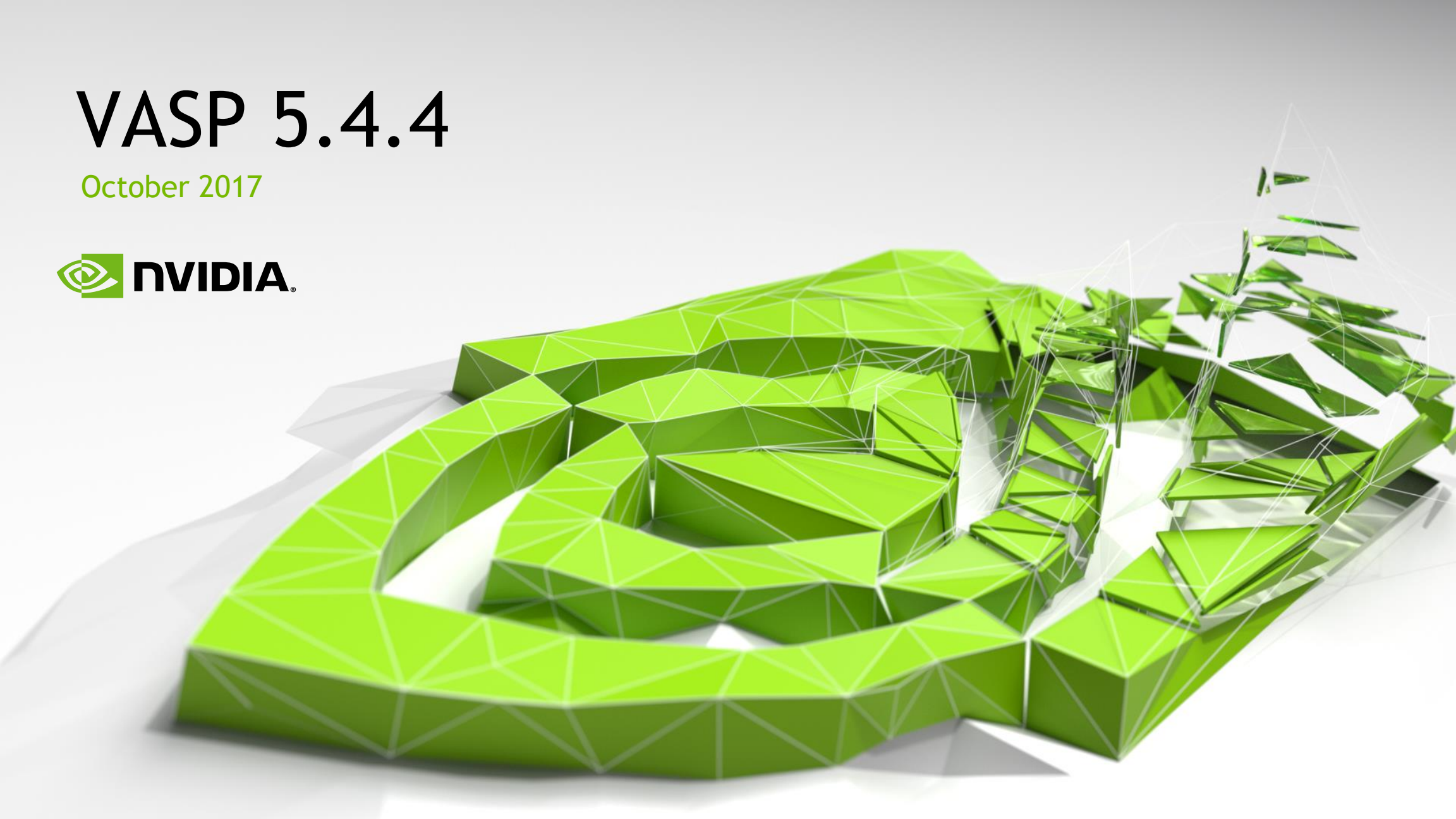
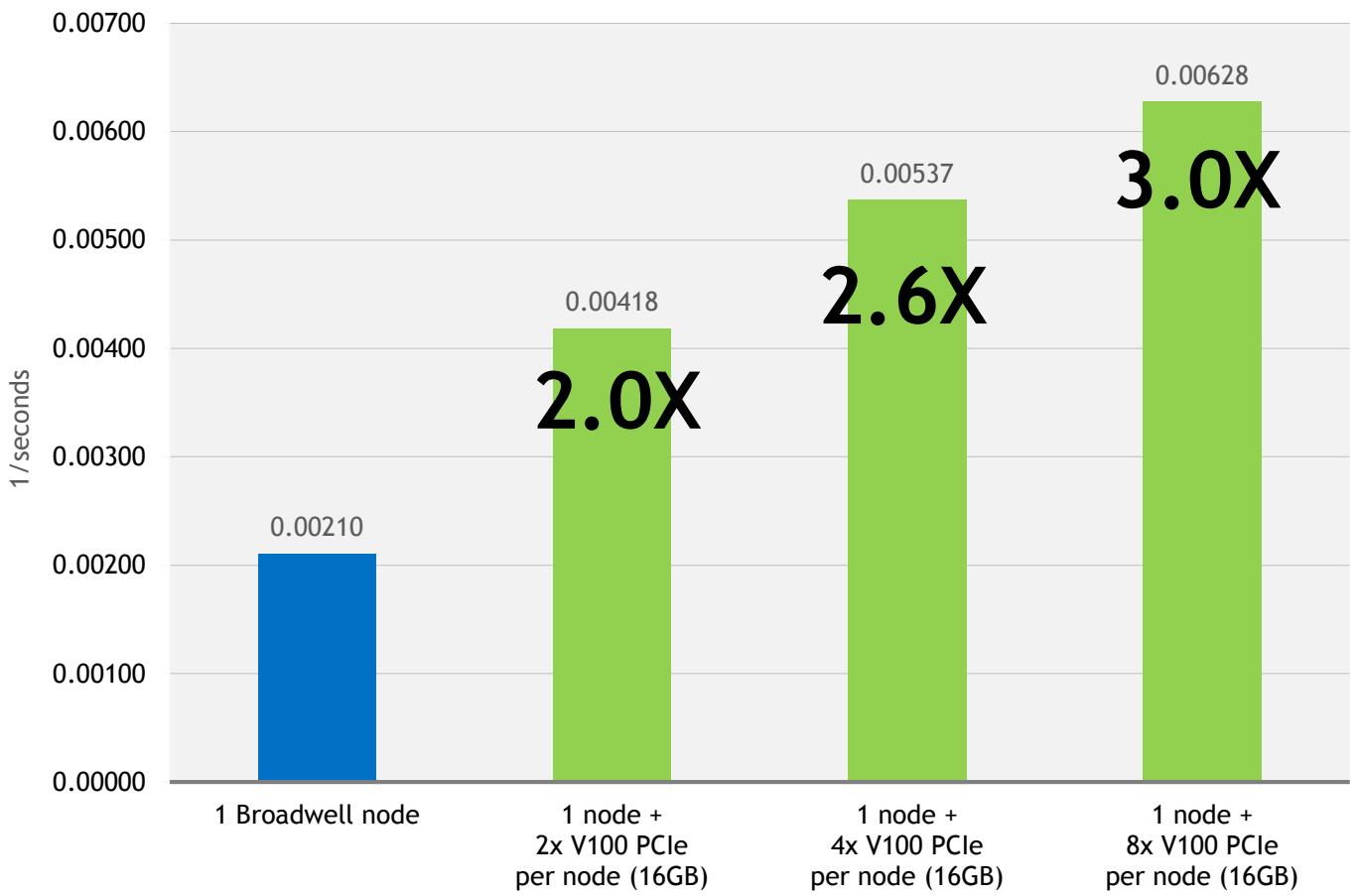
VASP 5.4.4

October 2017



Silica IFPEN on V100s PCIe



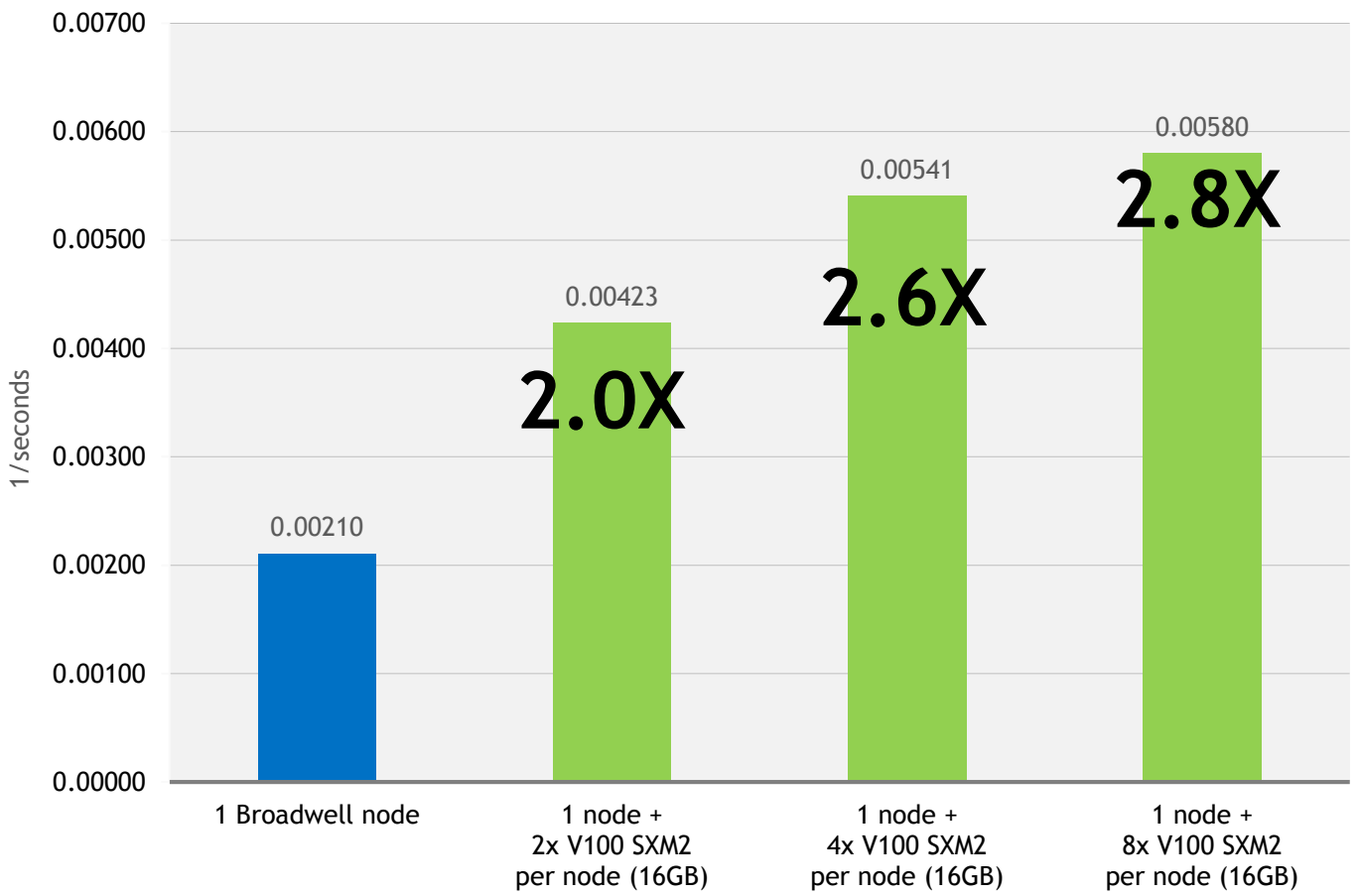
(Untuned on Volta)
Running VASP version 5.4.4

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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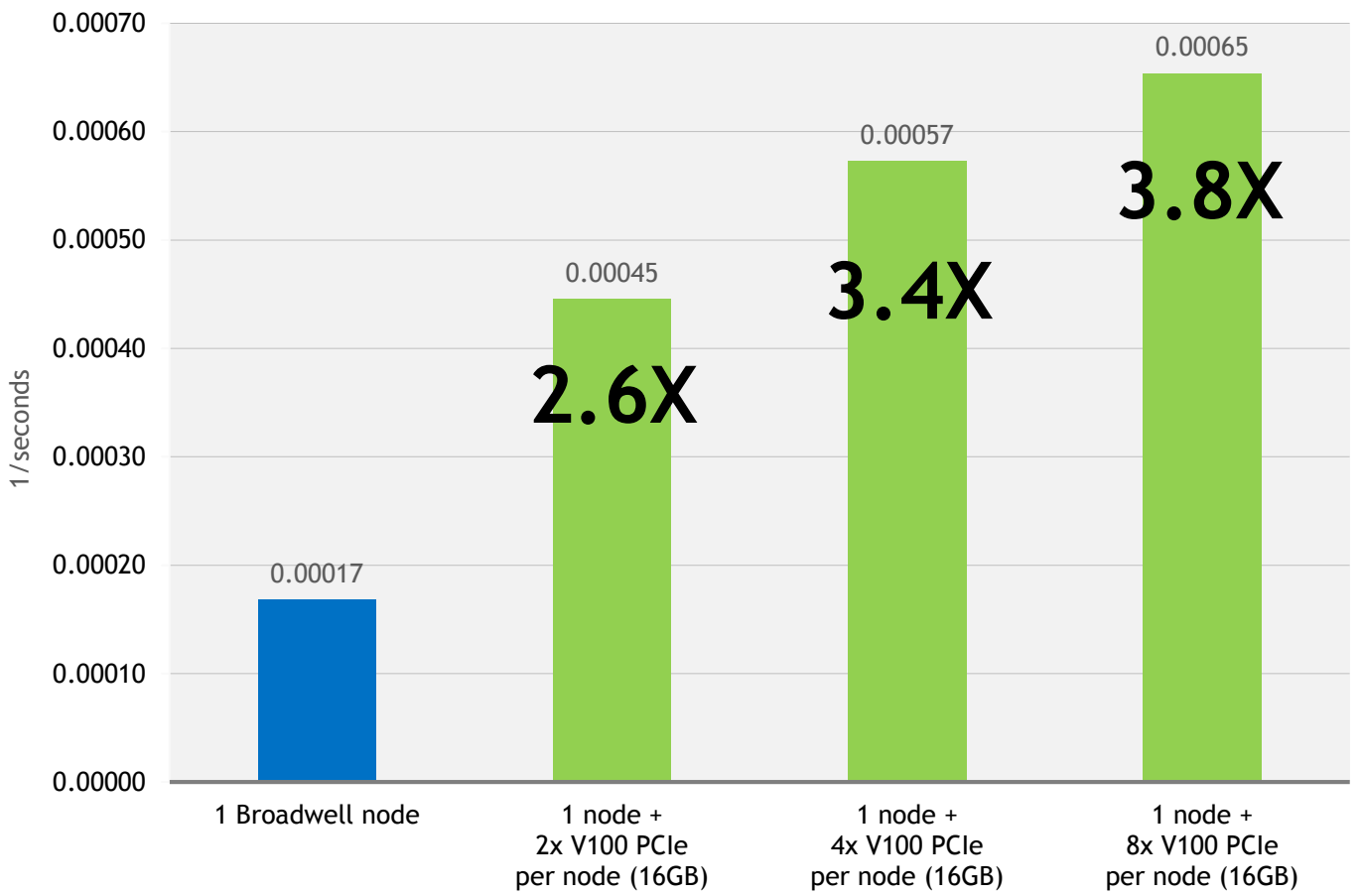
Si-Huge on V100s PCIe



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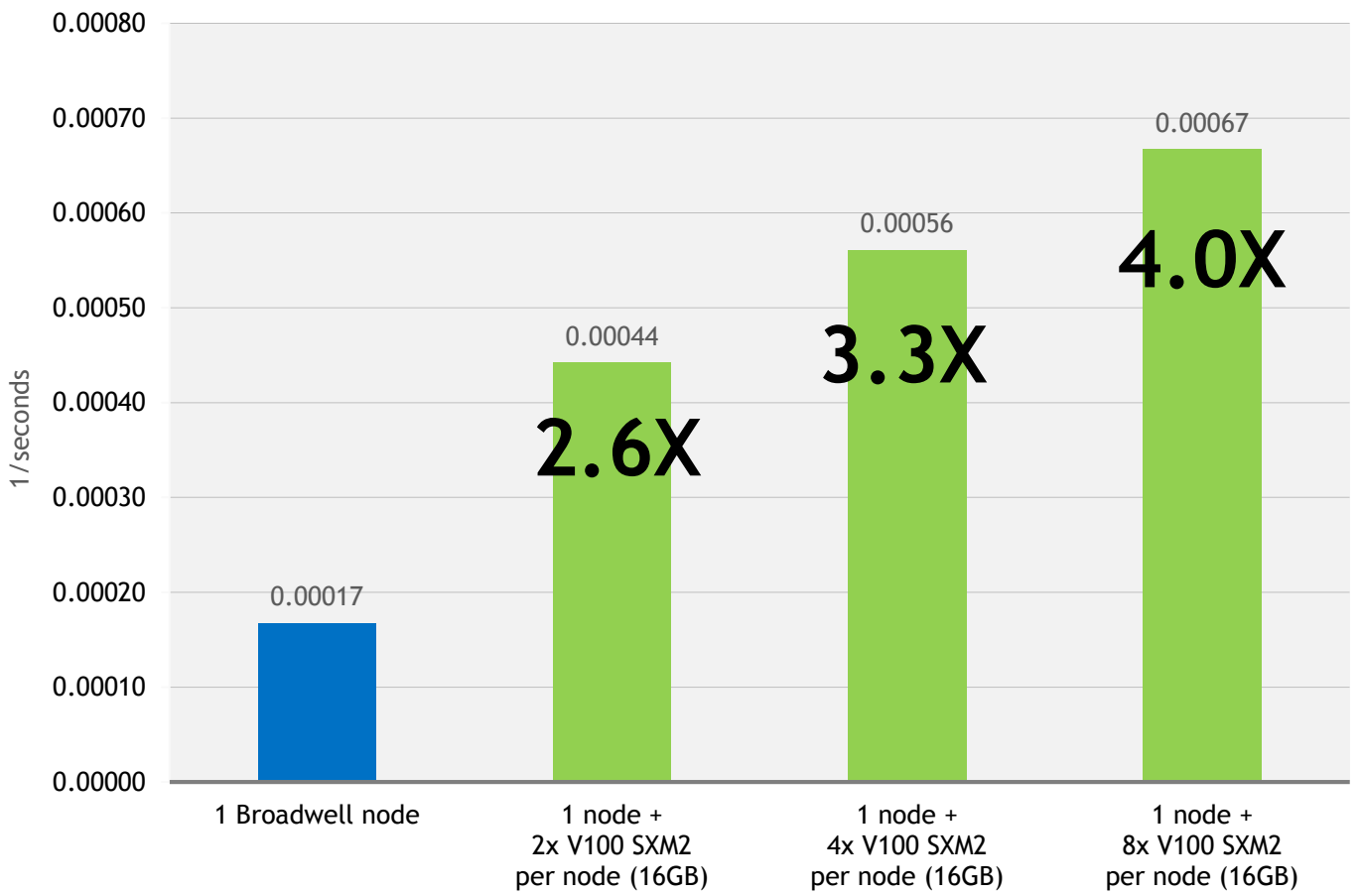
512 Si atoms
1282 bands
864000 Plane Waves
Algo = Normal (blocked Davidson)

Si-Huge on V100s SXM2



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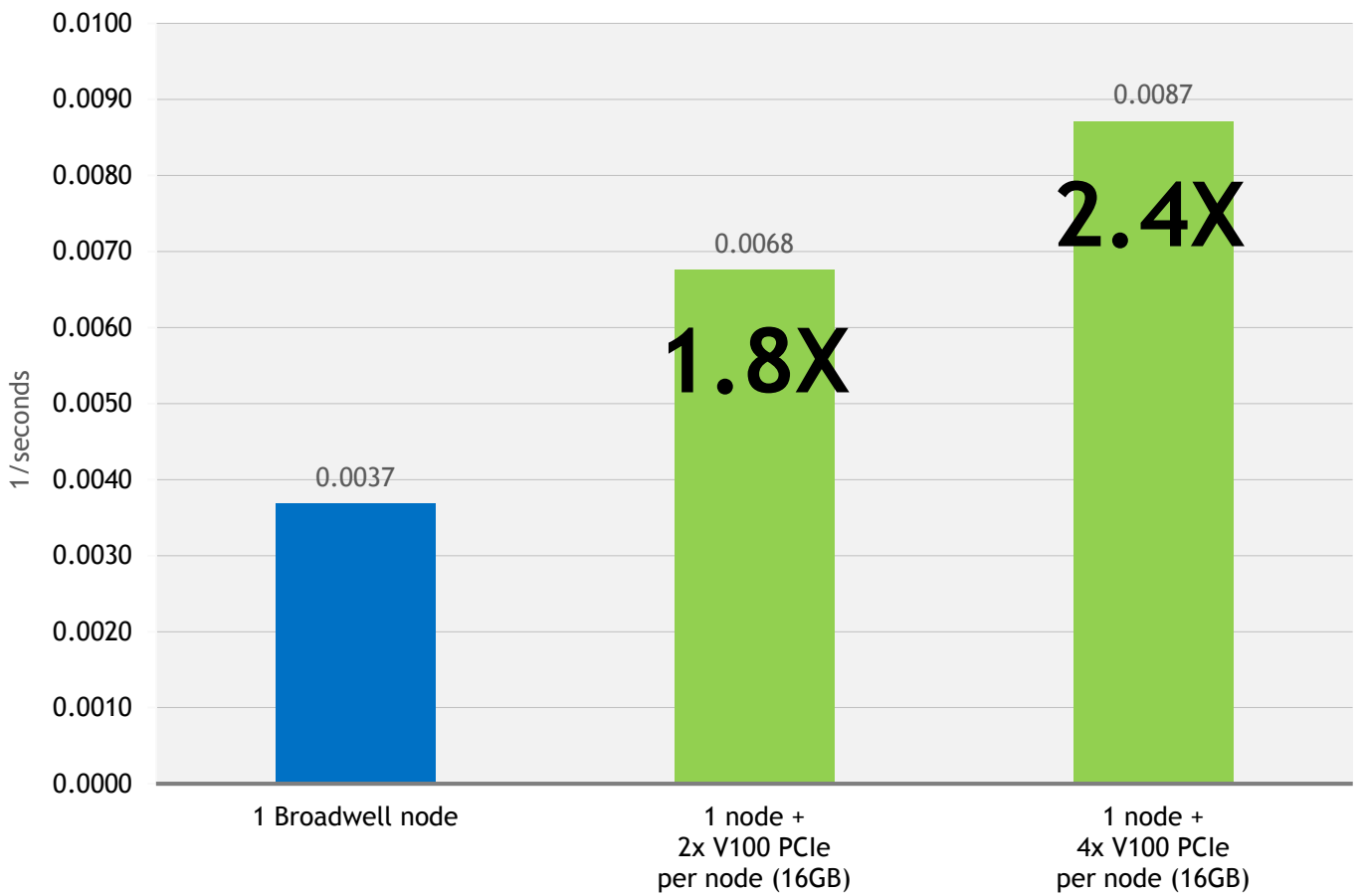
SupportedSystems on V100s PCIe



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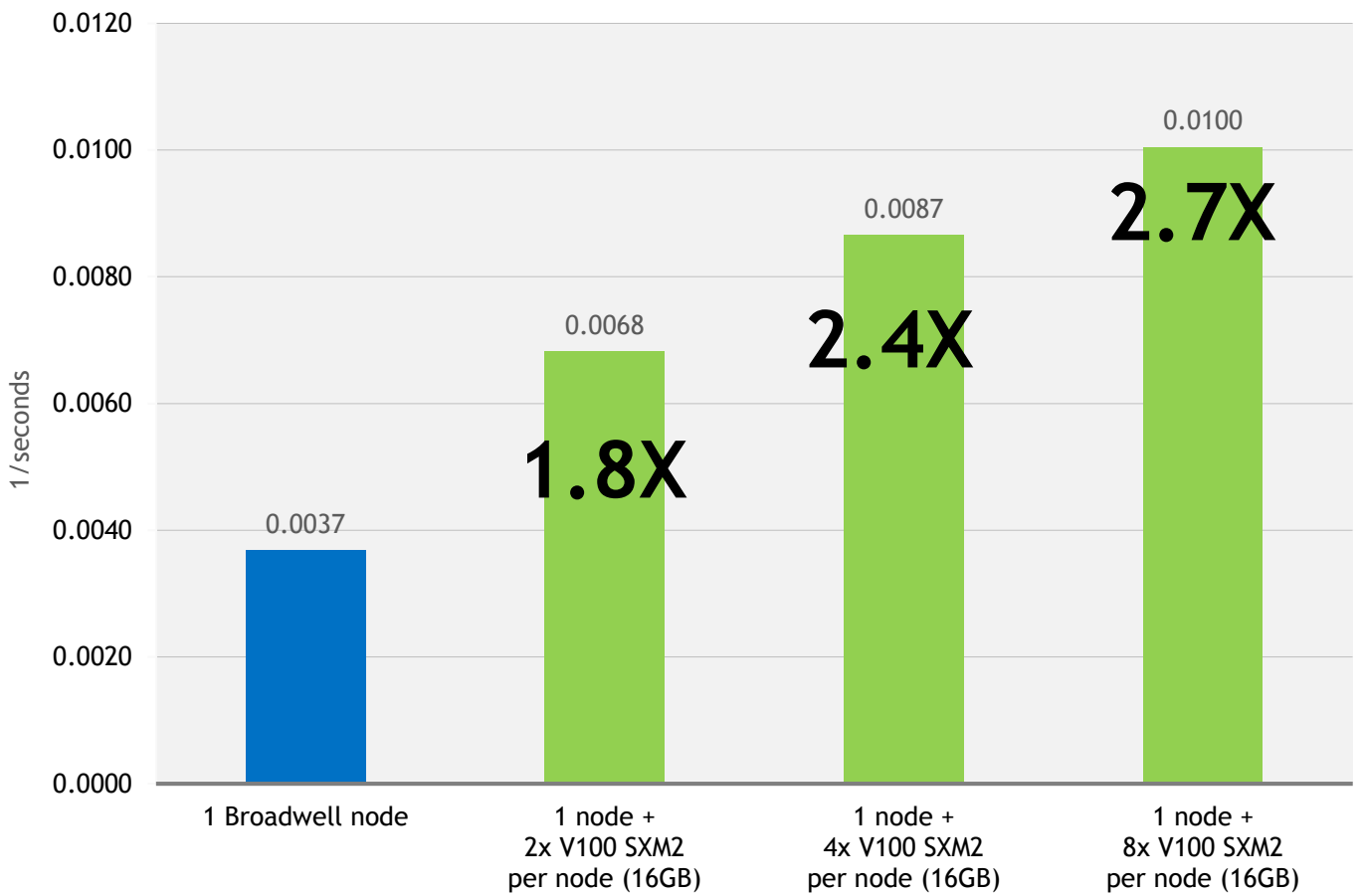
267 ions
788 bands
762048 plane waves
ALGO = Fast (Davidson + RMM-DIIS)

SupportedSystems on V100s SXM2



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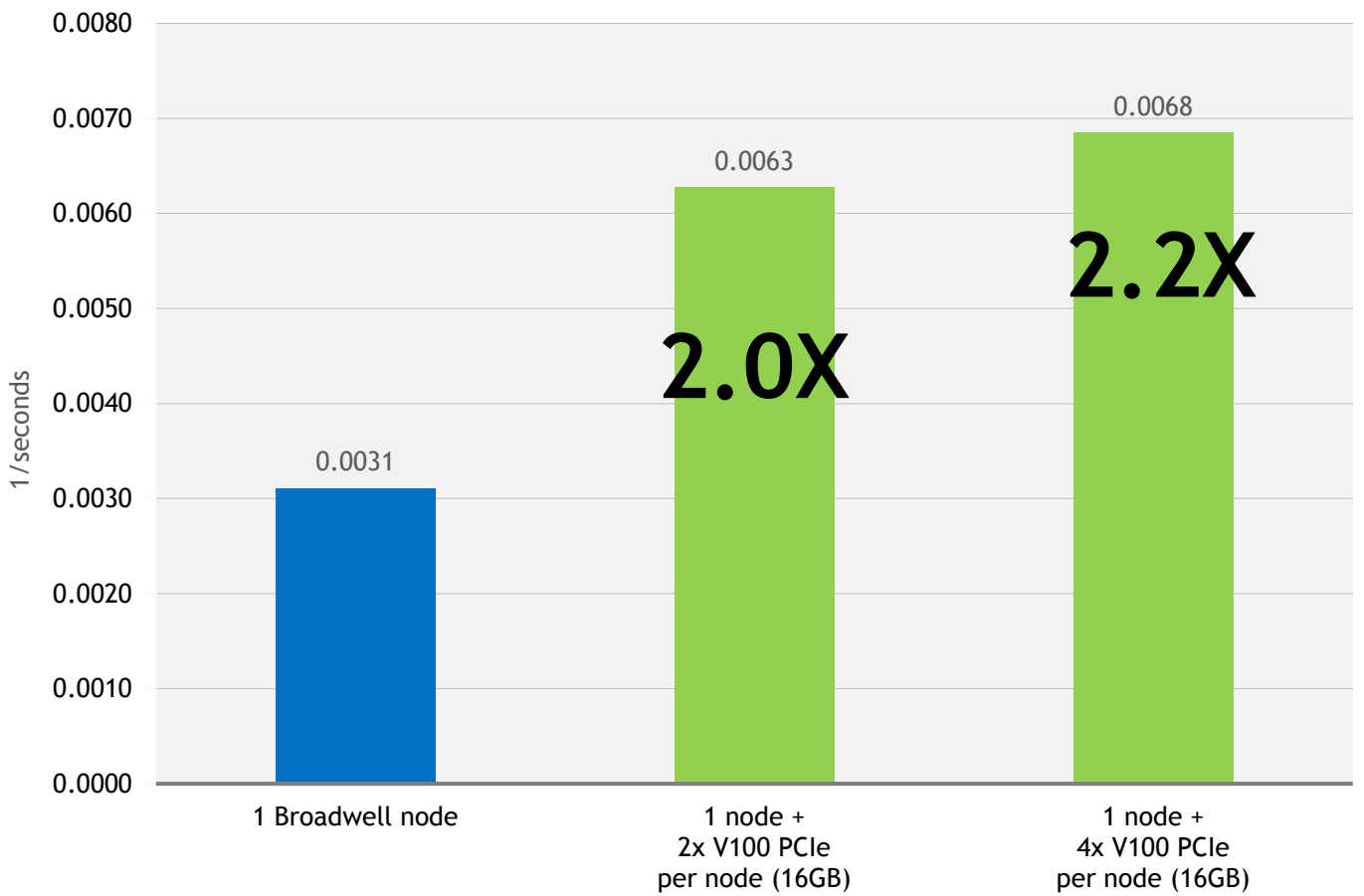
267 ions
788 bands
762048 plane waves
ALGO = Fast (Davidson + RMM-DIIS)

NiAl-MD on V100s PCIe



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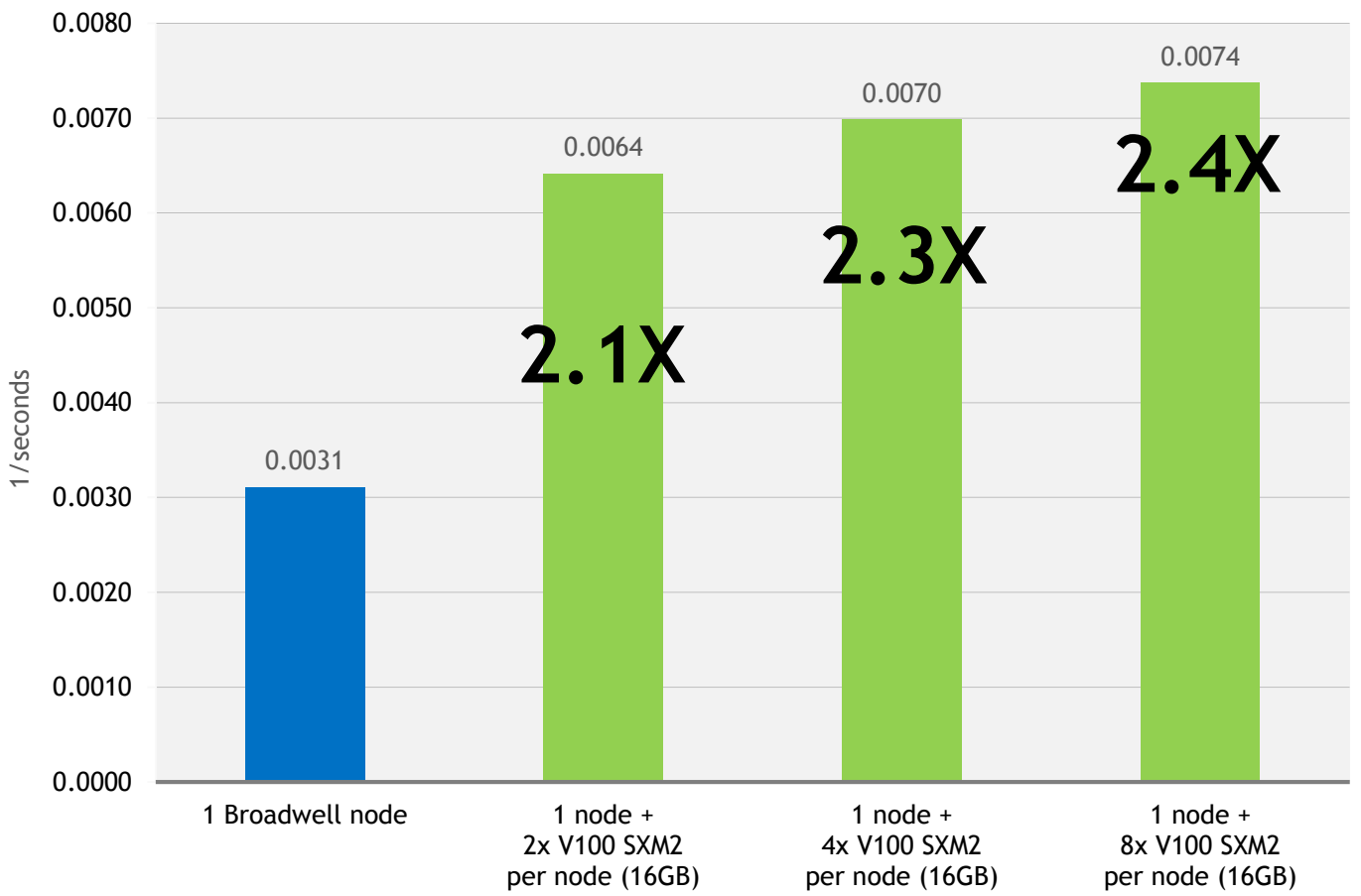
The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla V100 PCIe (16GB) GPUs

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

NiAl-MD on V100s SXM2



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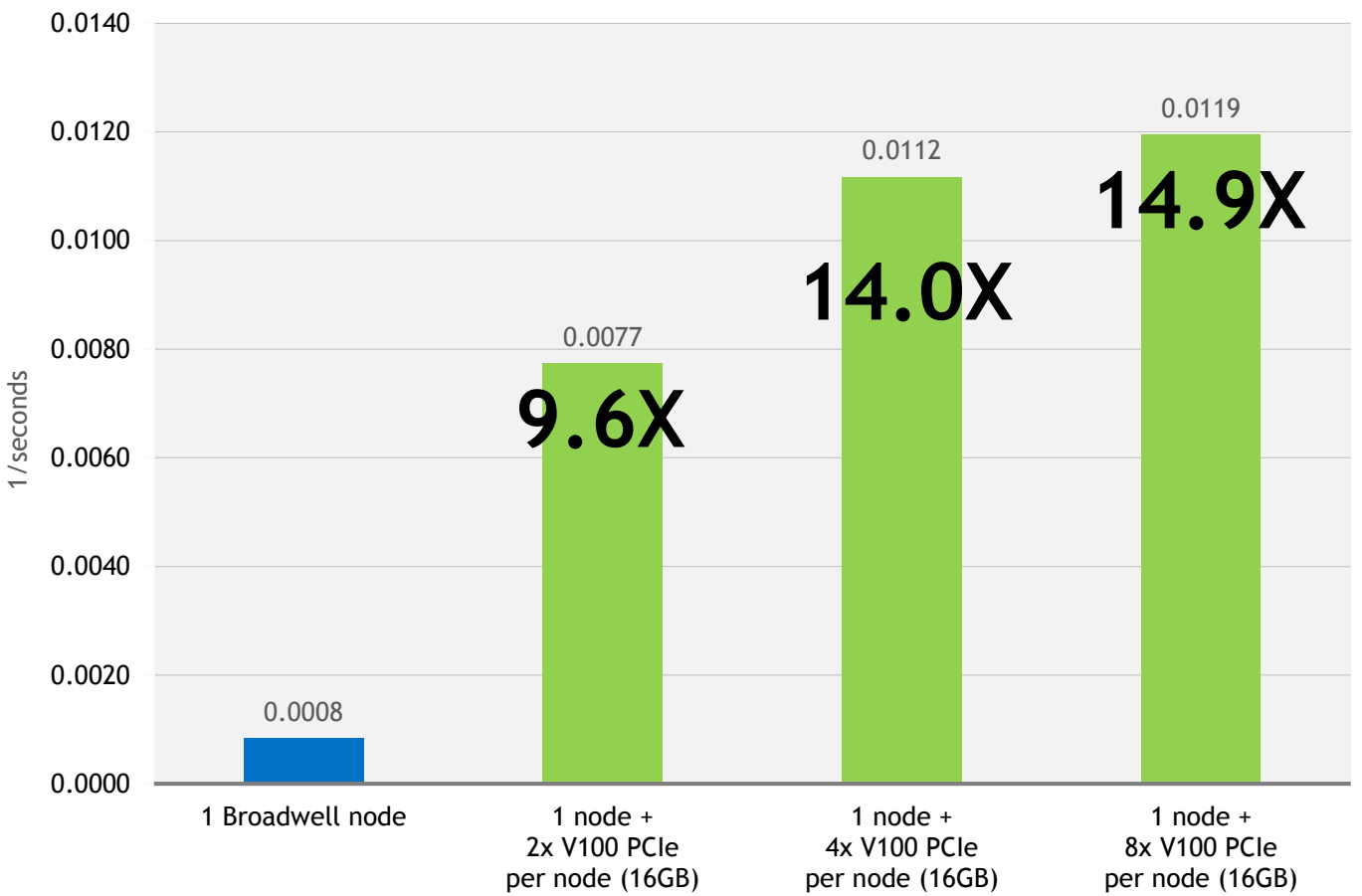
500 ions
3200 bands
729000 plane waves
ALGO = Fast (Davidson + RMM-DIIS)

B.hR105 on V100s PCIe



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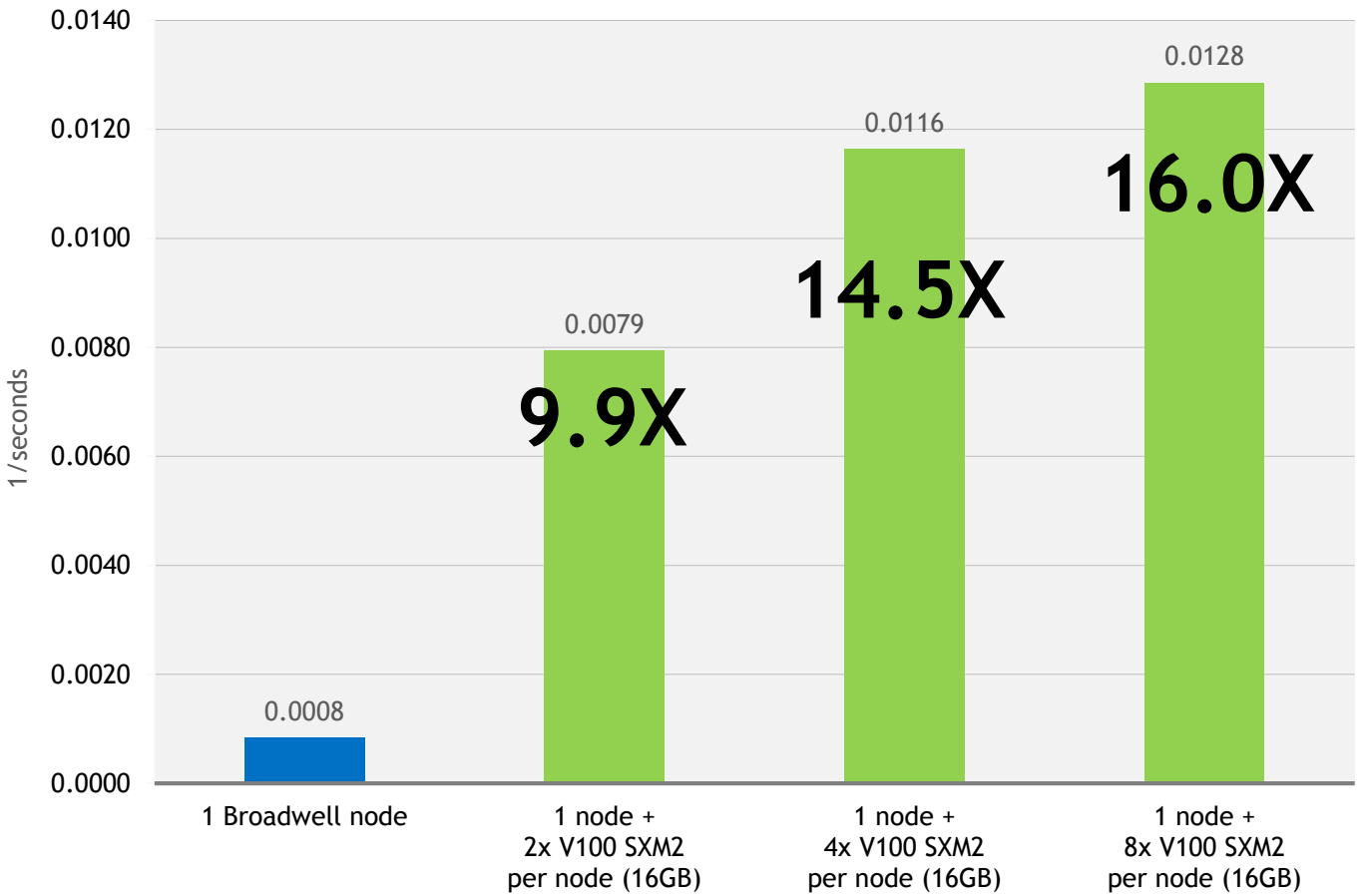
The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla V100 PCIe (16GB) GPUs

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

B.hR105 on V100s SXM2



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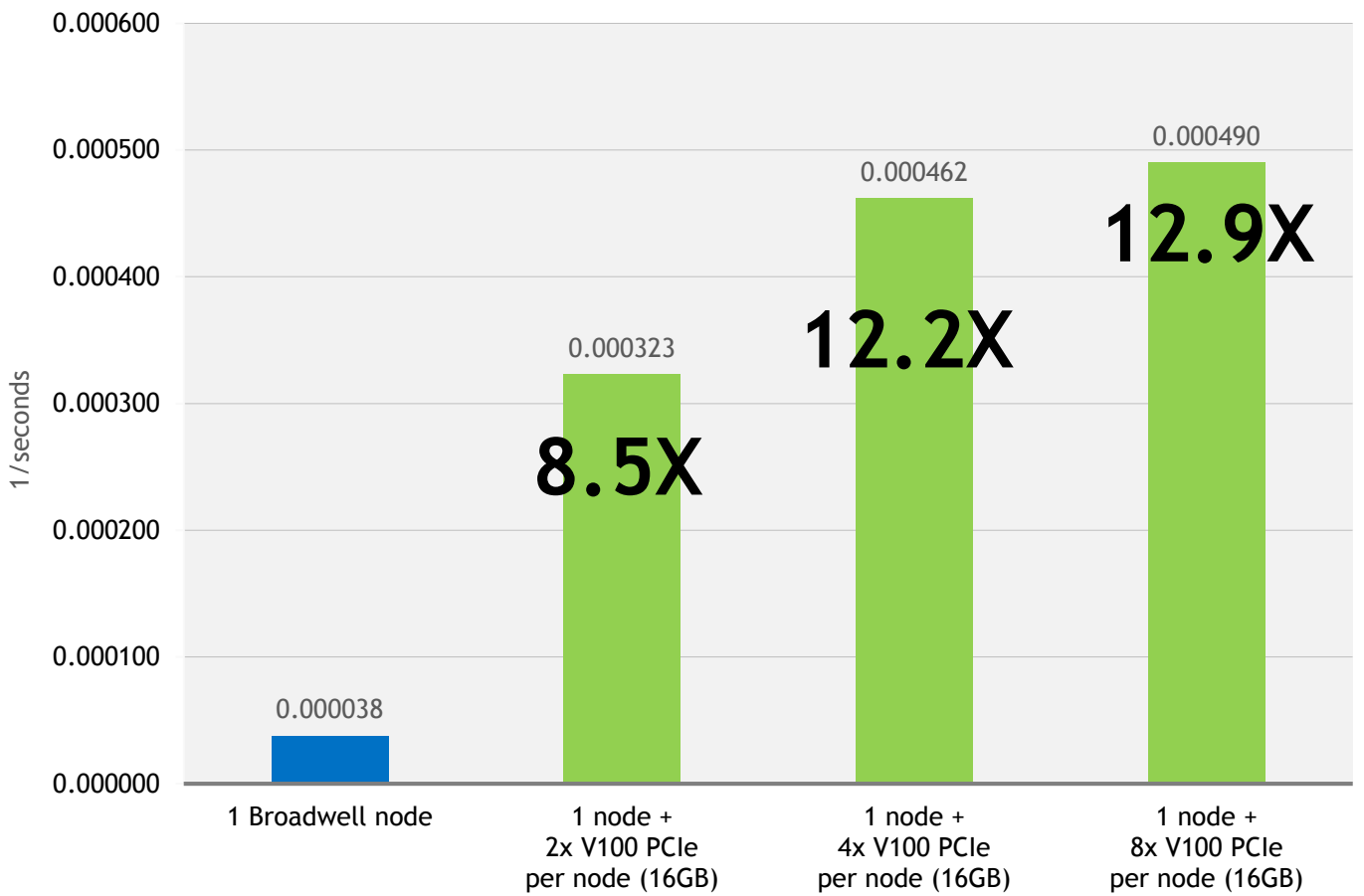
105 Boron atoms (B-rhombohedral structure)
216 bands
110592 plane waves
Hybrid Functional with blocked Davicson (ALGO=Normal)
LHFCALC=.True. (Exact Exchange)

B.aP107 on V100s PCIe



(Untuned on Volta)
Running VASP version 5.4.4

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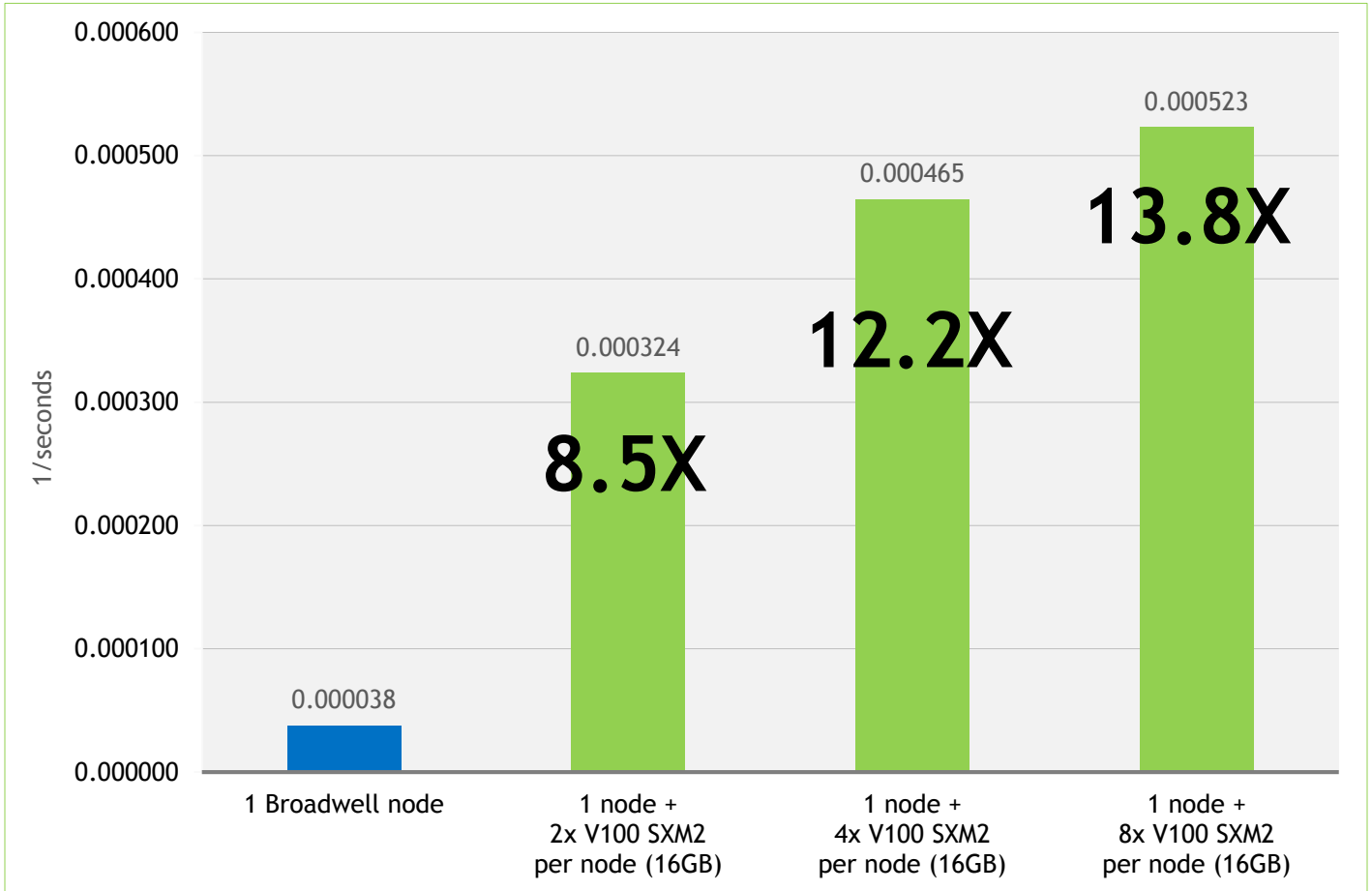
The green nodes contain Dual Intel Xeon E5-2690 v4@2.6GHz [3.5GHz Turbo] (Broadwell) CPUs + Tesla V100 PCIe (16GB) GPUs

107 Boron atoms (symmetry broken 107-atom 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 V100s SXM2



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