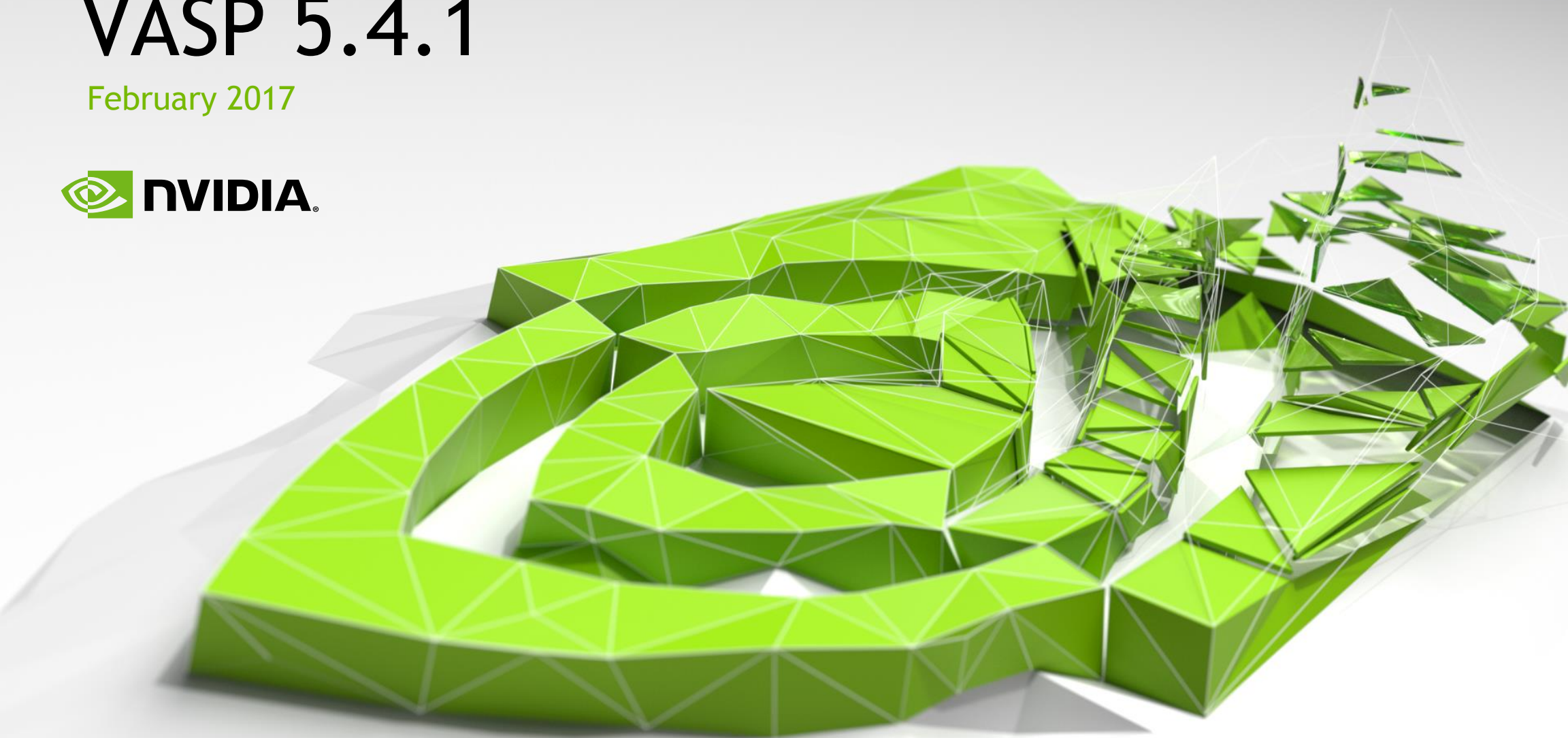
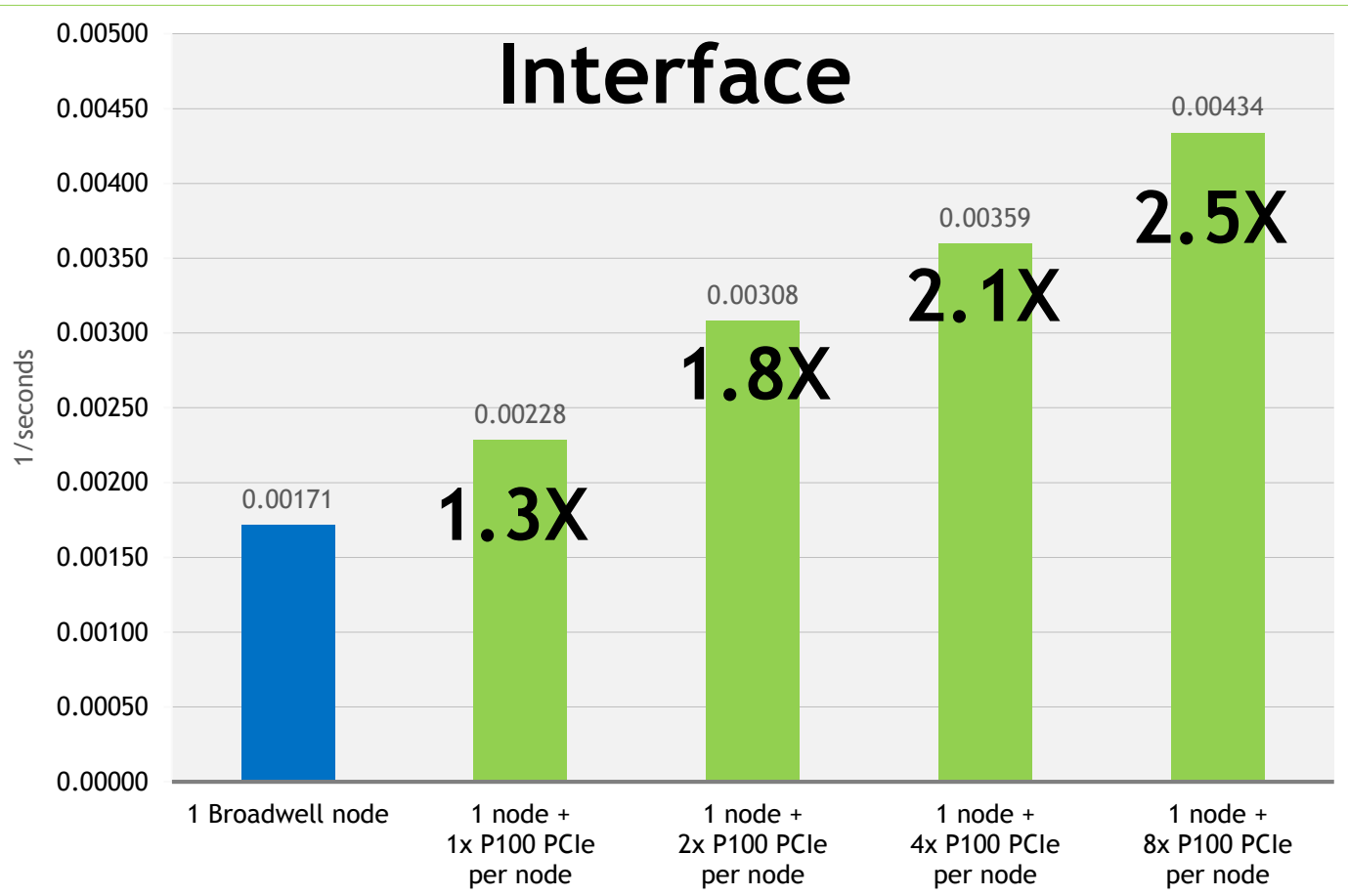


VASP 5.4.1

February 2017



Interface on P100s PCIe



Running **VASP** version 5.4.1

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

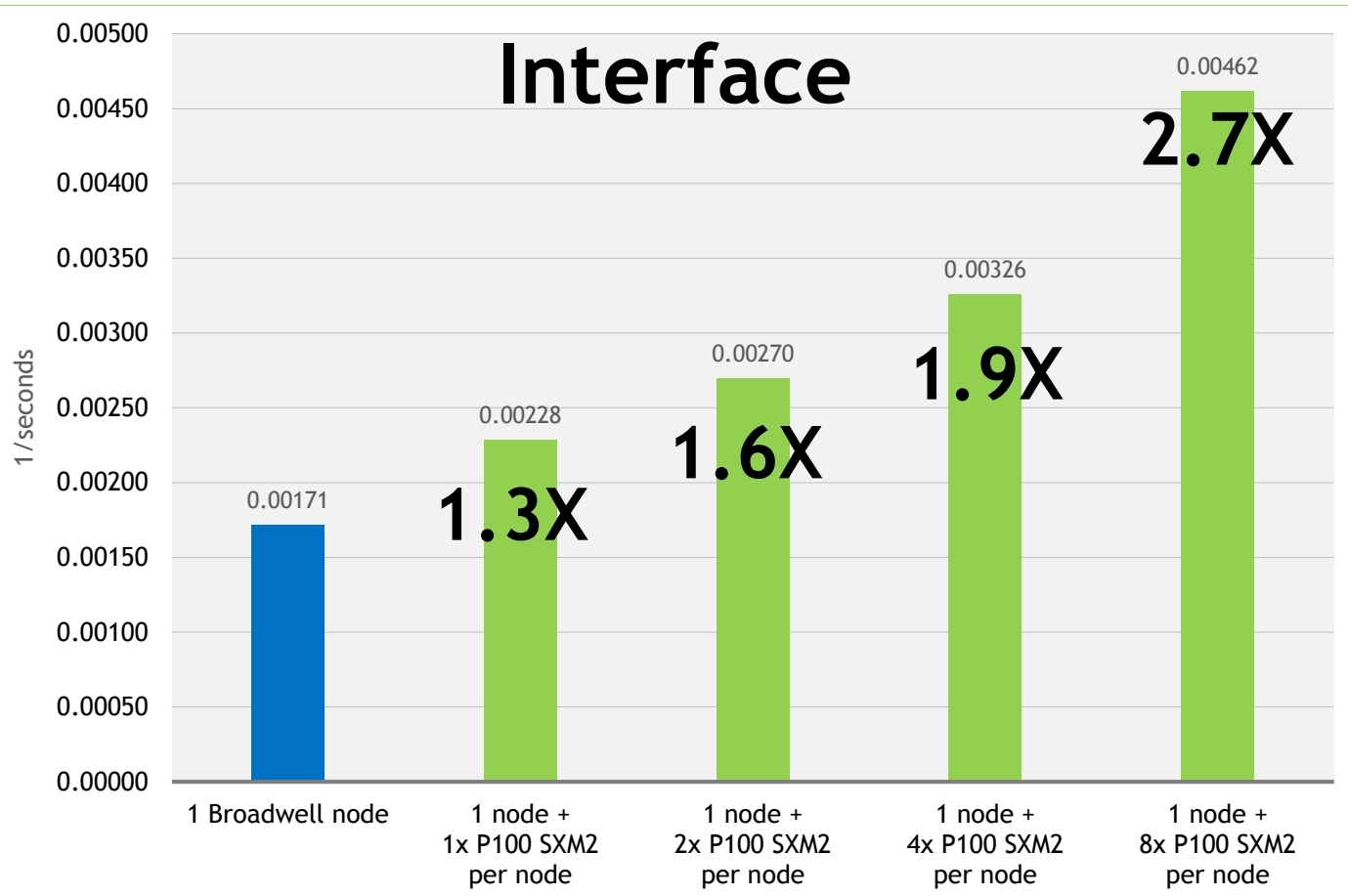
The **green nodes** contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

➤ 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

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

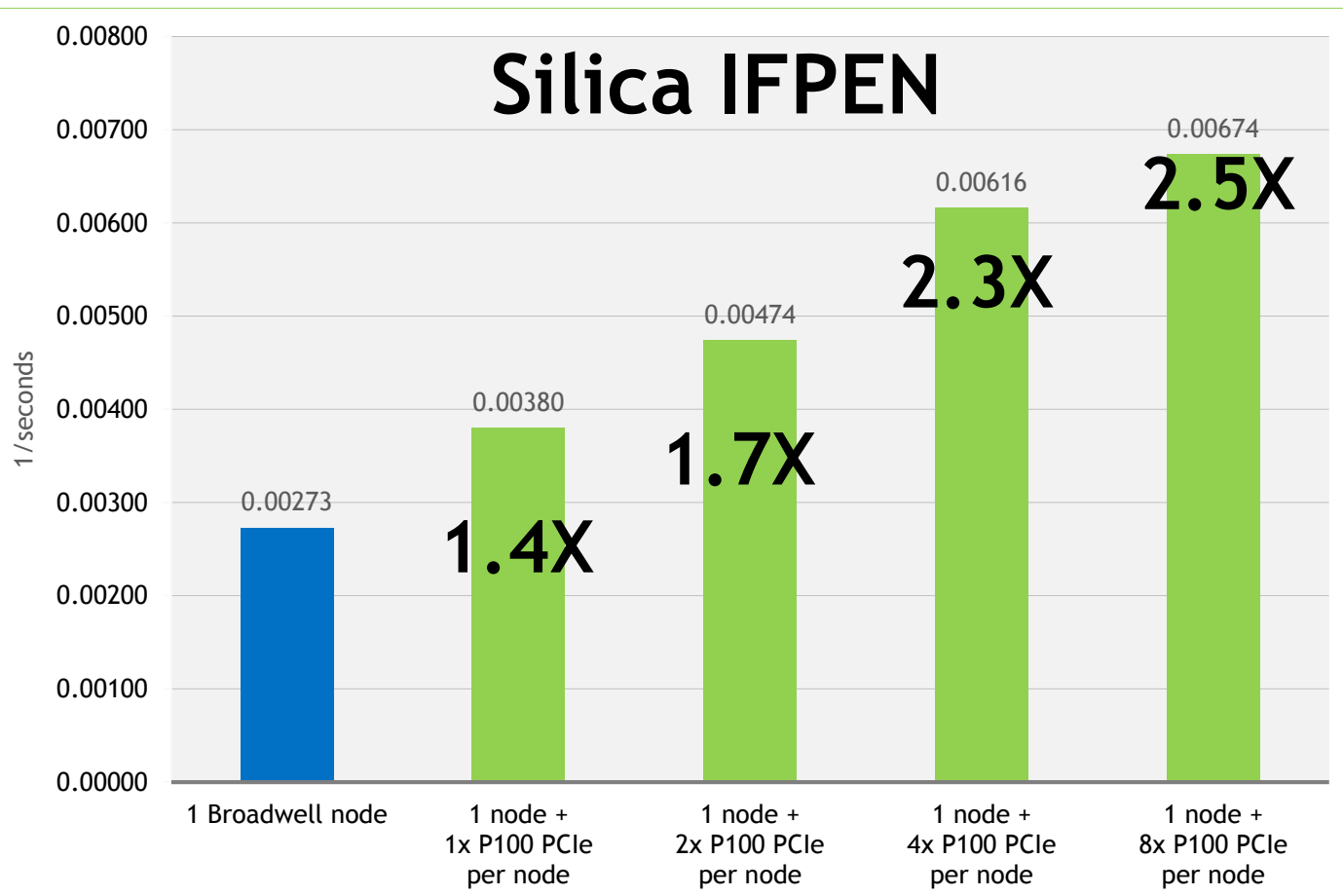
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Interface between a platinum slab Pt(111) (108 atoms) and liquid water (120 water molecules) (468 ions)

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

Silica IFPEN on P100s PCIe



Running **VASP** version 5.4.1

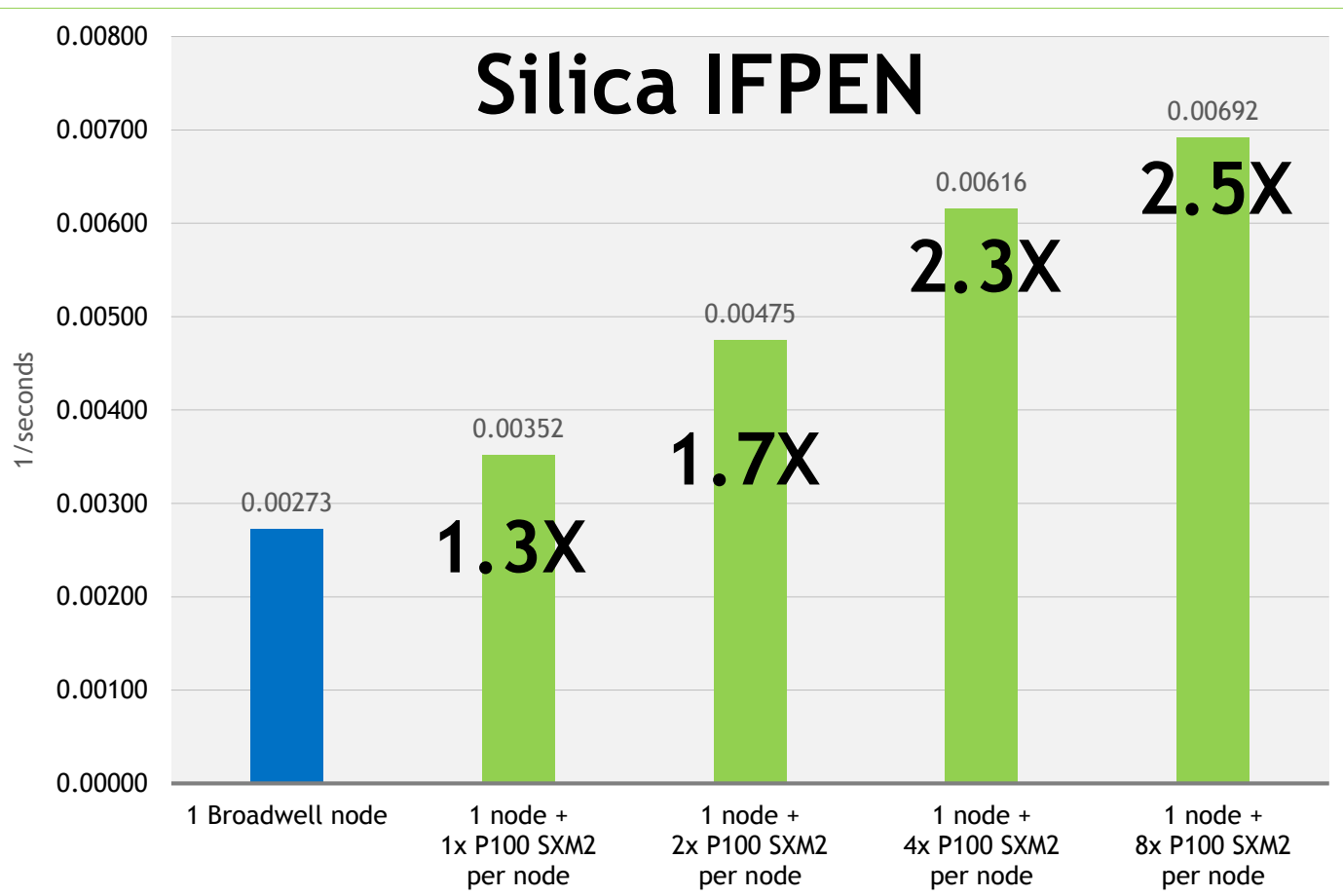
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➤ 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

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

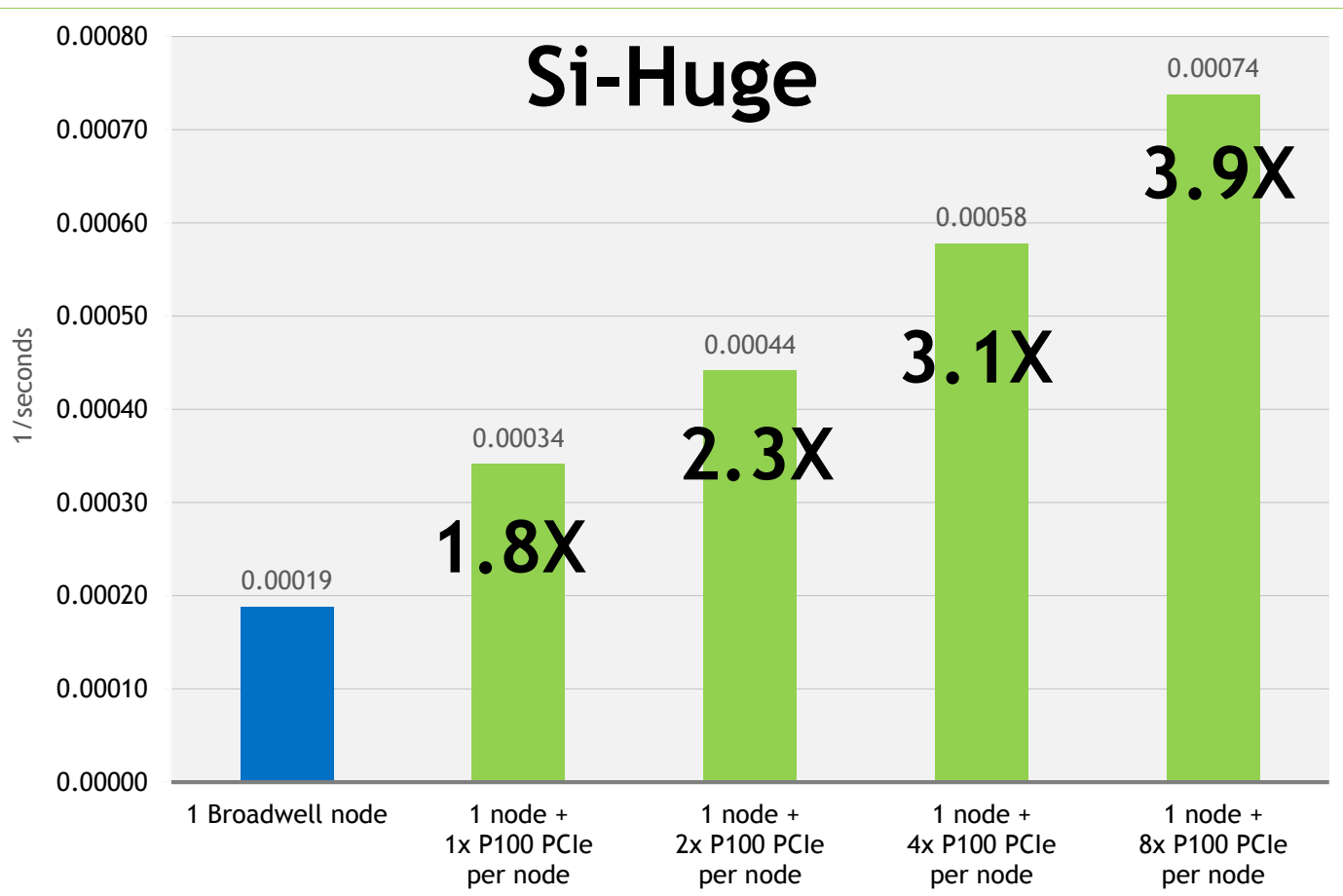
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240 ions, cristobalite (high) bulk
720 bands
? plane waves
ALGO = Very Fast (RMM-DIIS)

Si-Huge on P100s PCIe



Running **VASP** version 5.4.1

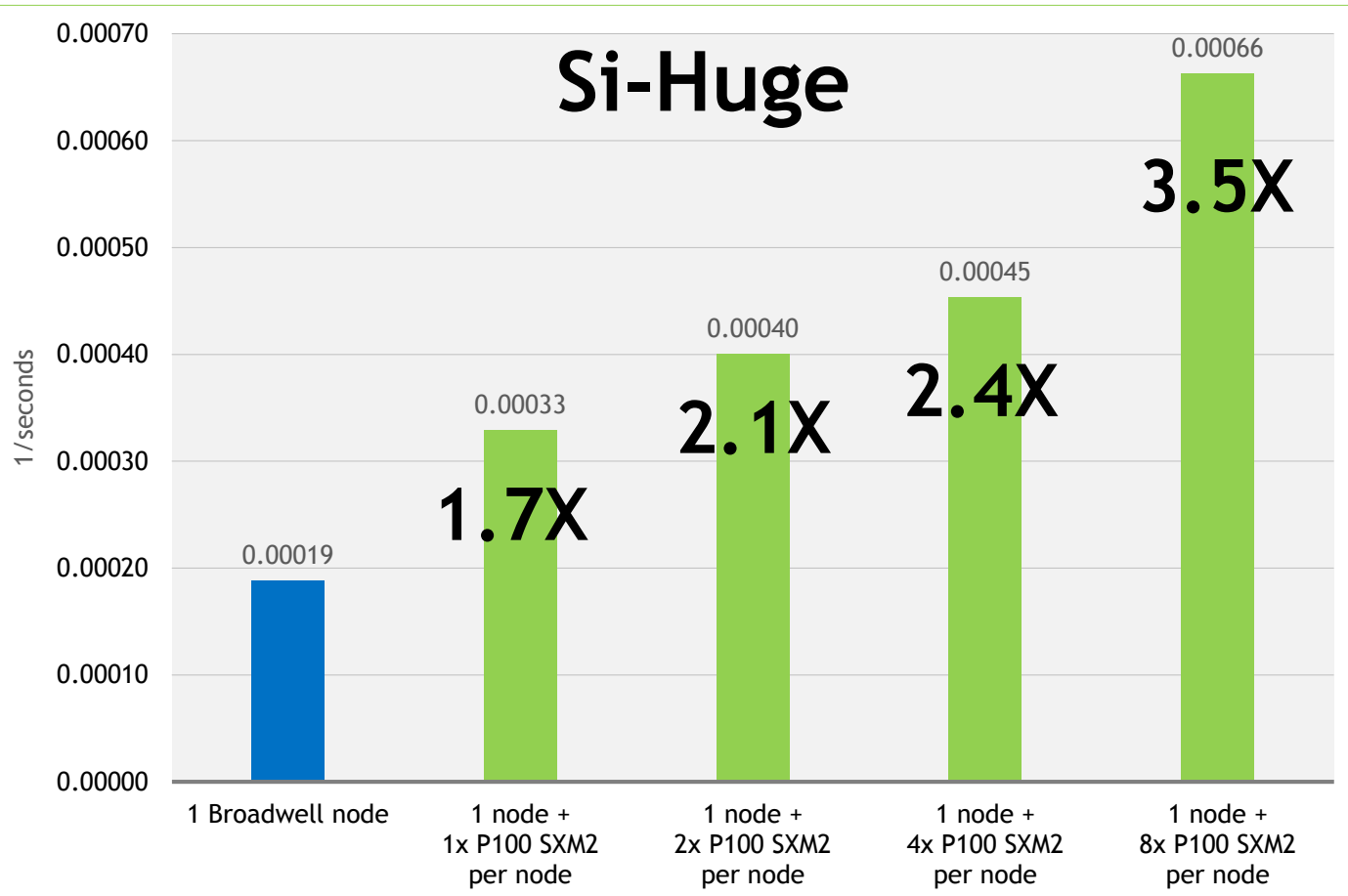
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➤ 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

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

Si-Huge on P100s SXM2



Running **VASP** version 5.4.1

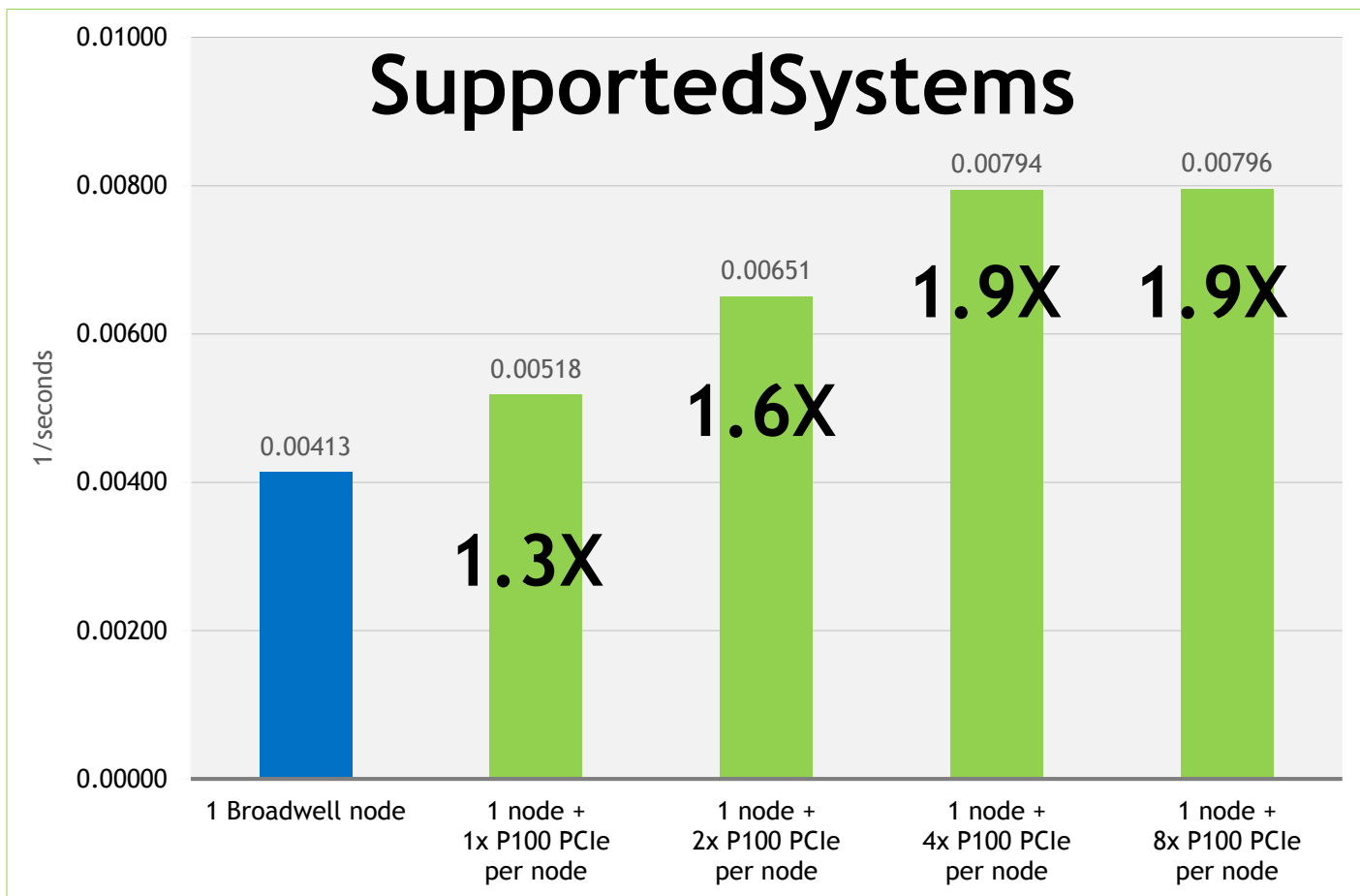
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512 Si atoms
1282 bands
864000 Plane Waves
Algo = Normal (blocked Davidson)

SupportedSystems on P100s PCIe



Running **VASP** version 5.4.1

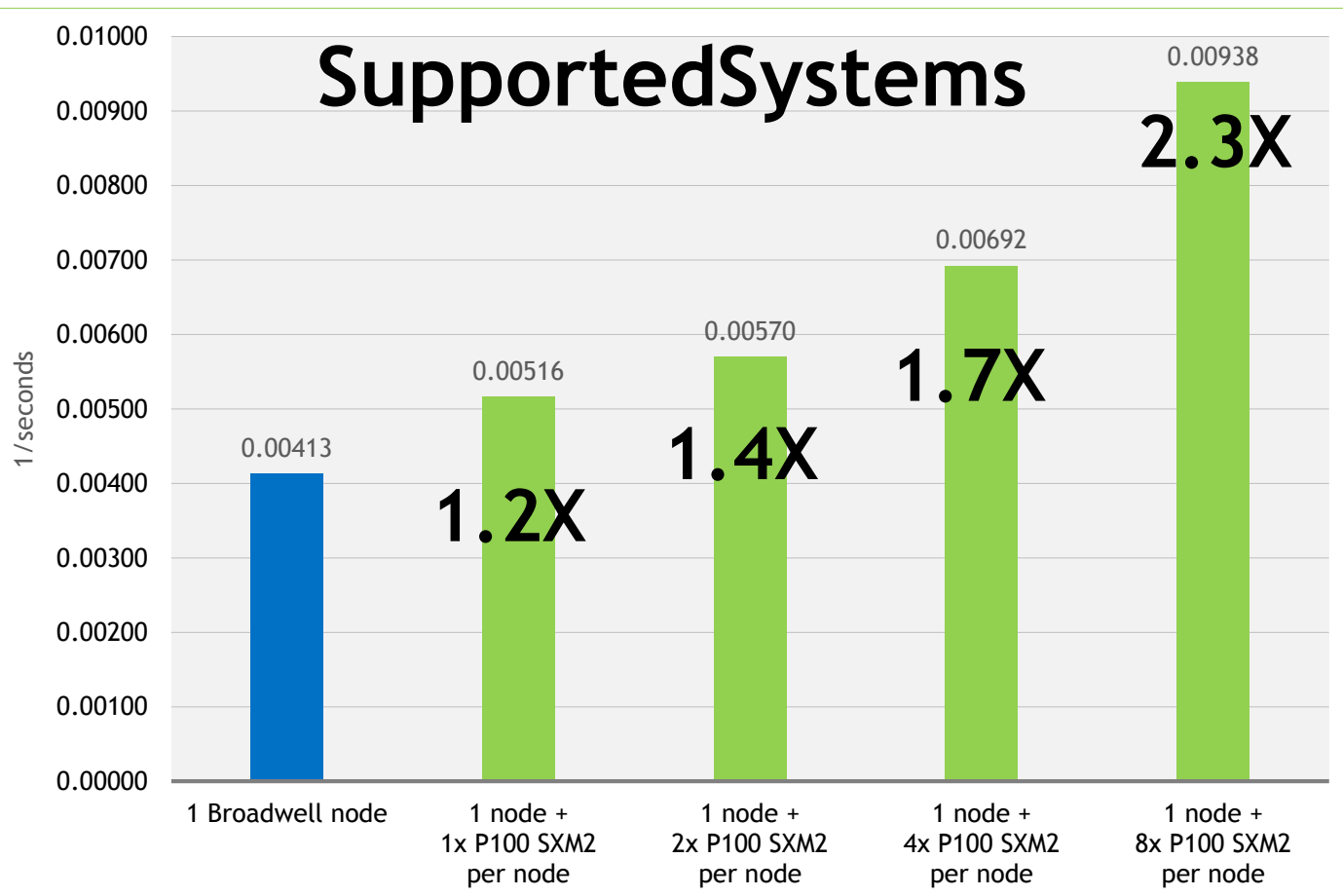
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➤ 1x P100 PCIe is paired with Single Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

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

SupportedSystems on P100s SXM2



Running **VASP** version 5.4.1

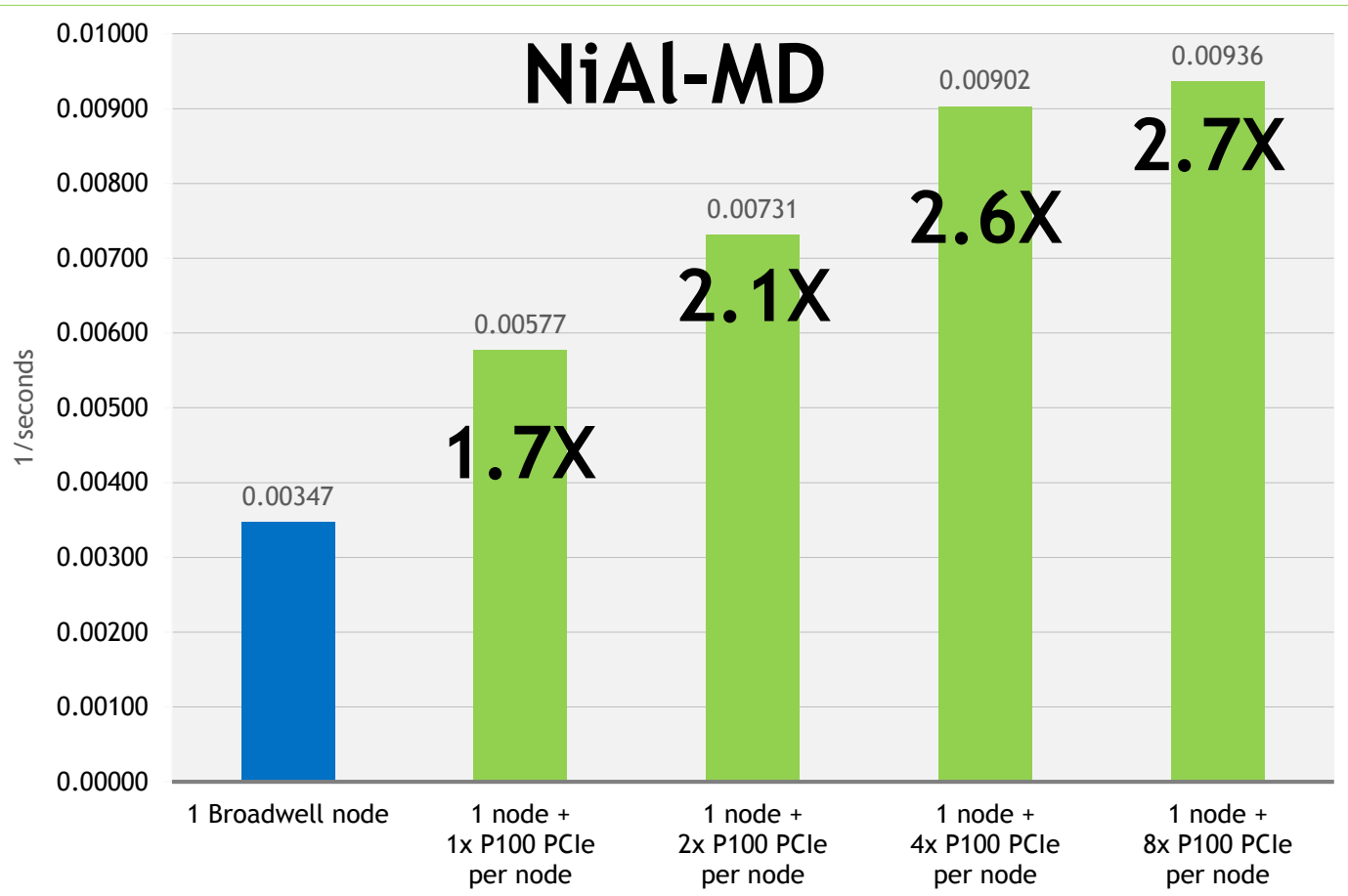
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*267 ions
788 bands
762048 plane waves
ALGO = Fast (Davidson + RMM-DIIS)*

NiAl-MD on P100s PCIe



Running **VASP** version 5.4.1

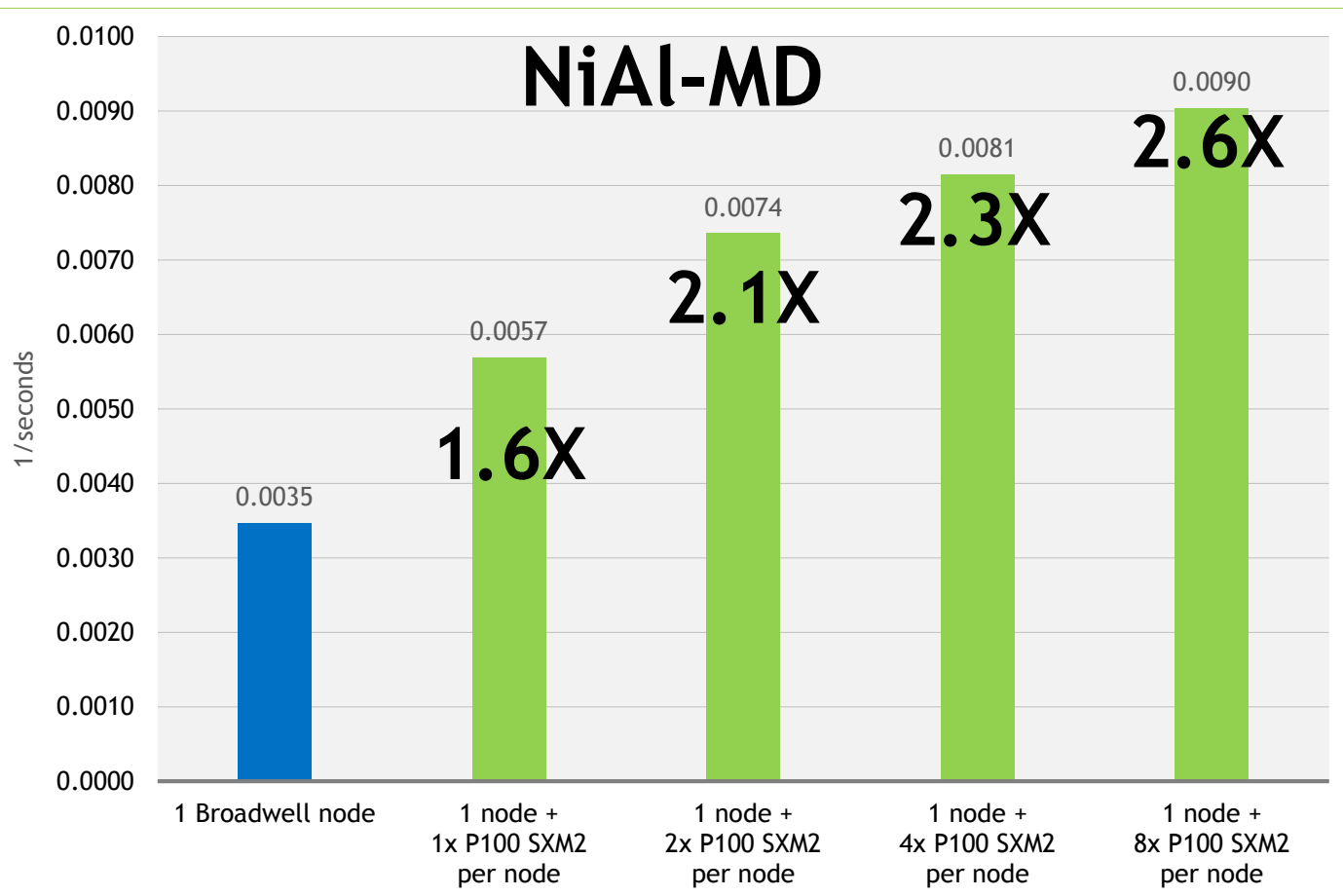
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The **green nodes** contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

➤ 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

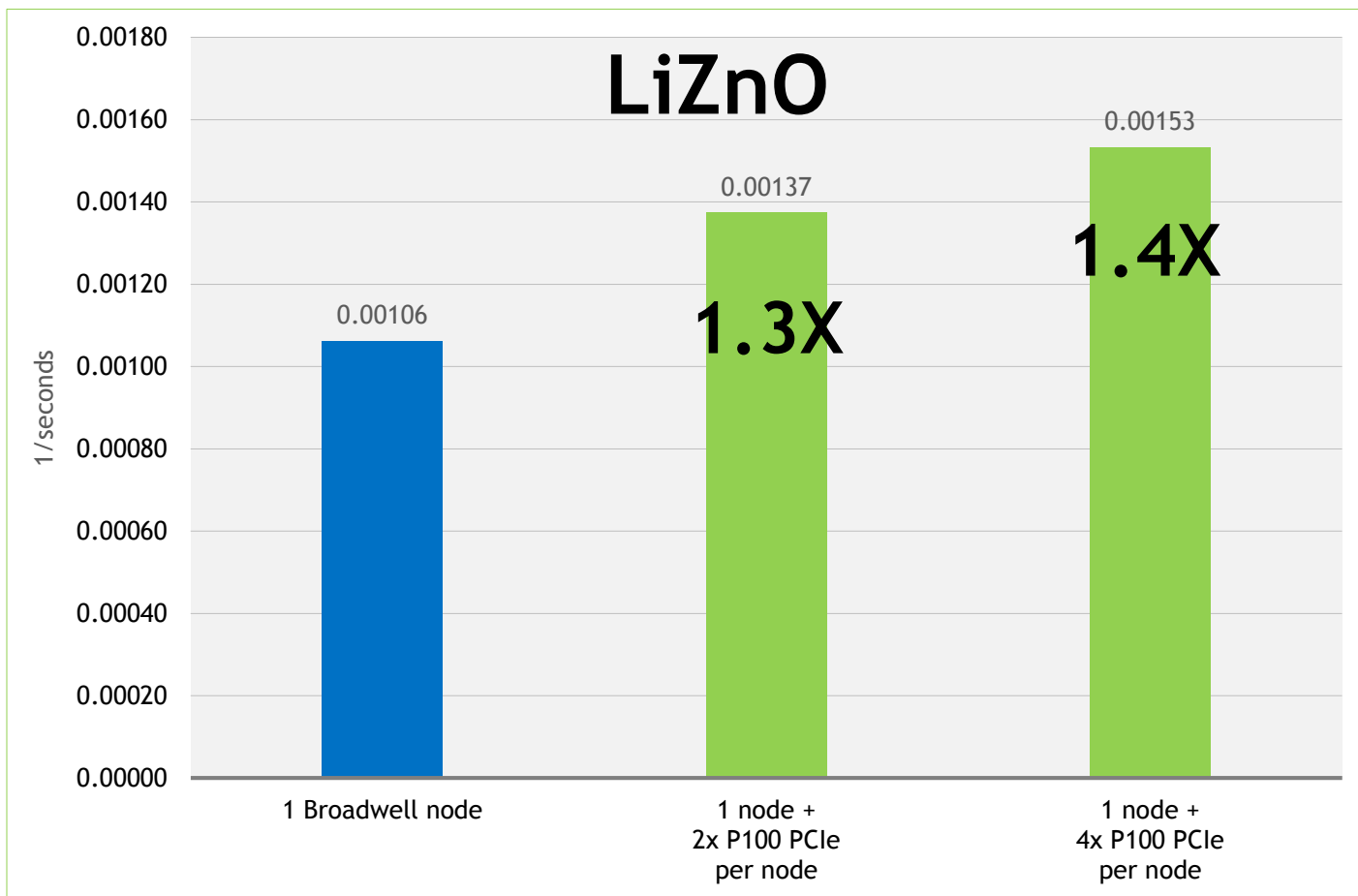
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- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

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

LiZnO on P100s PCIe



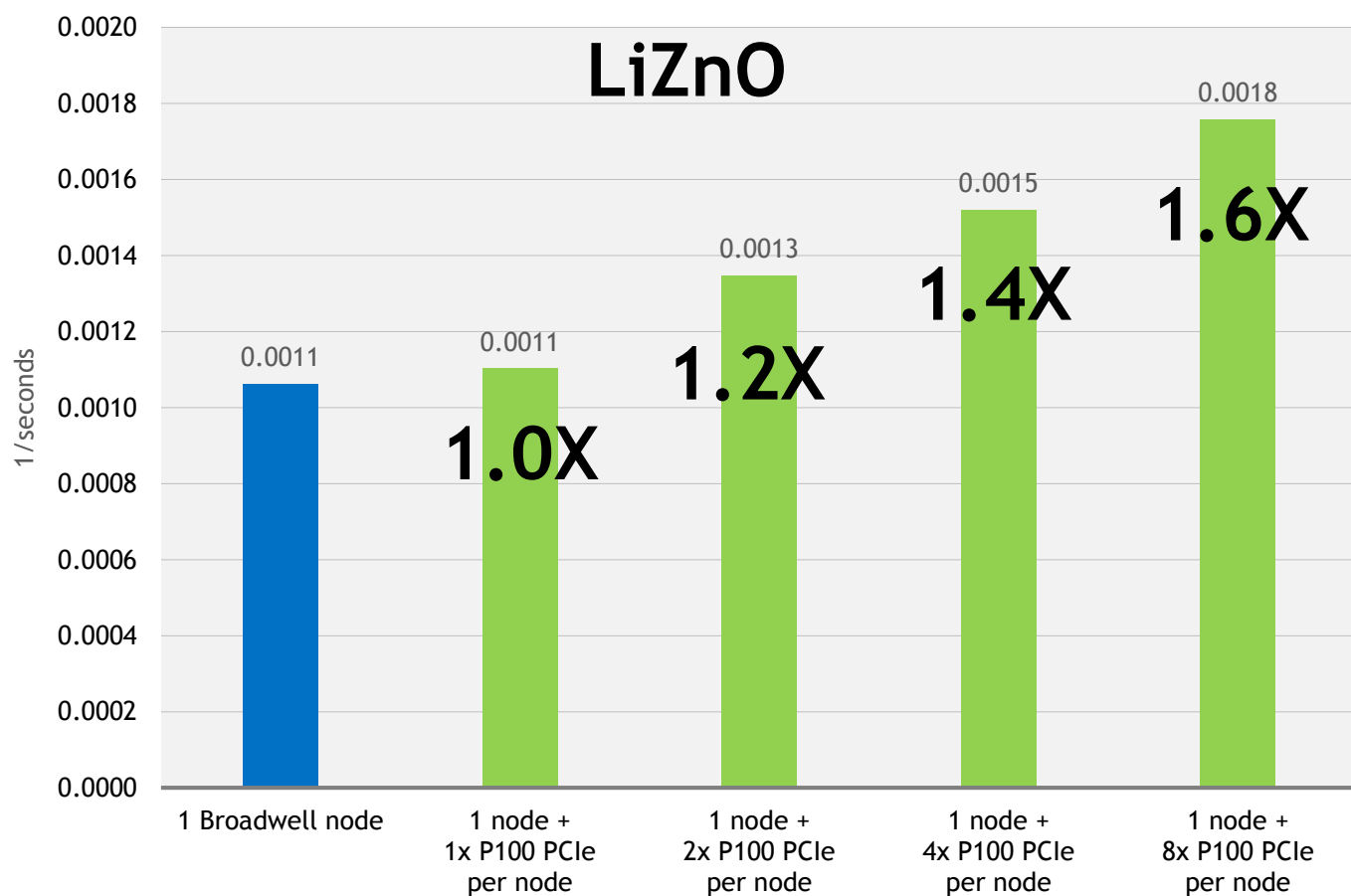
Running **VASP** version 5.4.1

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The **green nodes** contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

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

LiZnO on P100s SXM2



Running **VASP** version 5.4.1

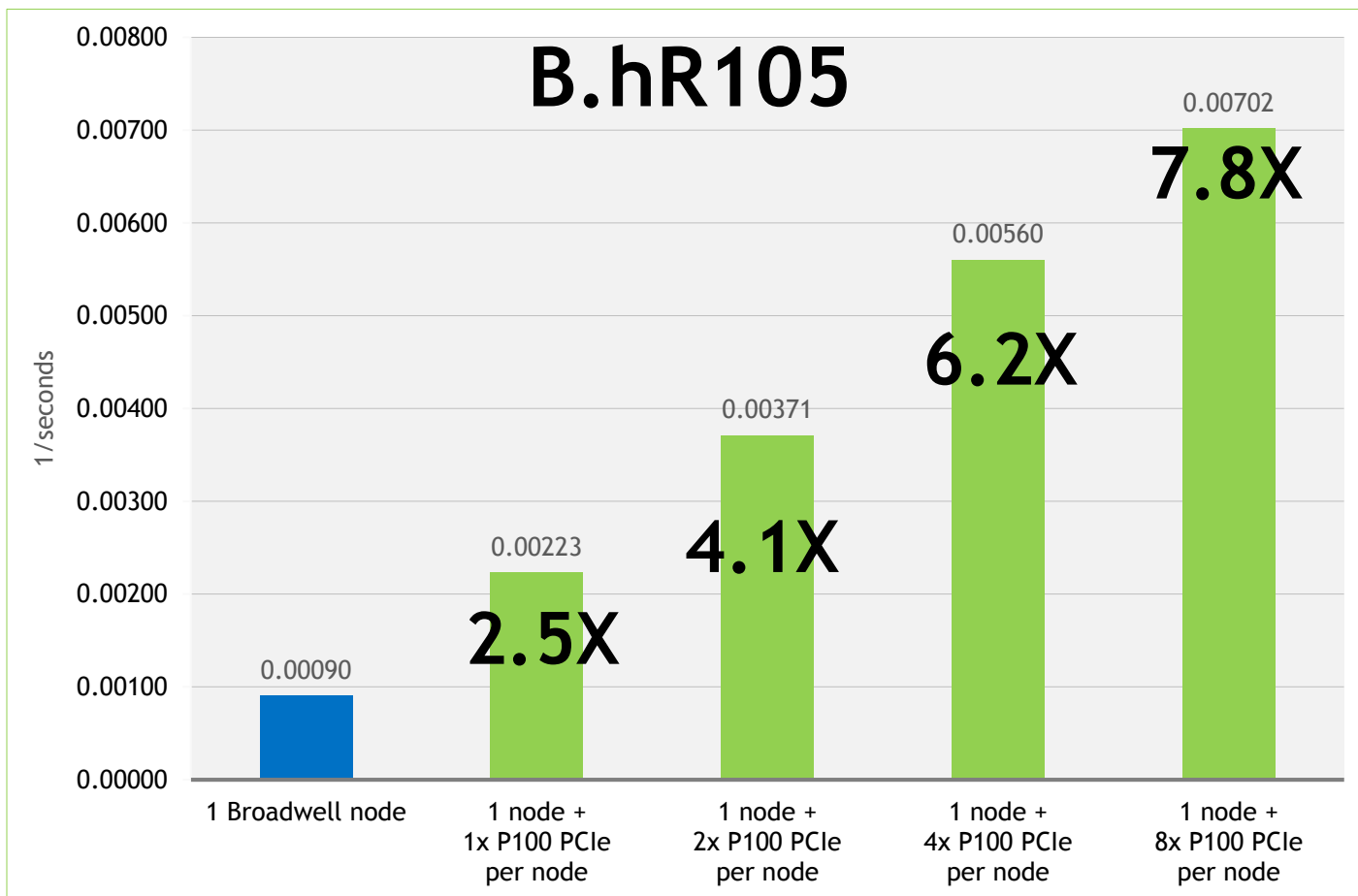
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- 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell)

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

B.hR105 on P100s PCIe



Running **VASP** version 5.4.1

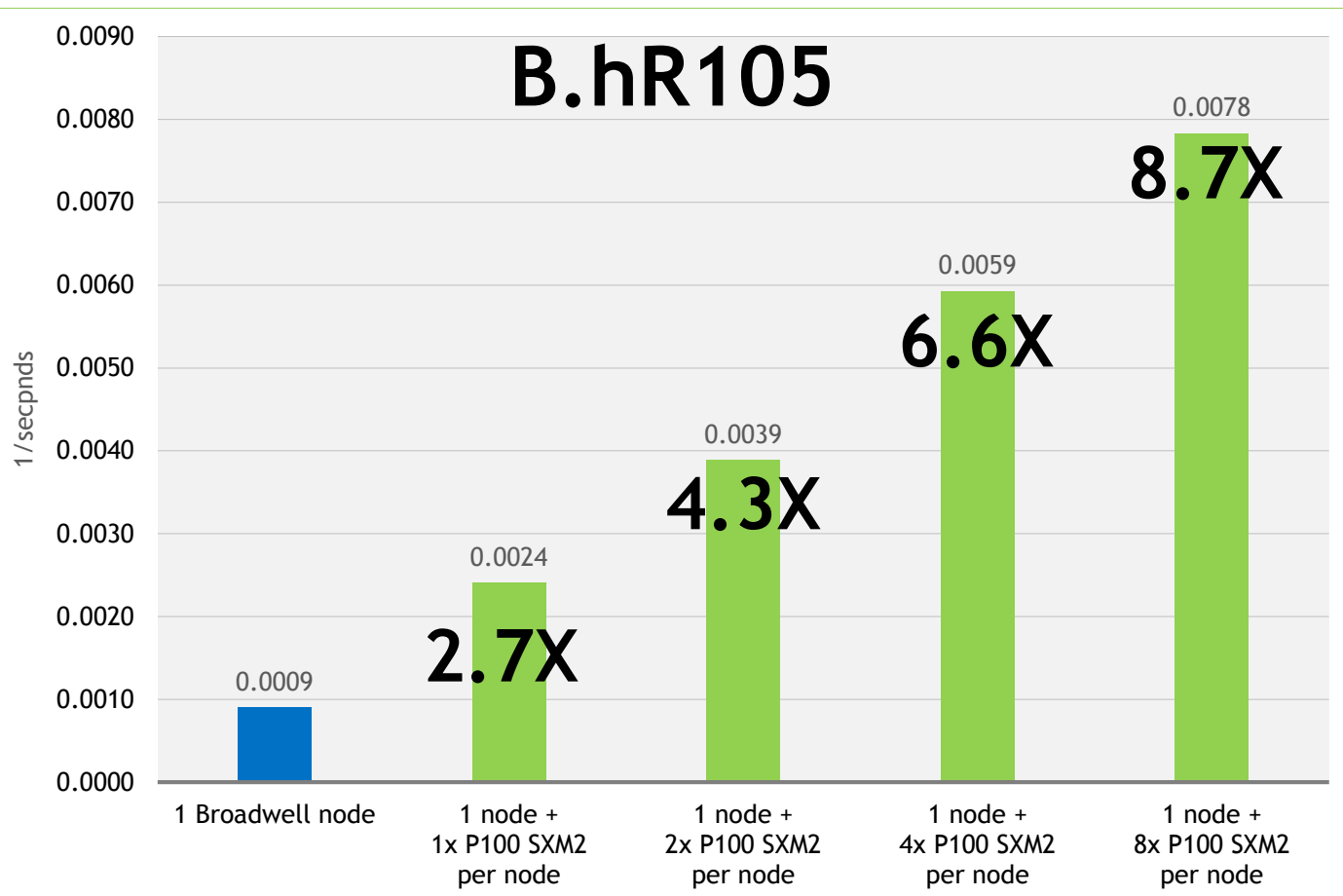
The **blue node** contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The **green nodes** contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

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

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

B.hR105 on P100s SXM2



Running **VASP** version 5.4.1

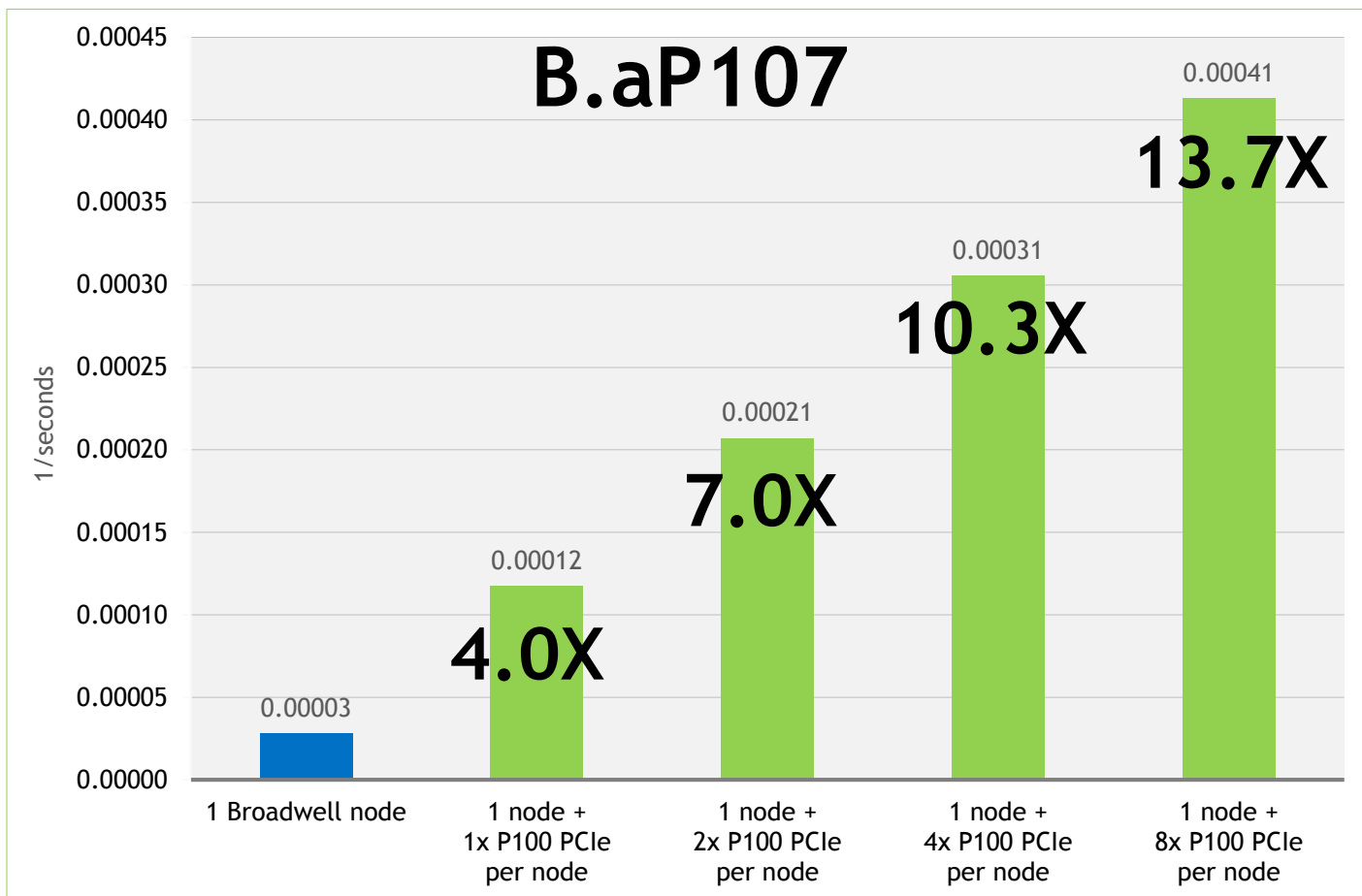
The **blue node** contains Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs

The **green nodes** contain Dual Intel Xeon E5-2698 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 SXM2 GPUs

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

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

B.aP107 on P100s PCIe



Running **VASP** version 5.4.1

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

The **green nodes** contain Dual Intel Xeon E5-2699 v4@2.2GHz [3.6GHz Turbo] (Broadwell) CPUs + Tesla P100 PCIe GPUs

➤ 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

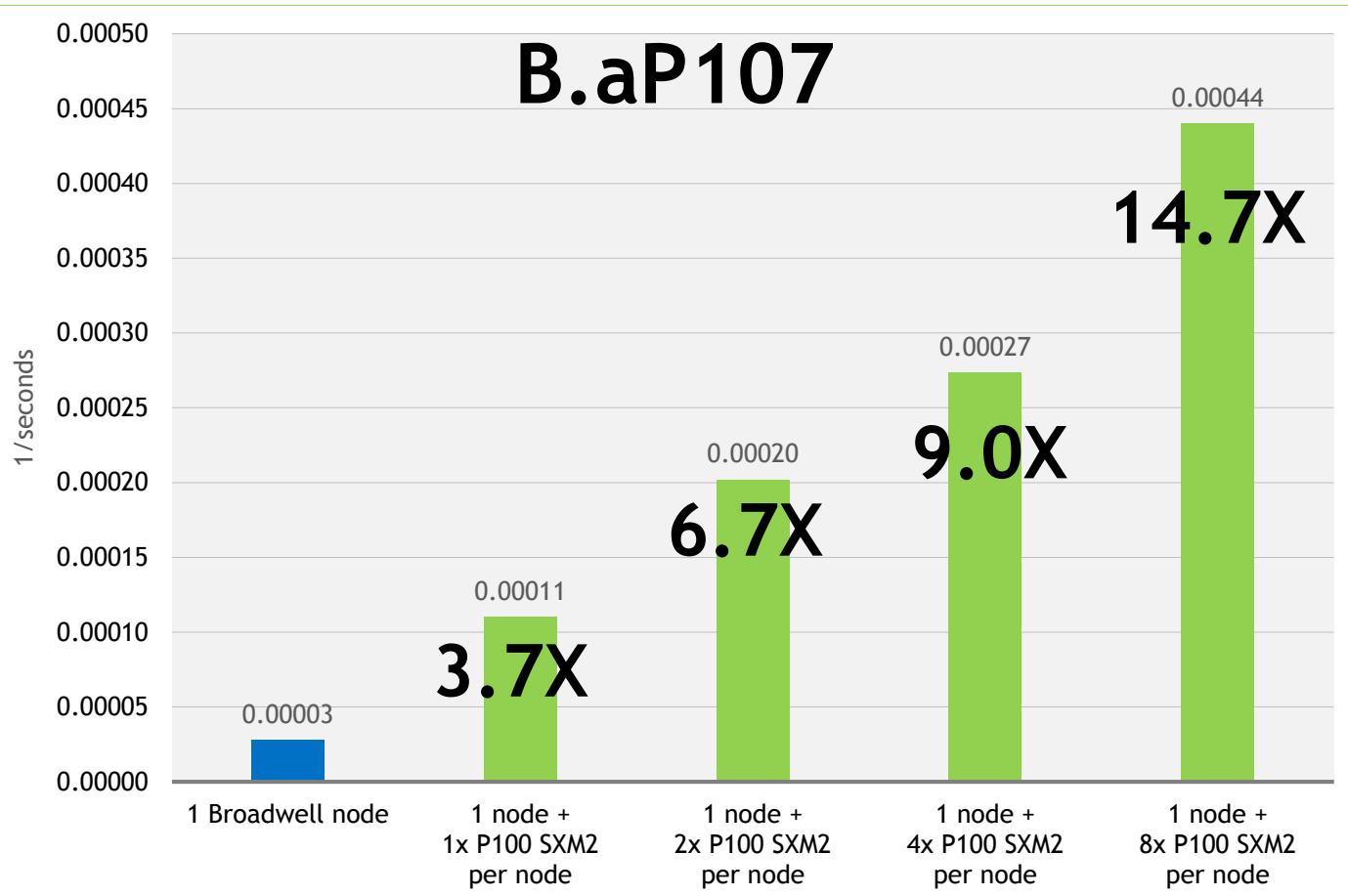
Hybrid functional calculation (exact exchange) with blocked Davidson. No KPoint parallelization.

Hybrid Functional with blocked Davidson

(ALGO=Normal)

LHFCALC=.True. (Exact Exchange)

B.aP107 on P100s SXM2



Running **VASP** version 5.4.1

The **blue node** contains Dual Intel Xeon E5-2699 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 P100 SXM2 GPUs

➤ 1x P100 SXM2 is paired with Single Intel Xeon E5-2698 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)