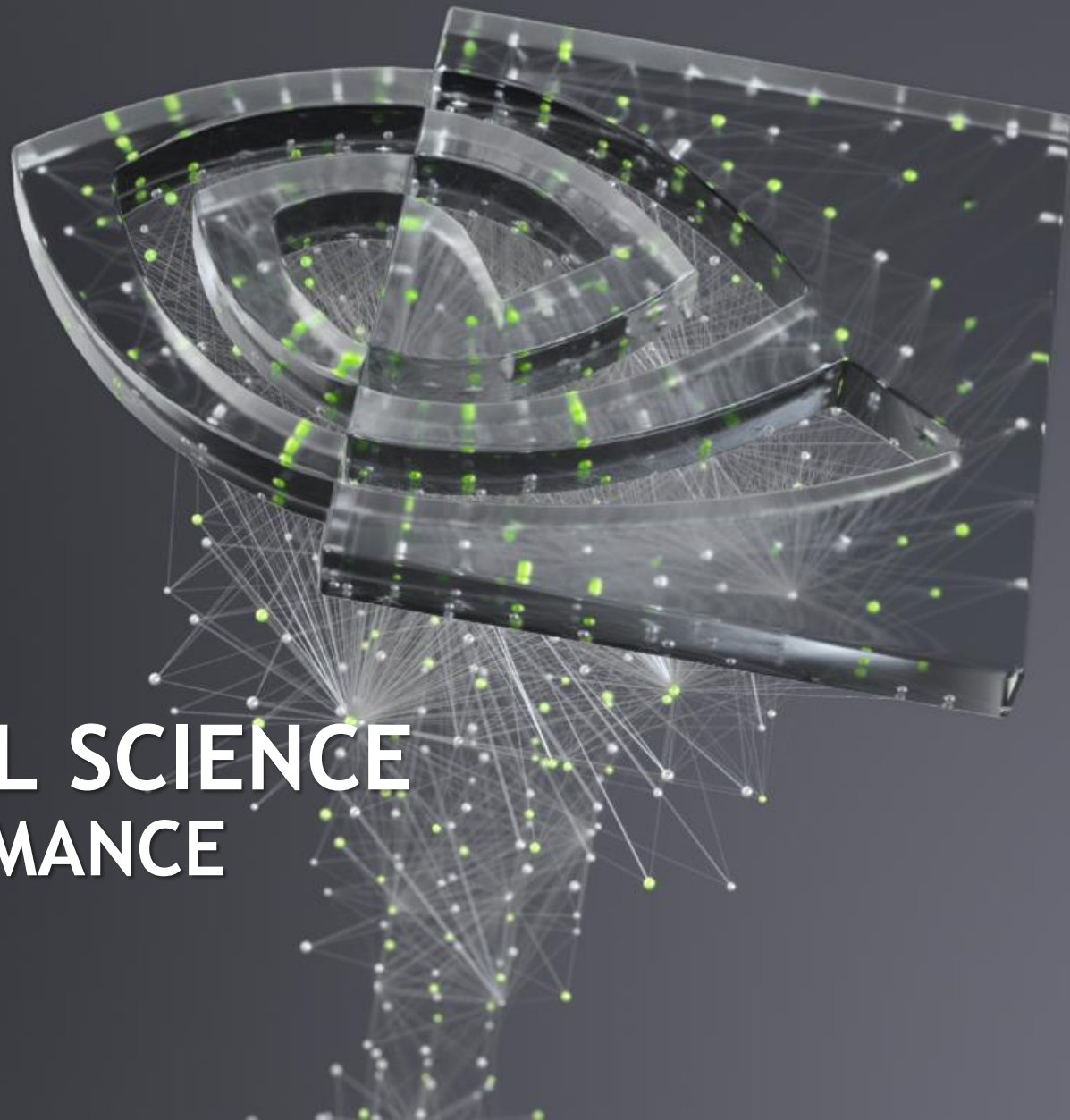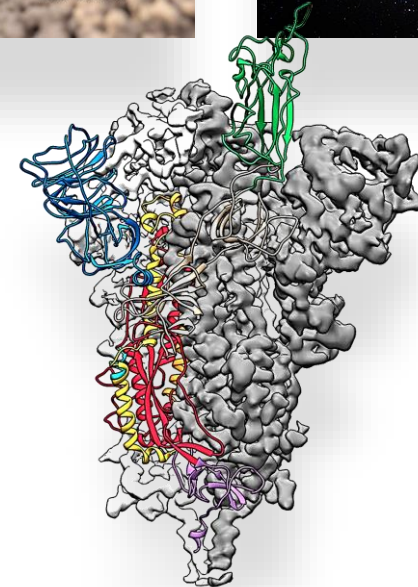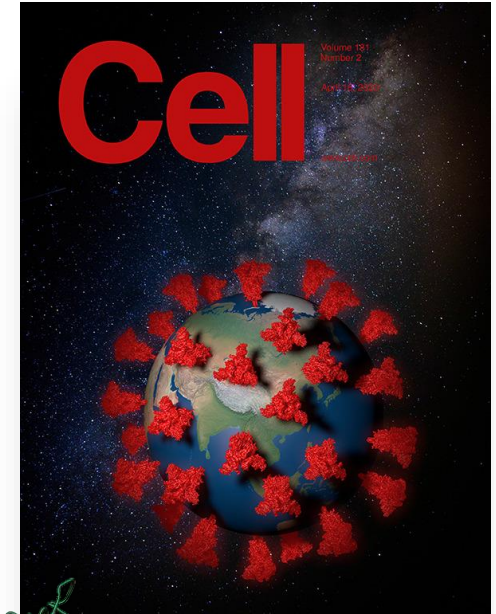# LIFE AND MATERIAL SCIENCE
APPLICATION PERFORMANCE

May 2020

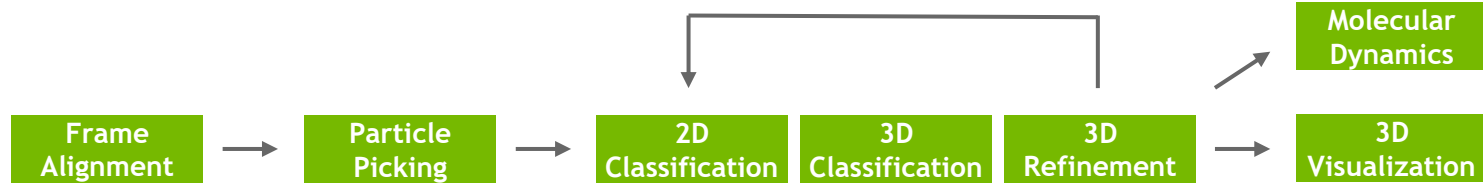# Critical COVID-19 Research Accelerated on NVIDIA GPUs

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

Frame Alignment → Particle Picking → 2D Classification — 3D Classification — 3D Refinement → 3D Visualization

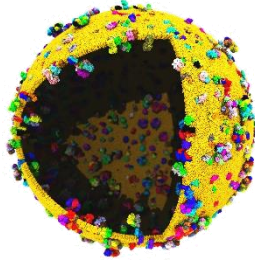Molecular Dynamics

GPU-accelerated apps

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

Cryo-EM Performance White Paper

NVIDIA

NVIDIA GPU Accelerated Cryo-EM Workflow

White Paper

3
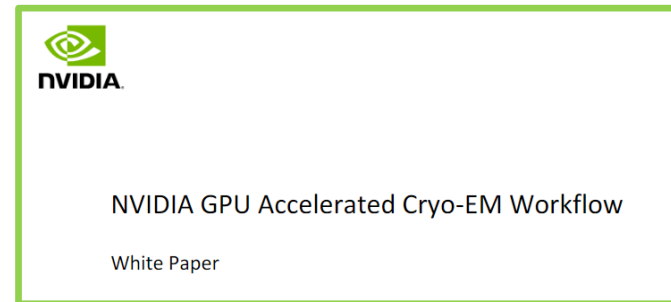
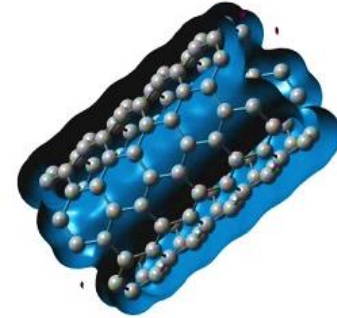# Overview of Life & Material Accelerated Apps

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
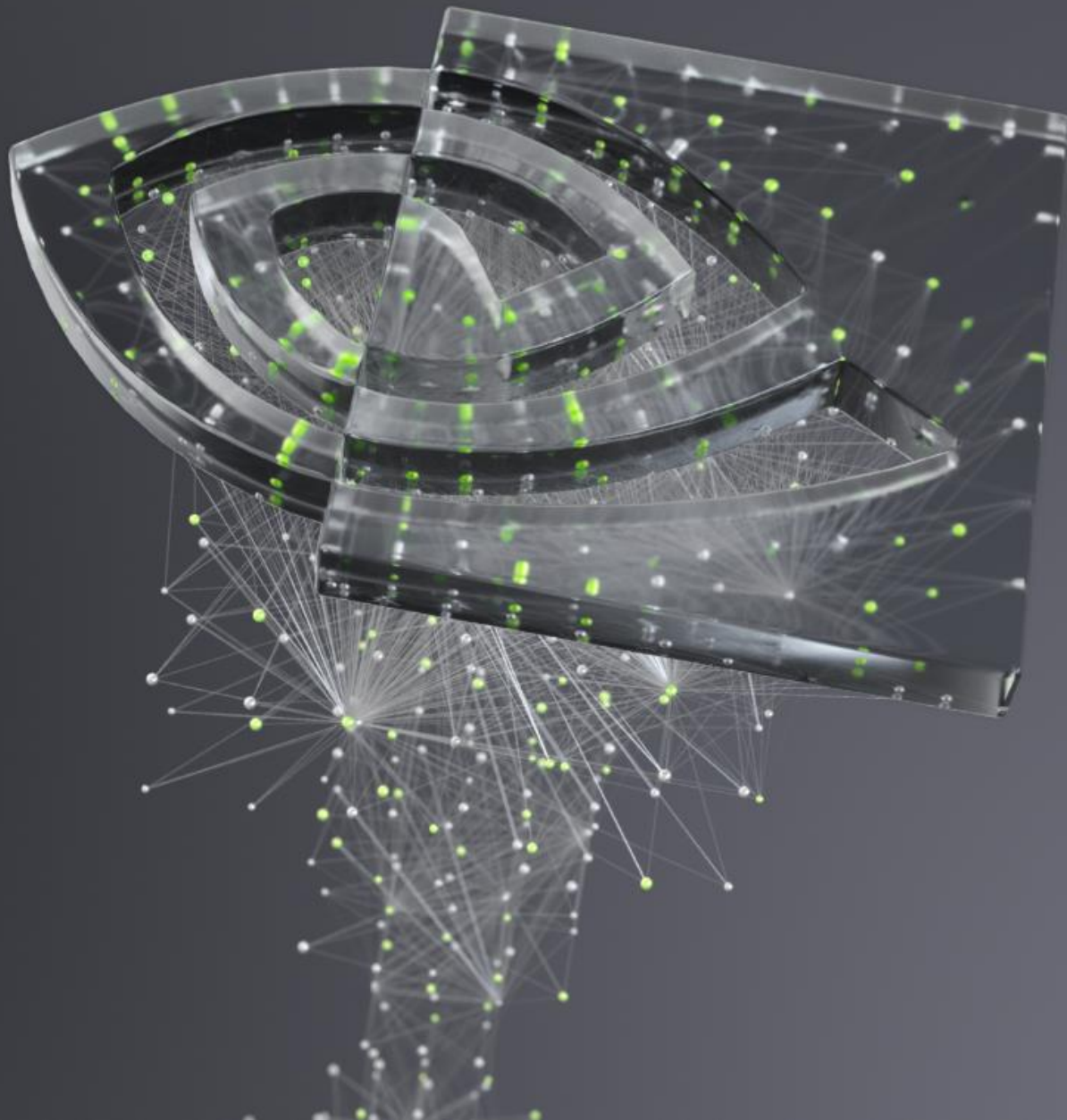
Active acceleration projects

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

NVIDIA.

AMBERMD 2020

May 2020

AmberMD 2020
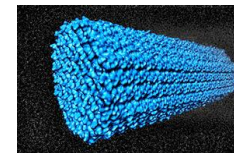
Performance Comparison - Cellulose 4fs

Cellulose
408,609 atoms

	1X	2X
-	Tesla T4 · Quadro RTX 6000 · Tesla V100-PCIE-32GB · A100-SXM4-40GB	Tesla T4 · Quadro RTX 6000 · Tesla V100-PCIE-32GB · A100-SXM4-40GB
Gold 6240		

Legend:
- Gold 6240
- Tesla T4
- Quadro RTX 6000
- Tesla V100-PCIE-32GB
- A100-SXM4-40GB

ns/day

Values:
- Gold 6240: NPT 4.7, NVE 4.7
- 1X Tesla T4: NPT 31.5, NVE 33.5
- 1X Quadro RTX 6000: NPT 72.5, NVE 80.0
- 1X Tesla V100-PCIE-32GB: NPT 89.0, NVE 98.8
- 1X A100-SXM4-40GB: NPT 129.5, NVE 151.9
- 2X Tesla T4: NPT 46.9, NVE 50.6
- 2X Quadro RTX 6000: NPT 66.0, NVE 72.6
- 2X Tesla V100-PCIE-32GB: NPT 97.2, NVE 110.7
- 2X A100-SXM4-40GB: NPT 174.7, NVE 219.9

AmberMD 2020

Performance Comparison - FactorIX 4fs

Factor IX
90,906 atoms
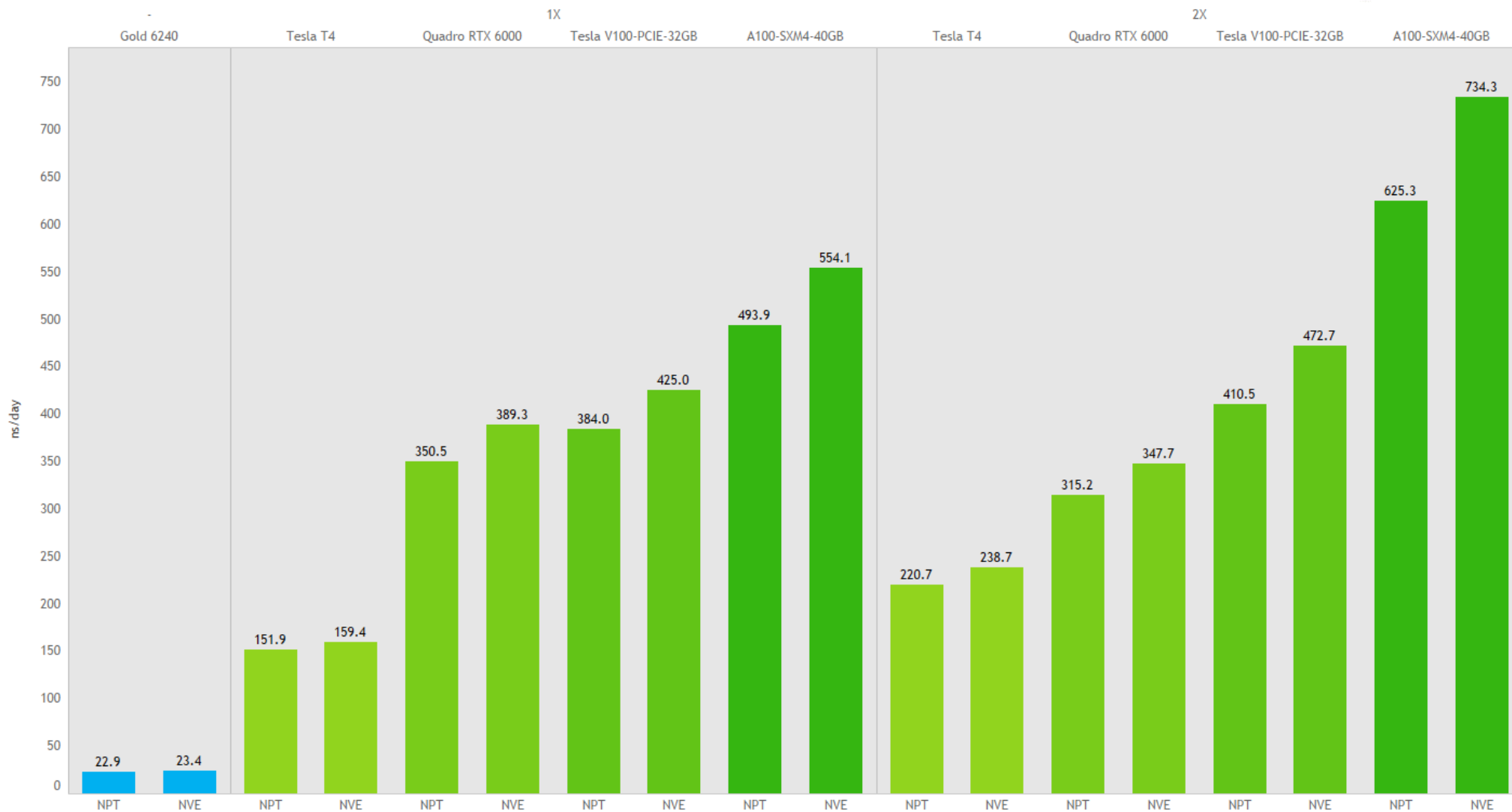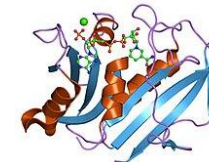
AmberMD 2020

Performance Comparison - JAC 4fs

DHFR 23,558 atoms
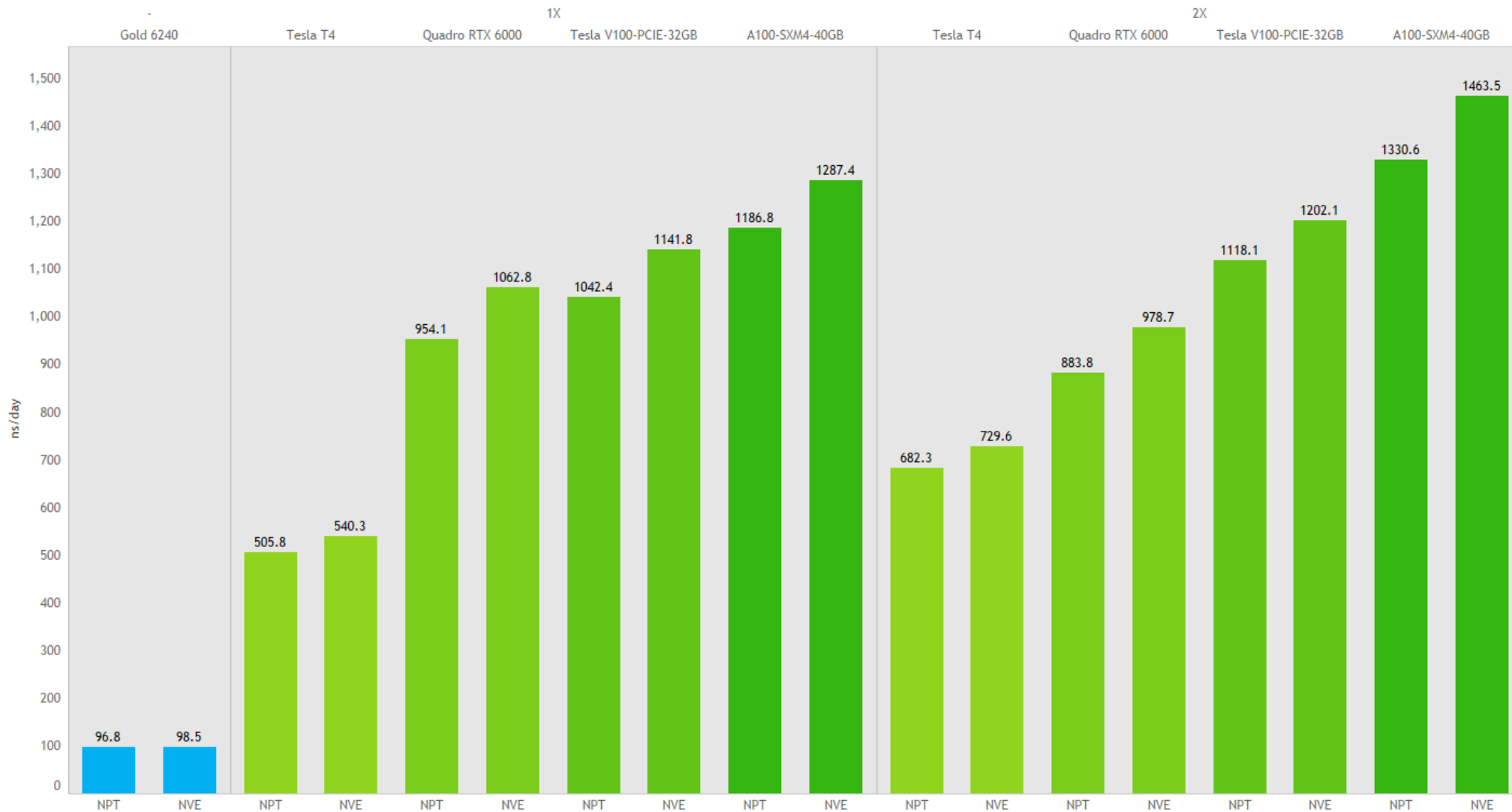
AmberMD 2020

Performance Comparison - STMV 4fs
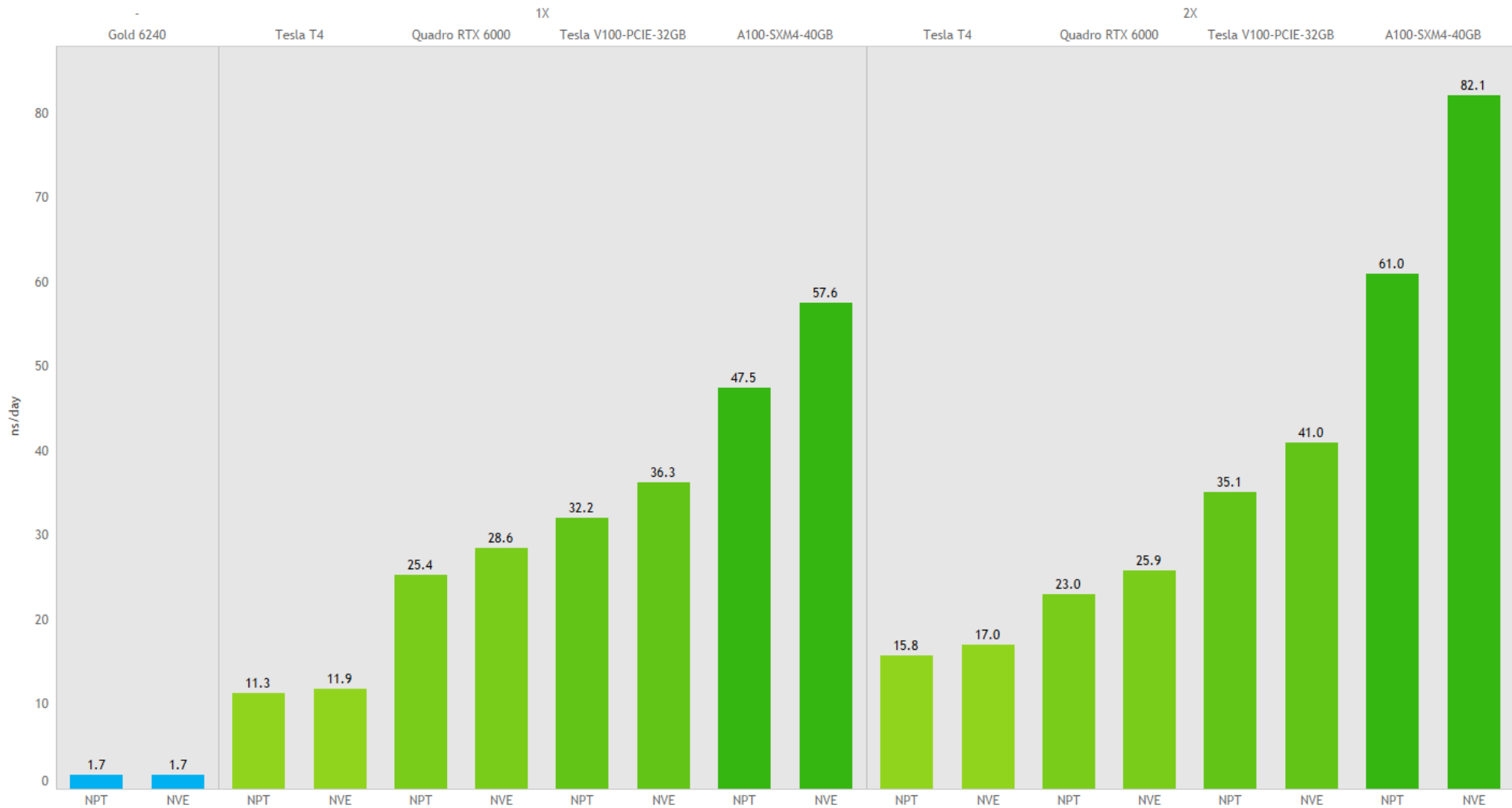
AmberMD

Benefit of NVSWITCH and NCCL - Average benchmark performance
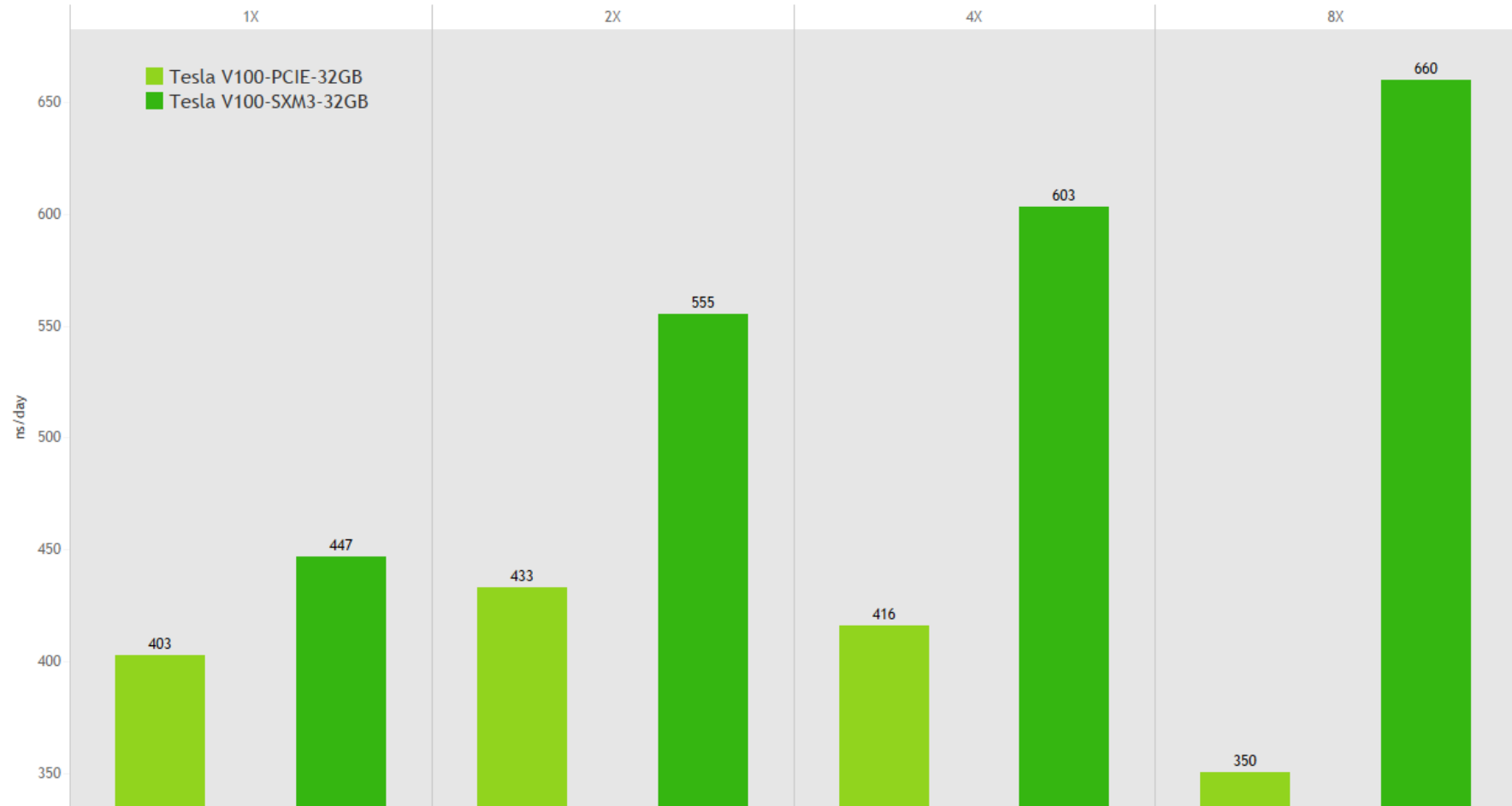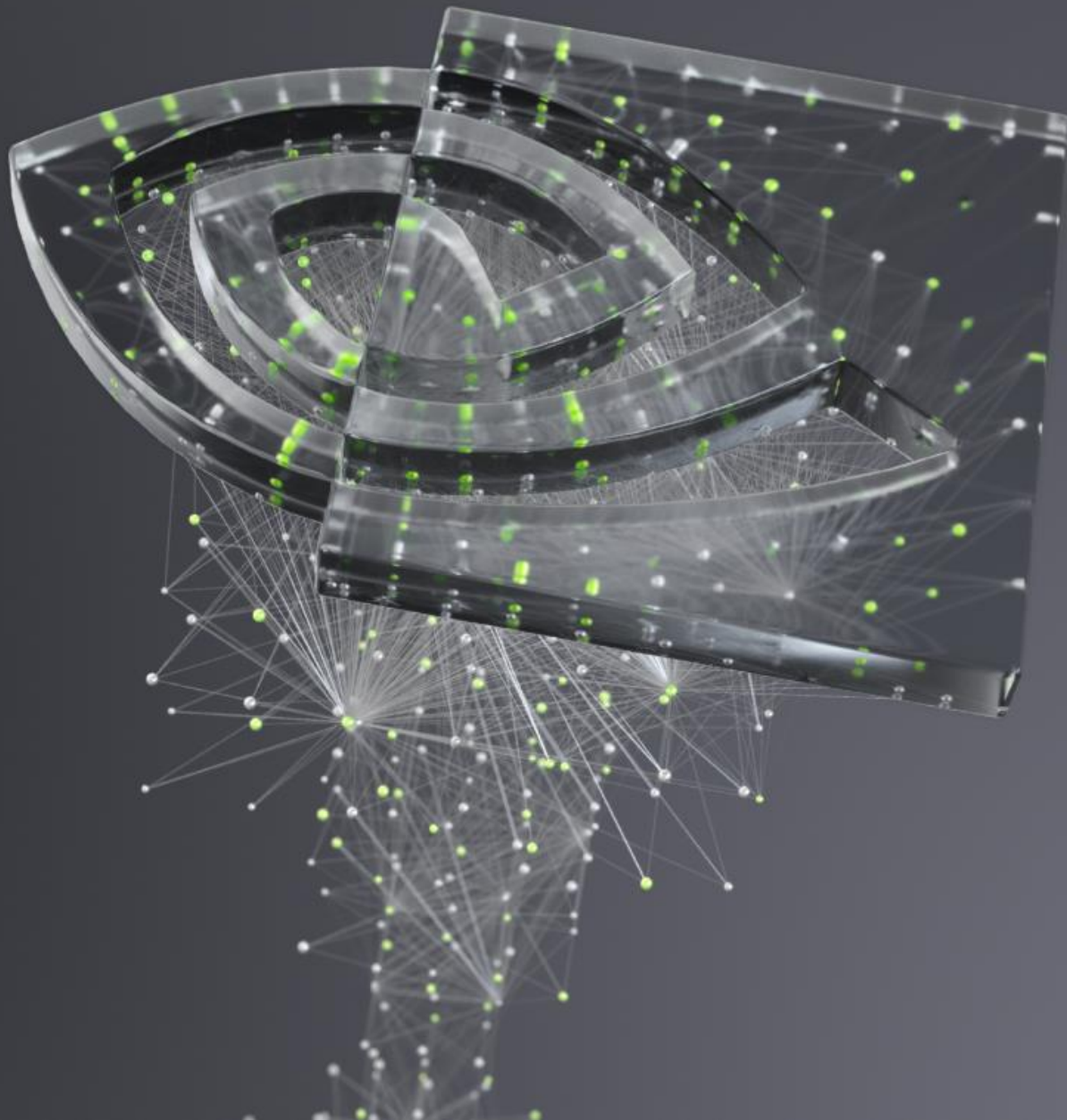
AmberMD recommended usage

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

May 2020

GROMACS - 2020

Performance Comparison - Average over Benchmarks

Legend:
- A100-SXM4-40GB
- Gold 6240
- Quadro RTX 6000 Passive
- Tesla T4
- Tesla V100-SXM3-32GB

y-axis: ns/day

Columns grouped: - , 1X, 2X, 4X

Values:
- 21.7 (ns/day)
- 1X: 39.3 (ns/day), 88.3 (ns/day), 94.2 (ns/day), 125.8 (ns/day)
- 2X: 57.5 (ns/day), 113.0 (ns/day), 126.2 (ns/day), 153.7 (ns/day)
- 4X: 94.5 (ns/day), 126.6 (ns/day), 215.2 (ns/day), 245.5 (ns/day)

GROMACS - 2020

Performance Comparison

Legend:
- Gold 6240
- A100-SXM4-40GB
- Quadro RTX 6000 Passive
- Tesla T4
- Tesla V100-SXM3-32GB

Y-axis: ns/day

Column groups: - | 1X | 2X | 4X

X-axis categories (repeating): STMV (h-bond), Cellulose (h-bond), ADH Dodec (h-bond)

Data values:

- group:
- STMV (h-bond): 3.5
- Cellulose (h-bond): 13.6
- ADH Dodec (h-bond): 48.1

1X group:
- STMV (h-bond): 18.0
- Cellulose (h-bond): 82.5
- ADH Dodec (h-bond): 276.8
- STMV (h-bond): 11.3
- Cellulose (h-bond): 52.5
- ADH Dodec (h-bond): 201.2
- STMV (h-bond): 4.4
- Cellulose (h-bond): 22.6
- ADH Dodec (h-bond): 91.0
- STMV (h-bond): 12.4
- Cellulose (h-bond): 61.1
- ADH Dodec (h-bond): 209.1

2X group:
- STMV (h-bond): 34.3
- Cellulose (h-bond): 122.4
- ADH Dodec (h-bond): 304.5
- STMV (h-bond): 23.9
- Cellulose (h-bond): 74.3
- ADH Dodec (h-bond): 240.9
- STMV (h-bond): 10.0
- Cellulose (h-bond): 39.3
- ADH Dodec (h-bond): 123.2
- STMV (h-bond): 27.7
- Cellulose (h-bond): 92.5
- ADH Dodec (h-bond): 258.4

4X group:
- STMV (h-bond): 51.0
- Cellulose (h-bond): 182.9
- ADH Dodec (h-bond): 502.7
- STMV (h-bond): 29.8
- Cellulose (h-bond): 78.5
- ADH Dodec (h-bond): 271.5
- STMV (h-bond): 16.6
- Cellulose (h-bond): 56.6
- ADH Dodec (h-bond): 210.2
- STMV (h-bond): 43.1
- Cellulose (h-bond): 154.3
- ADH Dodec (h-bond): 448.3

GROMACS recommended usage

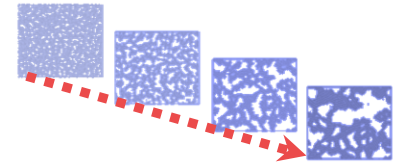| Motherboard and CPU	Dual-socket CPU server
System memory	>=16GB
GPUs	V100 / A100 with SXM2/3/4
GPUs per socket	1 to 4
GPUs per task	1 - 4

LAMMPS PATCH_20NOV2019

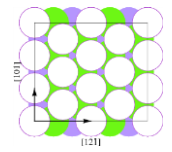May 2020
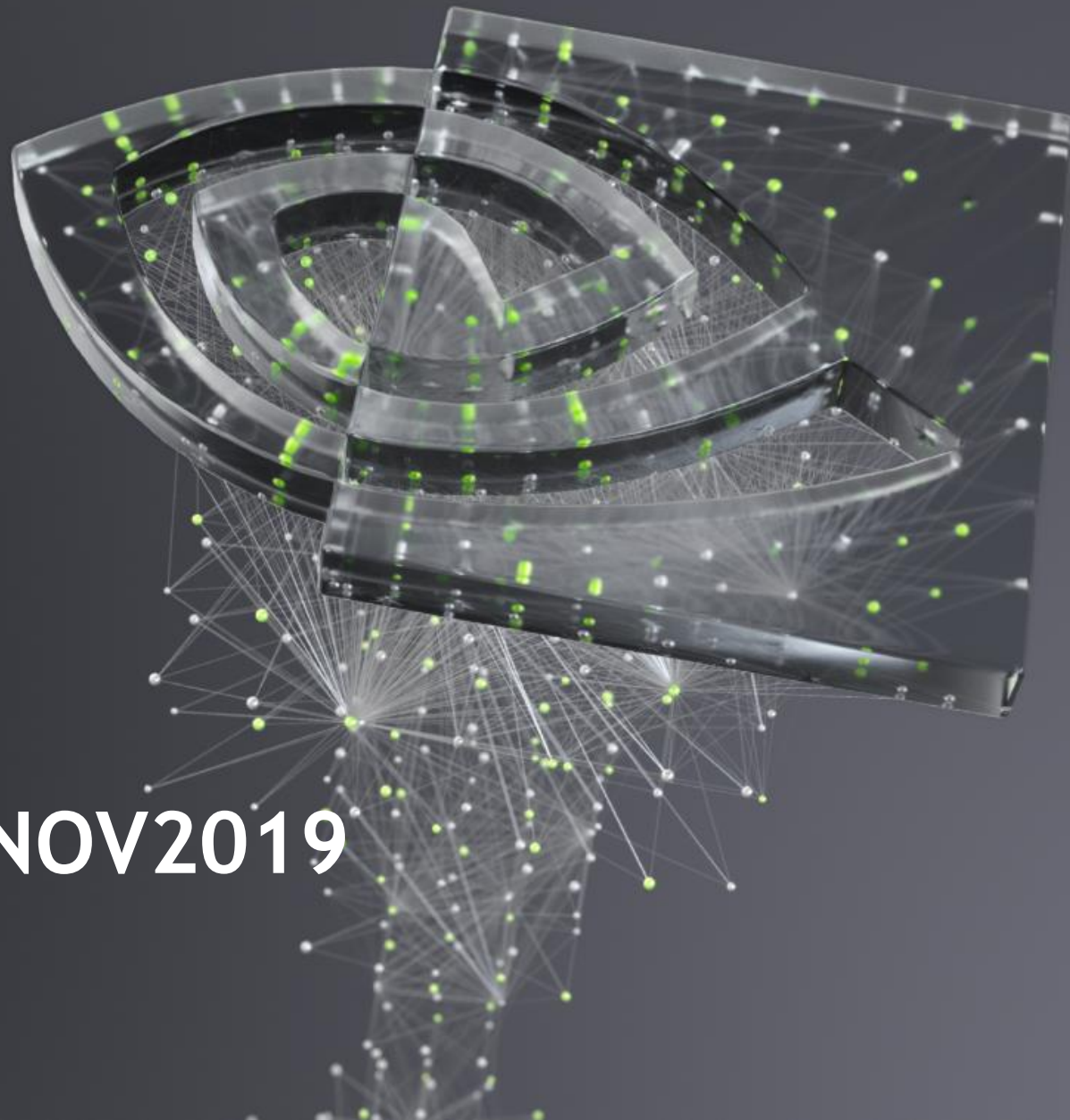
LAMMPS - patch_20Nov2019

Performance Comparison - Atomic-Fluid Lennard-Jones 2.5 Cutoff

Legend:
- Gold 6240
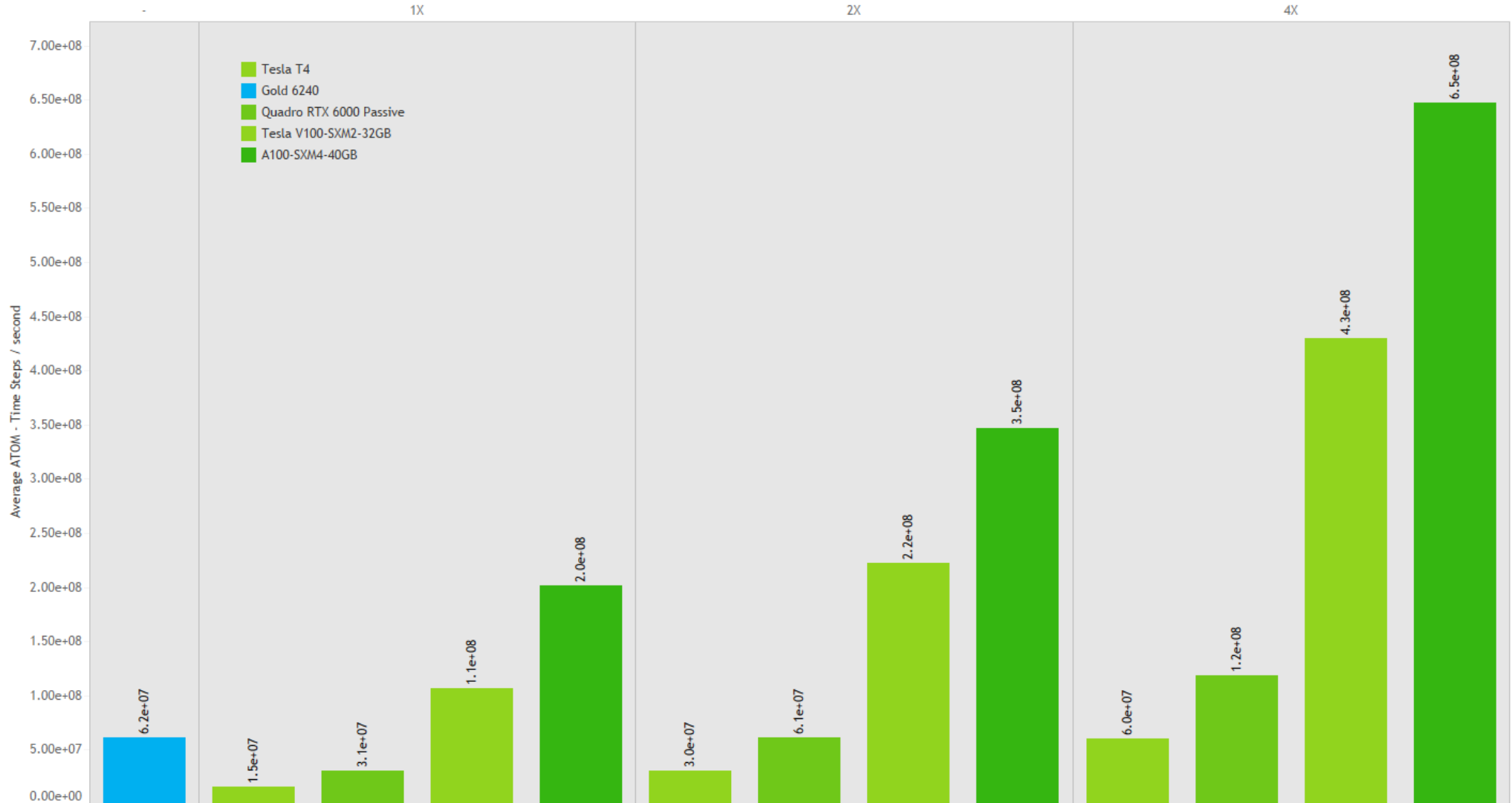- Tesla T4
- Quadro RTX 6000 Passive
- Tesla V100-SXM2-32GB
- A100-SXM4-40GB

Y-axis: Average ATOM - Time Steps / second

Configuration	Gold 6240	Tesla T4	Quadro RTX 6000 Passive	Tesla V100-SXM2-32GB	A100-SXM4-40GB
-	1.2e+08				
1X		4.9e+07	8.8e+07	2.9e+08	5.5e+08
2X		8.1e+07	1.7e+08	5.3e+08	1.0e+09
4X		1.7e+08	3.4e+08	1.2e+09	1.8e+09
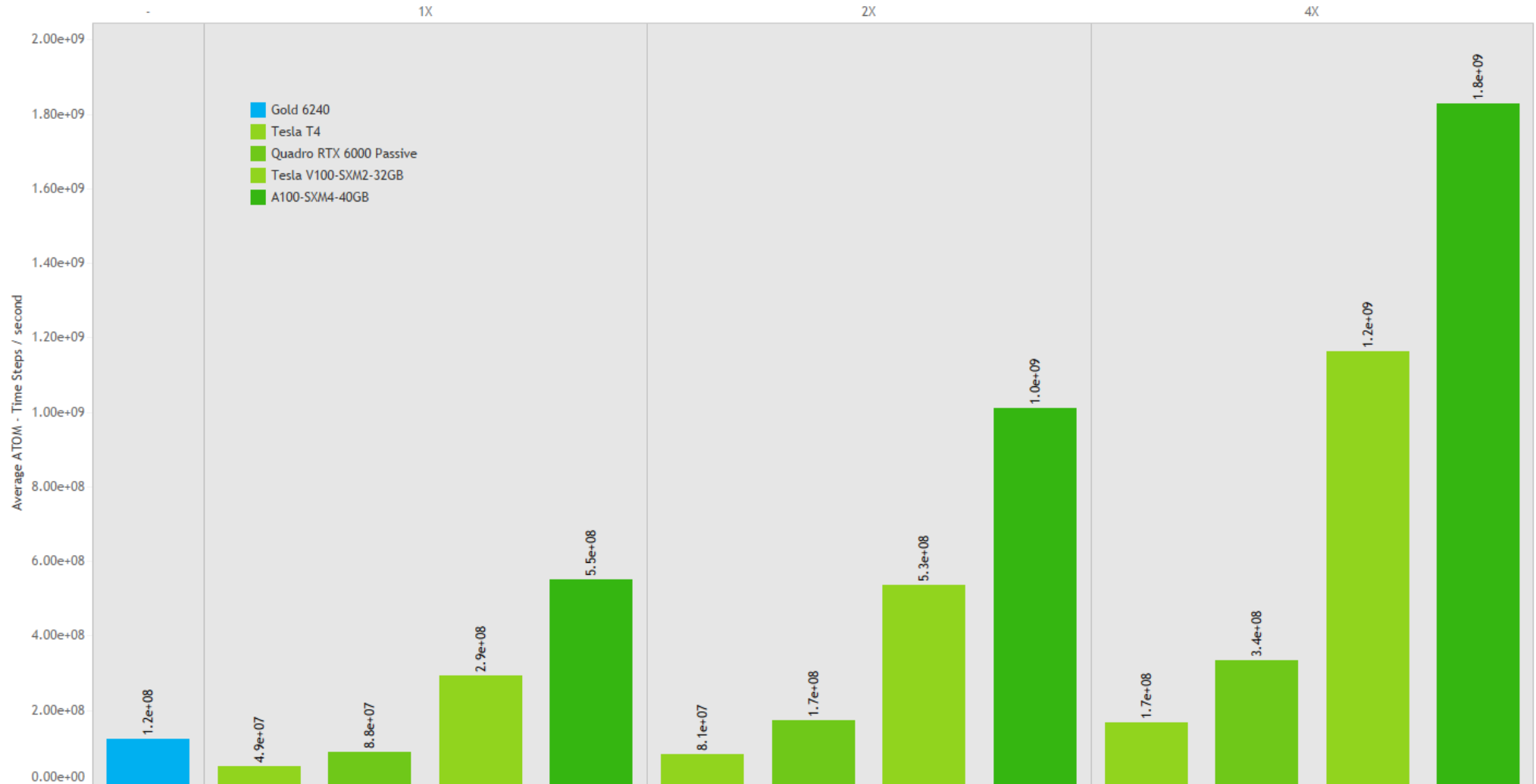
LAMMPS - patch_20Nov2019

Bulk Cu lattice

Performance Comparison - EAM

Legend:
- Tesla T4
- Gold 6240
- Quadro RTX 6000 Passive
- Tesla V100-SXM2-32GB
- A100-SXM4-40GB

Y-axis: Average ATOM - Time Steps / second (0.00e+00 to 7.00e+08)

Groups: - , 1X , 2X , 4X

Data labels:
- (-): 6.2e+07
- 1X: 1.5e+07, 3.1e+07, 1.1e+08, 2.0e+08
- 2X: 3.0e+07, 6.1e+07, 2.2e+08, 3.5e+08
- 4X: 6.0e+07, 1.2e+08, 4.3e+08, 6.5e+08
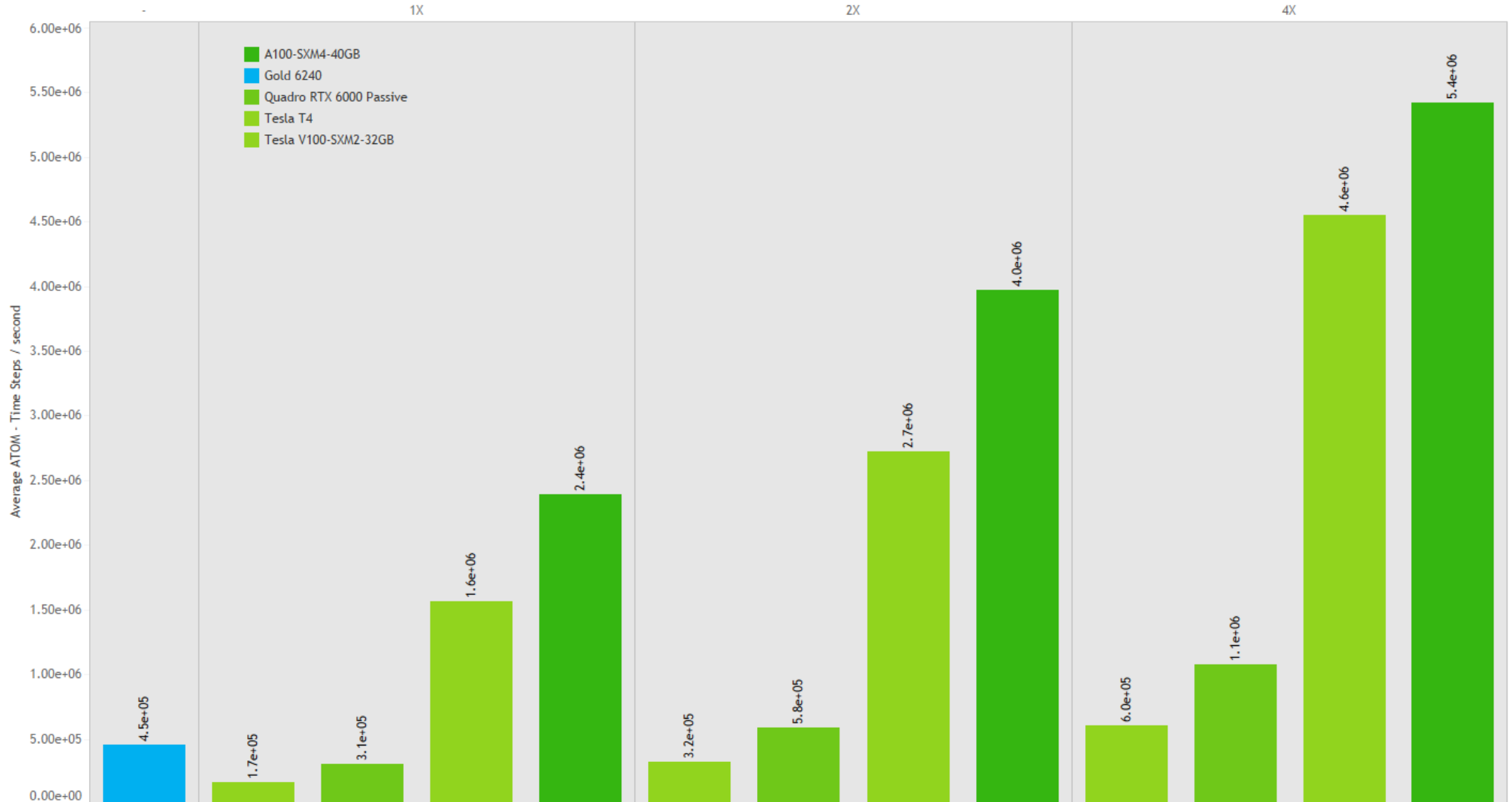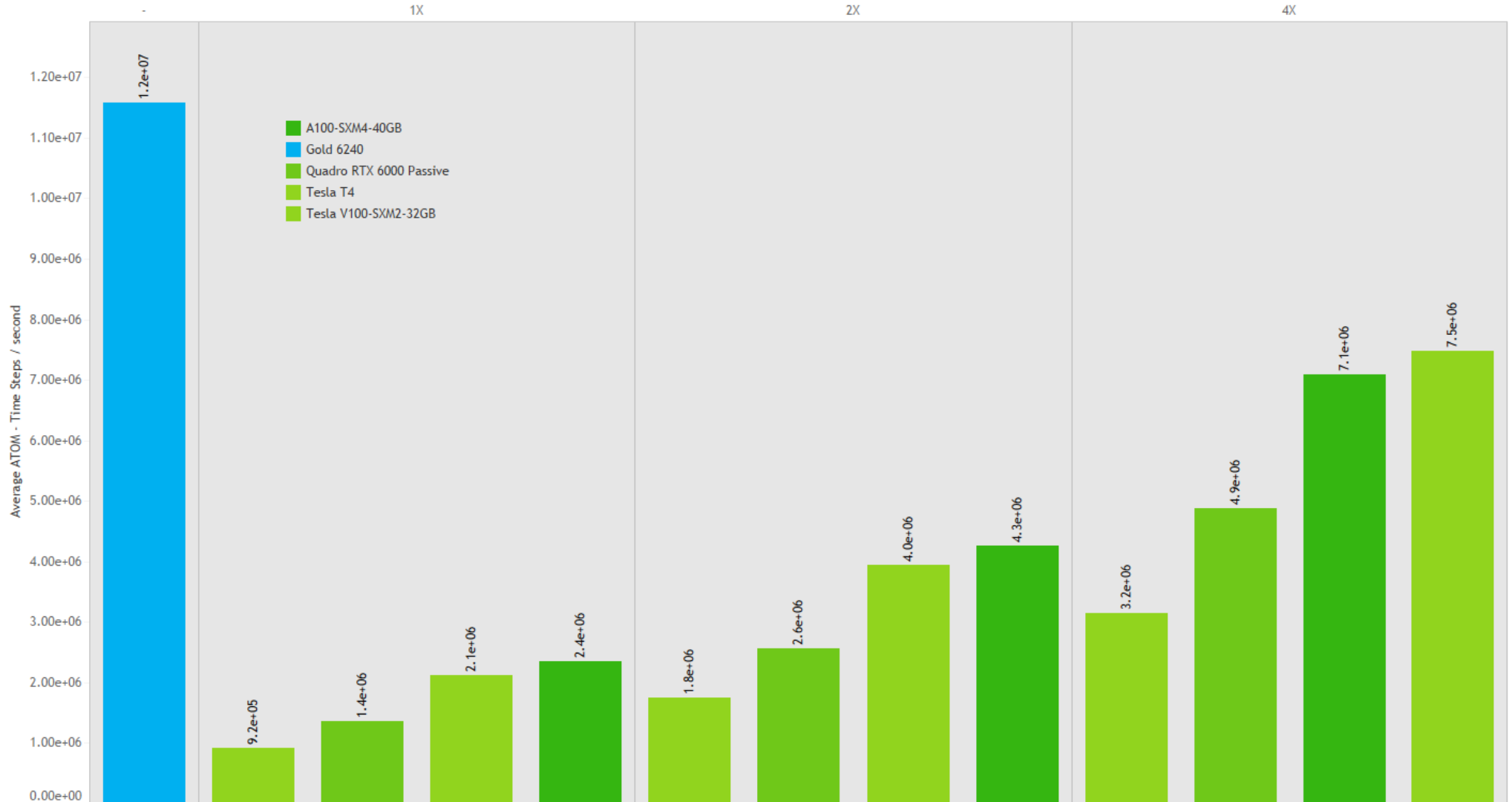
LAMMPS - patch_20Nov2019

Performance Comparison - ReaxFF/C

LAMMPS - patch_20Nov2019

Performance Comparison - Rhodopsin

Legend:
- A100-SXM4-40GB
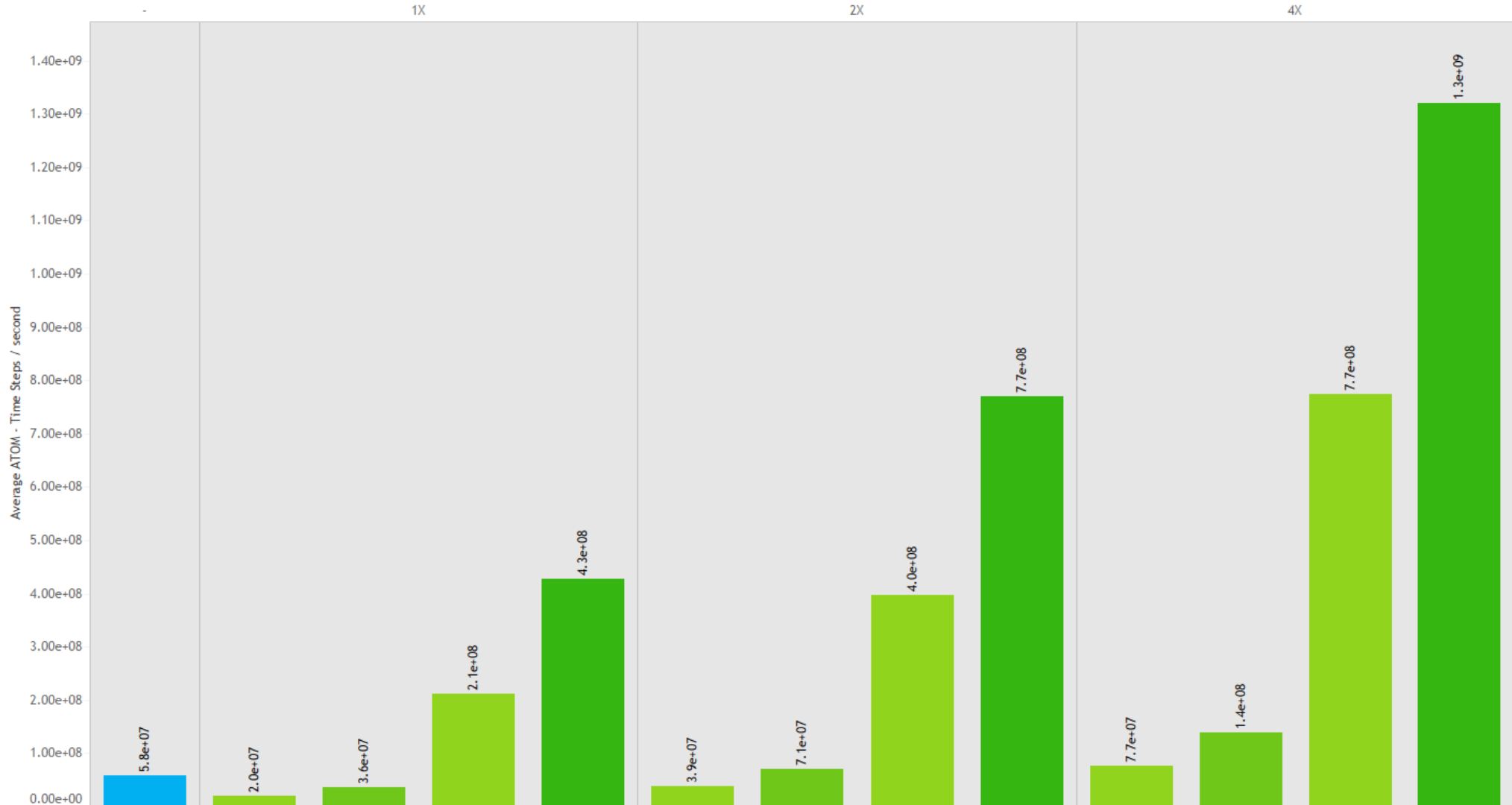- Gold 6240
- Quadro RTX 6000 Passive
- Tesla T4
- Tesla V100-SXM2-32GB

Y-axis: Average ATOM - Time Steps / second

Panel "-":
- Gold 6240: 1.2e+07

Panel "1X":
- 9.2e+05
- 1.4e+06
- 2.1e+06
- 2.4e+06

Panel "2X":
- 1.8e+06
- 2.6e+06
- 4.0e+06
- 4.3e+06

Panel "4X":
- 3.2e+06
- 4.9e+06
- 7.1e+06
- 7.5e+06

LAMMPS - patch_20Nov2019

Si crystallization
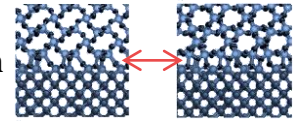
Performance Comparison - Tersoff

Average ATOM - Time Steps / second

- : 5.8e+07
- 1X: 2.0e+07, 3.6e+07, 2.1e+08, 4.3e+08
- 2X: 3.9e+07, 7.1e+07, 4.0e+08, 7.7e+08
- 4X: 7.7e+07, 1.4e+08, 7.7e+08, 1.3e+09
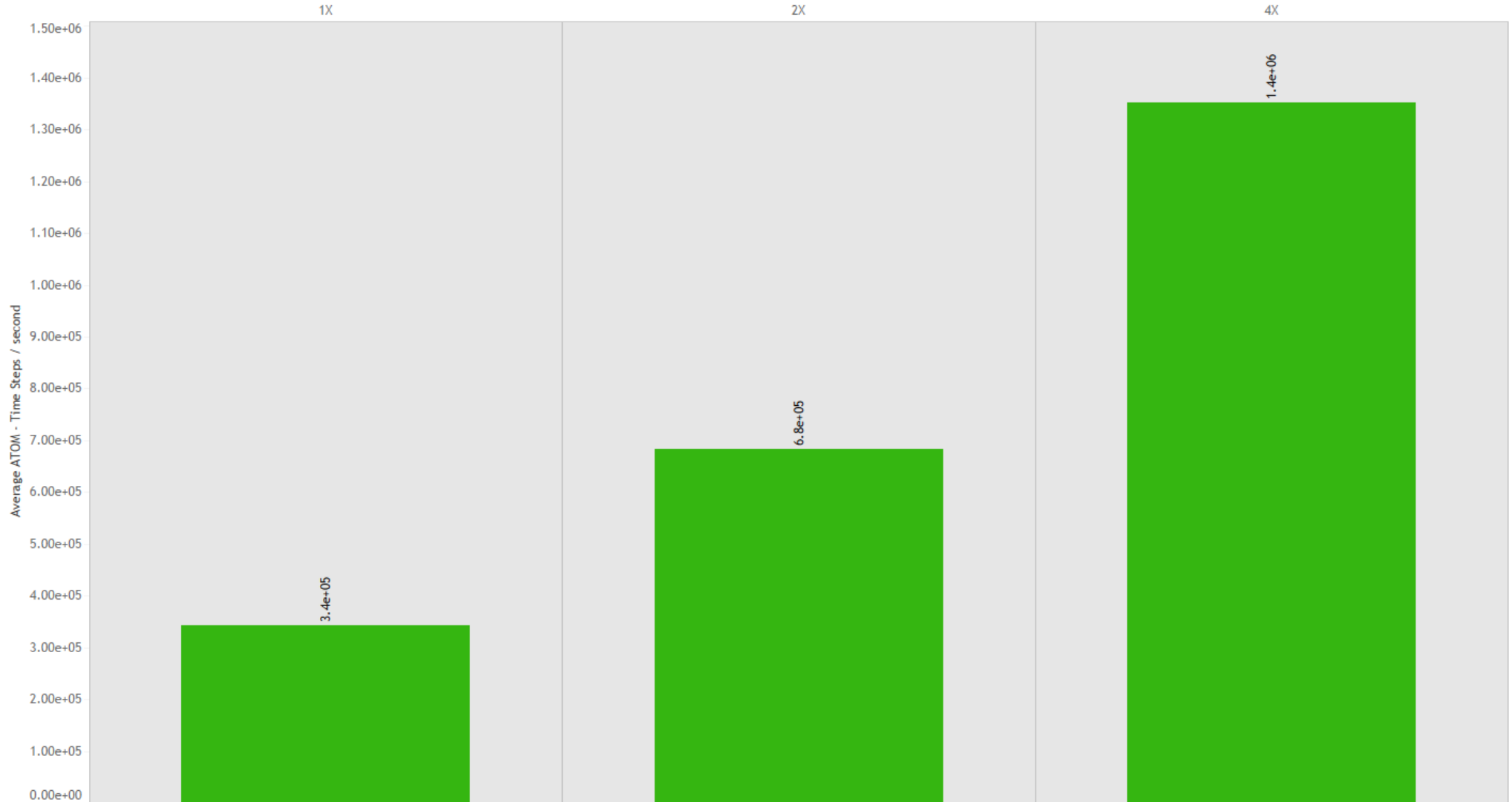
LAMMPS - patch_20Nov2019

Performance Comparison - SNAP

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

May 2020

NAMD - 3.0a1

Performance Comparison - Average Performance

	1X	2X	4X
Tesla V100-SXM2-32GB	52.3	104.1	207.5
A100-SXM4-40GB	67.9	135.0	268.4

AVG ns/day
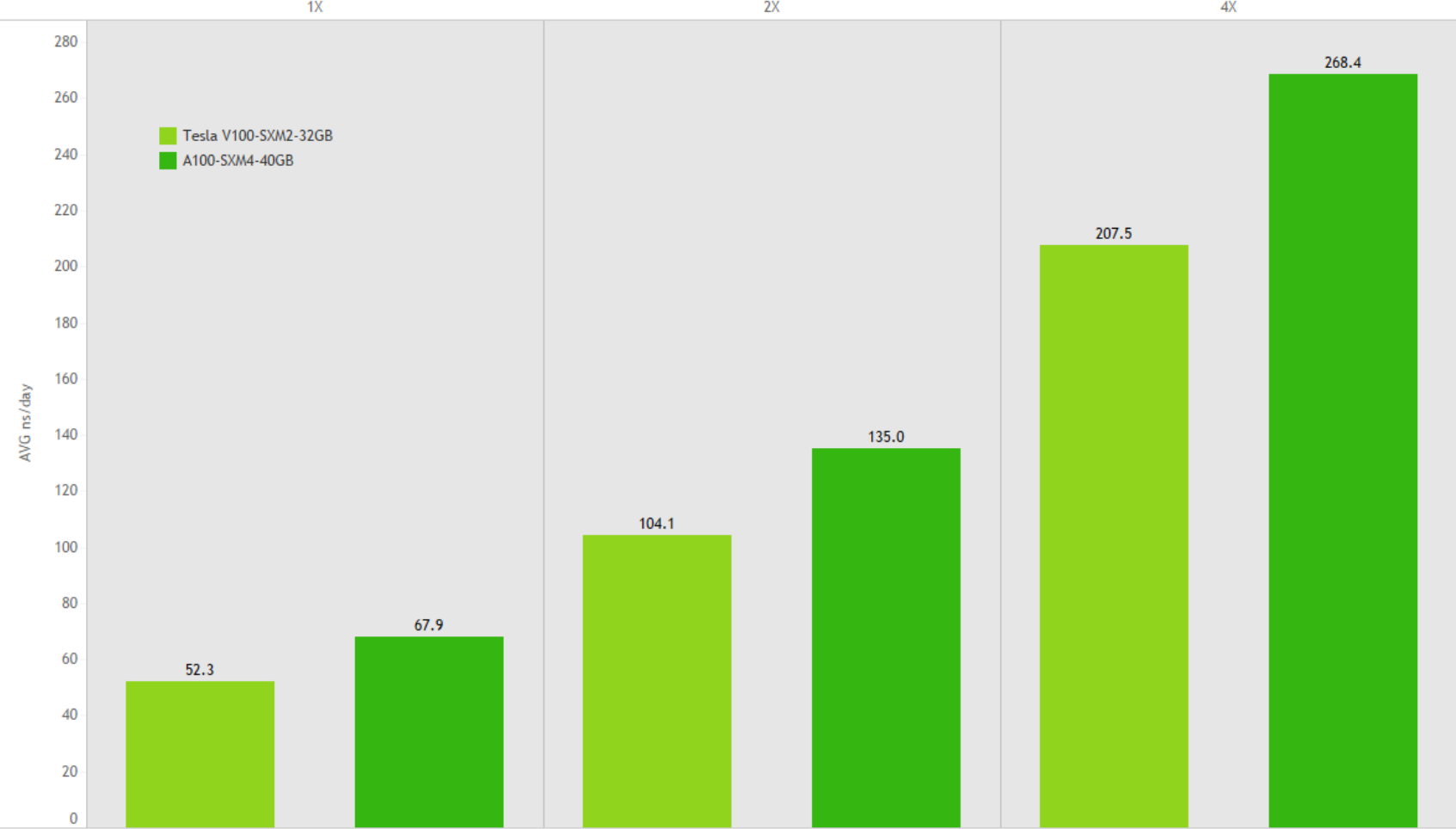
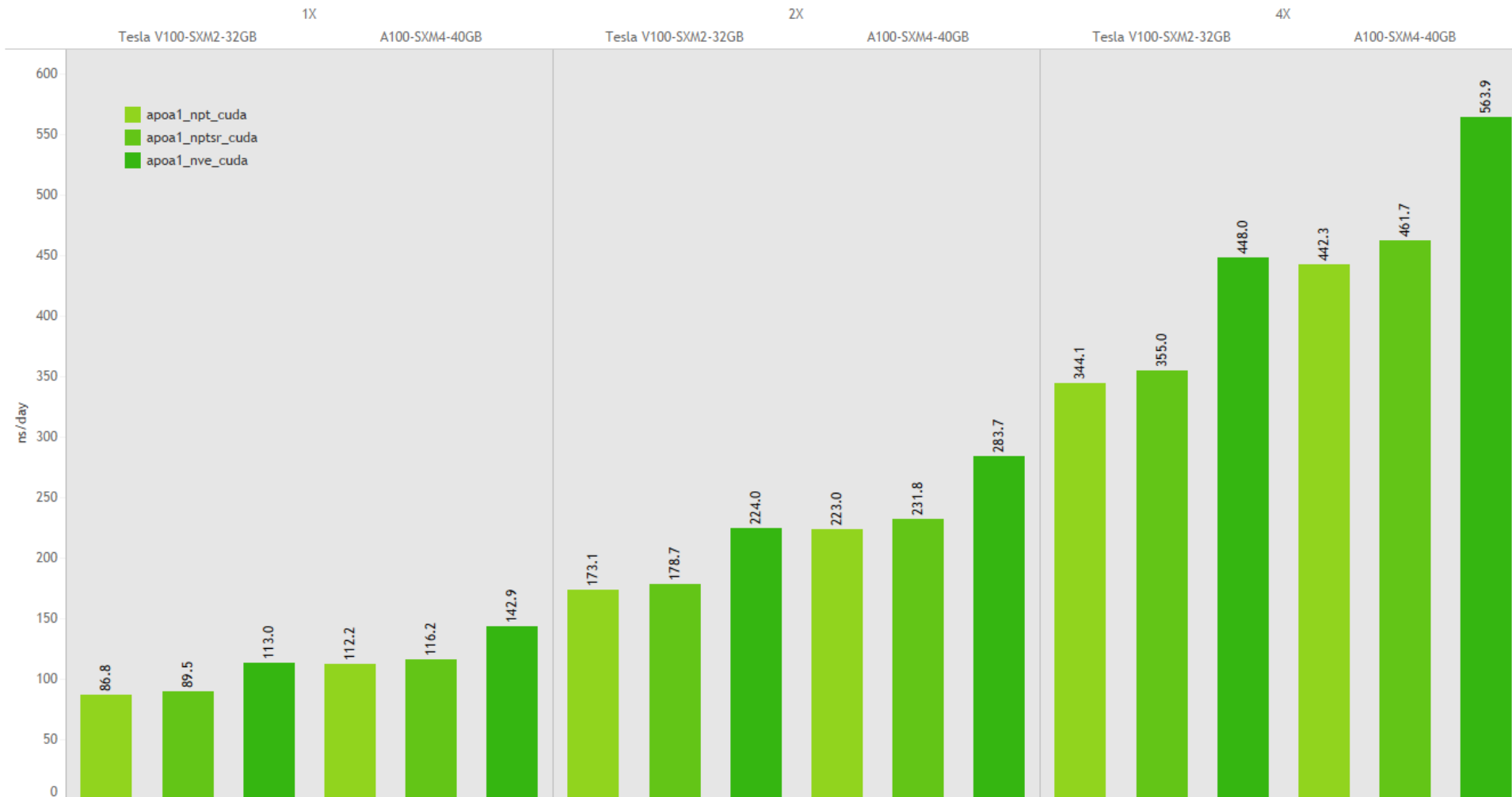# NAMD - 3.0a1

ApoA1
92,224 atoms
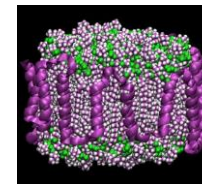
Performance Comparison of APOA1 benchmarks

NAMD - 3.0a1
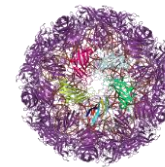
Performance Comparison of STMV benchmarks

STMV
1,067,095 atoms

	1X			2X			4X	
Tesla V100-SXM2-32GB		A100-SXM4-40GB	Tesla V100-SXM2-32GB		A100-SXM4-40GB	Tesla V100-SXM2-32GB		A100-SXM4-40GB

ns/day

Values (left to right):
- 1X: 7.7, 7.9, 8.9, 11.3, 11.5, 13.1
- 2X: 15.4, 15.8, 17.8, 22.5, 23.0, 26.1
- 4X: 30.8, 31.5, 35.5, 44.8, 46.0, 51.9
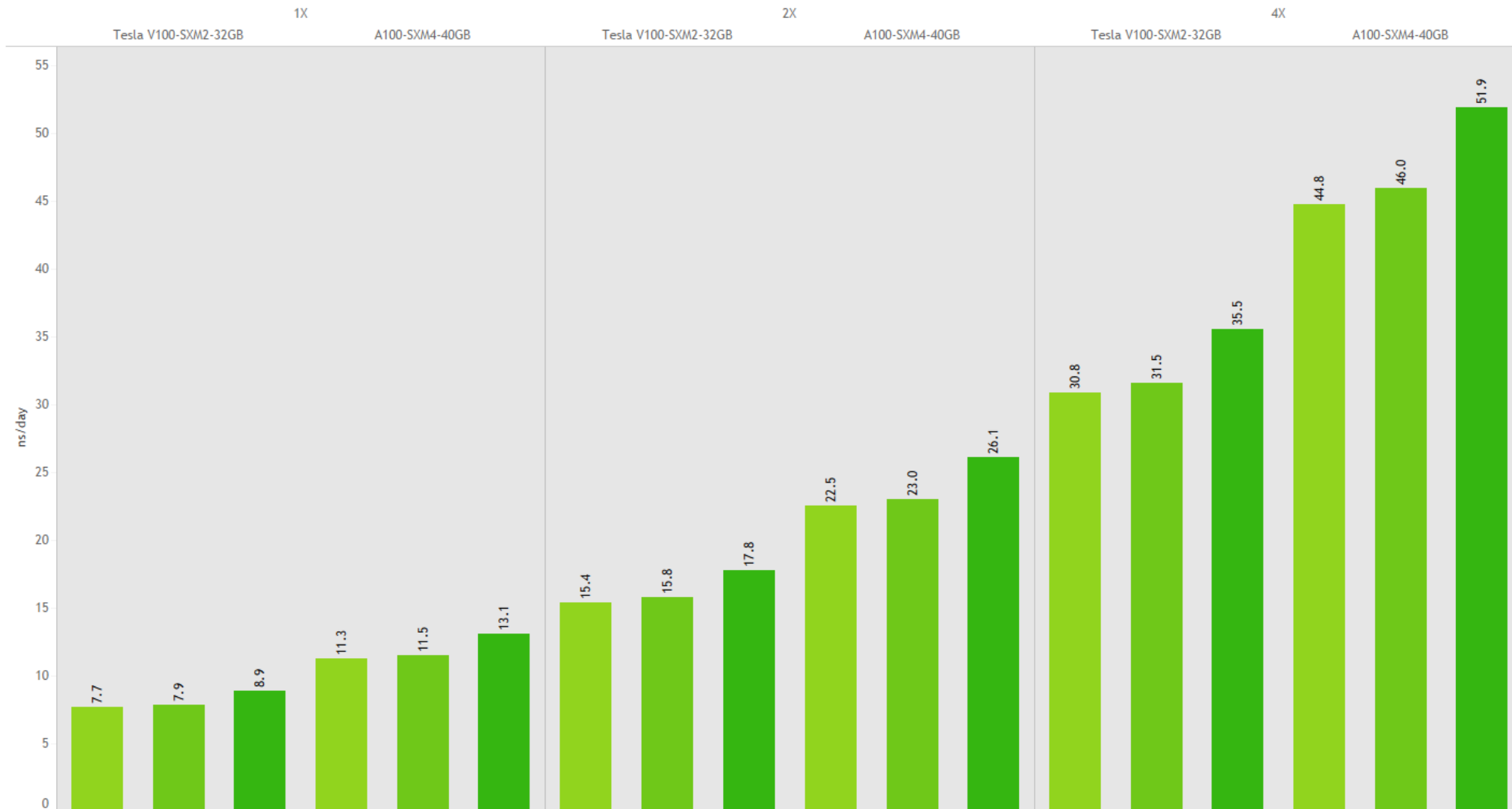
NAMD recommended usage

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

May 2020
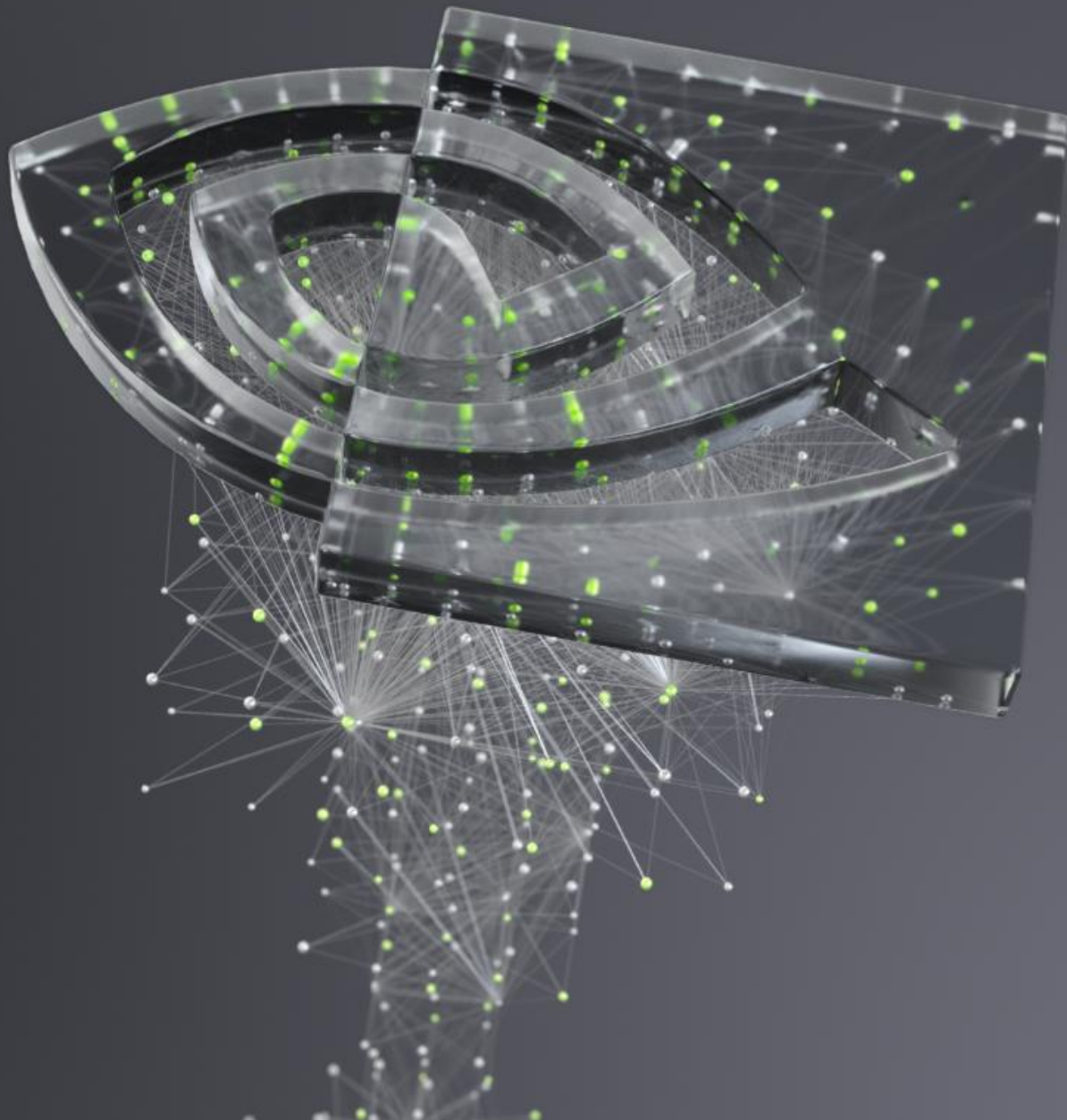
RELION - 3.0.8

Performance Comparison - 3D Refinement

Legend:
- Gold 6240
- Tesla T4
- Quadro RTX 6000 Passive
- Tesla V100-SXM2-32GB

Config	Gold 6240	Tesla T4	Quadro RTX 6000 Passive	Tesla V100-SXM2-32GB
-	13156 sec			
1X		8190 sec	6115 sec	5748 sec
2X		4706 sec	3846 sec	3463 sec
4X		3549 sec	3016 sec	2748 sec
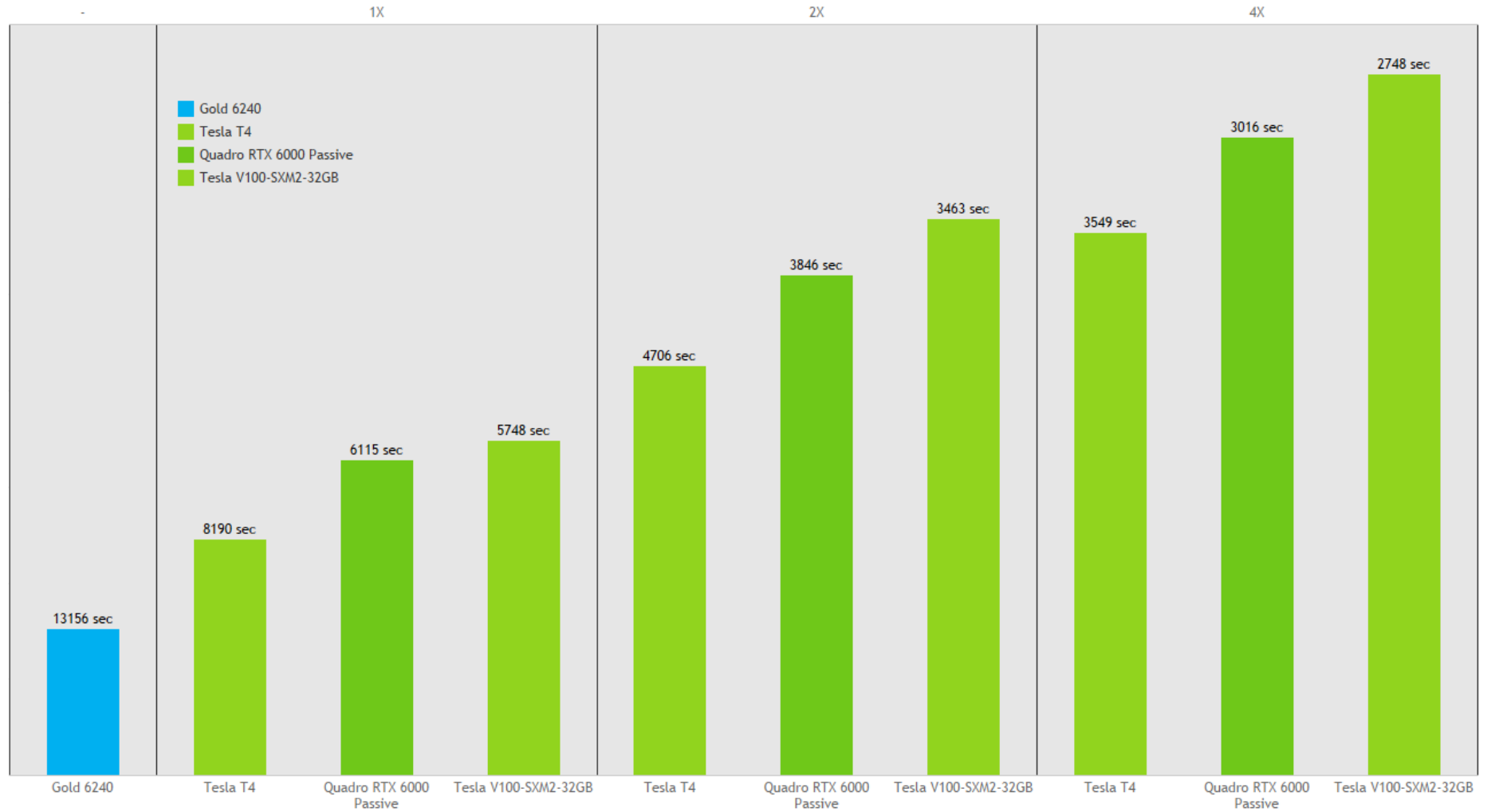
RELION RECOMMENDED USAGE

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