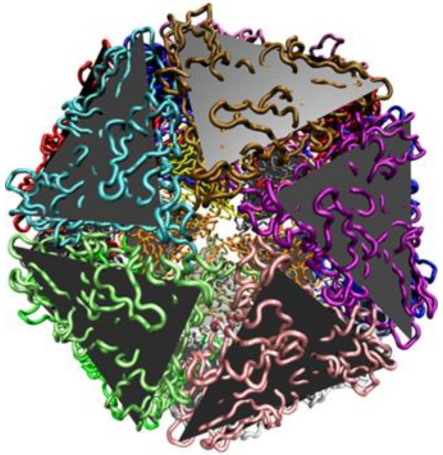
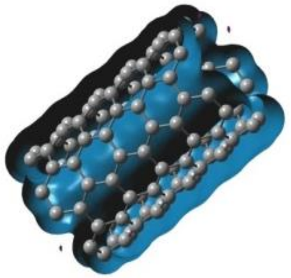
Quantum Chemistry (QC) on GPUs

October 2017

NVIDIA

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, HTMD, 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

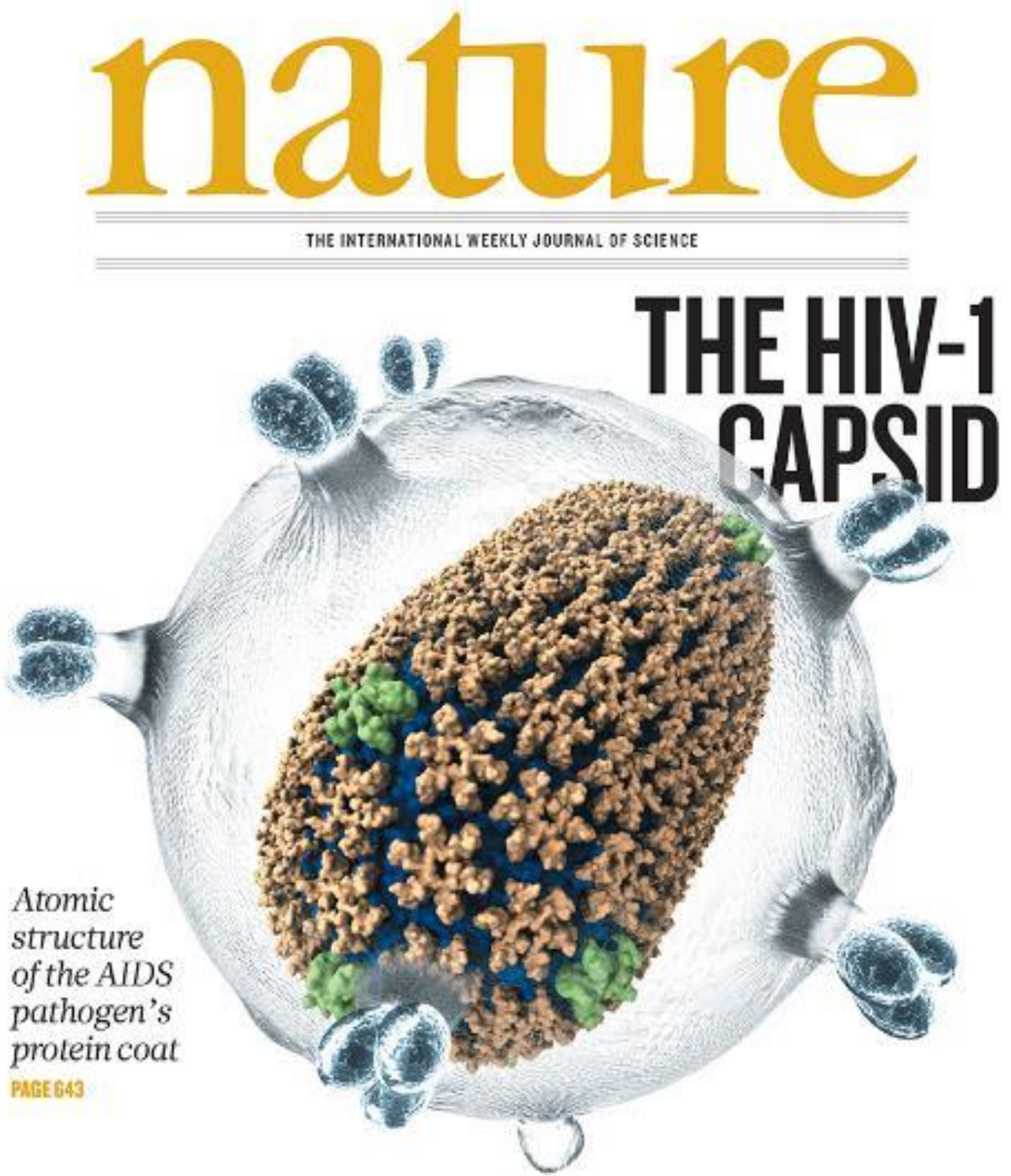
MD vs. QC on GPUs

"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 (Accademics), Tesla (Servers)	Tesla recommended
ECC off	ECC on

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.



GPU-Accelerated Quantum Chemistry Apps

Green Lettering Indicates Performance Slides Included

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

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

ABINIT

ABINIT on GPUS

- Speed in the parallel version:
  - For ground-state calculations, GPUs can be used. This is based on CUDA+MAGMA
  - For ground-state calculations, the wavelet part of ABINIT (which is BigDFT) is also very well parallelized : MPI band parallelism, combined with GPUs

BigDFT

BigDFT
http://bigdft.org

Multiscale Modelling Methods for Applications in Materials Science CECAM JÜLICH, GERMANY

Introduction to Electronic Structure Calculations with BigDFT

Thierry Deutsch, Damien Caliste, Luigi Genovese

L_Sim - CEA Grenoble

17 September 2013

Courtesy of BigDFT team @ CEA

BigDFT version 1.7: capabilities

http://bigdft.org

- Free, surface and periodic boundary conditions
- Geometry optimizations (with constraints)
- Born-Oppenheimer Molecular Dynamics
- Saddle point searches (Nudged-Elastic Band Method)
- Vibrations
- External electric fields
- Unoccupied KS orbitals
- Collinear and Non-collinear magnetism
- All XC functionals of the ABINIT package
- Hybrid functionals
- Empirical van der Waals interactions (many flavors)
- Also available within the ABINIT package

Courtesy of BigDFT team @ CEA

BigDFT version 1.7: capabilities

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- Also available within the ABINIT package

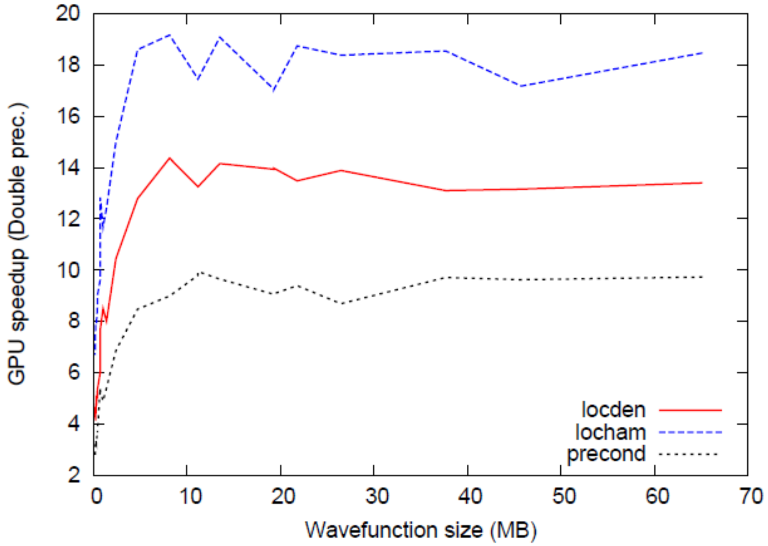
Courtesy of BigDFT team @ CEA

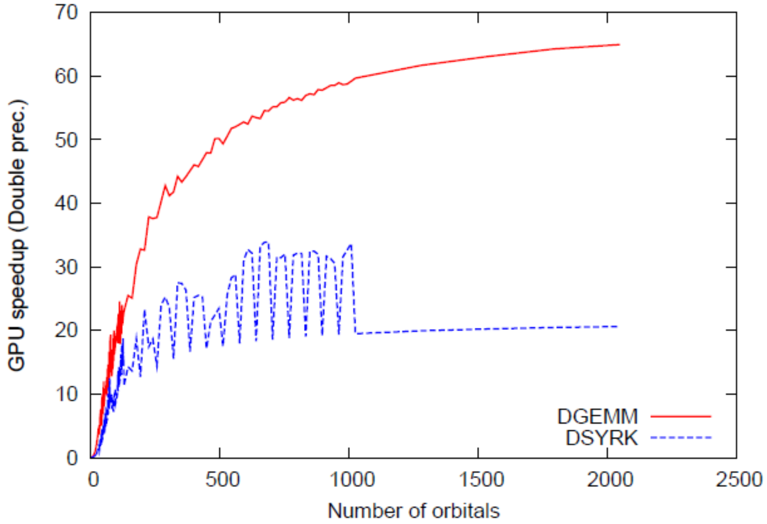
GPU-ported operations in BigDFT (double precision)

BigDFT
http://bigdft.org

Convolutions (OpenCL rewritten)

GPU speedups between 10 and 20 can be obtained for different sections





Linear algebra (CUBLAS library)

The interfacing with CUBLAS is immediate, with considerable speedups

Courtesy of BigDFT team @ CEA

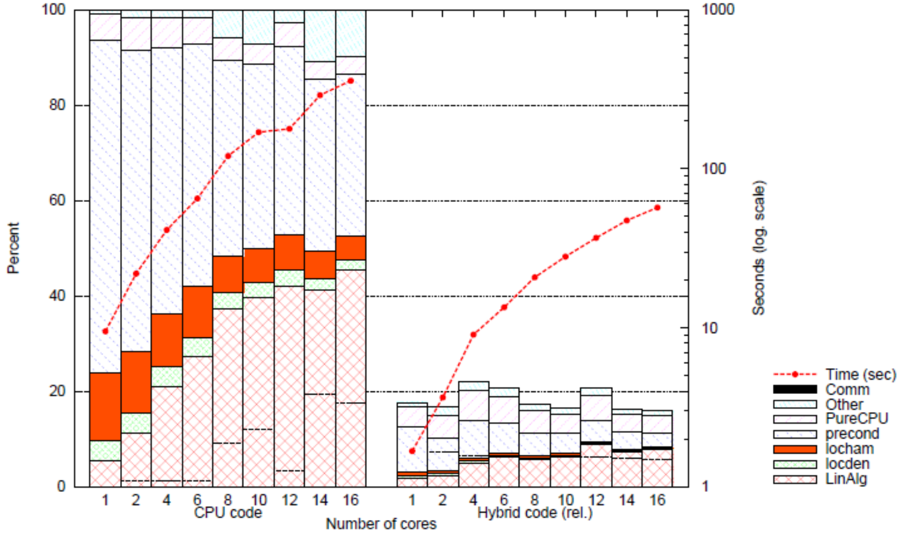
BigDFT code on Hybrid architectures

BigDFT
http://bigdft.org

BigDFT code can run on hybrid CPU/GPU supercomputers
In multi-GPU environments, double precision calculations

No Hot-spot operations

Different code sections can be ported on GPU
up to 20x speedup for some operations,
7x for the full parallel code



Courtesy of BigDFT team @ CEA

Hands on

See

http://bigdft.org/Wiki/index.php?title=Category:Tutorials

- First runs with BigDFT
- Basis-set convergence
- Acceleration example on different platforms:
  Kohn-Sham DFT Operation with GPU acceleration

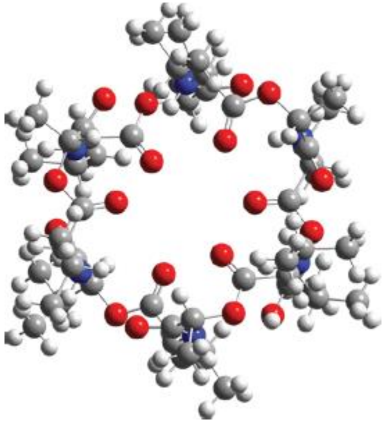
Courtesy of BigDFT team @ CEA

Gaussian 16

April 2017

GAUSSIAN 16

A Leading Computation Chemistry Code



Valinomycin
wB97xD/6-311+(2d,p) Freq
2.25X speedup

Hardware: HPE server with dual Intel Xeon E5-2698 v3 CPUs (2.30GHz ; 16 cores/chip), 256GB memory and 4 Tesla K80 dual GPU boards (boost clocks: MEM 2505 and SM 875). Gaussian source code compiled with PGI Accelerator Compilers (16.5) with OpenACC (2.5 standard).

PGI

Mike Frisch, Ph.D.
President and CEO
Gaussian, Inc.

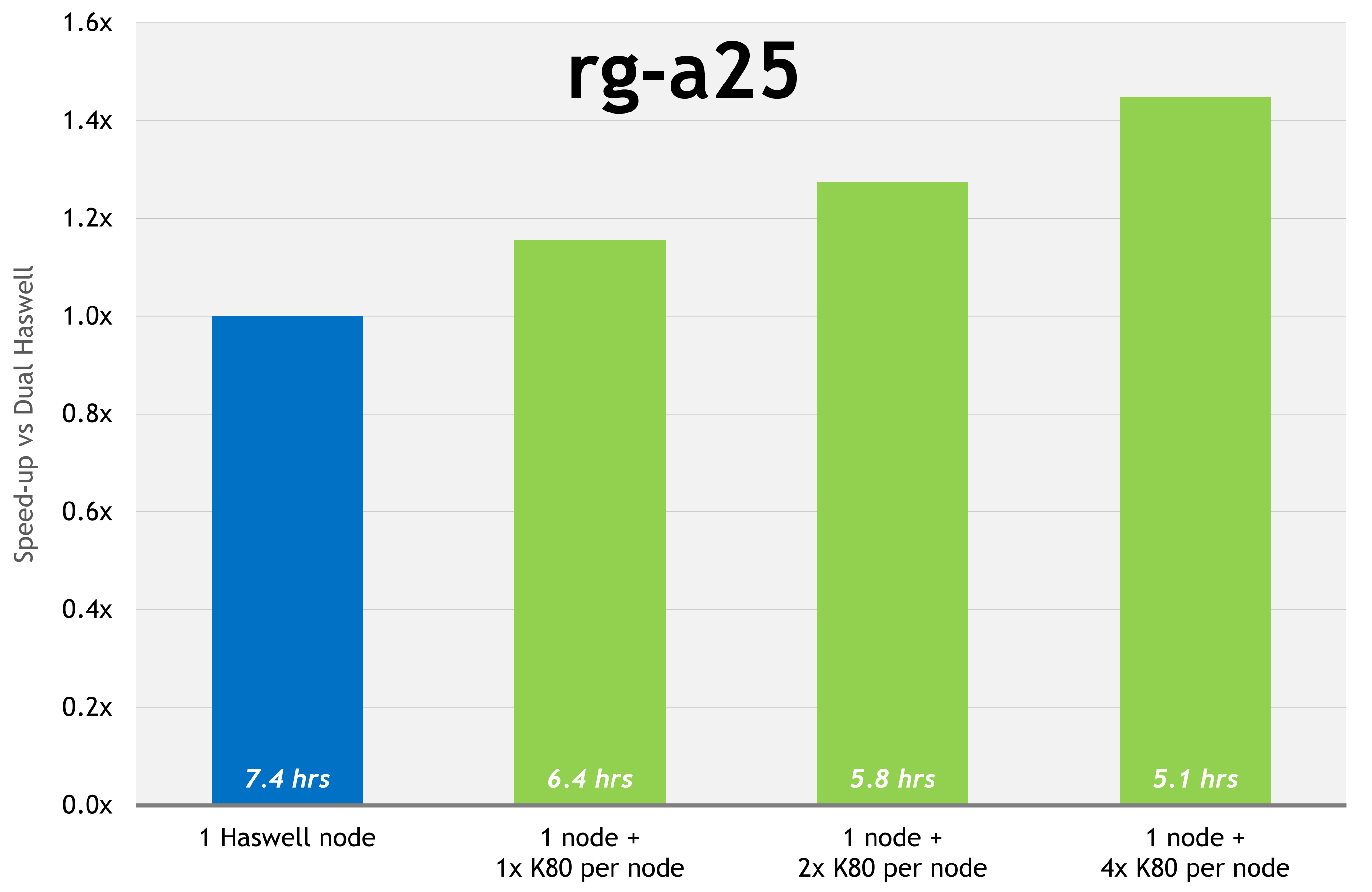
“Using OpenACC allowed us to continue development of our fundamental algorithms and software capabilities simultaneously with the GPU-related work. In the end, we could use the same code base for SMP, cluster/ network and GPU parallelism. PGI's compilers were essential to the success of our efforts.”

GPU-ACCELERATED GAUSSIAN 16 AVAILABLE

100% PGI OpenACC Port (no CUDA)

- Gaussian is a Top Ten HPC (Quantum Chemistry) Application.
- **80-85% of use cases are GPU-accelerated** (Hartree-Fock and DFT: energies, 1^{st} derivatives (gradients) and 2^{nd} derivatives). More functionality to come.
- K40, K80 support; P100 support coming as a minor release, performance "good", **faster wall clock times**. Early P100 results promising.
- **No pricing difference** between Gaussian CPU and GPU versions.
- Existing Gaussian 09 **customers under maintenance contract get (free) upgrade**.
- Existing non-maintenance customers required to pay upgrade fee.
- To get the bits or to ask about the upgrade fee, please contact Gaussian, Inc.'s Jim Hess, Operations Manager; jhess@gaussian.com.

rg-a25 on K80s

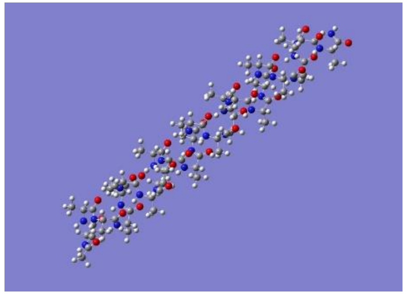


Running Gaussian version 16

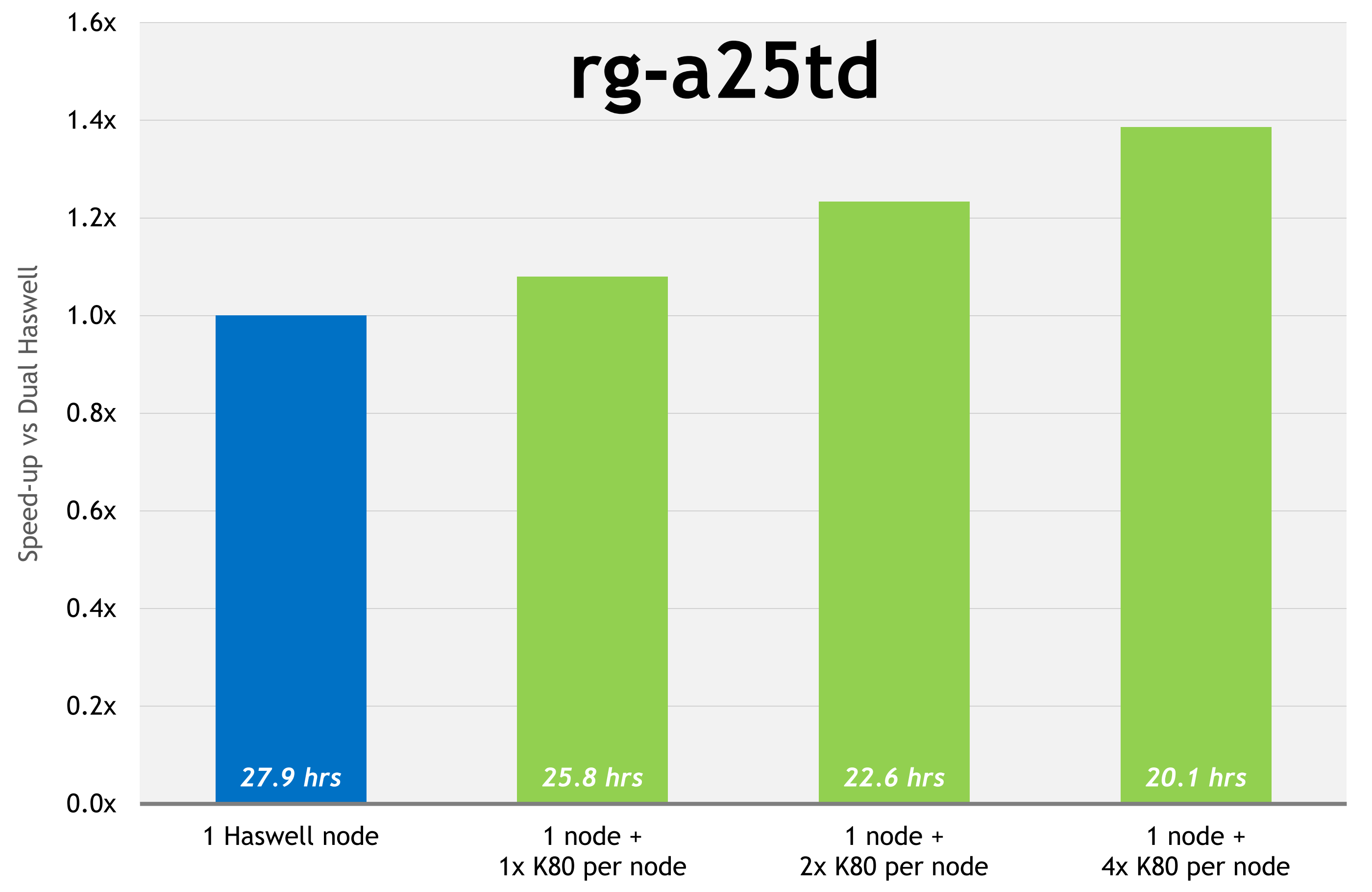
The blue node contains Dual Intel Xeon E5-2698 v3@2.3GHz (Haswell) CPUs

The green nodes contain Dual Intel Xeon E5-2698 v3@2.3GHz (Haswell) CPUs + Tesla K80 (autoboost) GPUs

Alanine 25. Two steps: Force and Frequency. APFD 6-31G*
nAtoms = 259, nBasis = 2195



rg-a25td on K80s



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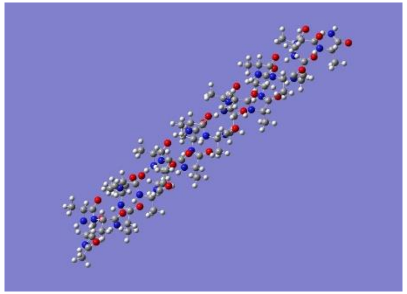
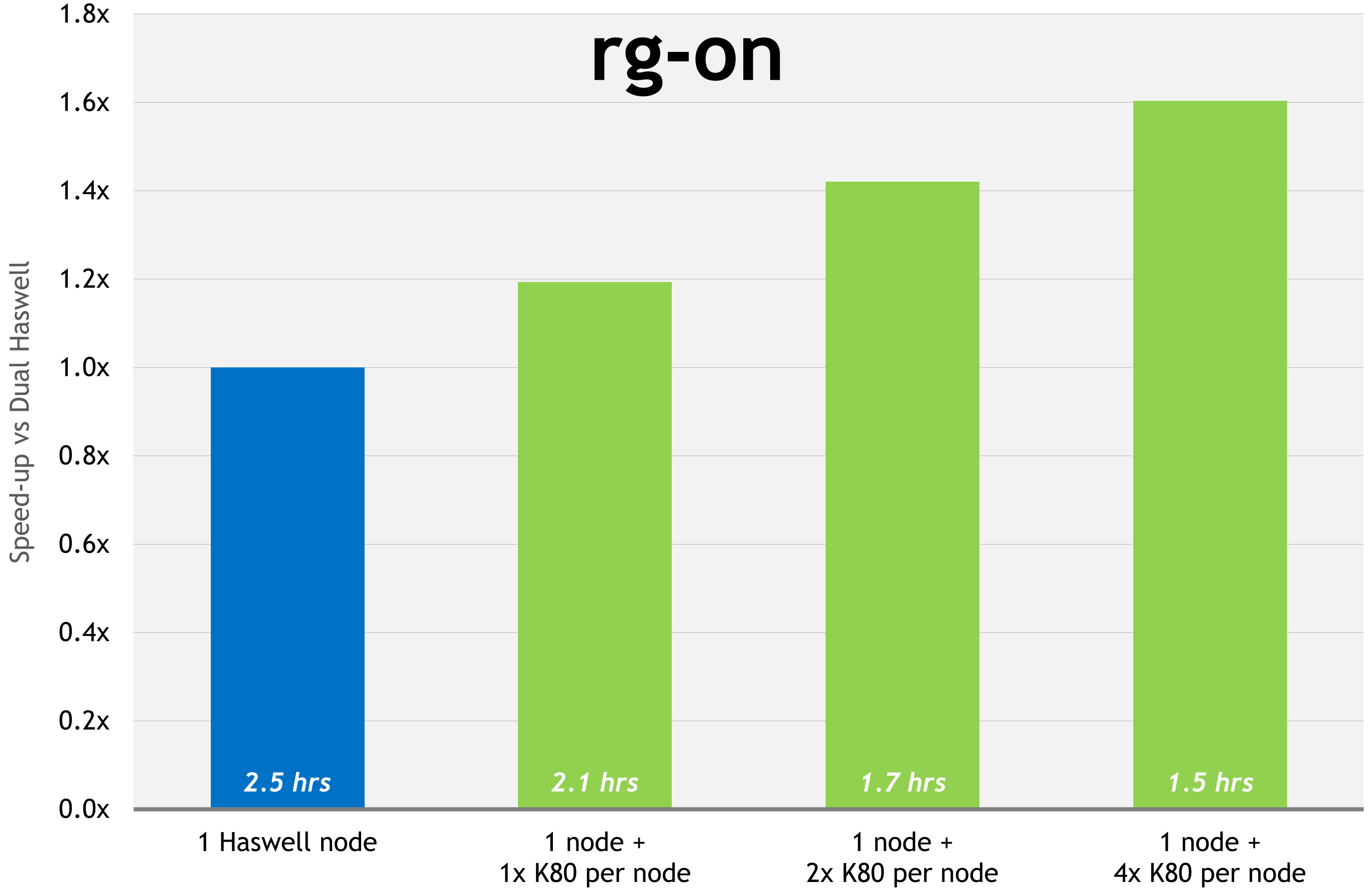
Alanine 25. Two Time-Dependent (TD) steps: Force and Frequency. APFD 6-31G*
nAtoms = 259, nBasis = 2195



rg-on on K80s



Running Gaussian version 16

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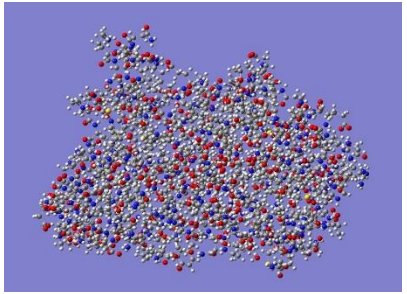
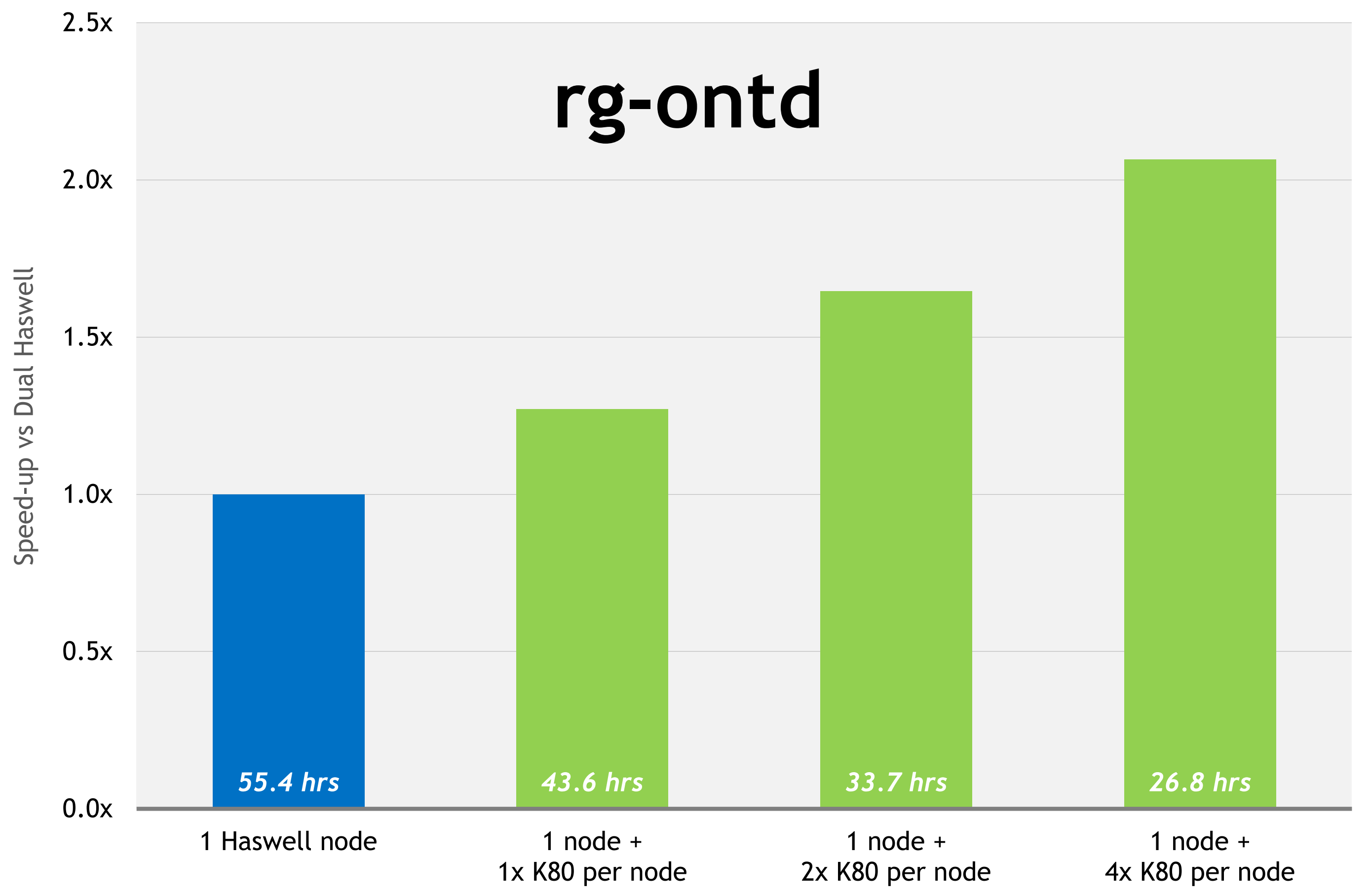
GFP ONIOM. Two steps: Force and Frequency. APFD/6-311+G(2d,p):amber=softfirst)=embed nAtoms = 3715 (48/3667), nBasis = 813



rg-ontd on K80s



Running Gaussian version 16

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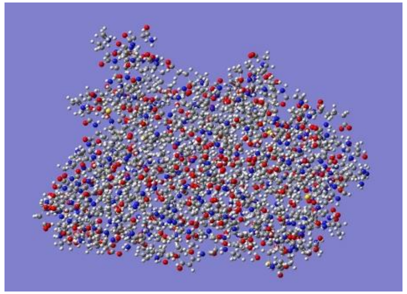
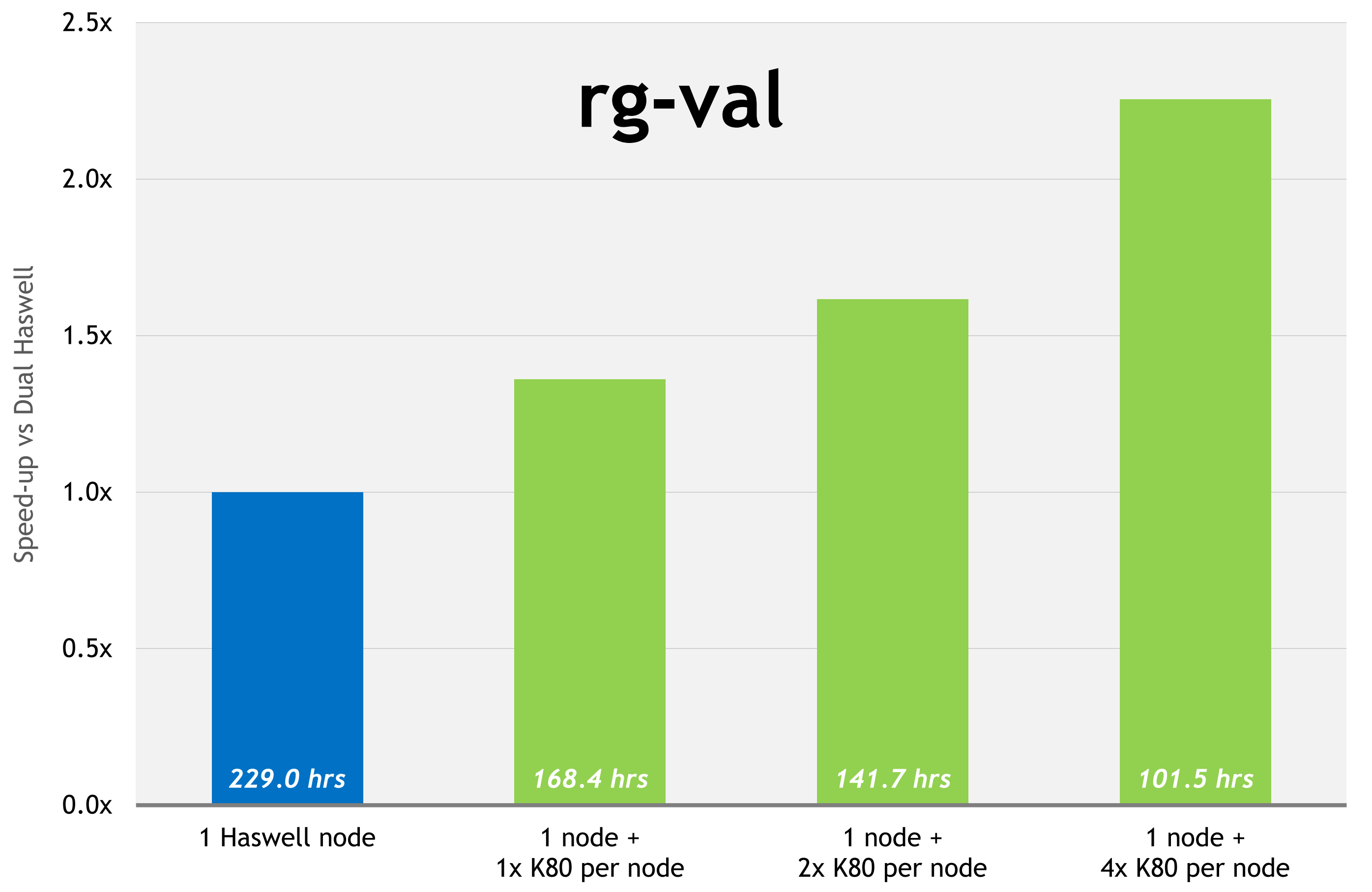


rg-val on K80s



Running Gaussian version 16

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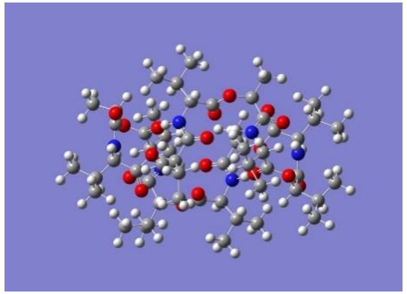
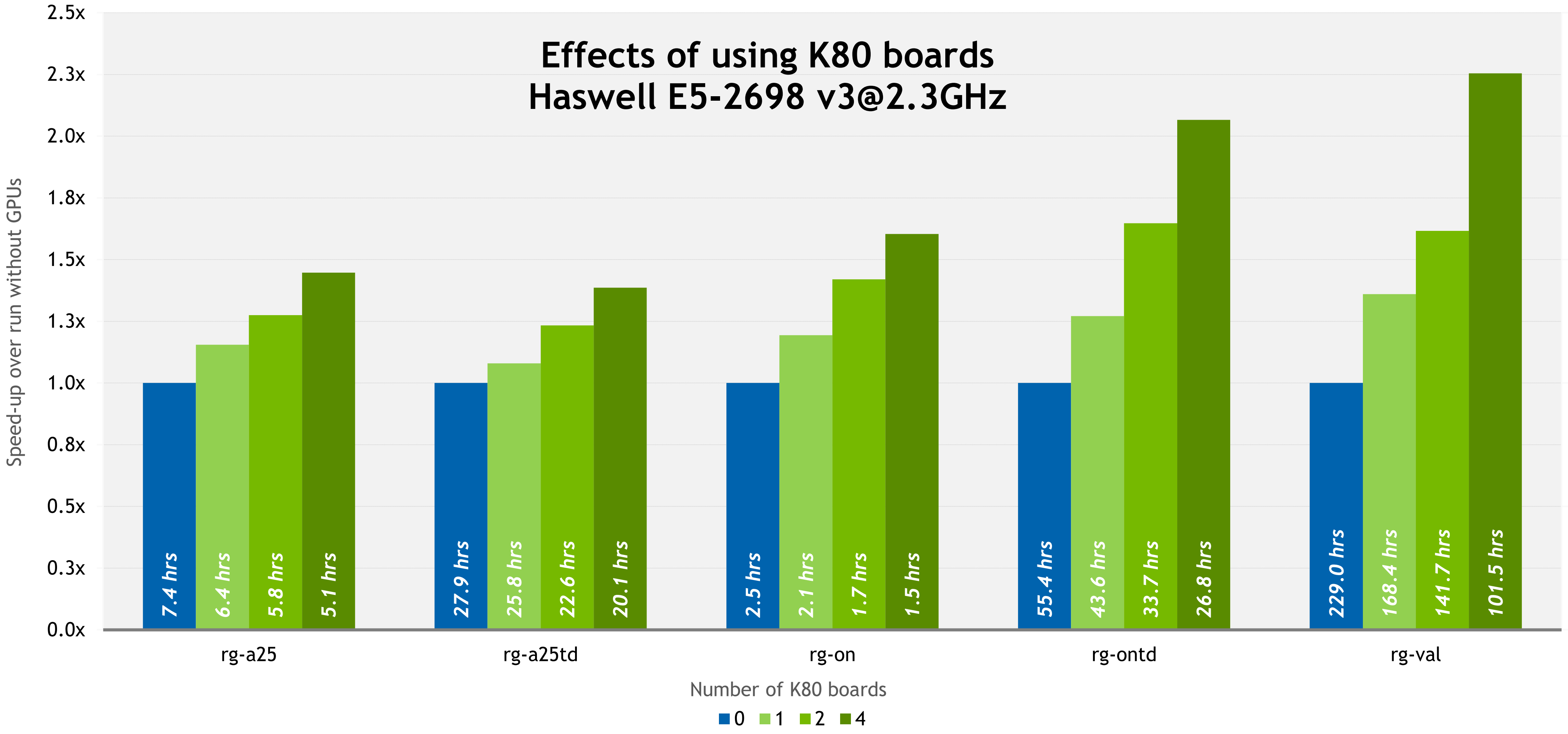
The green nodes contain Dual Intel Xeon E5-2698 v3@2.3GHz (Haswell) CPUs + Tesla K80 (autoboost) GPUs

Valinomycin. Two steps: Force and Frequency. APFD 6-311+G(2d,p) nAtoms = 168, nBasis = 2646



Effects of using K80s



Gaussian 16 Supported Platforms

- 4-way collaboration; Gaussian, Inc., PGI, NVIDIA and HPE
- HPE, NVIDIA and PGI is the development platform
- All released/certified x86_64 versions of Gaussian 16 use the PGI compilers
- Certified versions of Gaussian 16 use Intel only for Itanium, XLF for some IBM platforms, Fujitsu compilers for some SPARC-based machines and PGI for the rest (including some Apple products)
- GINC is collaborating with IBM, PGI (and NVIDIA) to release an OpenPower version of Gaussian that also uses the PGI compiler
- See Gaussian Supported Platforms for more details: http://gaussian.com/g16/g16_plat.pdf

CLOSING REMARKS

Significant Progress has been made in enabling Gaussian on GPUs with OpenACC

OpenACC is increasingly becoming more versatile

Significant work lies ahead to improve performance

Expand feature set:

- PBC, Solvation, MP2, ONIOM, triples-Corrections

ACKNOWLEDGEMENTS

Development is taking place with:

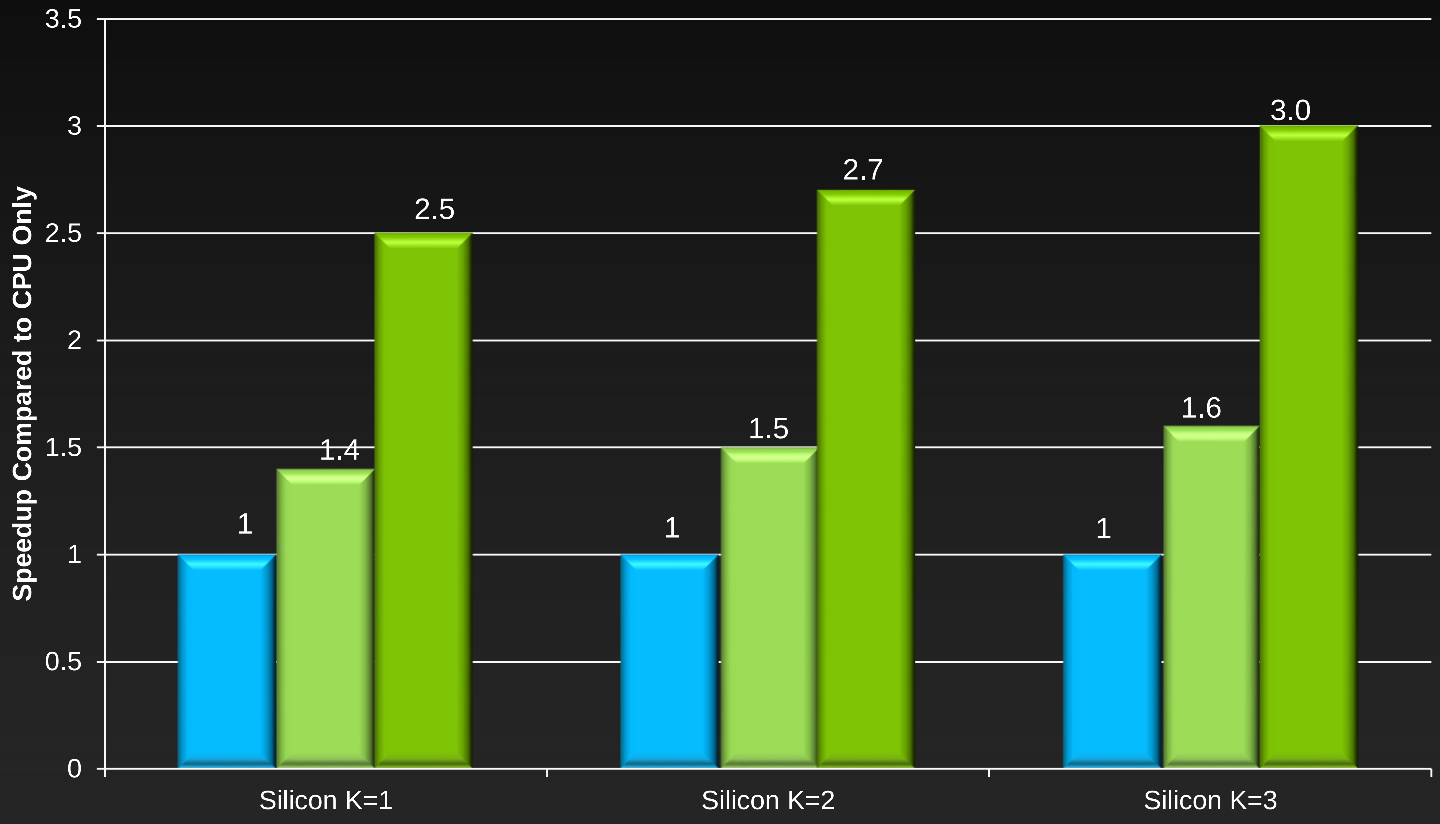
Hewlett-Packard (HP) Series SL2500 Servers (Intel® Xeon® E5-2680 v2 (2.8GHz/10-core/25MB/8.0GT-s QPI/115W, DDR3-1866)

NVIDIA® Tesla® GPUs (K40 and later)

PGI Accelerator Compilers (16.x) with OpenACC (2.5 standard)

GPAW

Increase Performance with Kepler

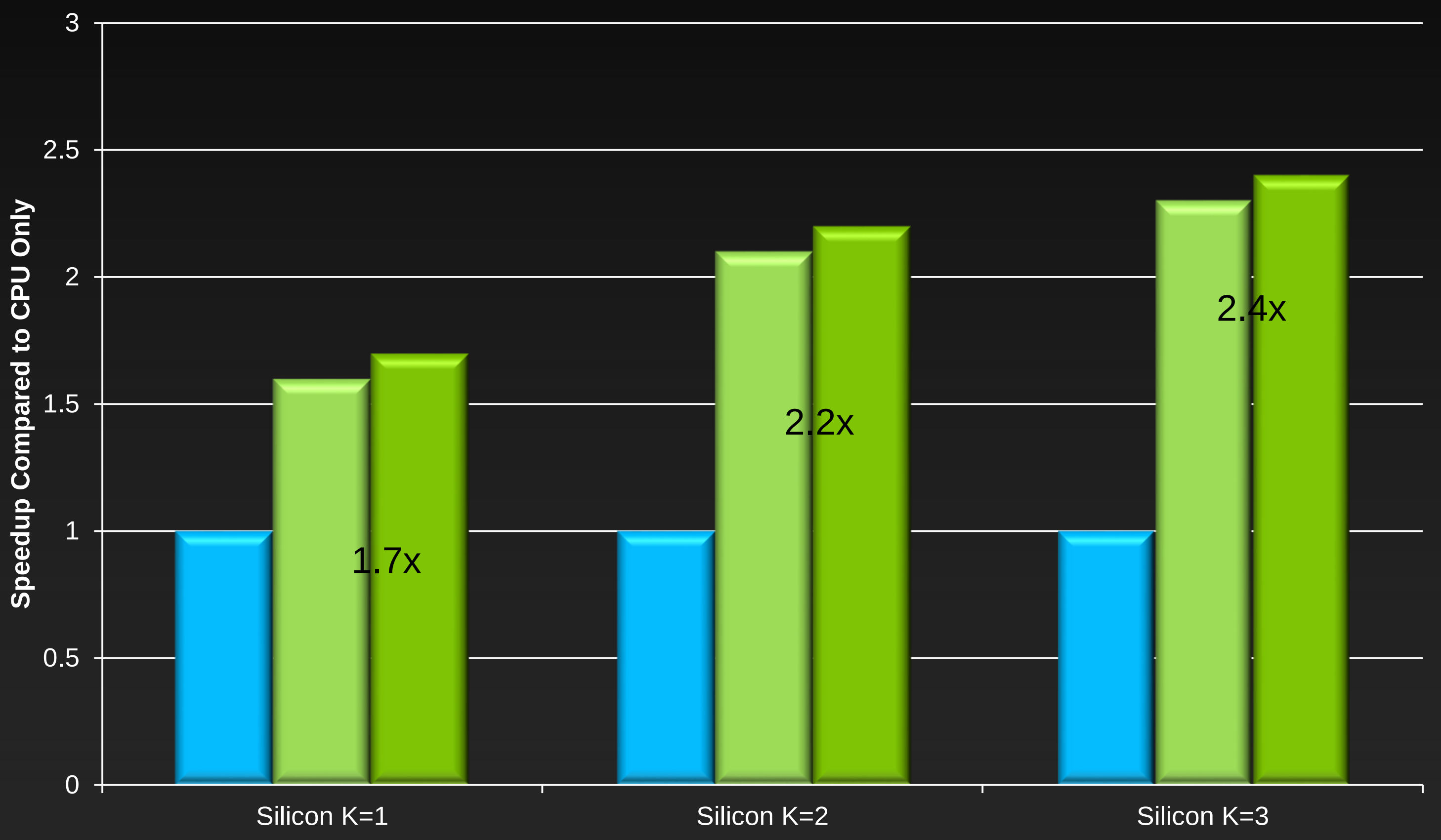


Running GPAW 10258

The blue nodes contain 1x E5-2687W CPU (8 Cores per CPU).

The green nodes contain 1x E5-2687W CPU (8 Cores per CPU) and 1x or 2x NVIDIA K20X for the GPU.

Increase Performance with Kepler



Running GPAW 10258

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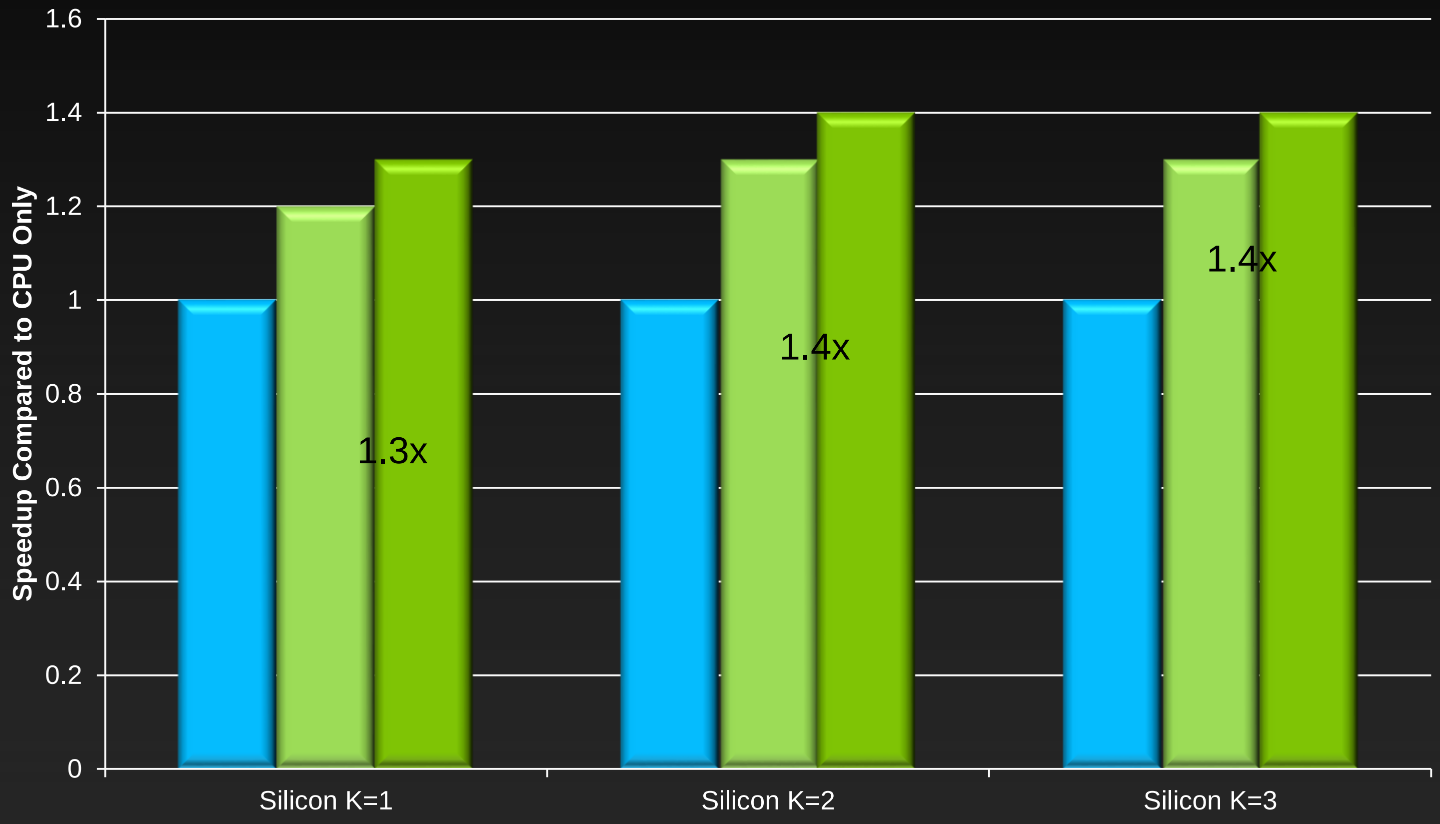
The green nodes contain 1x E5-2687W CPUs (8 Cores per CPU) and 2x NVIDIA K20 or K20X for the GPU.

Increase Performance with Kepler



Running GPAW 10258

The blue nodes contain 2x E5-2687W CPUs (8 Cores per CPU).

The green nodes contain 2x E5-2687W CPUs (8 Cores per CPU) and 2x NVIDIA K20 or K20X for the GPU.

Multi-GPU Accelerated Large Scale Electronic Structure Calculations

Used with permission from Samuli Hakala

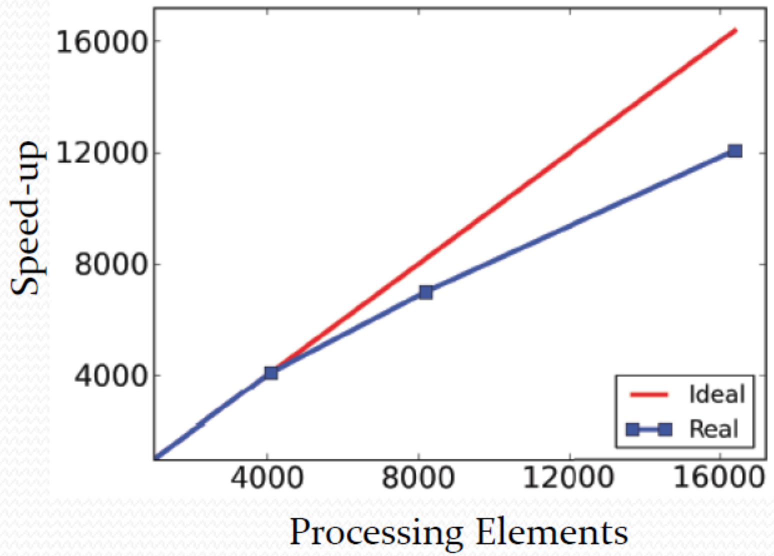
Samuli Hakala
COMP Centre of Excellence
Department of Applied Physics
Aalto University School of Science
Email: samuli.hakala@aalto.fi

GPU Technology Conference, March 2013

Aalto University
School of Science

GPAW

- Density Functional Theory (DFT) program package for electronic structure calculations
- Time-Dependent Density Functional Theory (TDDFT) is implemented in the linear response and time propagation schemes
- Can use real-space grids, atom centered basis functions or plane waves
- Random Phase Approximation (RPA) also available
- Scales to thousands of cores and suitable for large scale calculations
- Open Source software licensed under GPL



Ground state DFT calculation of 561 Au atom cluster on Blue Gene/P.

LibXC on GPUs

- A reusable library of >250 exchange-correlation functionals
- Used by 15 different codes (Abinit, GPAW, BigDFT, etc.)
- Can be a performance bottleneck for small systems
- Can "clone" existing functionals for GPU use with fairly minimal changes to existing LibXC code and parallelizes well over grid points
- More information:
  - https://confluence.slac.stanford.edu/display/SUNCAT/libxc+on+GPUs
- Work by Lin Li, Jun Yan, Christopher O'Grady (Stanford/SLAC)

Functional	Type	Speedup ((GPU+CPU)/CPU)
PW, PW Mode, OB PW, PW RPA	LDA Correlation	23,23,23,37
PBE, PBE sol, xPBE, PBE JRGX, RGE2, APBE	GGA Correlation	56, 58, 58, 58, 58, 58
RPBE	GGA Exchange	95
TPSS	MGGA Exchange	51

Ground State Performance

Bulk Silicon

- 95 atoms with periodic boundary conditions, 380 bands and 1 k-point. Grid size: 56x56x80.
- Time is in seconds per one SCF iteration.
- Intel Xeon X5650, NVIDIA Tesla M2070

Si95	CPU	GPU	%	S-Up
Poisson Solver	1.8	0.13	1%	**14**
Orthonormalization	23	3.0	23%	**7.7**
Precondition	9.4	0.77	6%	**12**
RMM-DIIS other	32	3.2	25%	**10**
Subspace Diag	23	2.1	16%	**11**
Other	2.7	2.7	21%	**1.0**
Total (SCF-Iter)	93	13		9.7/7.7

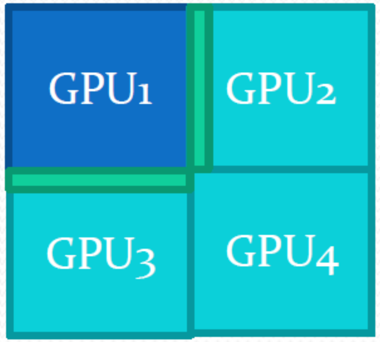
Fullerene

- C60 molecule with 240 valence electrons. Grid size: 84x84x84
- Intel Xeon X5650, NVIDIA Tesla M2070

C60	CPU	GPU	%	S-Up
	13	0.64	7%	**20**
	11	1.2	13%	**9.2**
	16	0.99	11%	**16**
	8.1	0.6	7%	**13**
	22	2.1	23%	**10**
	3.5	3.2	35%	**1.1**
	76	9.1		13/8.3

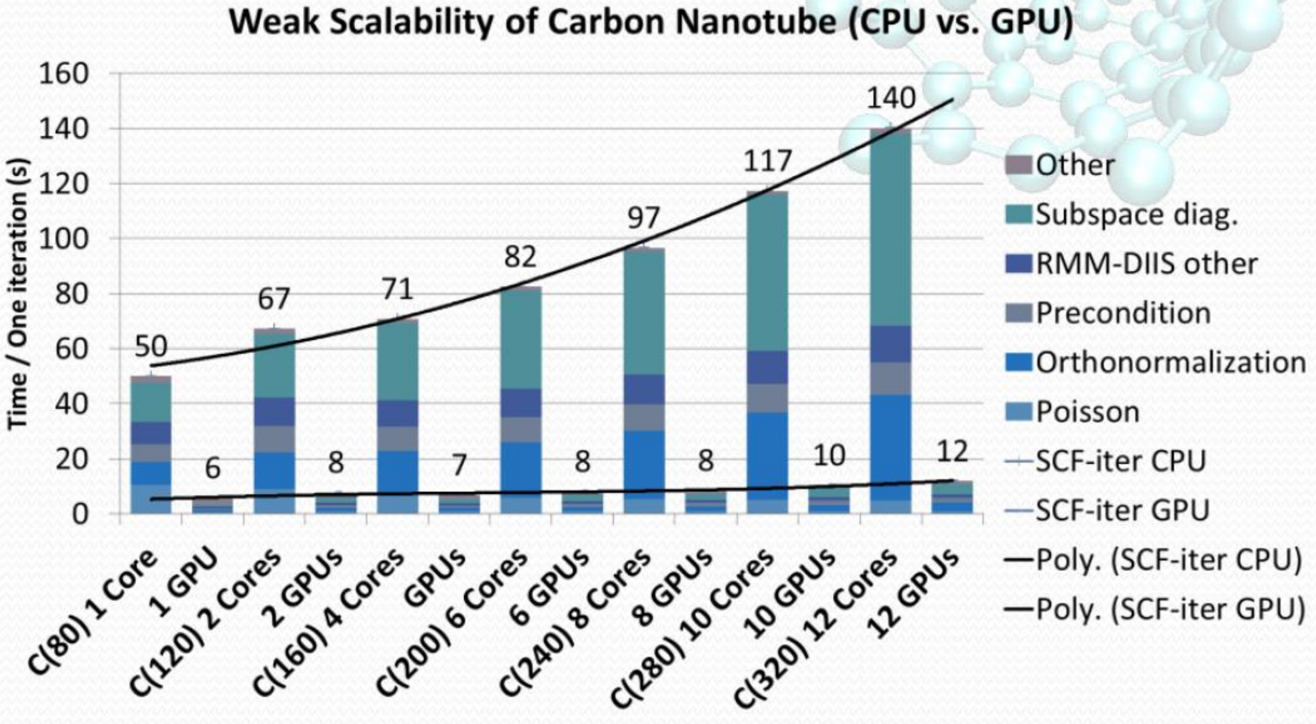
Multi-GPU Parallelization

- Parallelization is done with MPI
- Multiple GPUs can be used by domain decomposition or parallelization over k-points or spins
- Domain decomposition for the stencil operations involves exchanging boundary regions between neighboring nodes
- Communications between nodes require data movement: device memory → host memory → destinations node host memory → destinations node device memory.
- Overlaps receives, sends and computations in the middle part of the grid, BUT this causes issues with small grids
  - Small grids: Synchronous transfers
  - Medium grids: Asynchronous transfers
  - Large grids: Overlap calculations and asynchronous transfers
  - Combine of several wave functions and boundary regions into few large transfers



Weak Scalability (Carbon)

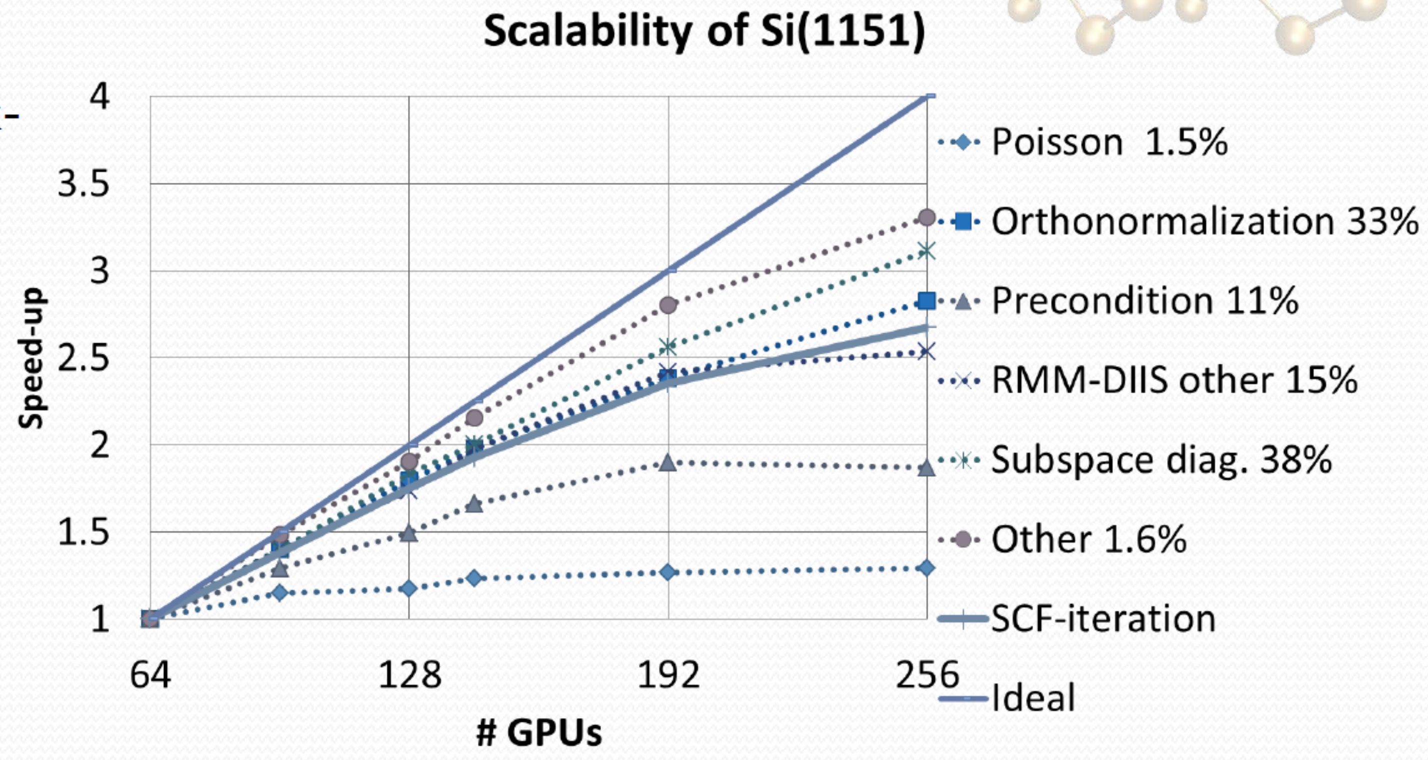
- The size of a carbon nanotube and the number of MPI tasks are varied from 80 atoms (240 states) to 320 atoms (1280 states) and 1 task to 12 tasks.
- Comparison between equal number of GPUs and CPU cores.
- CPU: Intel Xeon X5650 GPU: NVIDIA Tesla M2070
- Calculations performed on Vuori cluster at CSC



# MPI tasks	1	2	4	6	8	10	12
Speed-Up	8.8	8.7	10.5	10.2	11.5	11.3	11.9

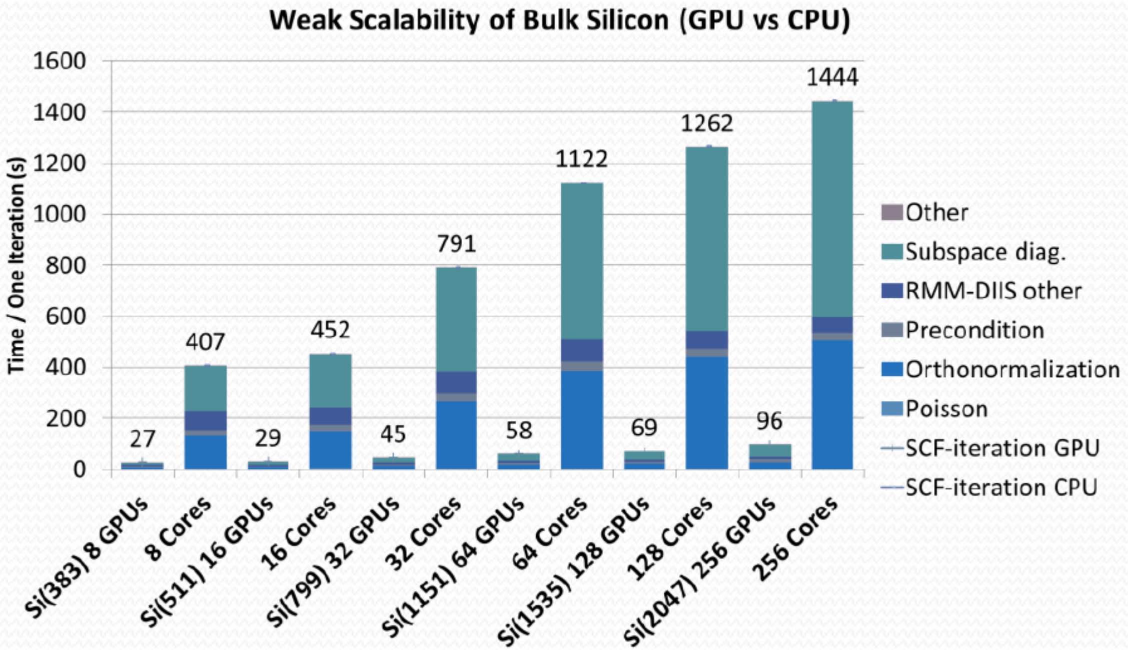
Strong Scalability

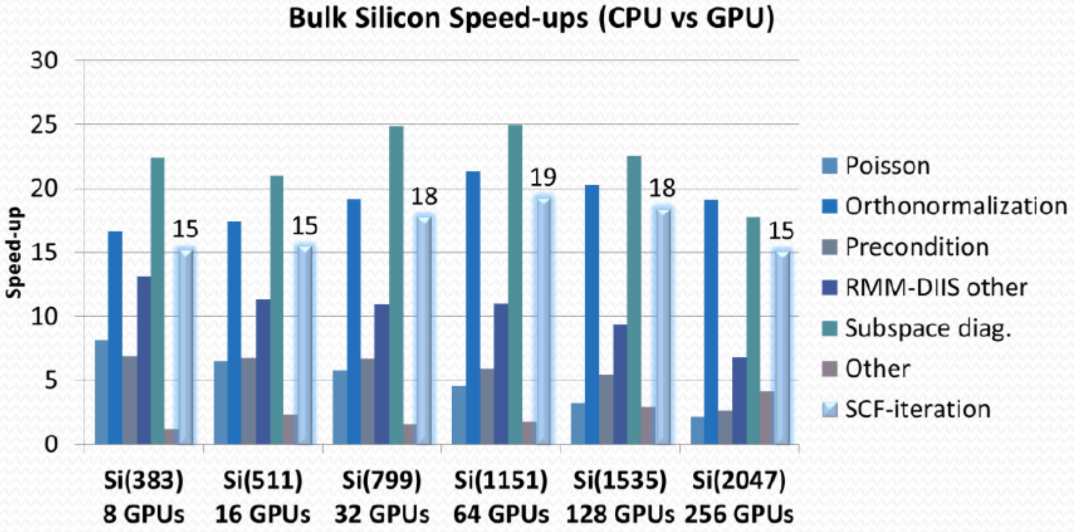
- Bulk silicon with 1151 atoms with periodic boundary conditions, 4604 bands and 1 k-point in the Brillouin zone.
- The number of GPUs is increased from 64 to 256.
- Grid size: 164x164x108
- Speed-up comparison to 64 GPUs.
- NVIDIA Tesla M2090
- Calculations performed on CURIE cluster in France at GENCI/CEA



Weak Scalability (Silicon)

- The size of bulk silicon system and the number of MPI tasks are varied from 383 atoms (1532 bands) to 2046 atoms (8188 bands) and 8 task to 256 tasks with periodic boundary conditions.
- The largest system requires about 1.3TB of memory for calculations.
- CPU: Intel Xeon E5640 GPU: NVIDIA Tesla M2090





Random Phase Approximation

GPAW Random Phase Approximation (RPA) code:

- 6000 lines of python, 1000 lines of C/CUDA (and re-uses many GPAW functions)
- Better than DFT for correlated materials, but more computationally expensive
- Useful for oxides, Van der Waals systems, etc.

GPU Techniques:

- Use BLAS3 "zherk" instead of BLAS2 "zher"
- Batch FFTs
- GPU kernels parallelized over atoms/bands/projector-functions
- No thunking: all calculations on GPU

Preliminary ((GPU+CPU)/CPU) speedup for 202-electron N_2-on-Ru: 30x

Work by Jun Yan, Lin Li, Christopher O'Grady (Stanford/SLAC)

Summary

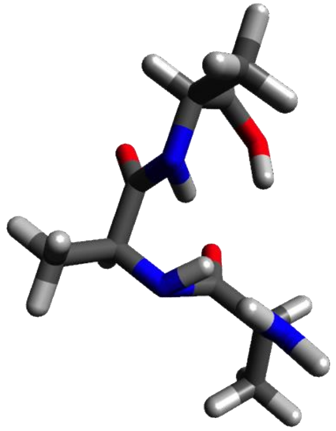
- We have accelerated the most numerically intensive parts of ground state DFT calculations
- Overall speed-ups in our tests varied from 8.8 to 19 depending on system size.
- Our multi-GPU implementation scales well even on large hybrid clusters.
- Code is available at GPAW Subversion repository.
- Acknowledgements to CSC and PRACE for computing resources

Hakala S., Havu V., Enkovaara J., Nieminen R. M. ”Parallel Electronic Structure Calculations Using Multiple Graphics Processing Units (GPUs)” In: Manninen, P., Öster, P. (eds.) PARA 2012. LNCS, vol. 7782, pp. 63--76. Springer, Heidelberg (2013)

LSDALTON

LSDALTON

Large-scale application for calculating high-accuracy molecular energies



"*OpenACC makes GPU computing approachable for domain scientists. Initial OpenACC implementation required only minor effort, and more importantly, no modifications of our existing CPU implementation.*"

Janus Juul Eriksen, PhD Fellow
qLEAP Center for Theoretical Chemistry, Aarhus University

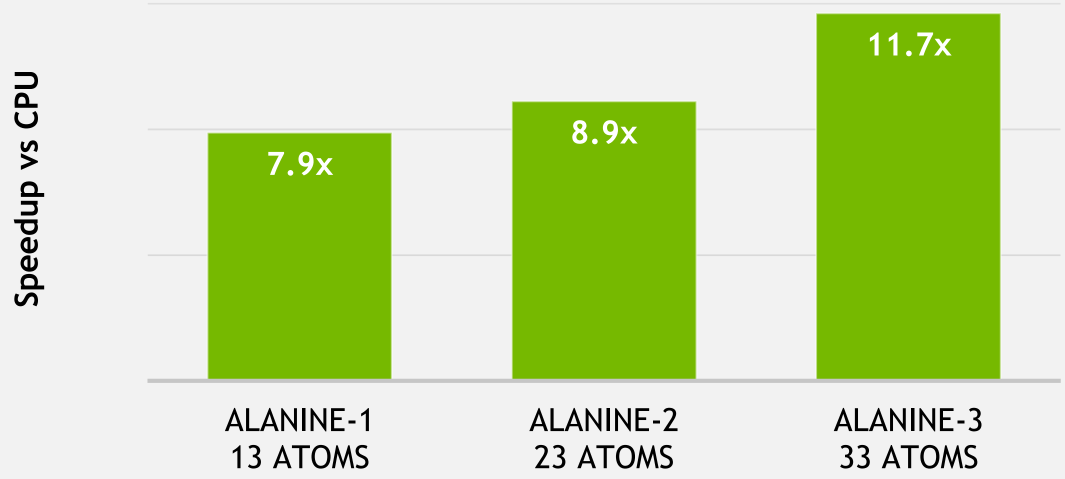
Minimal Effort

Lines of Code Modified	# of Weeks Required	# of Codes to Maintain
<100 Lines	1 Week	1 Source

Big Performance

LS-DALTON CCSD(T) Module

Benchmarked on Titan Supercomputer (AMD CPU vs Tesla K20X)



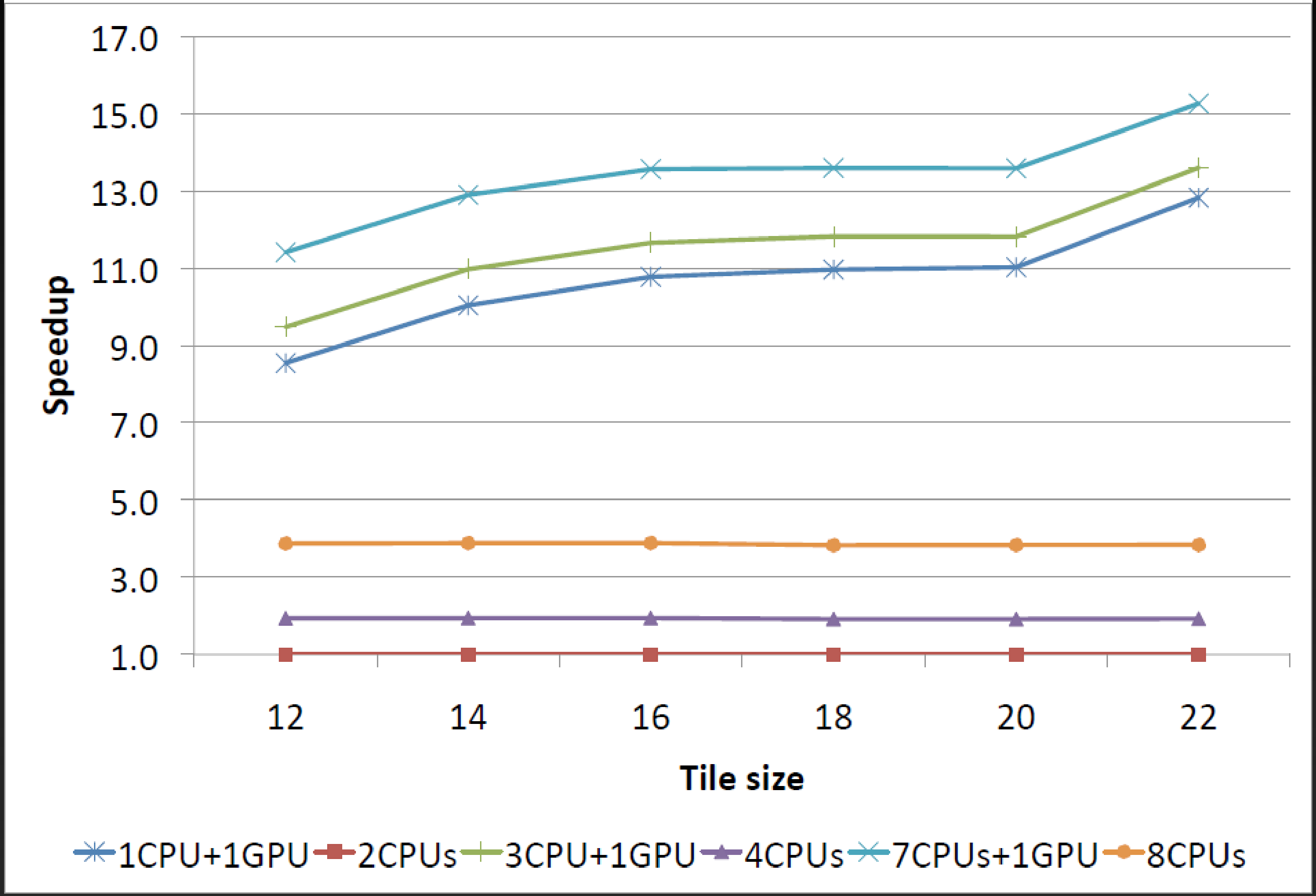
https://developer.nvidia.com/openacc/success-stories

NWChem

NWChem 6.3 Release with GPU Acceleration

- Addresses large complex and challenging molecular-scale scientific problems in the areas of catalysis, materials, geochemistry and biochemistry on highly scalable, parallel computing platforms to obtain the fastest time-to-solution
- Researchers can for the first time be able to perform large scale coupled cluster with perturbative triples calculations utilizing the NVIDIA GPU technology. A highly scalable multi-reference coupled cluster capability will also be available in NWChem 6.3.
- The software, released under the Educational Community License 2.0, can be downloaded from the NWChem website at www.nwchem-sw.org

NWChem - Speedup of the non-iterative calculation for various configurations/tile sizes



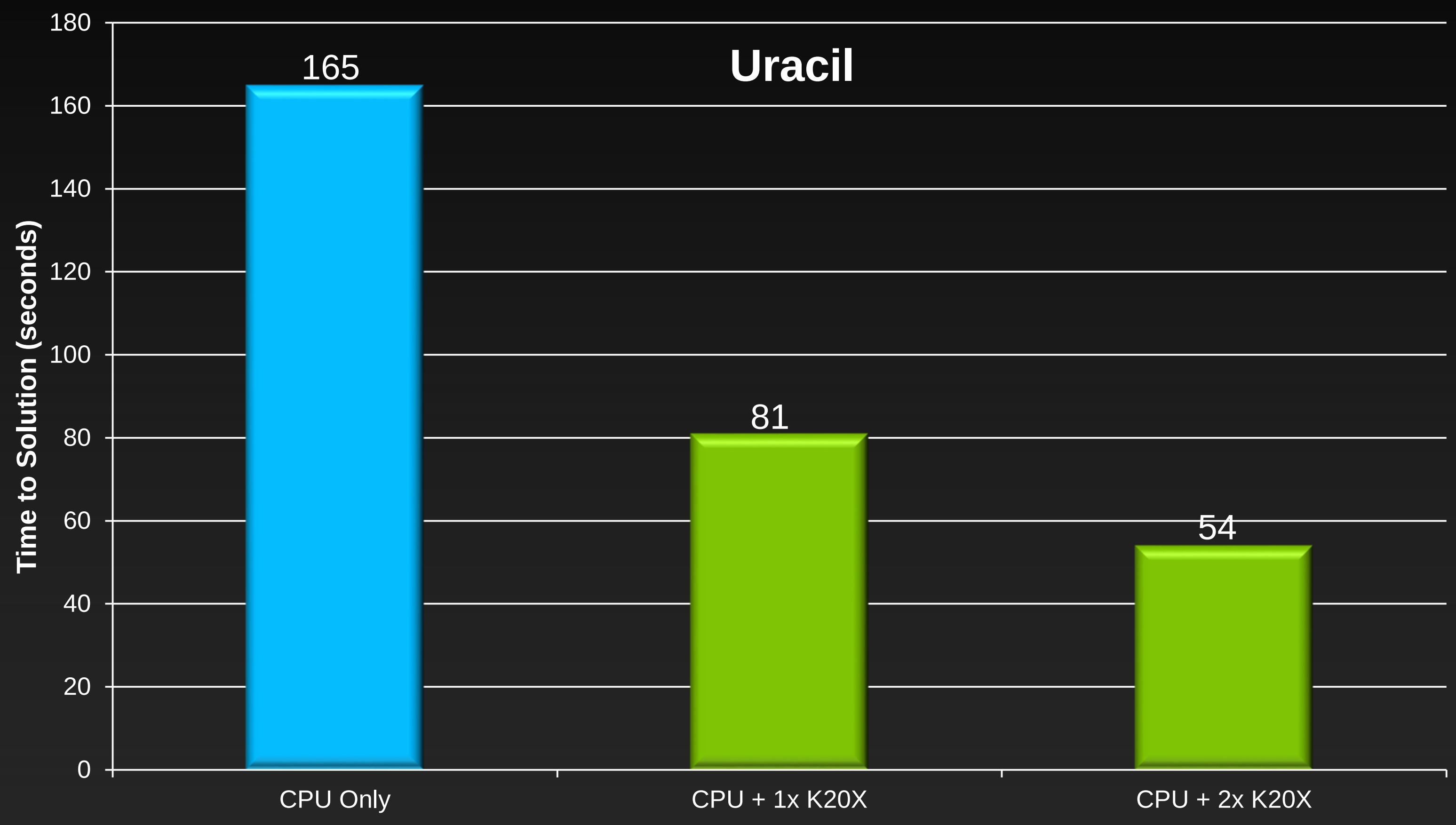
System: cluster consisting of dual-socket nodes constructed from:

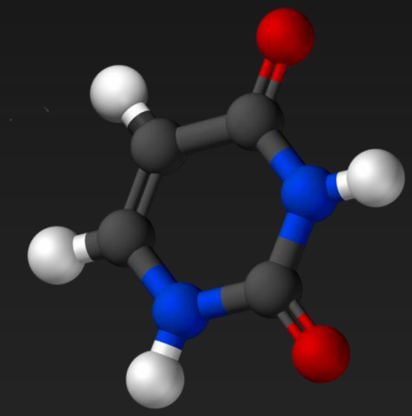
- 8-core AMD Interlagos processors
- 64 GB of memory
- Tesla M2090 (Fermi) GPUs

The nodes are connected using a high-performance QDR Infiniband interconnect

Courtesy of Kowolski, K., Bhaskaran-Nair, at al @ PNNL, JCTC (submitted)

Kepler, Faster Performance (NWChem)





Uracil Molecule

Performance improves by 2x with one GPU and by 3.1x with 2 GPUs

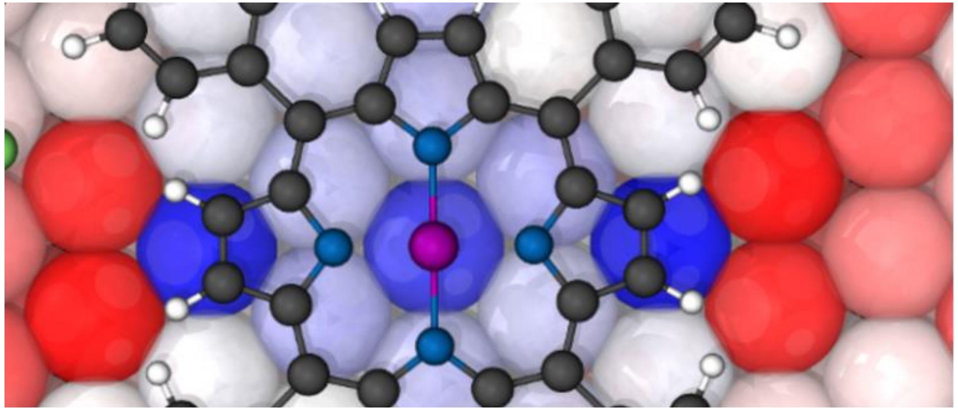
Quantum Espresso 5.4.0

December 2016

NVIDIA

QUANTUM ESPRESSO

Quantum Chemistry Suite



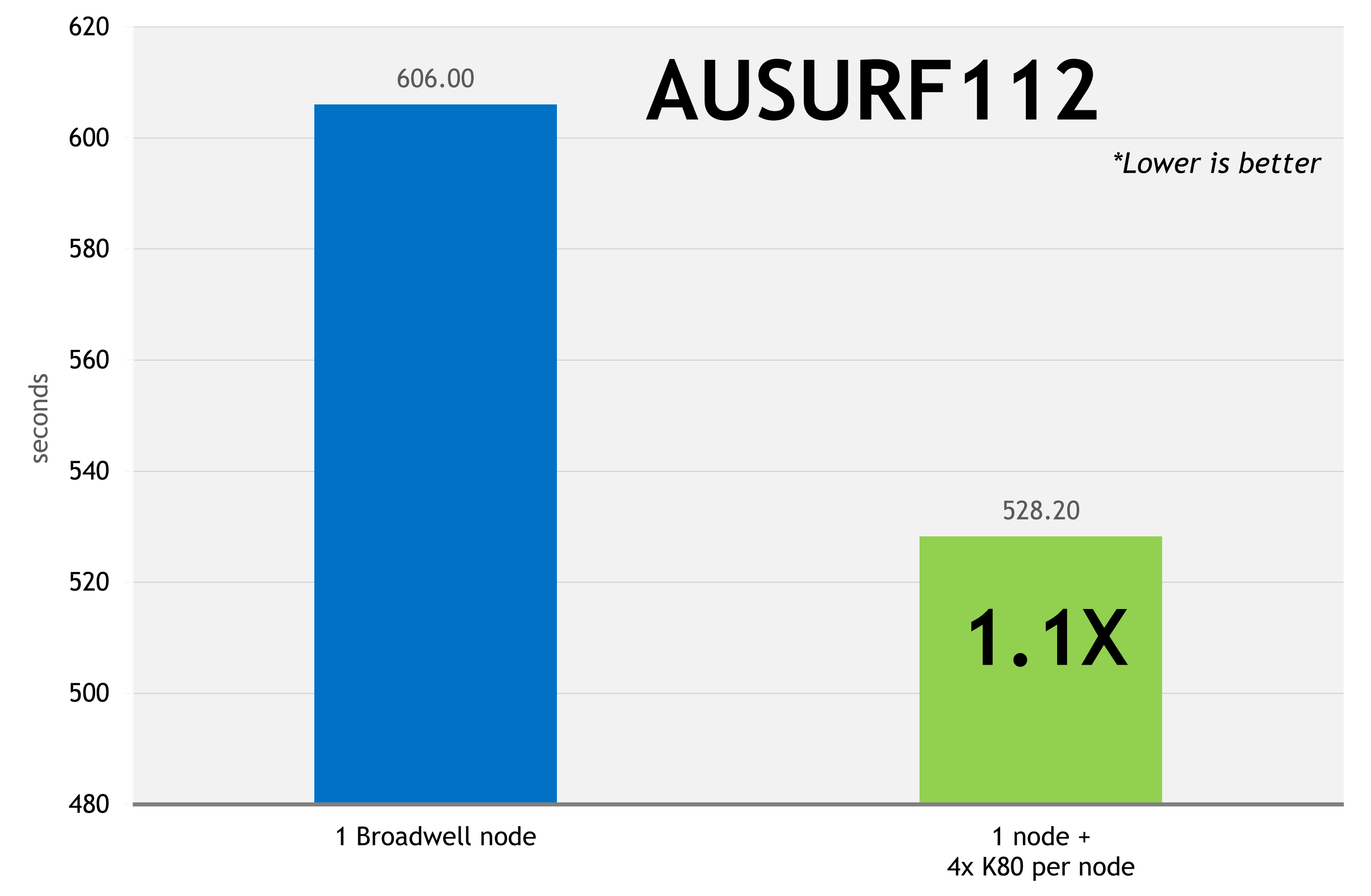
QUANTUMESPRESSO

www.quantum-espresso.org

Filippo Spiga
Head of Research Software Engineering
University of Cambridge

"CUDA Fortran gives us the full performance potential of the CUDA programming model and NVIDIA GPUs. !$CUF KERNELS directives give us productivity and source code maintainability. It's the best of both worlds."

AUSURF112 on K80s

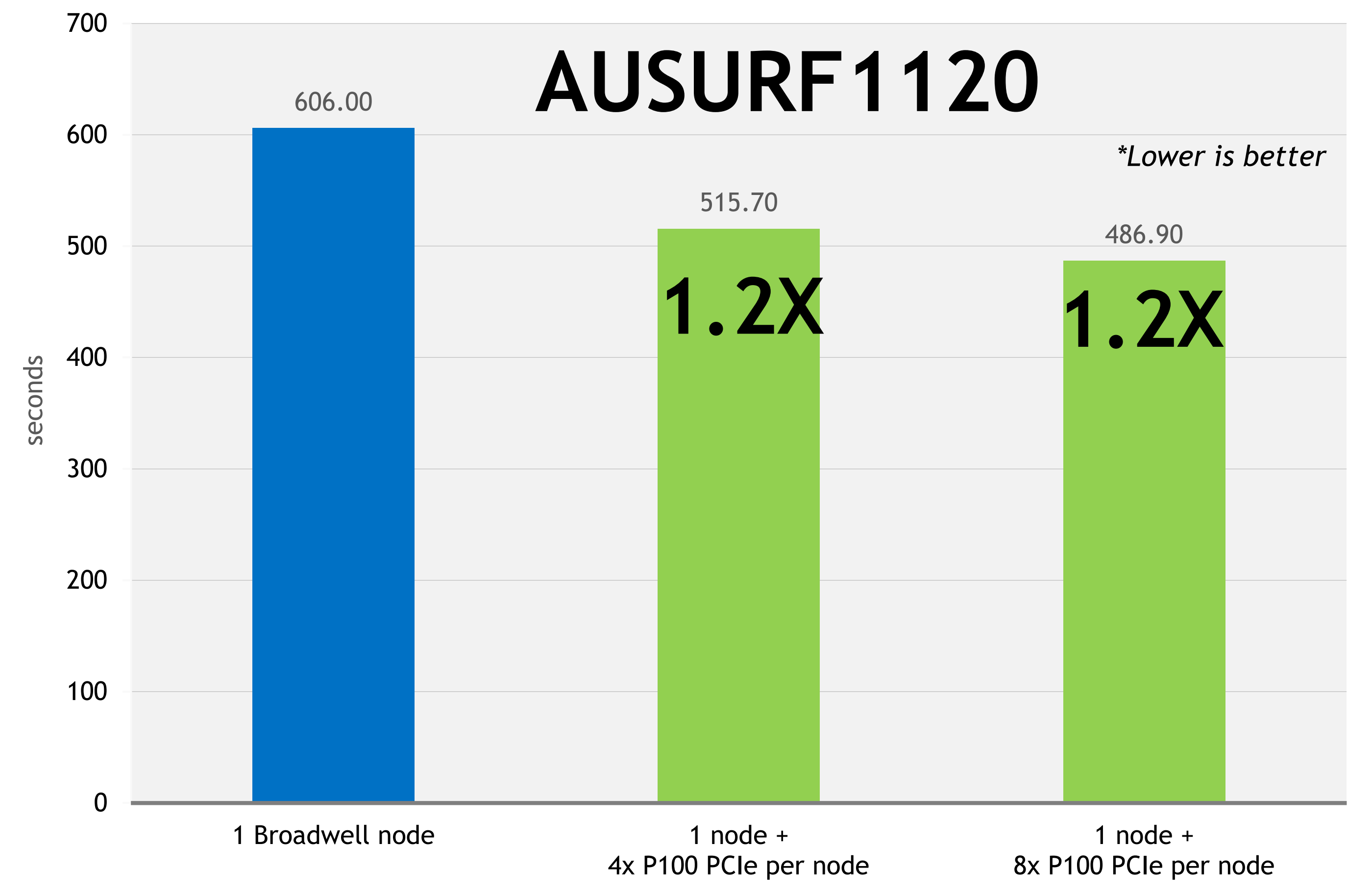


Running Quantum Espresso version 5.4.0

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

The green node contains Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla K80 (autoboost) GPUs

AUSURF112 on P100s PCIe



Running Quantum Espresso version 5.4.0

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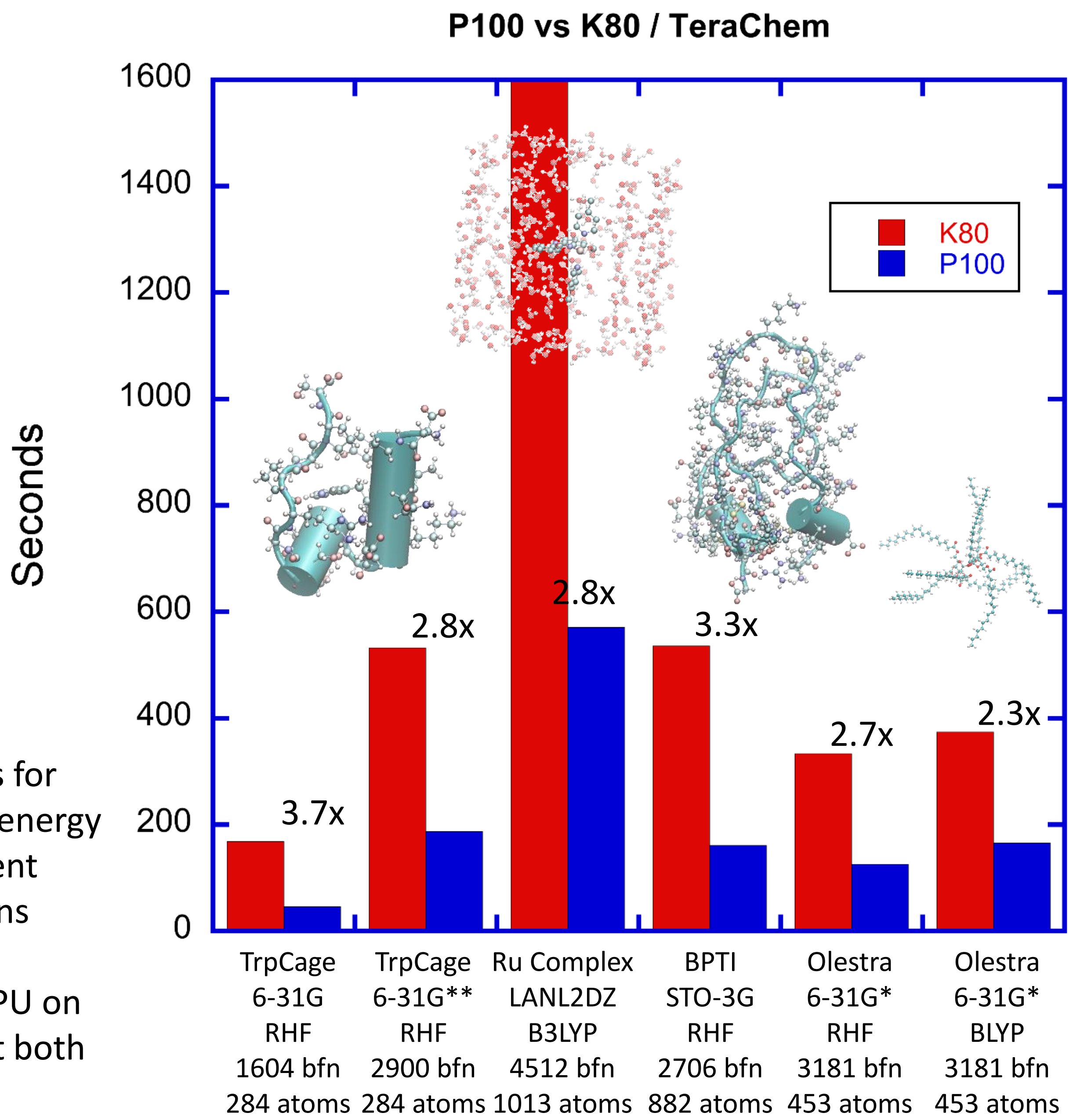
The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

TeraChem 1.5K

Speaker, Date

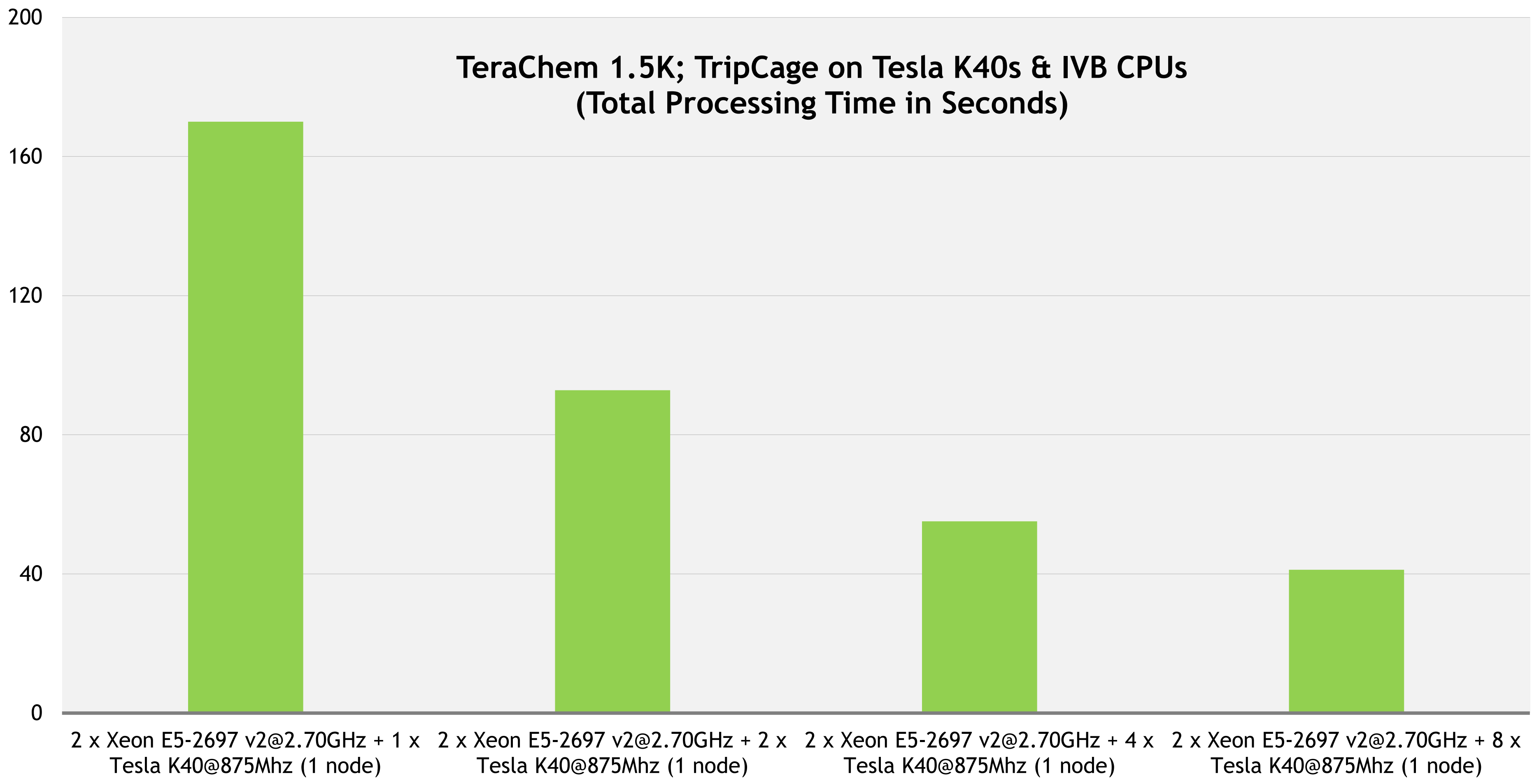


All timings for complete energy and gradient Calculations

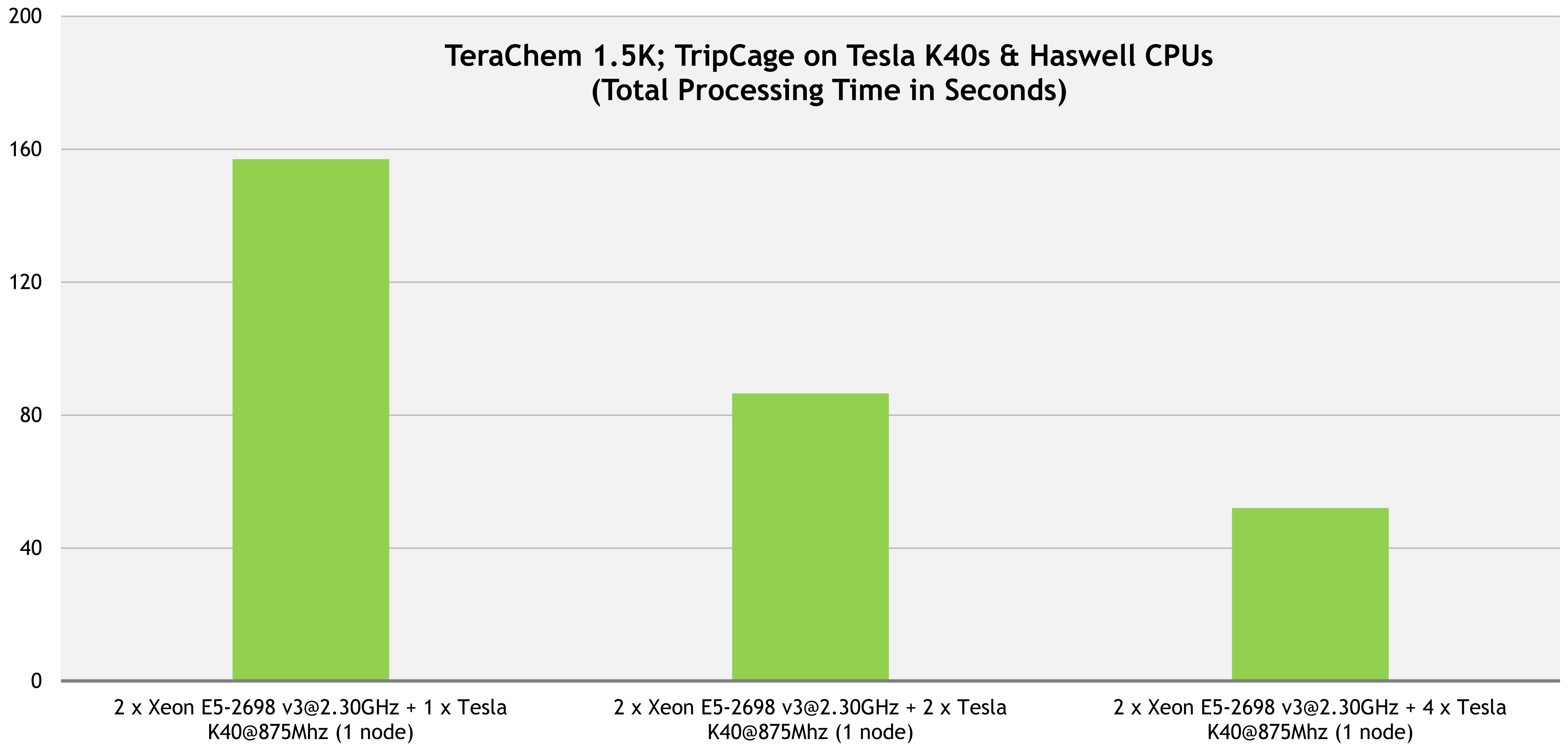
K80 = 1 GPU on Board, not both

Slide courtesy of PetaChem LLC / Todd Martinez

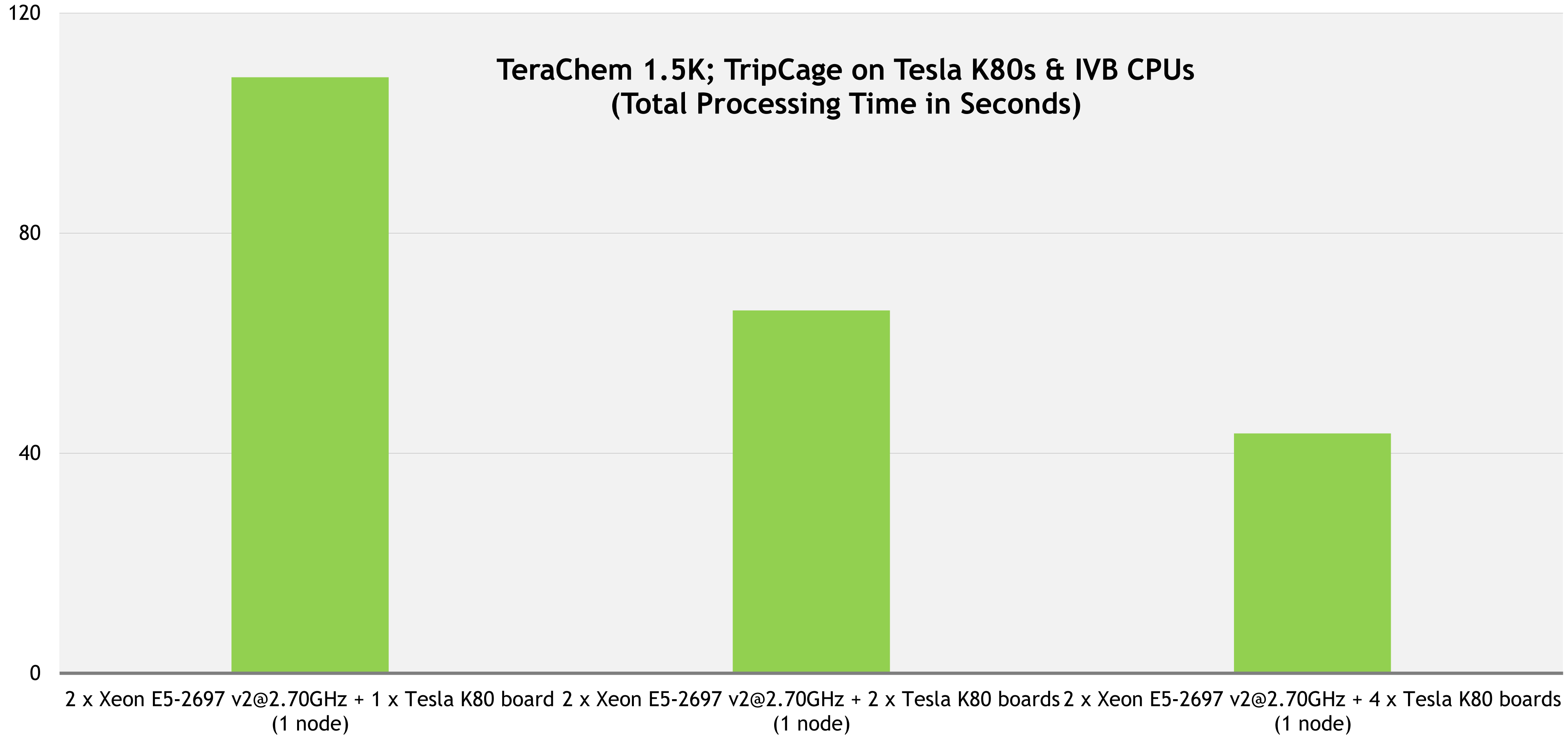
TERACHEM 1.5K; TRIPCAGE ON TESLA K40S



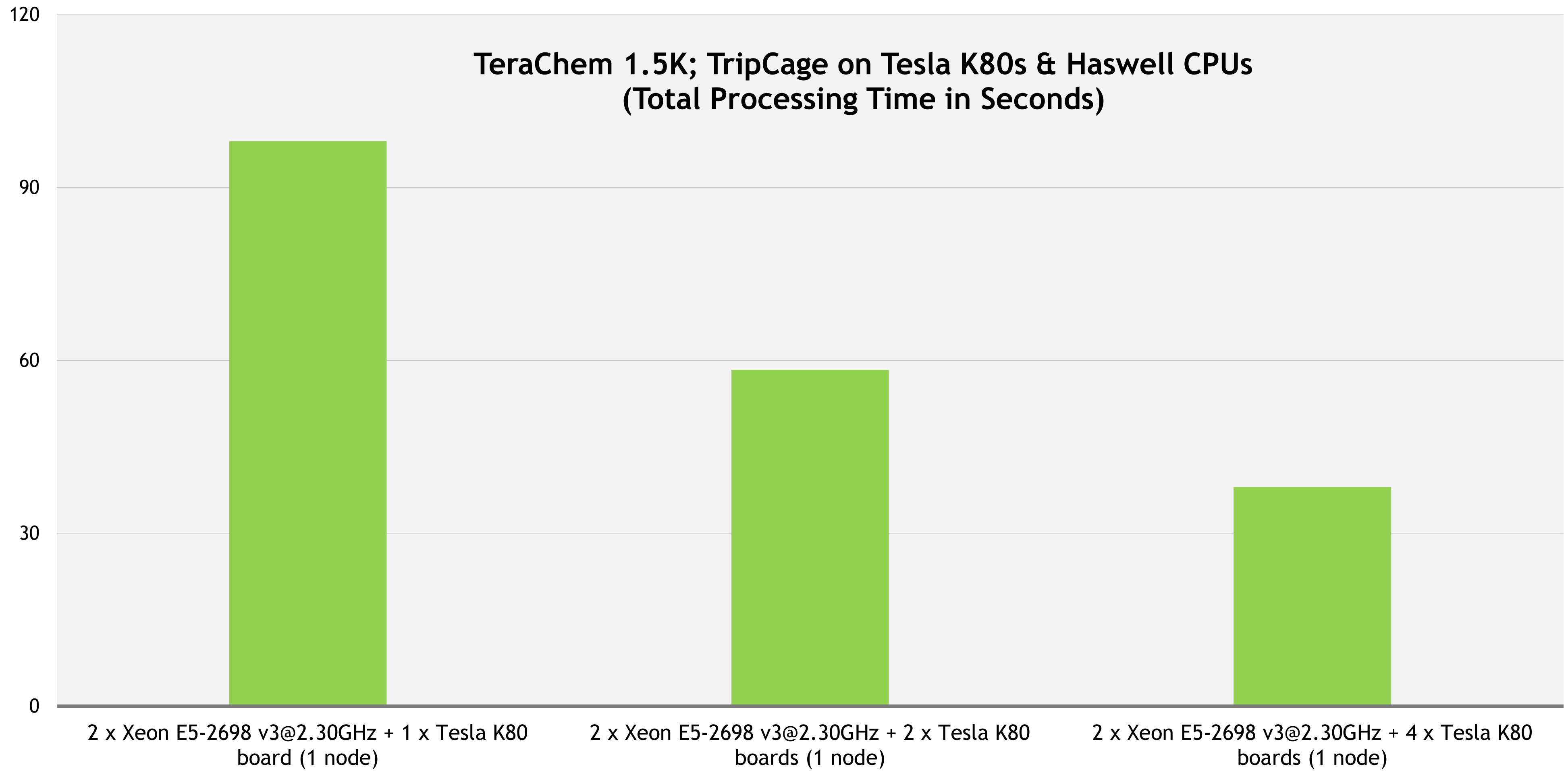
TERACHEM 1.5K; TRIPCAGE ON TESLA K40S & HASWELL CPUS



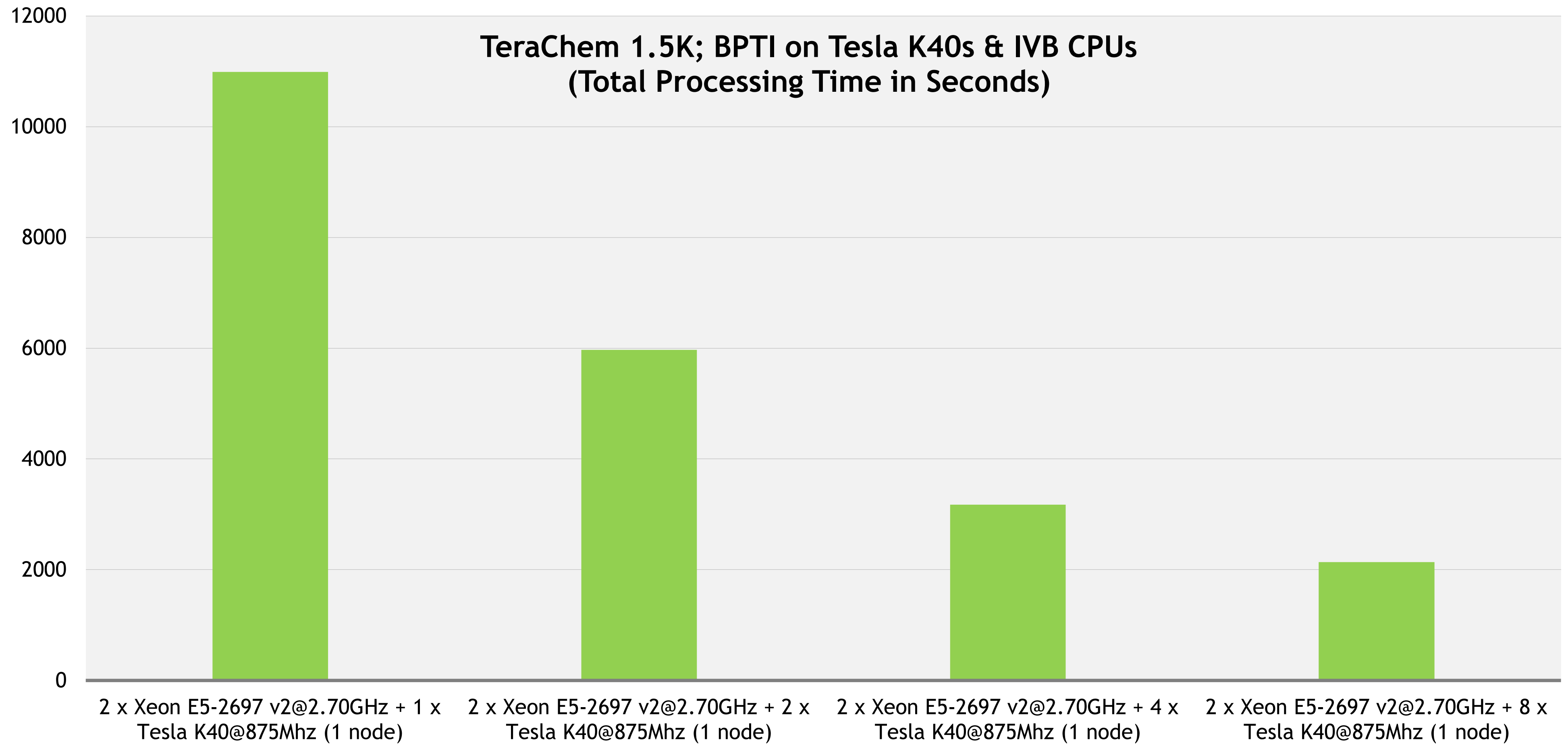
TERACHEM 1.5K; TRIPCAGE ON TESLA K80S & IVB CPUS



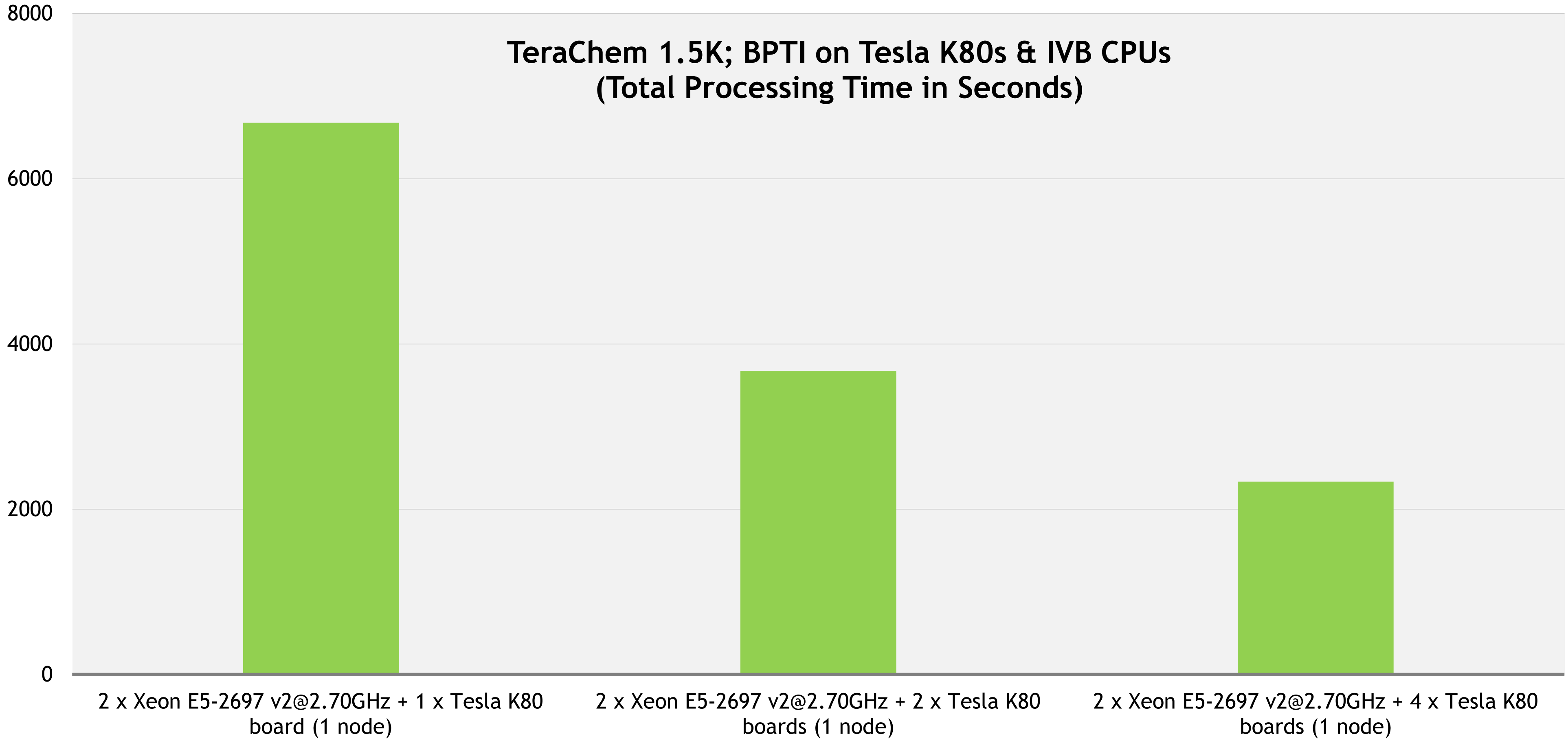
TERACHEM 1.5K; TRIPCAGE ON TESLA K80S & HASWELL CPUS



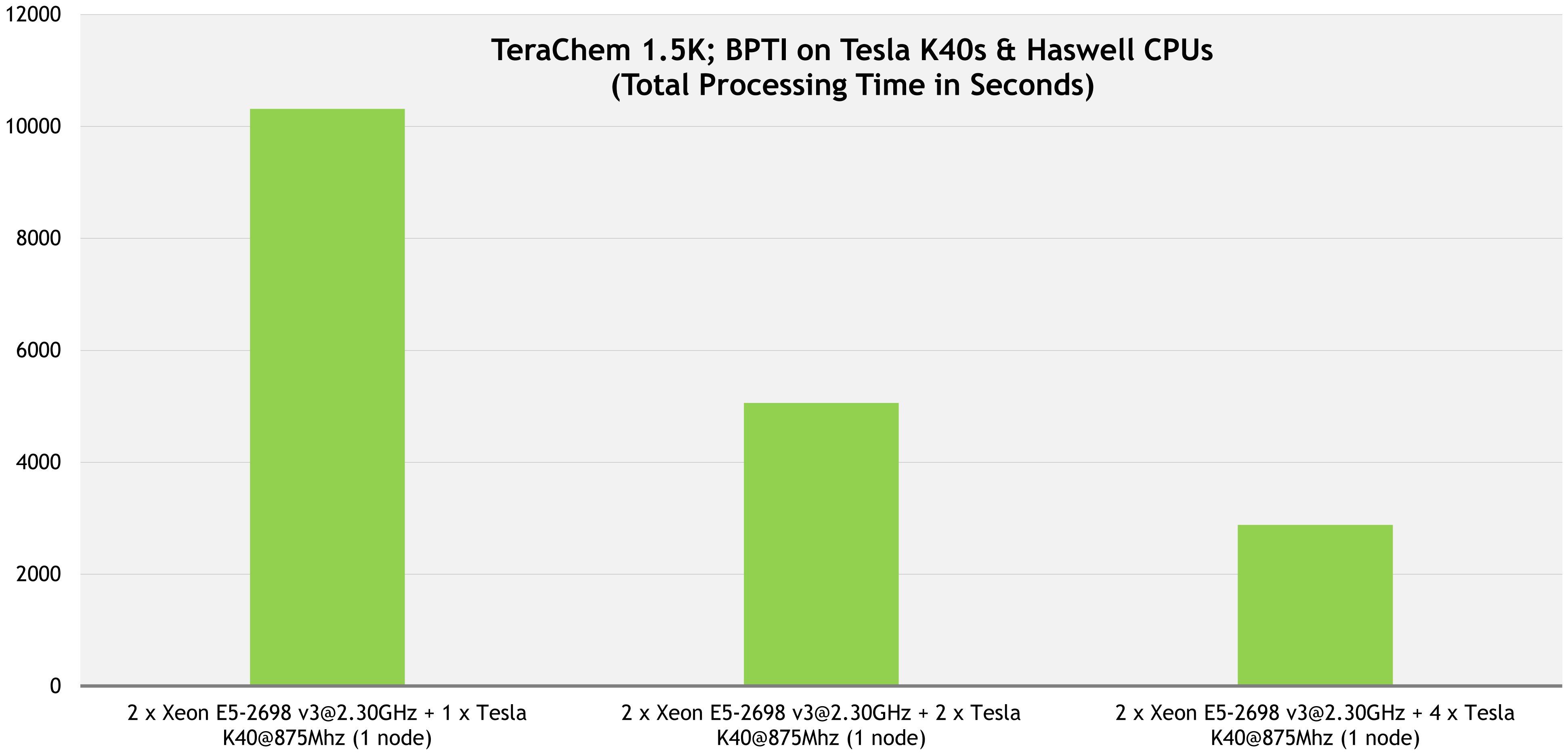
TERACHEM 1.5K; BPTI ON TESLA K40S & IVB CPUS



TERACHEM 1.5K; BPTI ON TESLA K80S & IVB CPUS



TERACHEM 1.5K; BPTI ON TESLA K40S & IVB CPUS



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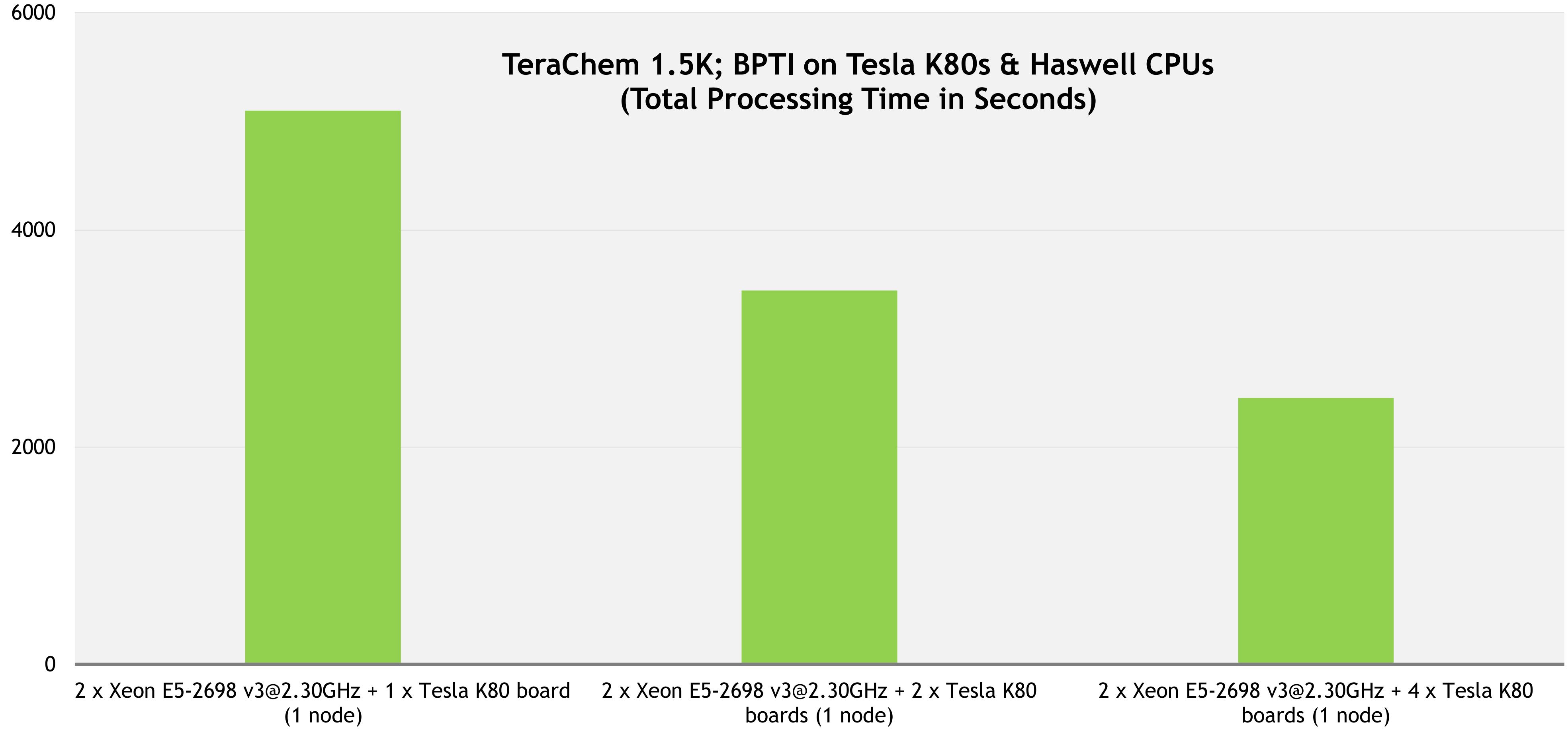
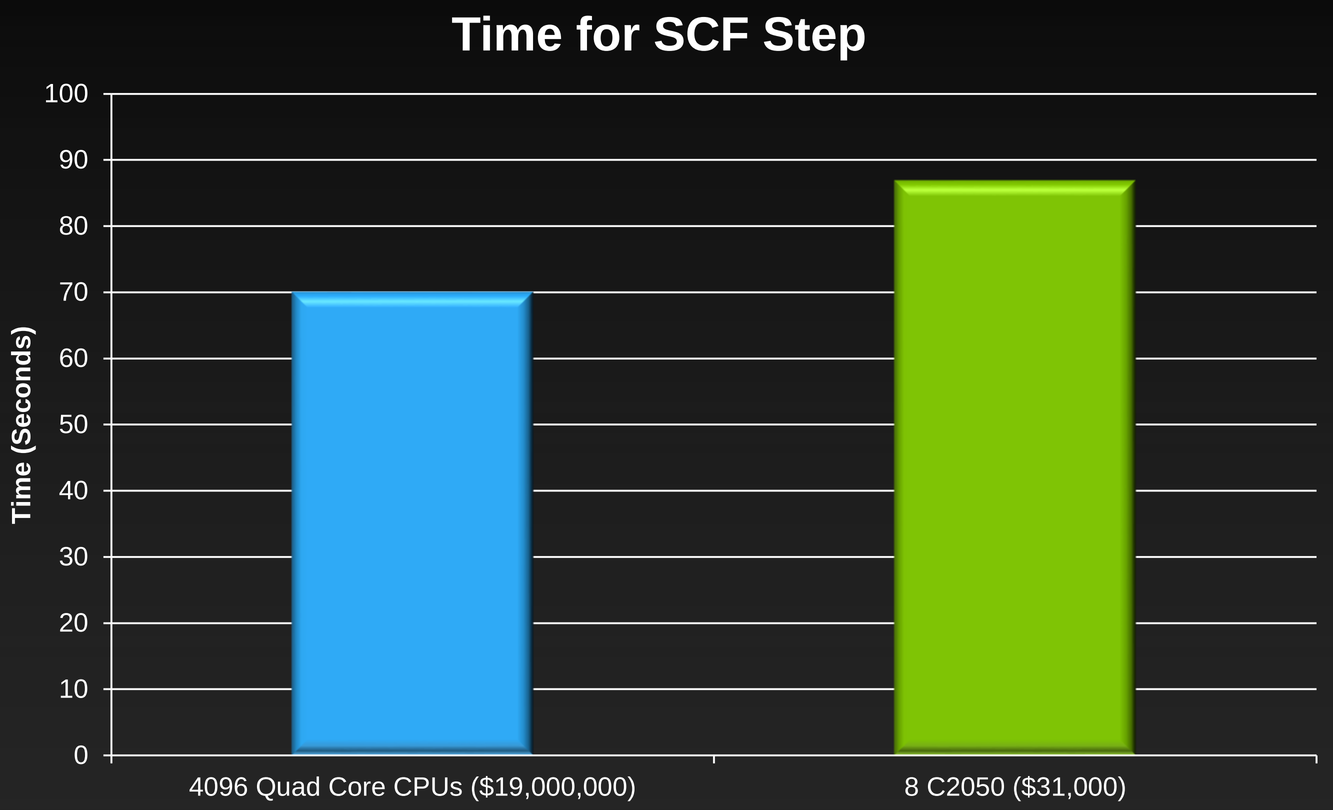


TeraChem
Supercomputer Speeds on GPUs

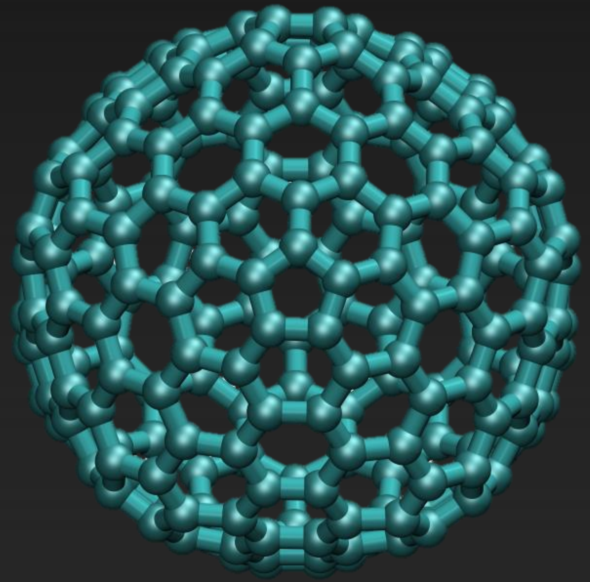


Similar performance from just a handful of GPUs

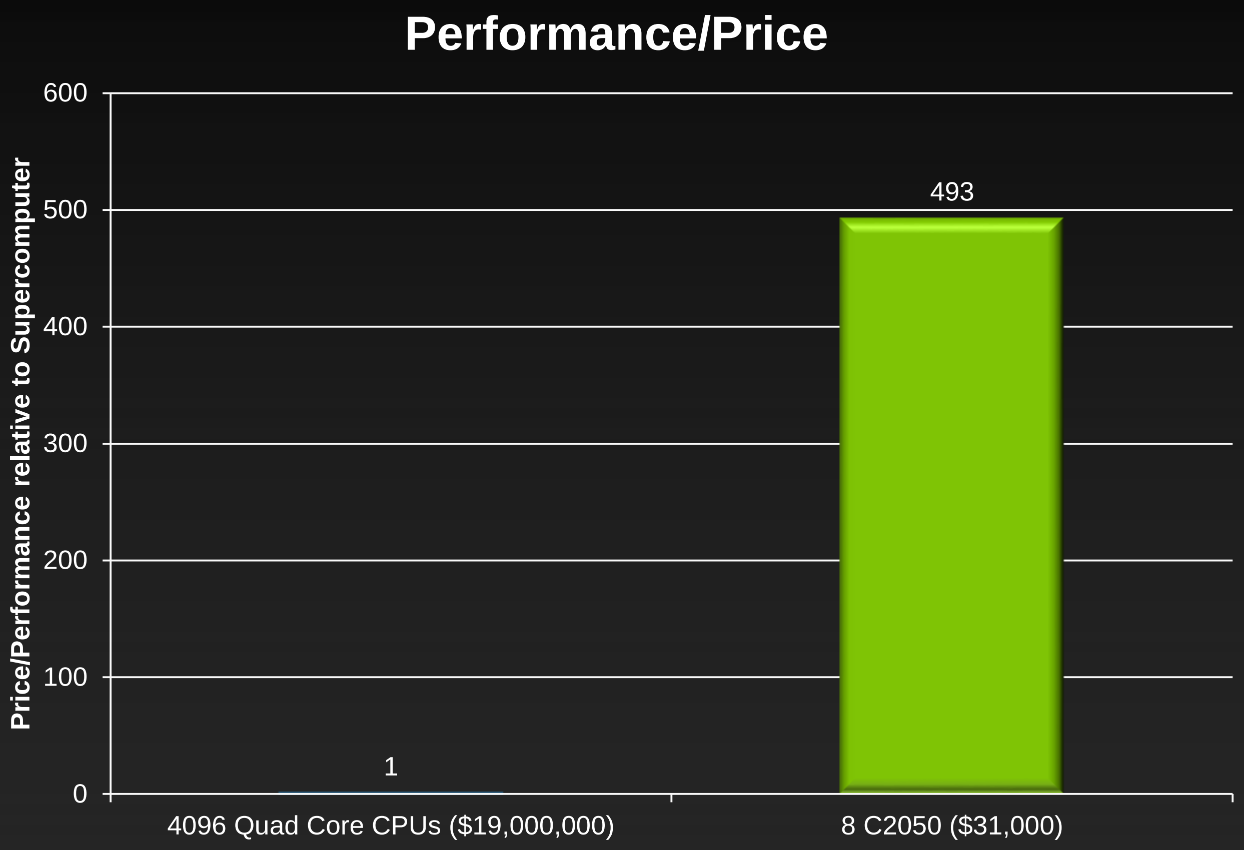
TeraChem running on 8 C2050s on 1 node

NWChem running on 4096 Quad Core CPUs
In the Chinook Supercomputer

Giant Fullerene C240 Molecule



TeraChem
Bang for the Buck

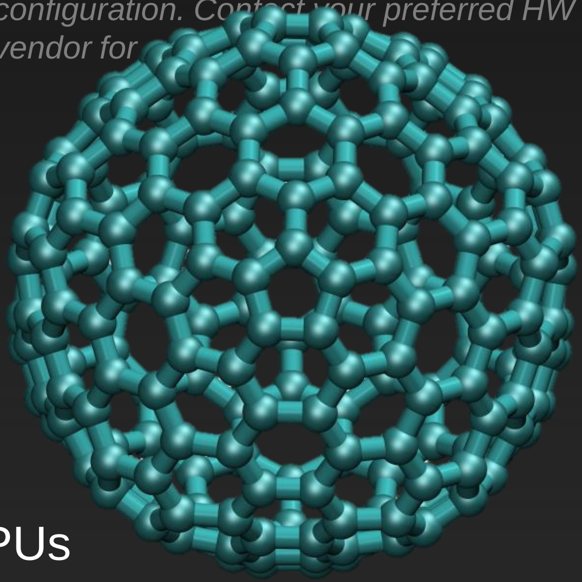


TeraChem running on 8 C2050s on 1 node

NWChem running on 4096 Quad Core CPUs
In the Chinook Supercomputer

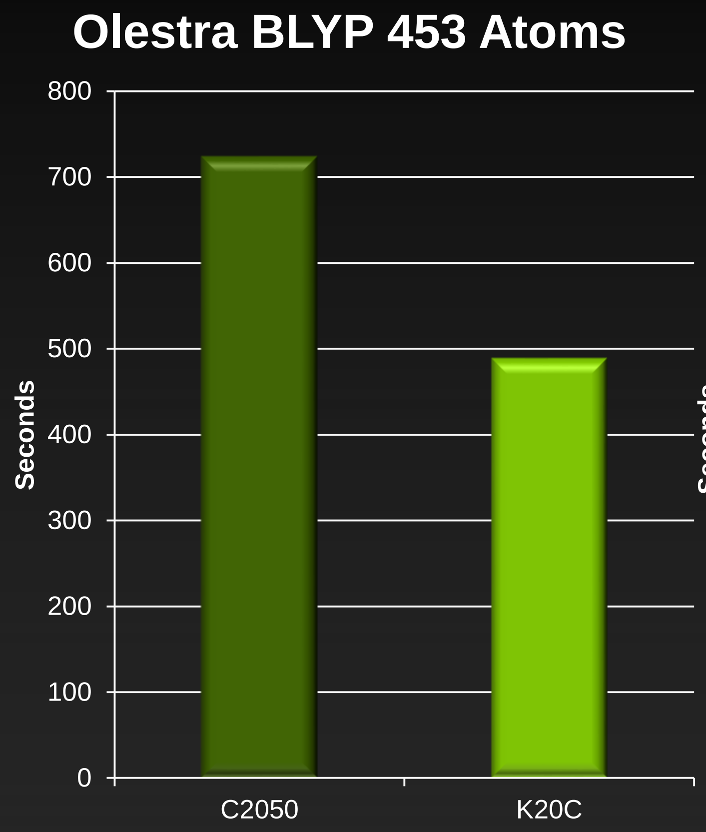
Giant Fullerene C240 Molecule

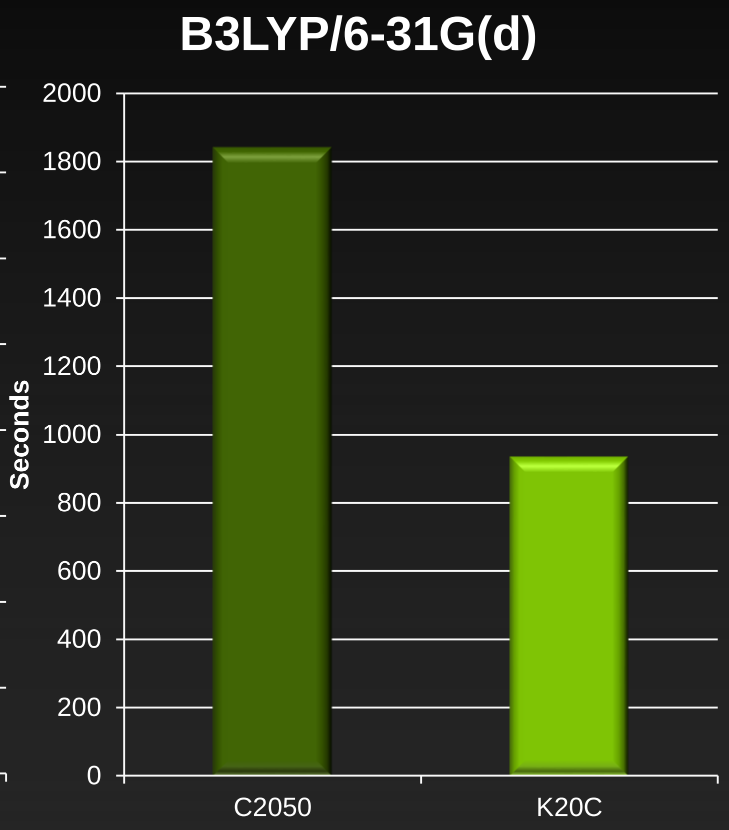
Note: Typical CPU and GPU node pricing used. Pricing may vary depending on node configuration. Contact your preferred HW vendor for



Dollars spent on GPUs do 500x more science than those spent on CPUs

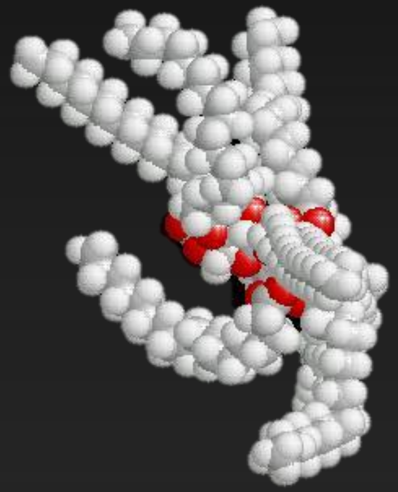
Kepler's Even Better





TeraChem running on C2050 and K20C

First graph is of BLYP/G-31(d)
Second is B3LYP/6-31G(d)

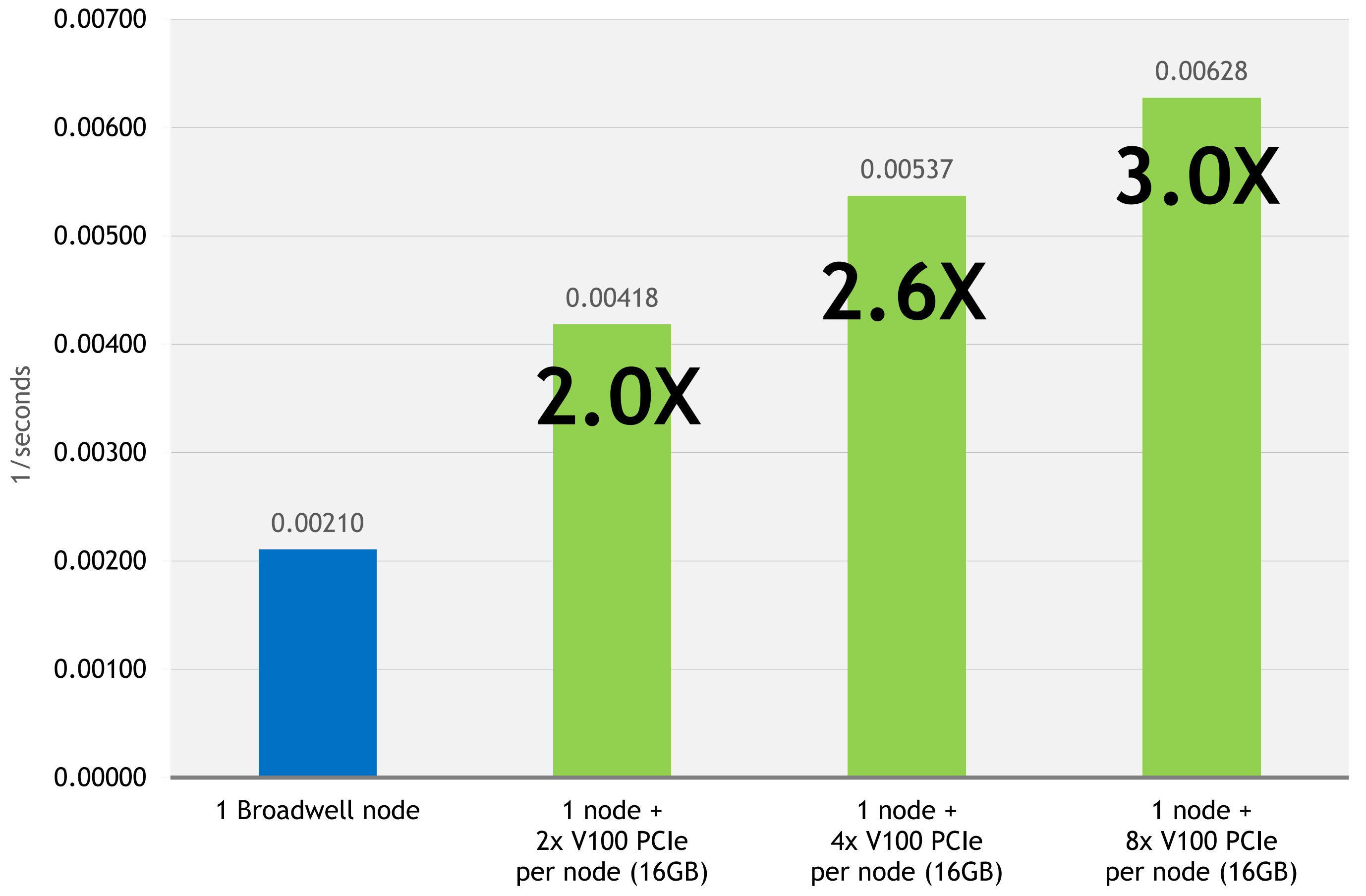


Kepler performs 2x faster than Tesla

VASP 5.4.4

October 2017

Silica IFPEN on V100s PCIe



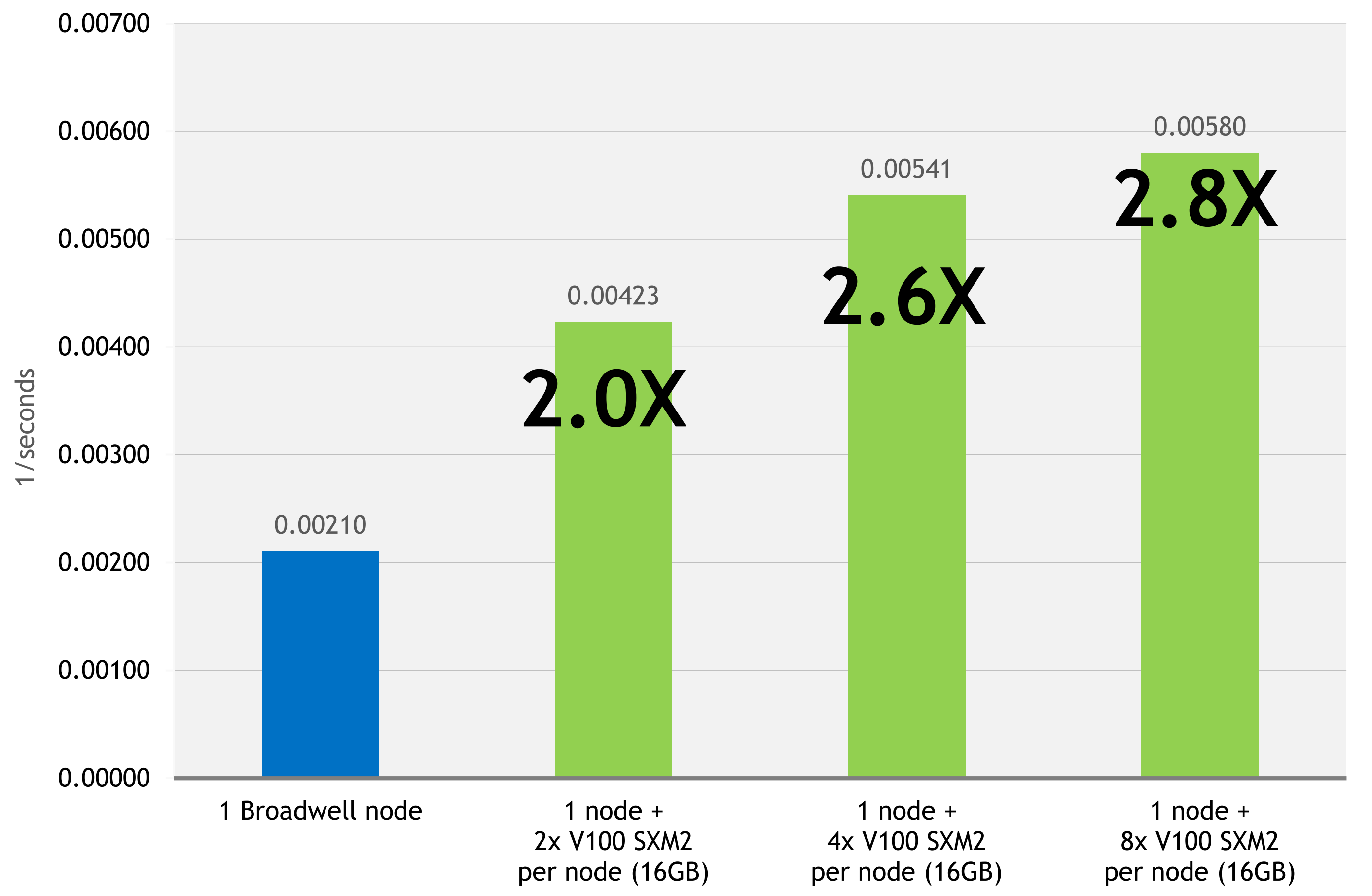
(Untuned on Volta)
Running VASP version 5.4.4

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

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

240 ions, cristobalite (high) bulk
720 bands
? plane waves
ALGO = Very Fast (RMM-DIIS)

Silica IFPEN on V100s SXM2



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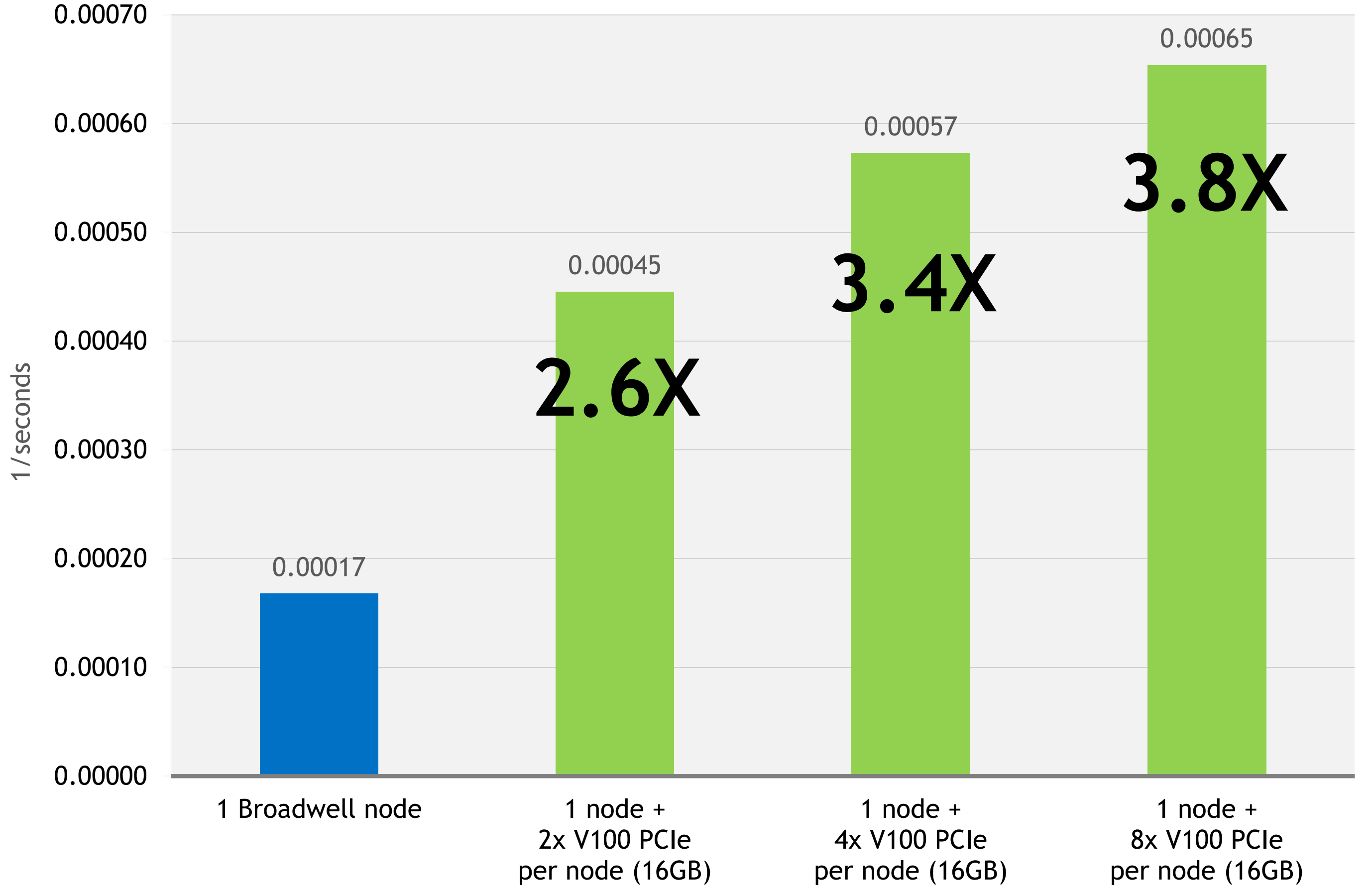
720 bands
? plane waves
ALGO = Very Fast (RMM-DIIS)

Si-Huge on V100s PCIe



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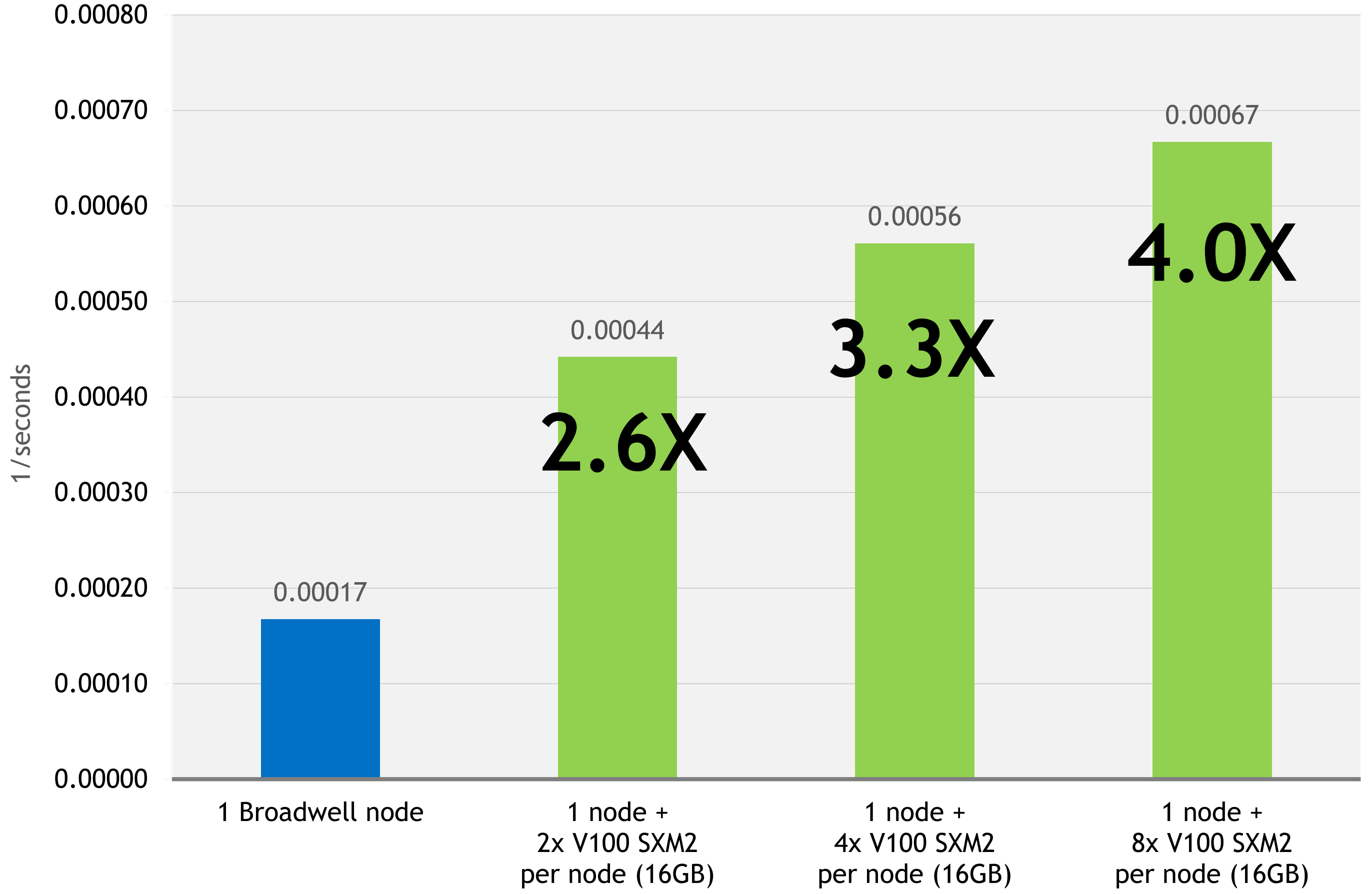
512 Si atoms
1282 bands
864000 Plane Waves
Algo = Normal (blocked Davidson)

Si-Huge on V100s SXM2



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1282 bands
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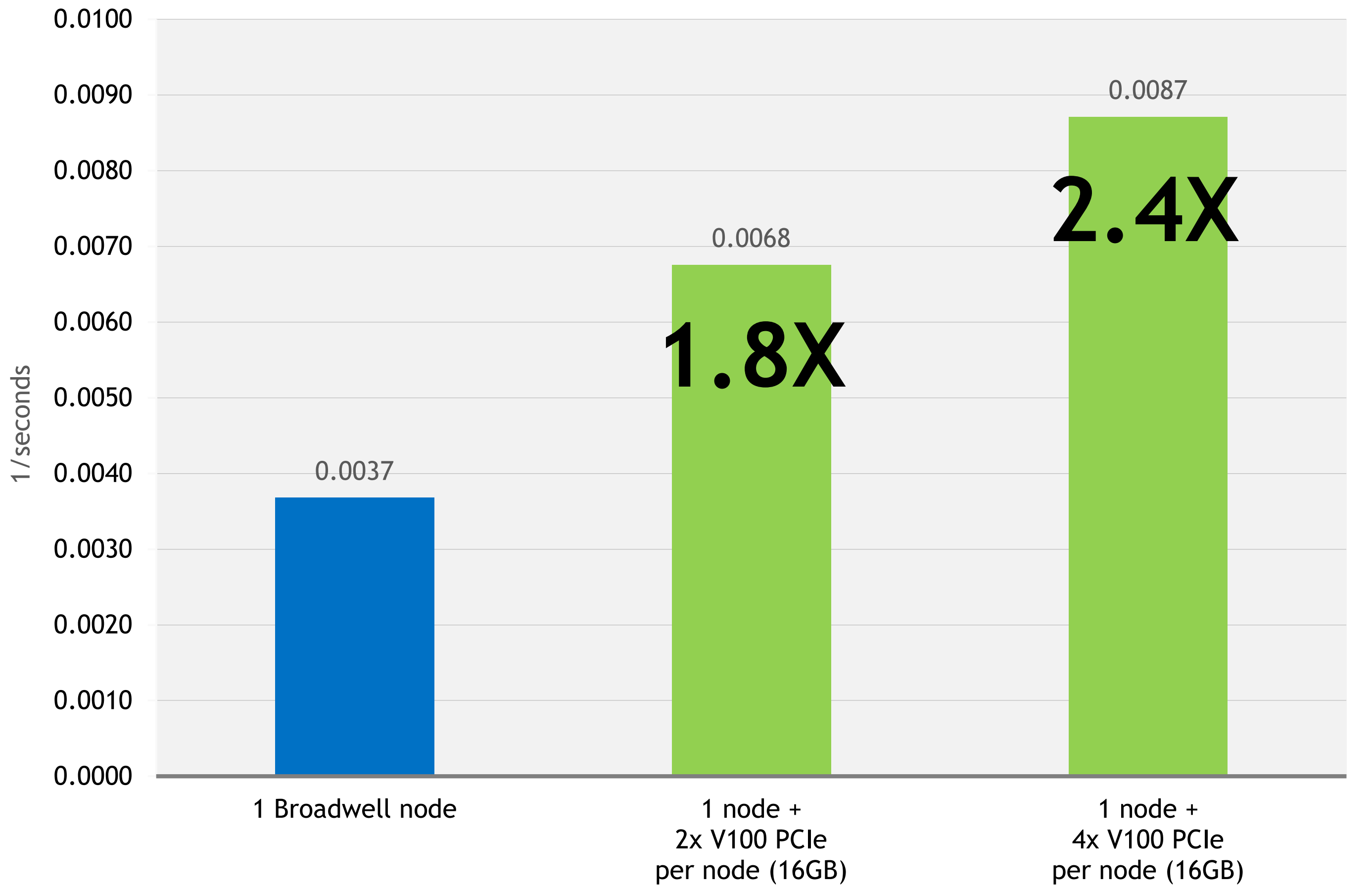
Algo = Normal (blocked Davidson)

SupportedSystems on V100s PCIe



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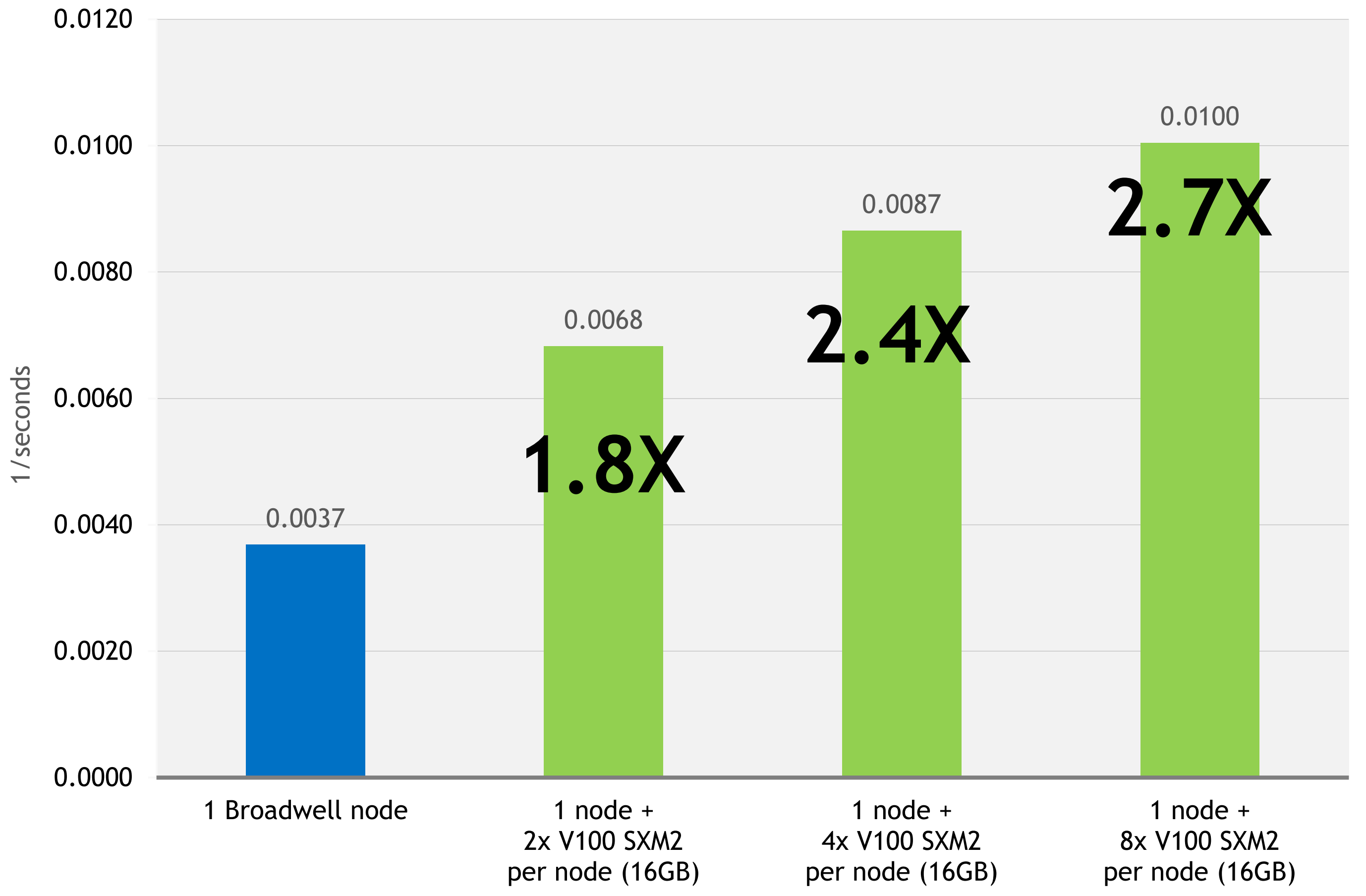
The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla V100 PCIe (16GB) GPUs

267 ions
788 bands
762048 plane waves
ALGO = Fast (Davidson + RMM-DIIS)

SupportedSystems on V100s SXM2



(Untuned on Volta)
Running VASP version 5.4.4

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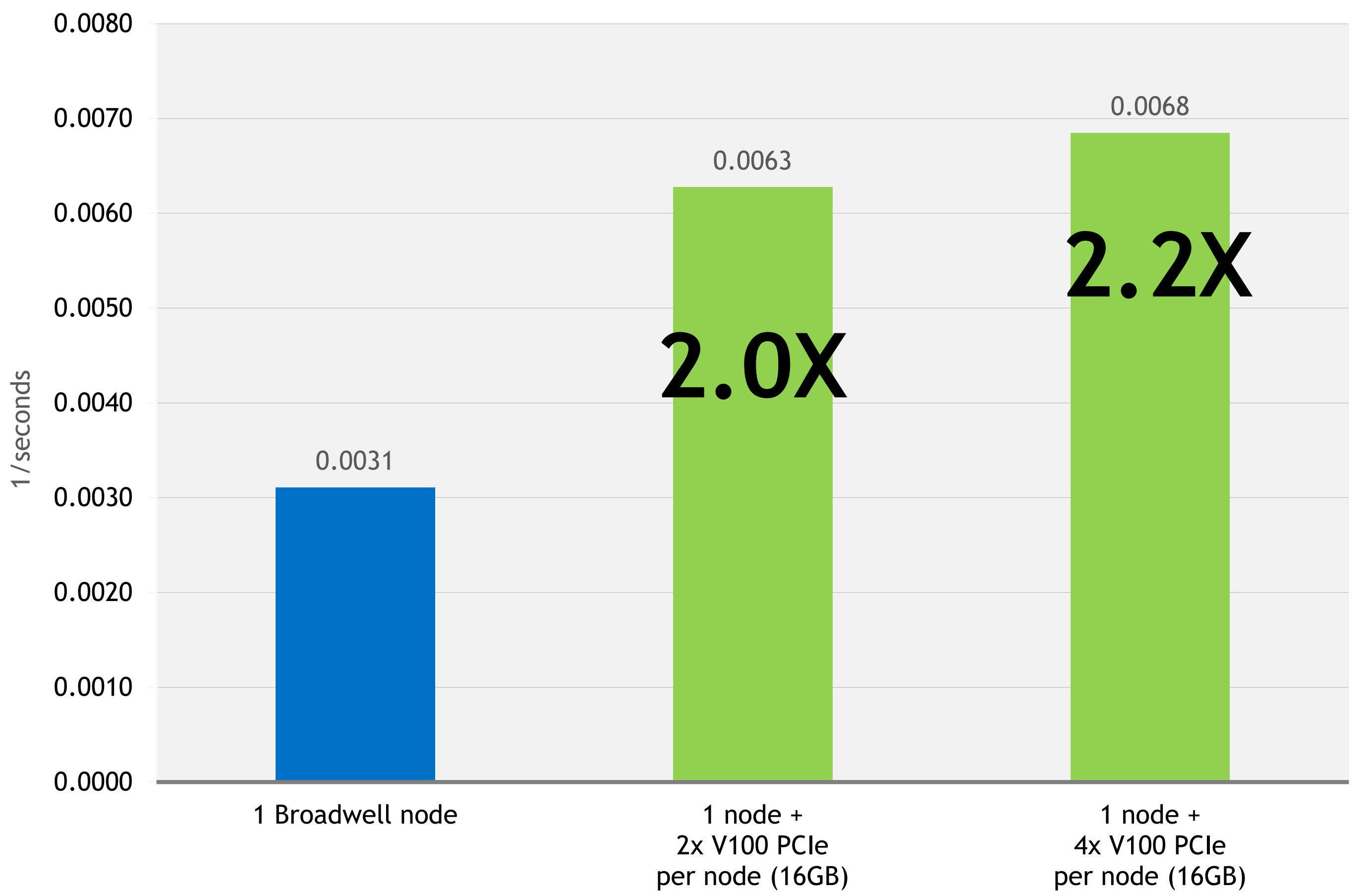
267 ions
788 bands
762048 plane waves
ALGO = Fast (Davidson + RMM-DIIS)

NiAl-MD on V100s PCIe



(Untuned on Volta)
Running VASP version 5.4.4

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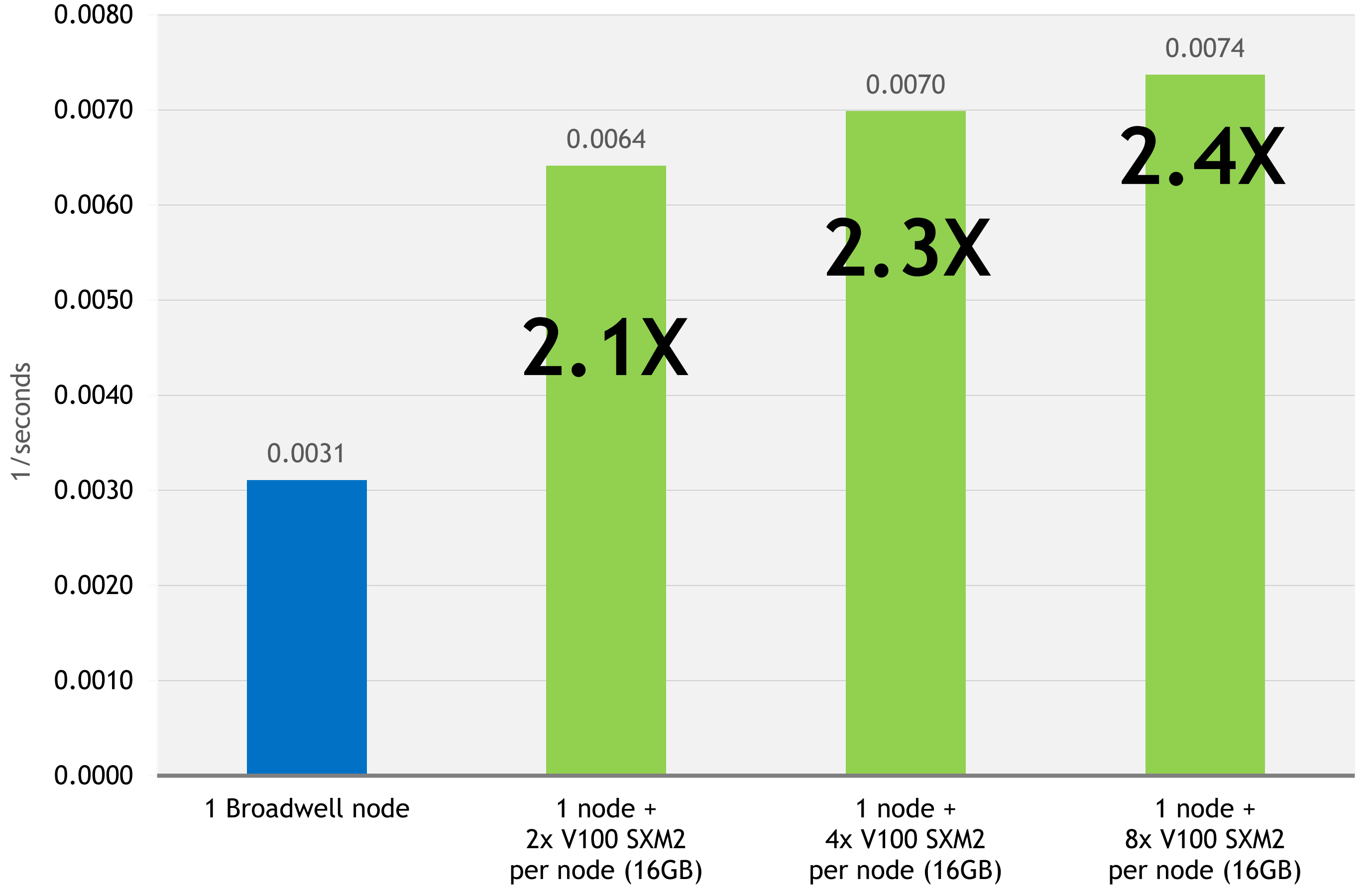
The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla V100 PCIe (16GB) GPUs

500 ions
3200 bands
729000 plane waves
ALGO = Fast (Davidson + RMM-DIIS)

NiAl-MD on V100s SXM2



(Untuned on Volta)
Running VASP version 5.4.4

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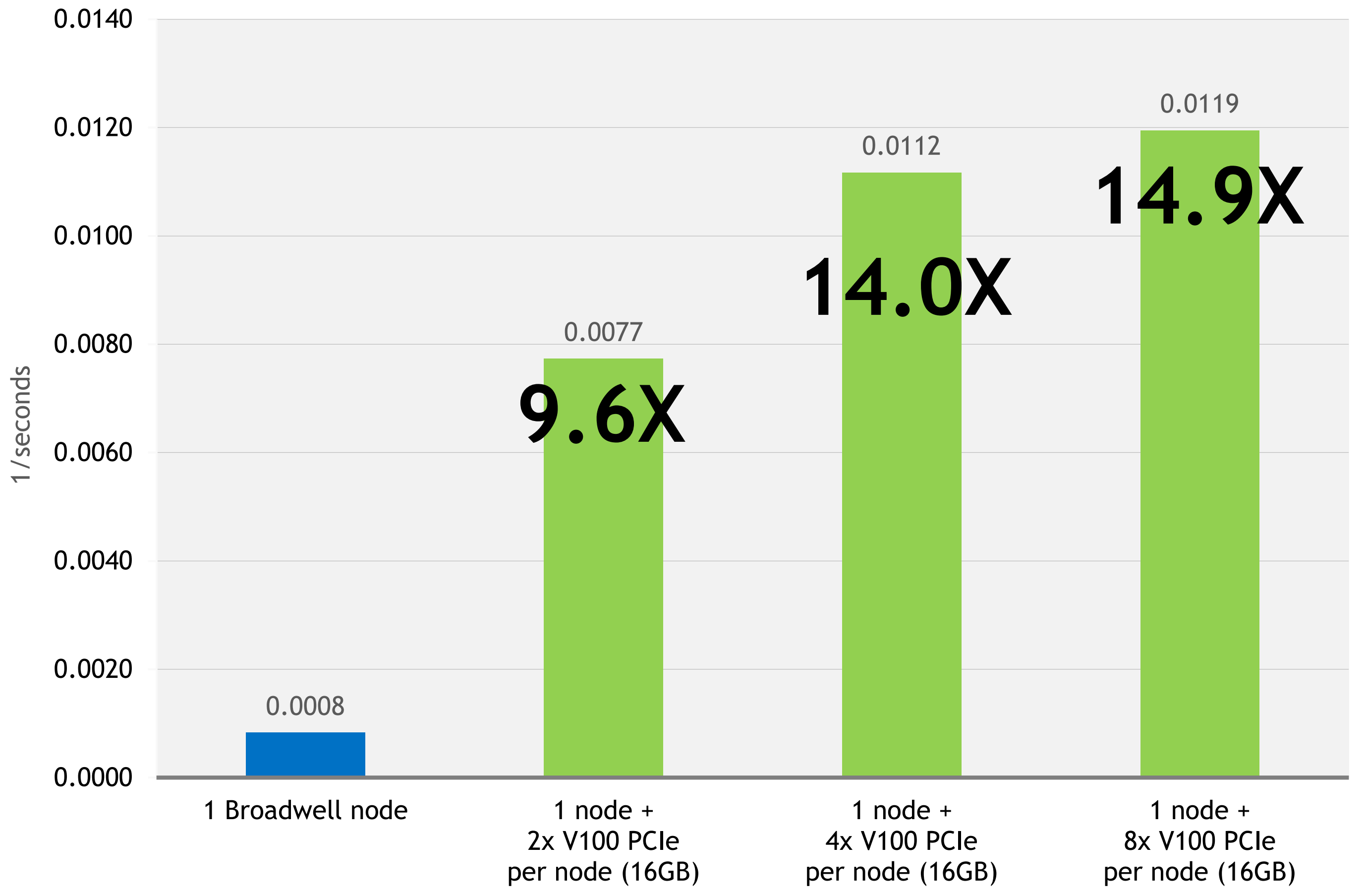
500 ions
3200 bands
729000 plane waves
ALGO = Fast (Davidson + RMM-DIIS)

B.hR105 on V100s PCIe



(Untuned on Volta)
Running VASP version 5.4.4

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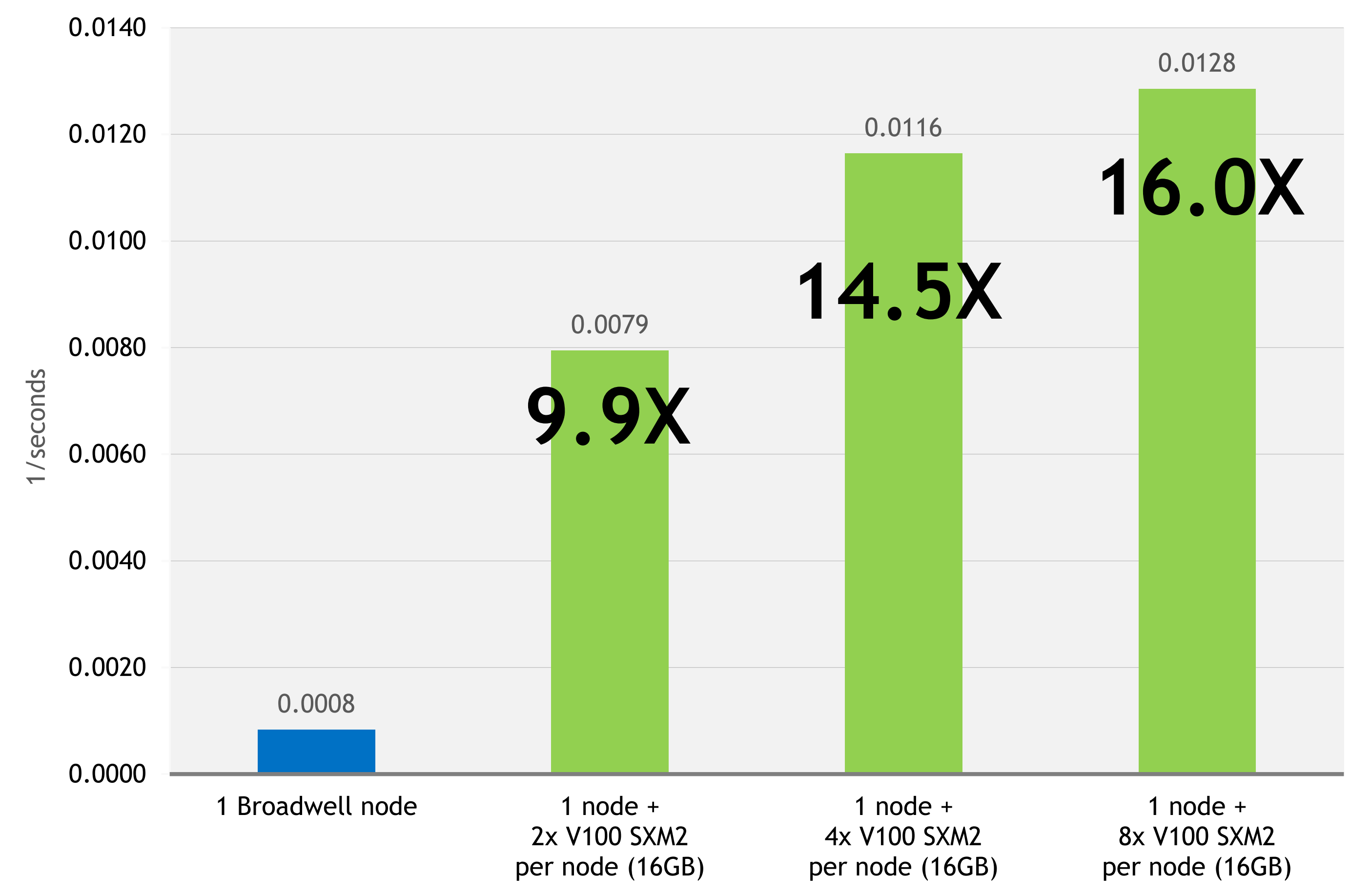
The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla V100 PCIe (16GB) GPUs

105 Boron atoms (β-rhombohedral structure)
216 bands
110592 plane waves
Hybrid Functional with blocked Davicson (ALGO=Normal)
LHFCALC=.True. (Exact Exchange)

B.hR105 on V100s SXM2



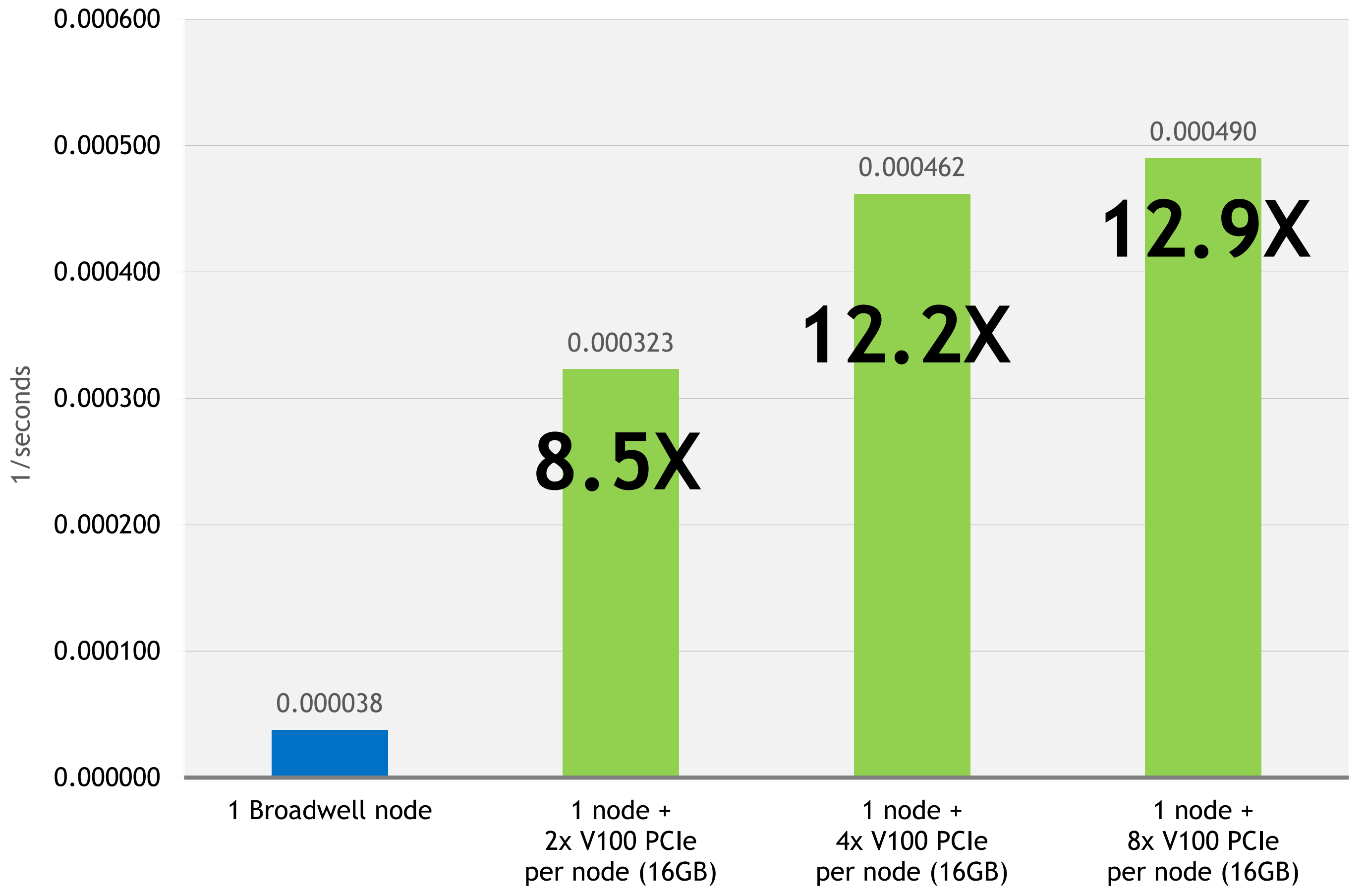
(Untuned on Volta)
Running VASP version 5.4.4

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

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

105 Boron atoms (β-rhombohedral structure)
216 bands
110592 plane waves
Hybrid Functional with blocked Davicson (ALGO=Normal)
LHFCALC=.True. (Exact Exchange)

B.aP107 on V100s PCIe



(Untuned on Volta)
Running VASP version 5.4.4

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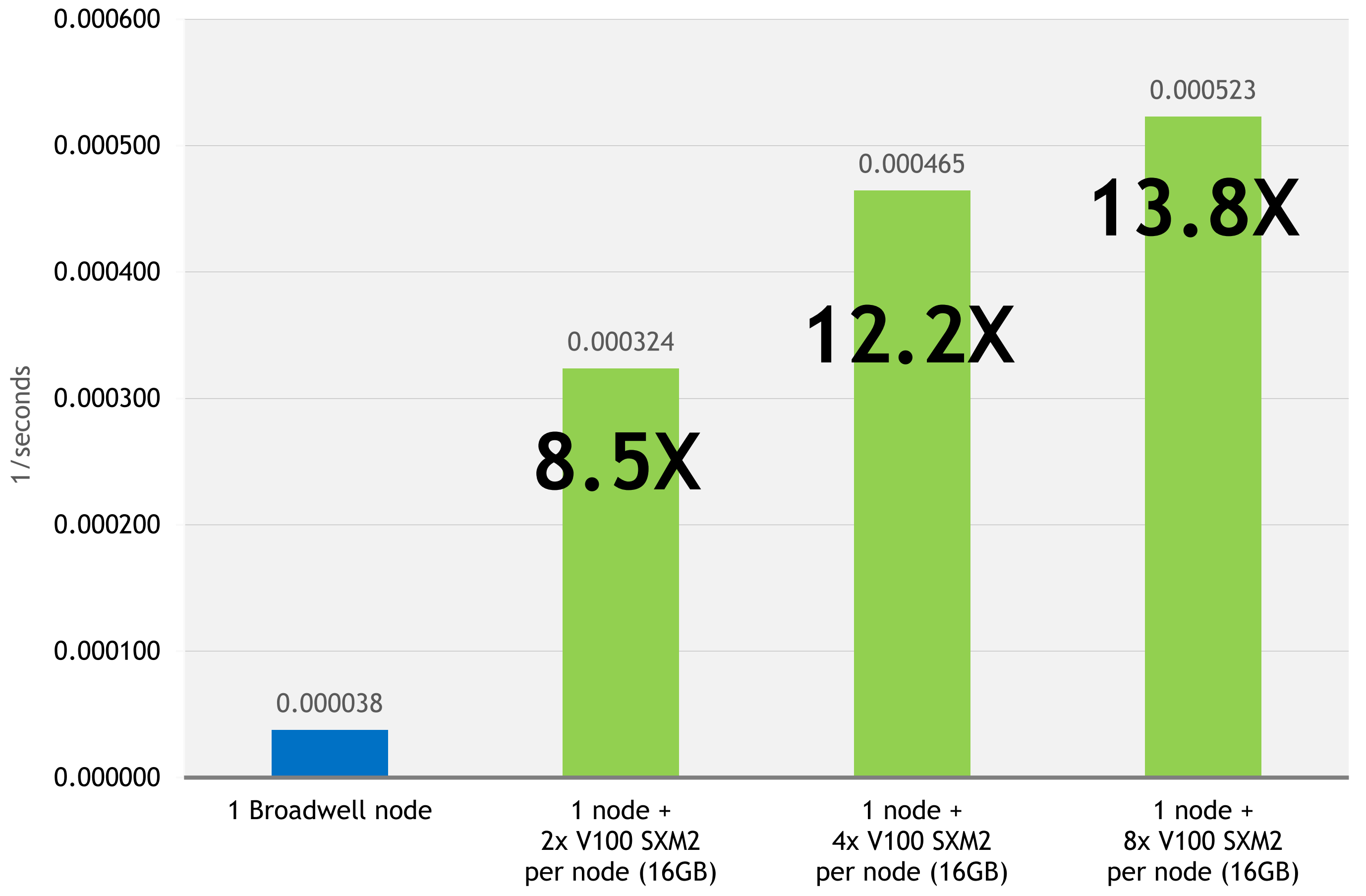
The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla V100 PCIe (16GB) GPUs

107 Boron atoms (symmetry broken 107-atom β′ variant)
216 bands
110592 plane waves
Hybrid functional calculation (exact exchange) with blocked Davidson. No KPoint parallelization.
Hybrid Functional with blocked Davidson (ALGO=Normal)
LHFCALC=.True. (Exact Exchange)

B.aP107 on V100s SXM2



(Untuned on Volta)
Running VASP version 5.4.4

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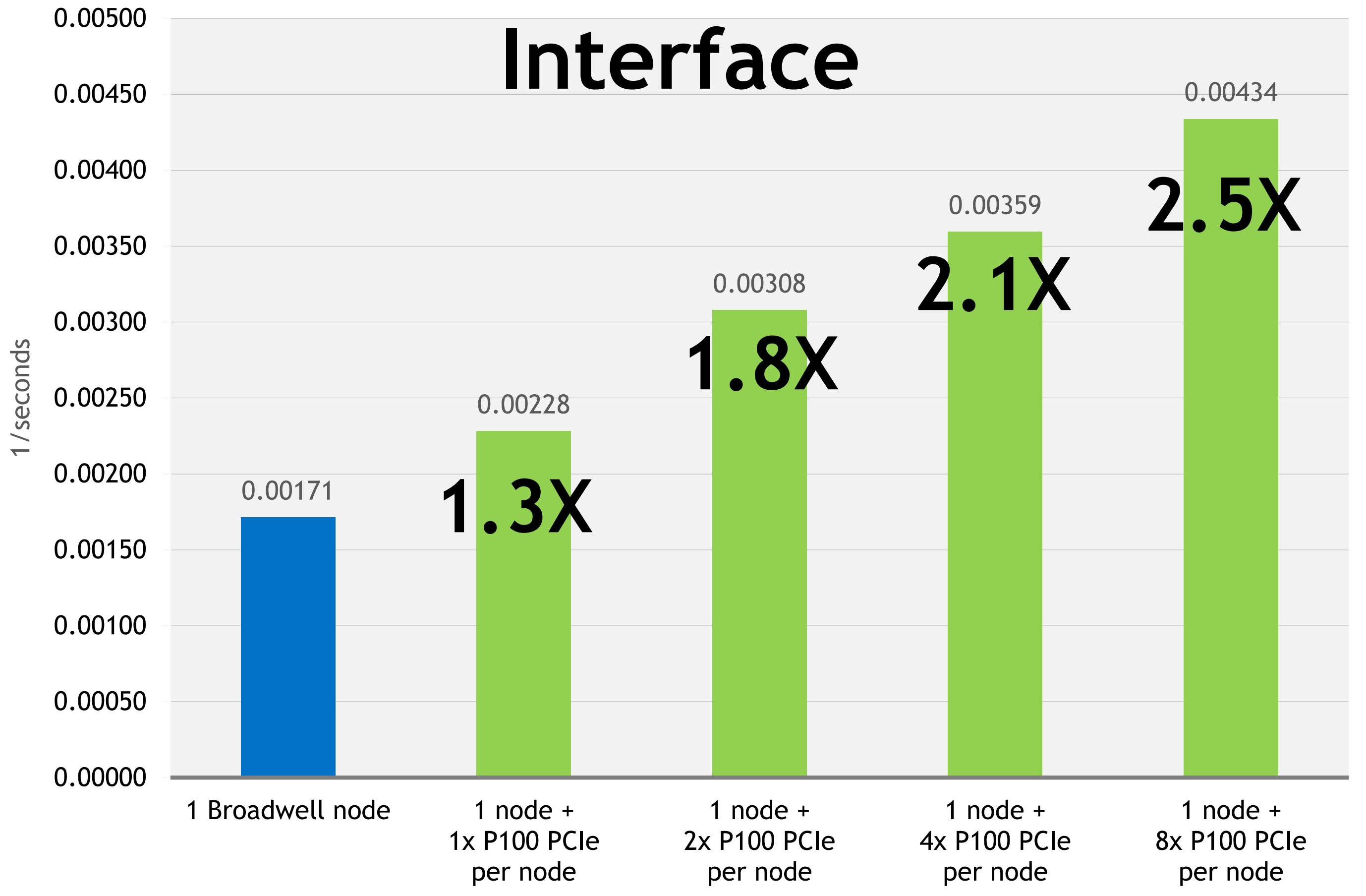
107 Boron atoms (symmetry broken 107-atom B′ variant)
216 bands
110592 plane waves
Hybrid functional calculation (exact exchange) with blocked Davidson. No KPoint parallelization.
Hybrid Functional with blocked Davidson (ALGO=Normal)
LHFCALC=.True. (Exact Exchange)

VASP 5.4.1

February 2017

NVIDIA.

Interface on P100s PCIe



Running VASP version 5.4.1

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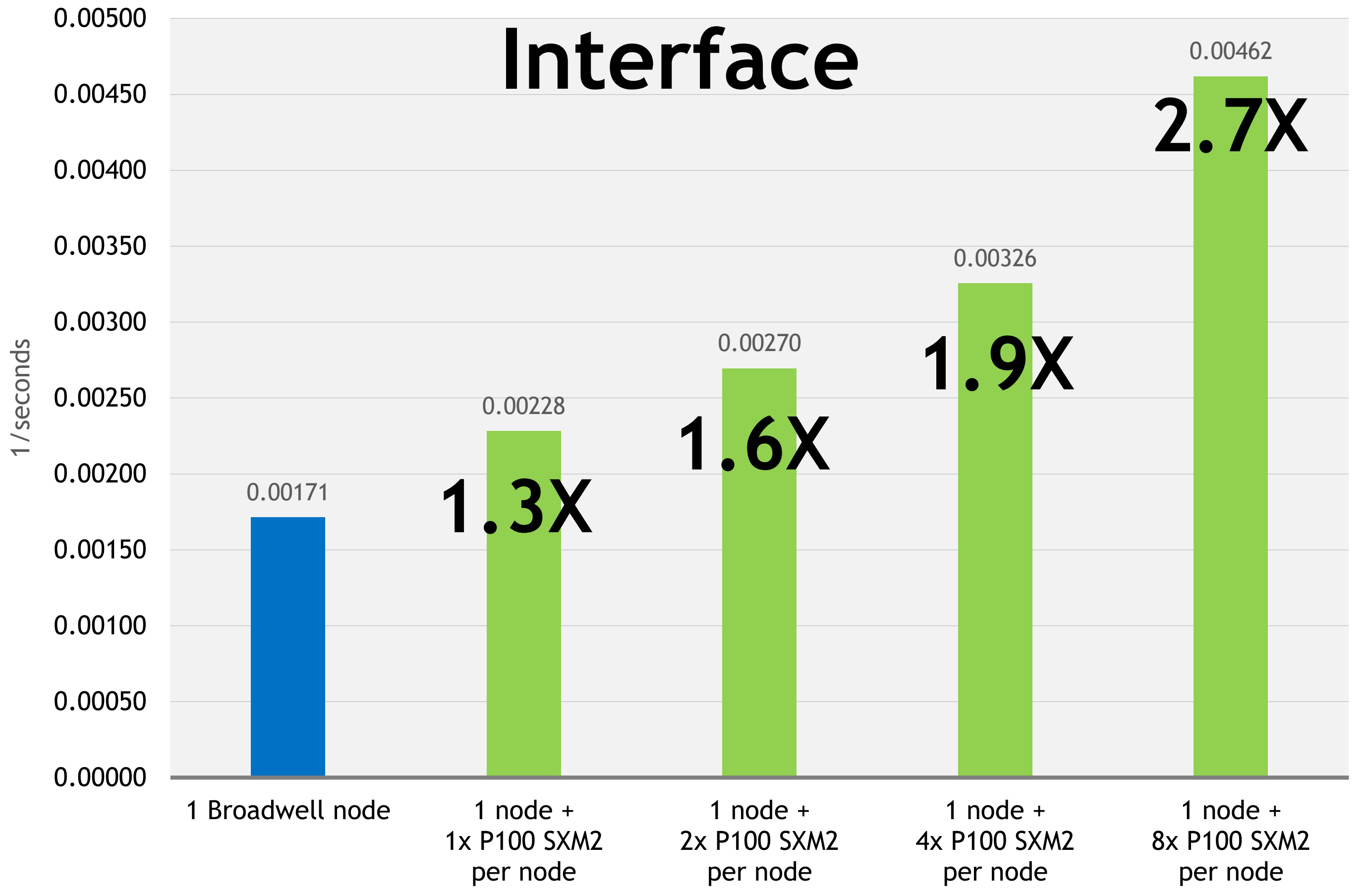
- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

Interface between a platinum slab Pt(111) (108 atoms) and liquid water (120 water molecules) (468 ions)

1256 bands
762048 plane waves
ALGO = Fast (Davidson + RMM-DIIS)

Interface on P100s SXM2



Running VASP version 5.4.1

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Interface between a platinum slab Pt(111) (108 atoms) and liquid water (120 water molecules) (468 ions)

1256 bands
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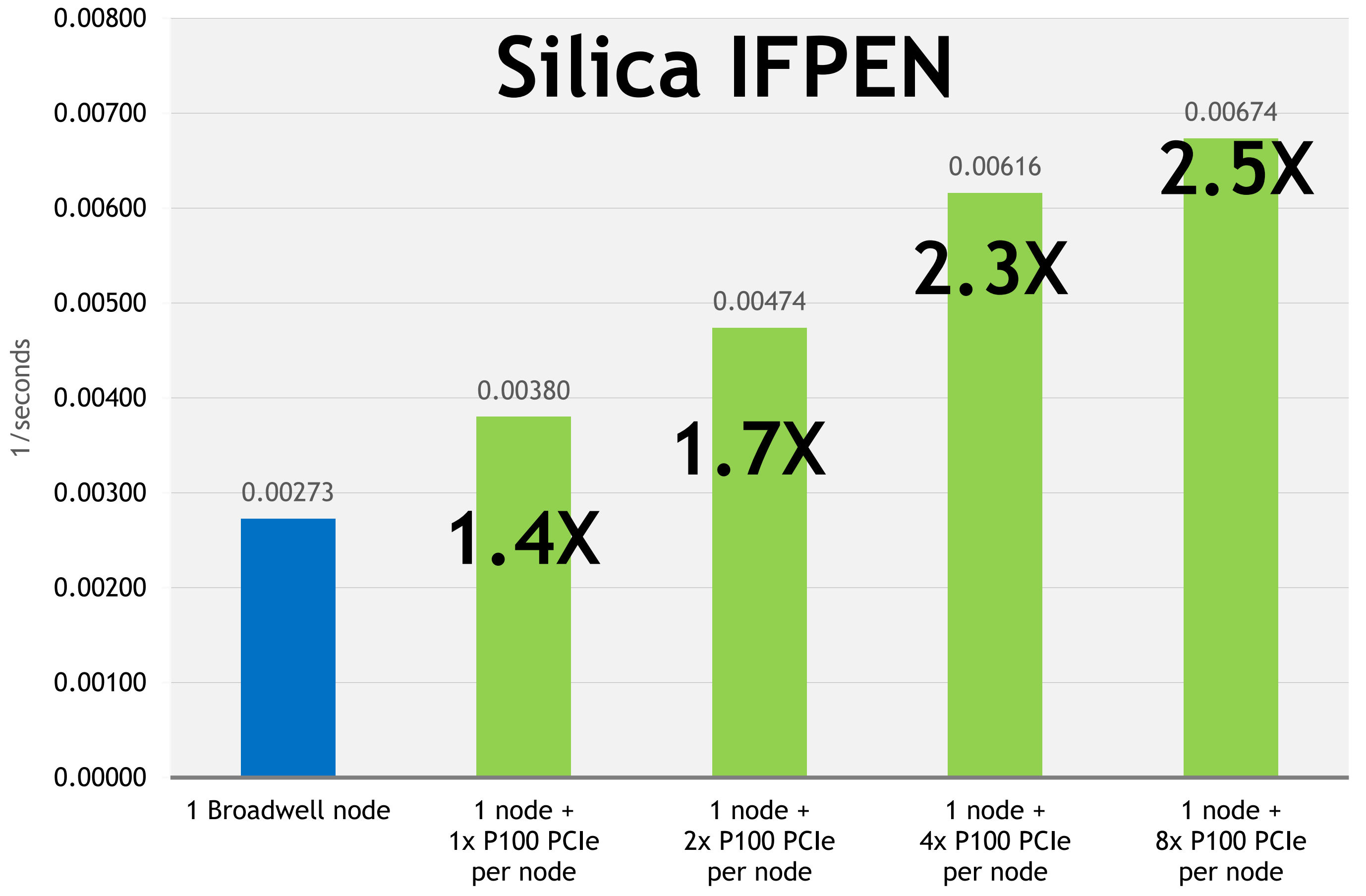
Silica IFPEN on P100s PCIe



Running VASP version 5.4.1

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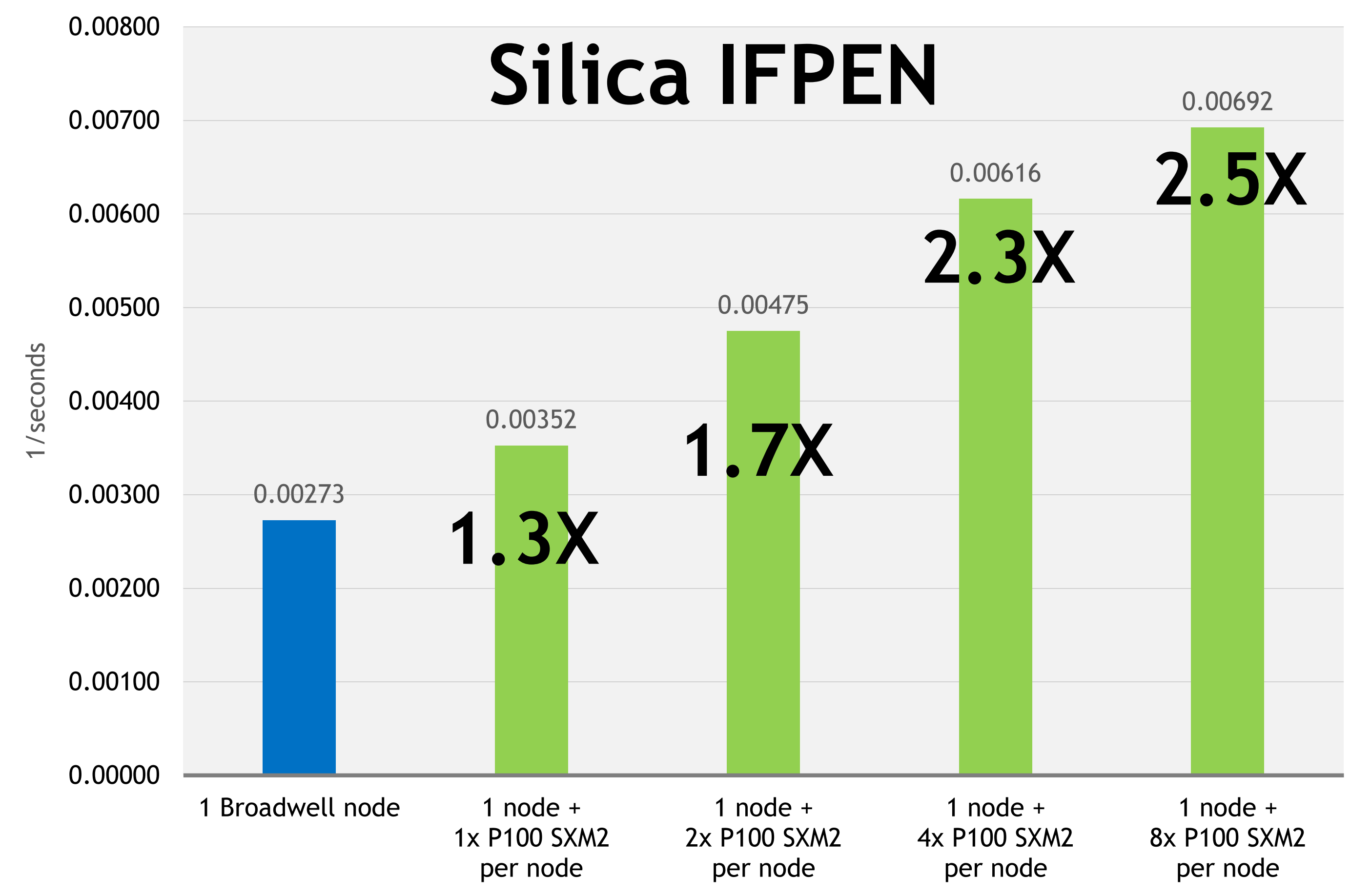
240 ions, cristobalite (high) bulk
720 bands
? plane waves
ALGO = Very Fast (RMM-DIIS)

Silica IFPEN on P100s SXM2



Running VASP version 5.4.1

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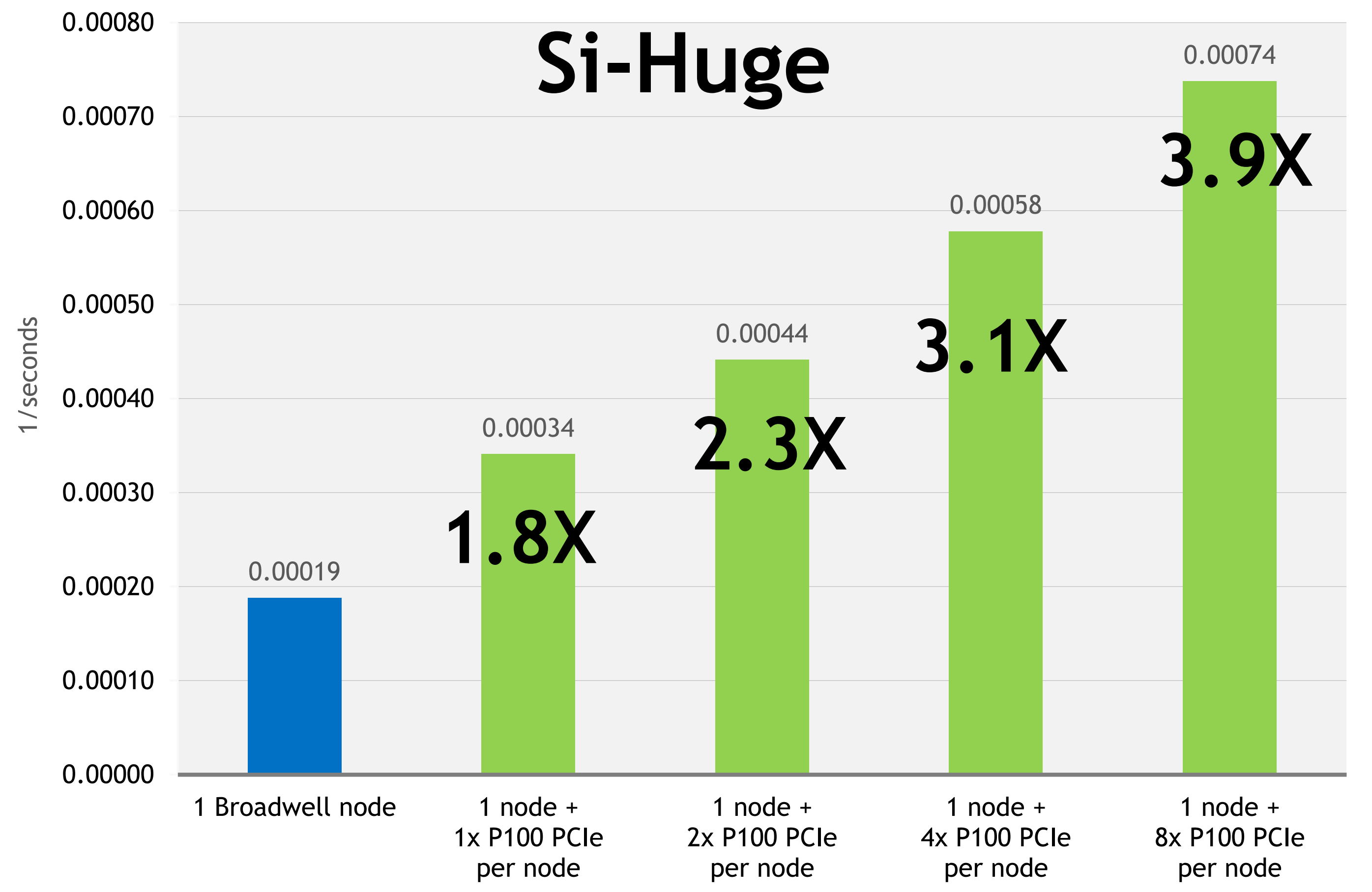
240 ions, cristobalite (high) bulk
720 bands
? plane waves
ALGO = Very Fast (RMM-DIIS)

Si-Huge on P100s PCIe



Running VASP version 5.4.1

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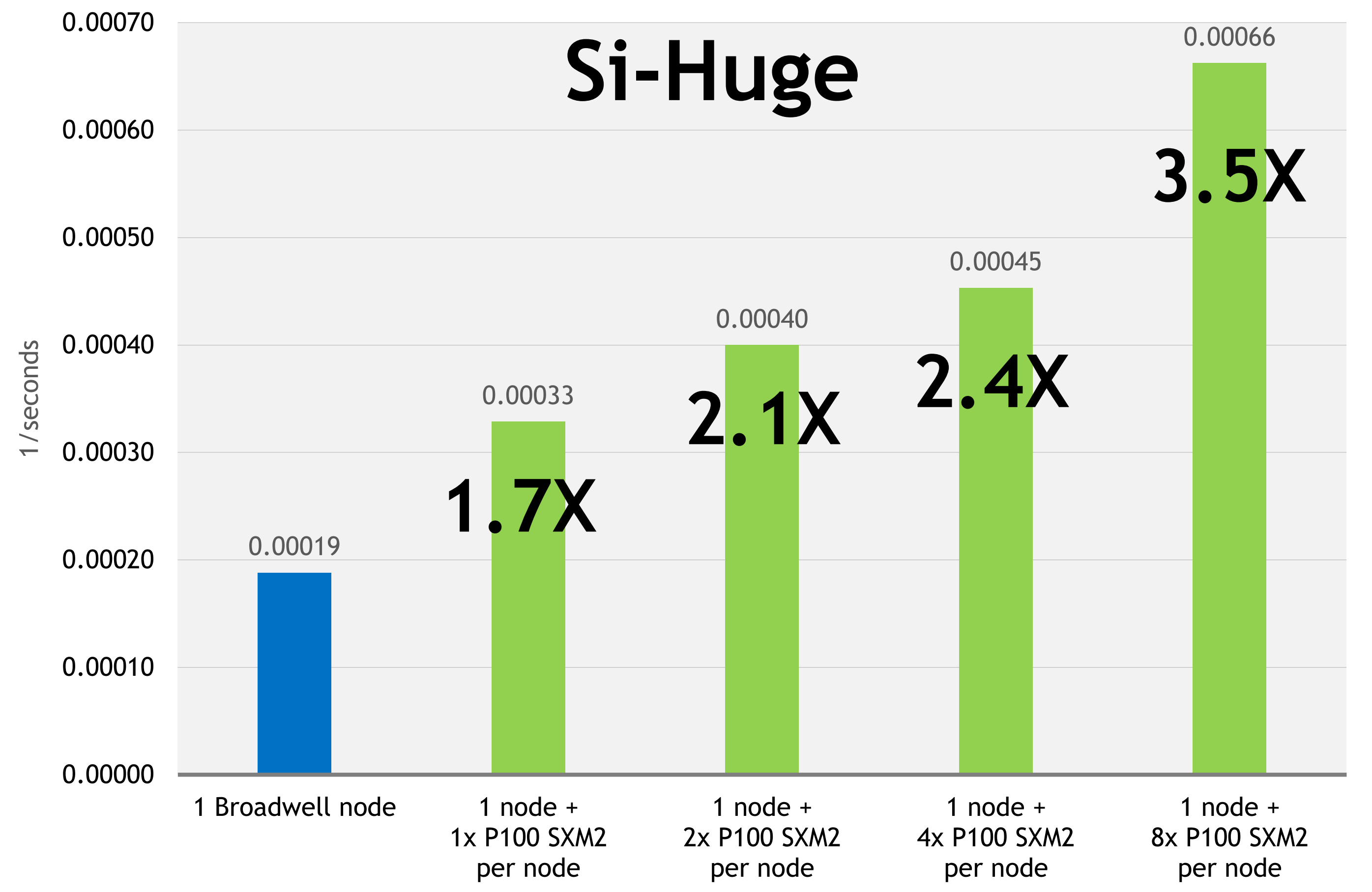
- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

512 Si atoms
1282 bands
864000 Plane Waves
Algo = Normal (blocked Davidson)

Si-Huge on P100s SXM2



Running VASP version 5.4.1

The blue node contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

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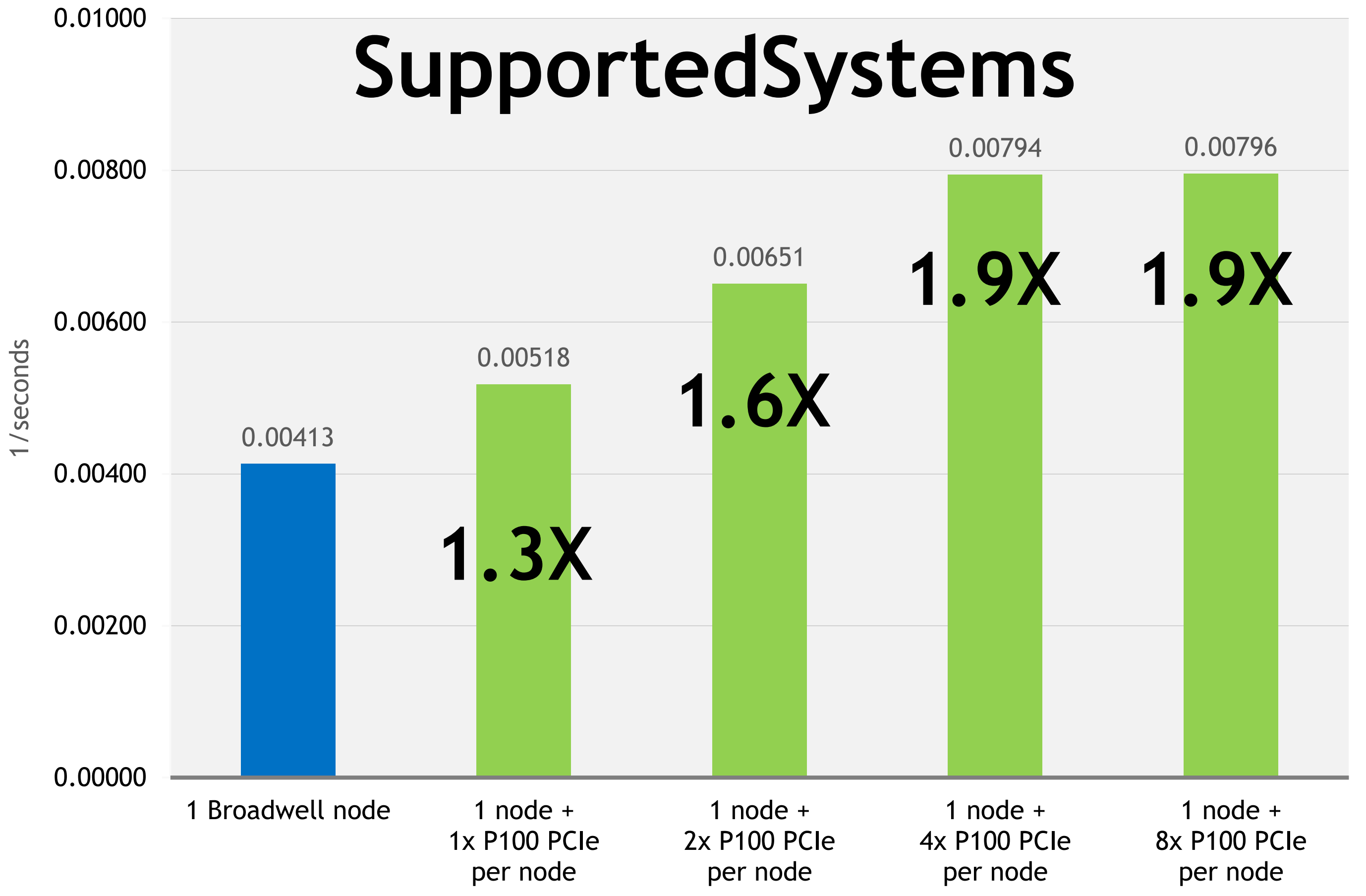
512 Si atoms
1282 bands
864000 Plane Waves
Algo = Normal (blocked Davidson)

SupportedSystems on P100s PCIe



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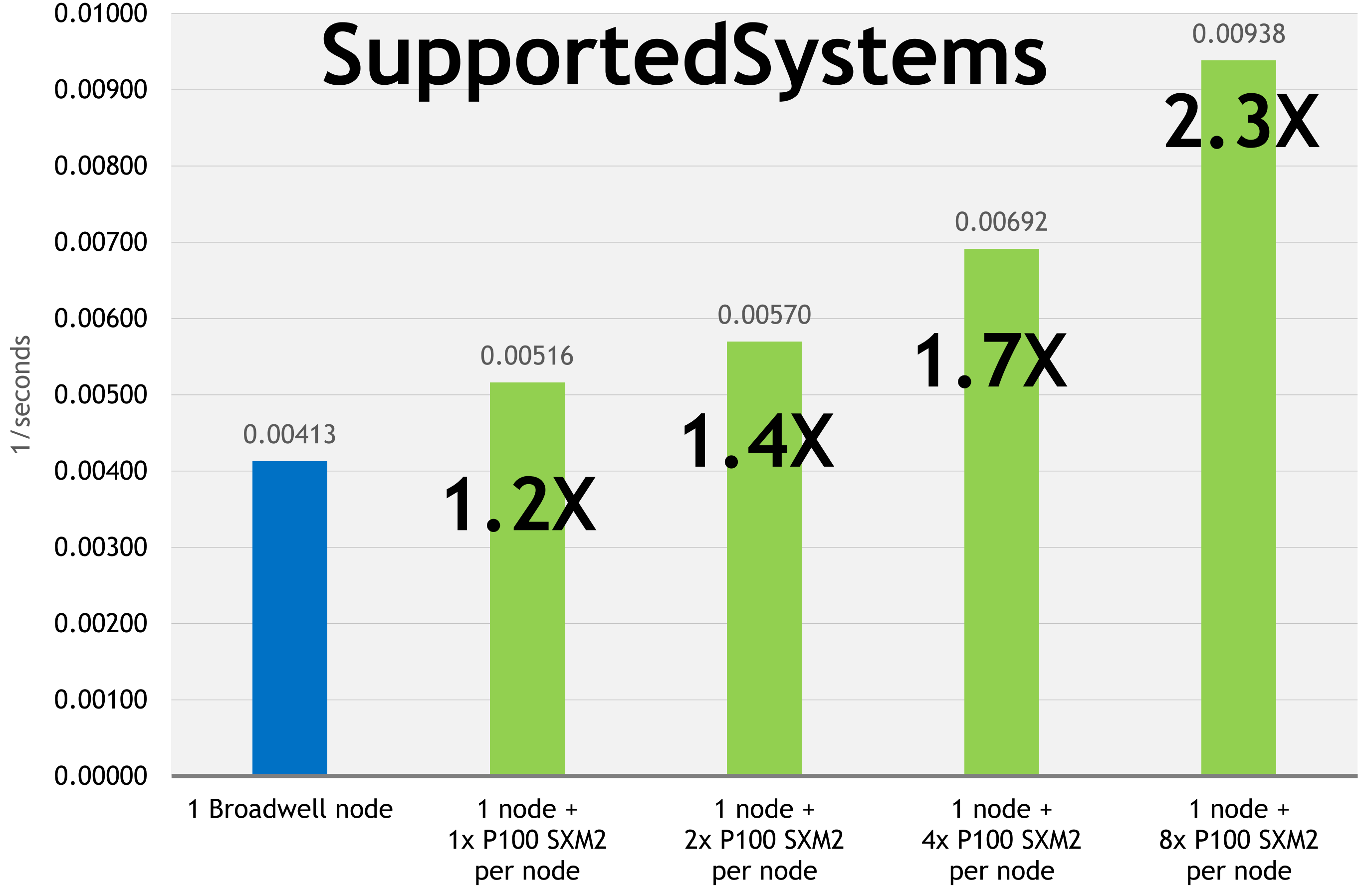
267 ions
788 bands
762048 plane waves
ALGO = Fast (Davidson + RMM-DIIS)

SupportedSystems on P100s SXM2



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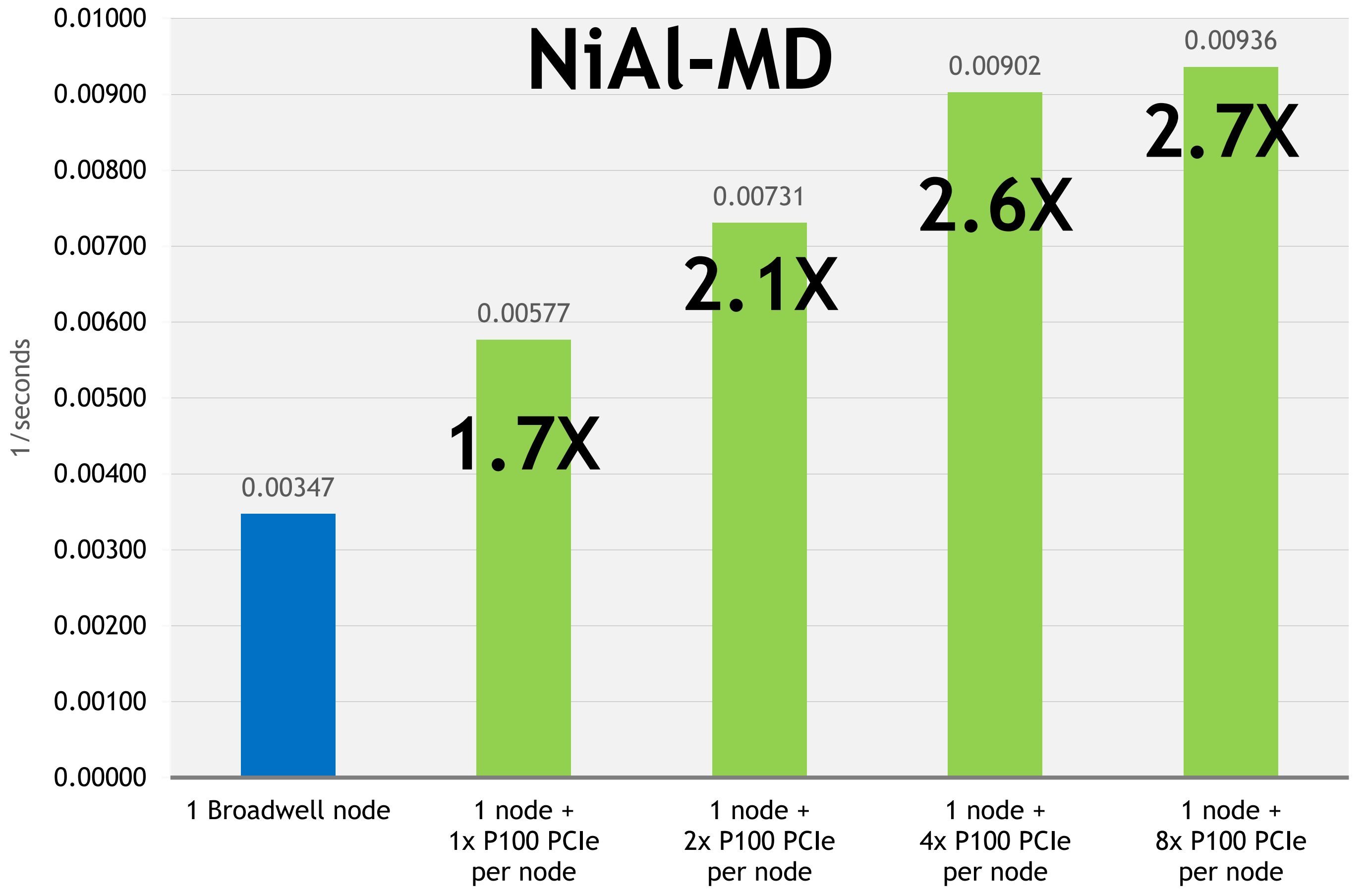
762048 plane waves
ALGO = Fast (Davidson + RMM-DIIS)

NiAl-MD on P100s PCIe



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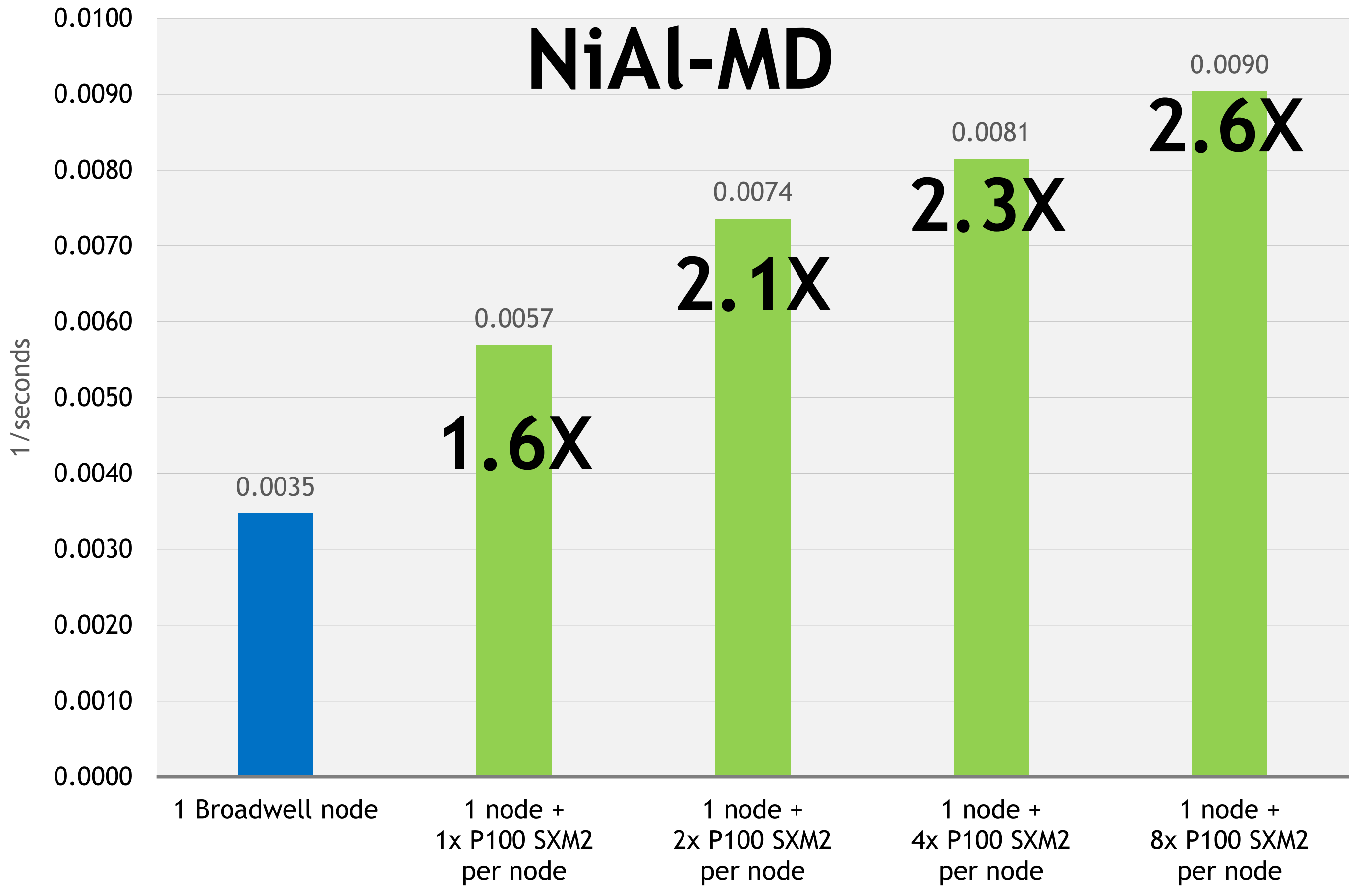
- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

500 ions
3200 bands
729000 plane waves
ALGO = Fast (Davidson + RMM-DIIS)

NiAl-MD on P100s SXM2



Running VASP version 5.4.1

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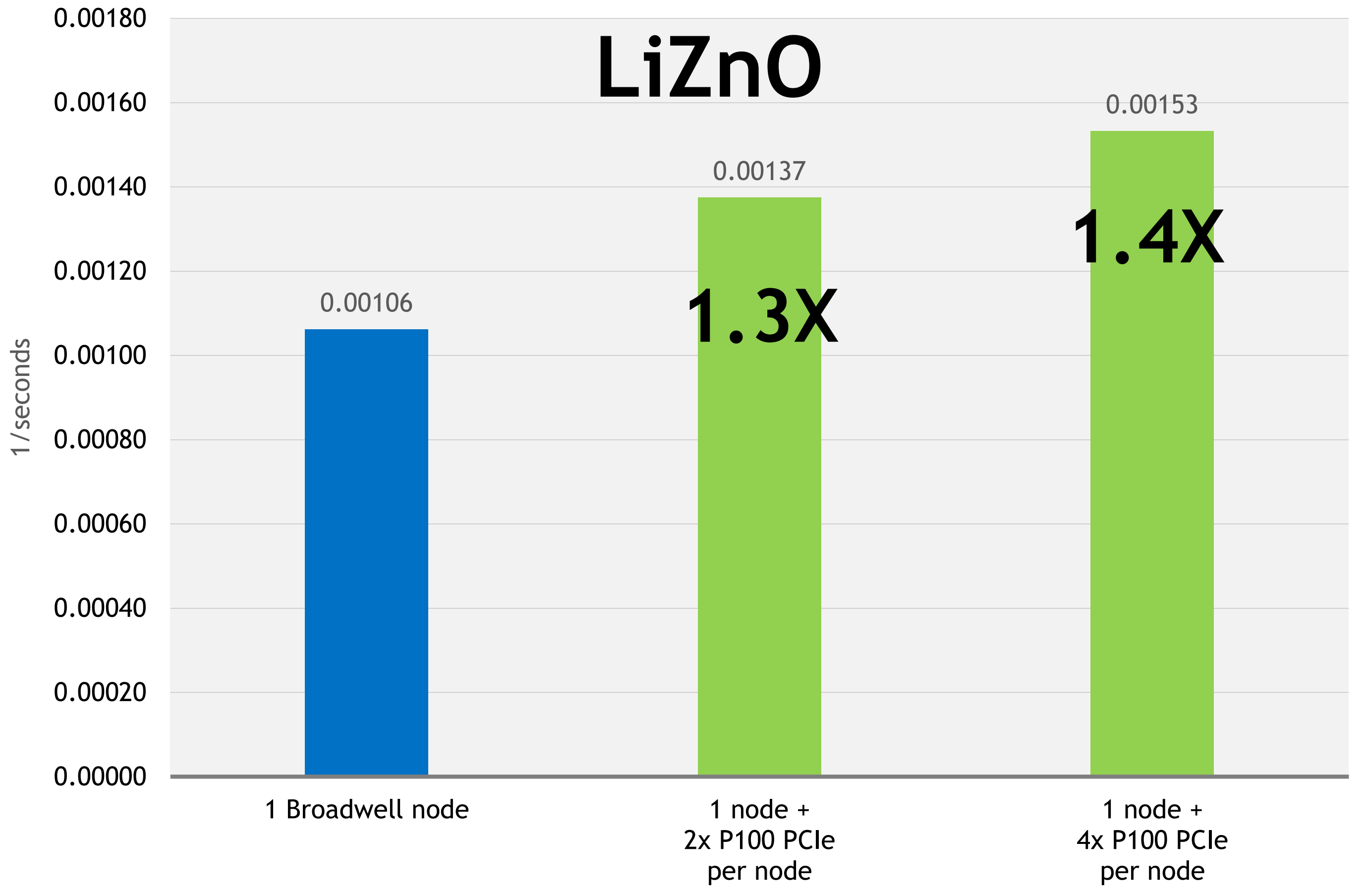
500 ions
3200 bands
729000 plane waves
ALGO = Fast (Davidson + RMM-DIIS)

LiZnO on P100s PCIe



Running VASP version 5.4.1

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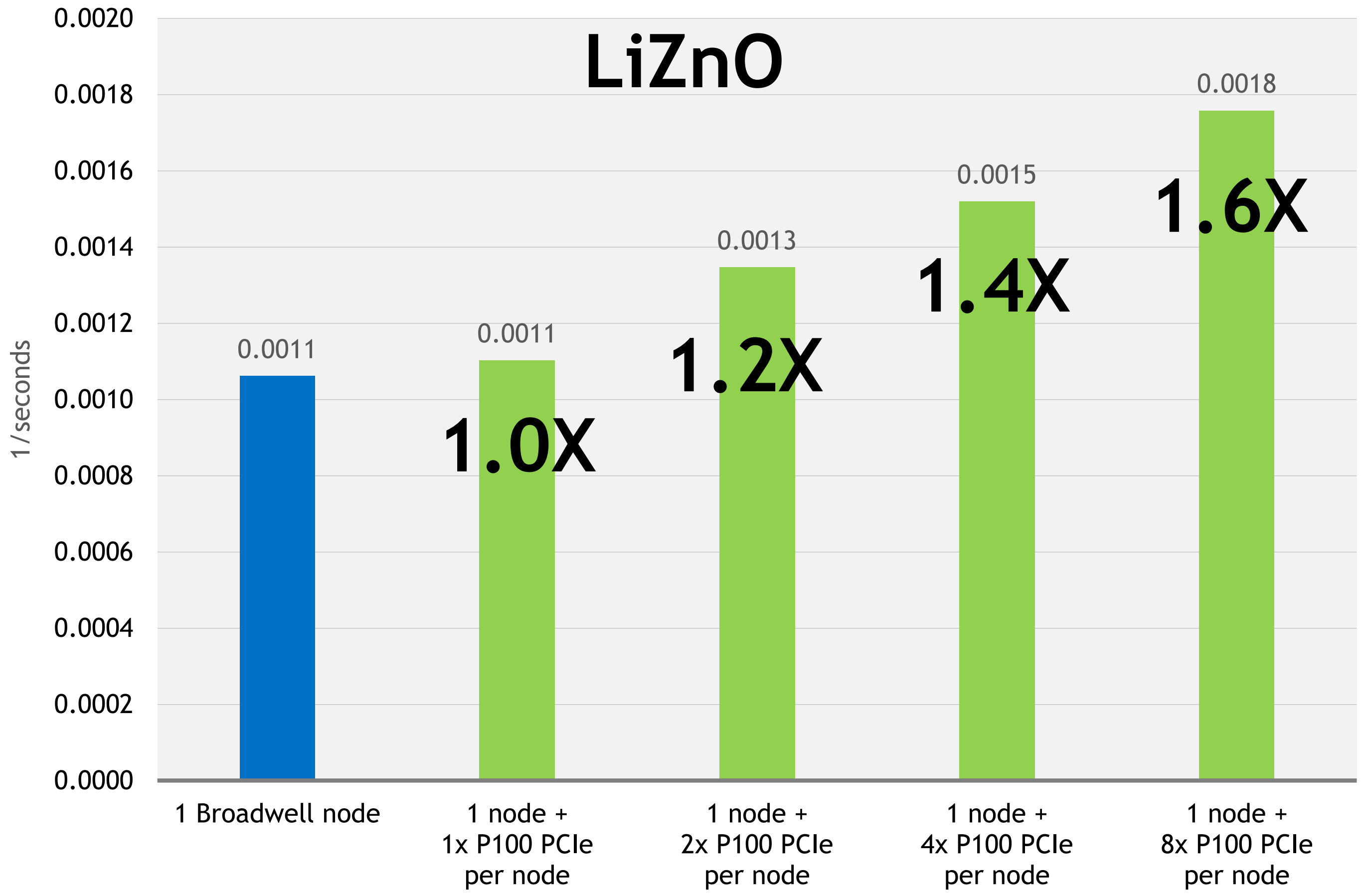
500 ions
3200 bands
729000 plane waves
ALGO = Fast (Davidson + RMM-DIIS)

LiZnO on P100s SXM2



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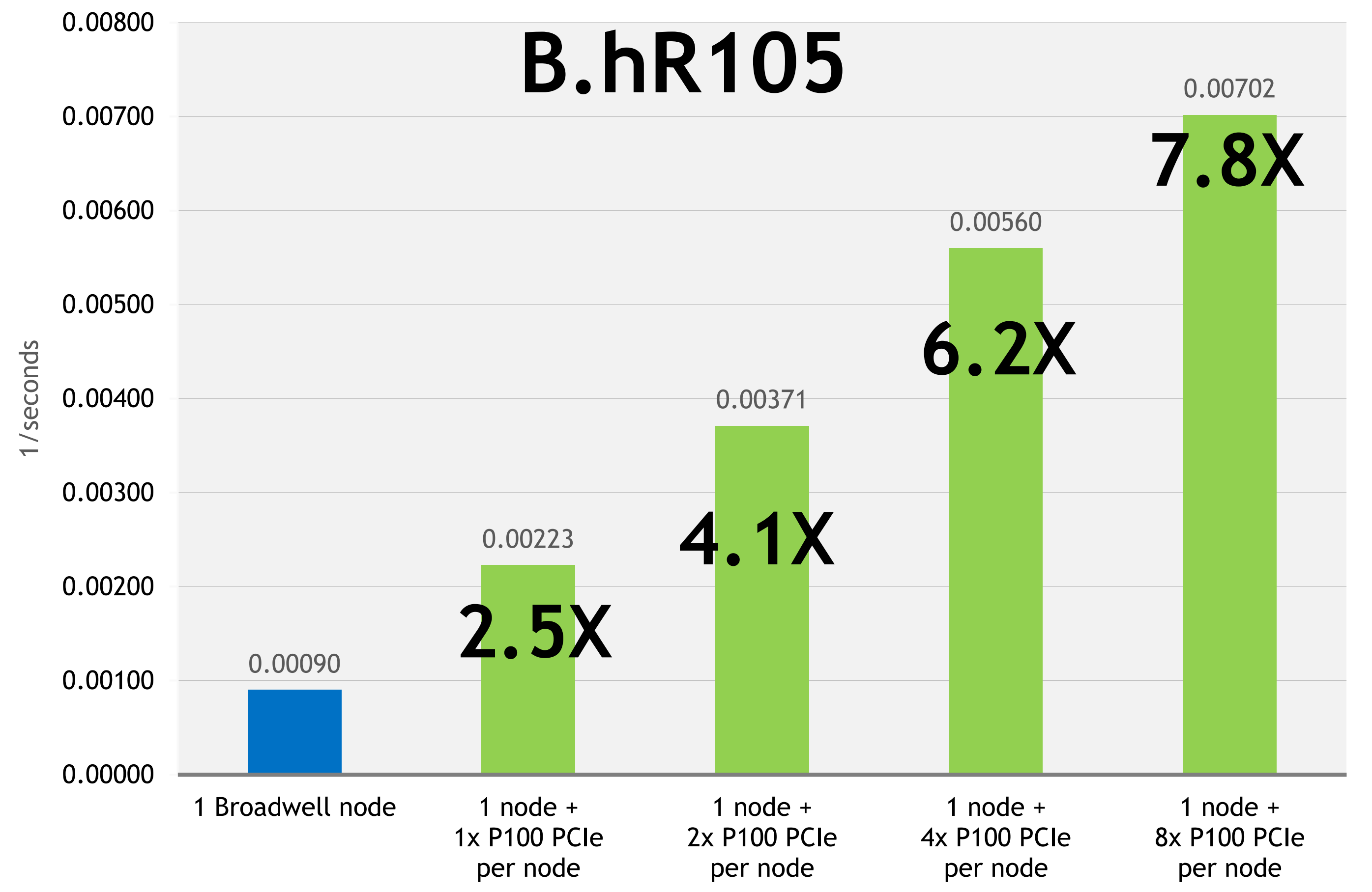
500 ions
3200 bands
729000 plane waves
ALGO = Fast (Davidson + RMM-DIIS)

B.hR105 on P100s PCIe



Running VASP version 5.4.1

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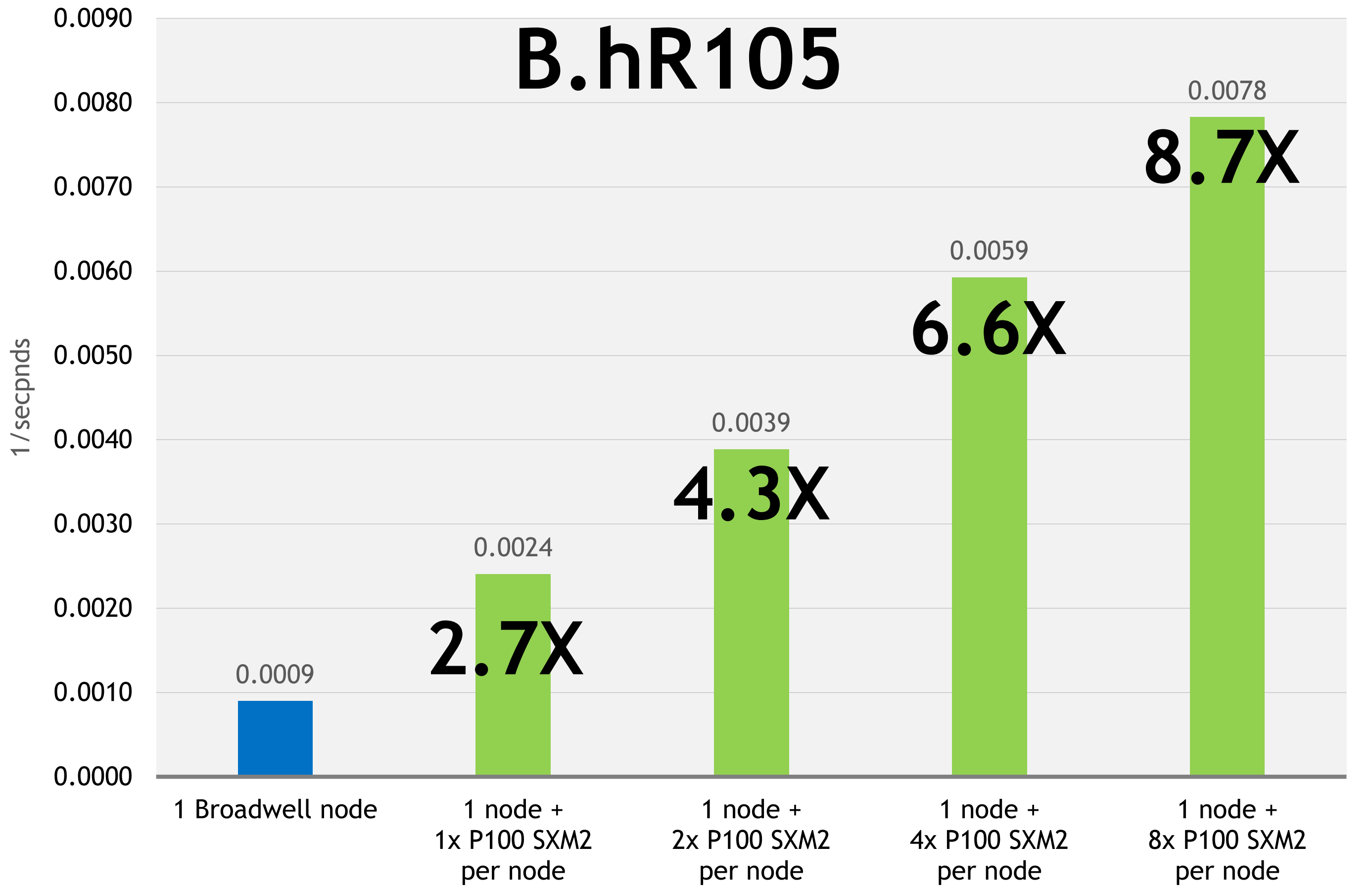
- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

105 Boron atoms (β-rhombohedral structure)
216 bands
110592 plane waves
Hybrid Functional with blocked Davicson (ALGO=Normal)
LHFCALC=.True. (Exact Exchange)

B.hR105 on P100s SXM2



Running VASP version 5.4.1

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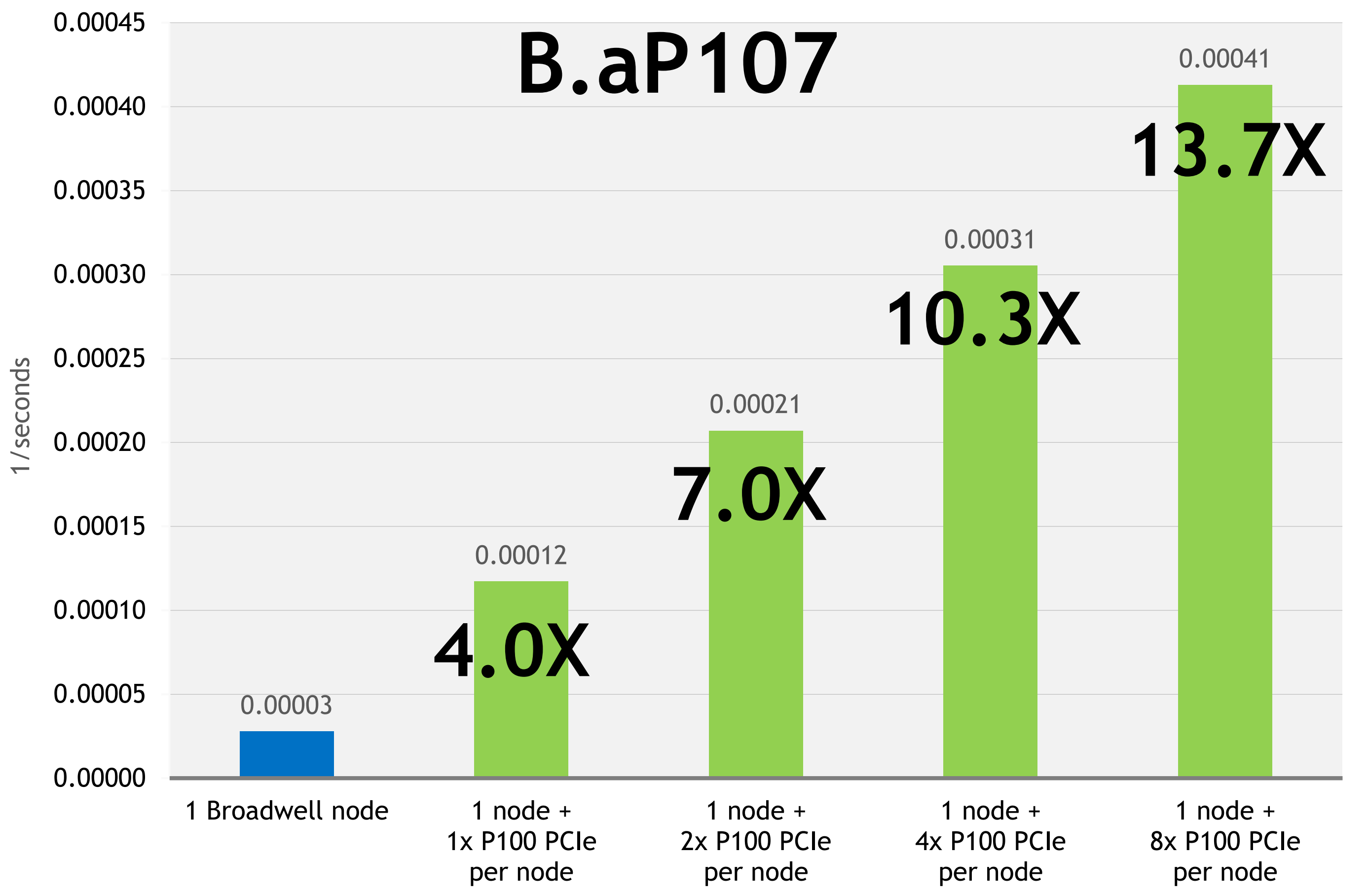
- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

105 Boron atoms (β-rhombohedral structure)
216 bands
110592 plane waves
Hybrid Functional with blocked Davicson (ALGO=Normal)
LHFCALC=.True. (Exact Exchange)

B.aP107 on P100s PCIe



Running VASP version 5.4.1

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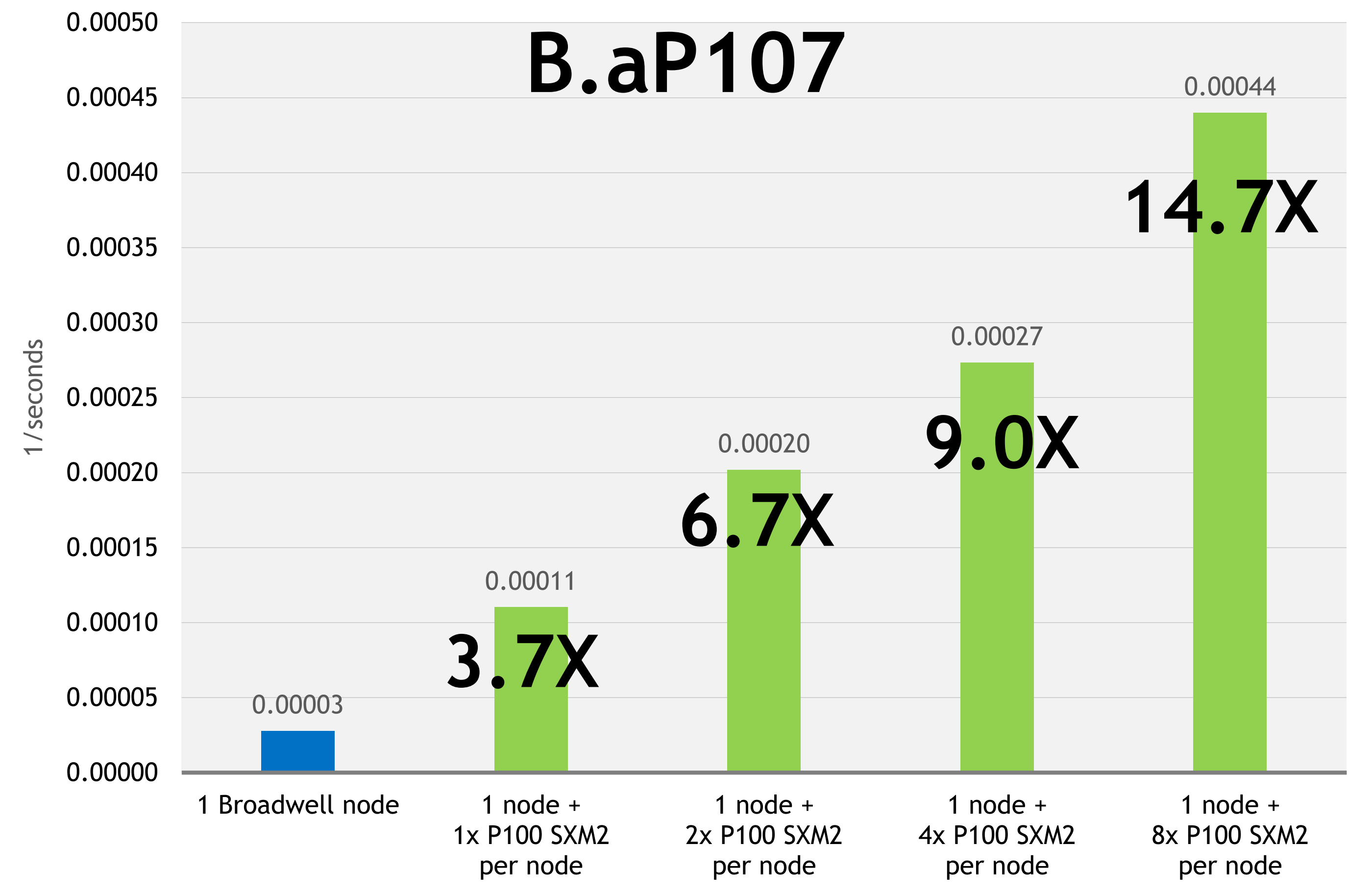
- 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

107 Boron atoms (symmetry broken 107-atom B′ variant)
216 bands
110592 plane waves
Hybrid functional calculation (exact exchange) with blocked Davidson. No KPoint parallelization.
Hybrid Functional with blocked Davidson (ALGO=Normal)
LHFCALC=.True. (Exact Exchange)

B.aP107 on P100s SXM2



Running VASP version 5.4.1

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Hybrid functional calculation (exact exchange) with blocked Davidson. No KPoint parallelization.
Hybrid Functional with blocked Davidson (ALGO=Normal)
LHFCALC=.True. (Exact Exchange)

Quantum Chemistry (QC) on GPUs

Dec, 19, 2016

GPU-Accelerated Molecular Dynamics Apps

Green Lettering Indicates Performance Slides Included

- ACEMD
- AMBER
- CHARMM
- DESMOND
- ESPResSO
- Folding@Home
- GENESIS
- GPUGrid.net
- GROMACS
- HALMD
- HOOMD-Blue
- HTMD
- LAMMPS
- mdcore
- MELD
- NAMD
- OpenMM
- PolyFTS

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