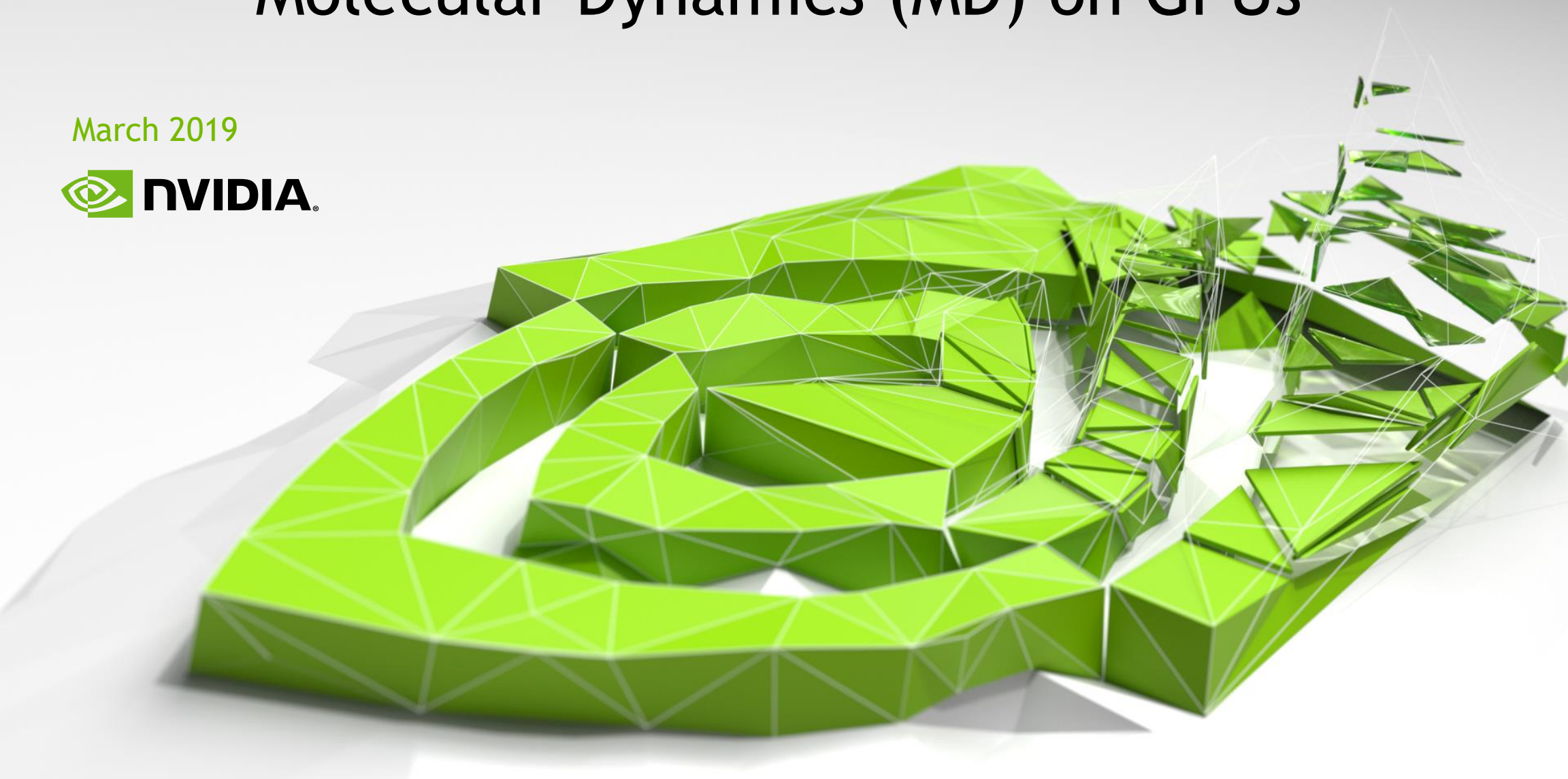
Molecular Dynamics (MD) on GPUs

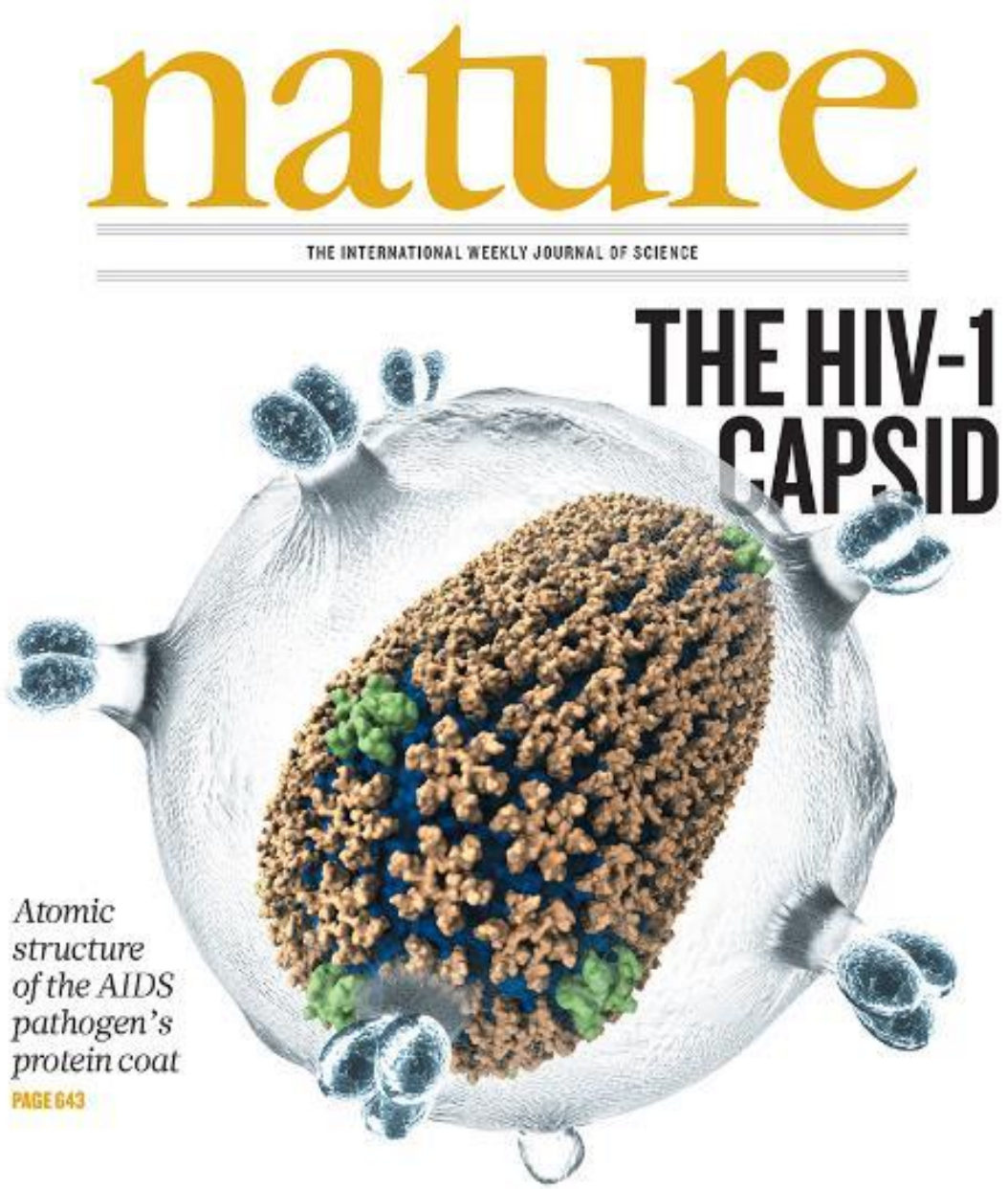
March 2019



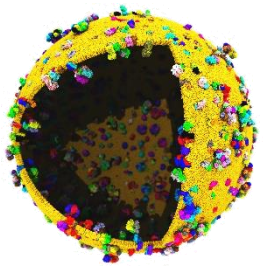
Accelerating Discoveries

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



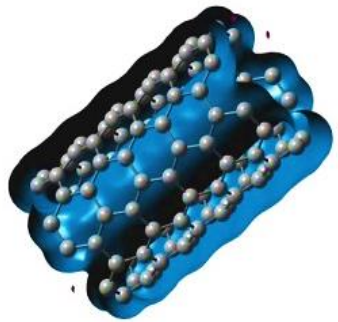
MD

All key codes are GPU-accelerated

Great multi-GPU, multi-node (dense) performance

GPU-accelerated apps

ACEMD*, AMBER*, 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

GPU-accelerated math libraries, OpenACC directives

GPU-accelerated apps

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 acceleration projects

CASTEP, GAMESS, Gaussian, ONETEP, Quantum Supercharger Library*, VASP & more

green* >90% of the workload is on GPU

MD vs. QC on GPUs

	Molecular Dynamics	Quantum Chemistry
Calculations	Simulates atomic positions over time Chemical-biological or chemical-material	Properties - electronic properties, ground state, excitation, spectra Examples: MO, PW, DFT, semi-emp
Forces	Simple empirical formulas No bond rearrangements	Electron wave function Bond rearrangements allowed
Atom count	Millions	Thousands
Solvent	Solvent included without difficulty	Solvent optional Classical QM/MM or implicit methods
Numeric precision	Primarily FP32	Primarily FP64
Software acceleration	CUDA - cuFFT	CUDA - cuBLAS, cuFFT Solvers – cuTensor, Eigen OpenACC
NVIDIA GPUs	Quadro for workstations Tesla for data center	Tesla for data center
Error correction (ECC)	Not required	Required

GPU-Accelerated Molecular Dynamics Apps

Performance Slides Available

- ACEMD
- AMBER/GTI
- Chameleon
- CHARMM
- GROMACS
- HOOMD-Blue
- LAMMPS
- NAMD

- DESMOND/FEP
- ESPResSO
- Folding@Home
- Genesis
- GPUGrid.net
- HALMD
- HTMD
- mdcore
- MELD
- OpenMM
- PolyFTS

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

MD Applications GPU-Accelerated Computing

Turbocharge your research!

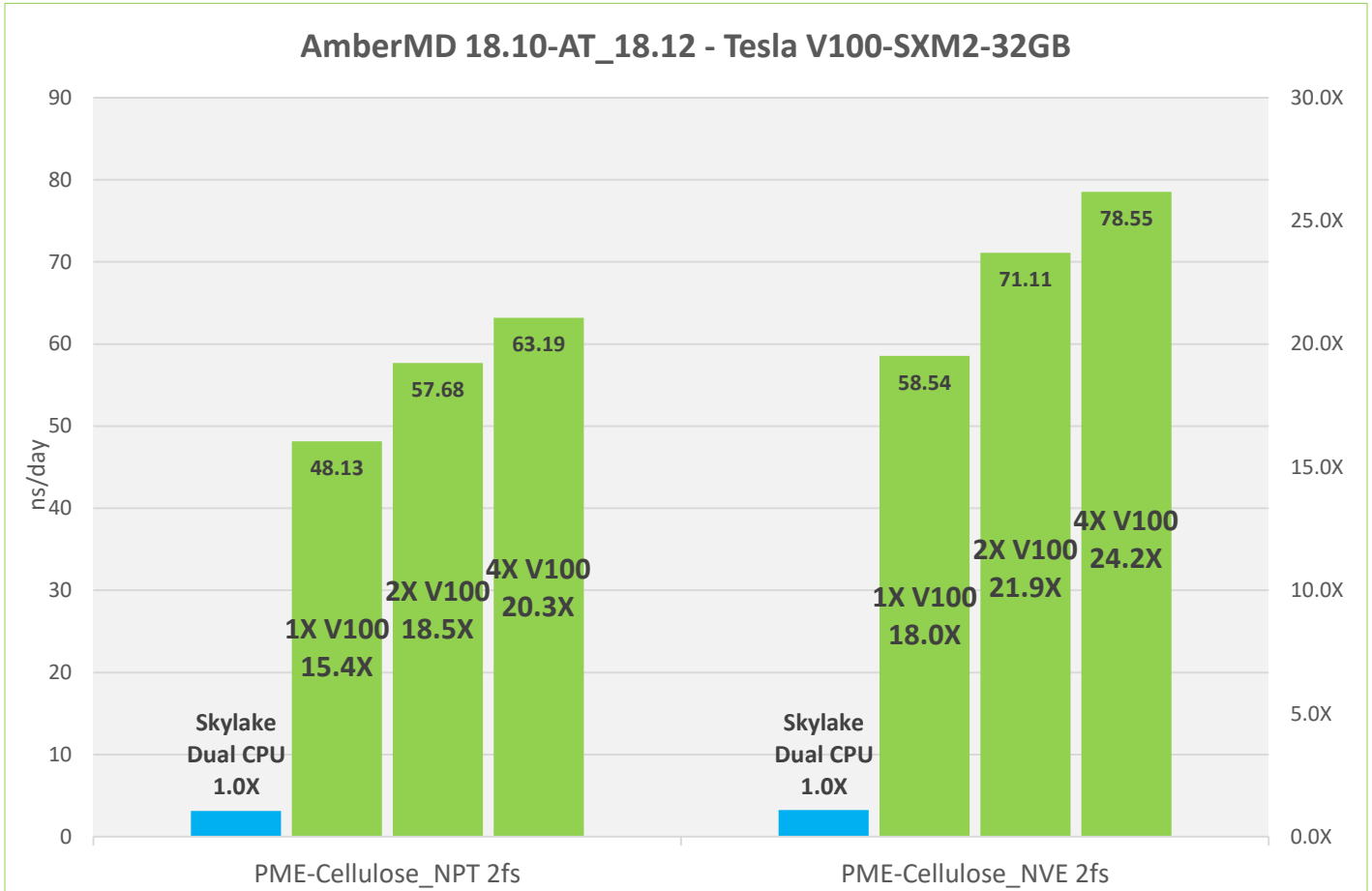
- Speedup of 3X-8X compared to CPU only in all tests (average)
- Majority of compute intensive for classical MD ported to GPUs
- Large performance boost and improve TCO for compute infrastructure
- Tesla GPUs are more energy efficient <50% of CPU-only computing
- GPUs scale well within a node and/or over multiple nodes
- Tesla V100 is highest performance GPU

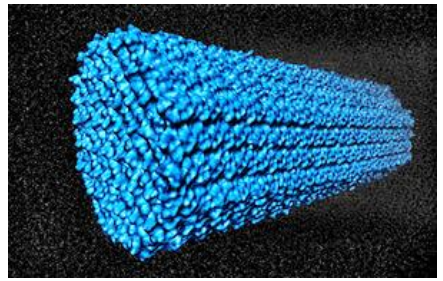
Try GPU accelerated MD apps for free – nvidia.com/GPUTestDrive

AmberMD 18.10-AT_18.12

March 2019

AmberMD 18.10_AT_18.12- PME-Cellulose





Cellulose
408,609 atoms

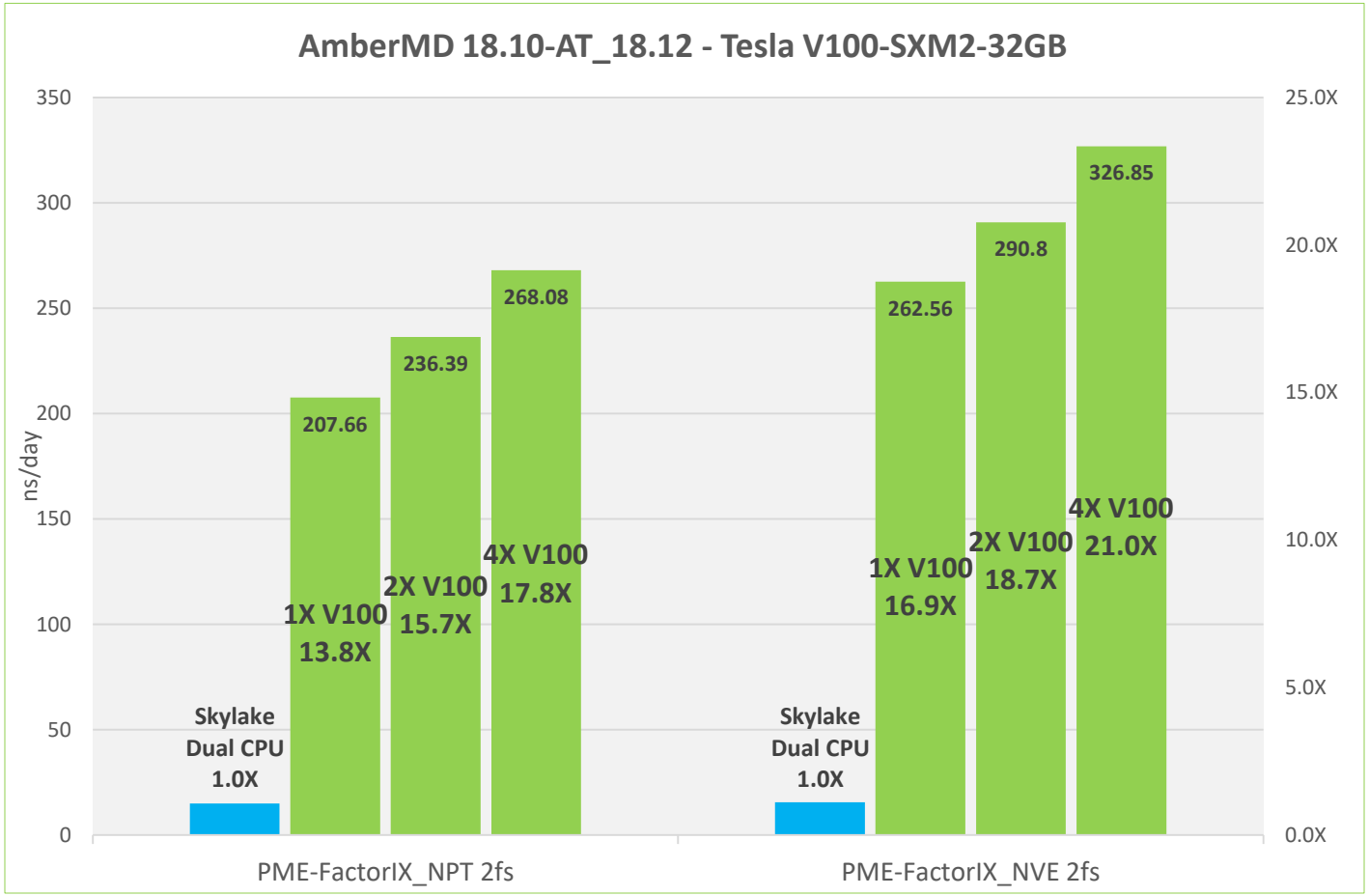
Running AmberMD 18.10_AT_18.12

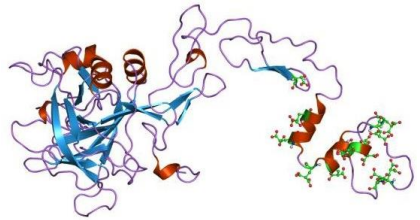
The blue node contains Dual Intel Xeon Gold 6140 (Skylake) CPUs

The green nodes contain Dual Intel Xeon Gold 6140 (Skylake) CPUs + Tesla V100 SXM2 (32GB) GPUs

Speed up over dual CPU node (X)

AmberMD 18.10_AT_18.12 - PME-FactorIX





Factor IX
90,906 atoms

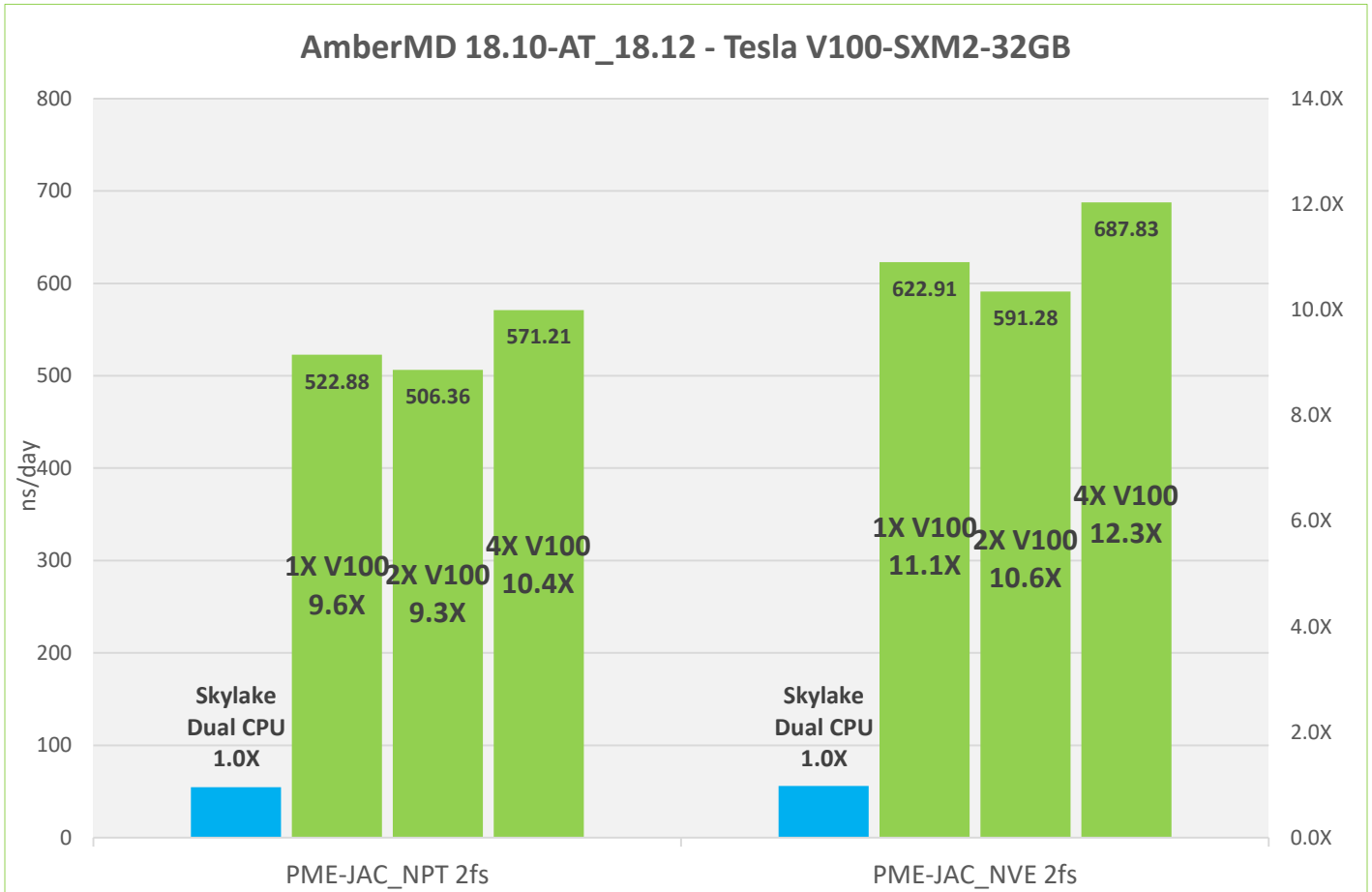
Running AmberMD 18.10_AT_18.12

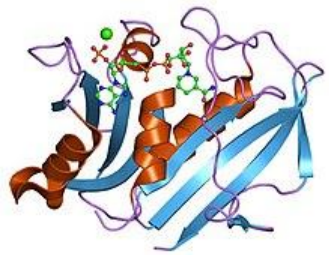
The blue node contains Dual Intel Xeon Gold 6140 (Skylake) CPUs

The green nodes contain Dual Intel Xeon Gold 6140 (Skylake) CPUs + Tesla V100 SXM2 (32GB) GPUs

Speed up over dual CPU node (X)

AmberMD 18.10_AT_18.12 - PME-JAC





DHFR
23,558 atoms

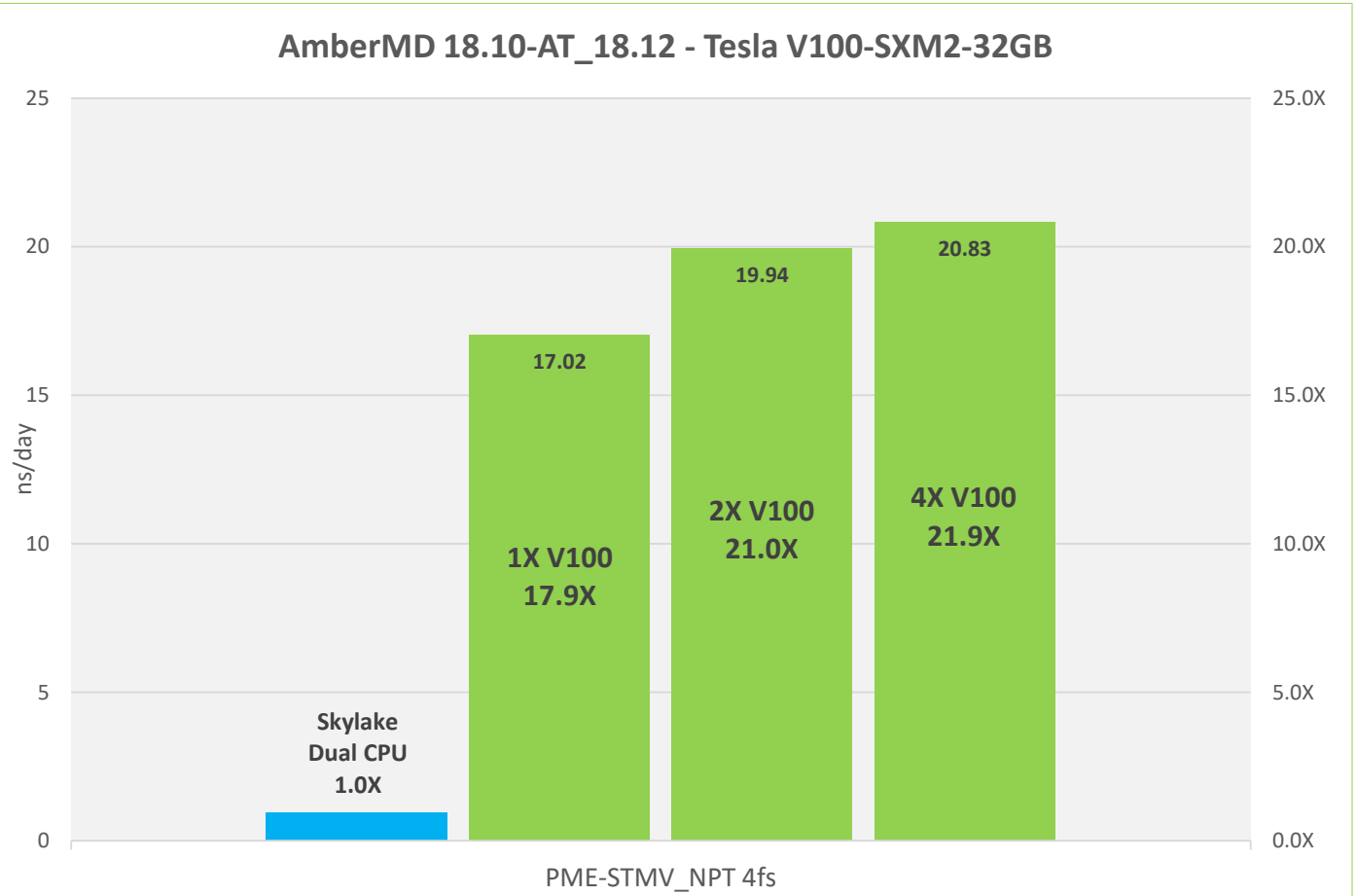
Running AmberMD 18.10_AT_18.12

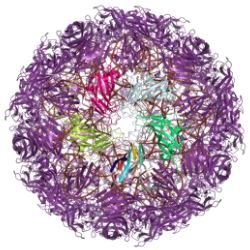
The blue node contains Dual Intel Xeon Gold 6140 (Skylake) CPUs

The green nodes contain Dual Intel Xeon Gold 6140 (Skylake) CPUs + Tesla V100 SXM2 (32GB) GPUs

Speed up over dual CPU node (X)

AmberMD 18.10_AT_18.12 - PME-STMV_NPT





Satellite Tobacco Mosaic Virus
1,067,095 atoms

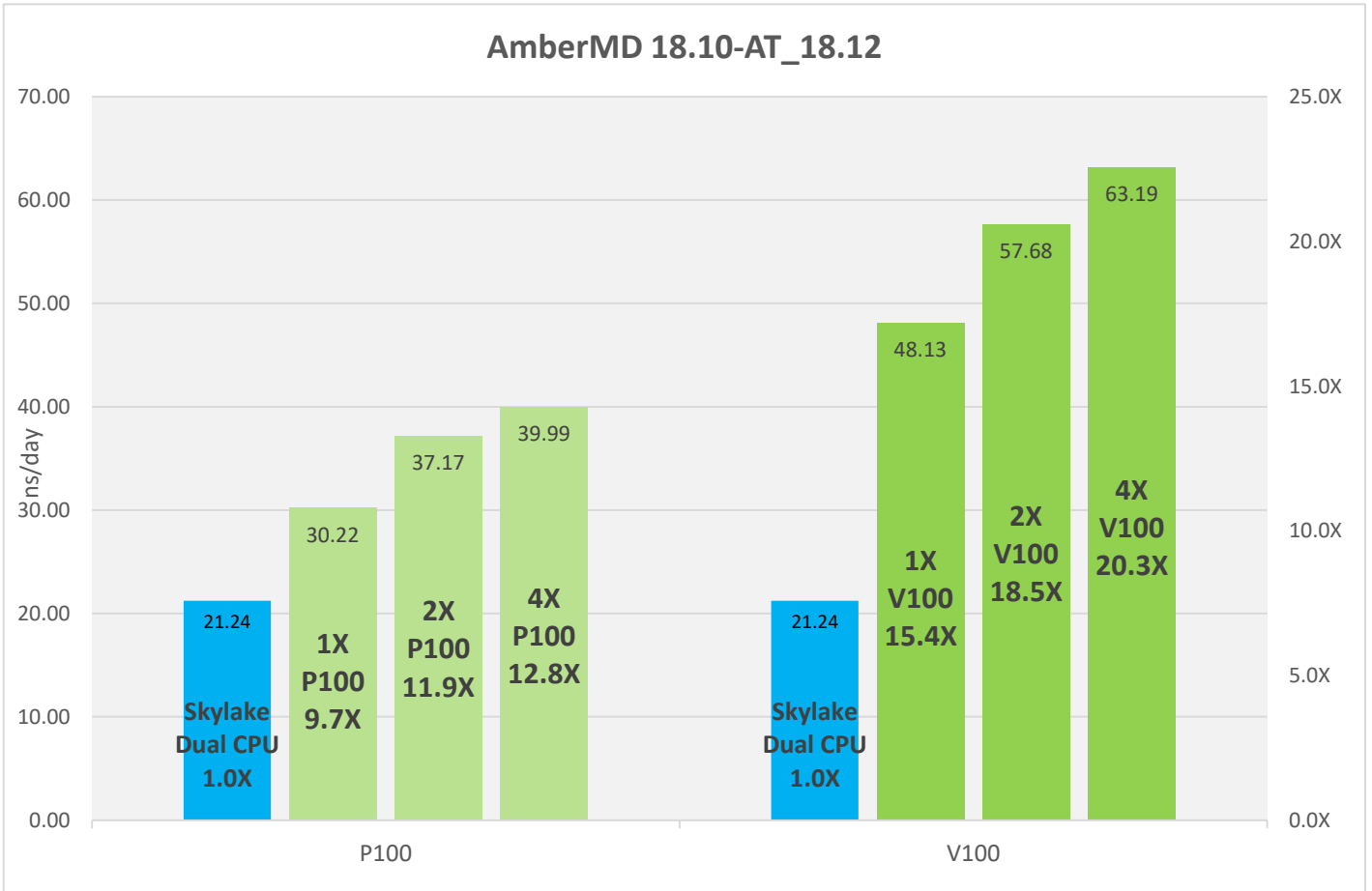
Running AmberMD 18.10_AT_18.12

The blue node contains Dual Intel Xeon Gold 6140 (Skylake) CPUs

The green nodes contain Dual Intel Xeon Gold 6140 (Skylake) CPUs + Tesla V100 SXM2 (32GB) GPUs

Speed up over dual CPU node (X)

AmberMD 18.10_AT_18.12 – P100 vs V100



All benchmarks compared as set Cellulose, FactorIX, JAC, STMV

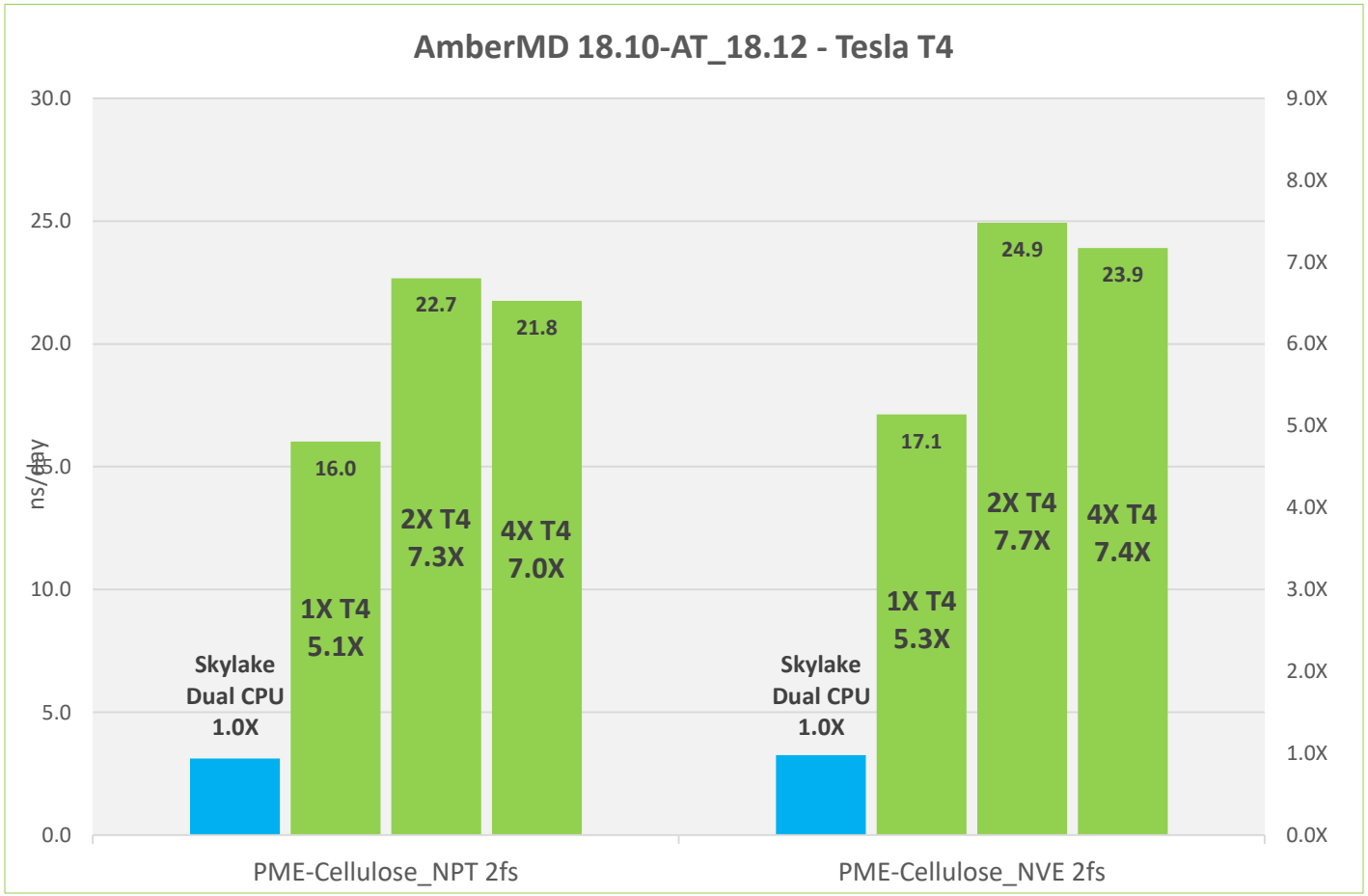
Running AmberMD 18.10_AT_18.12

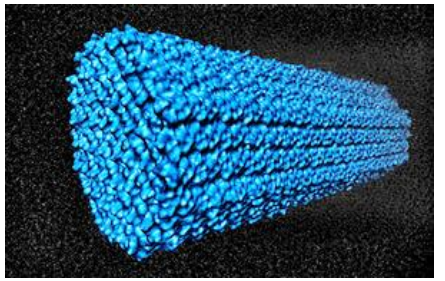
The blue node contains Dual Intel Xeon Gold 6140 (Skylake) CPUs

The green nodes contain Dual Intel Xeon Gold 6140 (Skylake) CPUs + Tesla P100 SXM2 (16GB) GPUs or Tesla V100 SXM2 (32GB) GPUs

Speed up over dual CPU node (X)

AmberMD 18.10_AT_18.12- PME-Cellulose





Cellulose
408,609 atoms

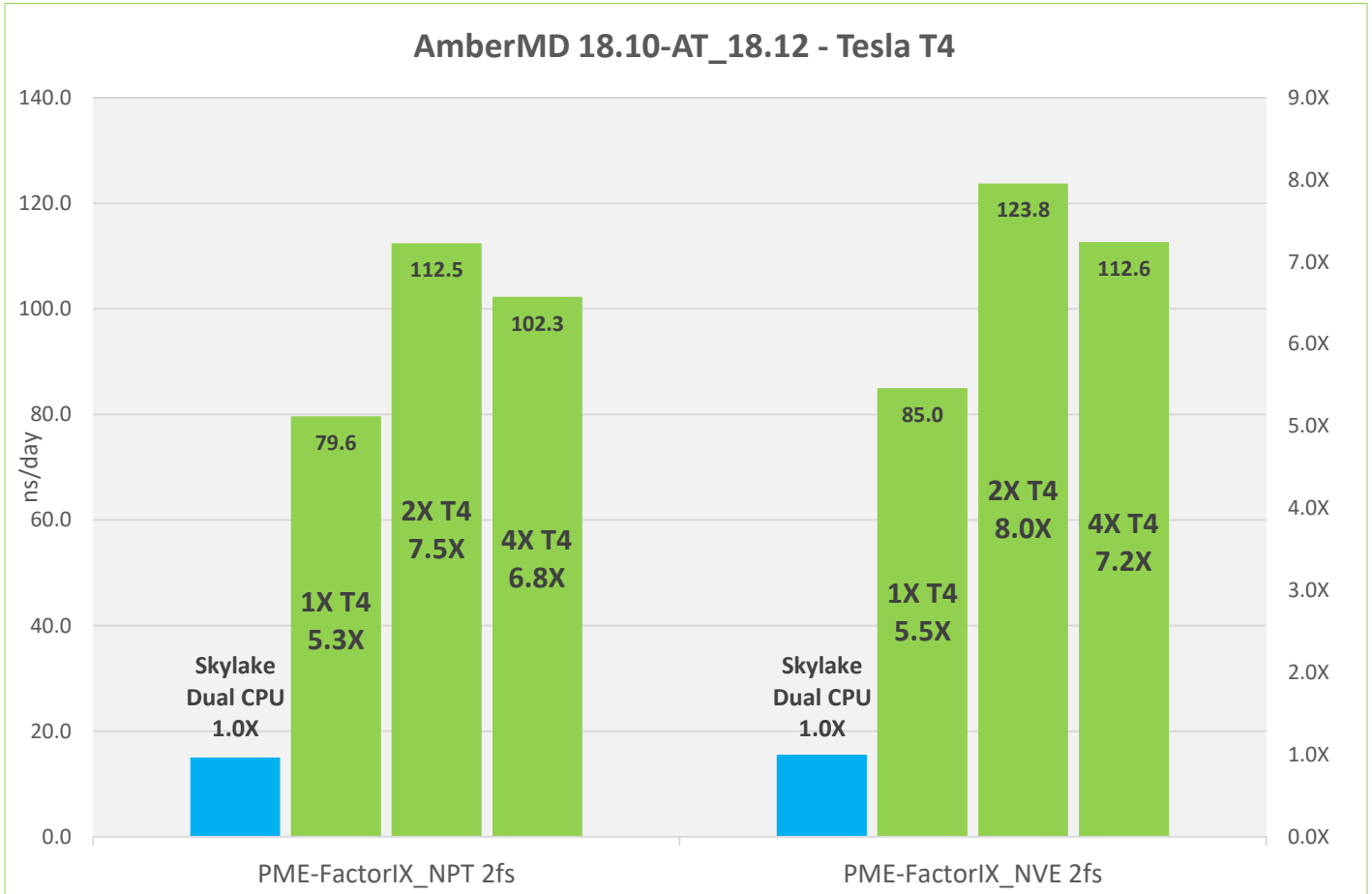
Running AmberMD 18.10_AT_18.12

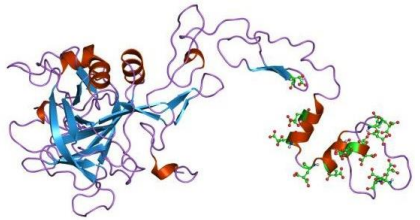
The blue node contains Dual Intel Xeon Gold 6140 (Skylake) CPUs

The green nodes contain Dual Intel Xeon Gold 6140 (Skylake) CPUs + Tesla T4 PCIe (16GB) GPUs

Speed up over dual CPU node (X)

AmberMD 18.10_AT_18.12 - PME-FactorIX





Factor IX
90,906 atoms

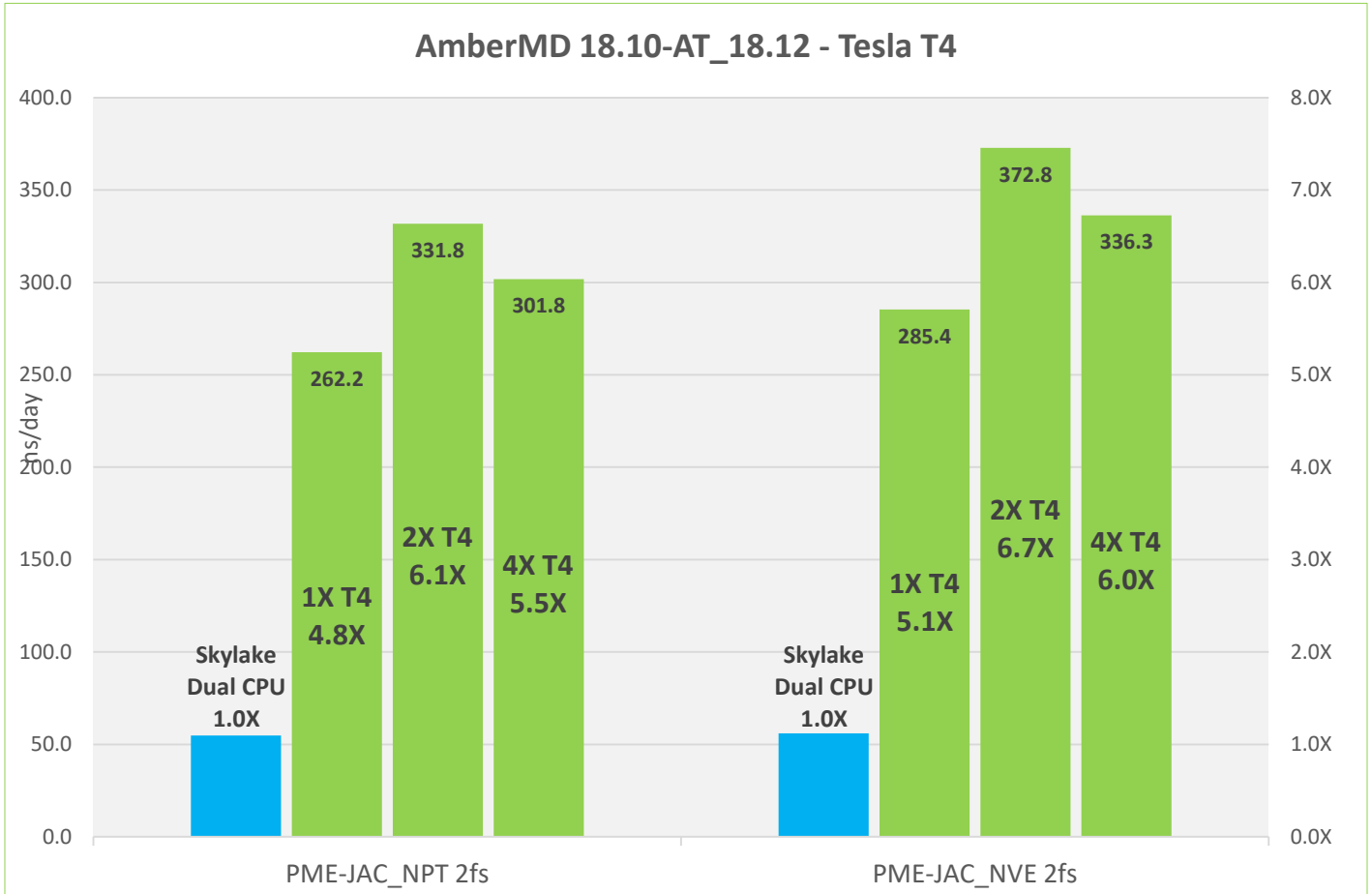
Running AmberMD 18.10_AT_18.12

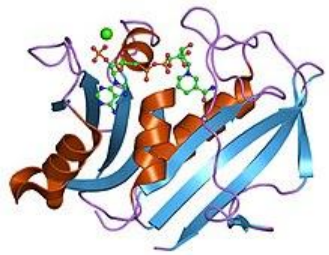
The blue node contains Dual Intel Xeon Gold 6140 (Skylake) CPUs

The green nodes contain Dual Intel Xeon Gold 6140 (Skylake) CPUs + Tesla T4 PCIe (16GB) GPUs

Speed up over dual CPU node (X)

AmberMD 18.10_AT_18.12 - PME-JAC





DHFR
23,558 atoms

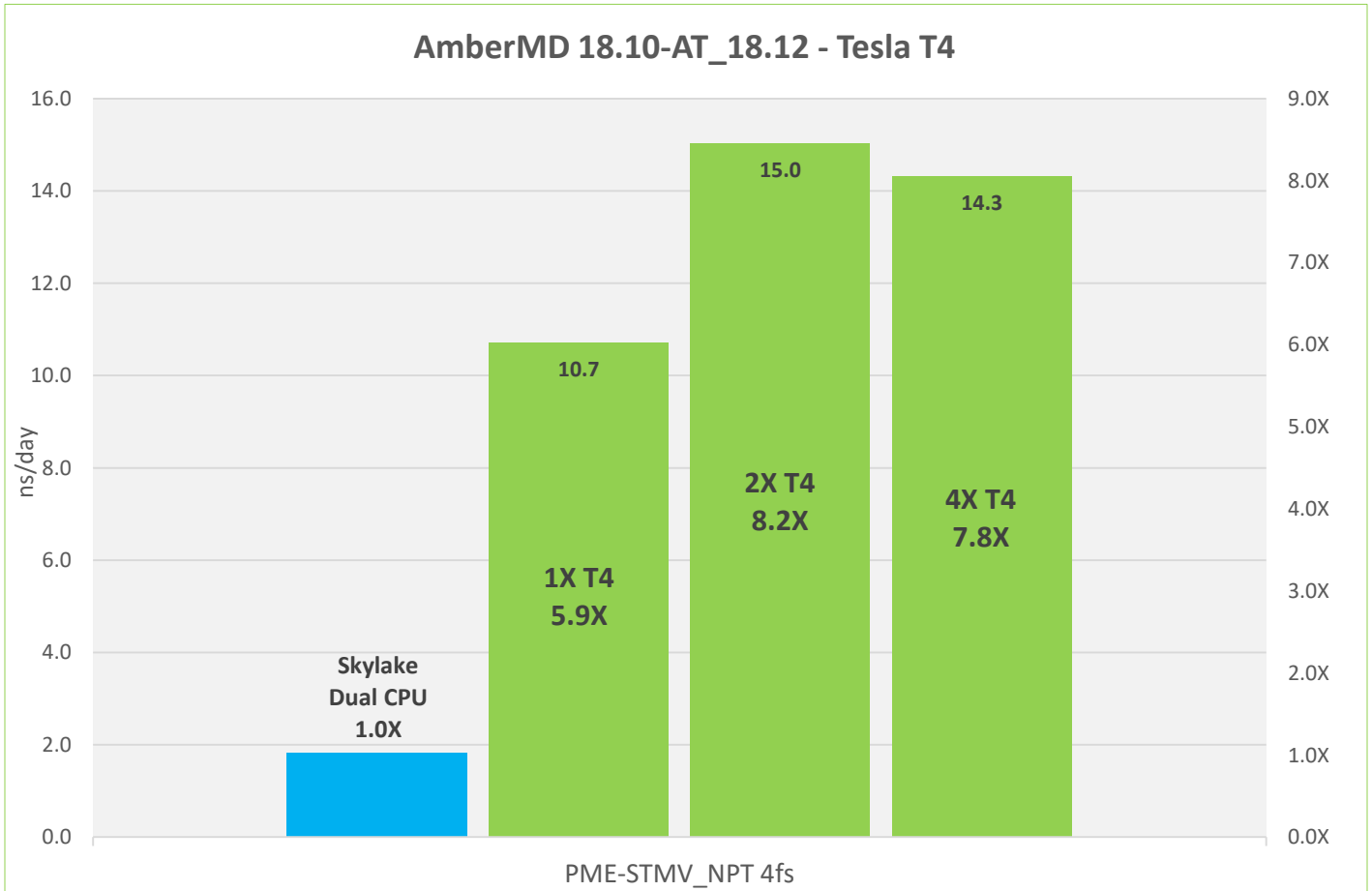
Running AmberMD 18.10_AT_18.12

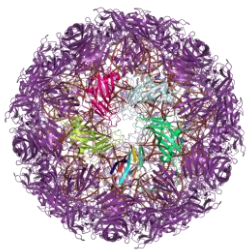
The blue node contains Dual Intel Xeon Gold 6140 (Skylake) CPUs

The green nodes contain Dual Intel Xeon Gold 6140 (Skylake) CPUs + Tesla T4 PCIe (16GB) GPUs

Speed up over dual CPU node (X)

AmberMD 18.10_AT_18.12 - PME-STMV_NPT





Satellite Tobacco Mosaic Virus
1,067,095 atoms

Running AmberMD 18.10_AT_18.12

The blue node contains Dual Intel Xeon Gold 6140 (Skylake) CPUs

The green nodes contain Dual Intel Xeon Gold 6140 (Skylake) CPUs + Tesla T4 PCIe (16GB) GPUs

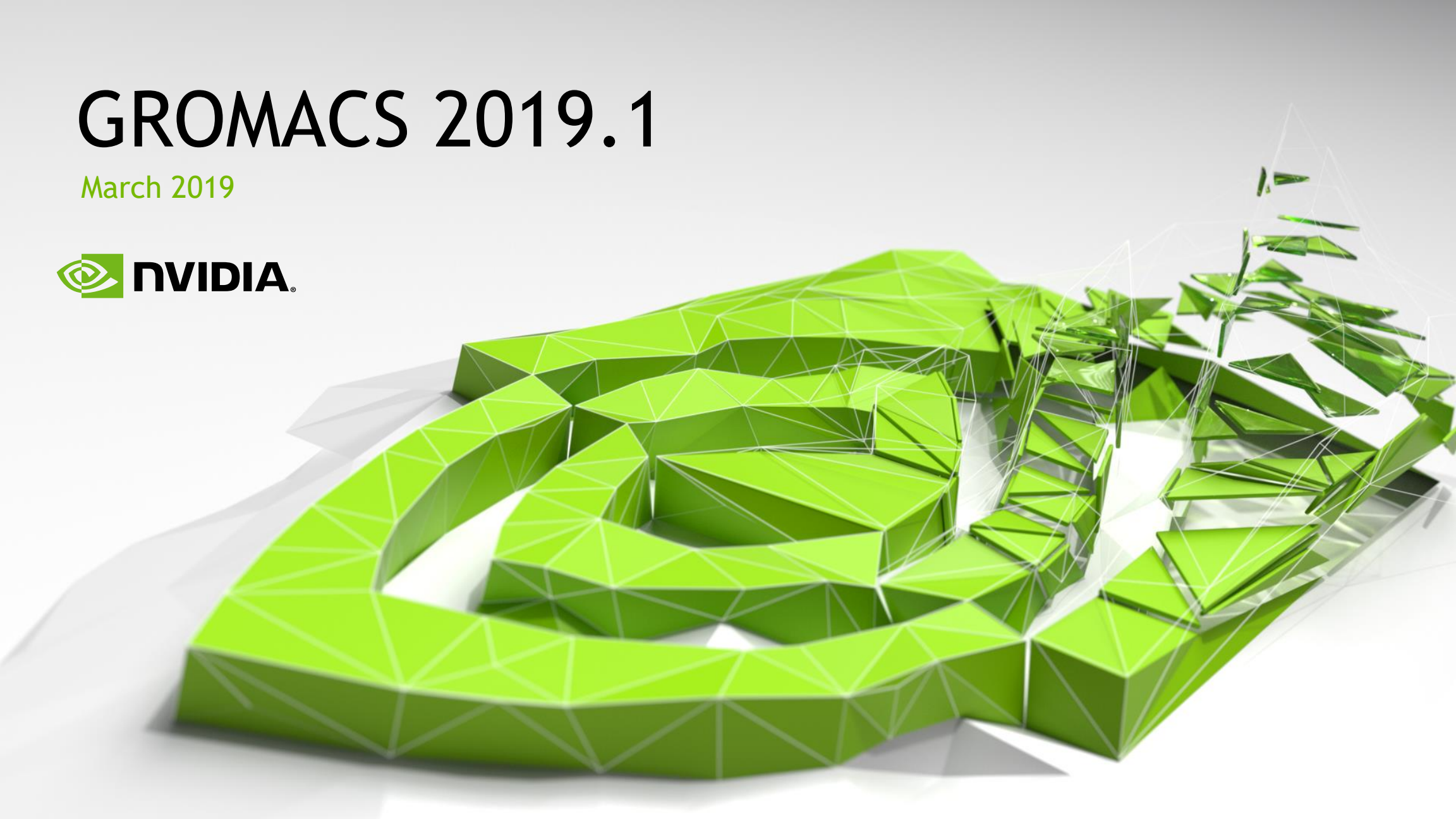
Speed up over dual CPU node (X)

AmberMD recommended usage

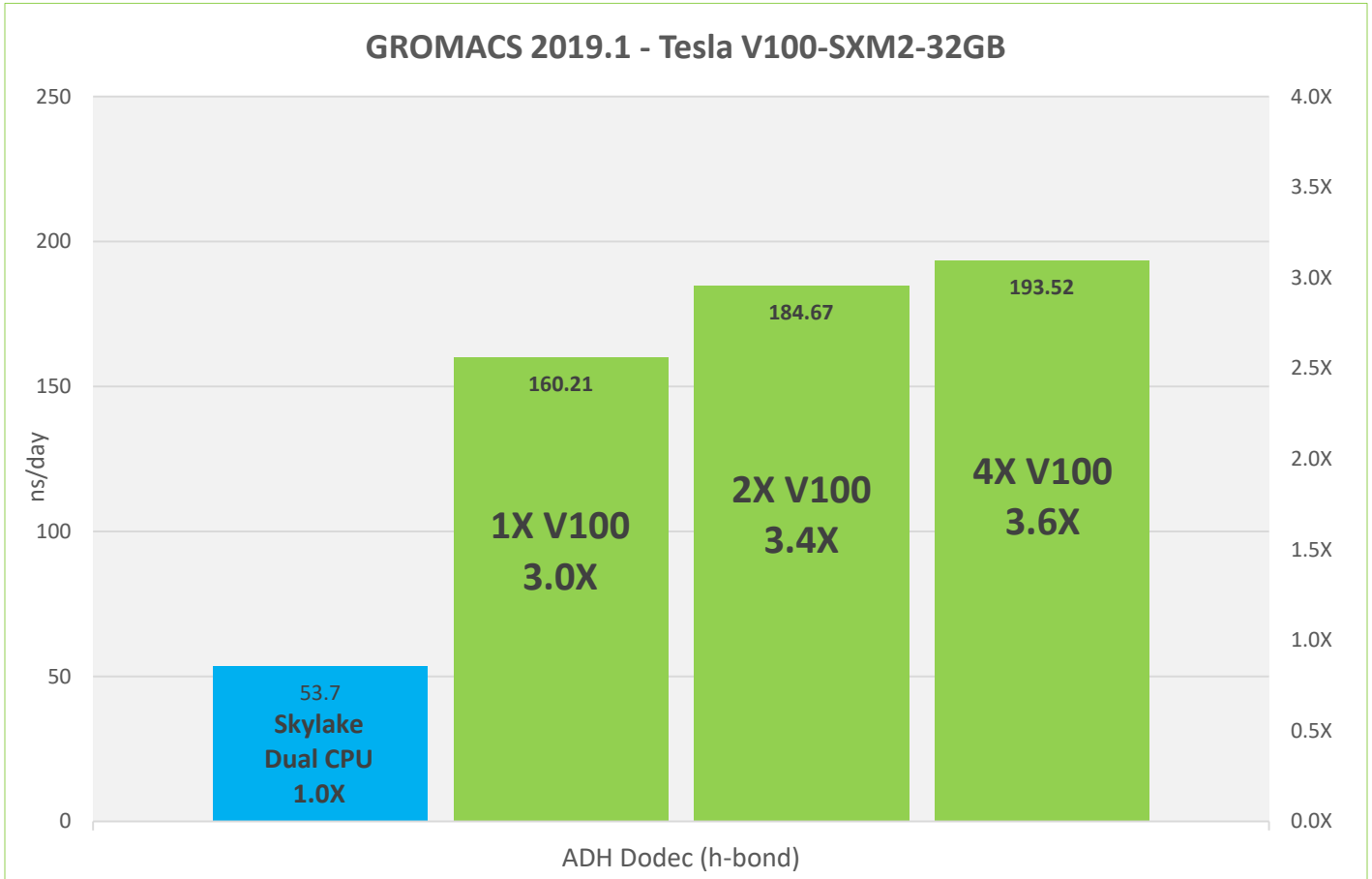
Motherboard and CPU	Dual-socket with server x86-64 CPU
System memory	>=16GB
GPUs	Tesla V100 SXM2
GPUs per socket	1 to 8
GPUs per task	1 – 4 (case dependent)

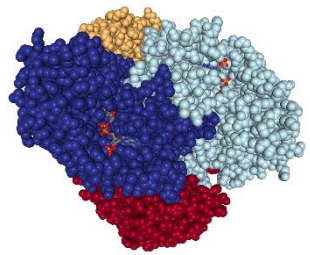
GROMACS 2019.1

March 2019



GROMACS 2019.1 - ADH Dodec





ADH
134,000 atoms

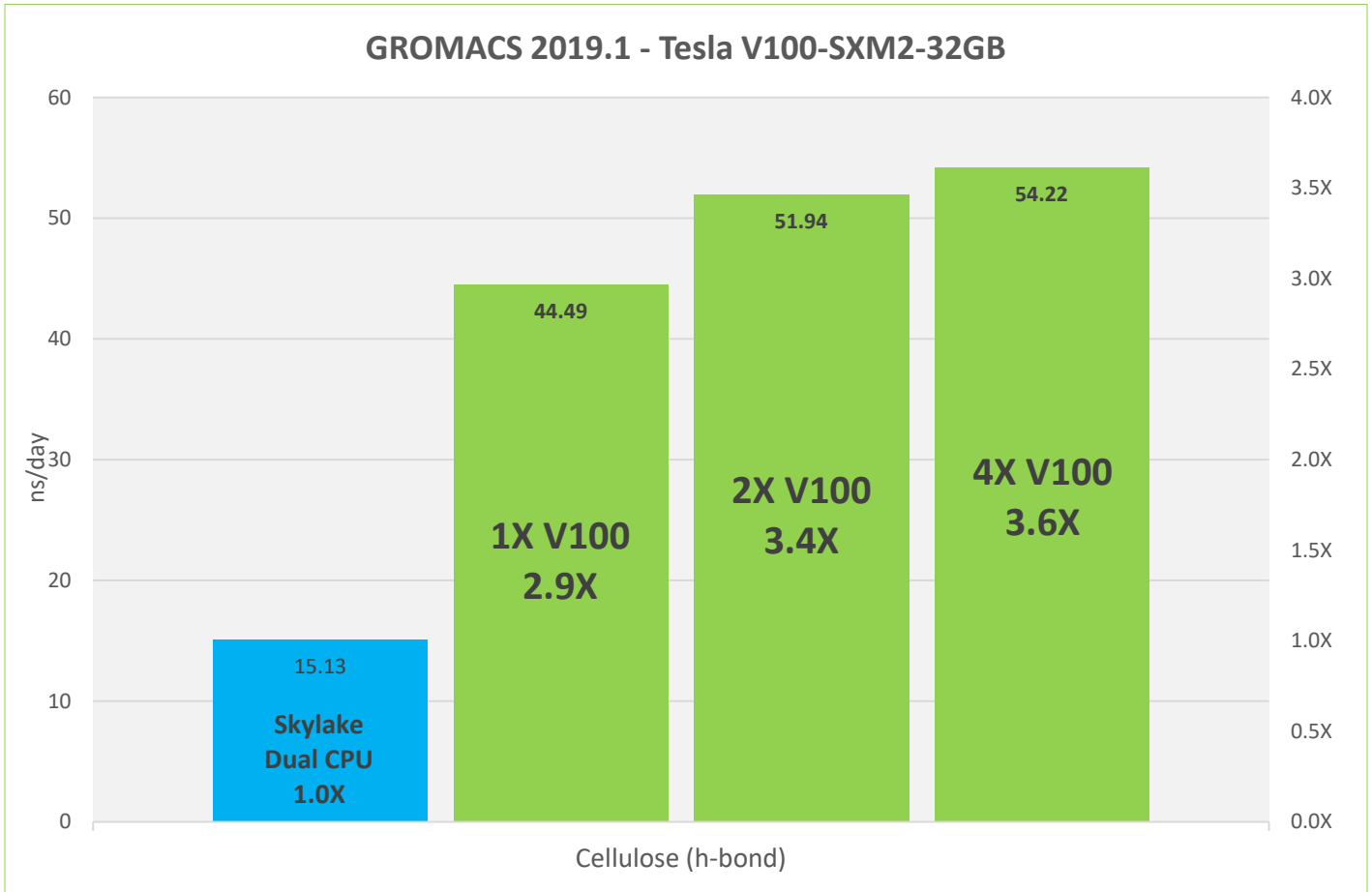
Running GROMACS 2019.1

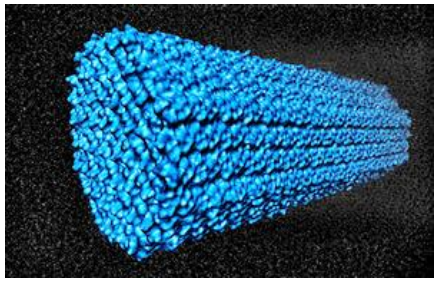
The blue node contains Dual Intel Xeon Gold 6140 (Skylake) CPUs

The green nodes contain Dual Intel Xeon Gold 6140 (Skylake) CPUs + Tesla V100 SXM2 (32GB) GPUs

Speed up over dual CPU node (X)

GROMACS 2019.1 - Cellulose





Cellulose
408,609 atoms

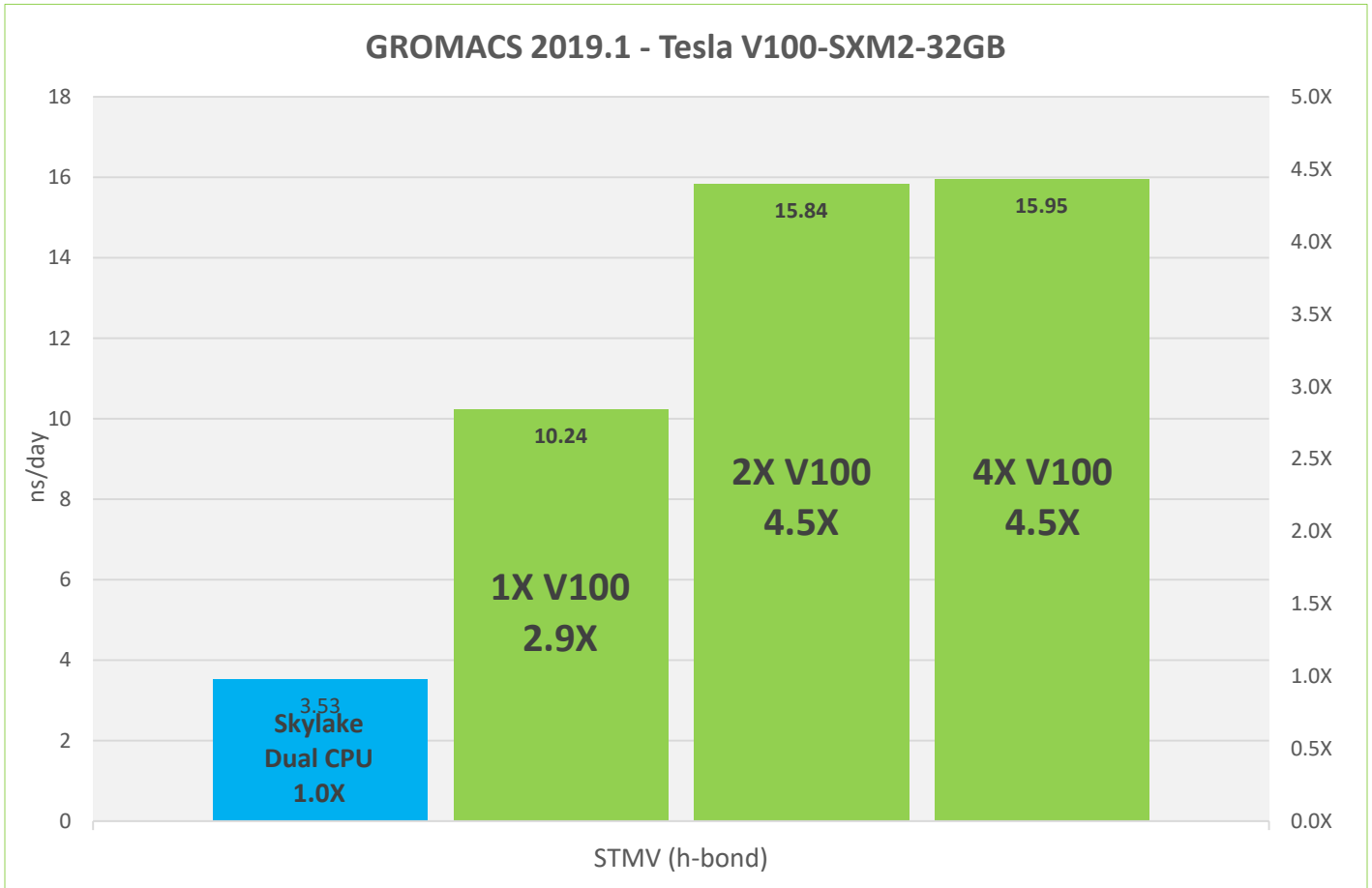
Running GROMACS 2019.1

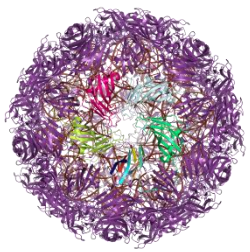
The blue node contains Dual Intel Xeon Gold 6140 (Skylake) CPUs

The green nodes contain Dual Intel Xeon Gold 6140 (Skylake) CPUs + Tesla V100 SXM2 (32GB) GPUs

Speed up over dual CPU node (X)

GROMACS 2019.1 - STMV





Satellite Tobacco Mosaic Virus
1,067,095 atoms

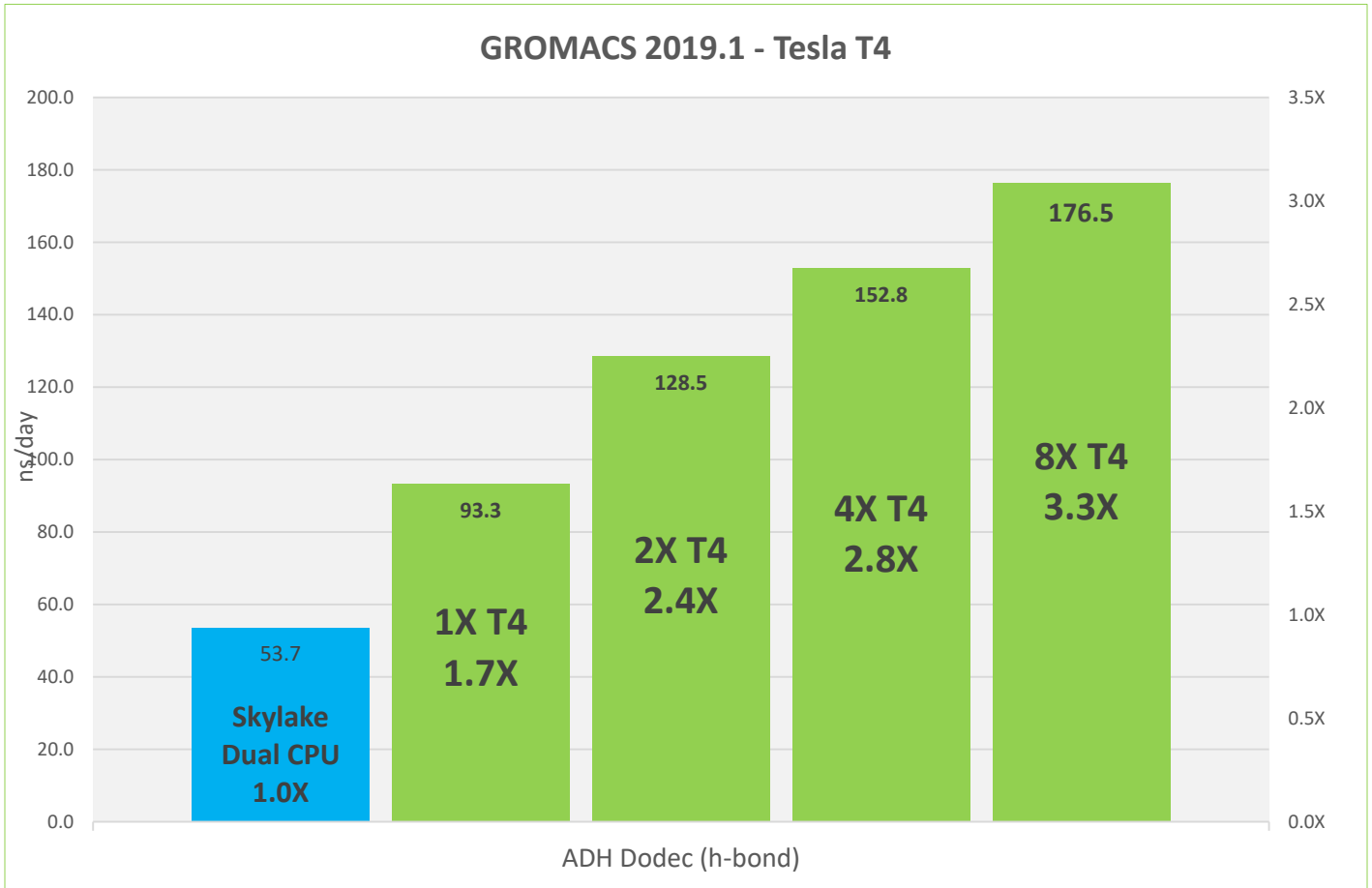
Running GROMACS 2019.1

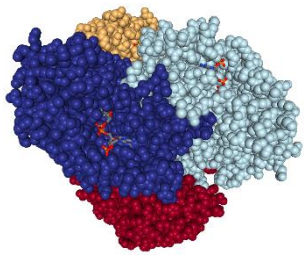
The blue node contains Dual Intel Xeon Gold 6140 (Skylake) CPUs

The green nodes contain Dual Intel Xeon Gold 6140 (Skylake) CPUs + Tesla V100 SXM2 (32GB) GPUs

Speed up over dual CPU node (X)

GROMACS 2019.1 - ADH Dodec





ADH
134,000 atoms

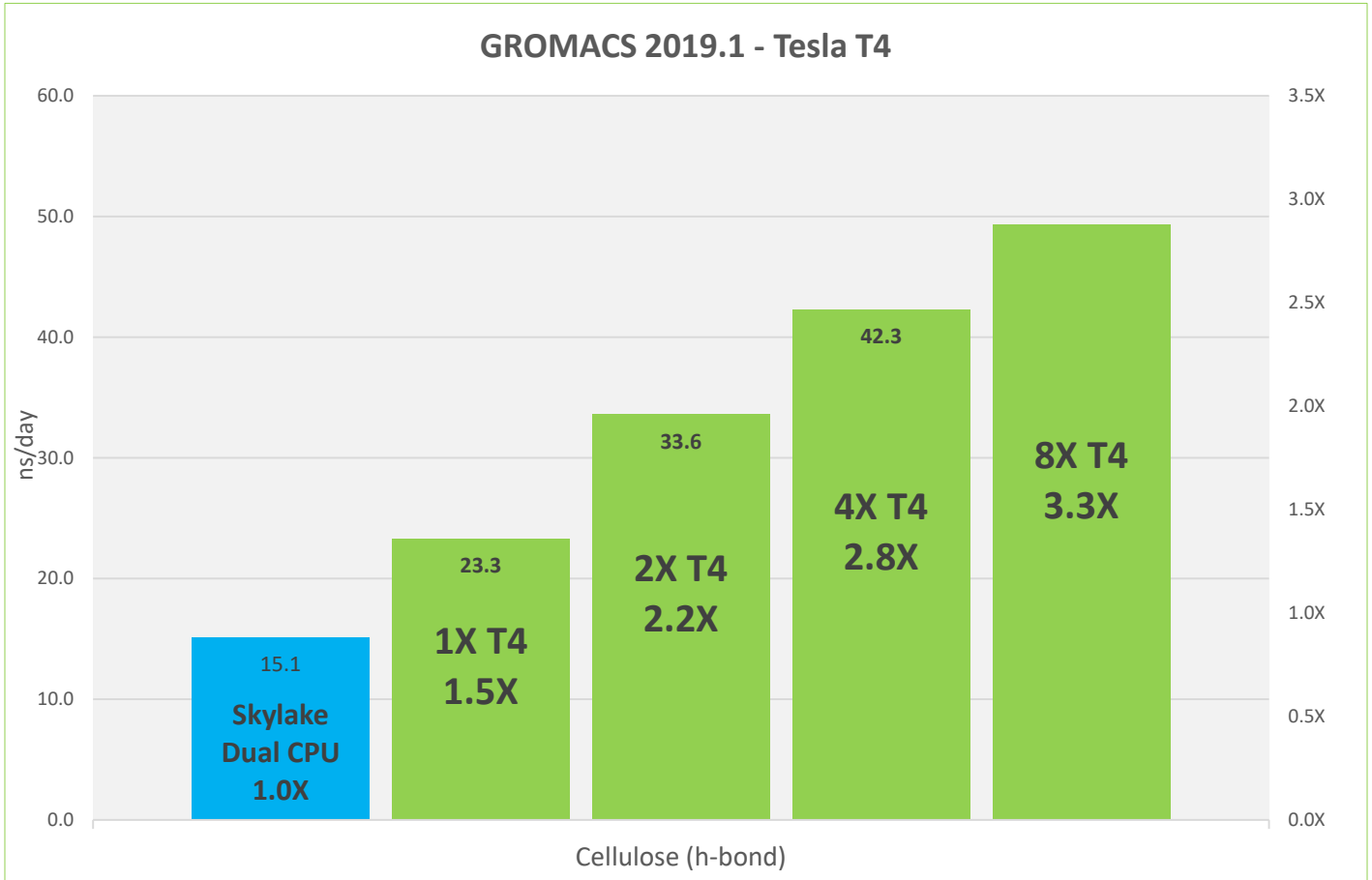
Running GROMACS 2019.1

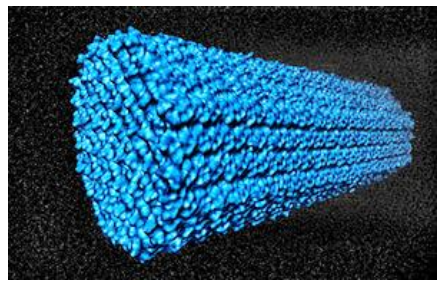
The blue node contains Dual Intel Xeon Gold 6140 (Skylake) CPUs

The green nodes contain Dual Intel Xeon Gold 6140 (Skylake) CPUs + Tesla T4 PCIe (16GB) GPUs

Speed up over dual CPU node (X)

GROMACS 2019.1 - Cellulose





Cellulose
408,609 atoms

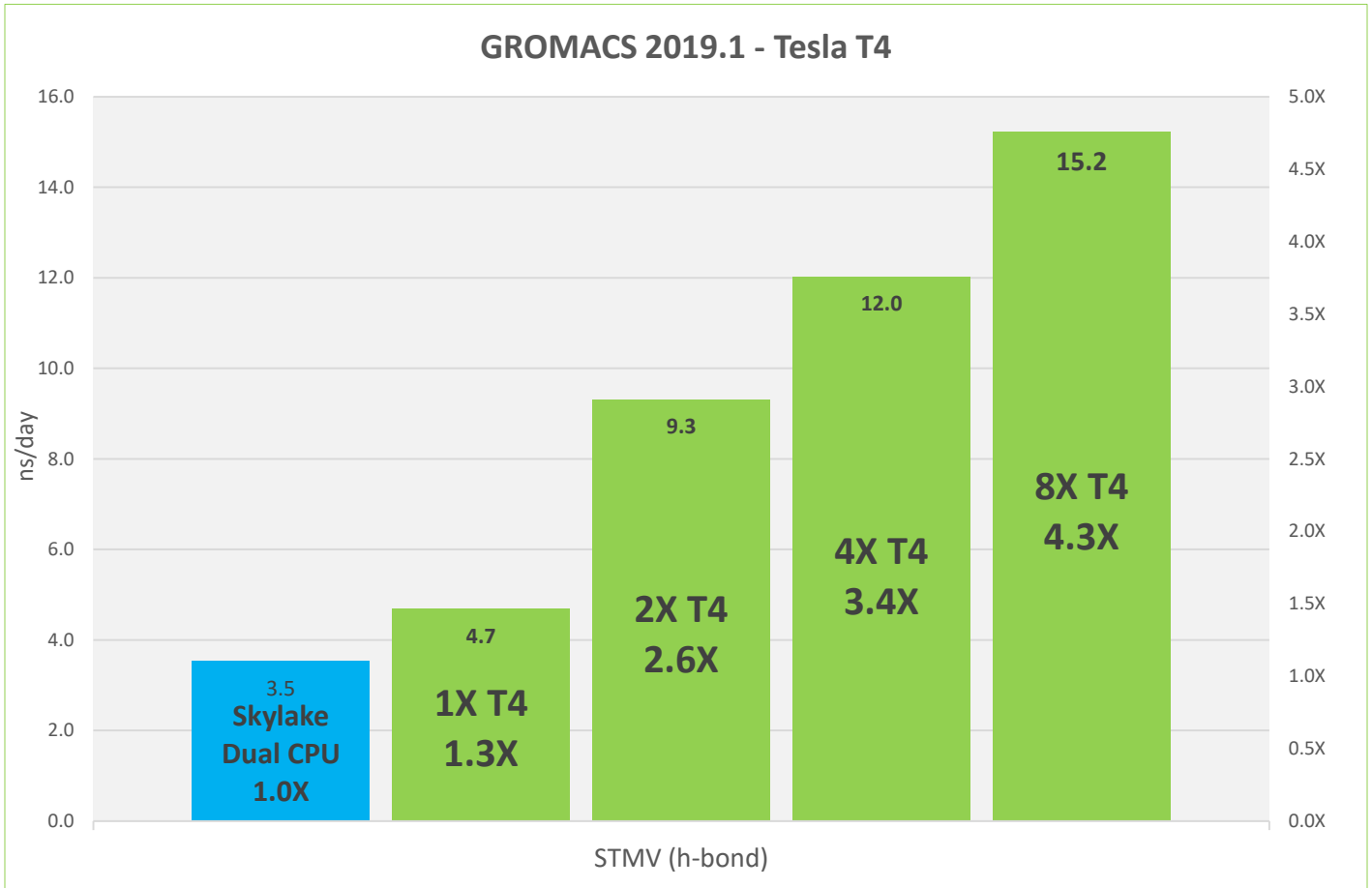
Running GROMACS 2019.1

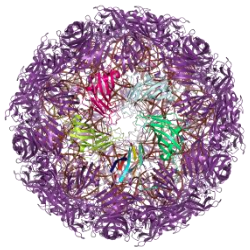
The blue node contains Dual Intel Xeon Gold 6140 (Skylake) CPUs

The green nodes contain Dual Intel Xeon Gold 6140 (Skylake) CPUs + Tesla T4 PCIe (16GB) GPUs

Speed up over dual CPU node (X)

GROMACS 2019.1 - STMV





Satellite Tobacco Mosaic Virus
1,067,095 atoms

Running GROMACS 2019.1

The blue node contains Dual Intel Xeon Gold 6140 (Skylake) CPUs

The green nodes contain Dual Intel Xeon Gold 6140 (Skylake) CPUs + Tesla T4 PCIe (16GB) GPUs

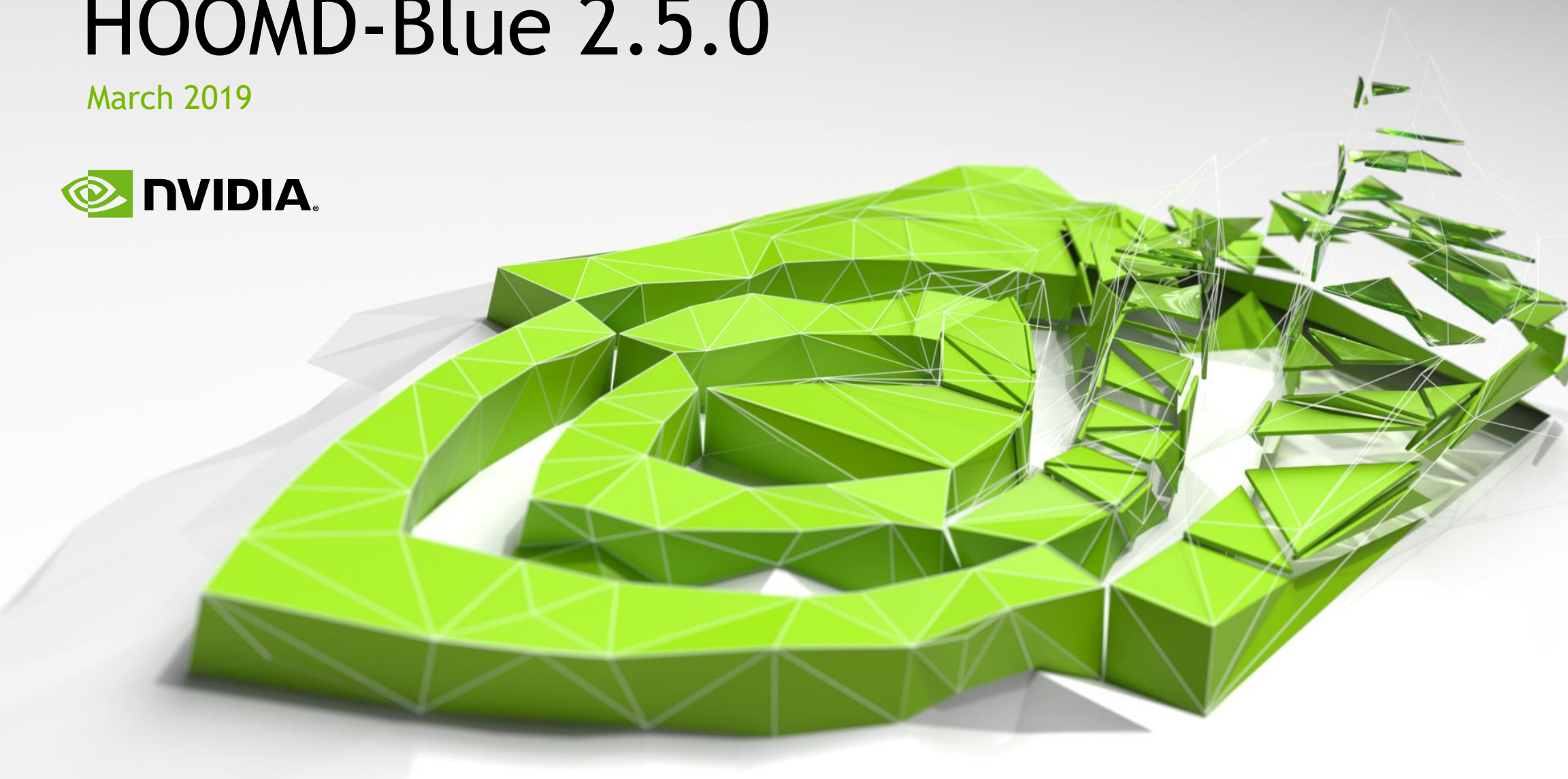
Speed up over dual CPU node (X)

GROMACS recommended usage

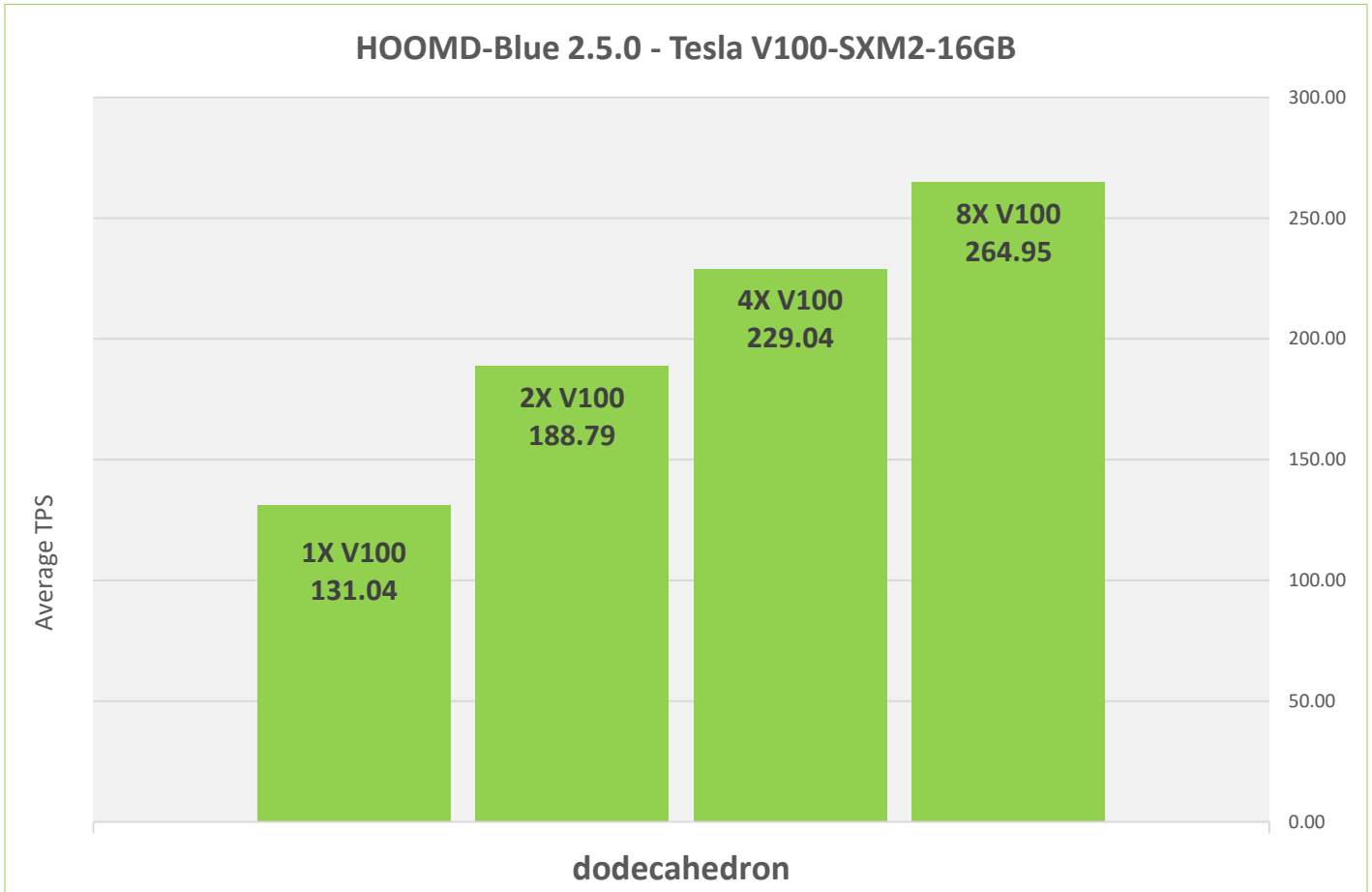
Motherboard and CPU	Dual-socket with server x86-64 CPU
System memory	>=16GB
GPUs	Tesla V100 SXM2
GPUs per socket	1 to 4
GPUs per task	1 - 2 (case dependent)

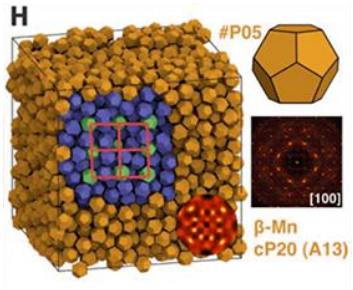
HOOMD-Blue 2.5.0

March 2019



HOOMD-Blue 2.5.0 - dodecahedron





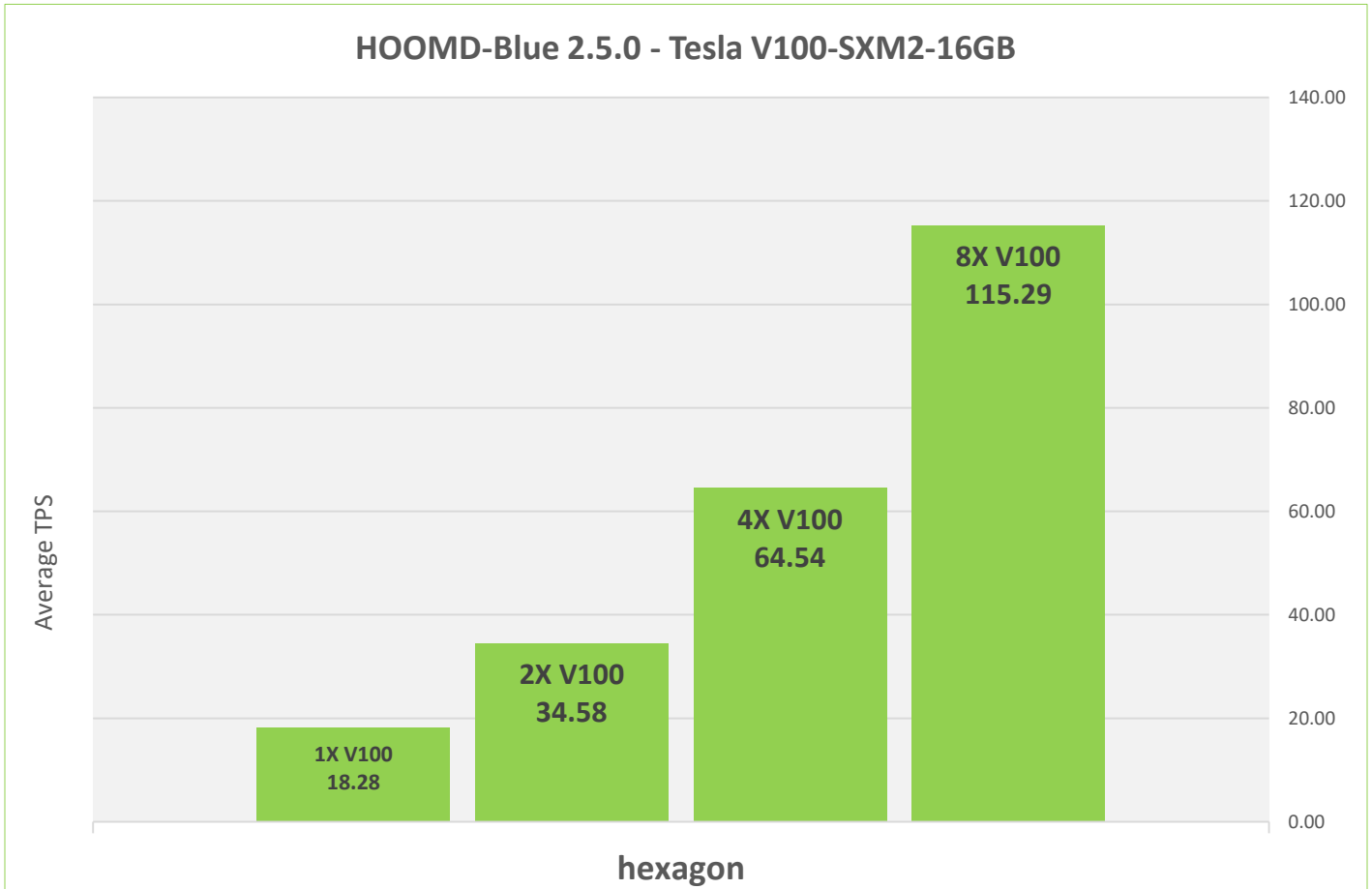
Hard particle Monte Carlo
131,072 atoms

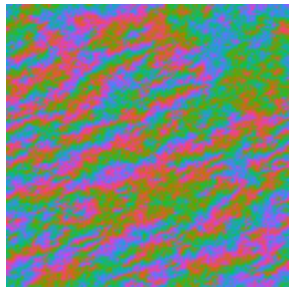
Running HOOMD-Blue 2.5.0

The blue node contains Dual Intel Xeon E5-2698 v4 (Broadwell) CPUs

The green nodes contain Dual Intel E5-2698 v4 (Broadwell) CPUs + Tesla V100 SXM2 (32GB) GPUs

HOOMD-Blue 2.5.0 - hexagon





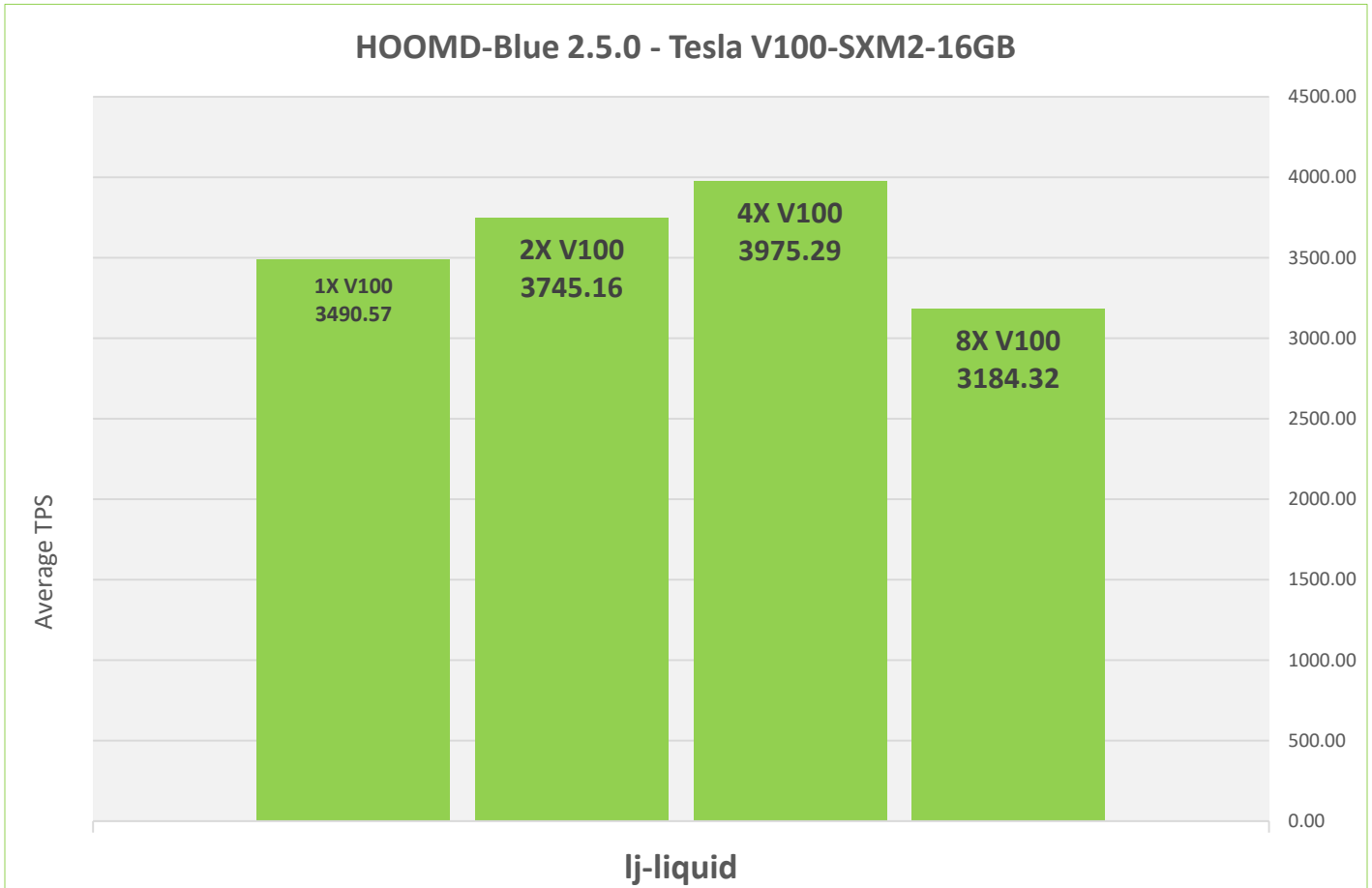
Hard particle Monte Carlo
1,048,576 atoms

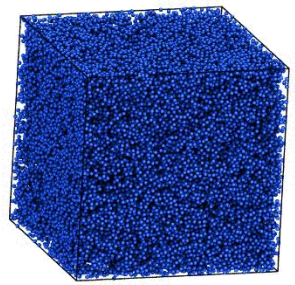
Running HOOMD-Blue 2.5.0

The blue node contains Dual Intel Xeon E5-2698 v4 (Broadwell) CPUs

The green nodes contain Dual Intel E5-2698 v4 (Broadwell) CPUs + Tesla V100 SXM2 (32GB) GPUs

HOOMD-Blue 2.5.0 - lj-liquid





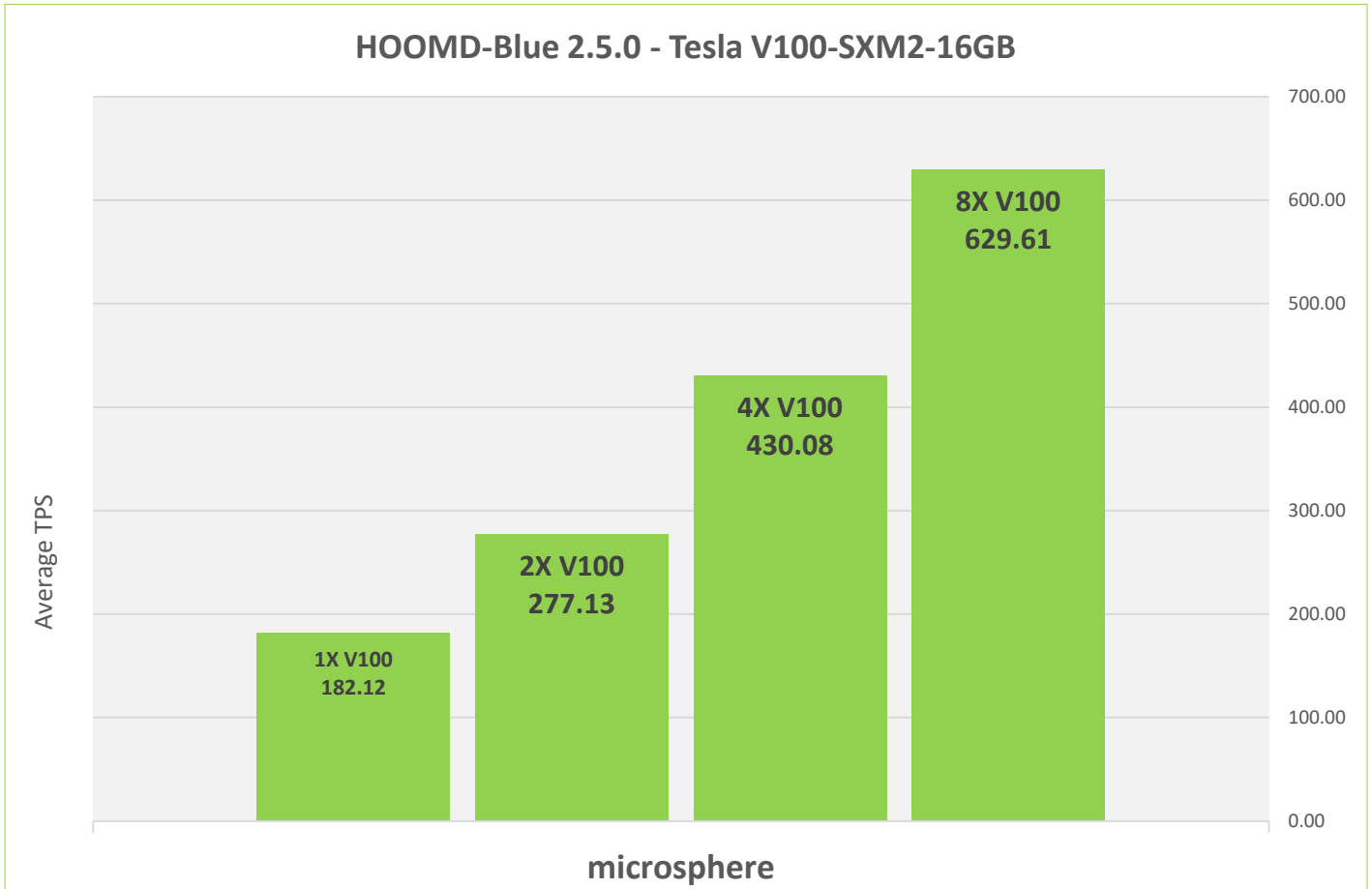
Lennard-Jones pair force
64000 atoms

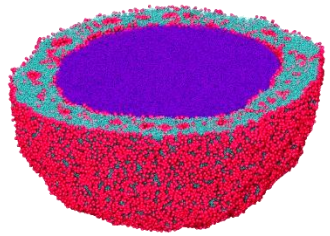
Running HOOMD-Blue 2.5.0

The blue node contains Dual Intel Xeon E5-2698 v4 (Broadwell) CPUs

The green nodes contain Dual Intel E5-2698 v4 (Broadwell) CPUs + Tesla V100 SXM2 (32GB) GPUs

HOOMD-Blue 2.5.0 - microsphere





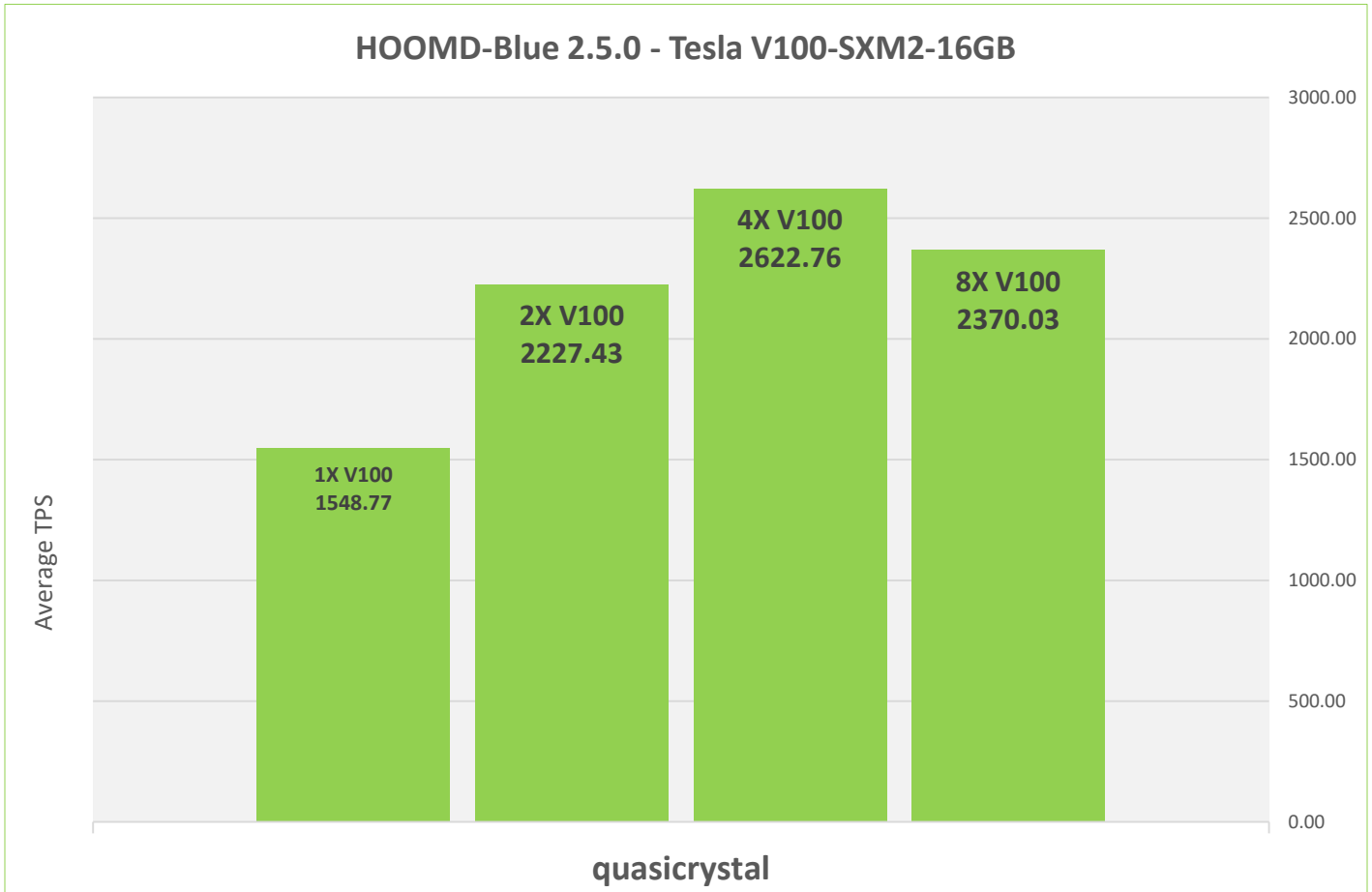
DPD pair force
1,428,364 atoms

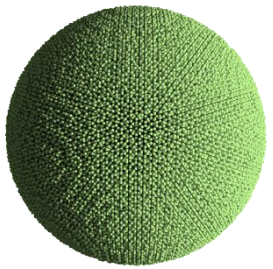
Running HOOMD-Blue 2.5.0

The blue node contains Dual Intel Xeon E5-2698 v4 (Broadwell) CPUs

The green nodes contain Dual Intel E5-2698 v4 (Broadwell) CPUs + Tesla V100 SXM2 (32GB) GPUs

HOOMD-Blue 2.5.0 - quasicrystal





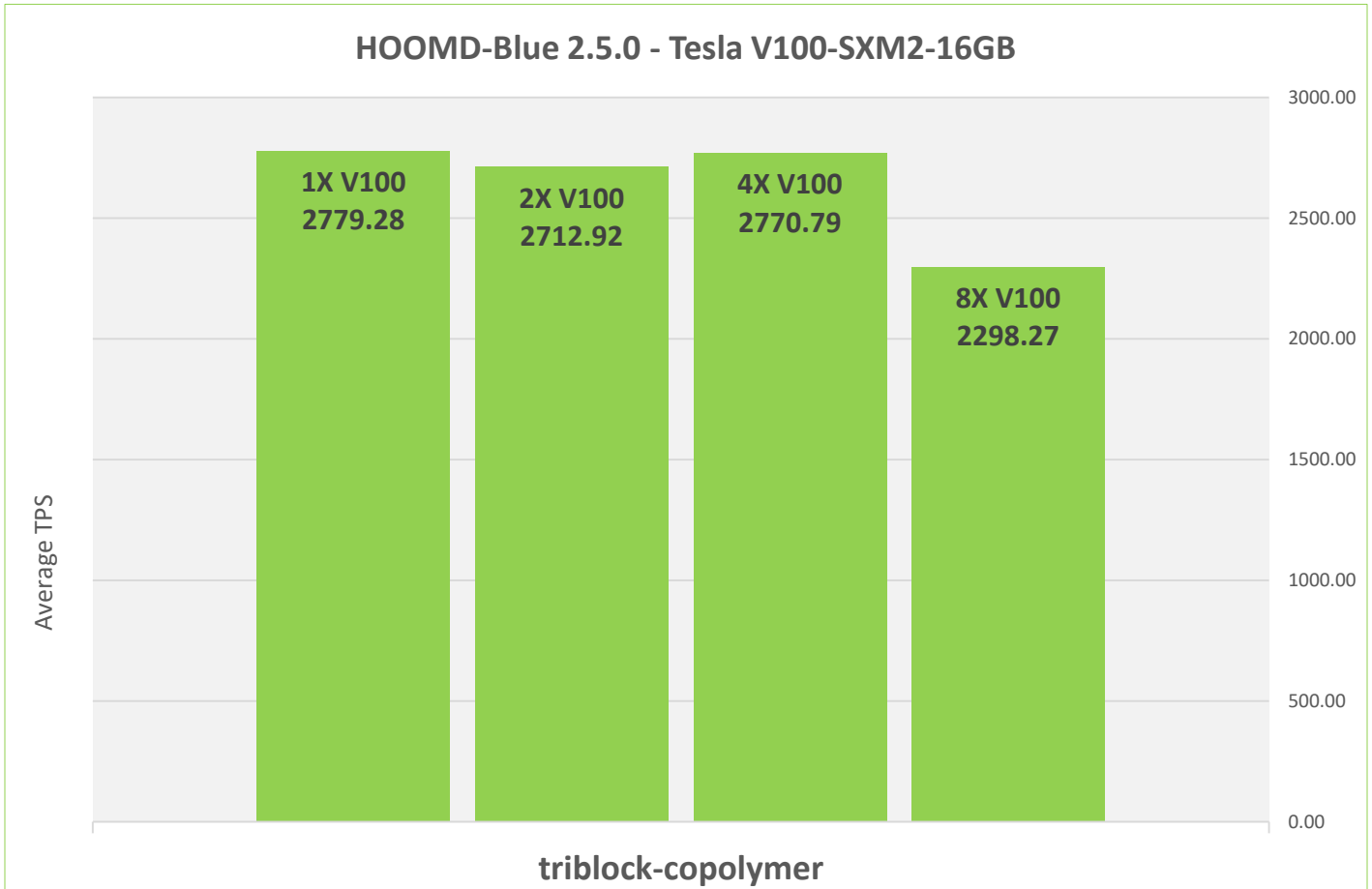
Oscillatory pair potential
100000 atoms

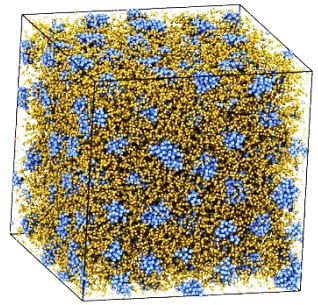
Running HOOMD-Blue 2.5.0

The blue node contains Dual Intel Xeon E5-2698 v4 (Broadwell) CPUs

The green nodes contain Dual Intel E5-2698 v4 (Broadwell) CPUs + Tesla V100 SXM2 (32GB) GPUs

HOOMD-Blue 2.5.0 - triblock-copolymer





LJ pair force - forms spherical micelles
64017 atoms

Running HOOMD-Blue 2.5.0

The blue node contains Dual Intel Xeon E5-2698 v4 (Broadwell) CPUs

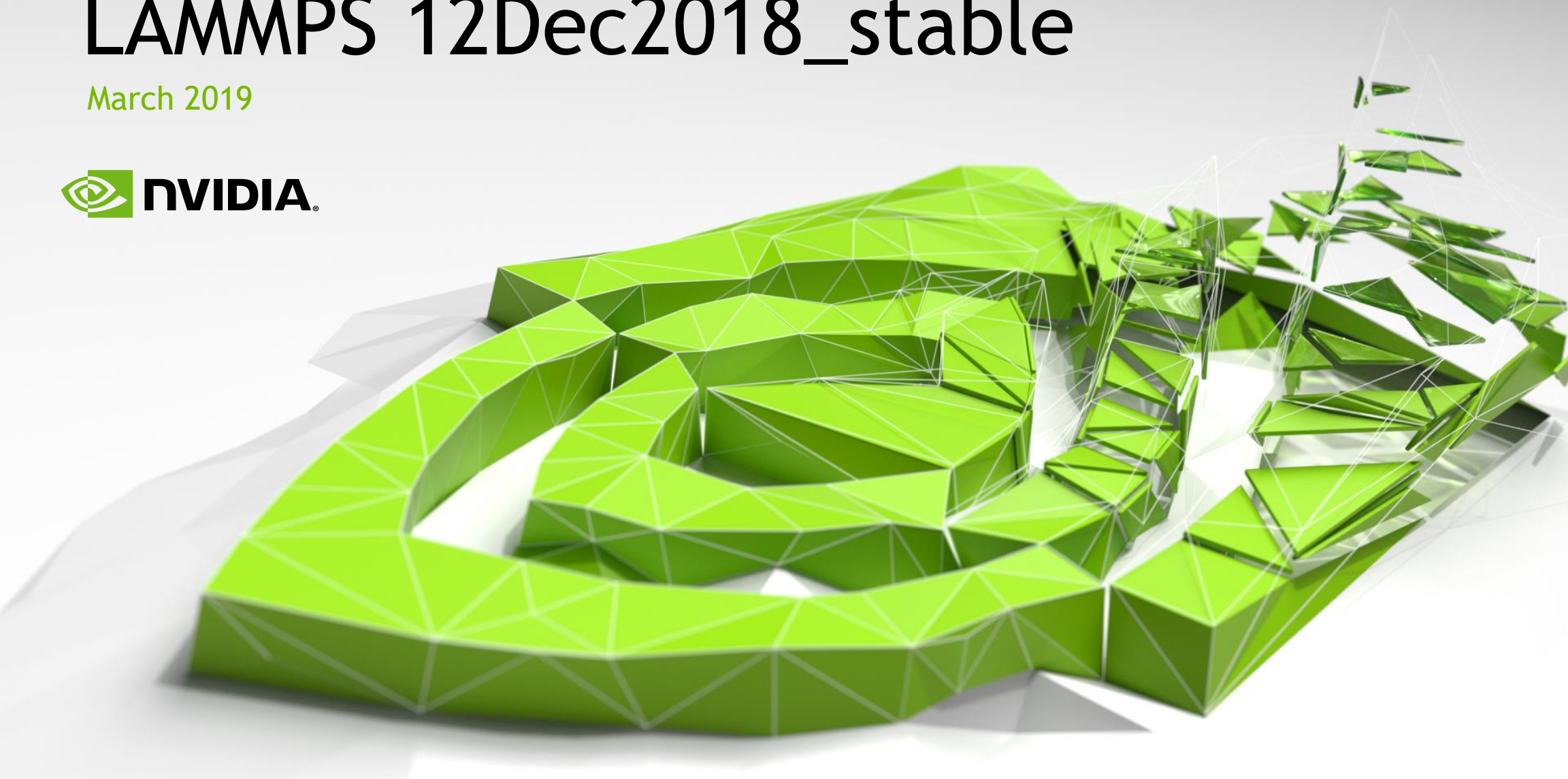
The green nodes contain Dual Intel E5-2698 v4 (Broadwell) CPUs + Tesla V100 SXM2 (32GB) GPUs

HOOMD-Blue recommended usage

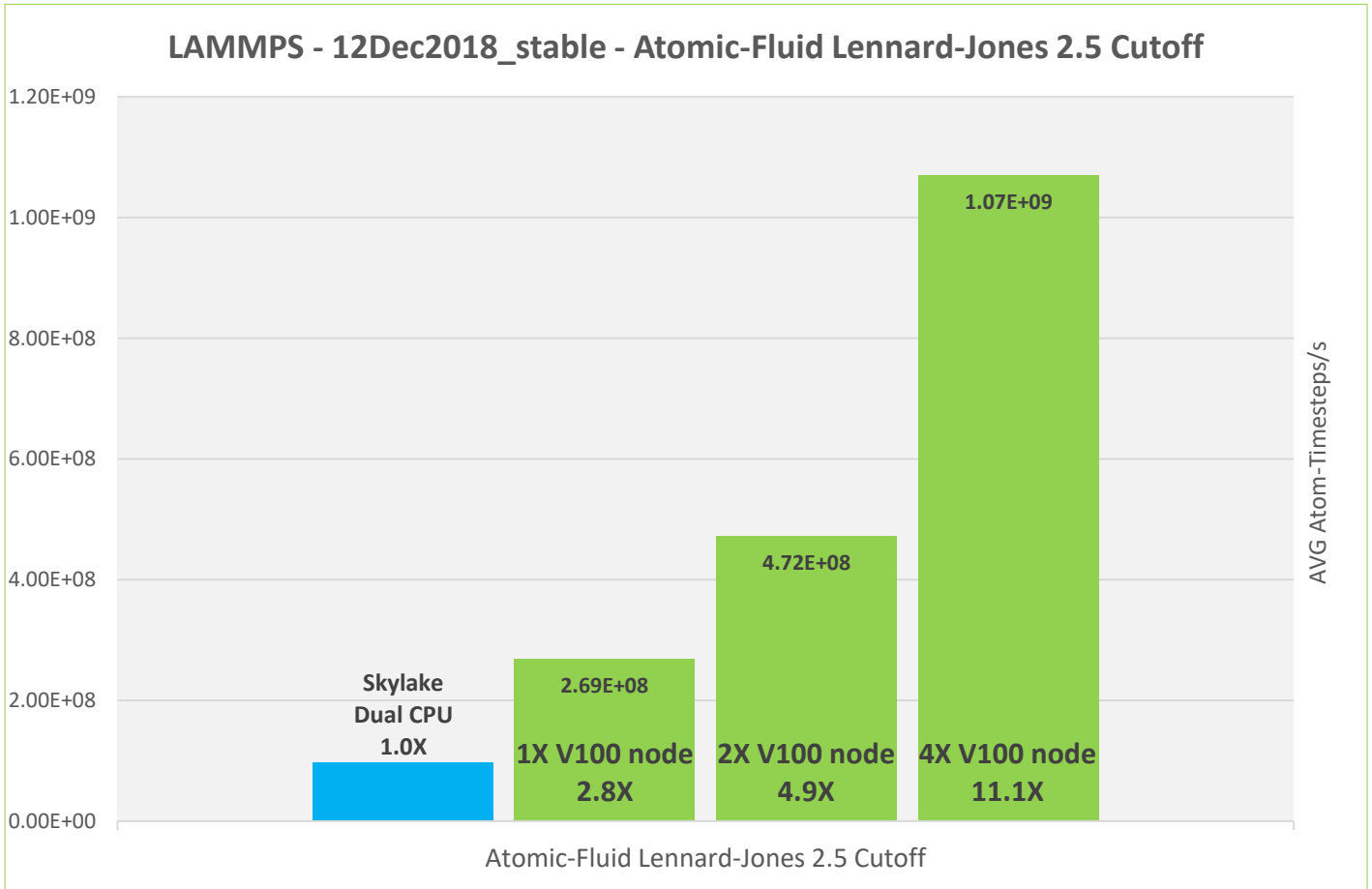
Motherboard and CPU	Dual-socket with server x86-64 CPU
System memory	>=32GB
GPUs	Tesla V100 SXM2
GPUs per socket	1 to 4
GPUs per task	1, 4, or 8 based on benchmarks

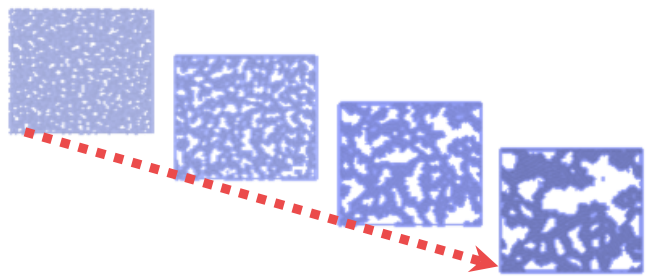
LAMMPS 12Dec2018_stable

March 2019



LAMMPS 12Dec2018_stable
Atomic-Fluid Lennard-Jones 2.5 Cutoff





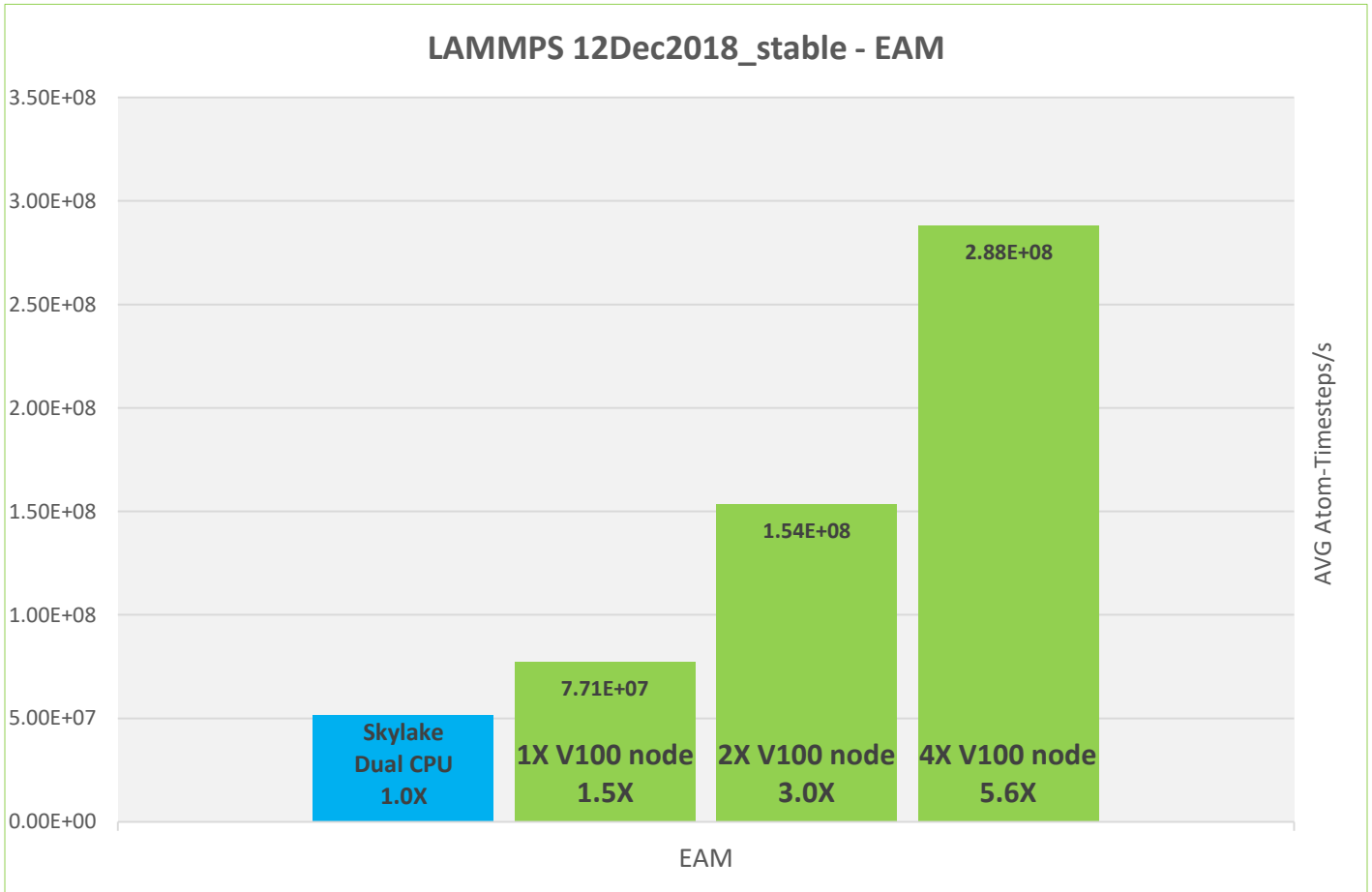
Running LAMMPS 12Dec2018_stable

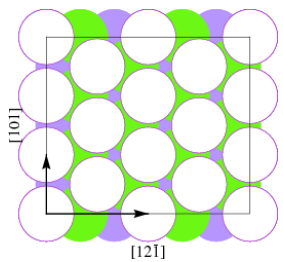
The blue node contains Dual Intel Xeon Gold 6140 (Skylake) CPUs

The green nodes contain Dual Intel Xeon Gold 6140 (Skylake) CPUs + Tesla V100 SXM2 (32GB) GPUs

Speed up over dual CPU node (X)

LAMMPS 12Dec2018_stable - EAM





Bulk Cu lattice

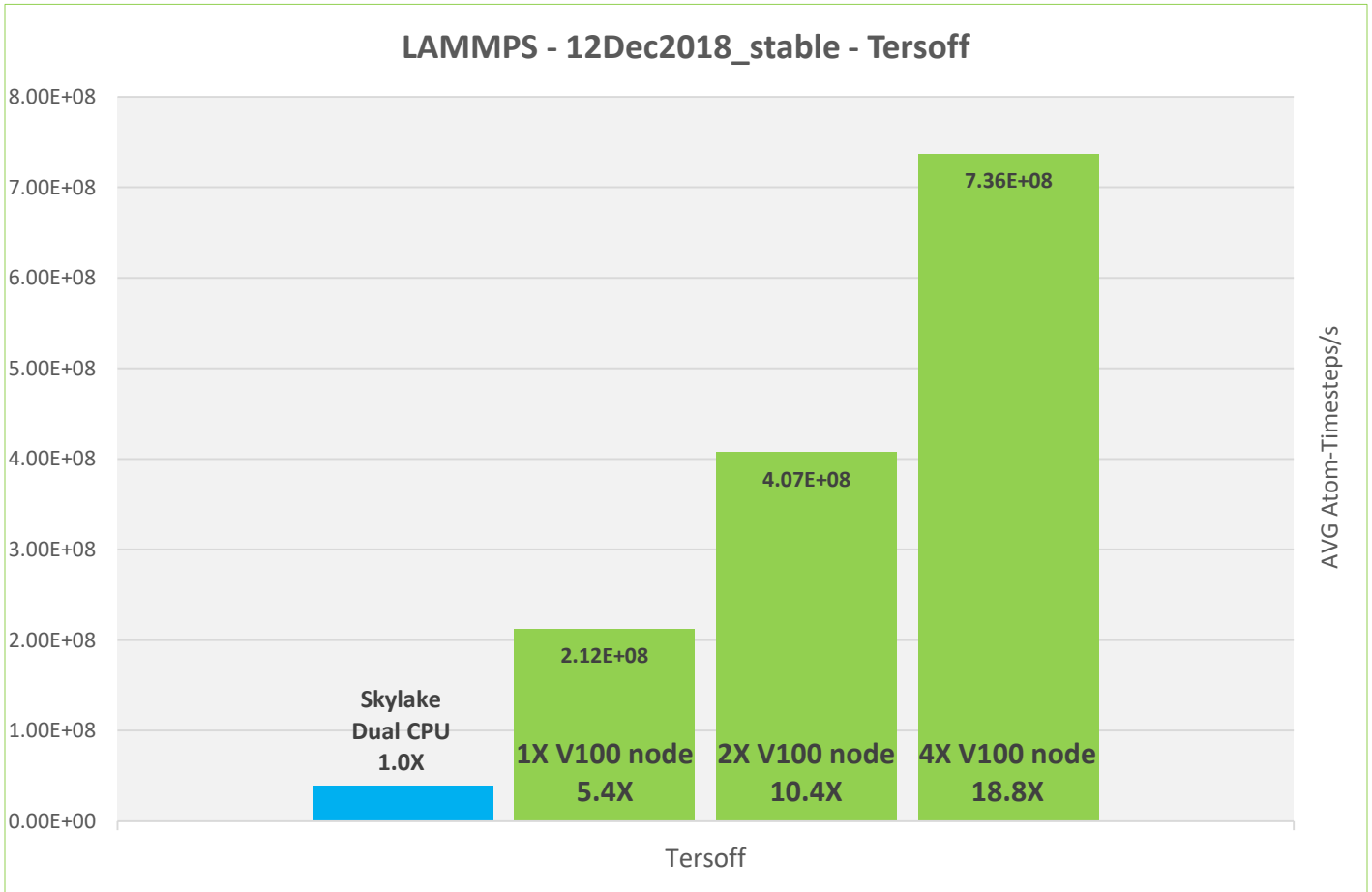
Running LAMMPS 12Dec2018_stable

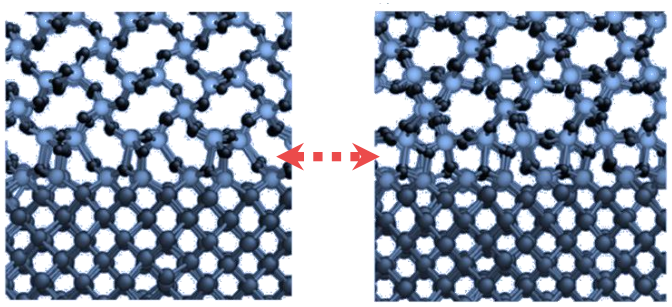
The blue node contains Dual Intel Xeon Gold 6140 (Skylake) CPUs

The green nodes contain Dual Intel Xeon Gold 6140 (Skylake) CPUs + Tesla V100 SXM2 (32GB) GPUs

Speed up over dual CPU node (X)

LAMMPS 12Dec2018_stable - Tersoff





Si crystallization

Running LAMMPS 12Dec2018_stable

The blue node contains Dual Intel Xeon Gold 6140 (Skylake) CPUs

The green nodes contain Dual Intel Xeon Gold 6140 (Skylake) CPUs + Tesla V100 SXM2 (32GB) GPUs

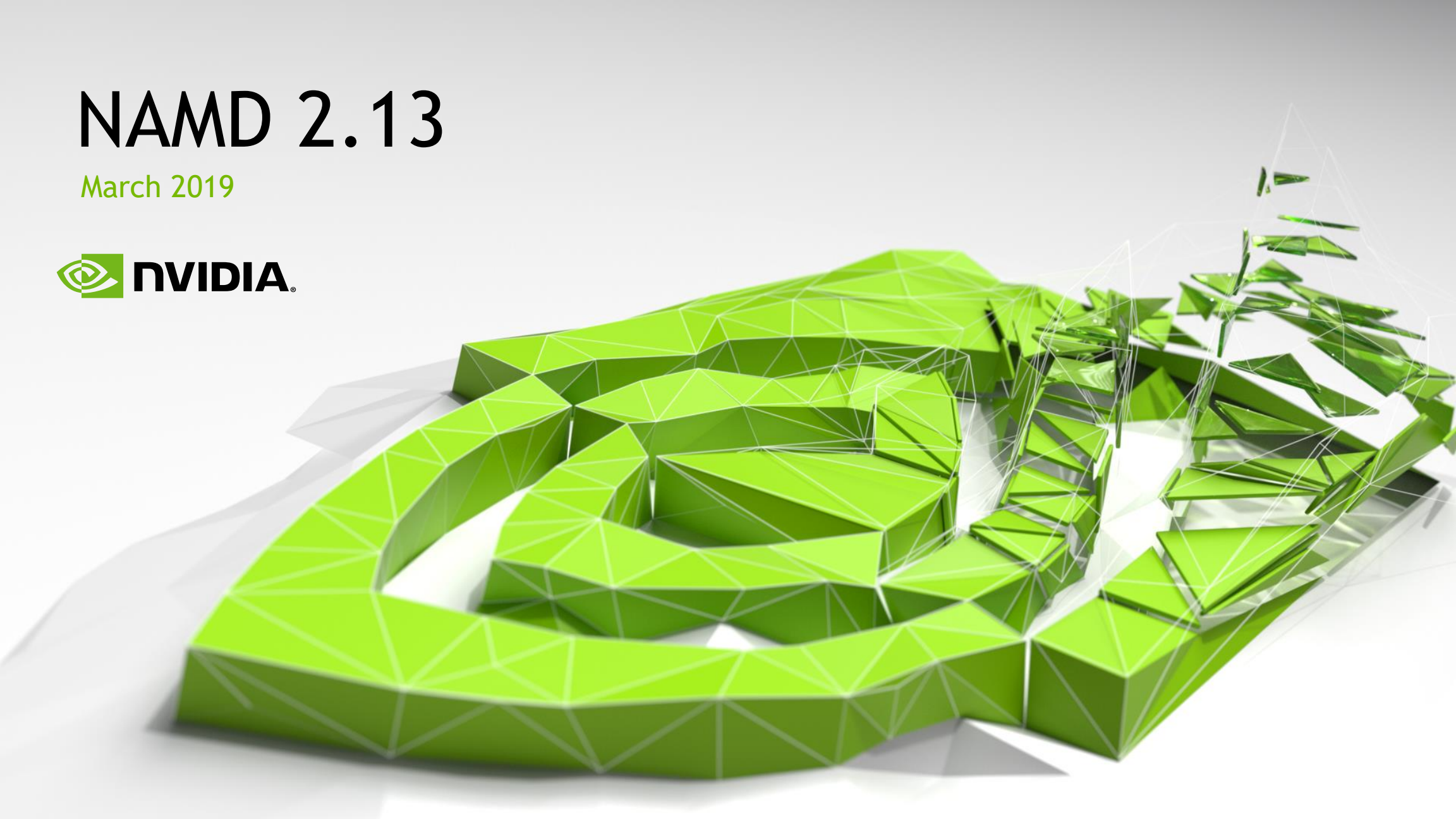
Speed up over dual CPU node (X)

LAMMPS recommended usage

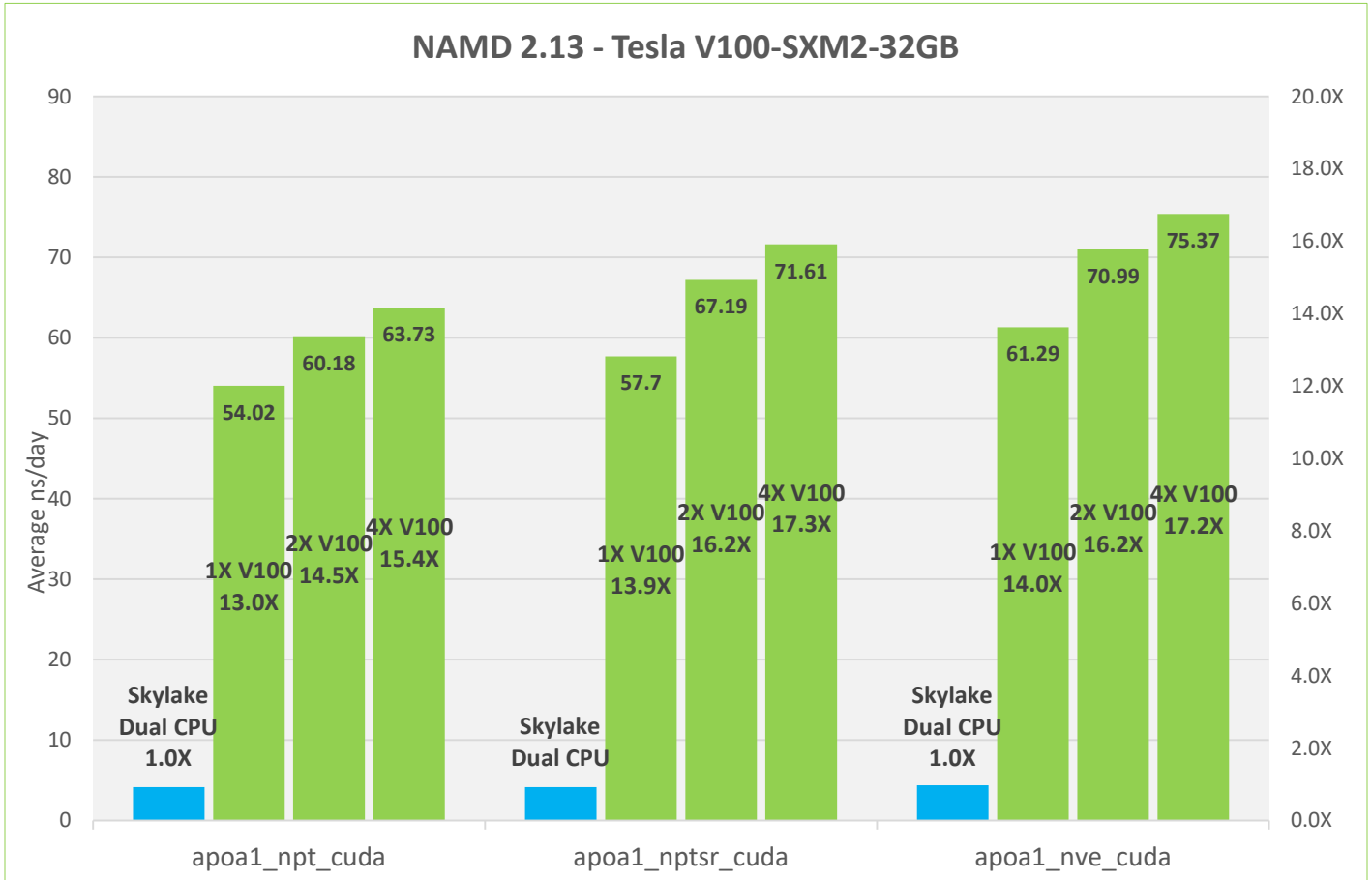
Motherboard and CPU	Dual-socket with server x86-64 CPU
System memory	>=32GB
GPUs	Tesla V100 SXM2
GPUs per socket	1 to 4
GPUs per task	4

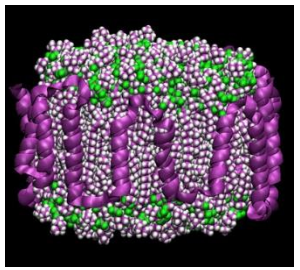
NAMD 2.13

March 2019



NAMD 2.13 - APO1





ApoA1
92,224 atoms

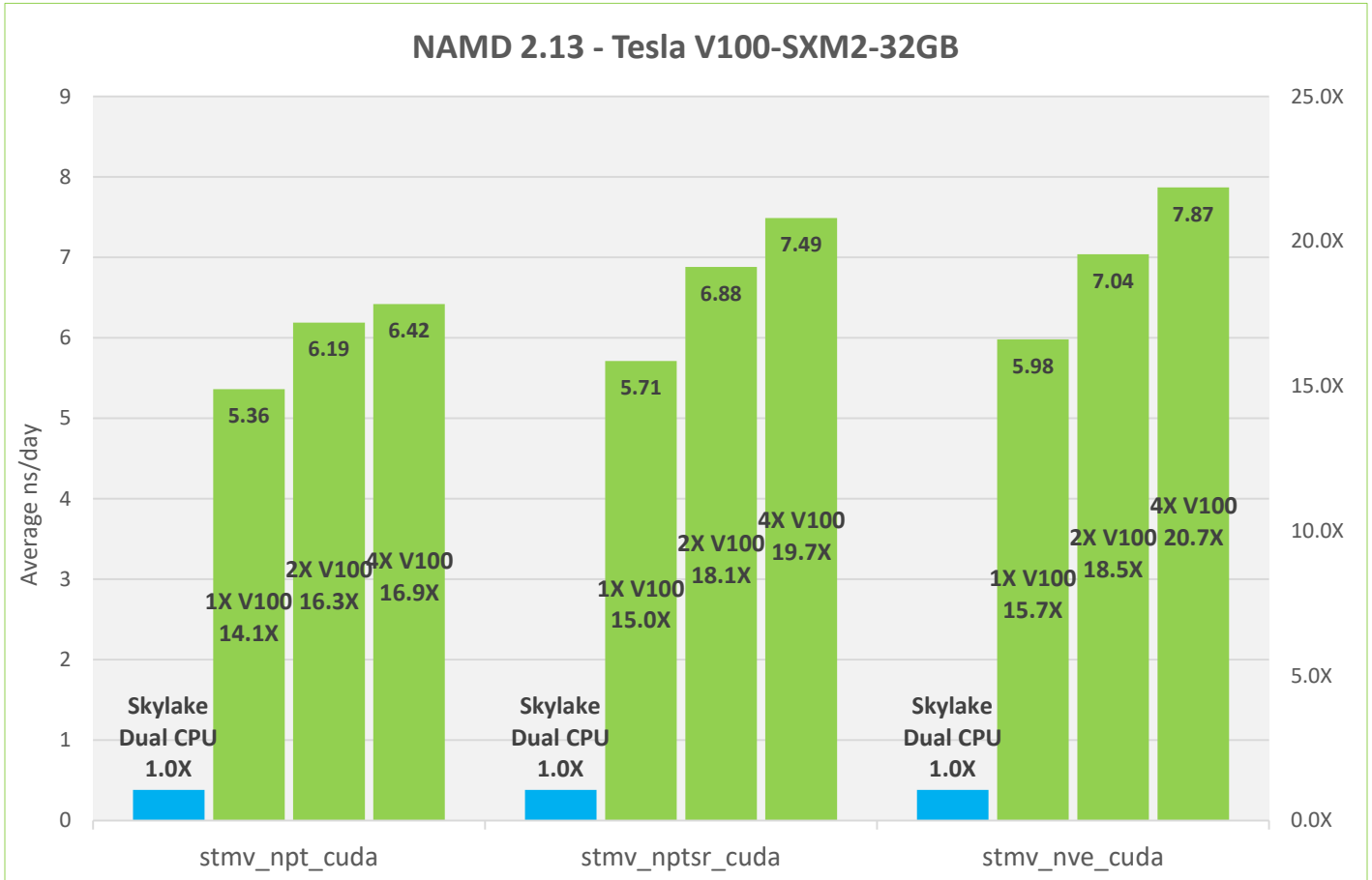
Running NAMD 2.13

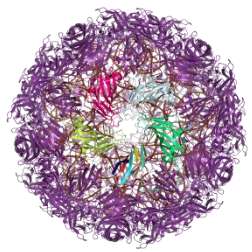
The blue node contains Dual Intel Xeon Gold 6140 (Skylake) CPUs

The green nodes contain Dual Intel Xeon Gold 6140 (Skylake) CPUs + Tesla V100 SXM2 (32GB) GPUs

Speed up over dual CPU node (X)

NAMD 2.13 - STMV





Satellite Tobacco Mosaic Virus
1,067,095 atoms

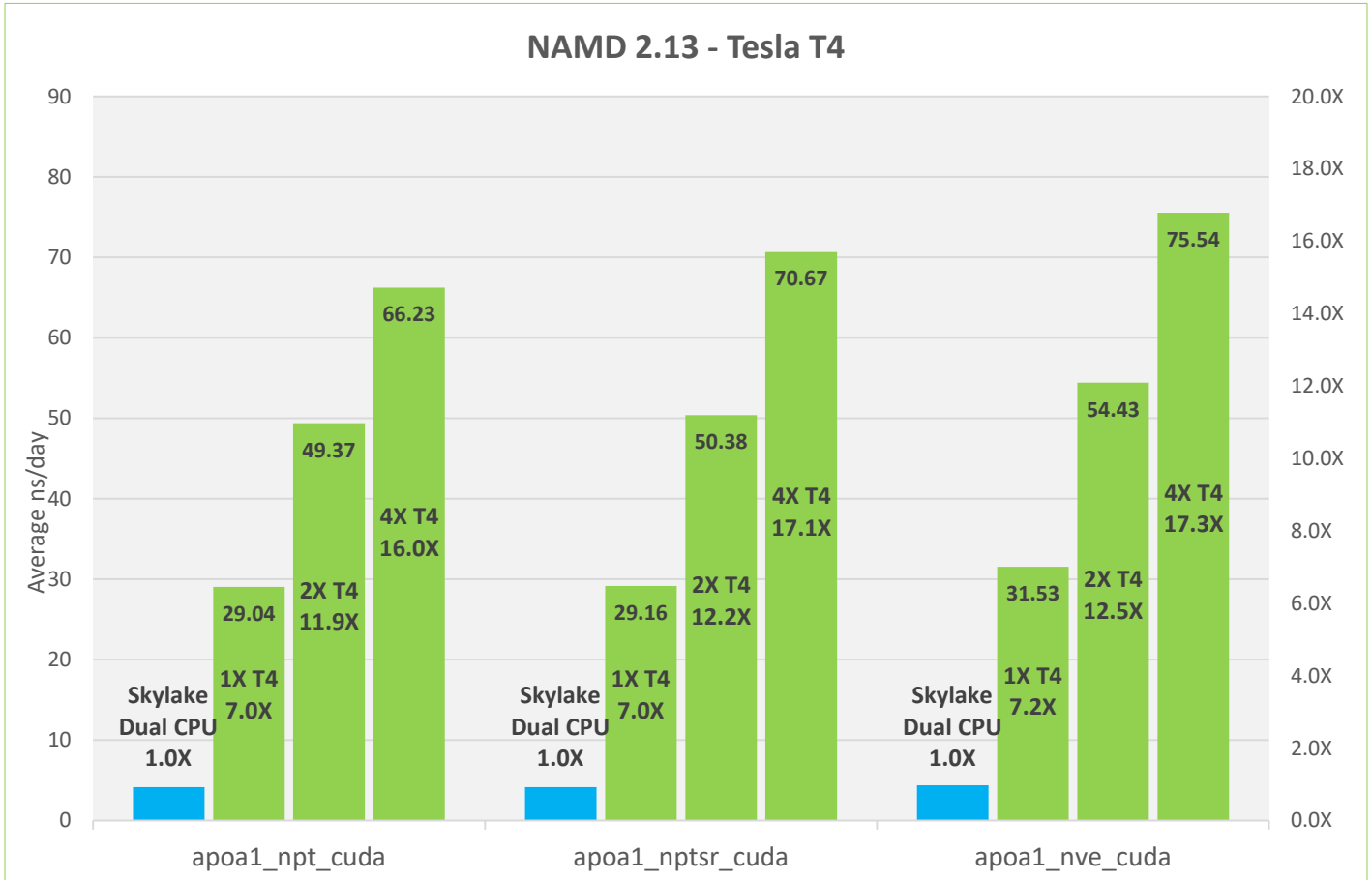
Running NAMD 2.13

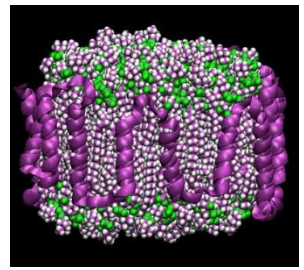
The blue node contains Dual Intel Xeon Gold 6140 (Skylake) CPUs

The green nodes contain Dual Intel Xeon Gold 6140 (Skylake) CPUs + Tesla V100 SXM2 (32GB) GPUs

Speed up over dual CPU node (X)

NAMD 2.13 - APO1





ApoA1
92,224 atoms

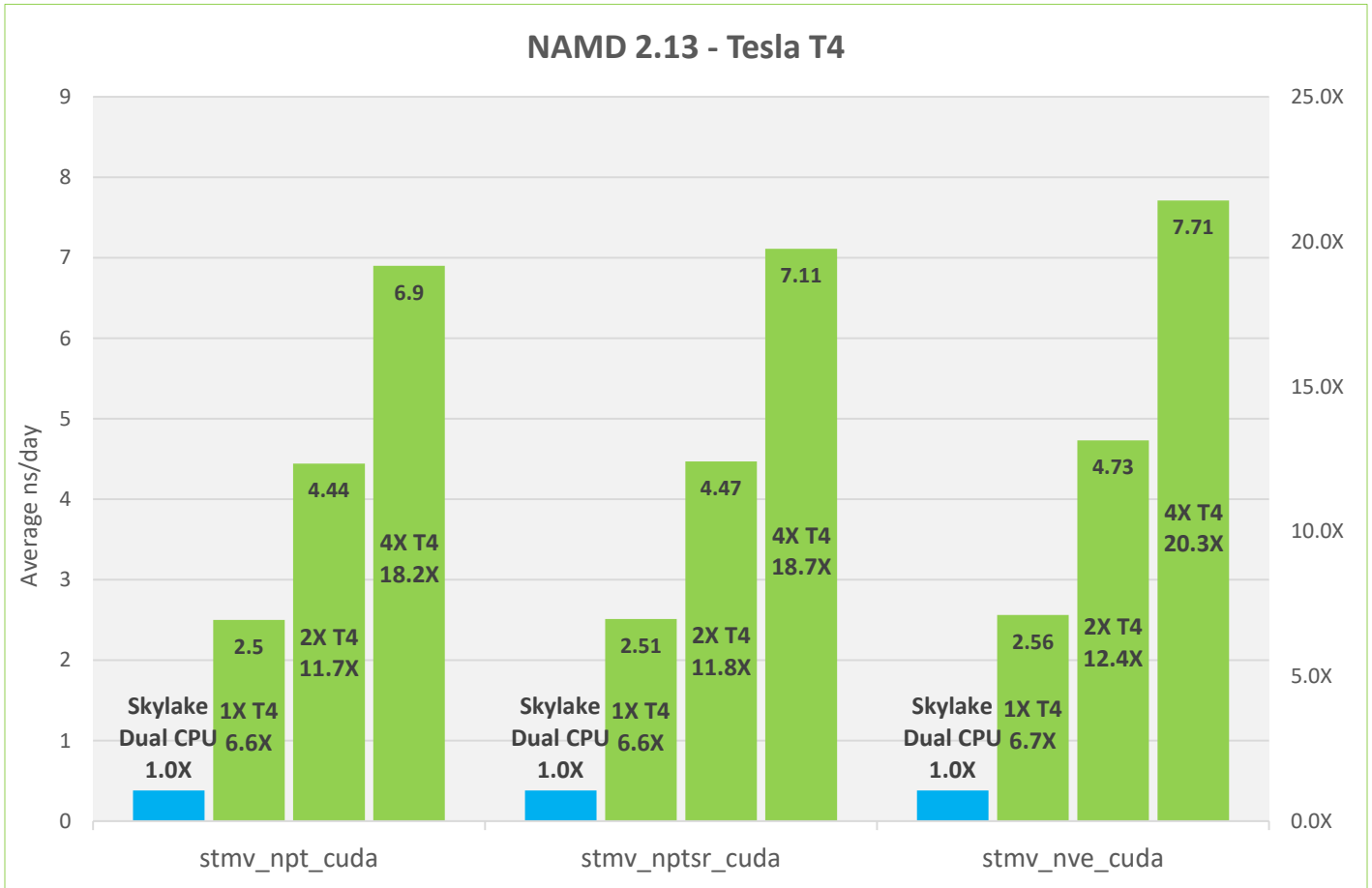
Running NAMD 2.13

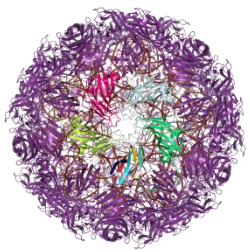
The blue node contains Dual Intel Xeon Gold 6140 (Skylake) CPUs

The green nodes contain Dual Intel Xeon Gold 6140 (Skylake) CPUs + Tesla T4 PCIe (16GB) GPUs

Speed up over dual CPU node (X)

NAMD 2.13 - STMV





Satellite Tobacco Mosaic Virus
1,067,095 atoms

Running NAMD 2.13

The blue node contains Dual Intel Xeon Gold 6140 (Skylake) CPUs

The green nodes contain Dual Intel Xeon Gold 6140 (Skylake) CPUs + Tesla T4 PCIe (16GB) GPUs

Speed up over dual CPU node (X)

NAMD recommended usage

Motherboard and CPU	Dual-socket with server x86-64 CPU
System memory	>=16GB
GPUs	Tesla V100 Tesla T4
GPUs per socket	1 to 4
GPUs per task	4

MD Applications GPU-Accelerated Computing

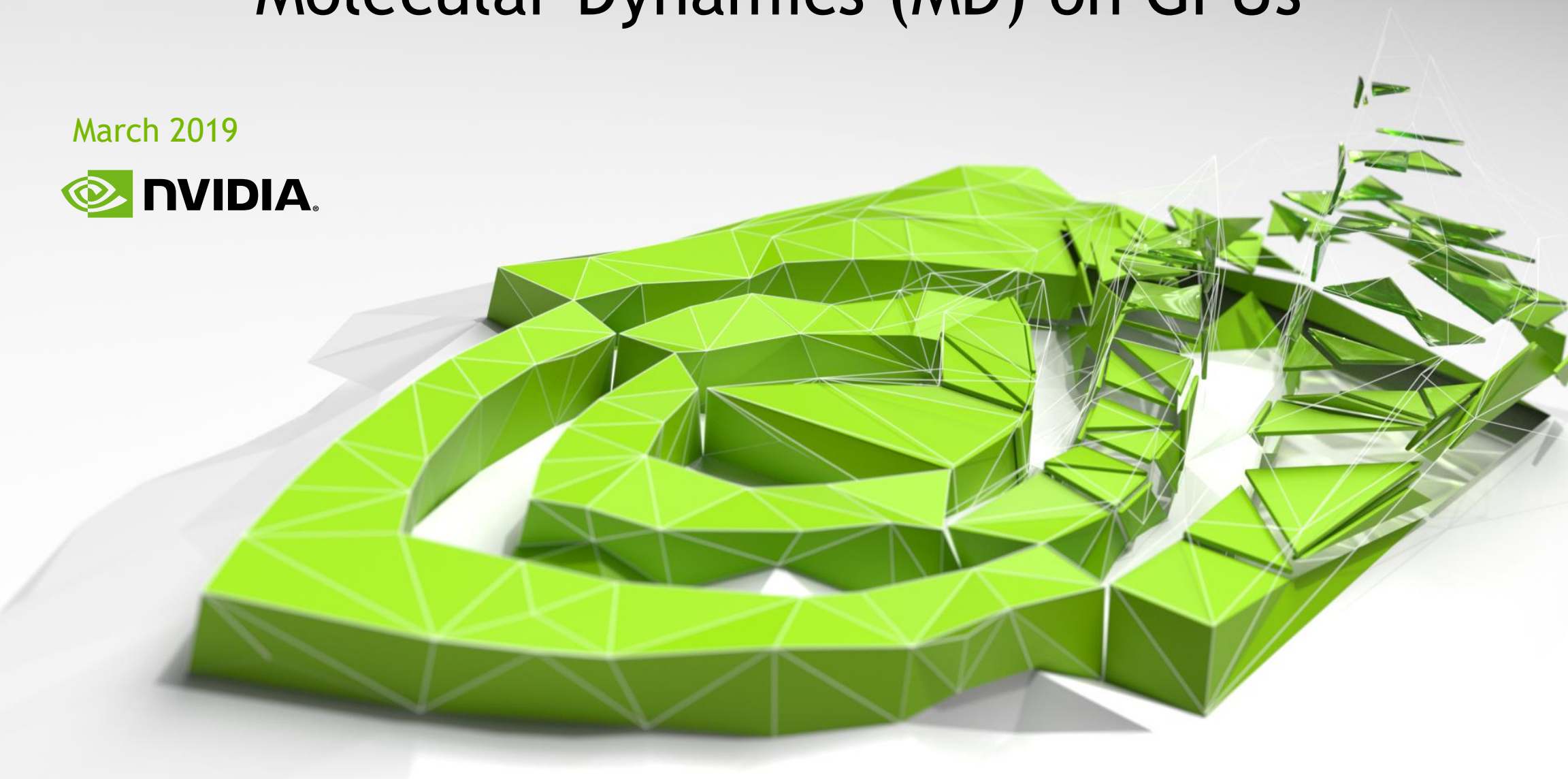
Turbocharge your research!

- Speedup of 3X-8X compared to CPU only in all tests (average)
- Majority of compute intensive for classical MD ported to GPUs
- Large performance boost and improve TCO for compute infrastructure
- Tesla GPUs are more energy efficient <50% of CPU-only computing
- GPUs scale well within a node and/or over multiple nodes
- Tesla V100 is highest performance GPU

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

Molecular Dynamics (MD) on GPUs

March 2019



GPU-Accelerated Quantum Chemistry Apps

Green Lettering Indicates Performance Slides Included

- Abinit
- ACES III
- ADF
- BigDFT
- CP2K
- DIRAC
- GAMESS-US
- Gaussian
- GPAW
- FHI-AIMS
- 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.