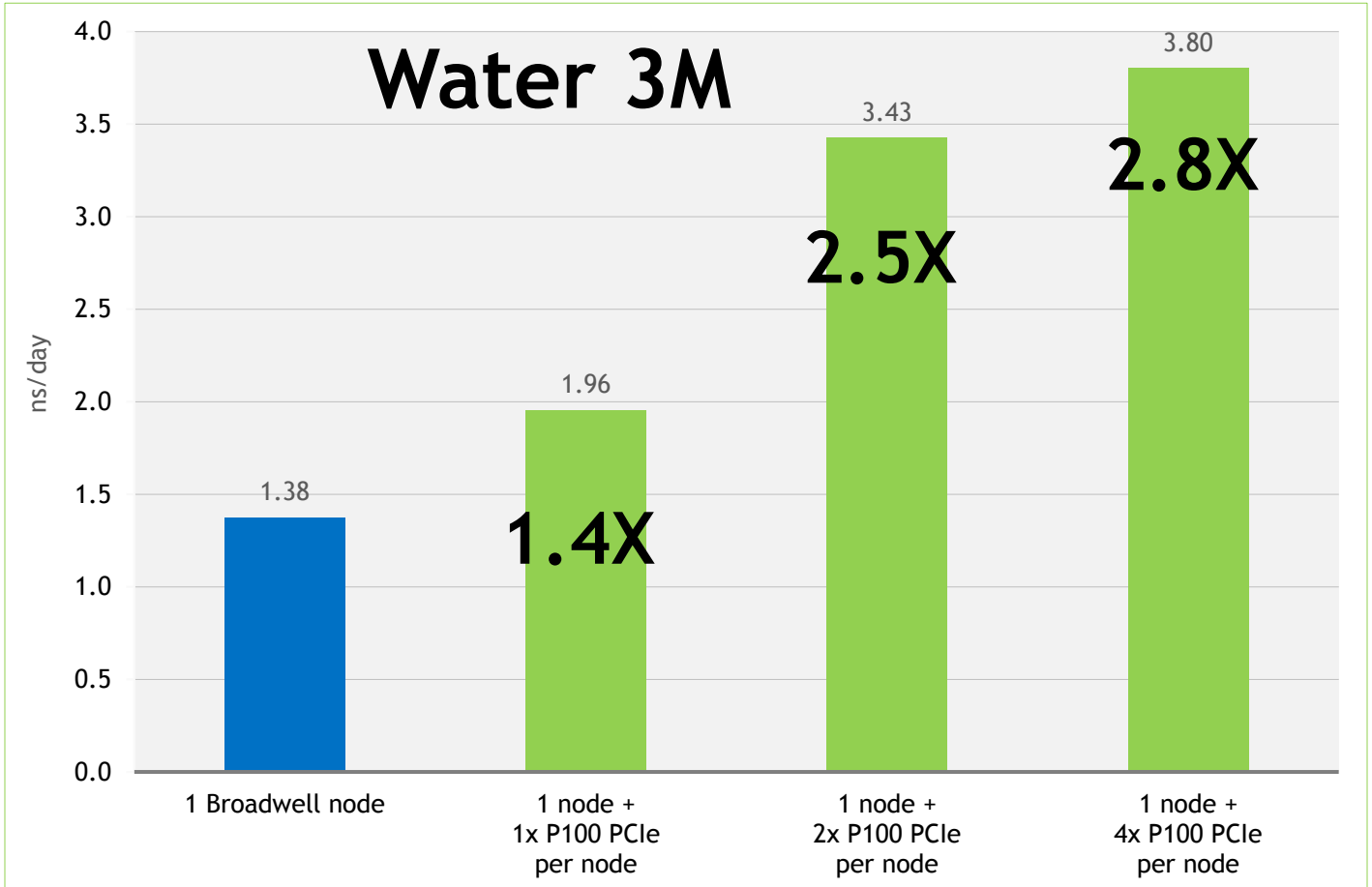
Running GROMACS version 5.1.2

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 K80 (autoboost) GPUs

- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

Water 3M on P100s PCIe



Running GROMACS version 5.1.2

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 GPUs

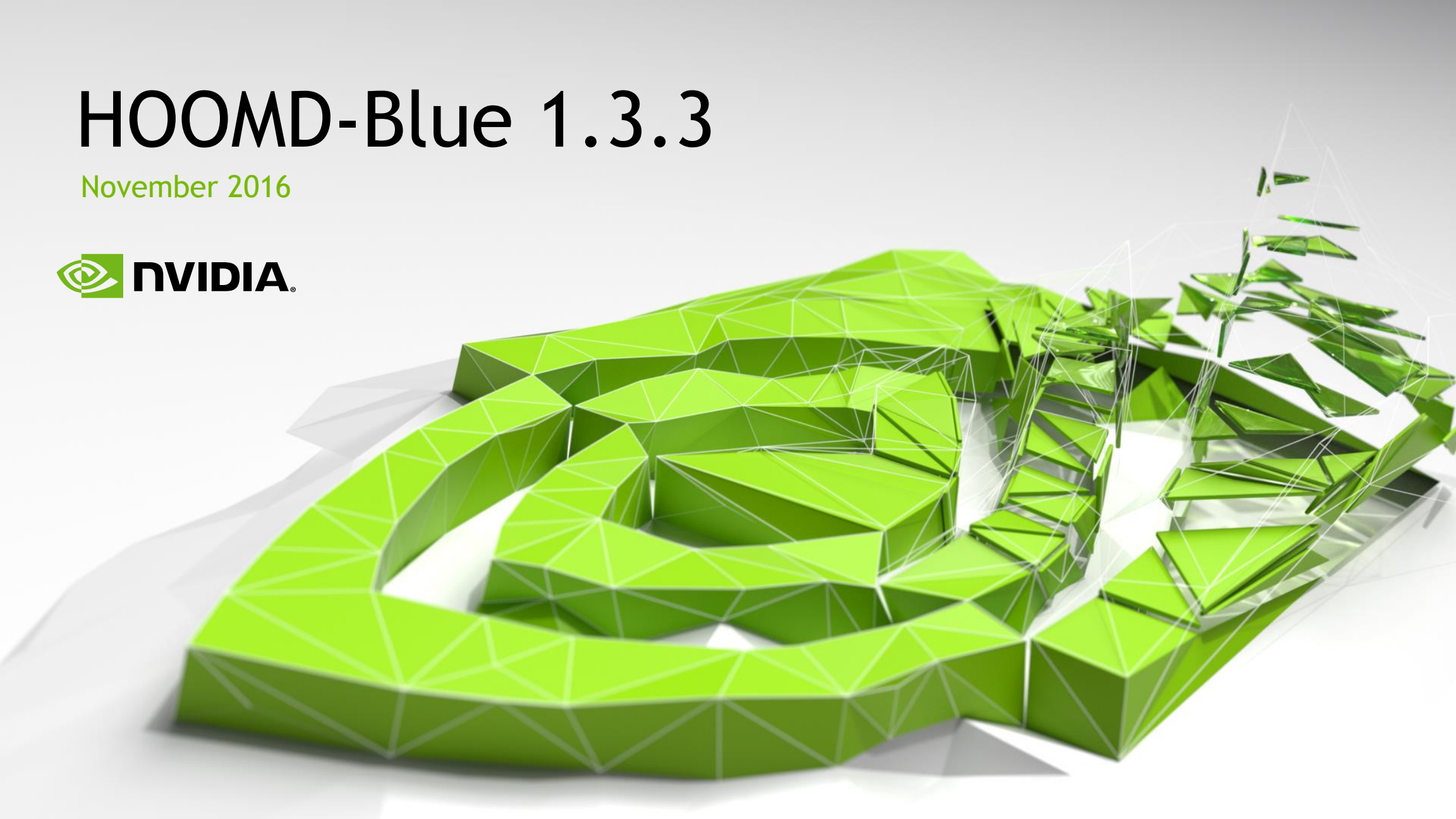
- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

Recommended GPU Node Configuration for GROMACS Computational Chemistry

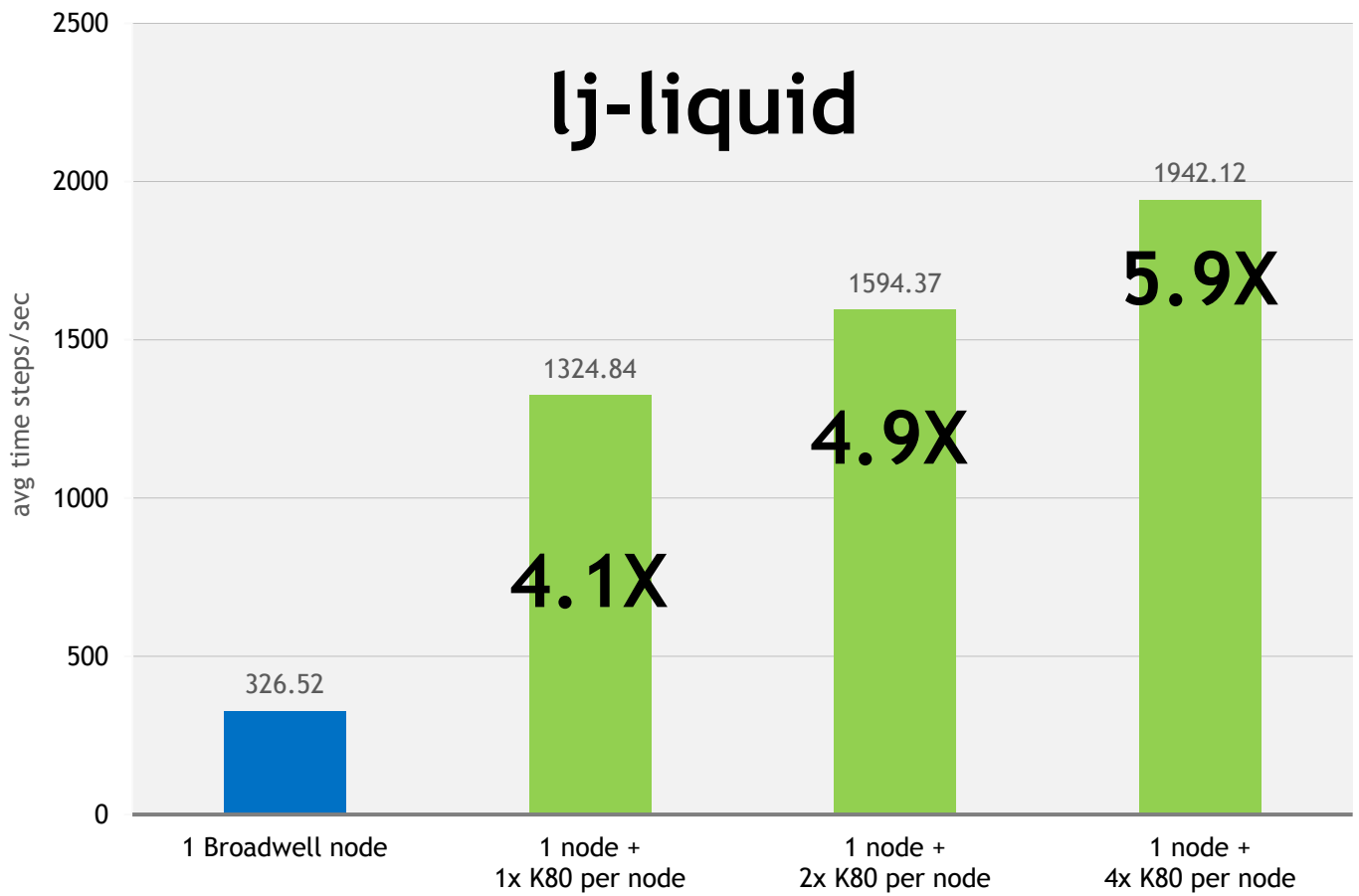
Workstation or Single Node Configuration	
# of CPU sockets	2
Cores per CPU socket	6+
CPU speed (Ghz)	2.66+
System memory per socket (GB)	32
GPUs	Kepler K20, K40, K80
# of GPUs per CPU socket	1x Kepler GPUs: need fast Sandy Bridge or Ivy Bridge, or high-end AMD Opterons
GPU memory preference (GB)	6
GPU to CPU connection	PCIe 3.0 or higher
Server storage	500 GB or higher
Network configuration	Gemini, InfiniBand

HOOMD-Blue 1.3.3

November 2016



lj-liquid on K80s



Running HOOMD-Blue version 1.3.3

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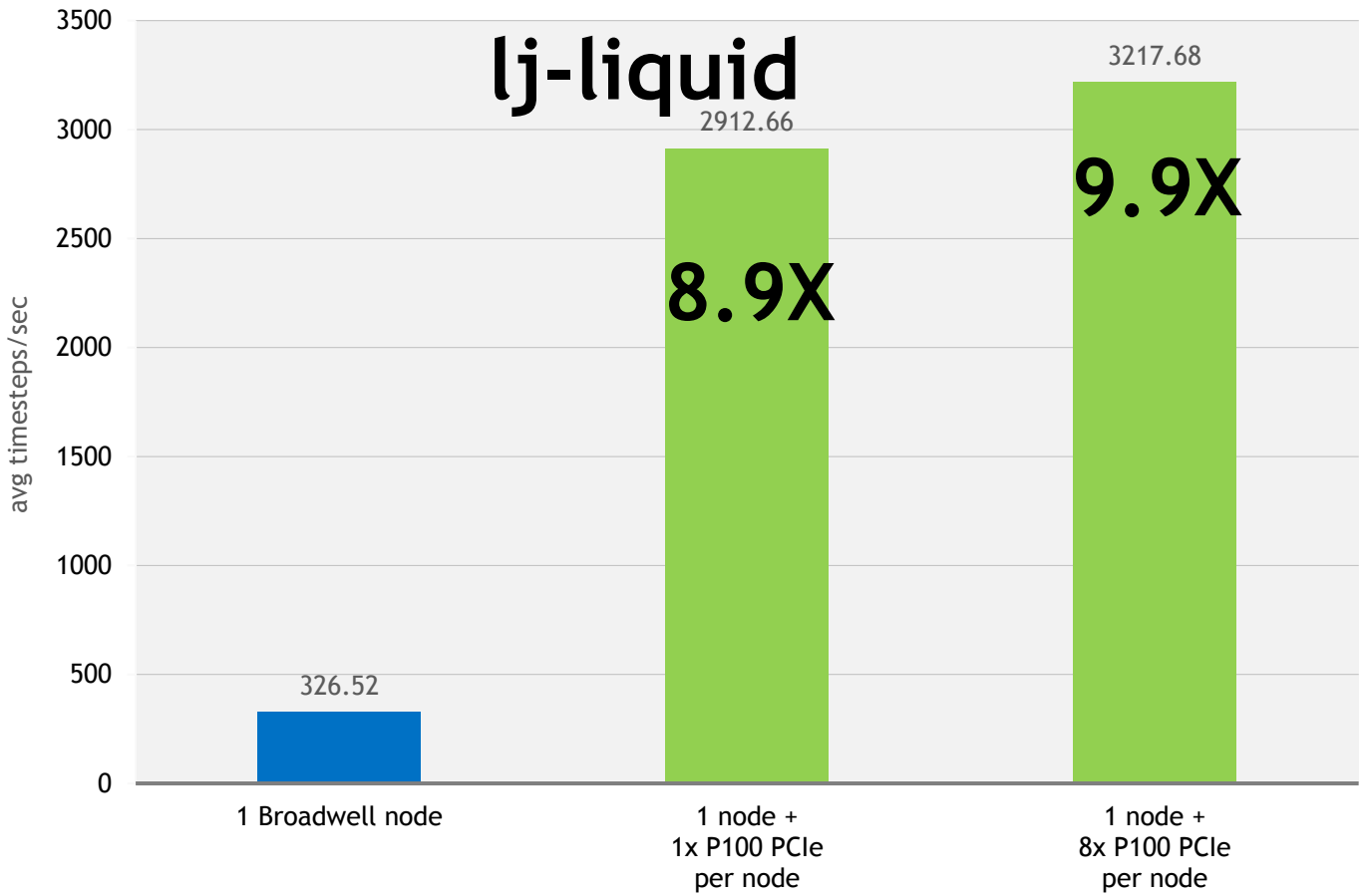
lj-liquid on P100s PCIe



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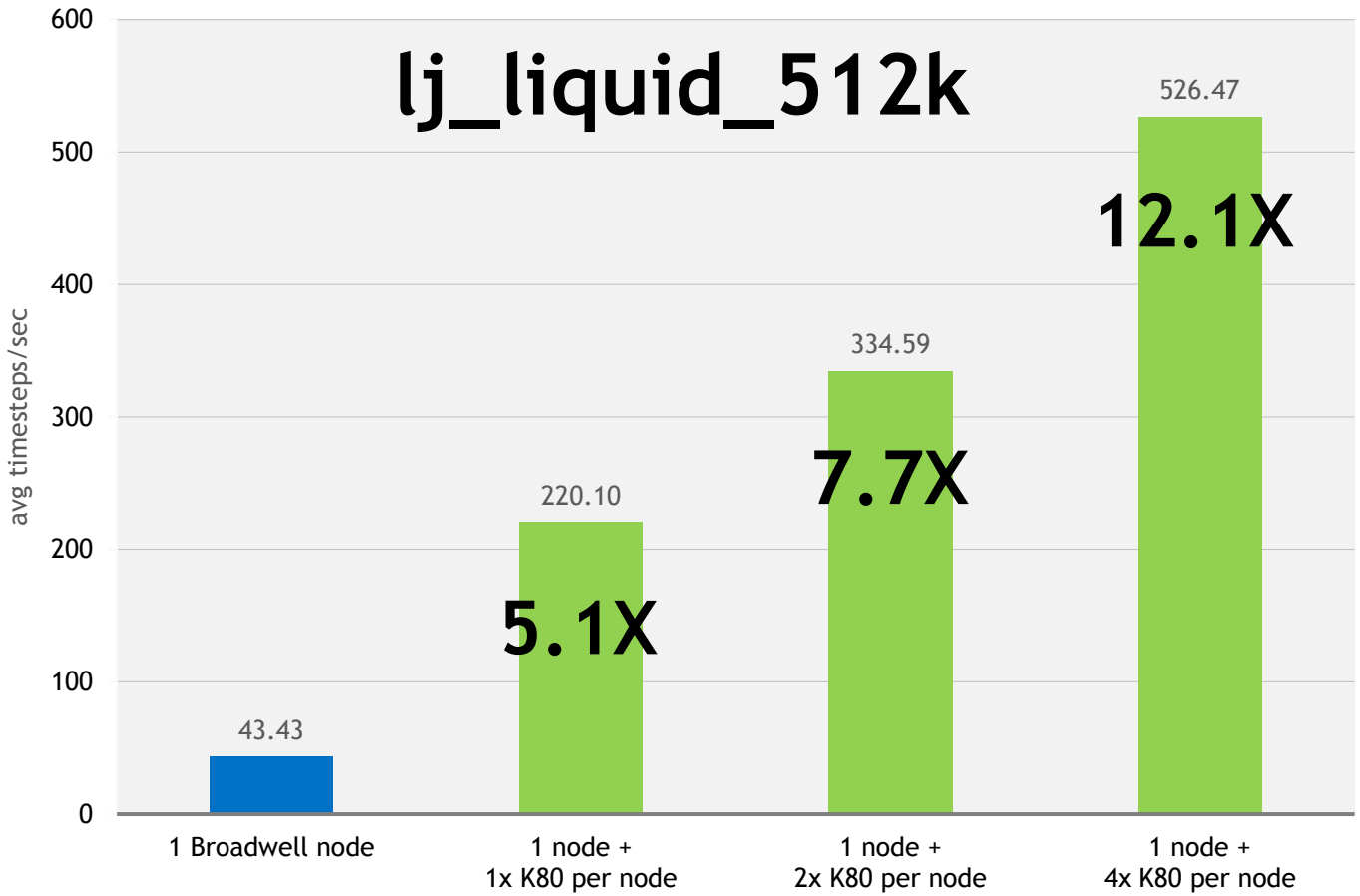
lj_liquid_512k on K80s



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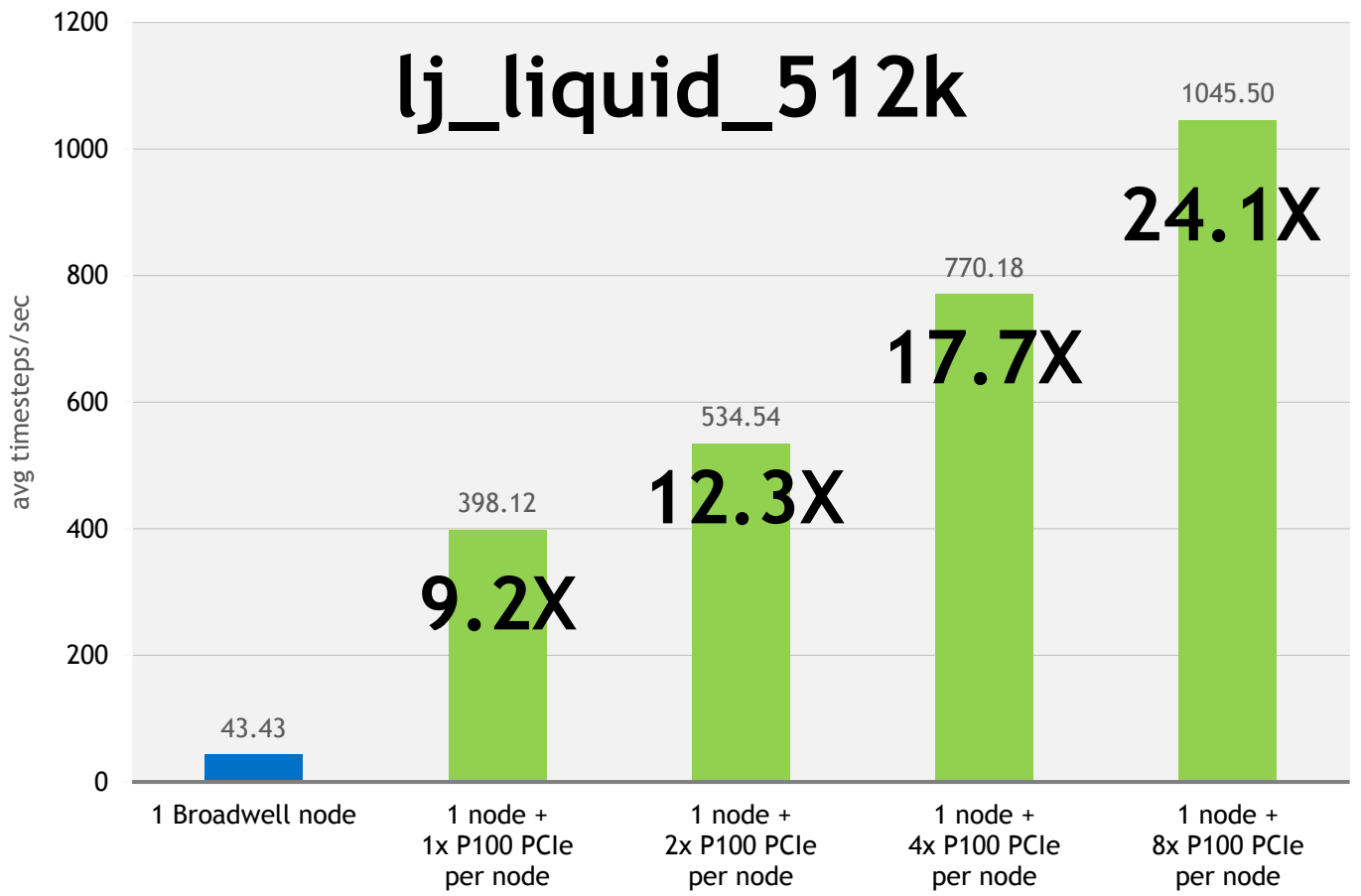
lj_liquid_512k on P100s PCIe



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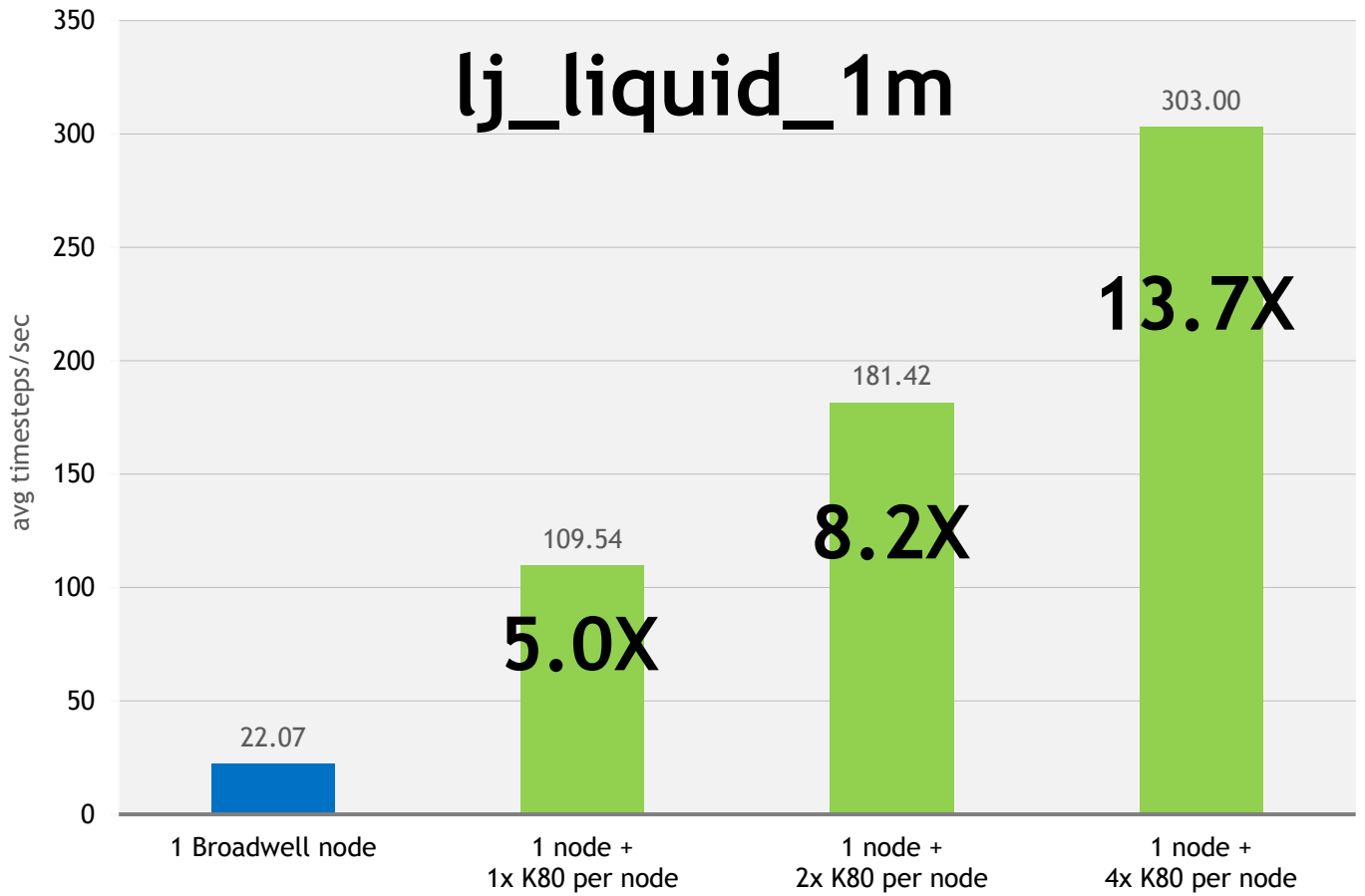
lj_liquid_1m on K80s



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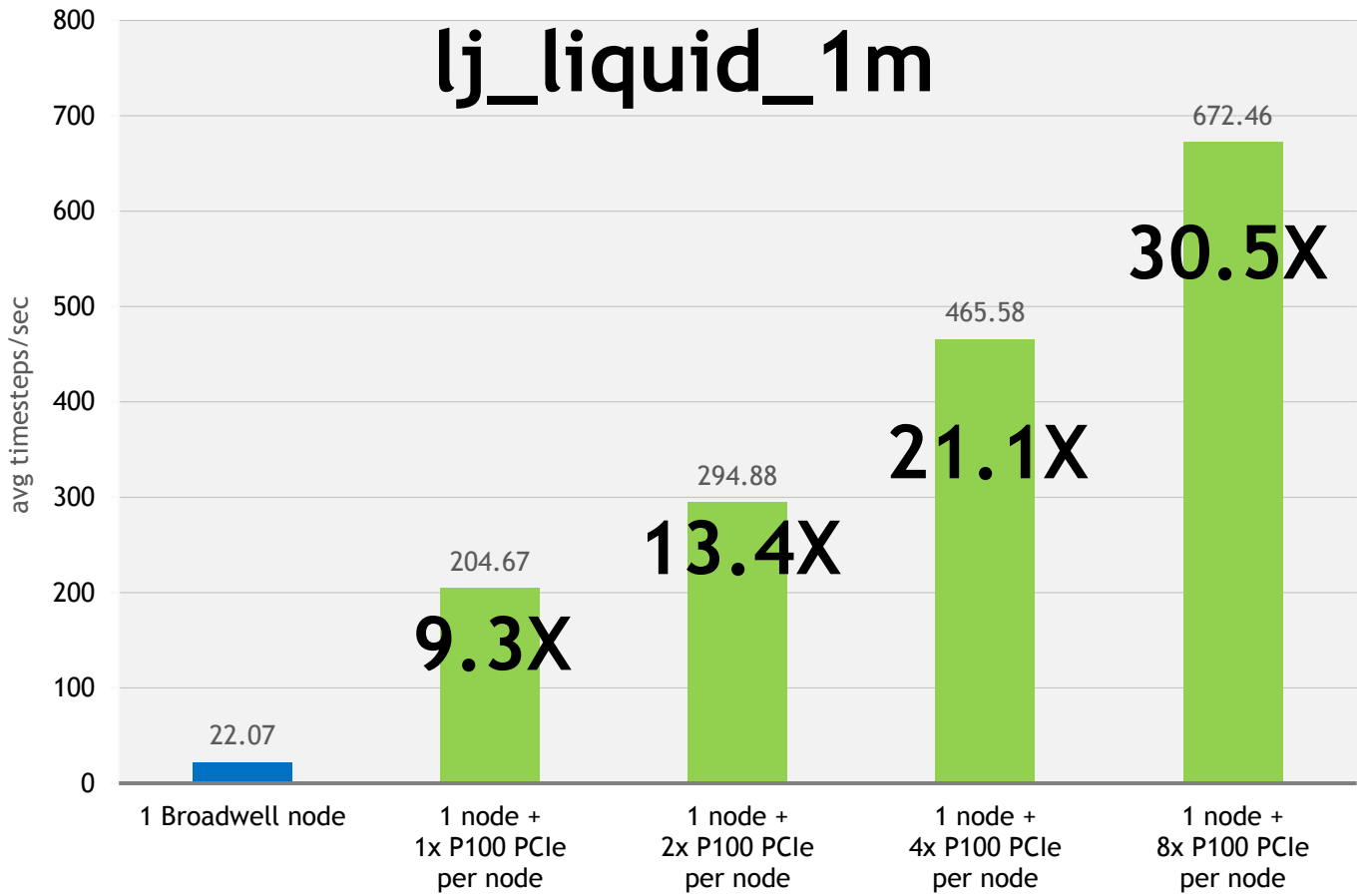
lj_liquid_1m on P100s PCIe



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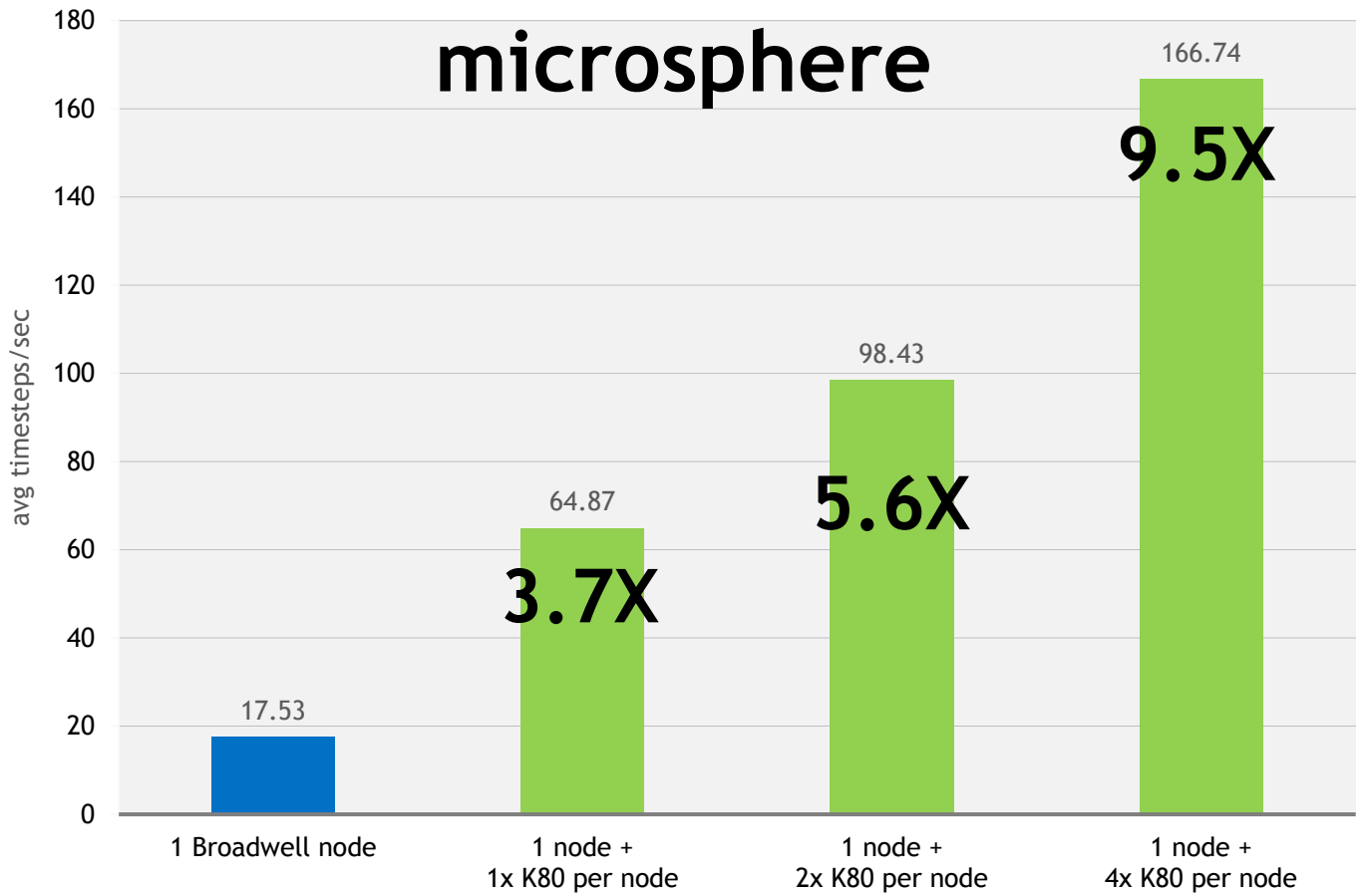
Microsphere on K80s



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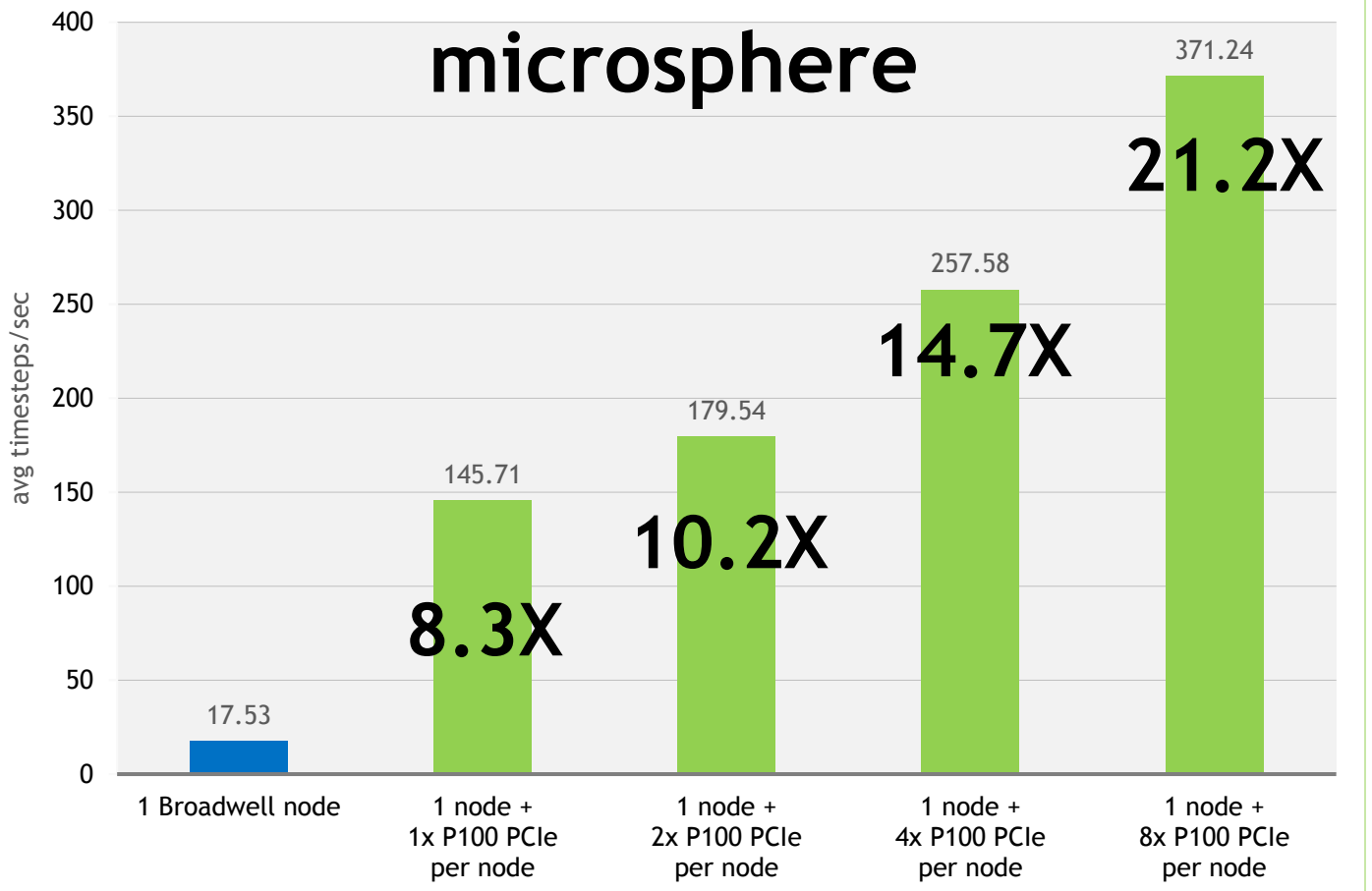
Microsphere on P100s PCIe



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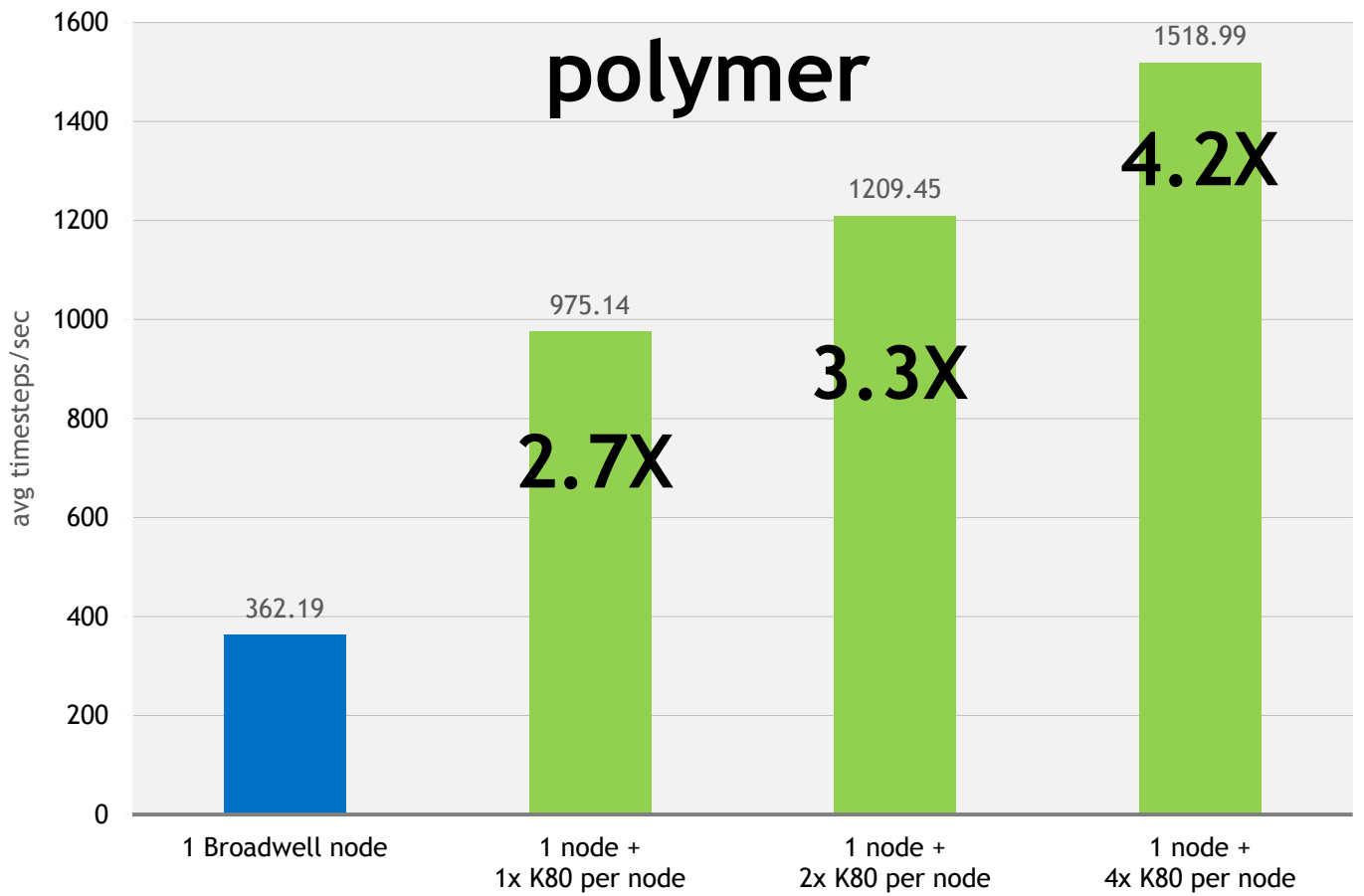
Polymer on K80s



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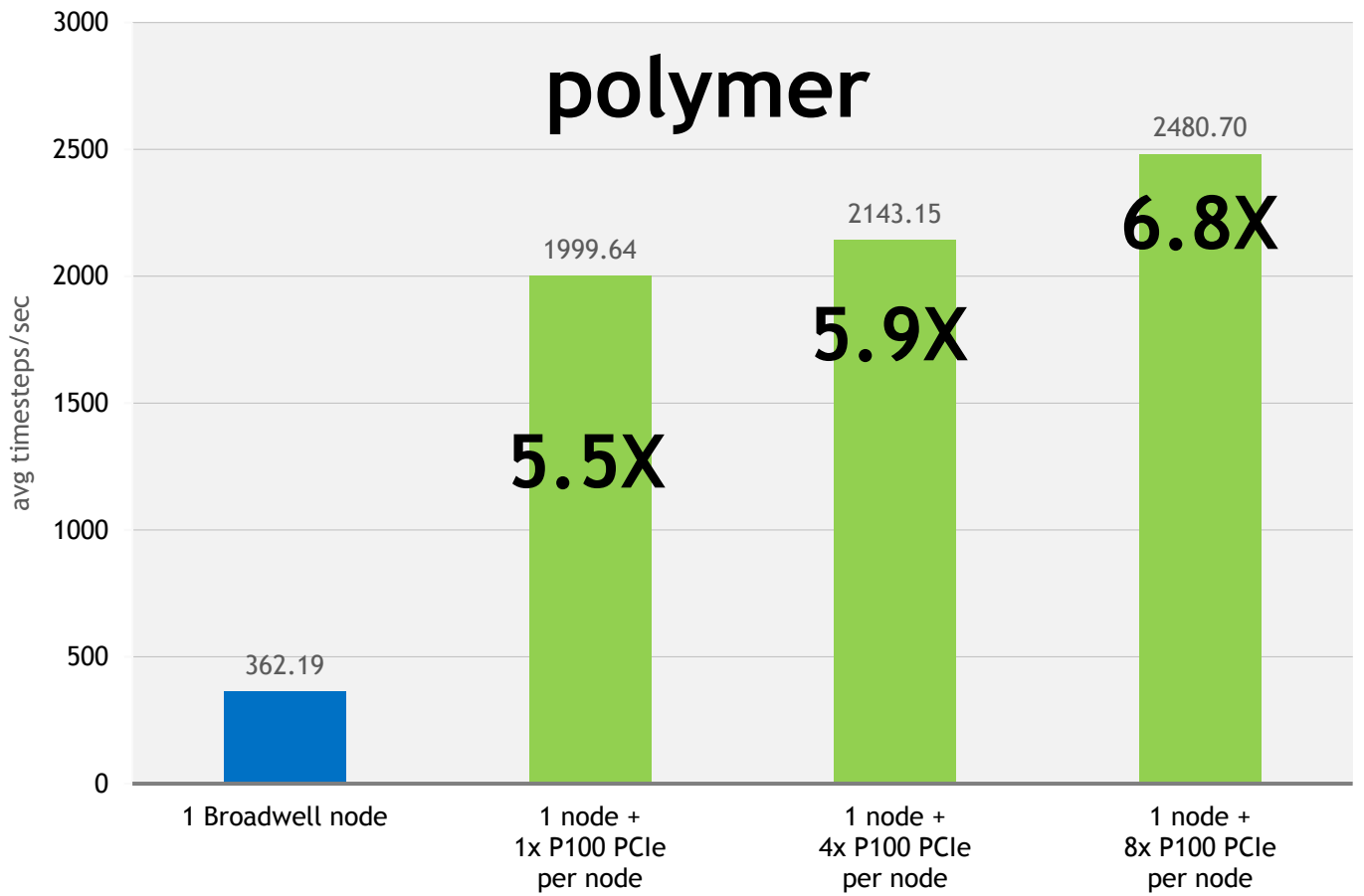
Polymer on P100s PCIe



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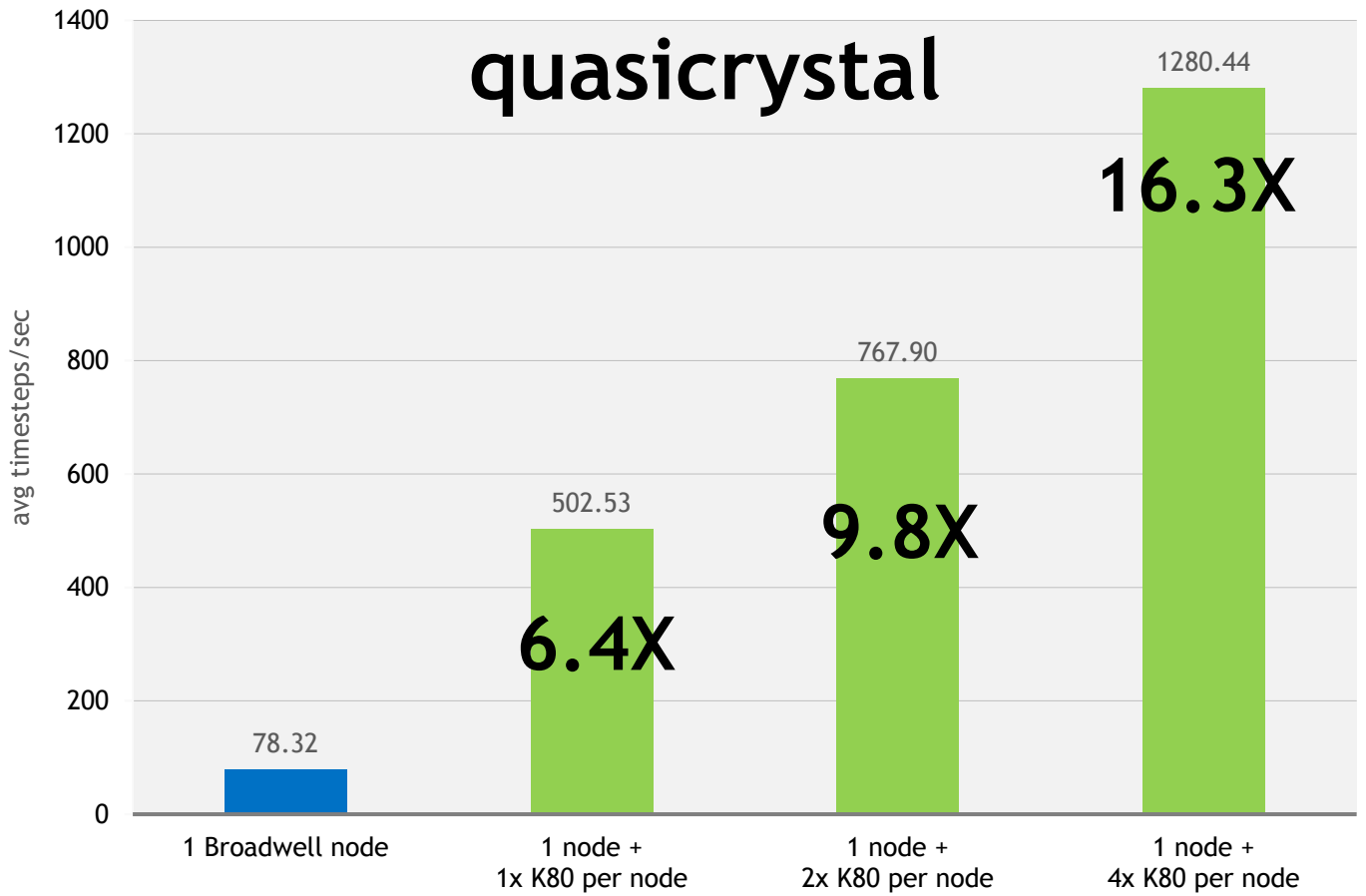
Quasicrystal on K80s



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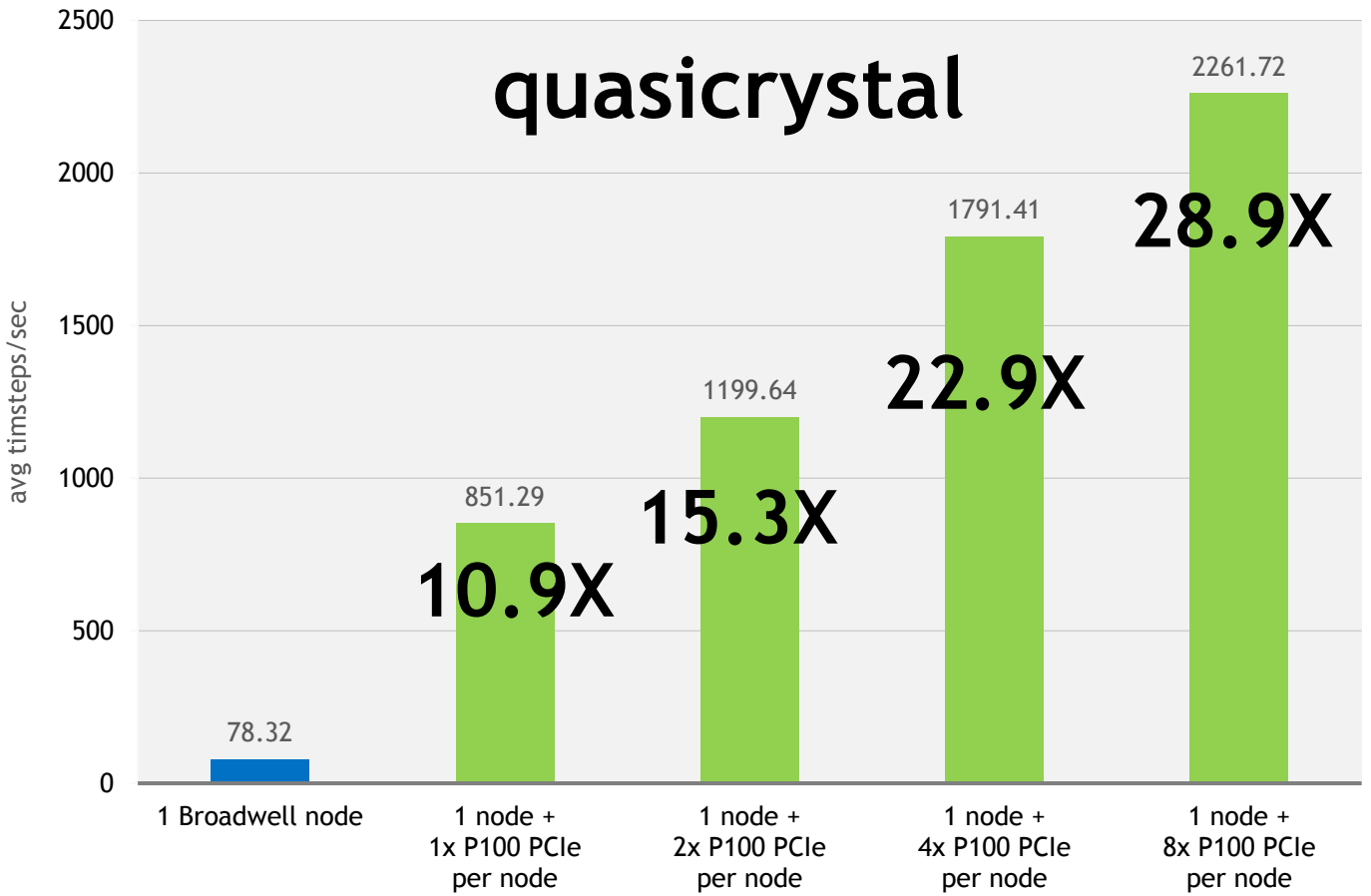
Quasicrystal on P100s PCIe



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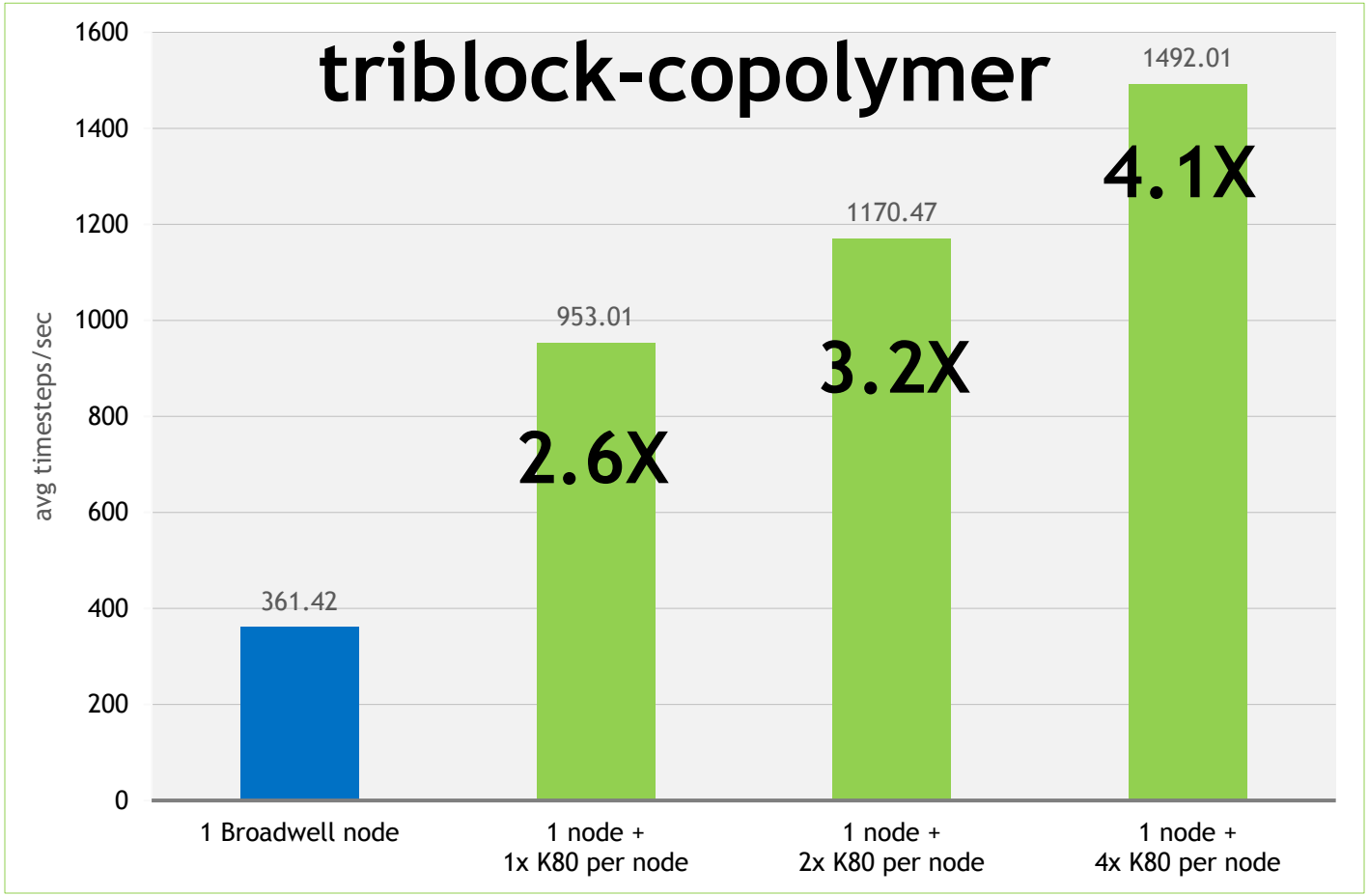
Triblock-copolymer on K80s



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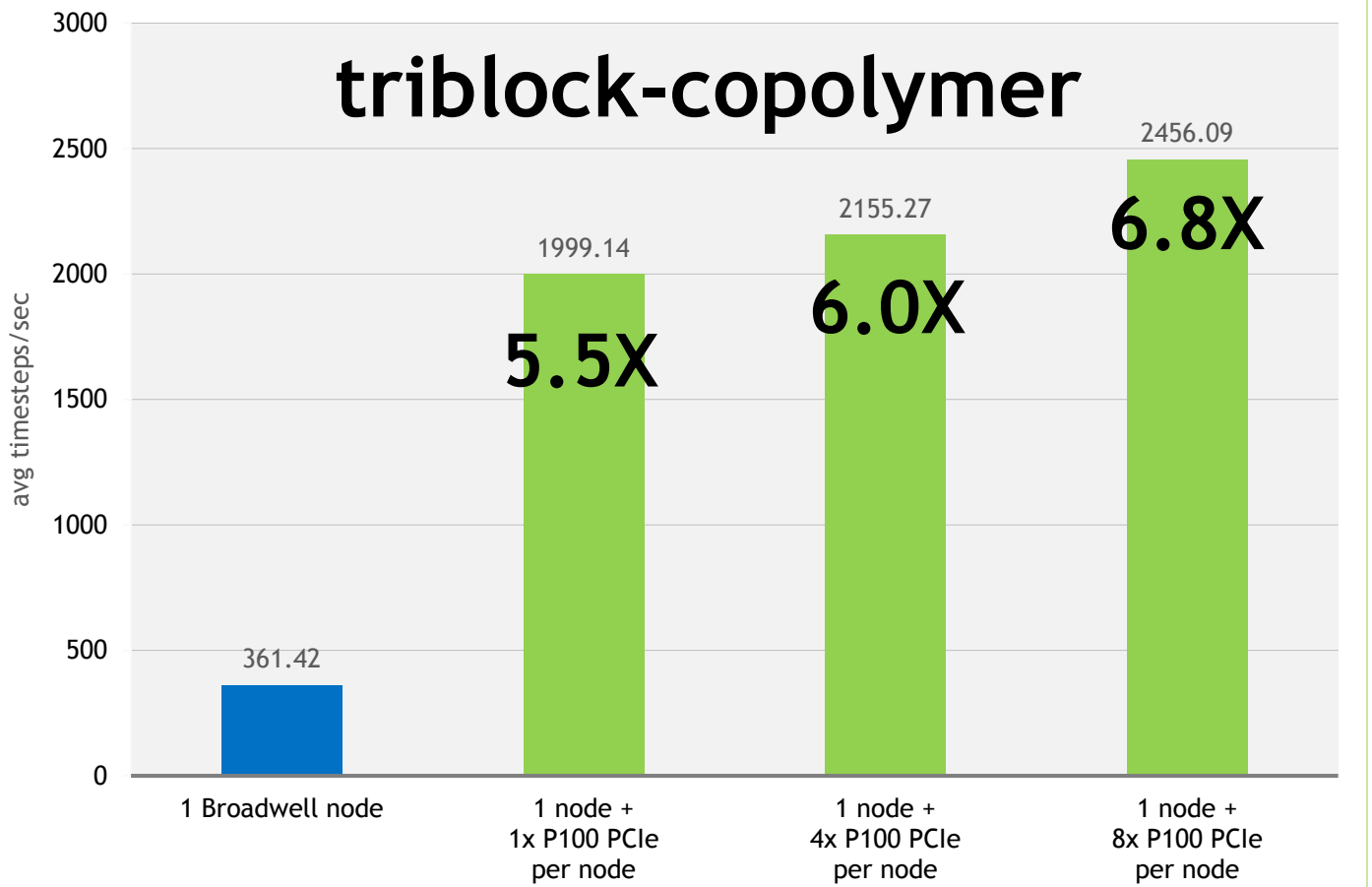
Triblock-copolymer on P100s PCIe



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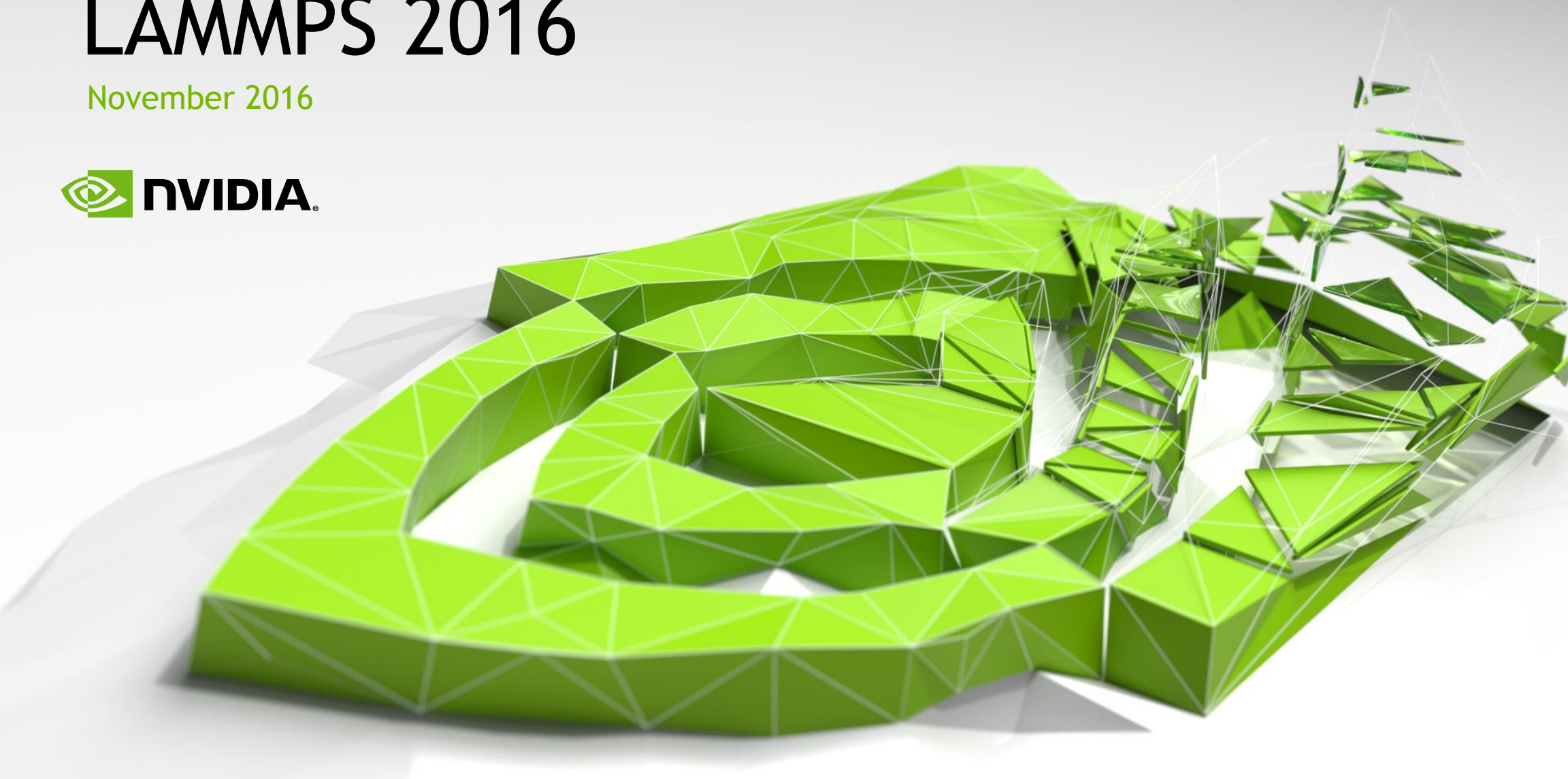
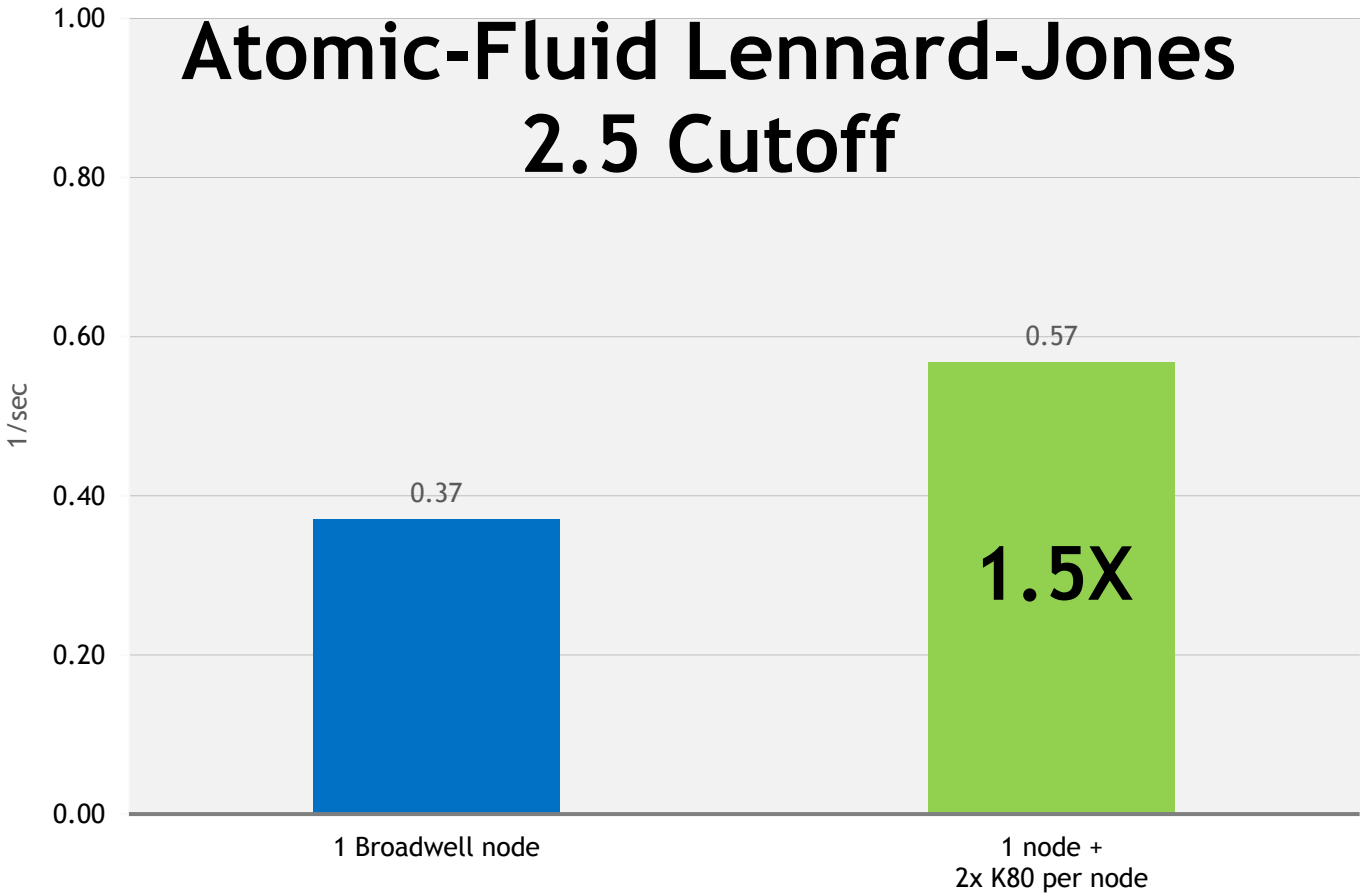
LAMMPS 2016

November 2016



Atomic-Fluid Lennard-Jones 2.5 Cutoff on K80s



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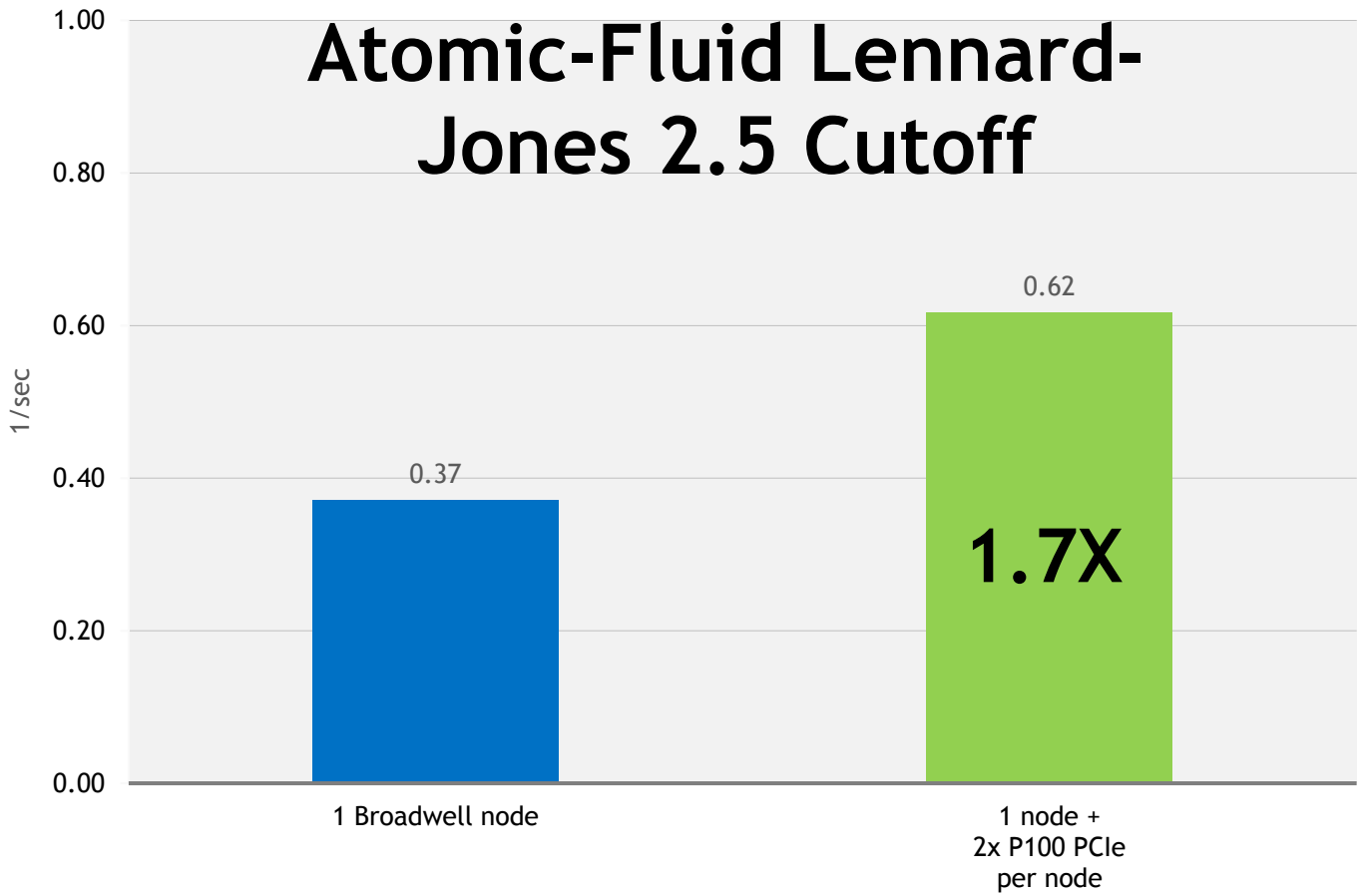
Atomic-Fluid Lennard-Jones 2.5 Cutoff on P100s PCIe



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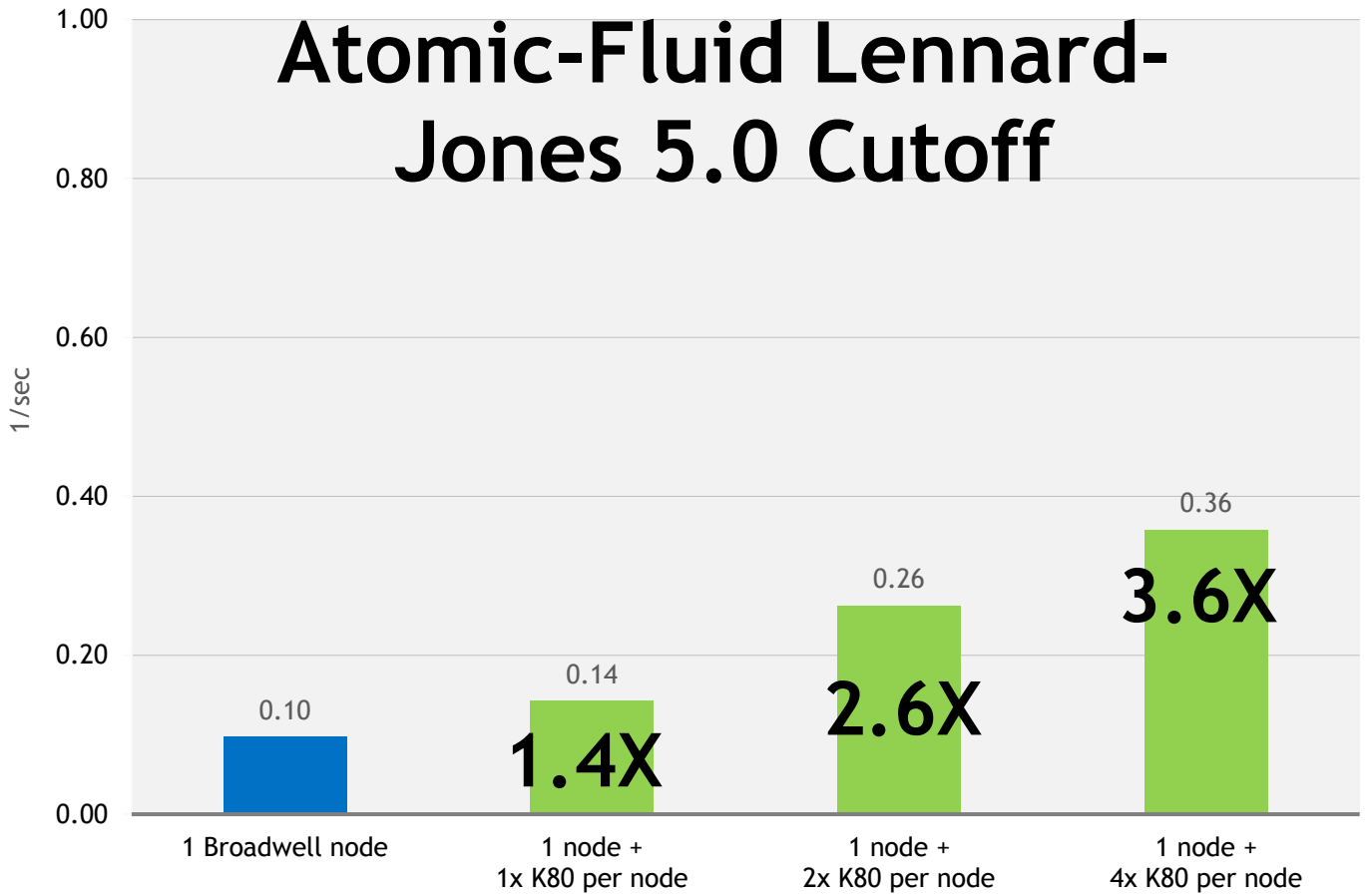
Atomic-Fluid Lennard-Jones 5.0 Cutoff on K80s



Running LAMMPS version 2016

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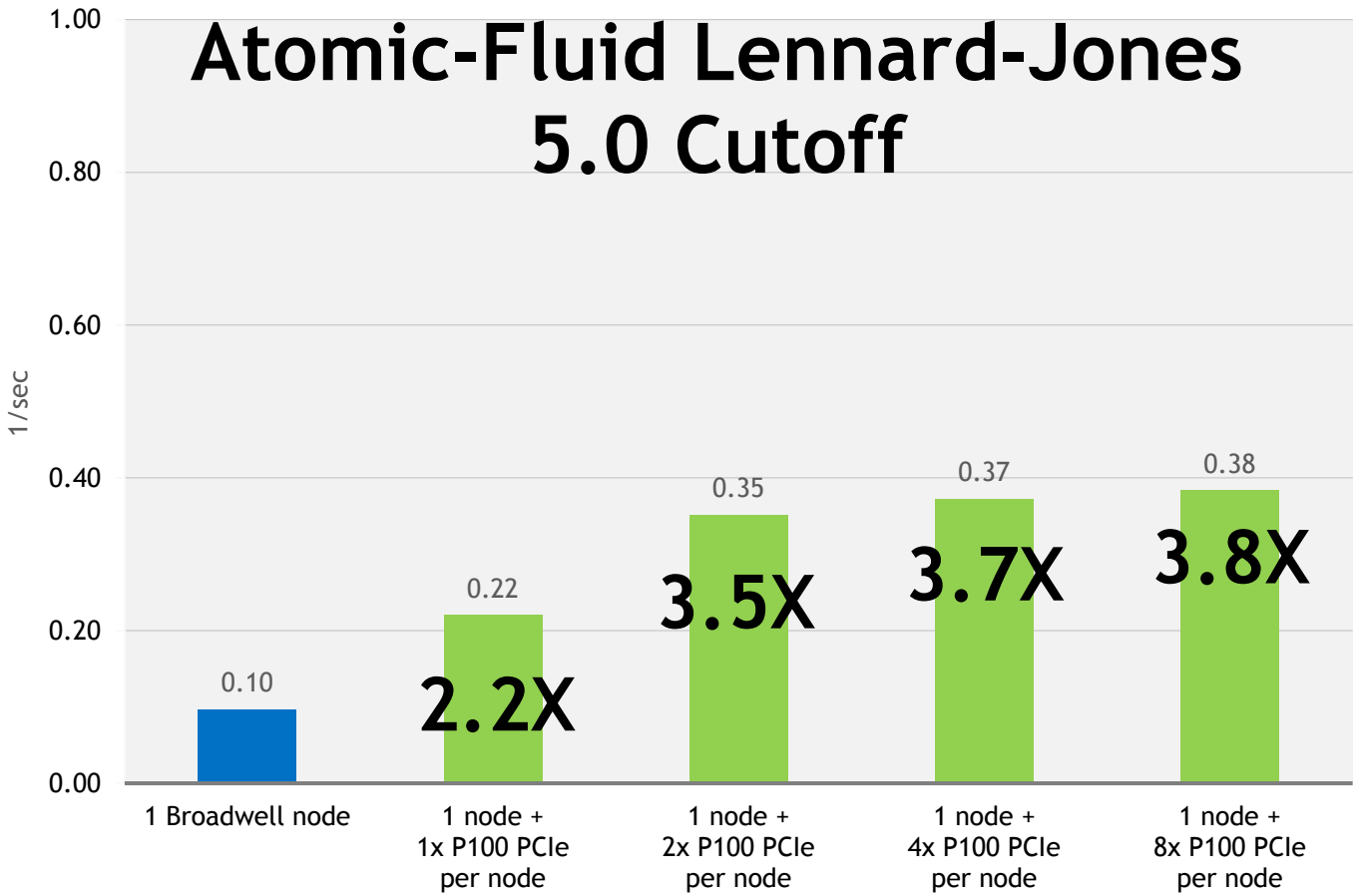
- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

Atomic-Fluid Lennard-Jones 5.0 Cutoff on P100s PCIe



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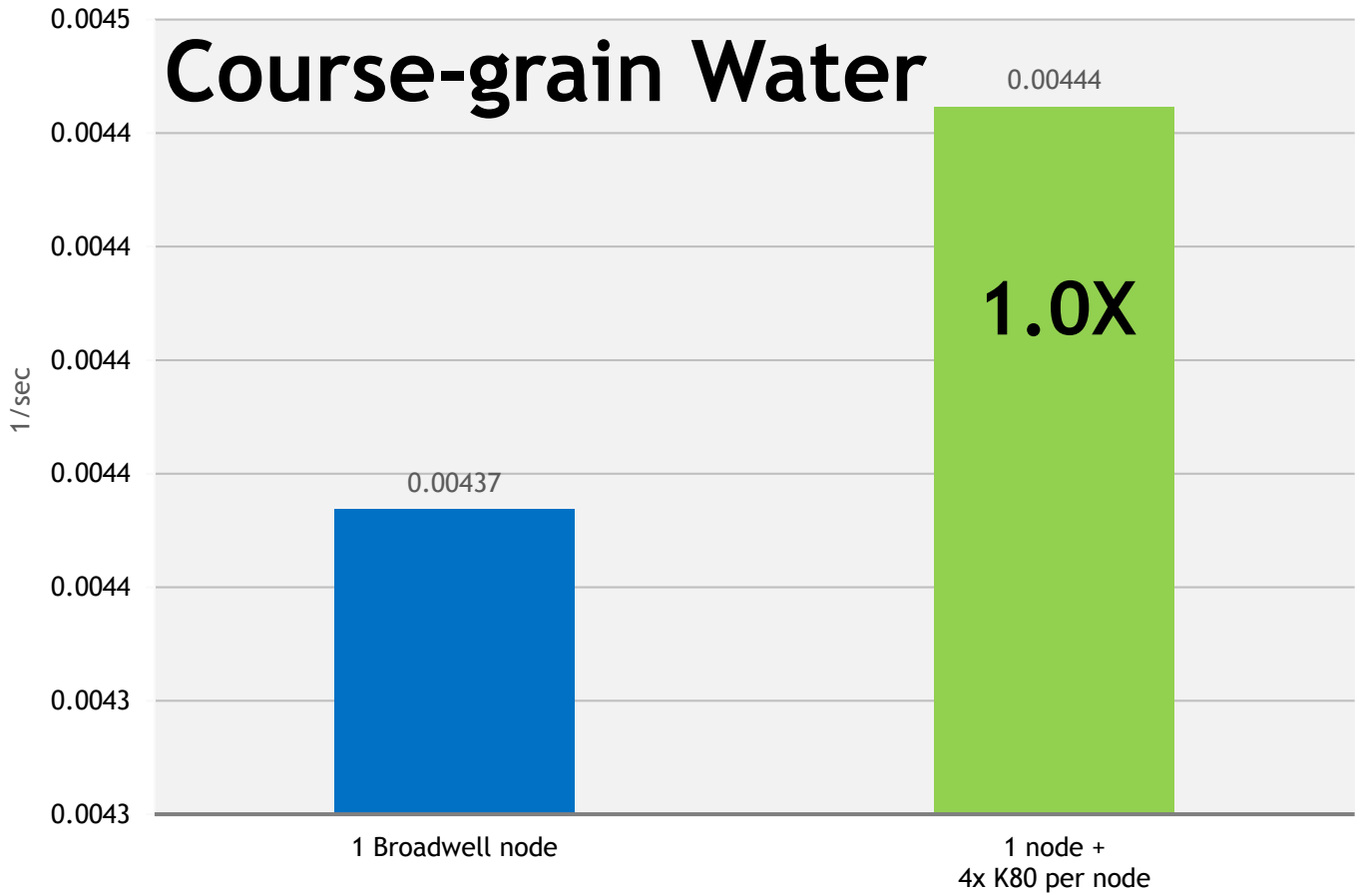
Course-grain Water on K80s



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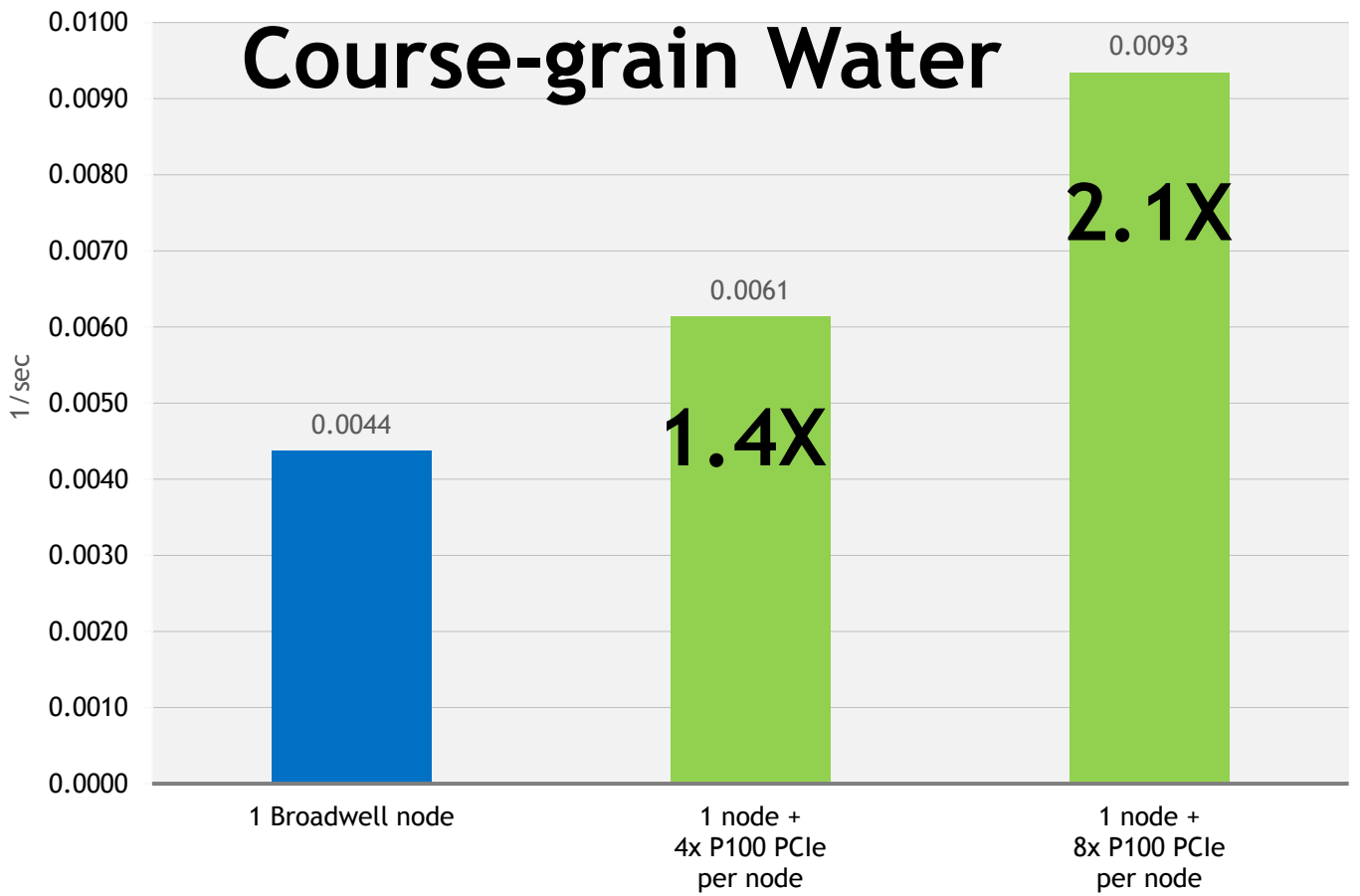
Course-grain Water on P100s PCIe



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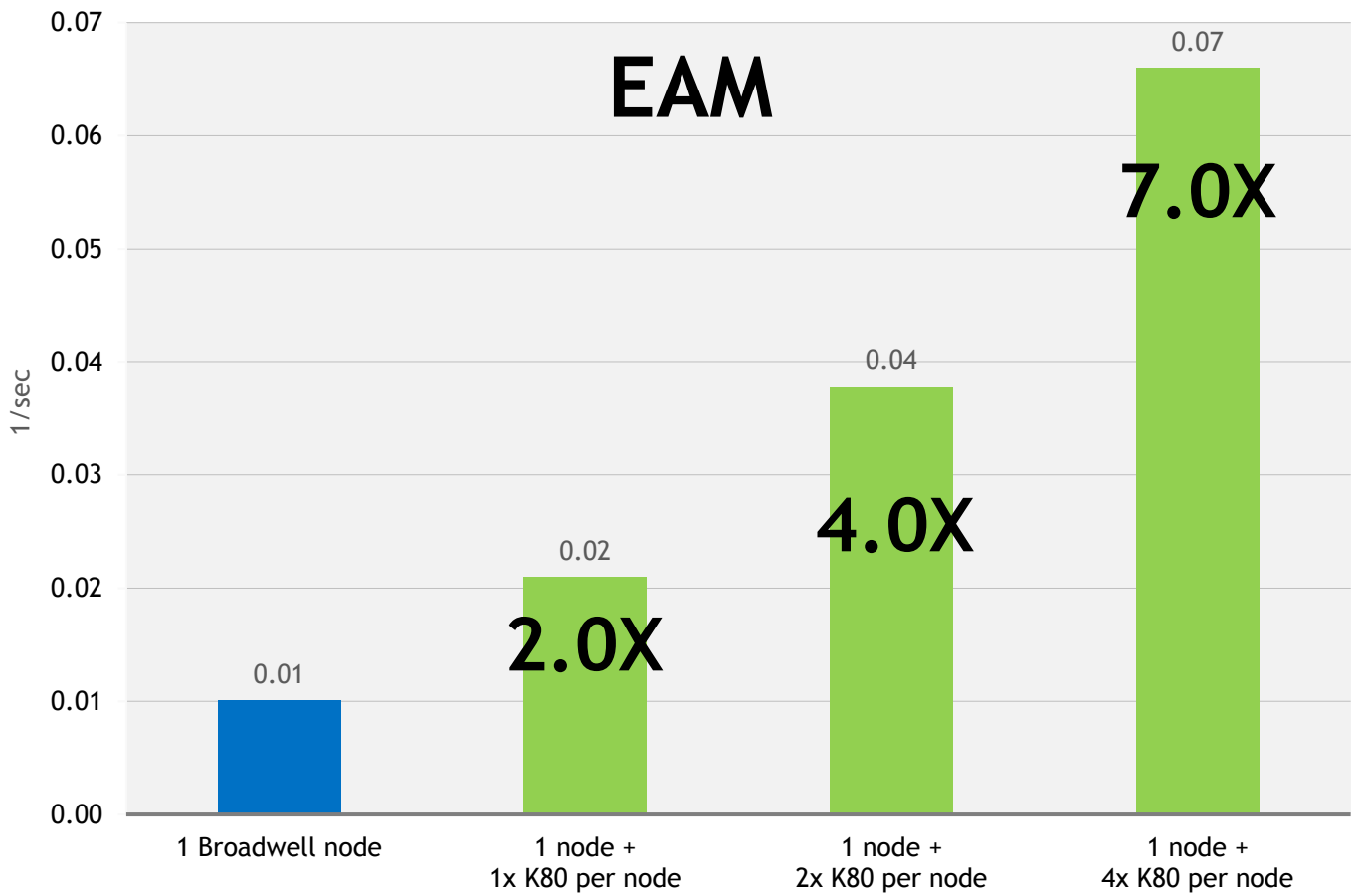
EAM on K80s



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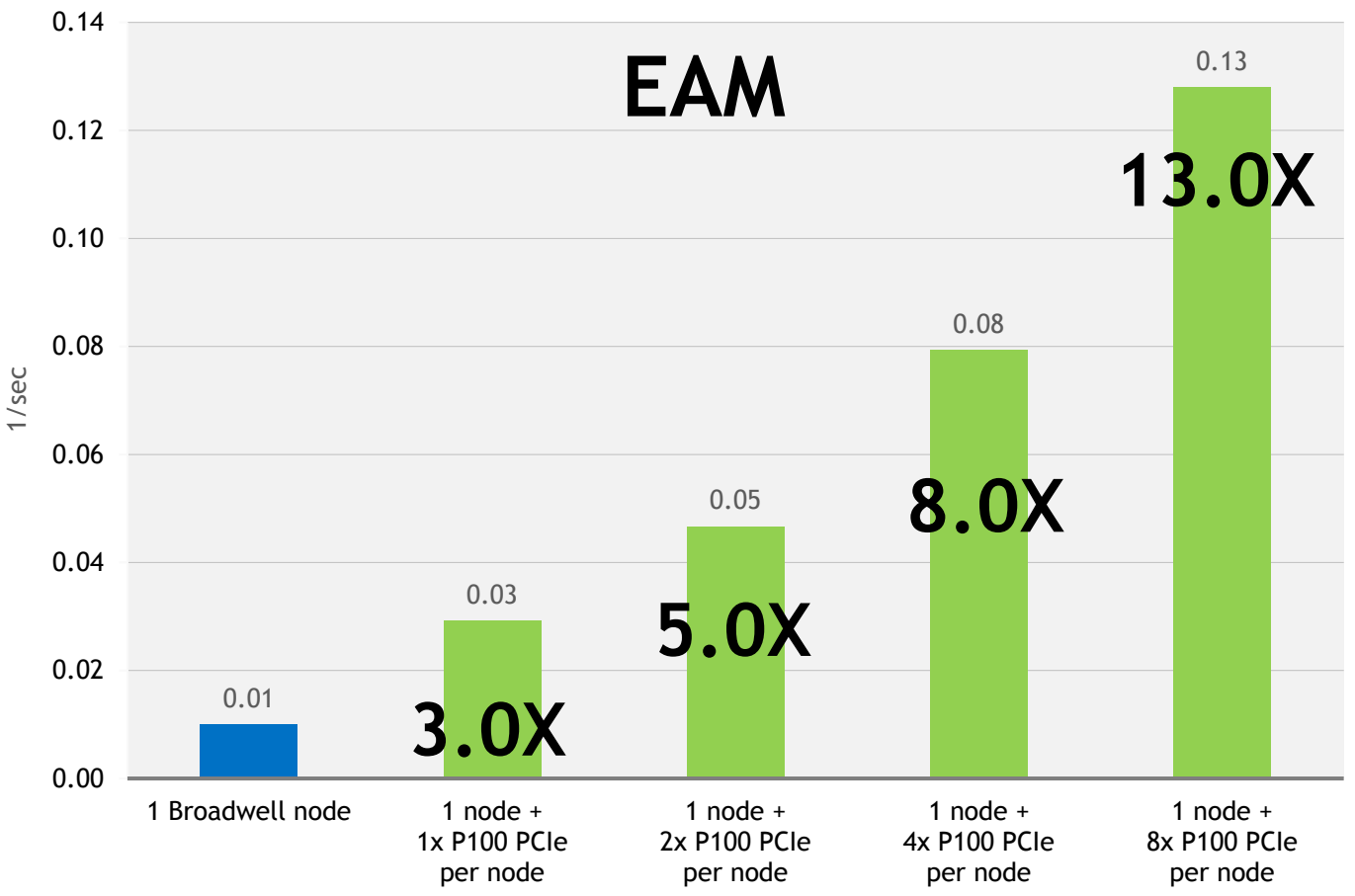
EAM on P100s PCIe



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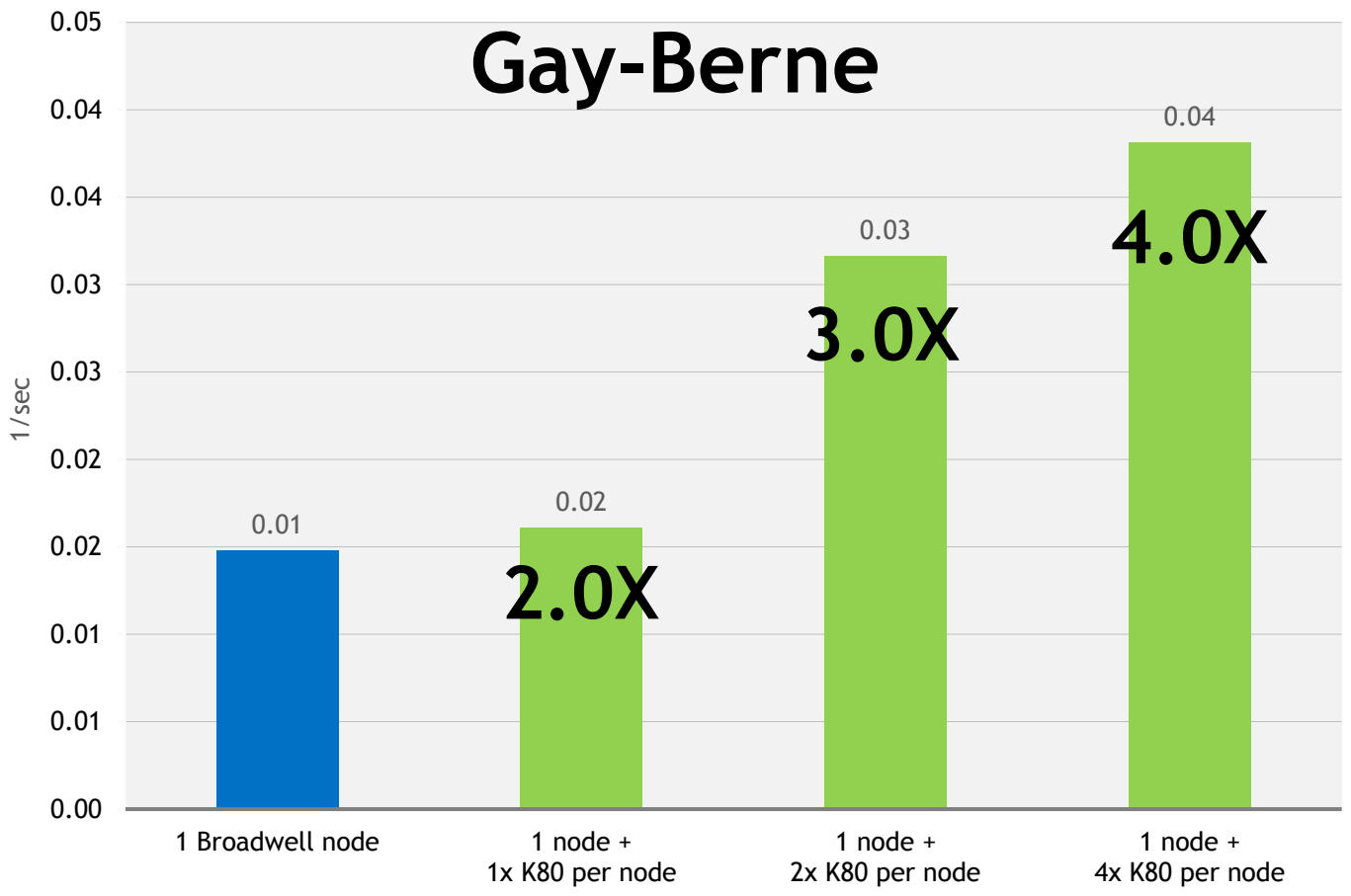
Gay-Berne on K80s



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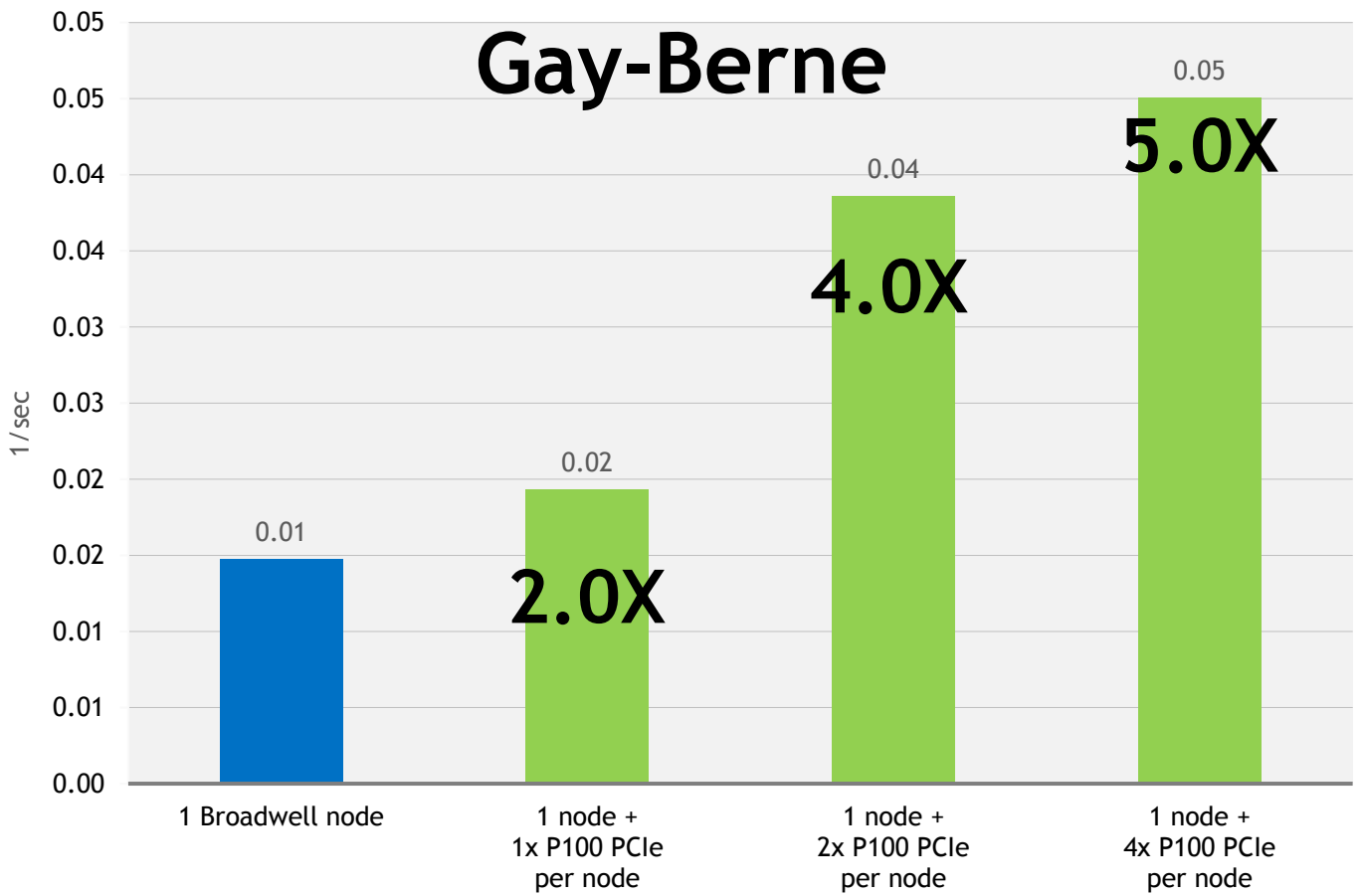
Gay-Berne on P100s PCIe



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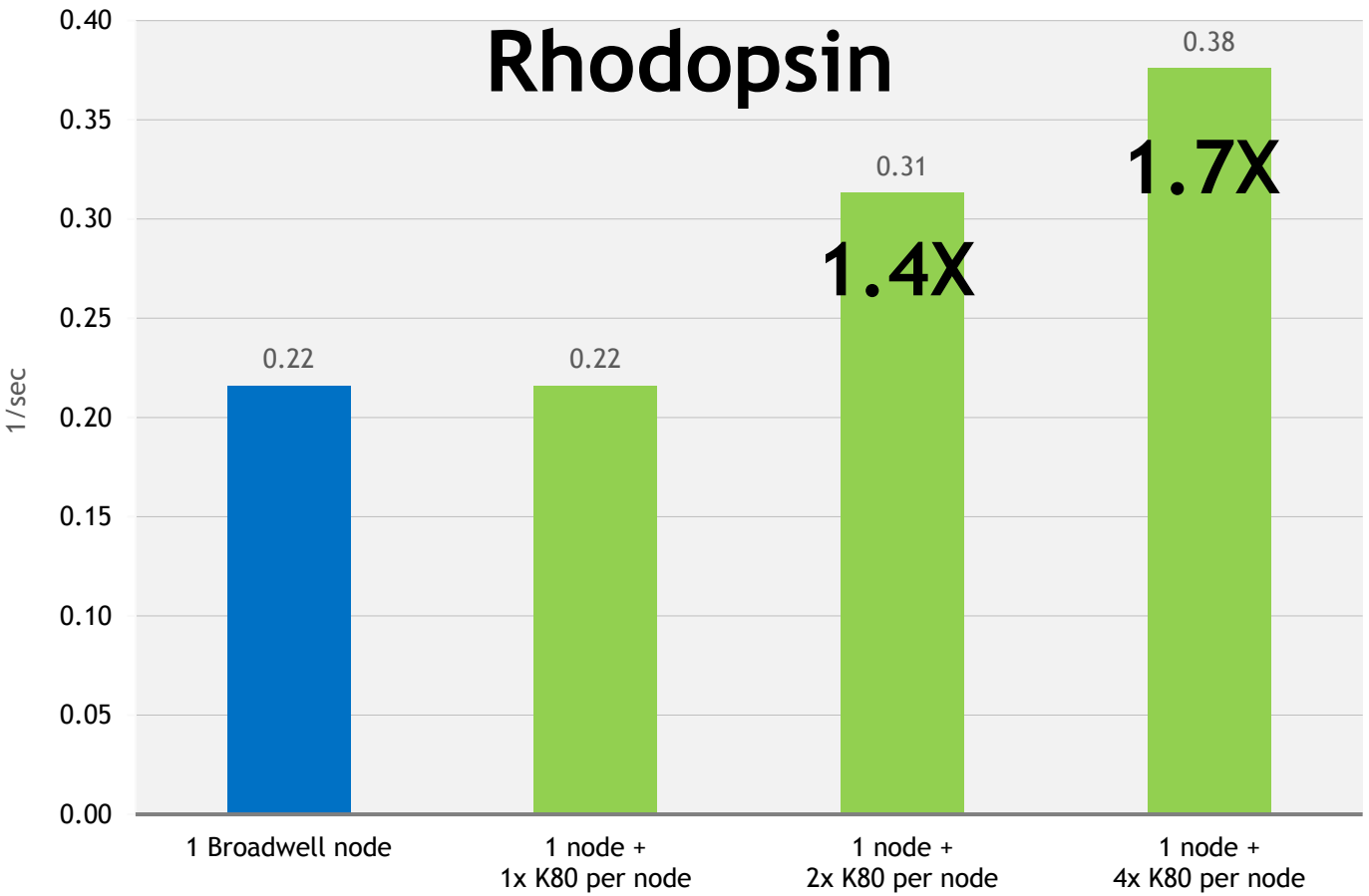
Rhodopsin on K80s



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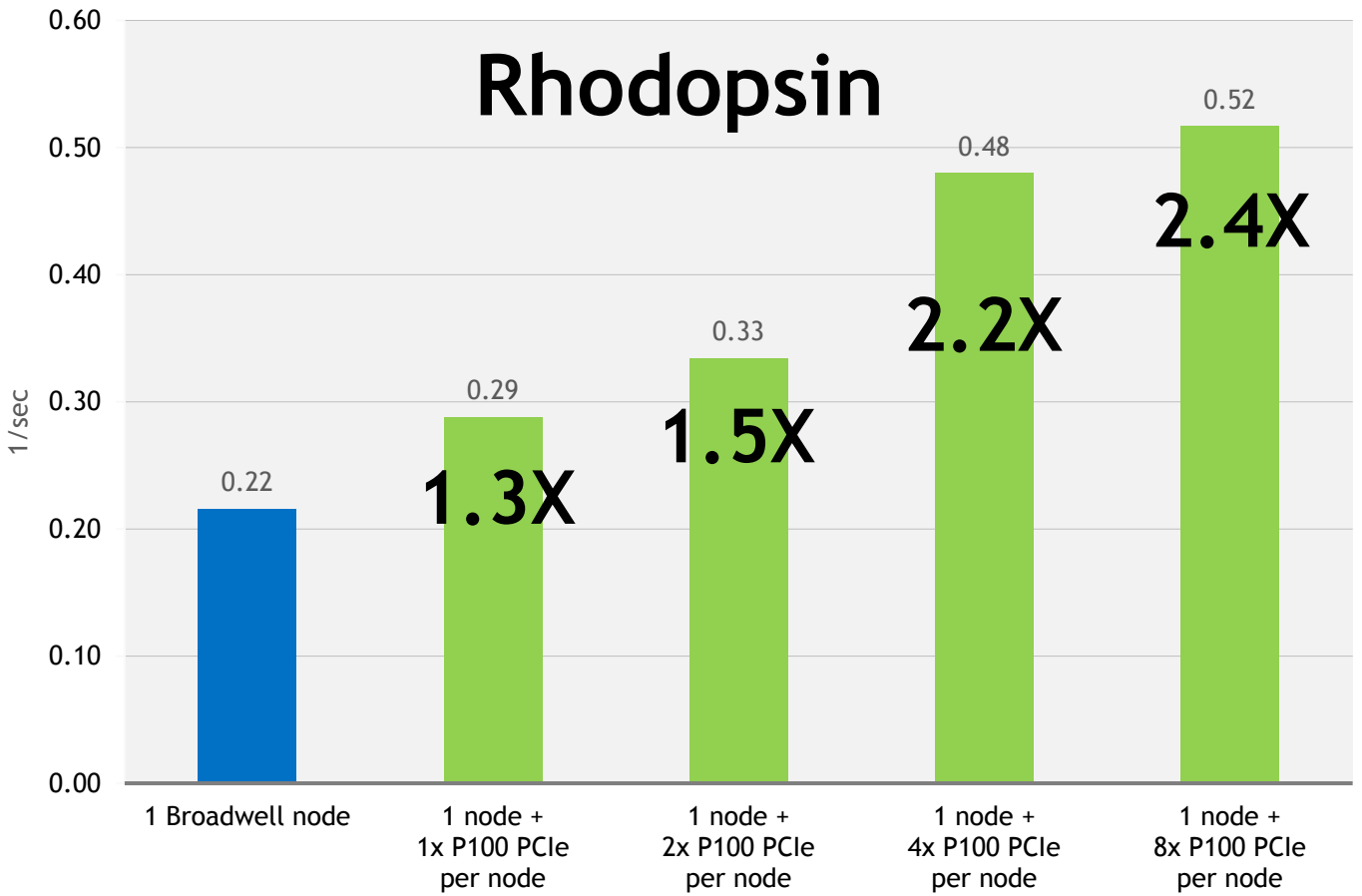
Rhodopsin on P100s PCIe



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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, Kepler K20, K40, K80, M40
# 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

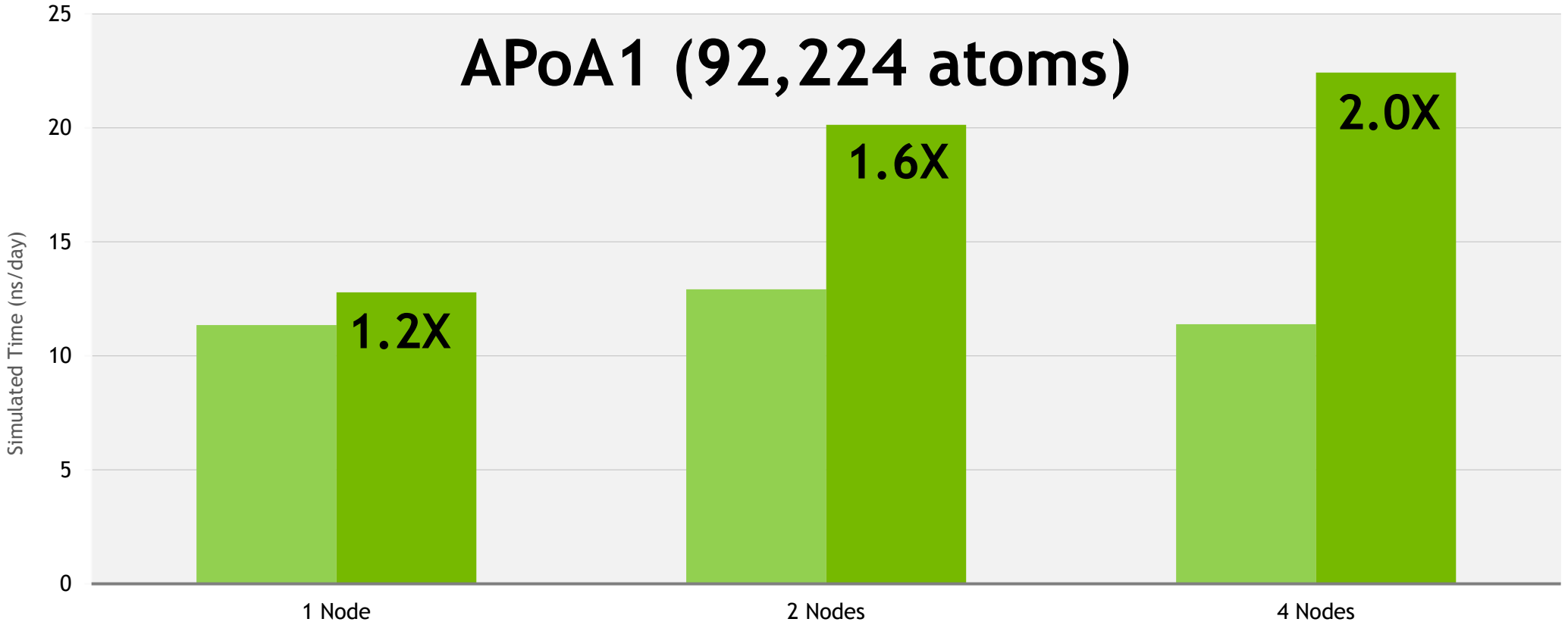
NAMD 2.11 – Up to 2X Faster

New GPU features in NAMD 2.11

Selected Text from the NAMD website

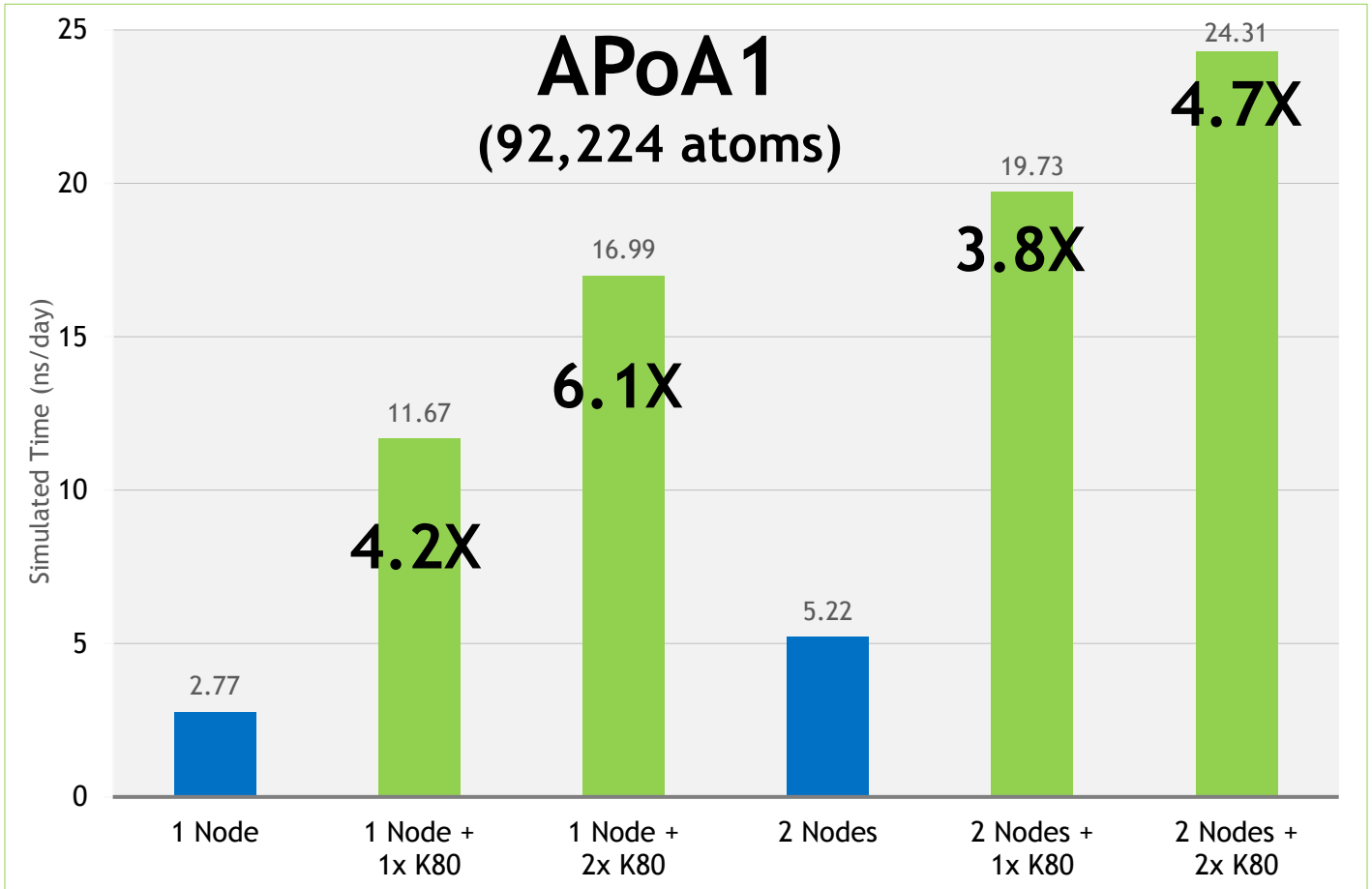
- **GPU-accelerated simulations up to twice as fast as NAMD 2.10**
- **Pressure calculation with fixed atoms on GPU works as on CPU**
- **Improved scaling for GPU-accelerated particle-mesh Ewald calculation**
  - CPU-side operations overlap better and are parallelized across cores.
- **Improved scaling for GPU-accelerated simulations**
  - Nonbonded force calculation results are streamed from the GPU for better overlap.
- **NVIDIA CUDA GPU-acceleration binaries for Mac OS X**

NAMD 2.11 is up to 2x faster



NAMD 2.10 & NAMD 2.11 contain Dual Intel E5-2697 v2@2.7GHz (IvyBridge) CPUs + 2 Tesla K80 (autoboost) GPUs

NAMD 2.11 APoA1 on 1 and 2 nodes



Running NAMD version 2.11

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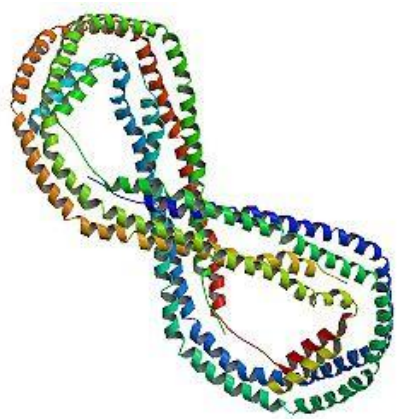
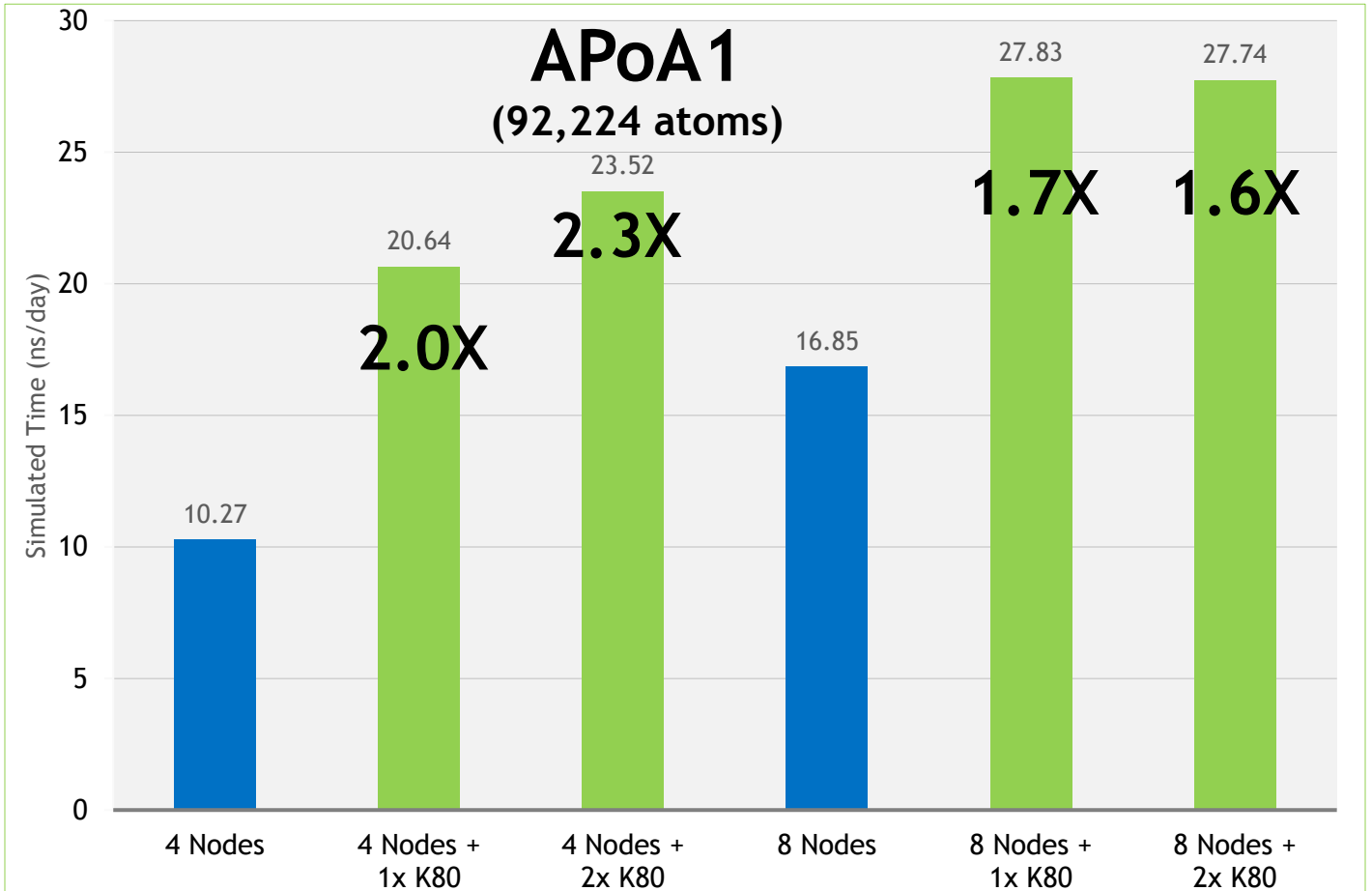


NAMD 2.11 APoA1 on 4 and 8 nodes



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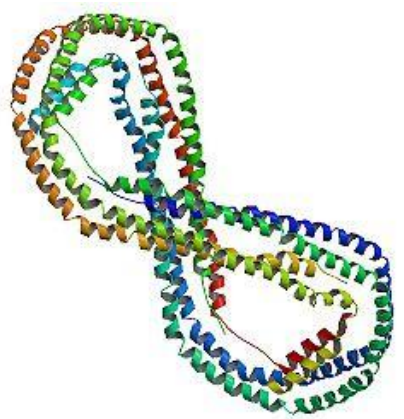
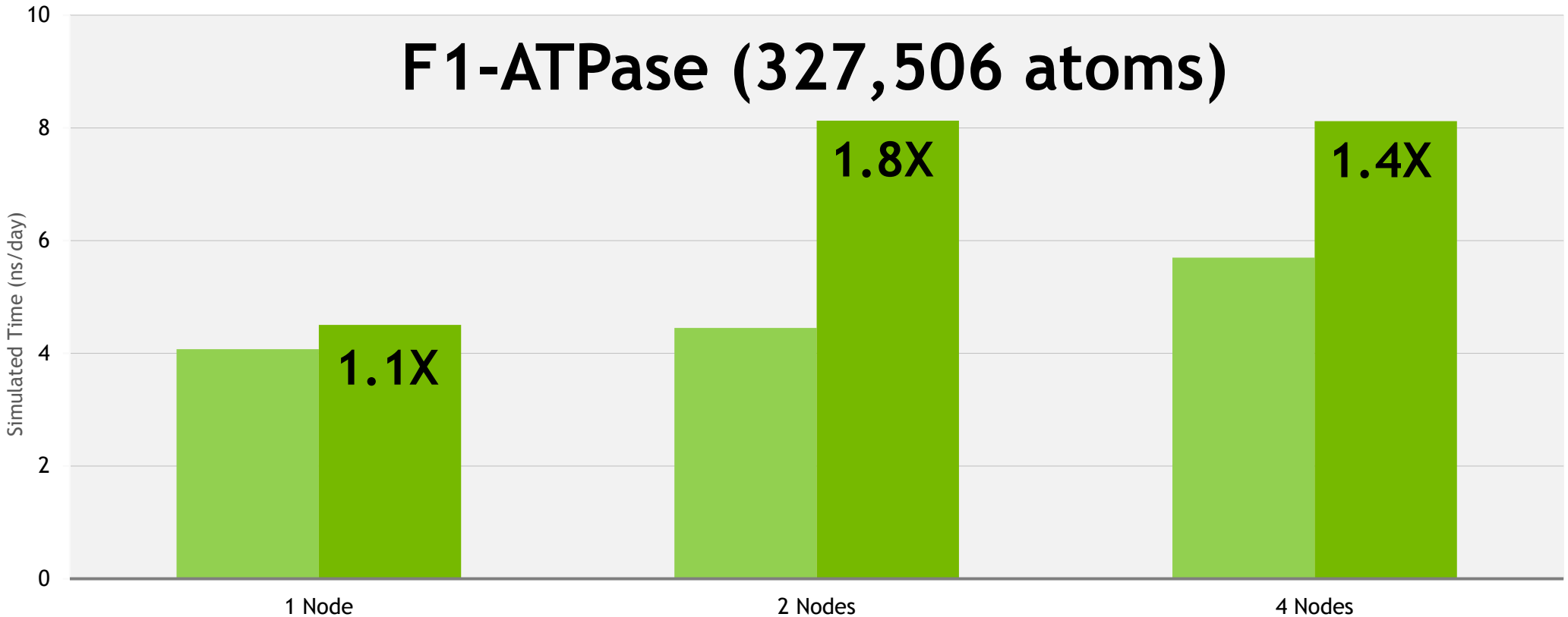


NAMD 2.11 is up to 1.8x faster



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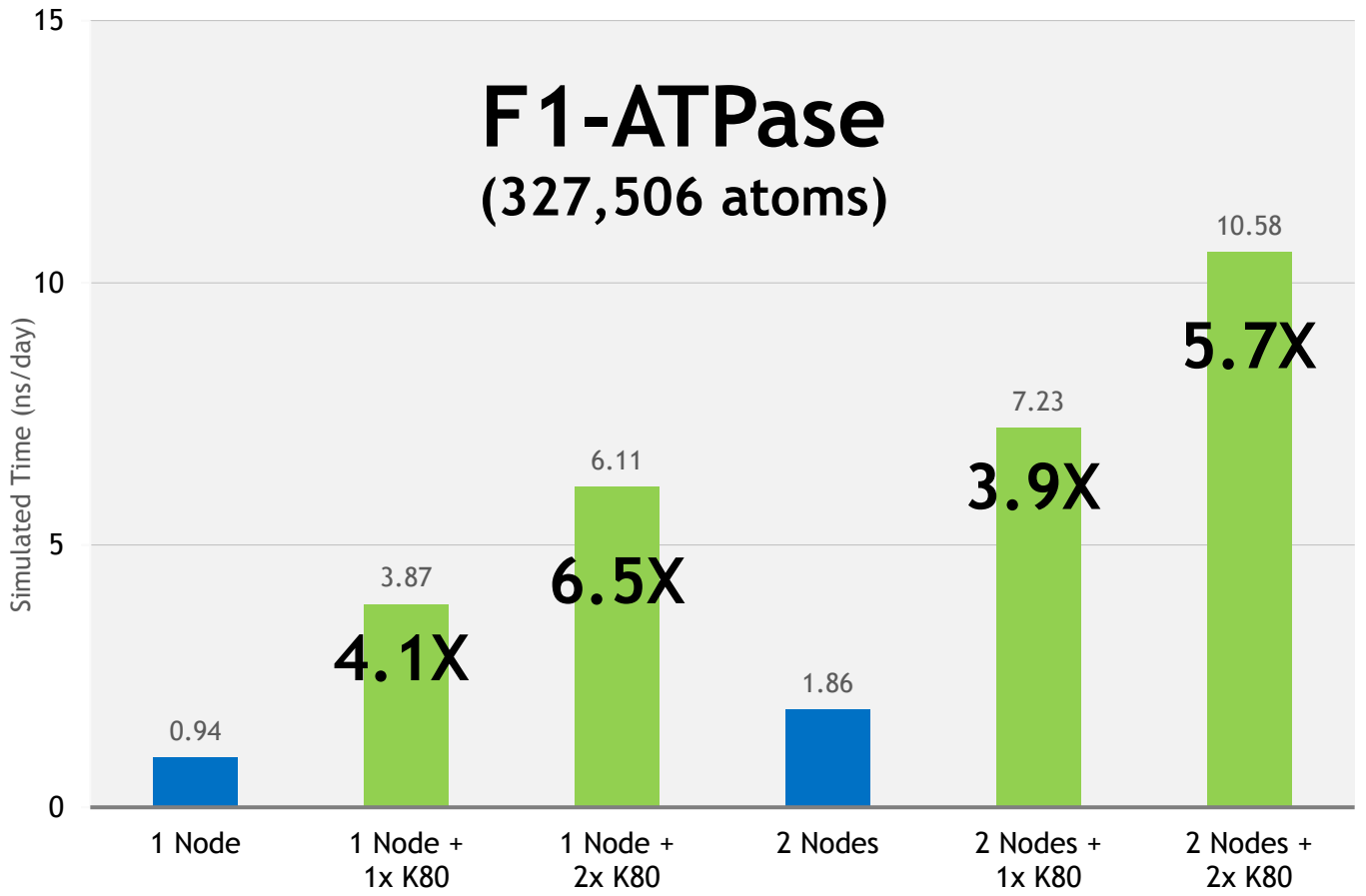
NAMD 2.11 F1-ATPase on 1 and 2 nodes



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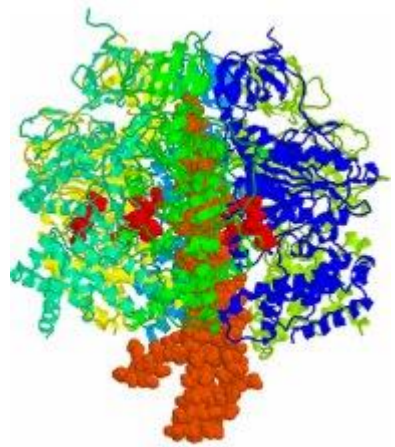
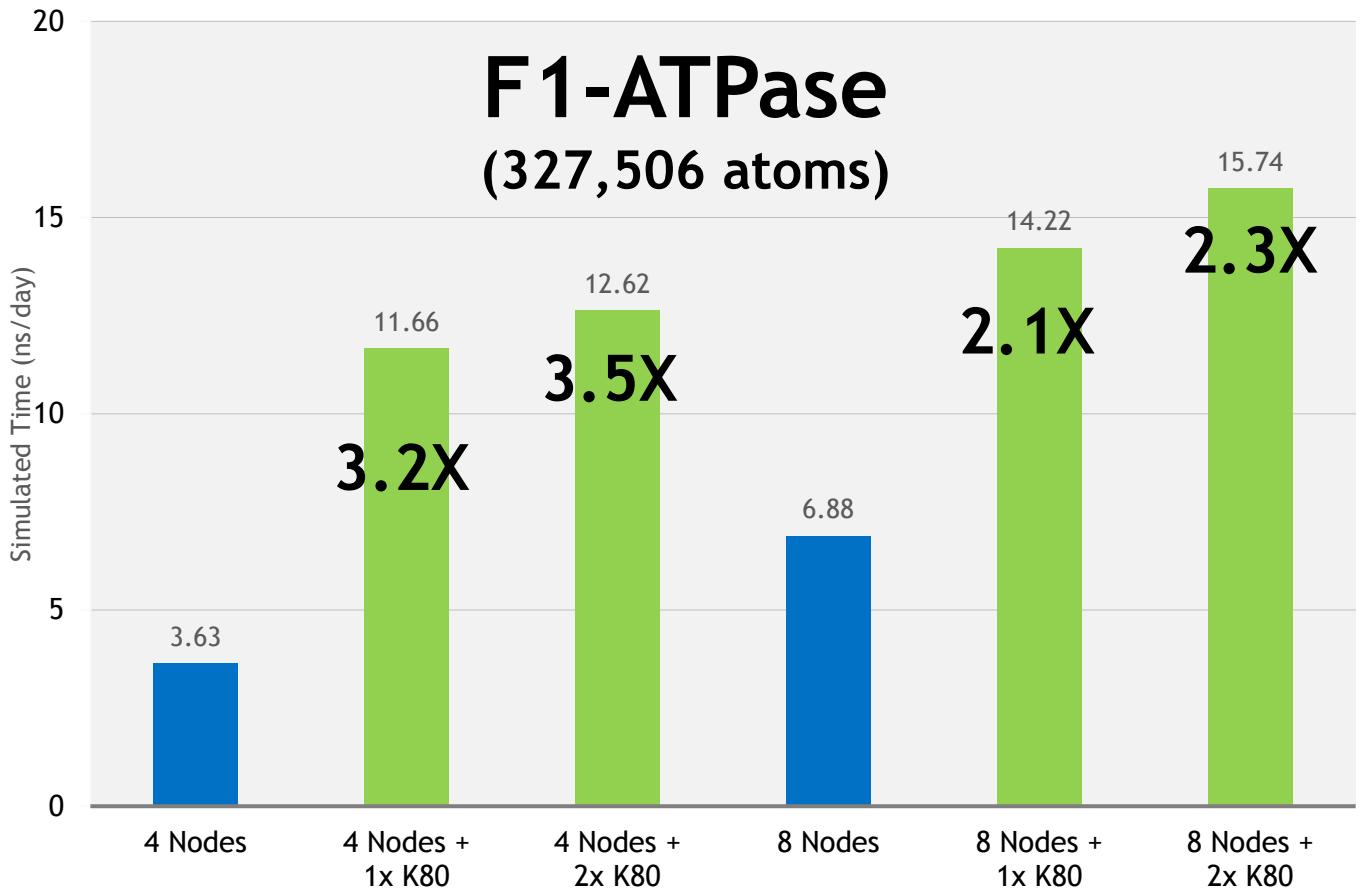


NAMD 2.11 F1-ATPase on 4 and 8 nodes



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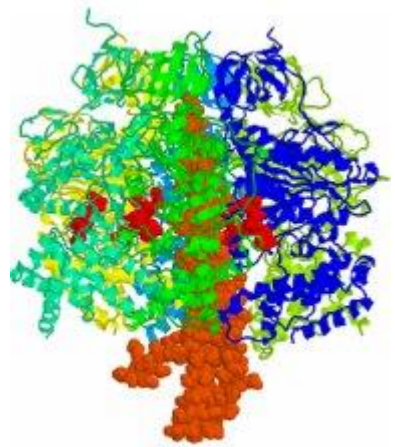
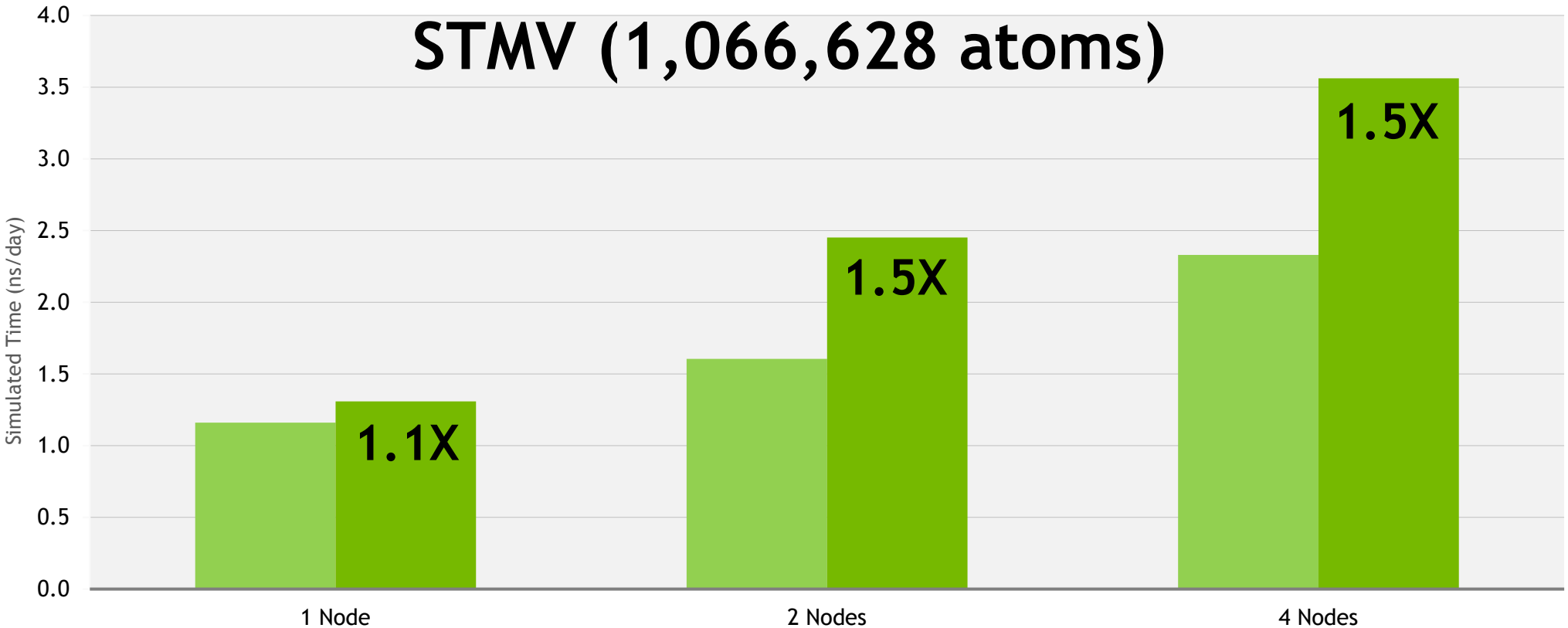


NAMD 2.11 is up to 1.5x faster



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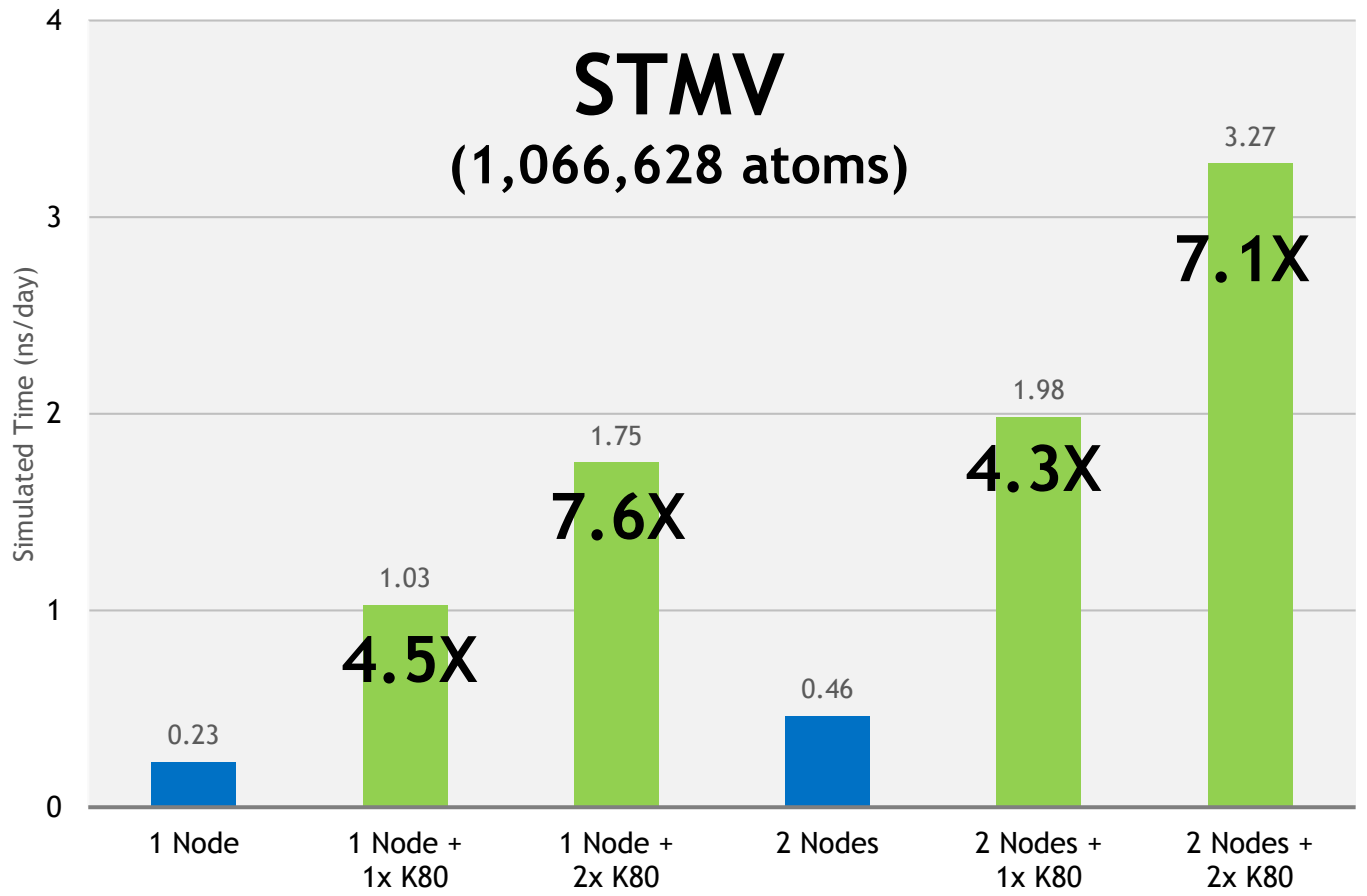
NAMD 2.11 STMV on 1 and 2 nodes



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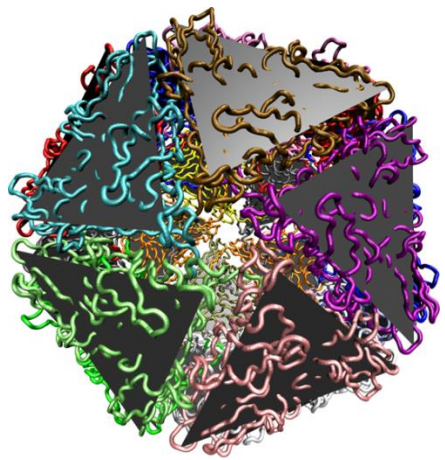
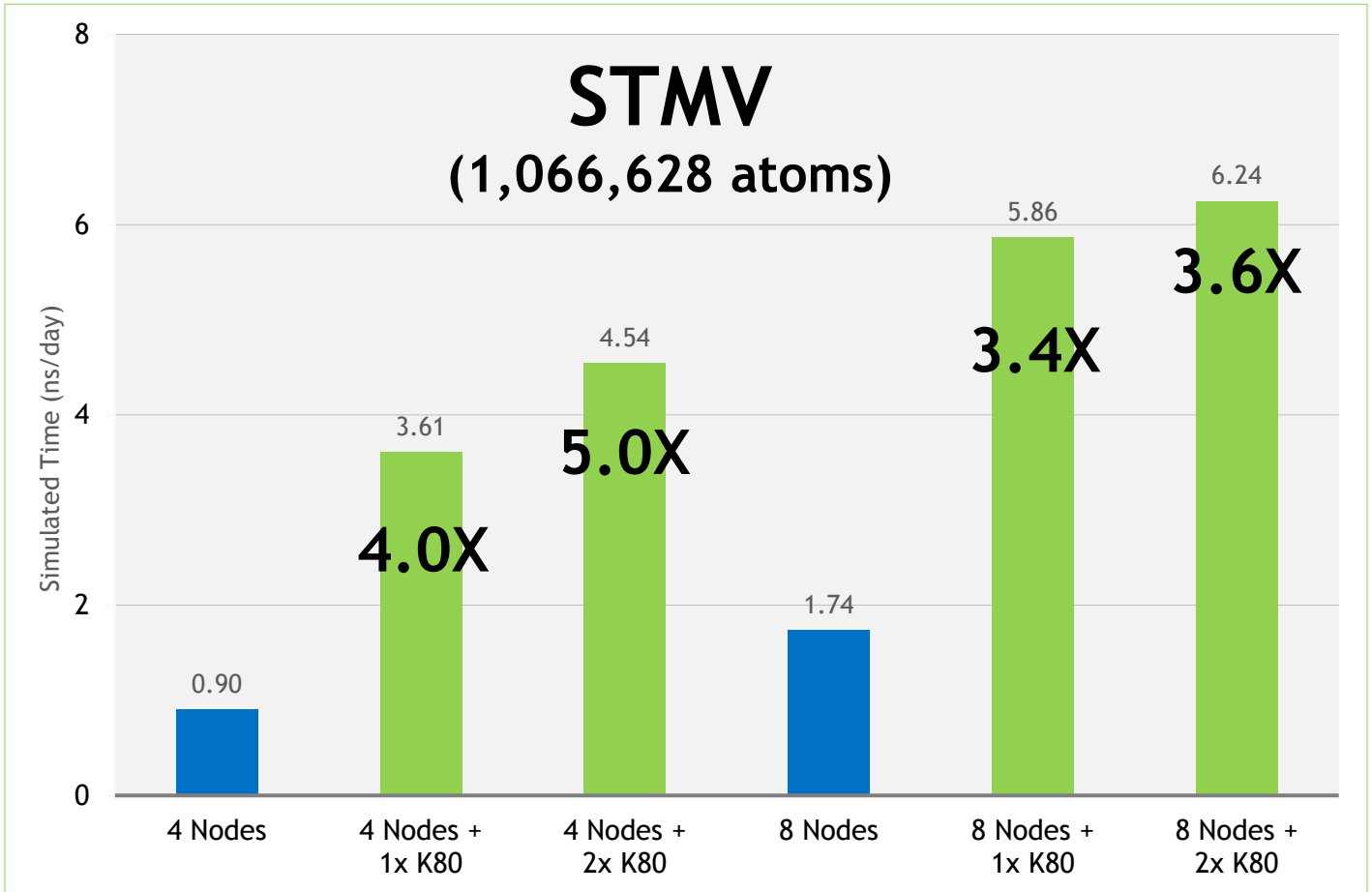


NAMD 2.11 STMV on 4 and 8 nodes



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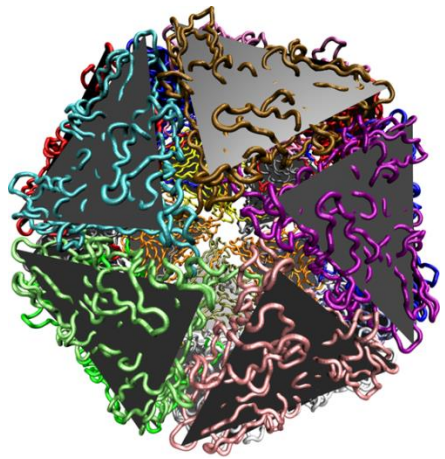
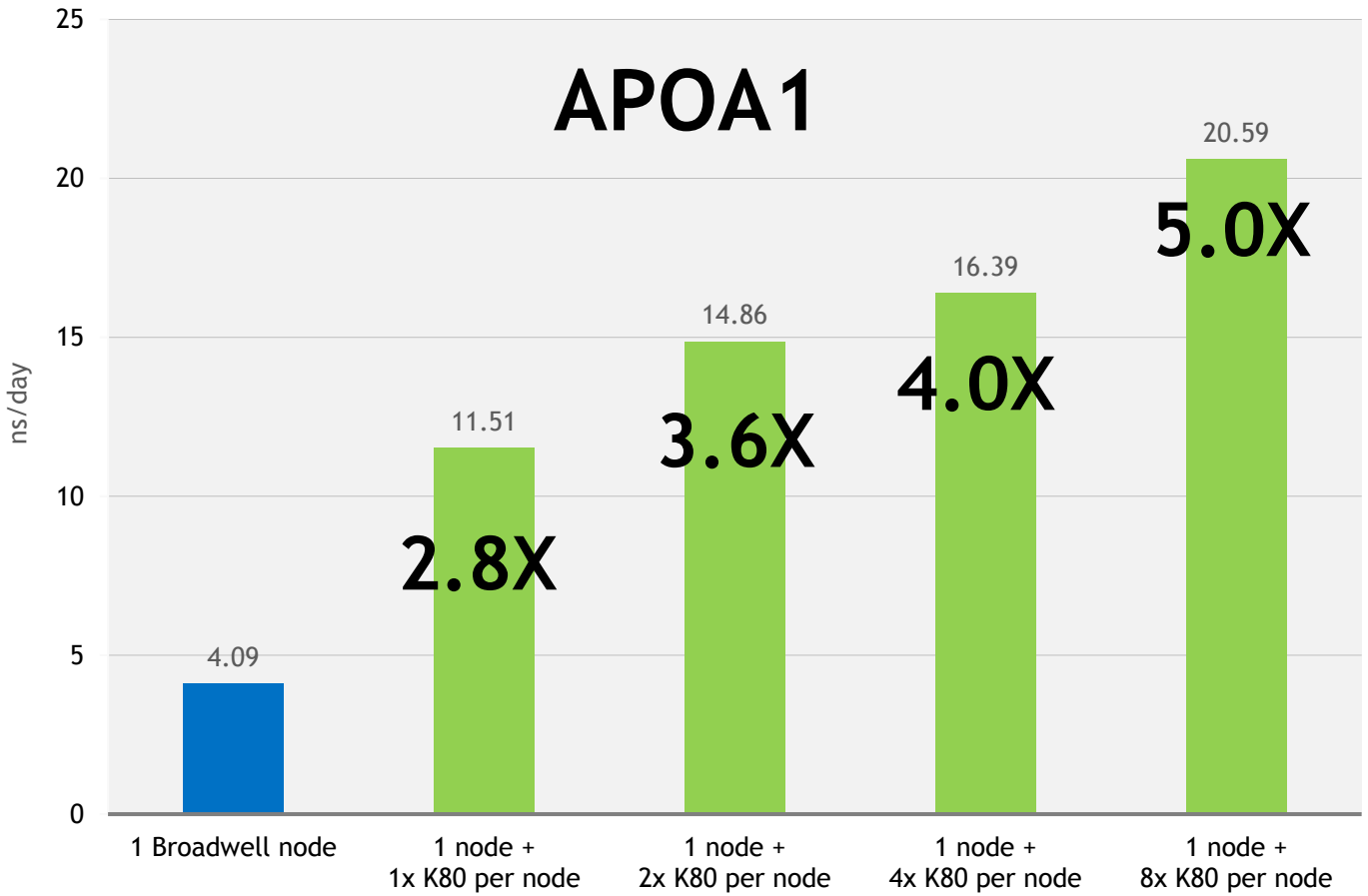


NAMD 2.11

November 2016

APOA1 on K80s



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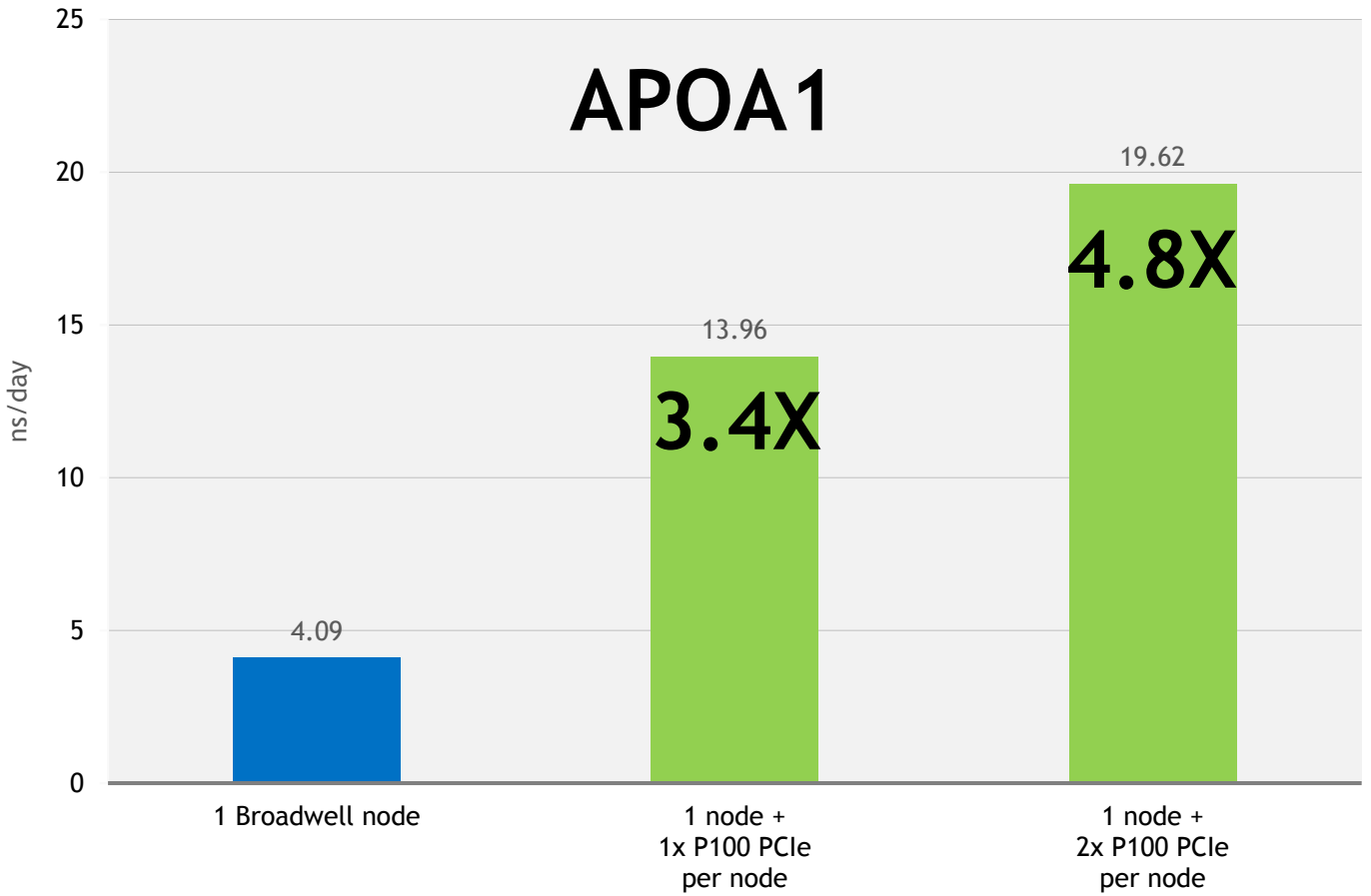
- 1x K80 is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

APOA1 on P100s PCIe



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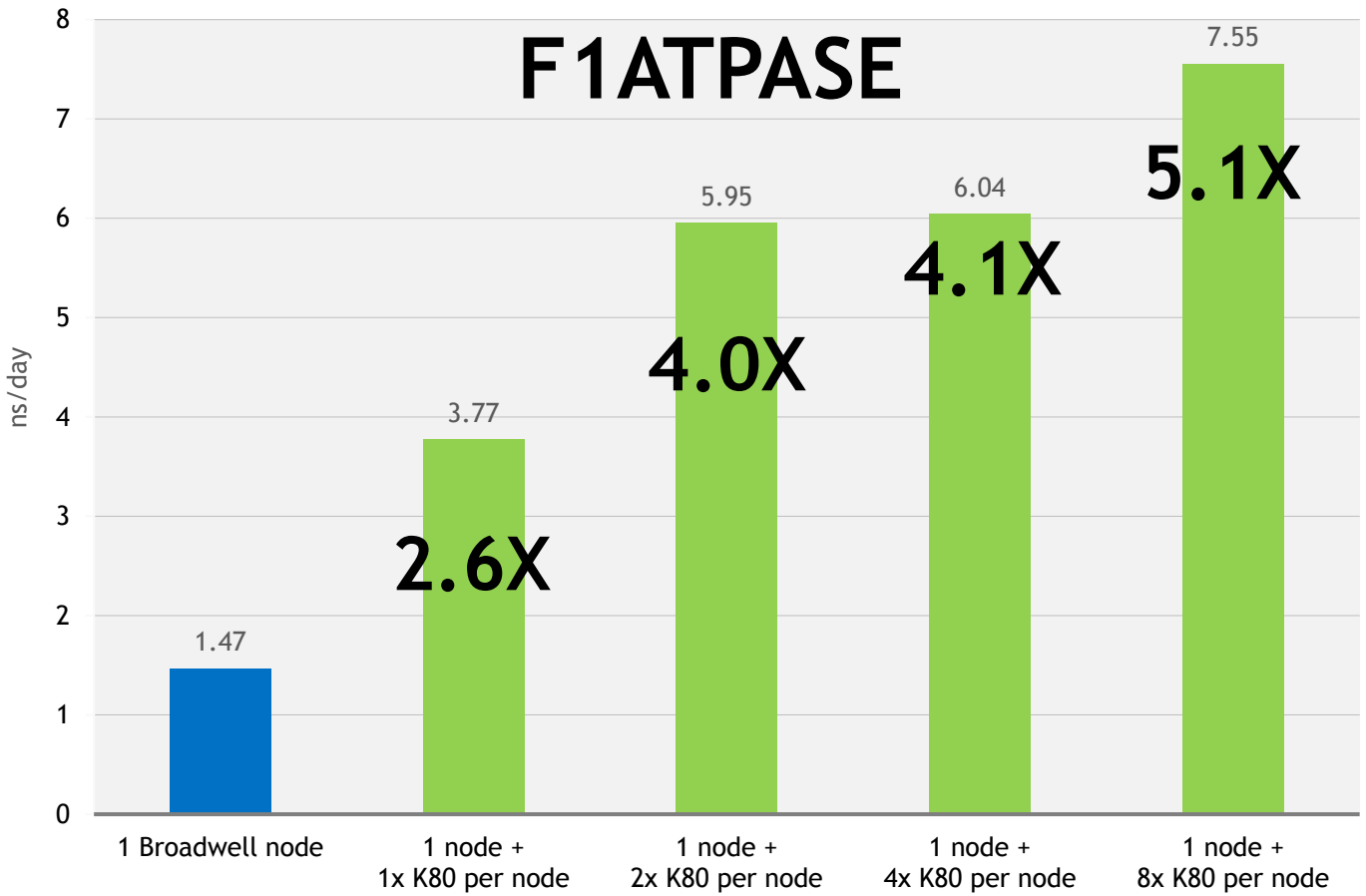
F1ATPASE on K80s



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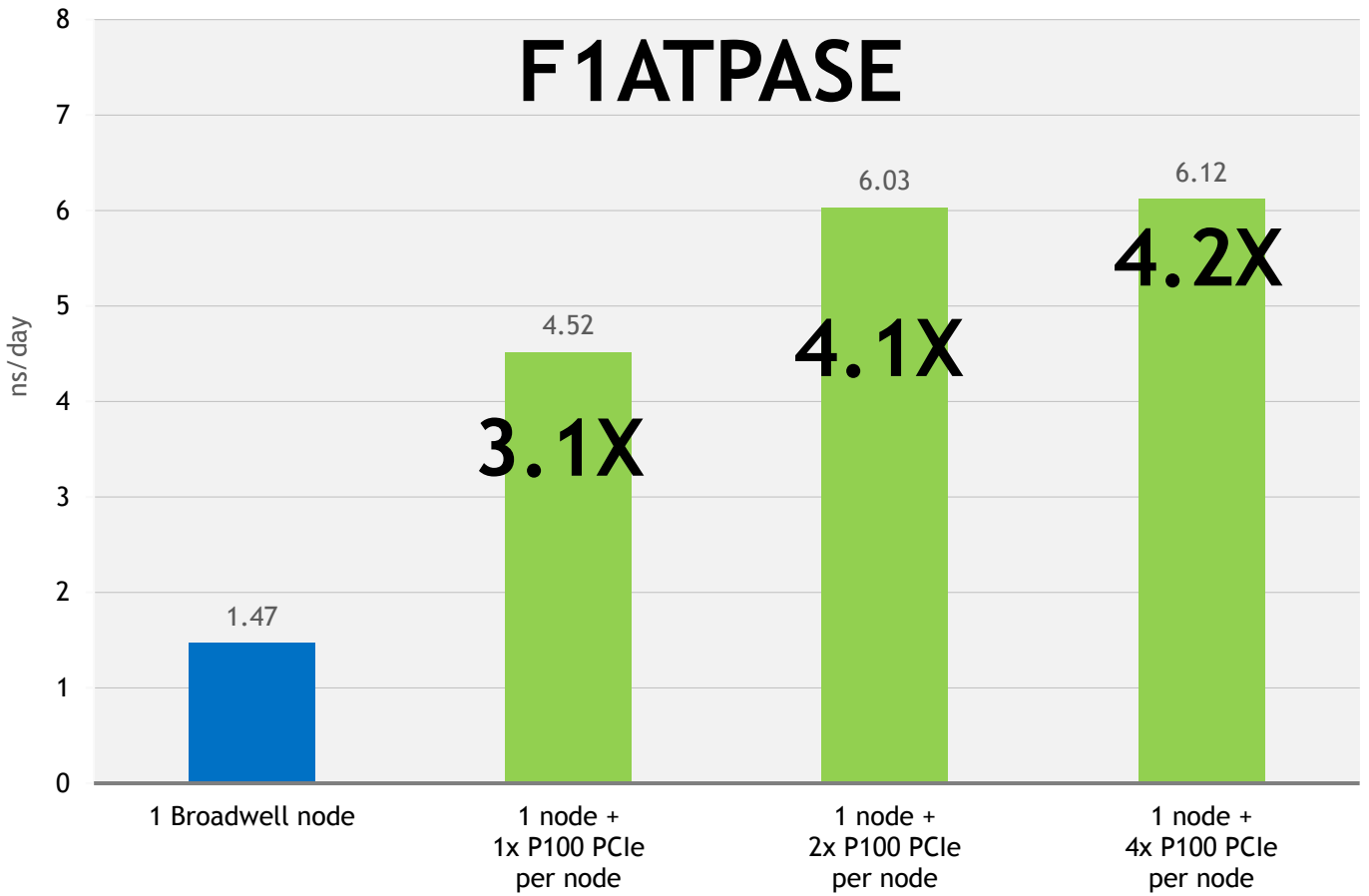

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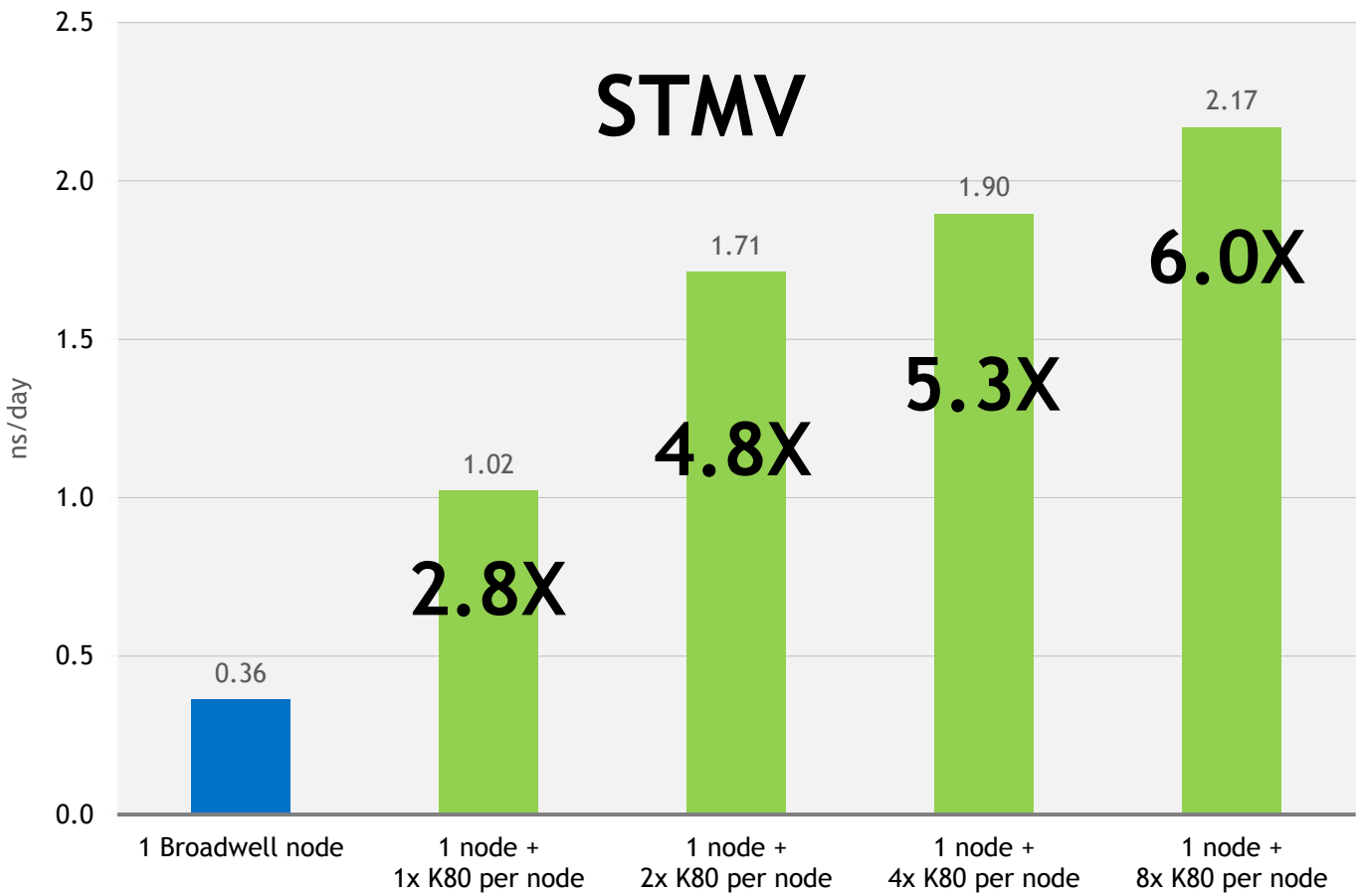
STMV on K80s



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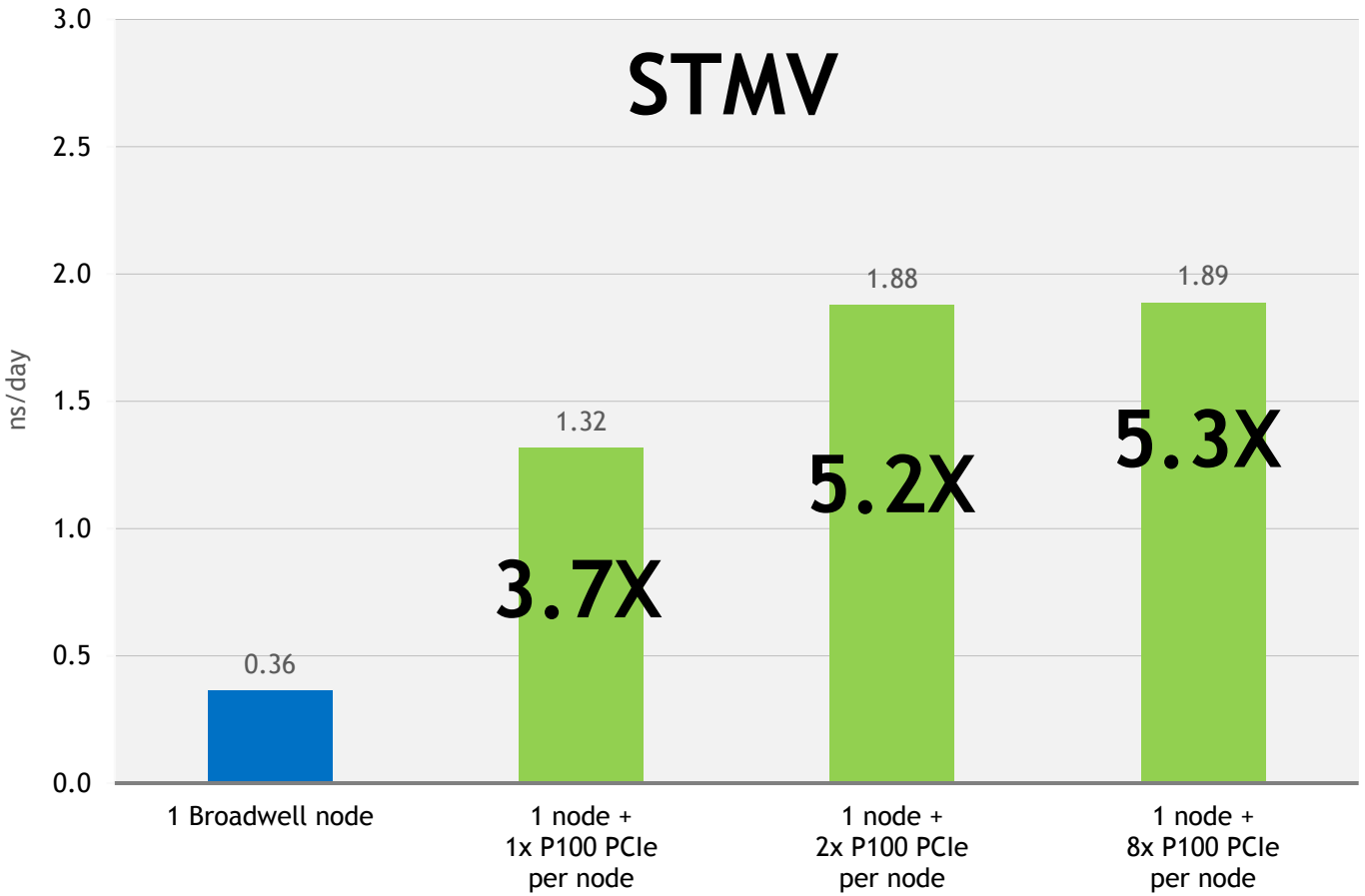

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Recommended GPU Node Configuration for NAMD Computational Chemistry

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	Kepler K20, K40, K80
# of GPUs per CPU socket	1-2
GPU memory preference (GB)	6-12
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

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 with marginal price increase
- 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