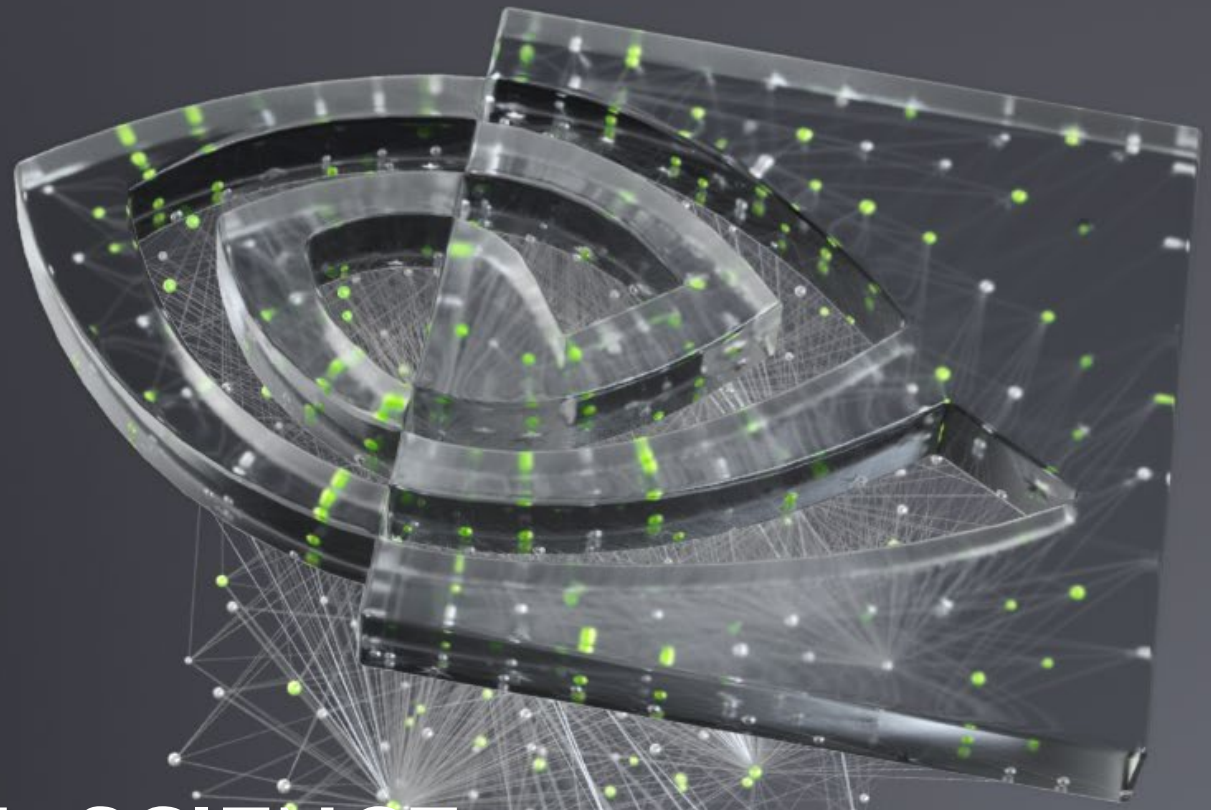


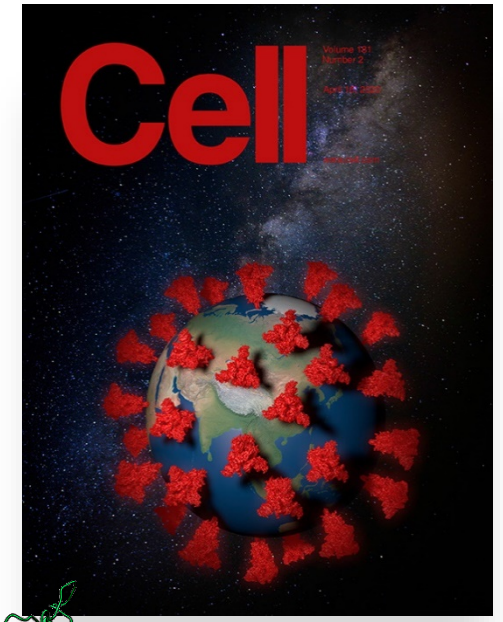
LIFE AND MATERIAL SCIENCE
APPLICATION PERFORMANCE

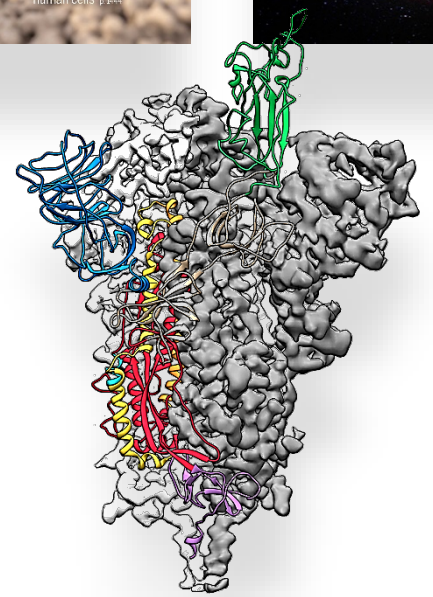
June 2020

Critical COVID-19 Research Accelerated on NVIDIA GPUs

NVIDIA GPUs accelerate today's most critical global health research efforts. In just under two weeks, researchers determined the first high resolution structure of the 2019-nCoV spike protein using Structura Bio application, cryoSPARC. The turnaround time came by ongoing improvements in computational throughput and more accurate methods. Over the past 5 years, today's cryo-EM pipelines take days rather than months.

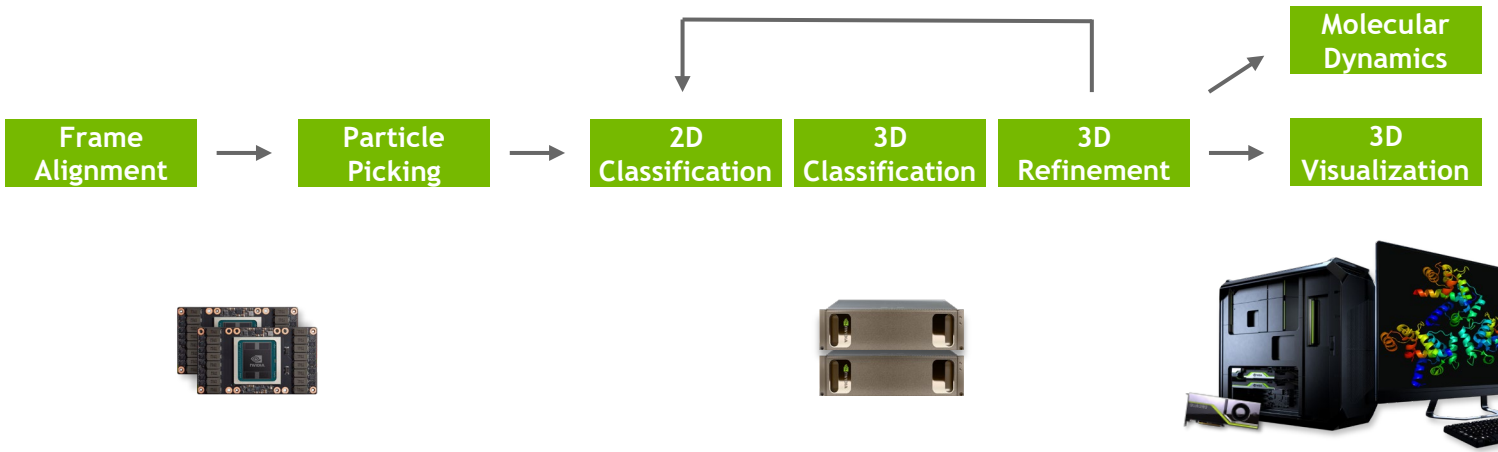
From real-time processing as data is acquired to advanced molecular simulations using HPC and AI, future vaccines and therapies will be ready to fight global health threats.





END TO END GPU ACCELERATED CRYO-EM

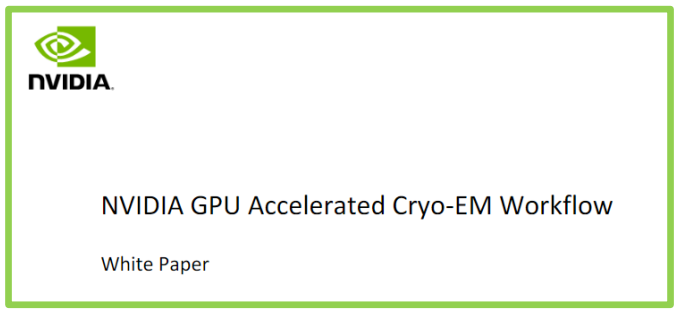
Single Compute Platform for AI, HPC, Visualization



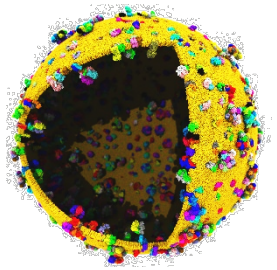
GPU-accelerated apps

- AMIRA
- BioEM
- cryoSPARC
- cyYOLO
- Dynamo
- EMAN2
- emClarity
- GCTF
- IMOD
- MotionCor2
- RELION
- Tomviz
- Topaz
- VMD
- Warp

Cryo-EM Performance White Paper



Overview of Life & Material Accelerated Apps



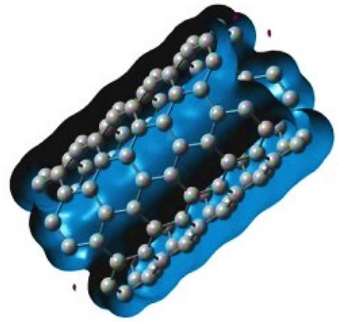
MD

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

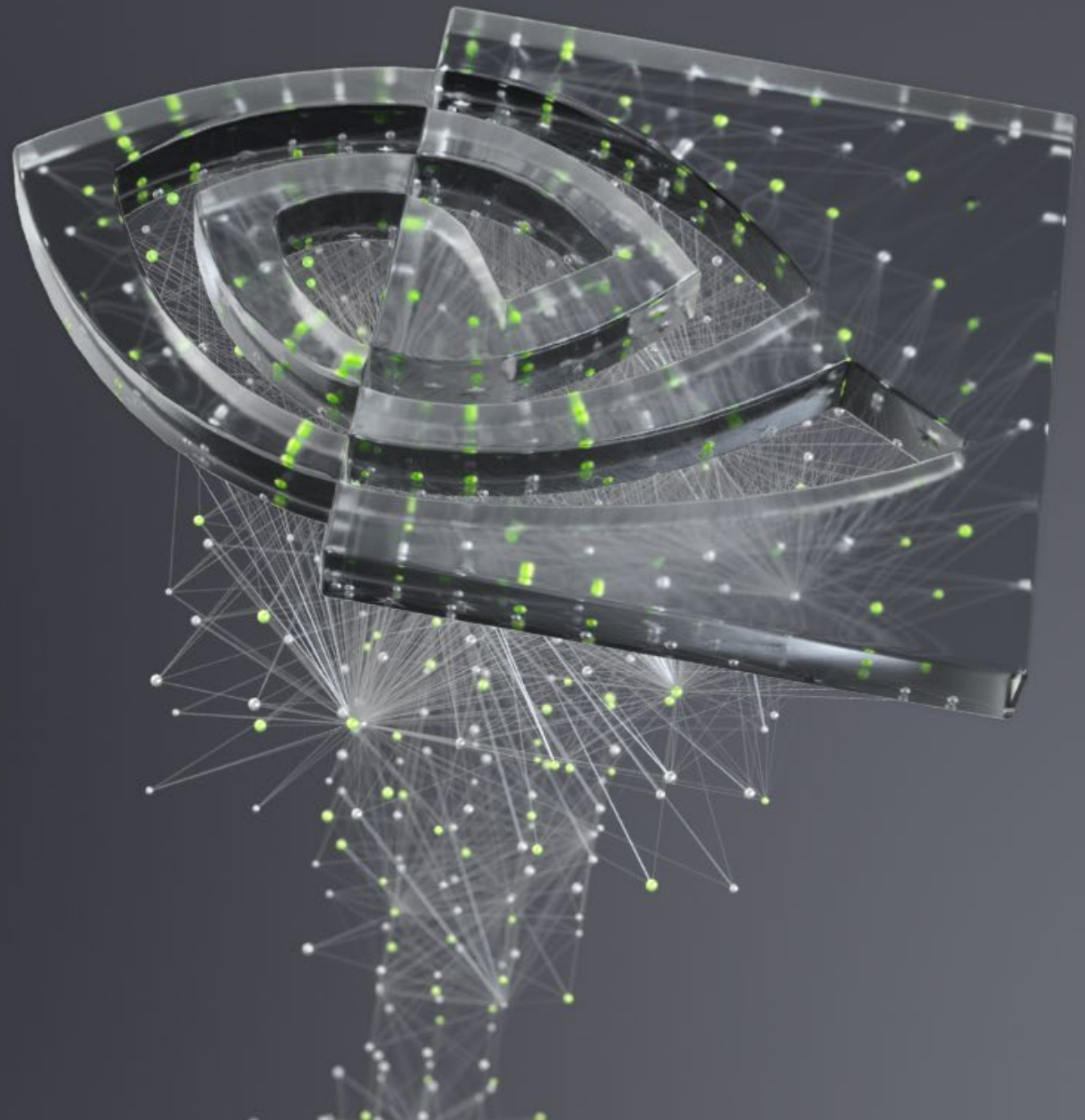
GPU-accelerated math libraries, OpenACC directives

GPU-accelerated apps

ABINIT, ACES III, ADF, BigDFT, CP2K, GAMESS, GAMESS-UK, GPAW, LATTE, LSDalton, LSMS, MOLCAS, MOPAC2012, NWChem, NWChemEx, OCTOPUS, PEtot, QUICK, Q-Chem, QMCPack, Quantum Espresso, QUICK, TeraChem, VASP

Active acceleration projects

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

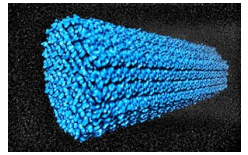


AMBERMD 2020

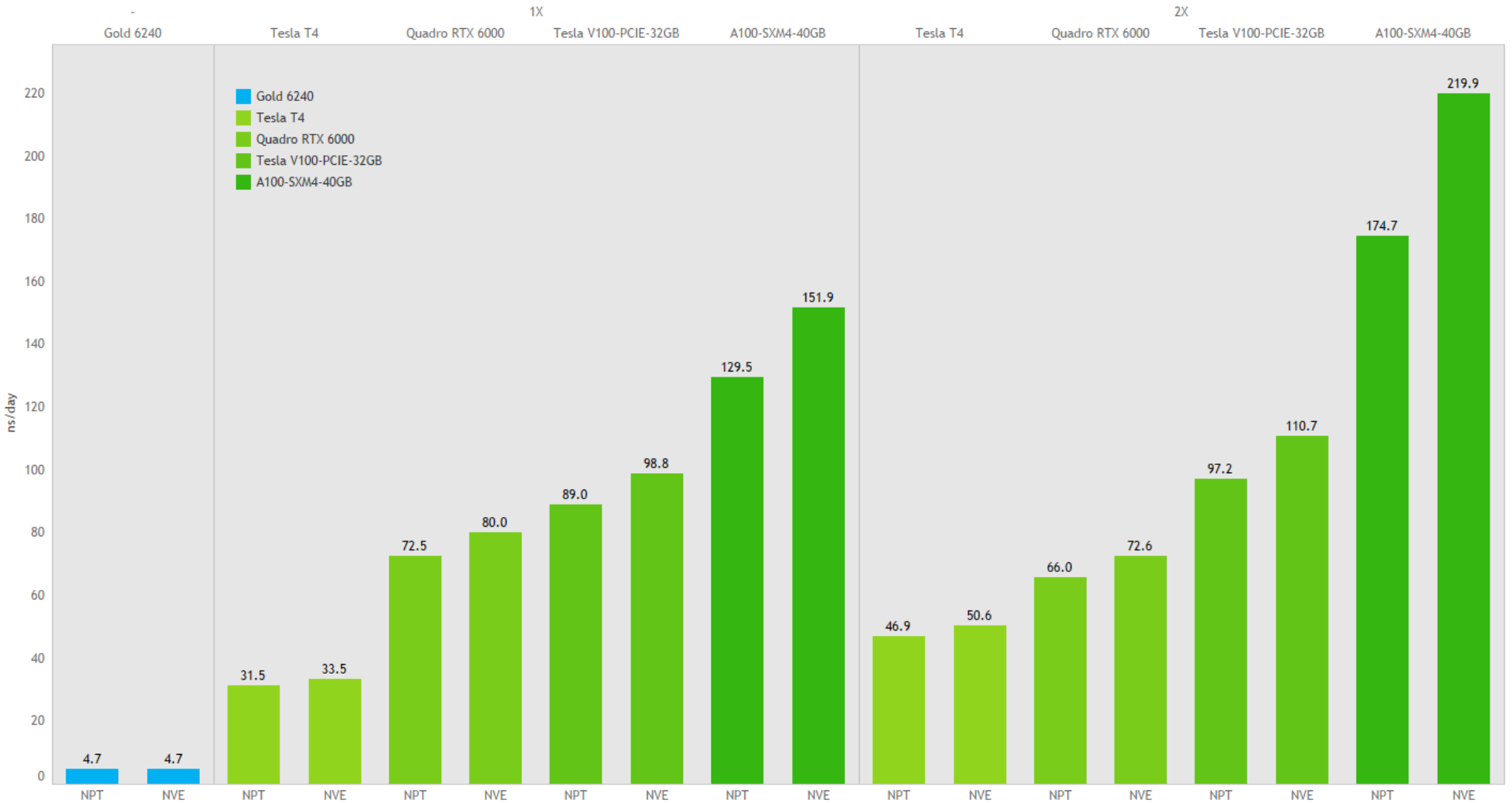
June 2020

AmberMD 2020

Cellulose
408,609 atoms

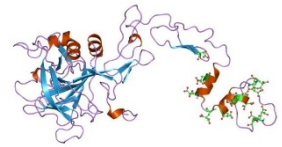


Performance Comparison - Cellulose 4fs

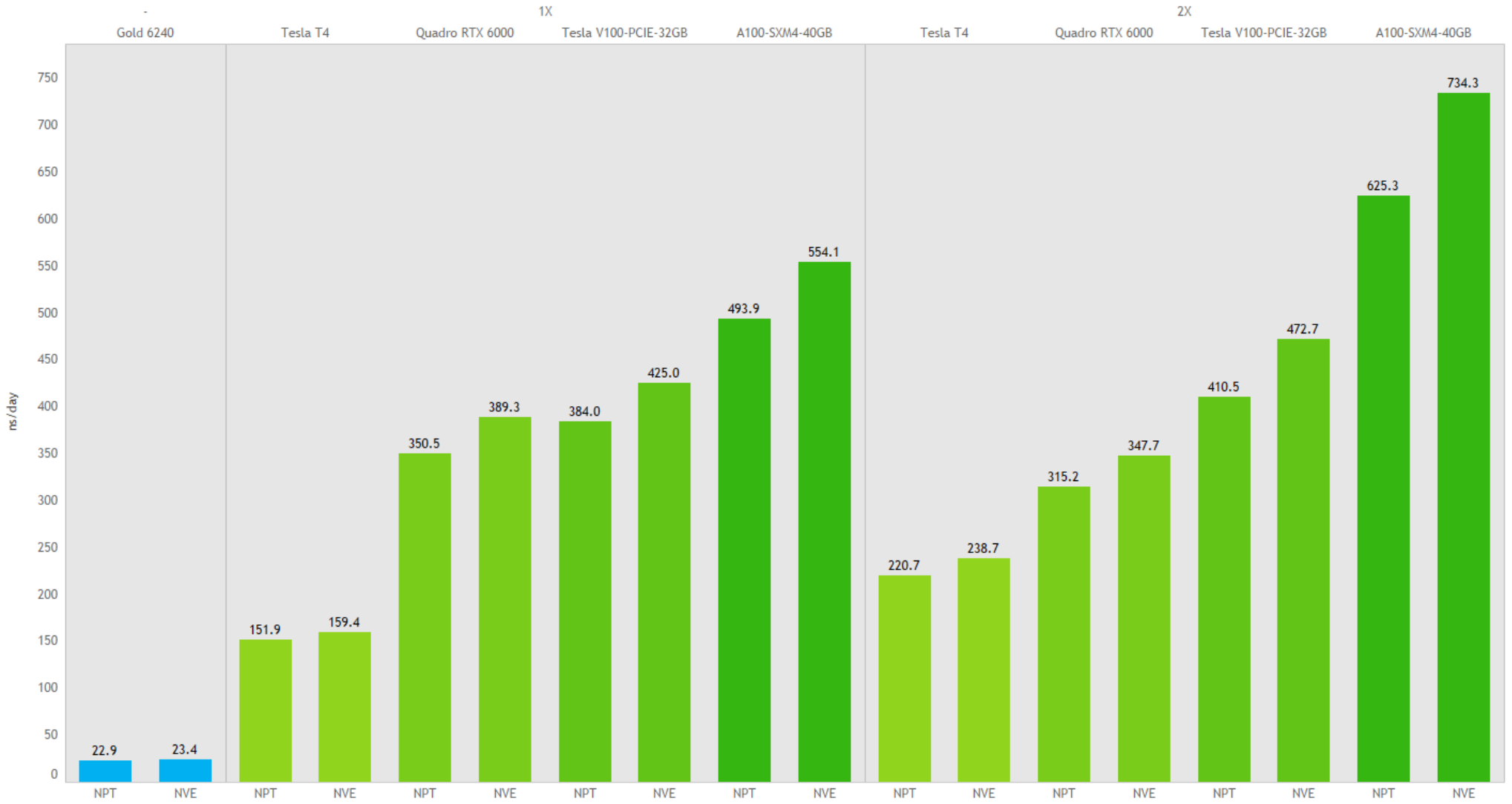


AmberMD 2020

Factor IX
90,906 atoms

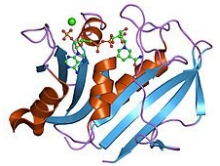


Performance Comparison - FactorIX 4fs

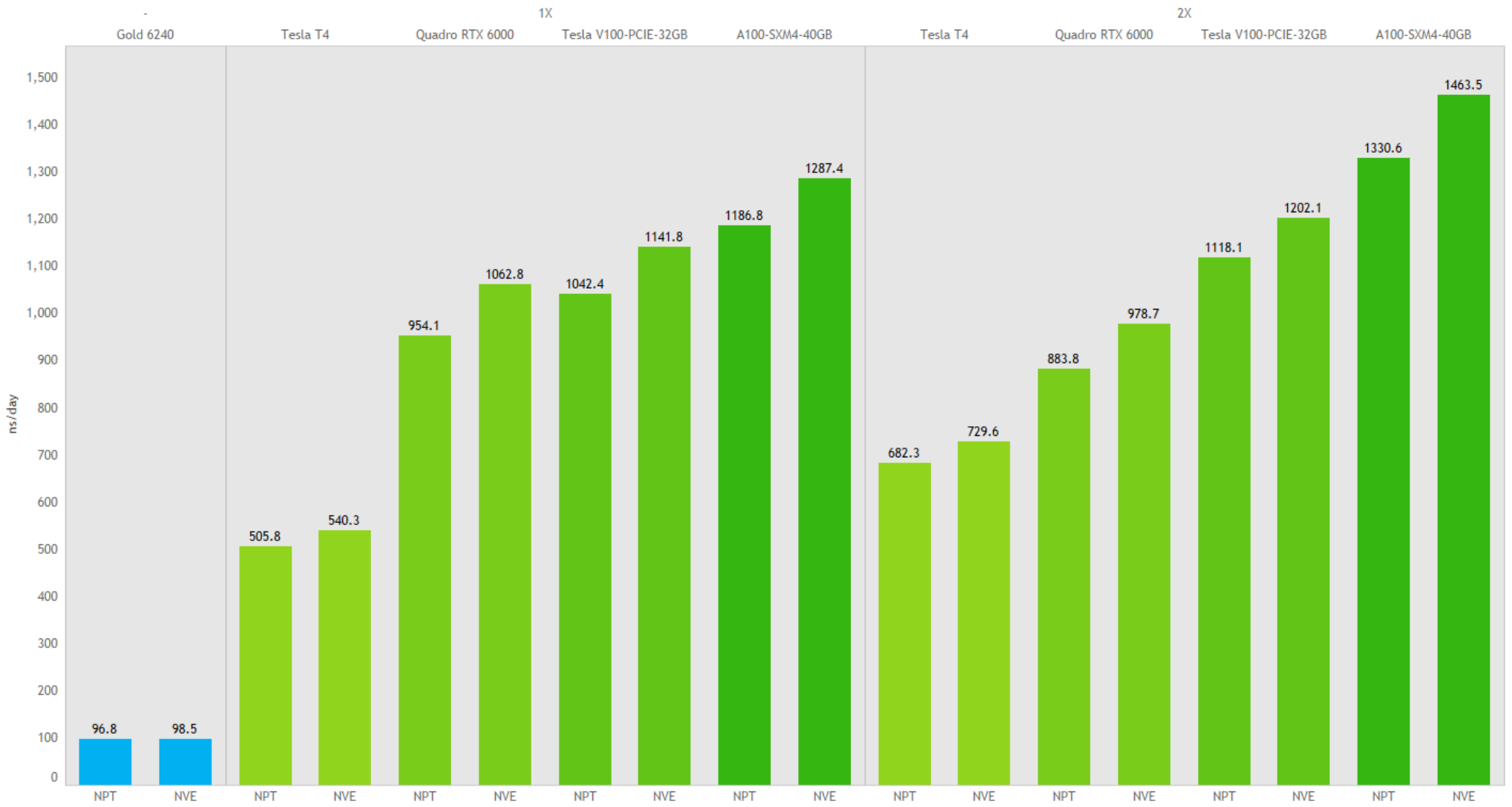


AmberMD 2020

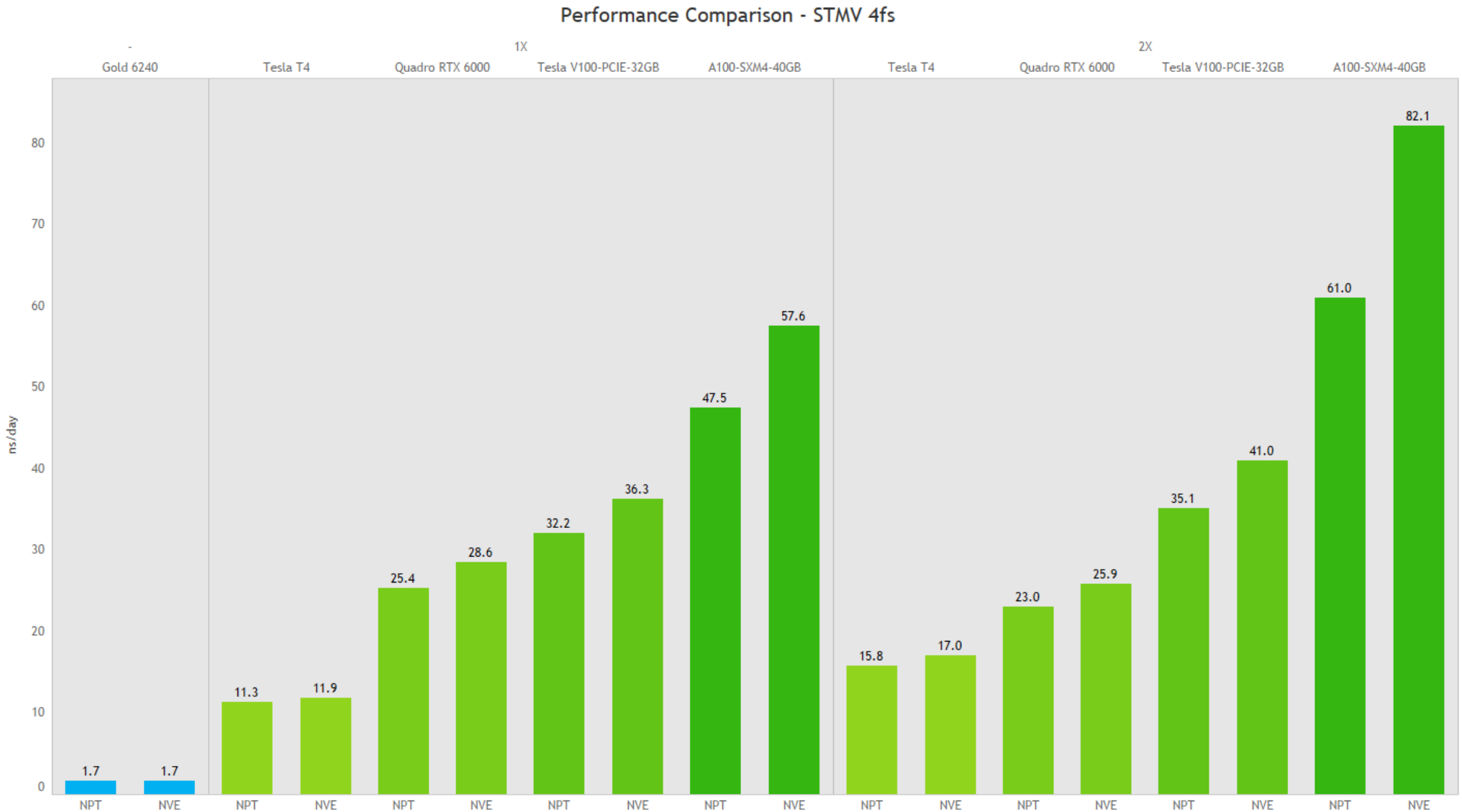
DHFR 23,558 atoms



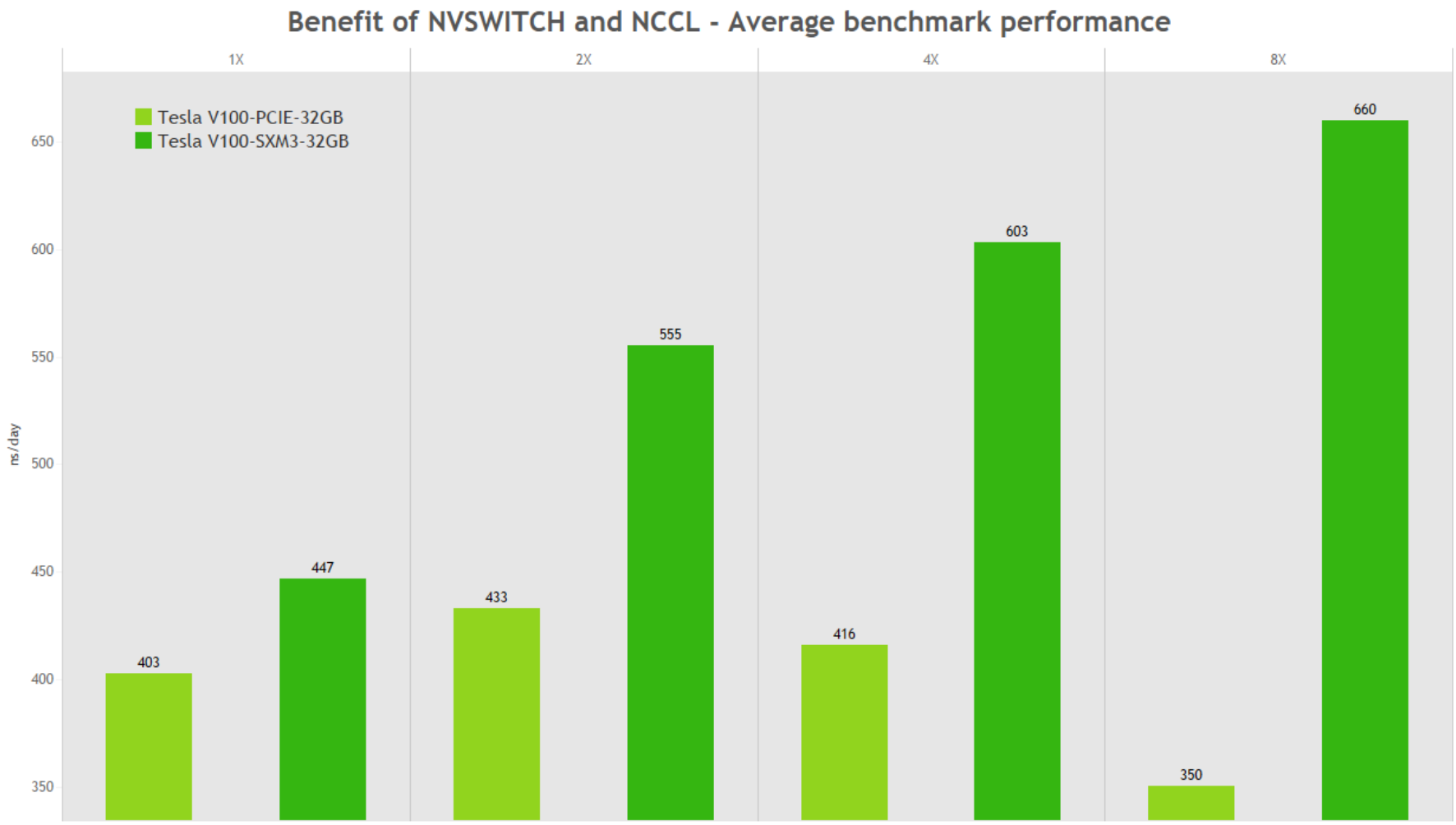
Performance Comparison - JAC 4fs



AmberMD 2020

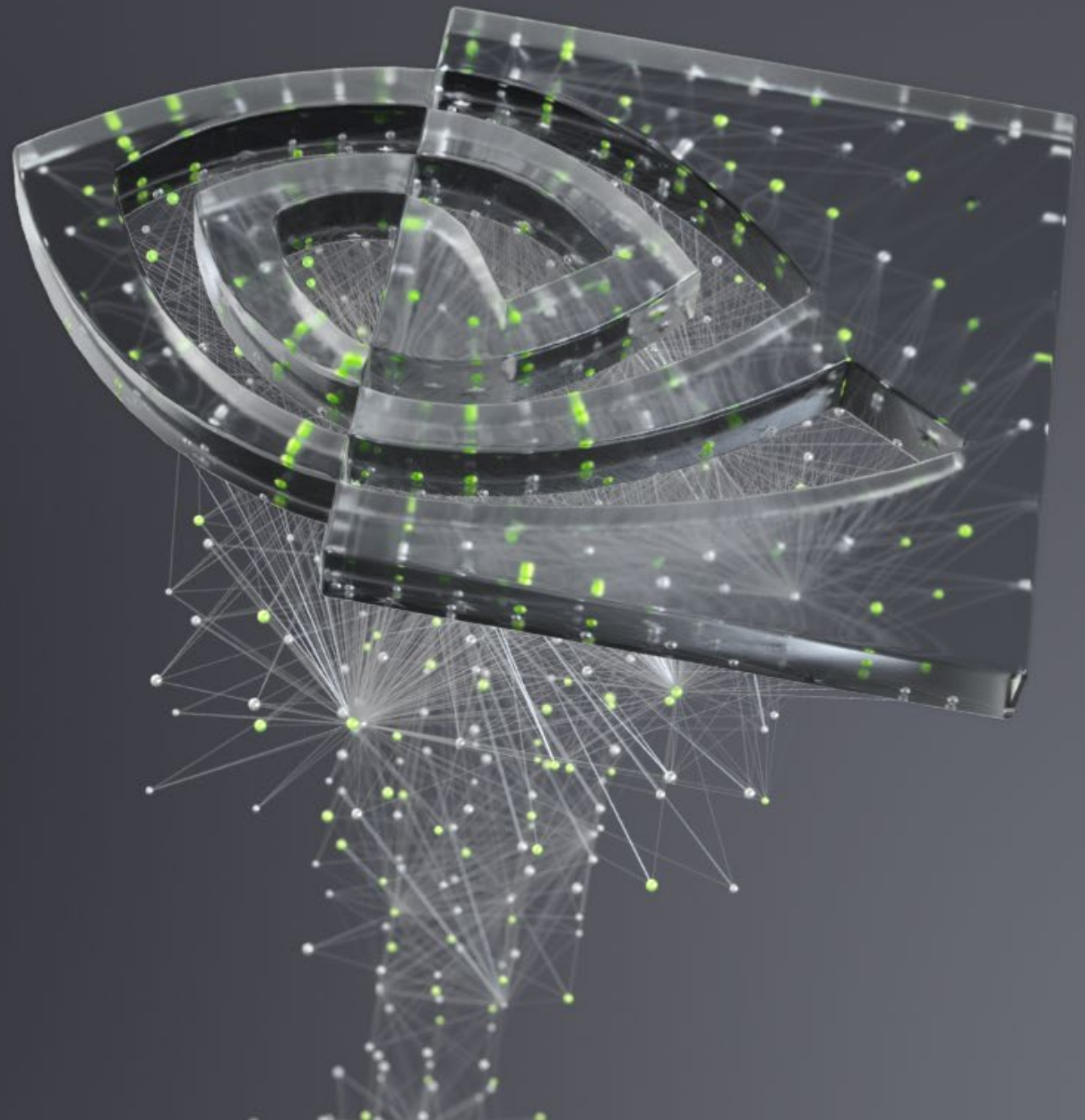


AmberMD


Benefit of NVSWITCH and NCCL - Average benchmark performance
1X
2X
4X
8X
Tesla V100-PCIE-32GB
Tesla V100-SXM3-32GB
ns/day
650
600
550
500
450
400
350
403
447
433
555
416
603
350
660

AmberMD recommended usage

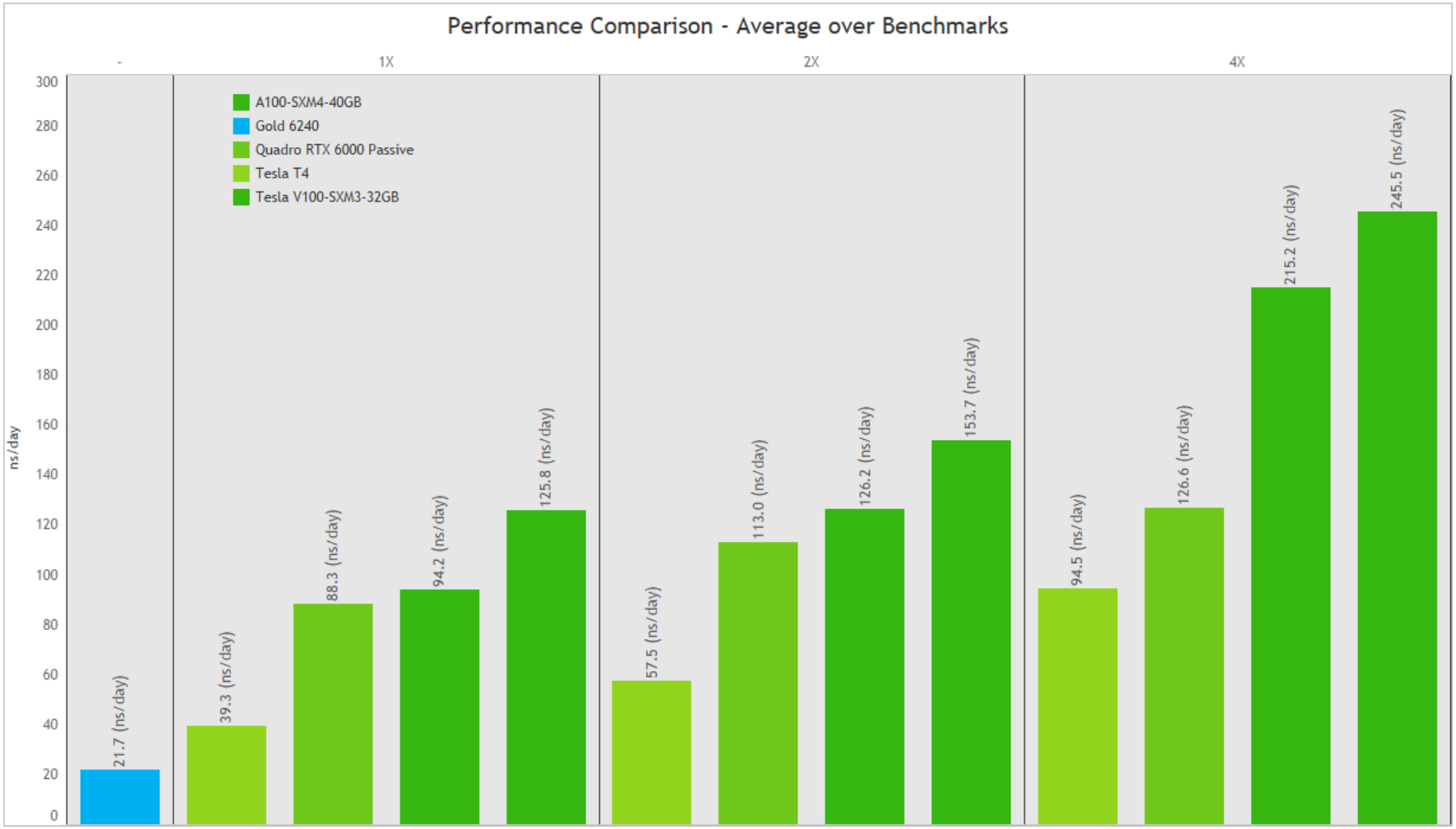
Motherboard and CPU	Dual-socket CPU with server
System memory	>=16GB
GPUs	V100 or A100 NVSWITCH
GPUs per socket	4 or 8
GPUs per task	1 – 4



GROMACS 2020

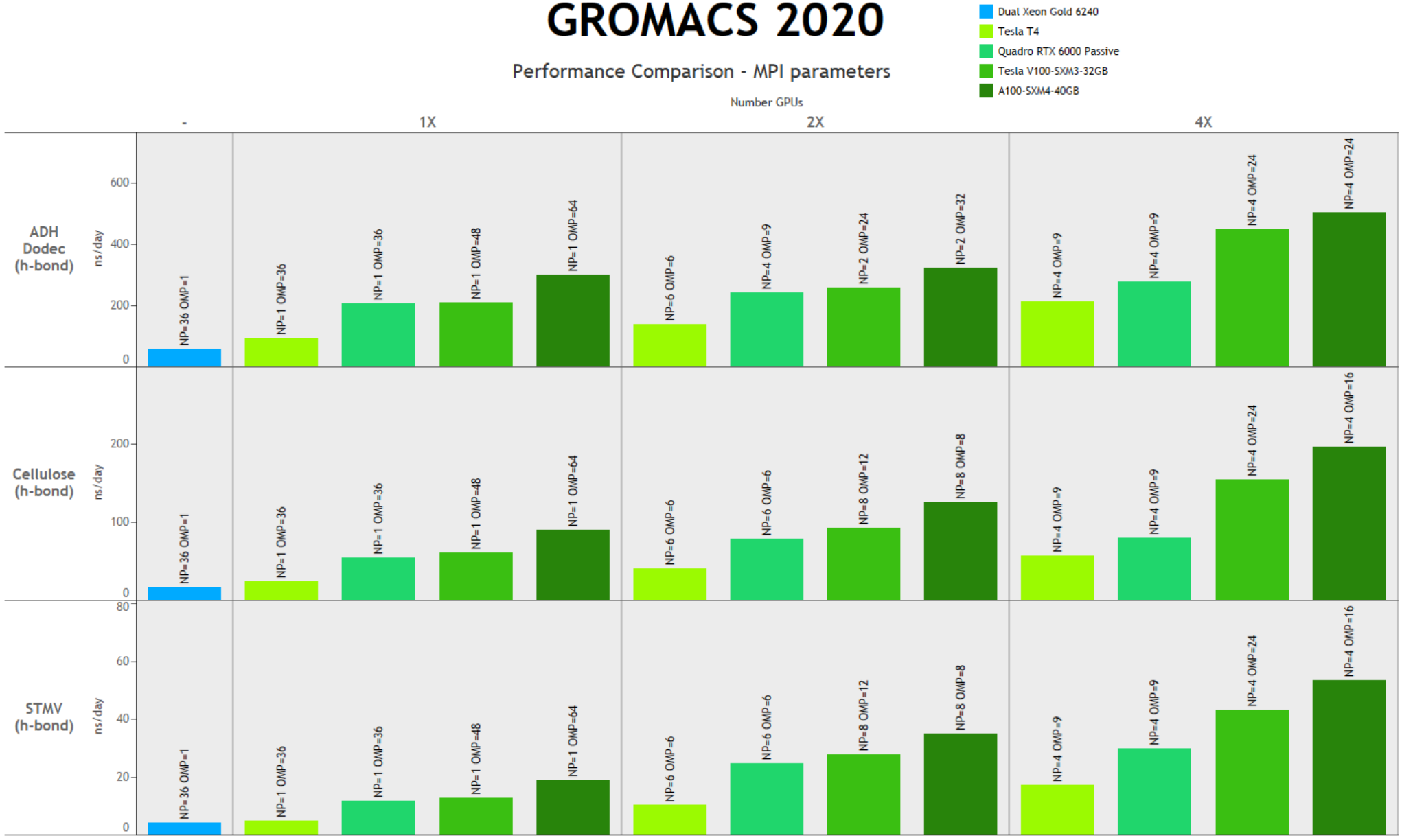
June 2020

GROMACS - 2020



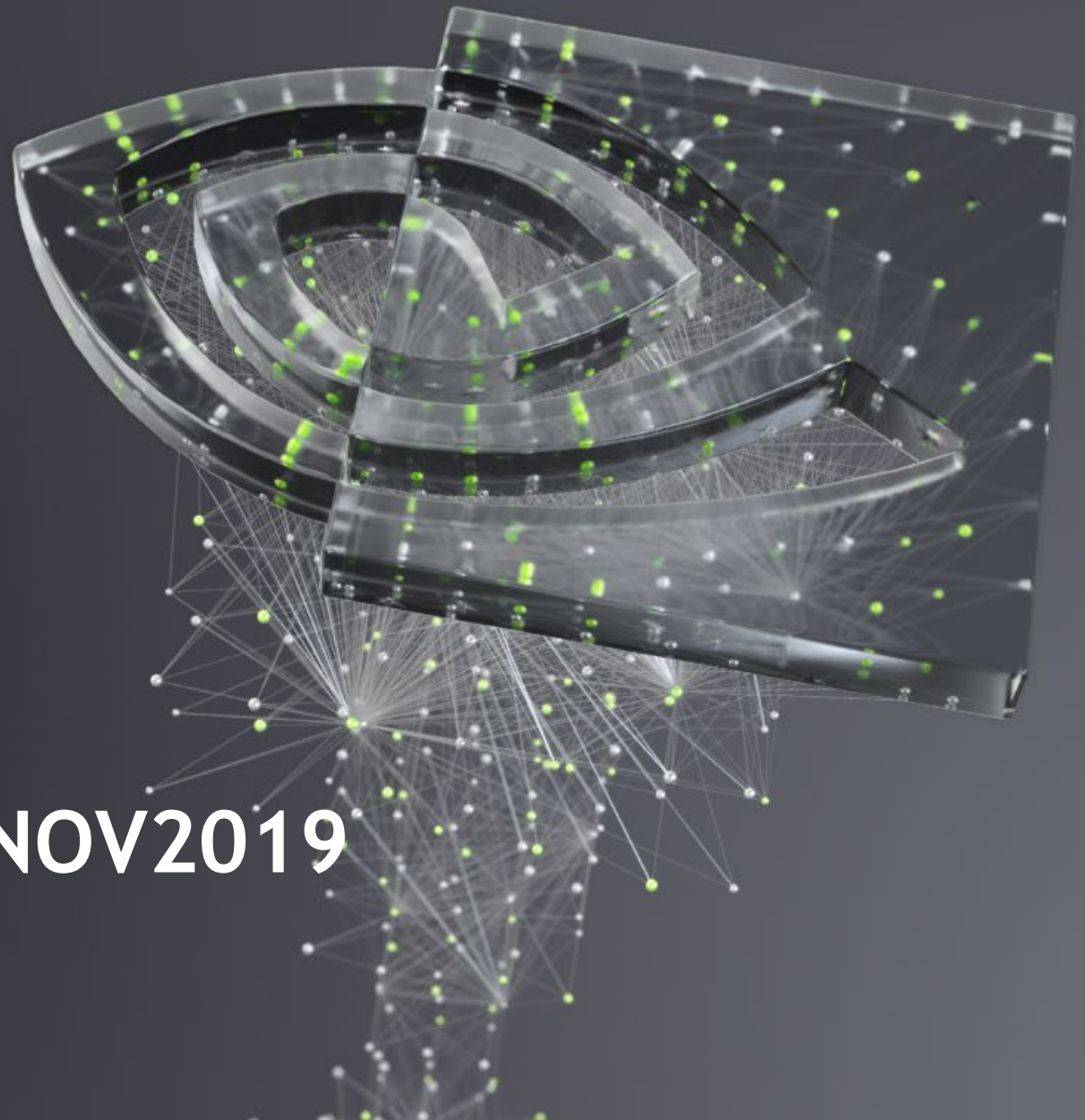
GROMACS 2020

Performance Comparison - MPI parameters



GROMACS recommended usage

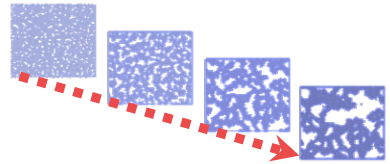
Motherboard and CPU	Dual-socket CPU server
System memory	>=16GB
GPUs	V100 / A100 with SXM2/3/4
GPUs per socket	1 to 4
GPUs per task	1 - 4



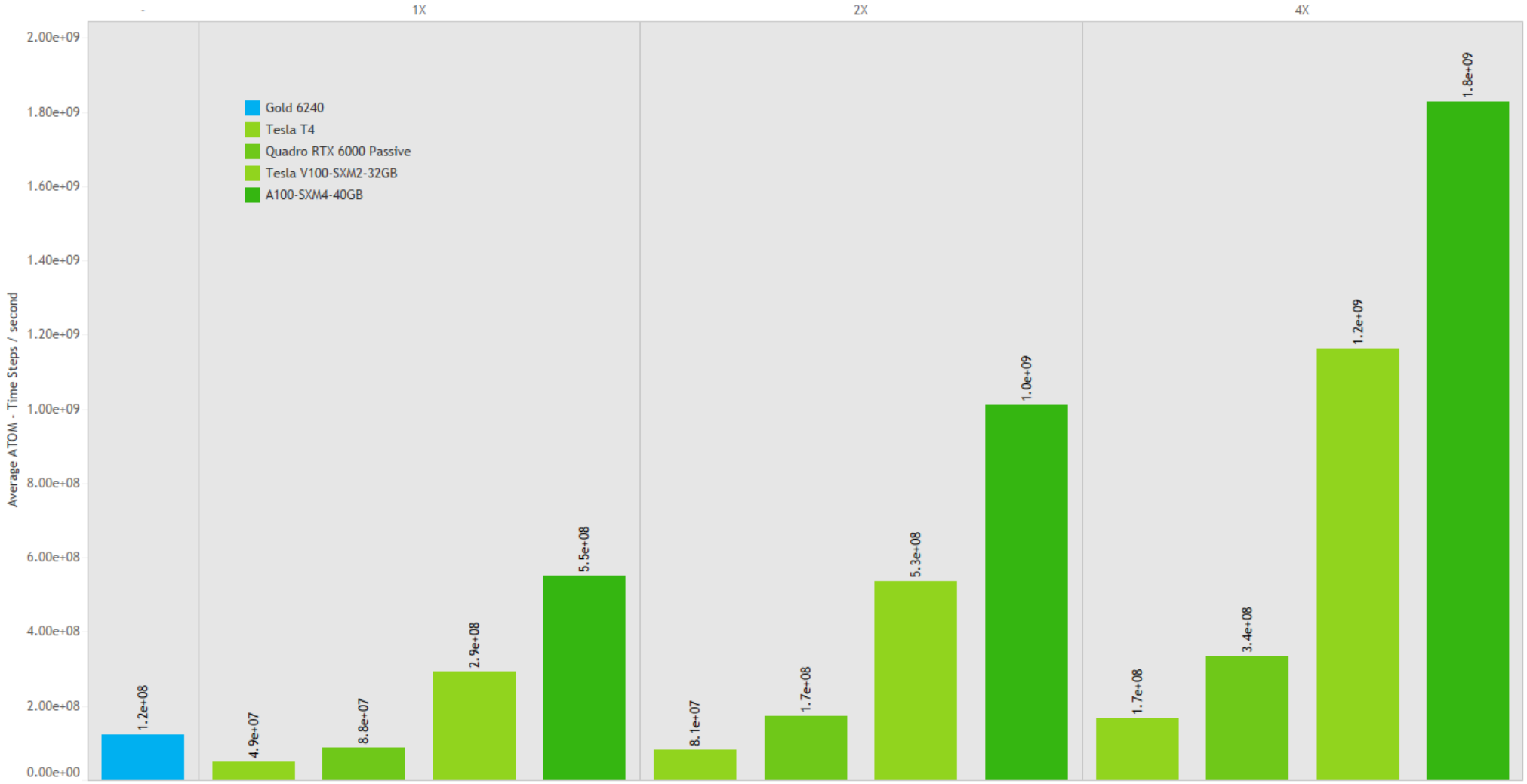
LAMMPS PATCH_20NOV2019

June 2020

LAMMPS - patch_20Nov2019

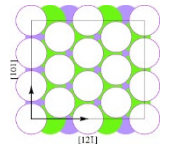


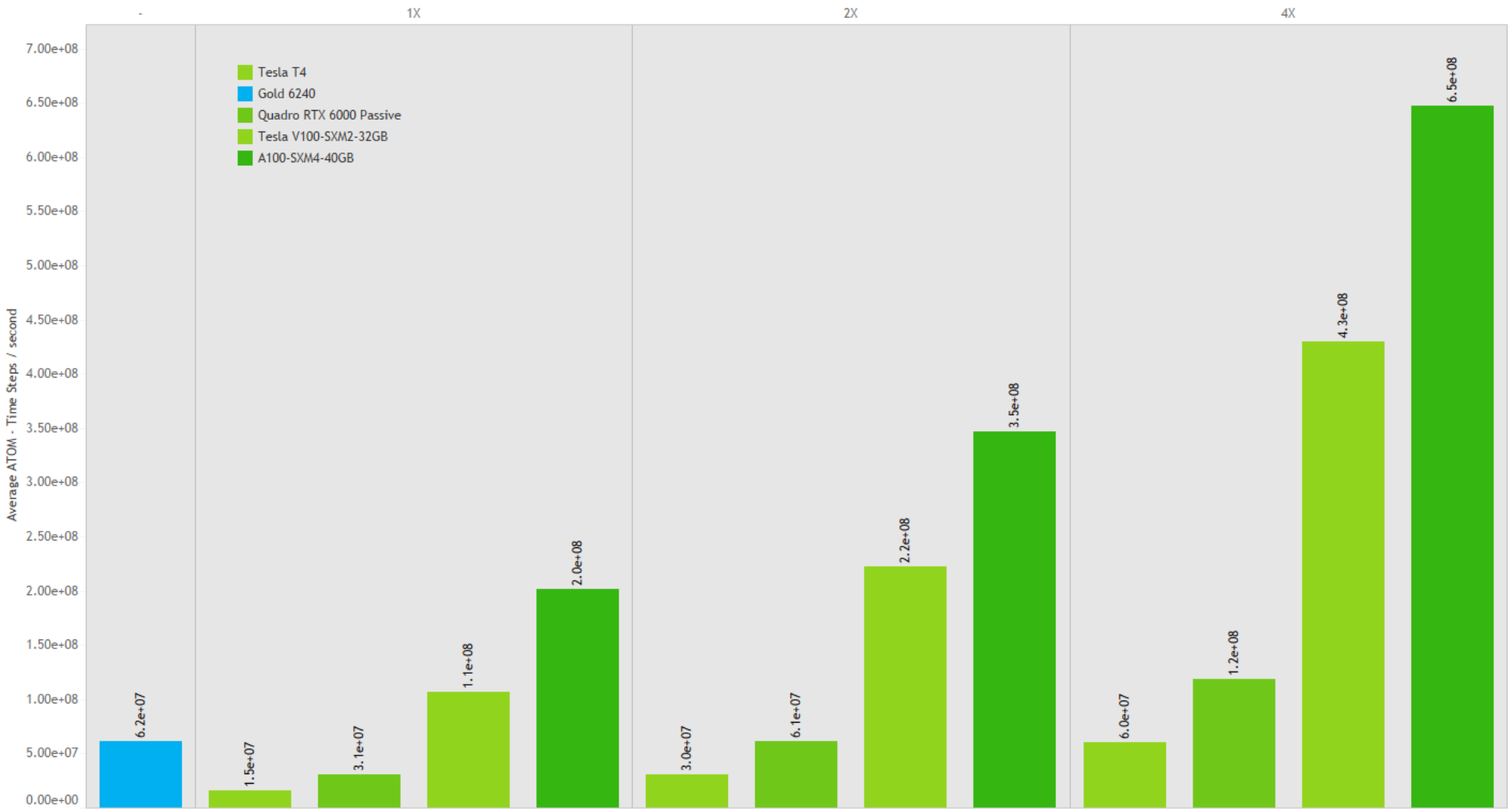
Performance Comparison - Atomic-Fluid Lennard-Jones 2.5 Cutoff



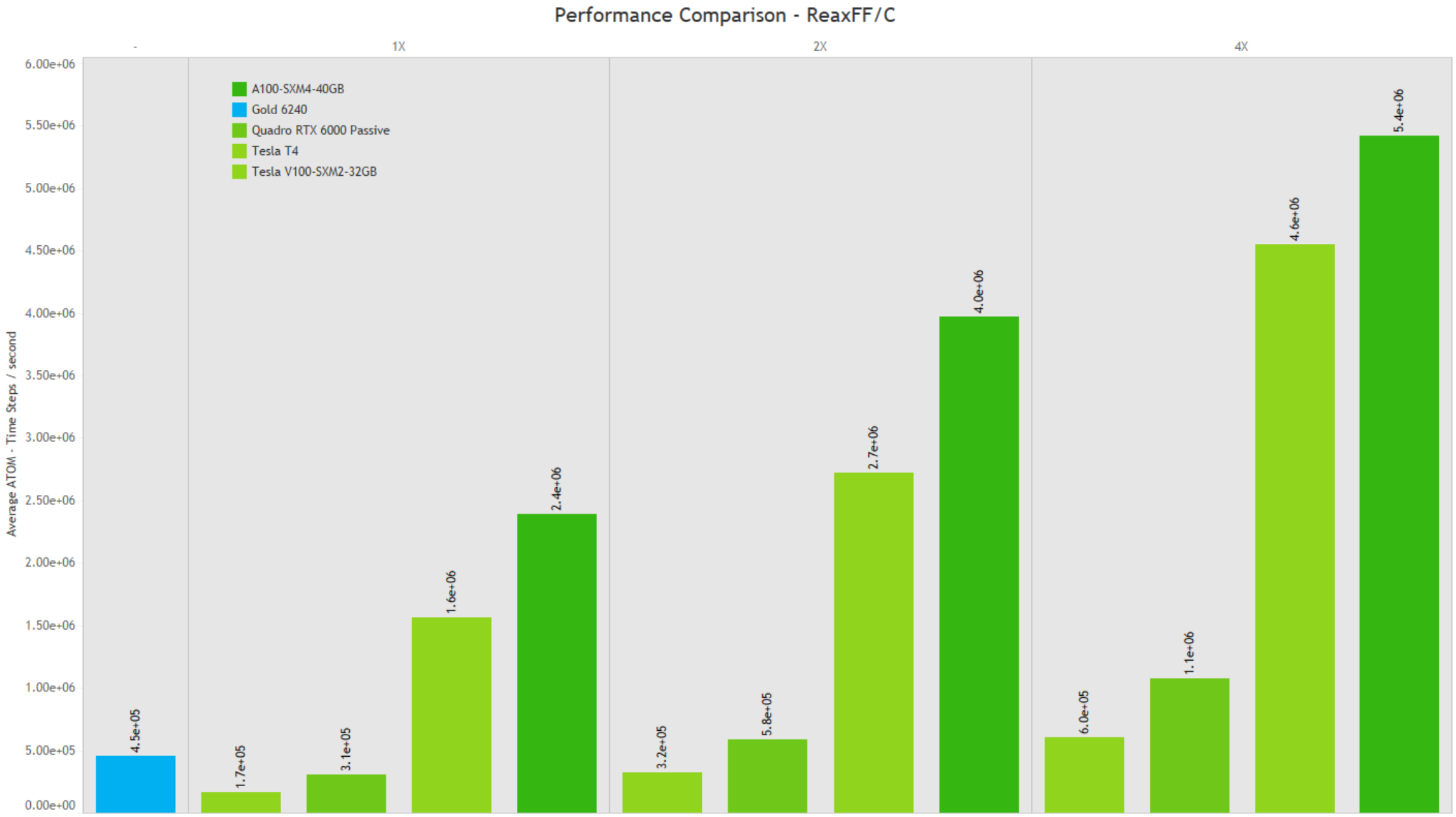
LAMMPS - patch_20Nov2019

Bulk Cu lattice

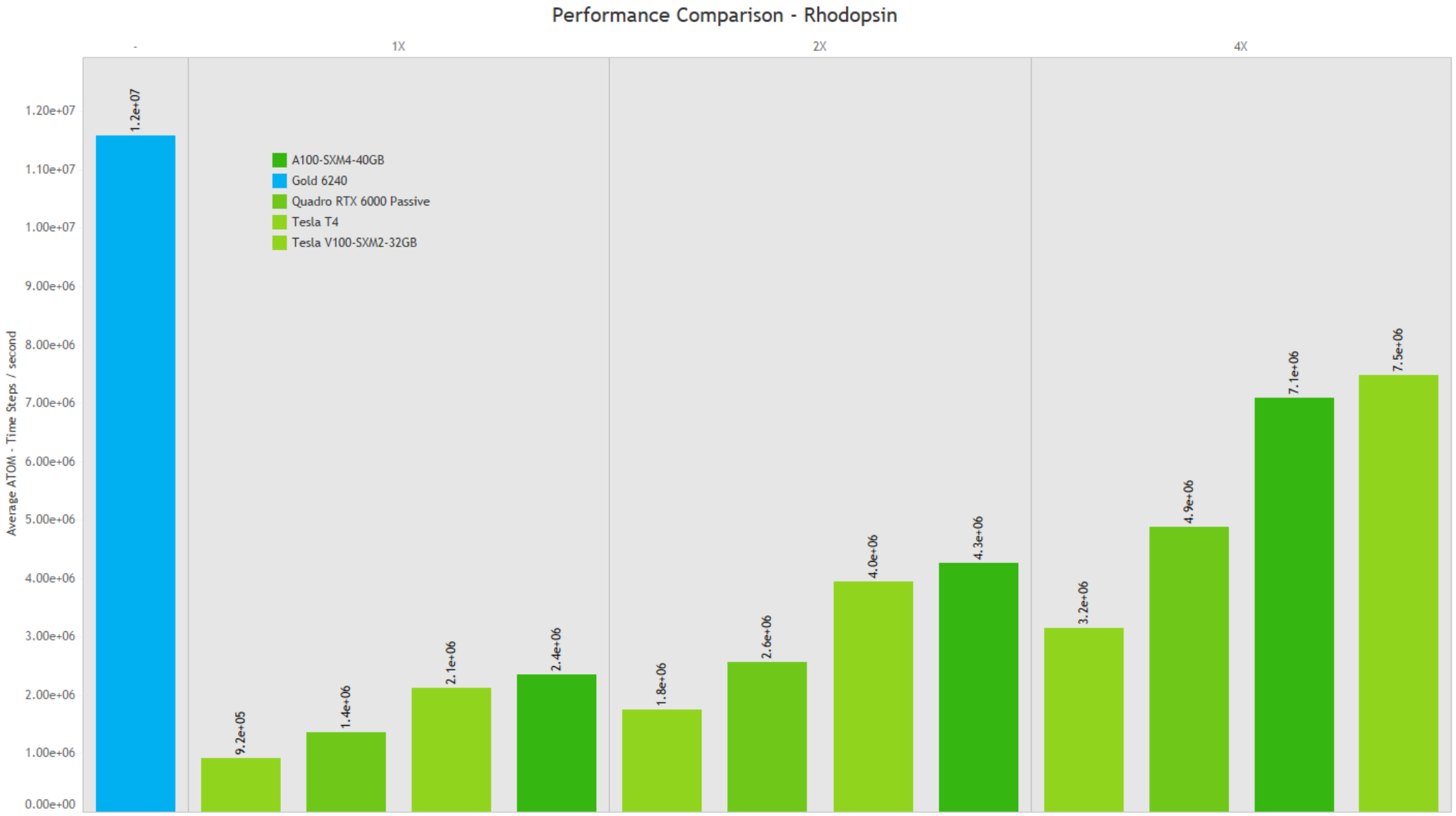




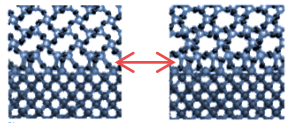
LAMMPS - patch_20Nov2019

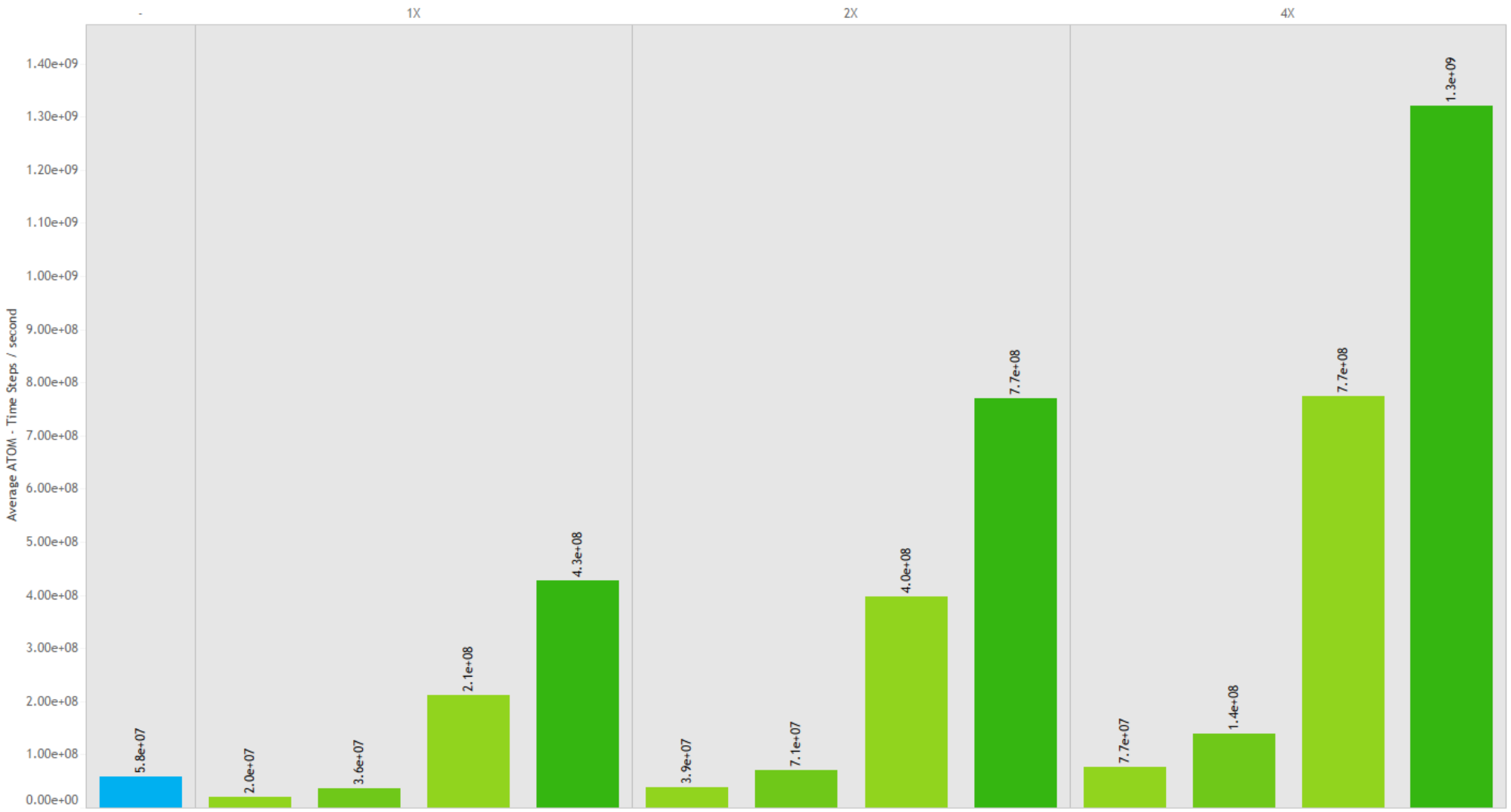


LAMMPS - patch_20Nov2019

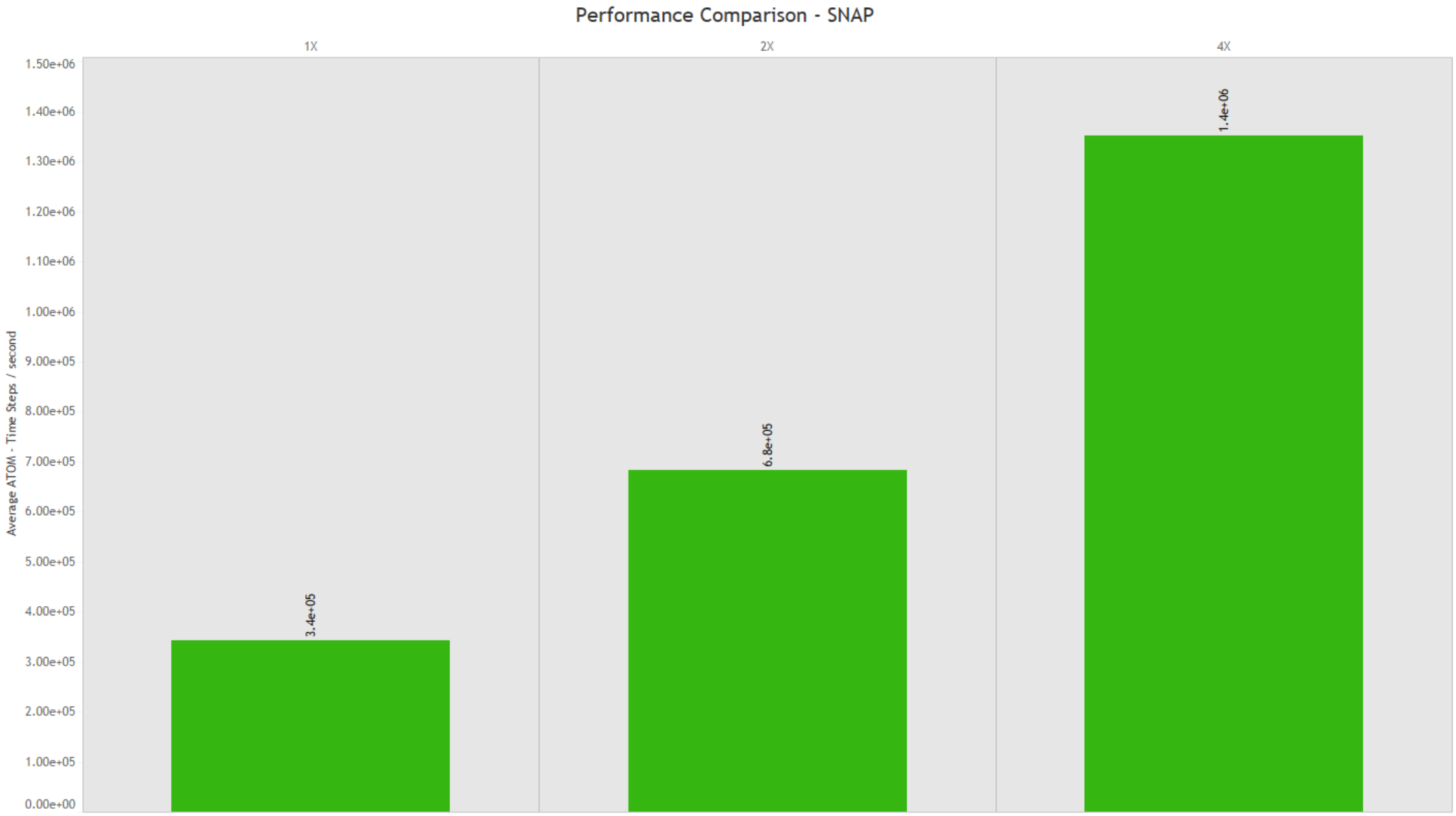


LAMMPS - patch_20Nov2019

Si crystallization 

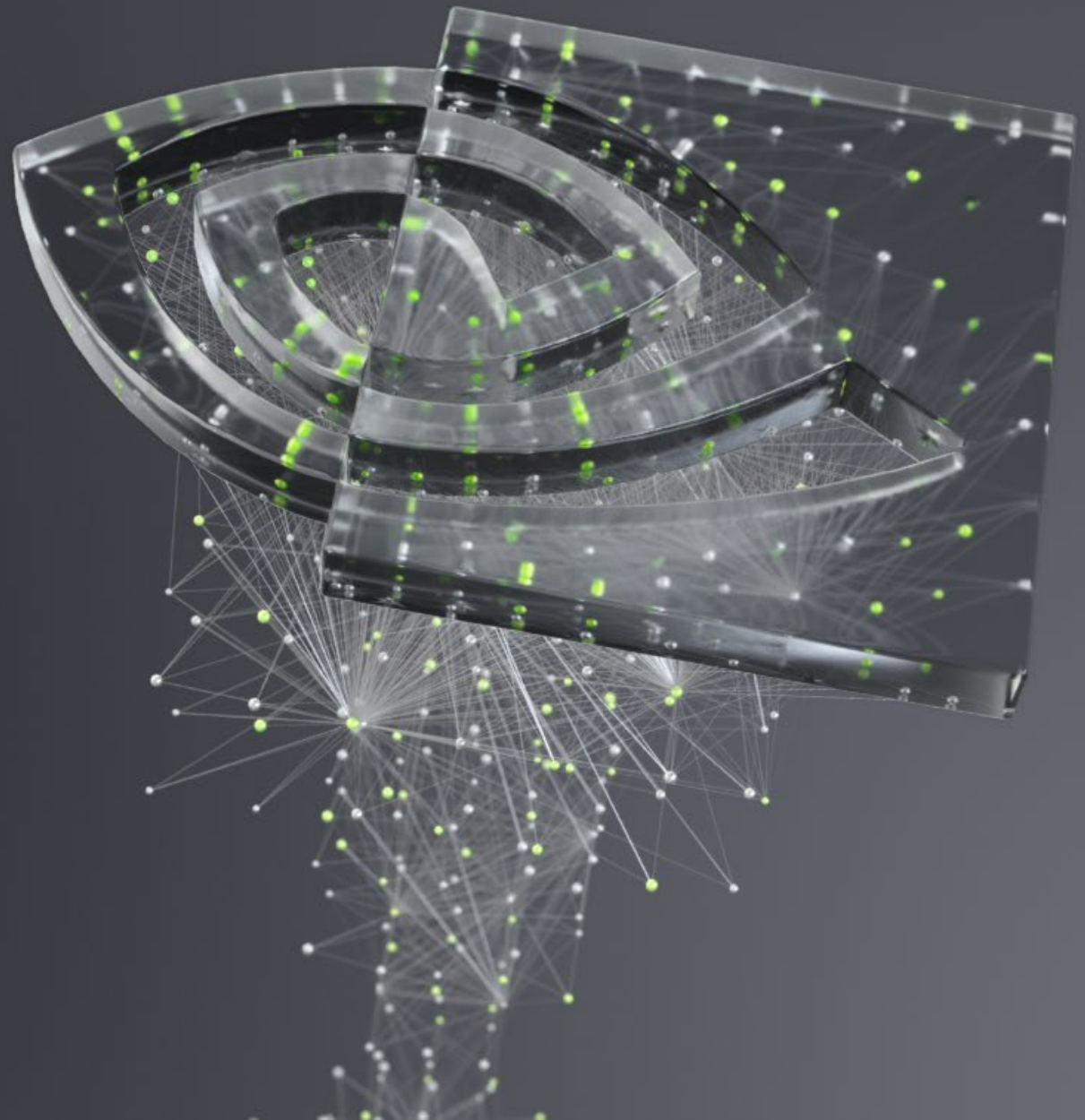


LAMMPS - patch_20Nov2019



LAMMPS recommended usage

Motherboard and CPU	Dual-socket CPU
System memory	>=32GB
GPUs	V100 / A100
GPUs per socket	1 to 4
GPUs per task	4



NAMD 3.0A

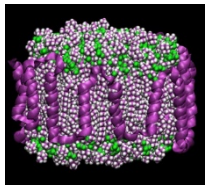
June 2020

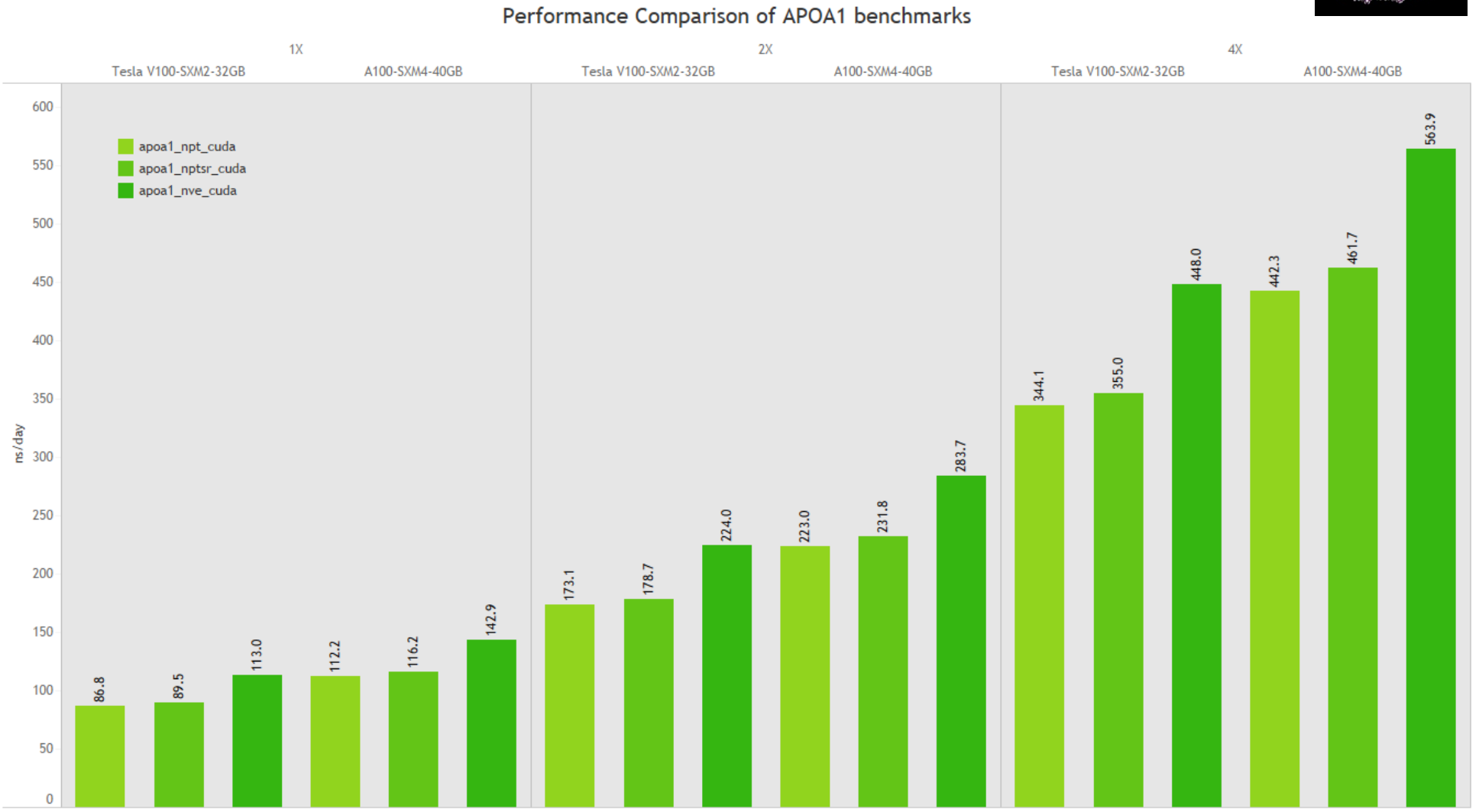
NAMD - 3.0a1


Performance Comparison - Average Performance
1X
2X
4X
AVG ns/day
280
260
240
220
200
180
160
140
120
100
80
60
40
20
0
Tesla V100-SXM2-32GB
A100-SXM4-40GB
52.3
67.9
104.1
135.0
207.5
268.4

NAMD - 3.0a1

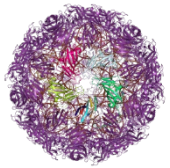
ApoA1
92,224 atoms



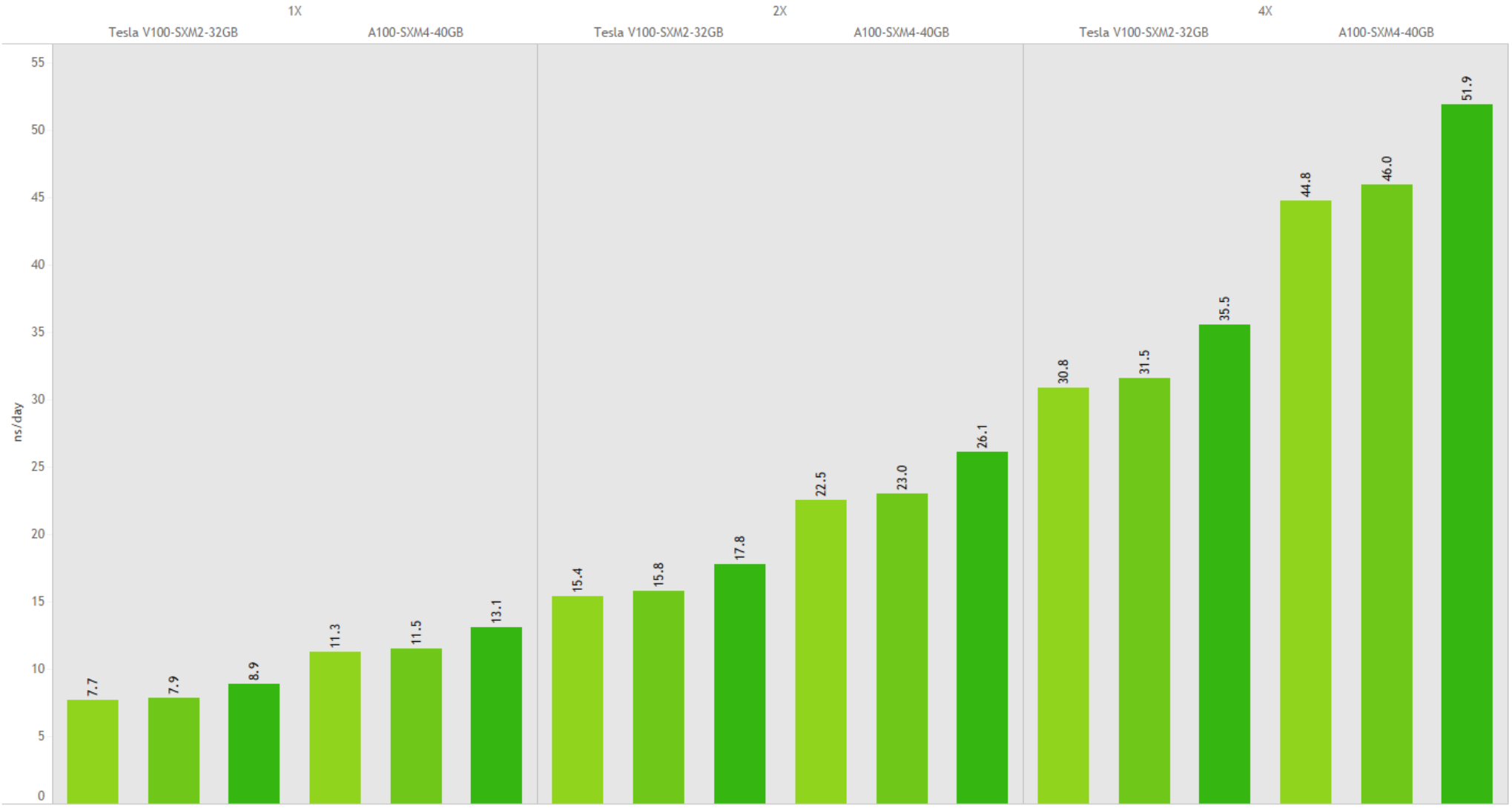


NAMD - 3.0a1

STMV
1,067,095 atoms



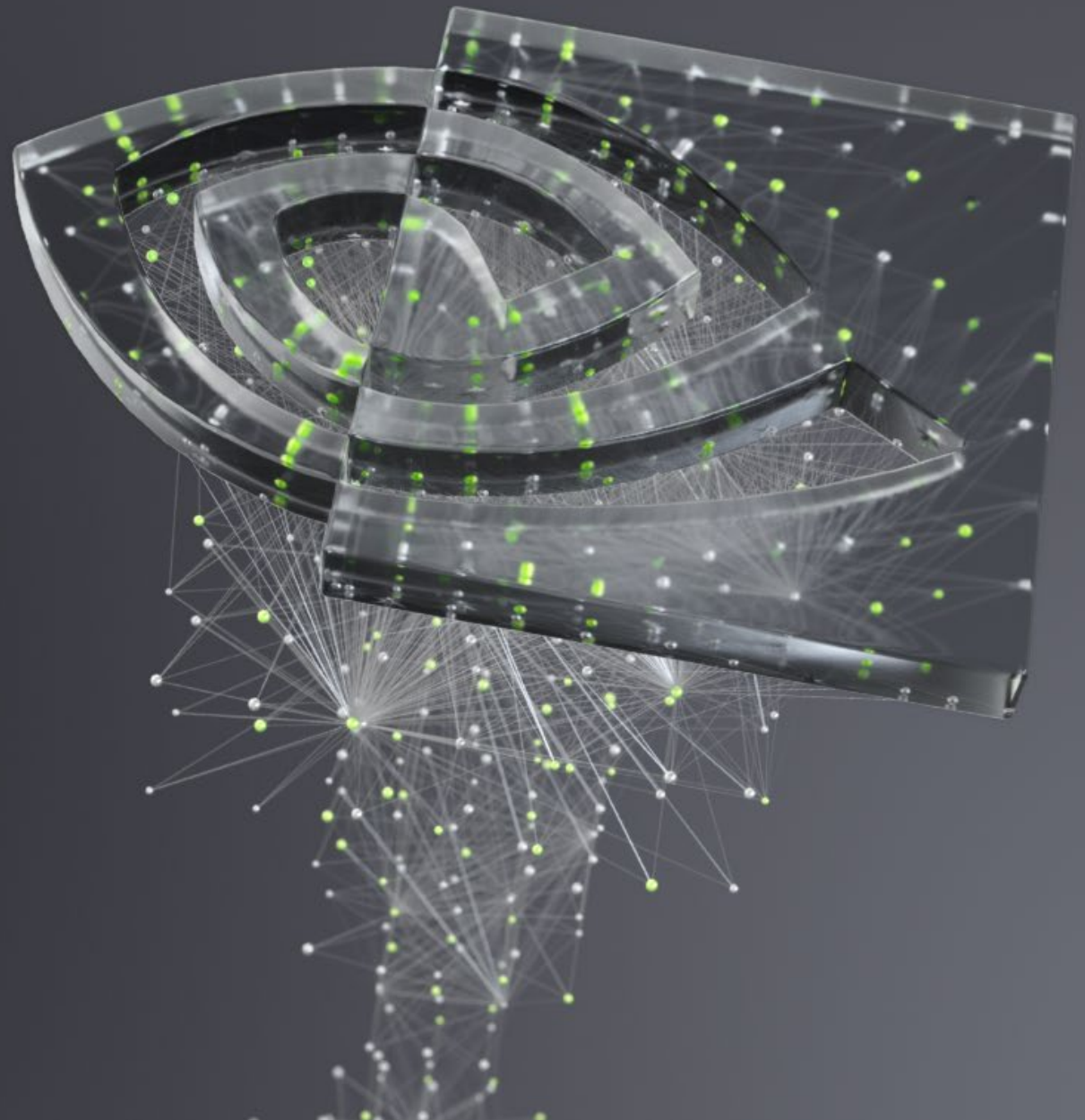
Performance Comparison of STMV benchmarks



NAMD recommended usage

v3.0a has strong single GPU performance

Motherboard and CPU	Dual-socket CPU server
System memory	>=16GB
GPUs	V100 / A100
GPUs per socket	1 to 4
GPUs per task	1



RELION 3.0.8

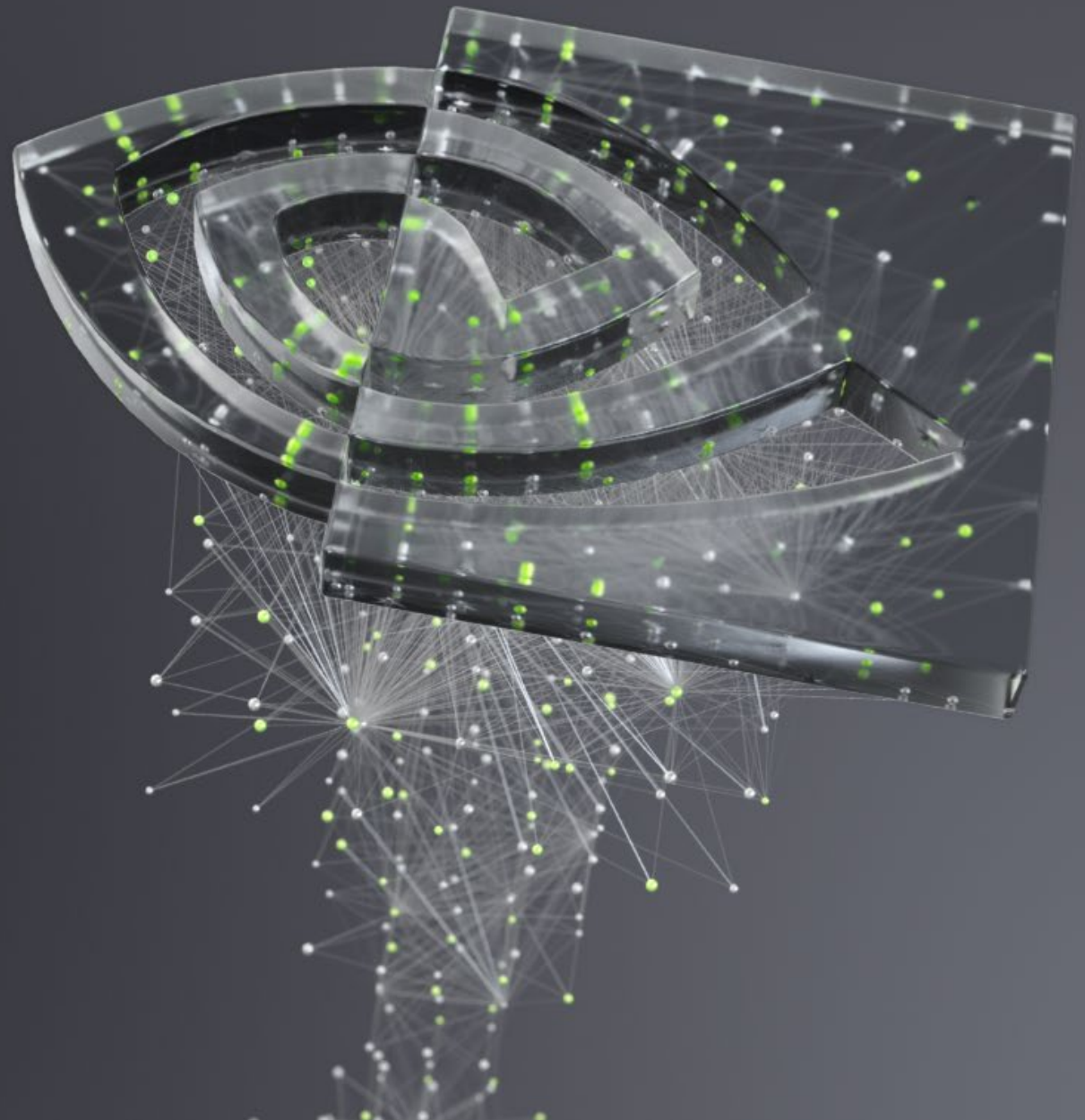
June 2020

RELION - 3.0.8


Performance Comparison - 3D Refinement
-
1X
2X
4X
Gold 6240
Tesla T4
Quadro RTX 6000 Passive
Tesla V100-SXM2-32GB
13156 sec
8190 sec
6115 sec
5748 sec
4706 sec
3846 sec
3463 sec
3549 sec
3016 sec
2748 sec
Gold 6240
Tesla T4
Quadro RTX 6000 Passive
Tesla V100-SXM2-32GB
Tesla T4
Quadro RTX 6000 Passive
Tesla V100-SXM2-32GB
Tesla T4
Quadro RTX 6000 Passive
Tesla V100-SXM2-32GB

RELION RECOMMENDED USAGE

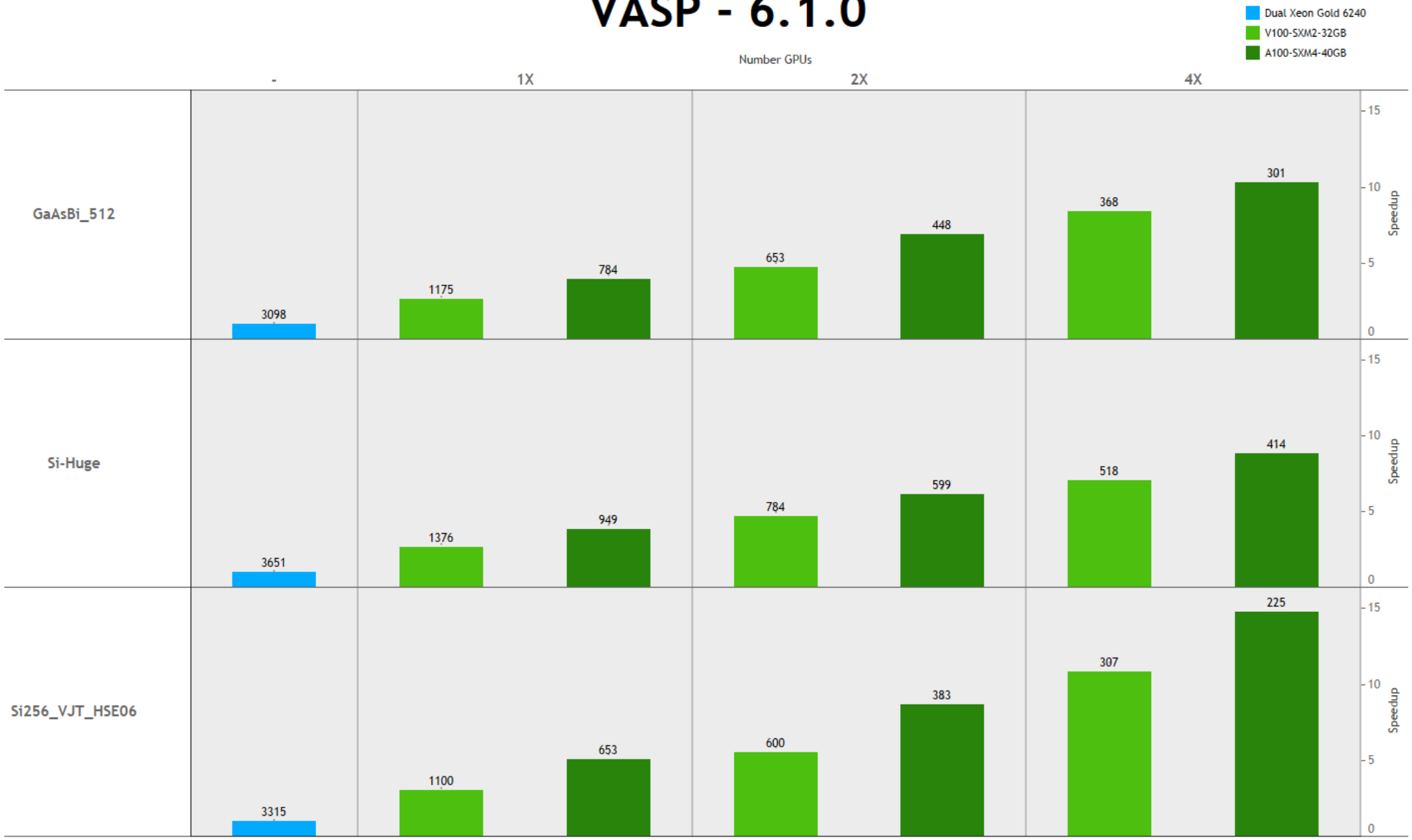
Motherboard and CPU	Dual-socket CPU
System memory	>=32GB
GPUs	RTX 6000 / RTX 8000 / V100 / A100
GPUs per socket	1 to 4
GPUs per task	1 to 4



VASP 6.1.0

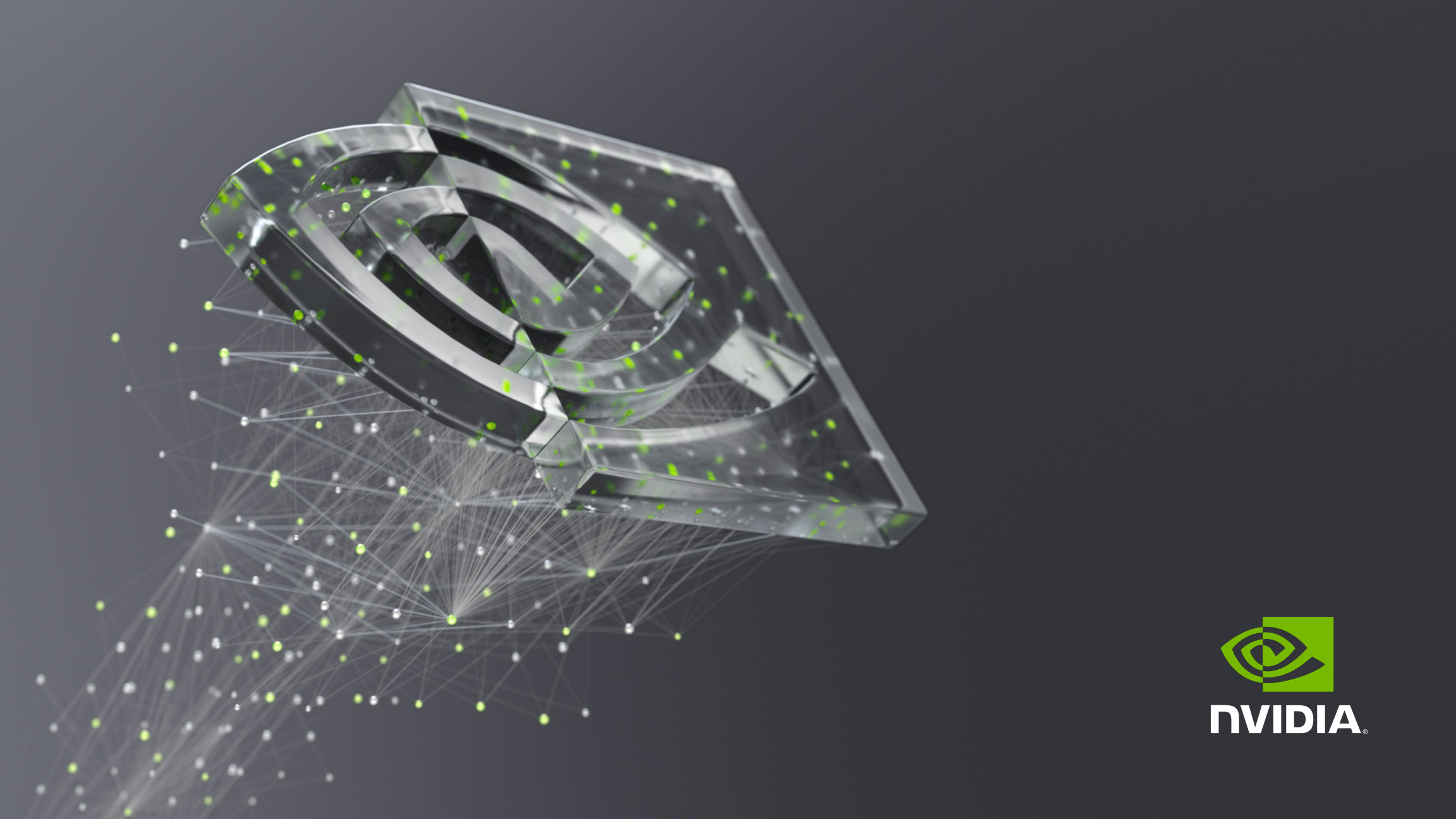
June 2020

VASP - 6.1.0


Dual Xeon Gold 6240
V100-SXM2-32GB
A100-SXM4-40GB
Number GPUs
-
1X
2X
4X
GaAsBi_512
3098
1175
784
653
448
368
301
Si-Huge
3651
1376
949
784
599
518
414
Si256_VJT_HSE06
3315
1100
653
600
383
307
225
Speedup
0
5
10
15

VASP RECOMMENDED USAGE

Motherboard and CPU	Dual-socket CPU
System memory	>=32GB
GPUs	V100 / A100
GPUs per socket	1 to 4
GPUs per task	1 to 4


NVIDIA