

TESLA V100 PERFORMANCE GUIDE

Deep Learning and HPC Applications

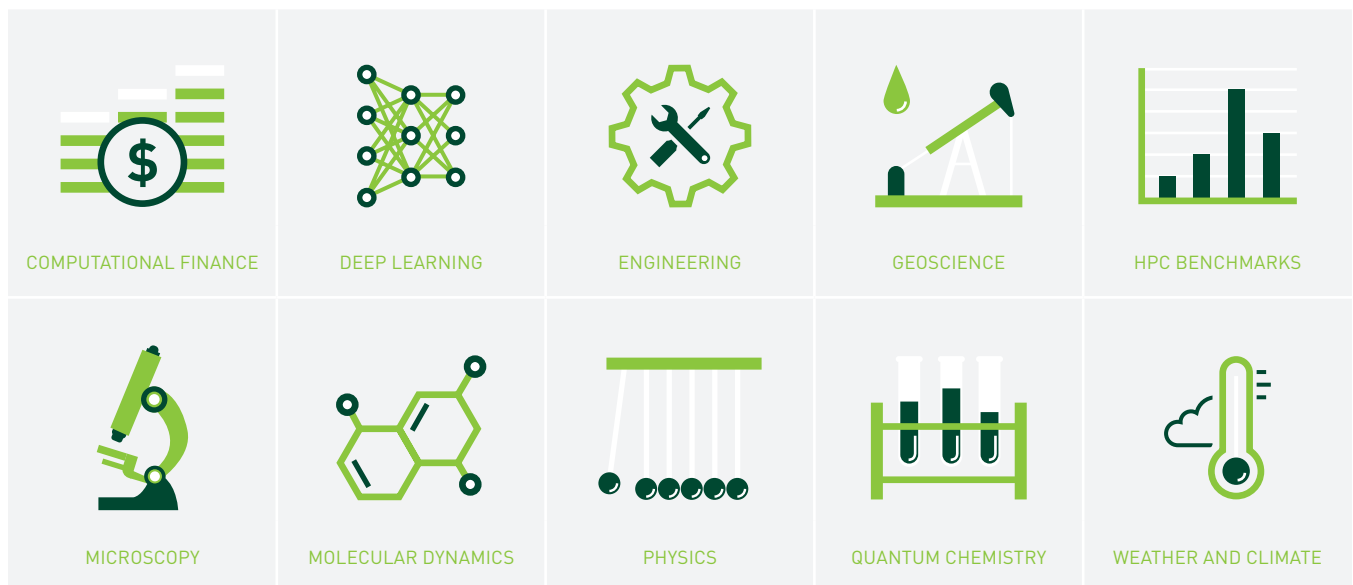


TESLA V100 PERFORMANCE GUIDE

Modern high performance computing (HPC) data centers are key to solving some of the world's most important scientific and engineering challenges. NVIDIA® Tesla® accelerated computing platform powers these modern data centers with the industry-leading applications to accelerate HPC and AI workloads. The Tesla V100 GPU is the engine of the modern data center, delivering breakthrough performance with fewer servers, less power consumption, and reduced networking overhead, resulting in total cost savings of 5X-10X. Each GPU-accelerated server provides the performance of dozens of commodity CPU servers, delivering a dramatic boost in application throughput. Improved performance and time-to-solution can also have significant favorable impacts on revenue and productivity.

Every HPC data center can benefit from the Tesla platform. Over 580 HPC applications in a broad range of domains are optimized for GPUs, including all 15 of the top 15 HPC applications and every major deep learning framework.

RESEARCH DOMAINS WITH GPU-ACCELERATED APPLICATIONS INCLUDE:



Over 580 HPC applications and all deep learning frameworks are GPU-accelerated.

- > To get the latest catalog of GPU-accelerated applications visit:
www.nvidia.com/teslaapps
- > To get up and running fast on GPUs with a simple set of instructions for a wide range of accelerated applications visit:
www.nvidia.com/gpu-ready-apps

COMPUTATIONAL FINANCE



Computational finance applications are essential to the success of global financial service firms when performing market and counterparty risk analytics, asset pricing, and portfolio risk management analysis. This analysis requires numerical methods that are computationally intensive. And because time is money in financial analysis, several of the leading computational finance applications are GPU-accelerated. Computational finance applications using Tesla V100 GPUs can improve performance by over 50X and save up to 80% in server and infrastructure acquisition costs.

KEY FEATURES OF THE TESLA PLATFORM AND V100 FOR COMPUTATIONAL FINANCE

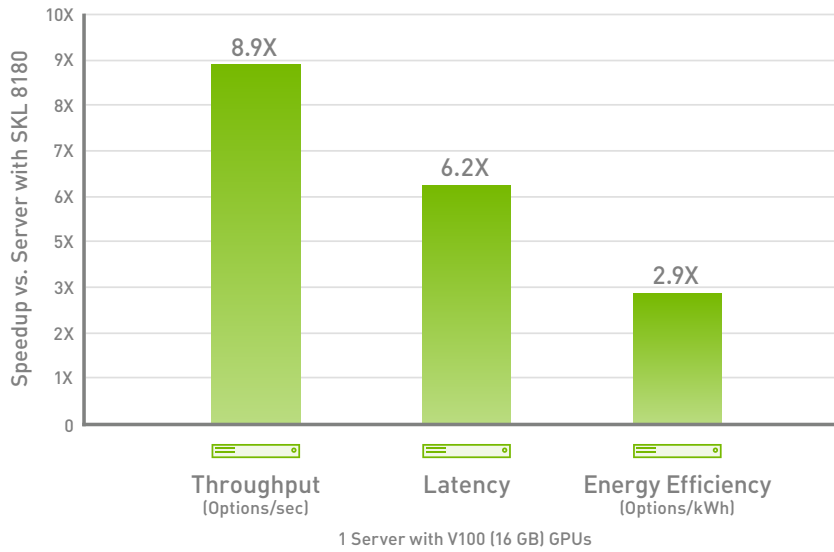
- > Servers with V100 outperform CPU servers by nearly 9X based on STAC-A2 benchmark results
- > Top Computational Finance applications are GPU-accelerated
- > Up to 7.8 TFLOPS per second of double precision performance per GPU
- > Up to 32 GB of memory capacity per GPU
- > Up to 900 GB/s memory bandwidth per GPU

View all related applications at:

www.nvidia.com/en-us/data-center/gpu-accelerated-applications/catalog

STAC-A2 Benchmark Performance Results

8X V100 GPU Server vs Dual Skylake Platinum 8180 Sever



System Configuration: GPU Server SUT ID: NVDA171020 | STAC-A2 Pack for CUDA (Rev D) | GPU Server: 8X NVIDIA® Tesla® V100 | GPU, 2X Intel® Xeon E5-2680 v4 @ 2.4 GHz | NVIDIA CUDA® Version 9.0 | Compared to: CPU Server SUT ID: INTC170920 | STAC-A2 Pack for Intel Composer XE (Rev K) | 2X 28-Core Intel Xeon Platinum 8180 @ 2.5GHz "Throughput" is STAC-A2.B2.HPORTFOLIO.SPEED, "Latency" is STAC-A2.B2.GREEKS.WARM, and "Energy Efficiency" is STAC-A2.B2.ENERG_EFF."STAC" and all STAC names are trademarks or registered trademarks of the Securities Technology Analysis Center, LLC.

STAC-A2

Financial risk management benchmark created by leading global banks working with the Securities Technology Analysis Center (STAC) used to assess financial compute solutions

VERSION

STAC-A2 (Beta 2)

ACCELERATED FEATURES

Full framework accelerated

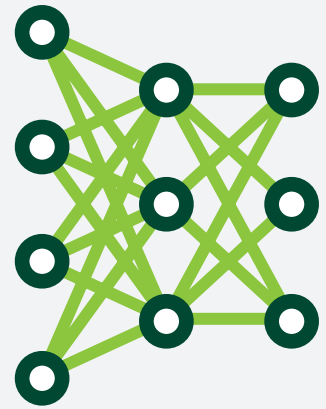
SCALABILITY

Multi-GPU

MORE INFORMATION

www.STACresearch.com/nvidia

DEEP LEARNING



Deep Learning is solving important scientific, enterprise, and consumer problems that seemed beyond our reach just a few years back. Every major deep learning framework is optimized for NVIDIA GPUs, enabling data scientists and researchers to leverage artificial intelligence for their work. When running deep learning training and inference frameworks, a data center with Tesla V100 GPUs can save over 90% in server and infrastructure acquisition costs.

KEY FEATURES OF THE TESLA PLATFORM AND V100 FOR DEEP LEARNING TRAINING

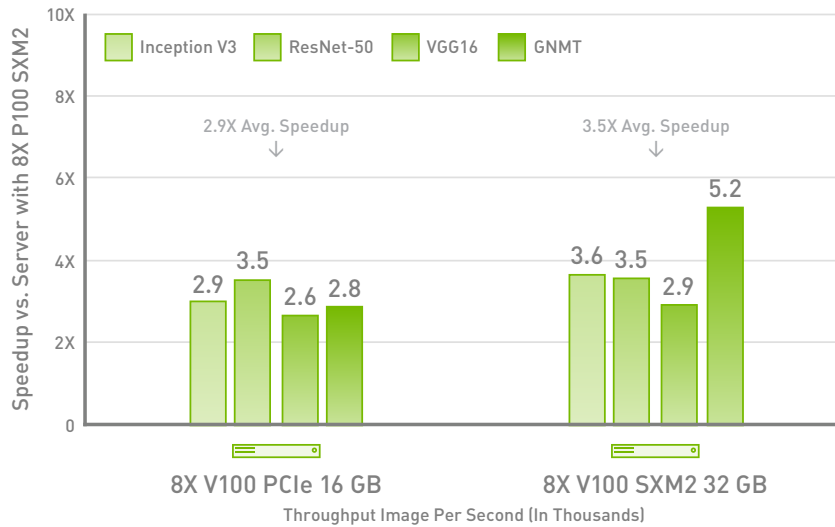
- > PyTorch, TensorFlow, and MxNet are up to 50x faster with Tesla V100 compared to P100
- > 100% of the top deep learning frameworks are GPU-accelerated
- > Up to 125 TFLOPS of TensorFlow operations per GPU
- > Up to 32 GB of memory capacity per GPU
- > Up to 900 GB/s memory bandwidth per GPU

View all related applications at:

www.nvidia.com/deep-learning-apps

PyTorch Deep Learning Framework

Training on 8X V100 GPU Server vs 8X P100 GPU Server



CPU Server: Dual-Socket Xeon E5-2698 v4 @ 3.6GHz, 512GB System Memory | GPU servers as shown
 Framework: PyTorch v0.4.1; Mixed Precision | NVIDIA CUDA® 10.0.130; NCCL 2.3.4, cuDNN 7.3.0.29; cuBLAS 10.0.130 | NVIDIA Driver: 384.145 | Batch sizes: V100 PCIe: Inception V3 192, ResNet-50 256, VGG16 192, GNMT 192; V100 SXM2: Inception V3 384, ResNet 256, VGG16 256, GNMT 192; P100 SXM2: Inception V3 96, ResNet-50 128, VGG16 96, GNMT 128.

PYTORCH

PyTorch is a deep learning framework that puts Python first

VERSION

0.4.1

ACCELERATED FEATURES

Full framework accelerated

SCALABILITY

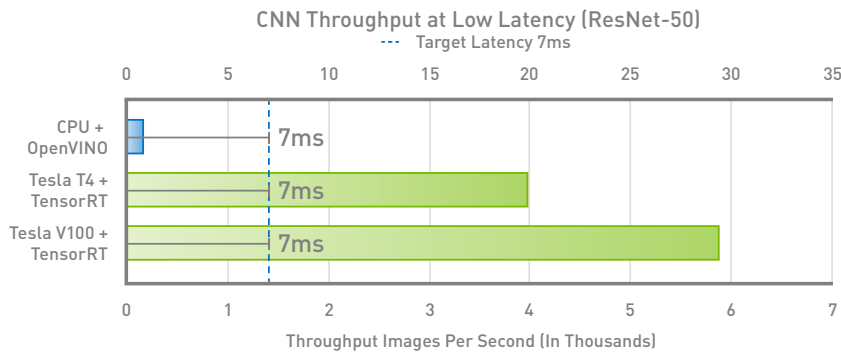
Multi-GPU

MORE INFORMATION

www.pytorch.org

NVIDIA TensorRT 4

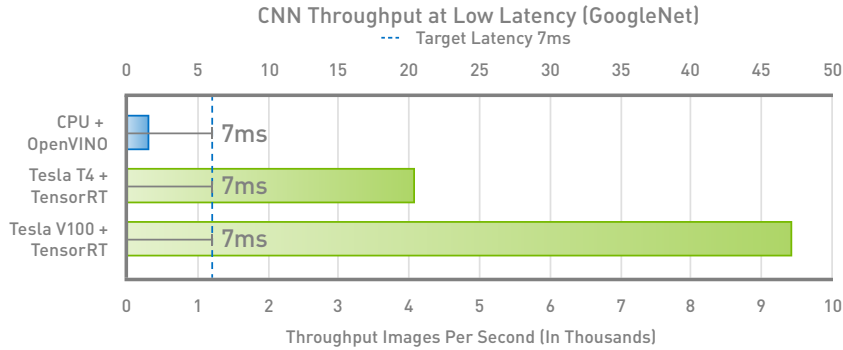
Massive Throughput at Low Latency



CPU throughput based on measured inference throughput performance on Skylake-based Xeon Scalable Processor Gold 6140 CPU | GPU Server config: Dual-socket Xeon Gold 6140 @ 2.30GHz, and a single NVIDIA® Tesla® T4 or V100; GPU running TensorRT 5 GA vs. Intel OpenVINO Toolkit | NVIDIA CUDA® 10.0.130; NCCL 2.3.4, cuDNN 7.3.0.29, cuBLAS 10.0.130 | NVIDIA Driver: 384.145 | Batch sizes: T4: ResNet-50 28, GoogleNet 29; V100: ResNet-50 41, GoogleNet 66.

NVIDIA TensorRT 4

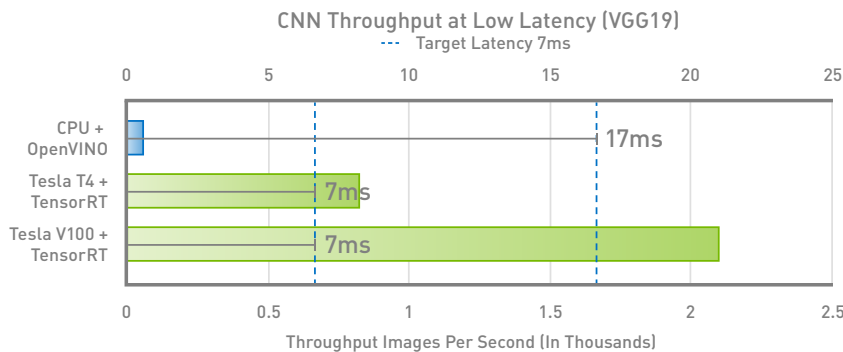
Massive Throughput at Low Latency



CPU throughput based on measured inference throughput performance on Skylake-based Xeon Scalable Processor Gold 6140 CPU | GPU Server config: Dual-socket Xeon Gold 6140 @ 2.30GHz, and a single NVIDIA® Tesla® T4 or V100; GPU running TensorRT 5 GA vs. Intel OpenVINO Toolkit | NVIDIA CUDA® 10.0.130; NCCL 2.3.4, cuDNN 7.3.0.29, cuBLAS 10.0.130 | NVIDIA Driver: 384.145 | Batch sizes: T4: ResNet-50 28, GoogleNet 29; V100: ResNet-50 41, GoogleNet 66.

NVIDIA TensorRT 4

Massive Throughput at Low Latency



CPU throughput based on measured inference throughput performance on Skylake-based Xeon Scalable Processor Gold 6140 CPU | GPU Server config: Dual-socket Xeon Gold 6140 @ 2.30GHz, and a single NVIDIA® Tesla® T4 or V100; GPU running TensorRT 5 GA vs. Intel OpenVINO Toolkit | NVIDIA CUDA® 10.0.130; NCCL 2.3.4, cuDNN 7.3.0.29 cuBLAS 10.0.130 | NVIDIA Driver: 384.145 | Batch sizes: T4: VGG19 6; V100: VGG19 13.

ENGINEERING



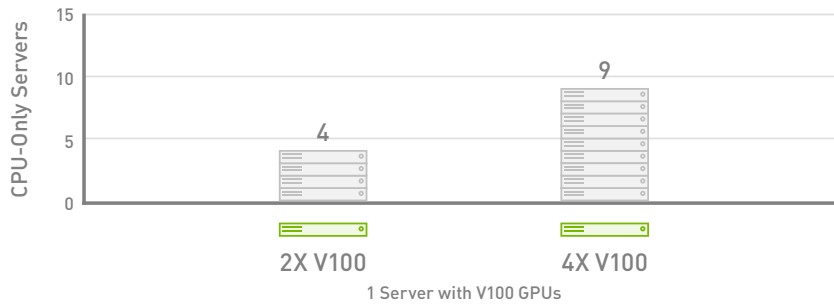
Engineering simulations are key to developing new products across industries by modeling flows, heat transfers, finite element analysis and more. Many of the top Engineering applications are accelerated with GPUs today. When running Engineering applications, a data center with NVIDIA® Tesla® V100 GPUs can save over 70% in software licensing costs and 60% in server and infrastructure acquisition costs.

KEY FEATURES OF THE TESLA PLATFORM AND V100 FOR ENGINEERING

- > Servers with Tesla V100 replace up to 34 CPU servers for applications such as FUN3D, SIMULIA Abaqus and ANSYS FLUENT
- > The top engineering applications are GPU-accelerated
- > Up to 7.8 TFLOPS of double precision floating point performance per GPU
- > Up to 32 GB of memory capacity per GPU
- > Up to 900 GB/s memory bandwidth per GPU

SIMULIA Abaqus Performance Equivalency

Single GPU Server vs Multiple Skylake CPU-Only Servers



CPU Server: Dual Xeon Gold 6140 @ 2.30GHz, GPU Servers: Same as CPU server with NVIDIA® Tesla® V100 PCIe | NVIDIA CUDA® Version: 7.5 | Dataset: LS-EPP-Combined-WC-Mkl (RR) | To arrive at CPU node equivalence, we use measured benchmark with up to 8 CPU nodes. Then we use linear scaling to scale beyond 8 nodes.

SIMULIA ABAQUS

Simulation tool for analysis of structures

VERSION

2017

ACCELERATED FEATURES

Direct sparse solver, AMS eigensolver, steady-state dynamics solver

SCALABILITY

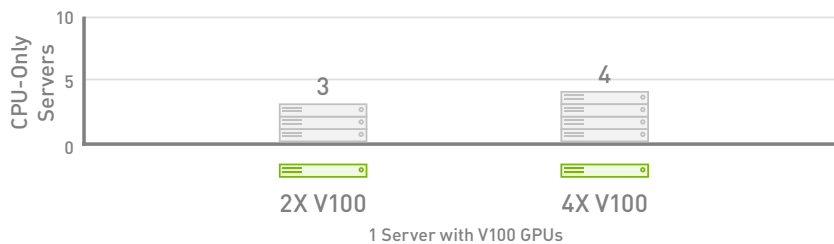
Multi-GPU and Multi-Node

MORE INFORMATION

<http://www.nvidia.com/simulia-abaqus>

ANSYS Fluent Performance Equivalency

Single GPU Server vs Multiple Skylake CPU-Only Servers



CPU Server: Dual Xeon Gold 6140 @ 2.30GHz, GPU Servers: Same as CPU server with NVIDIA® Tesla® V100 PCIe | NVIDIA CUDA® Version: 6.0 | Dataset: Water Jacket | To arrive at CPU node equivalence, we use measured benchmark with up to 8 CPU nodes. Then we use linear scaling to scale beyond 8 nodes.

ANSYS FLUENT

General purpose software for the simulation of fluid dynamics

VERSION

18

ACCELERATED FEATURES

Pressure-based Coupled Solver and Radiation Heat Transfer

SCALABILITY

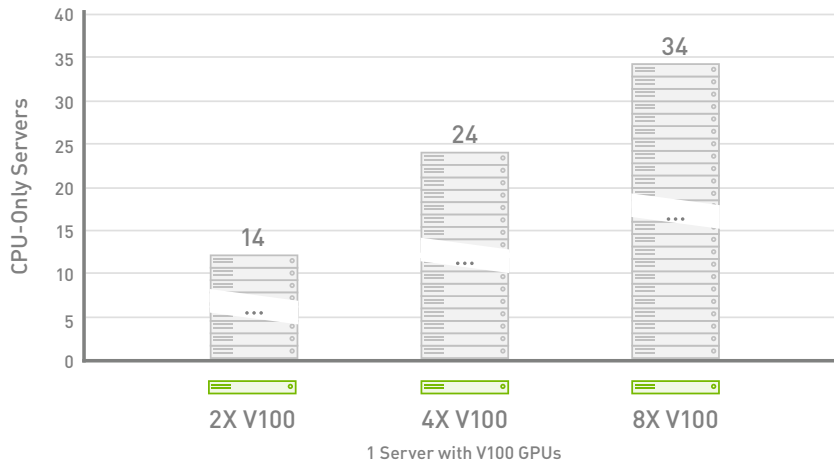
Multi-GPU and Multi-Node

MORE INFORMATION

www.nvidia.com/ansys-fluent

FUN3D Performance Equivalence

Single GPU Server vs Multiple Skylake CPU-Only Servers



CPU Server: Dual Xeon Gold 6140 @ 2.30GHz, GPU Servers: Same as CPU server with NVIDIA® Tesla® V100 PCIe or V100 SXM2 on 8X V100 config | NVIDIA CUDA® Version: 9.2.148 | Dataset: dpw_wbt0_crs-3.6Mn_5.merged | To arrive at CPU node equivalence, we use linear scaling to scale beyond 1 node.

FUN3D

Suite of tools for modeling fluid flow, actively developed at NASA for Aeronautics and Space Technology

VERSION

13.3

ACCELERATED FEATURES

Full range of Mach number regimes for the Reynolds-averaged Navier Stokes (RANS) formulation

SCALABILITY

Multi-GPU and Multi-Node

MORE INFORMATION

<https://fun3d.larc.nasa.gov>

GEOSCIENCE



Geoscience simulations are key to the discovery of oil and gas and performing geological modeling. Many of the top geoscience applications are accelerated with GPUs today. When running Geoscience applications, a data center with Tesla V100 GPUs can save over 90% in server and infrastructure acquisition costs.

KEY FEATURES OF THE TESLA PLATFORM AND V100 FOR GEOSCIENCE

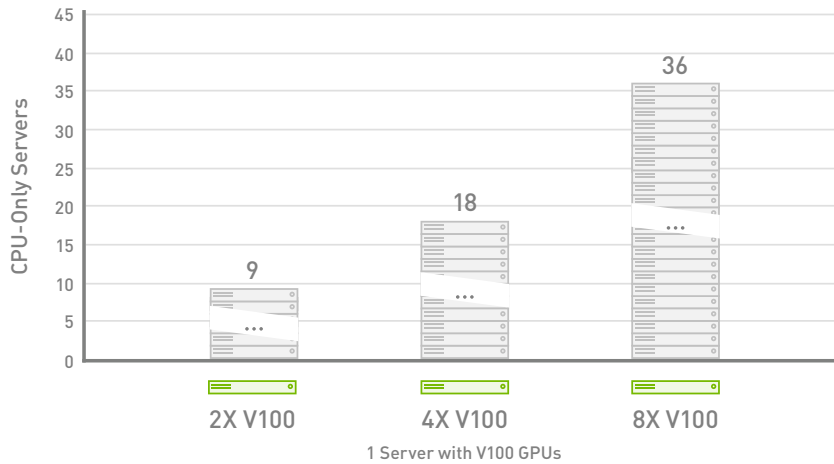
- > Servers with V100 replace up to 124 CPU servers for applications such as RTM and SPECFEM3D
- > Top Geoscience applications are GPU-accelerated
- > Up to 15.7 TFLOPS of single precision floating point performance
- > Up to 32 GB of memory capacity per GPU
- > Up to 900 GB/s memory bandwidth per GPU

View all related applications at:

www.nvidia.com/oil-and-gas-apps

RTM Performance Equivalence

Single GPU Server vs Multiple Skylake CPU-Only Servers



CPU Server: Dual Xeon Gold 6140 @ 2.30GHz, GPU Servers: Same as CPU server with NVIDIA® Tesla® V100 PCIe or V100 SXM2 on 8X V100 config | NVIDIA CUDA® Version: 9.2.148 | Dataset: Isotropic Radius 4 | To arrive at CPU node equivalence, we use linear scaling to scale beyond 1 node.

RTM

Reverse time migration (RTM) modeling is a critical component in the seismic processing workflow of oil and gas exploration

VERSION

2018

ACCELERATED FEATURES

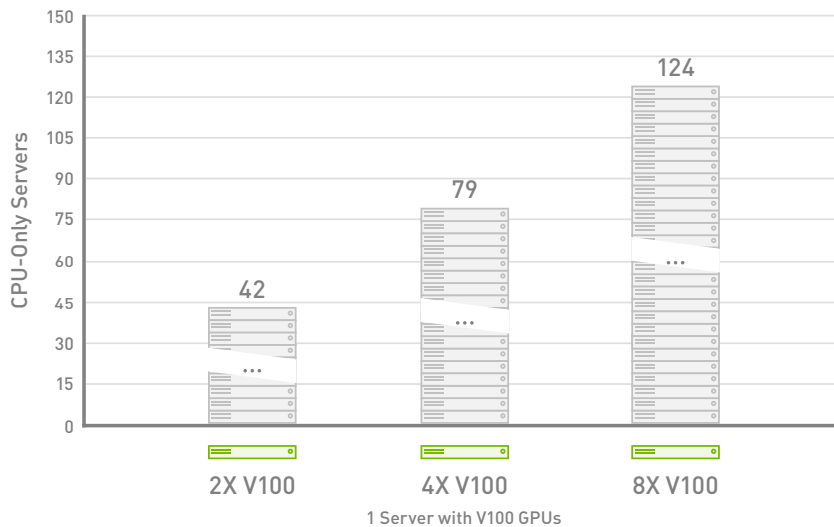
Batch algorithm

SCALABILITY

Multi-GPU and Multi-Node

SPECFEM3D Performance Equivalence

Single GPU Server vs Multiple Skylake CPU-Only Servers



CPU Server: Dual Xeon Gold 6140 @ 2.30 GHz, GPU Servers: Same as CPU server with NVIDIA® Tesla® V100 PCIe | NVIDIA CUDA® Version: 10.0.130 | Dataset: four_material_simple_model | To arrive at CPU node equivalence, we use linear scaling to scale beyond 1 node.

SPECFEM3D

Simulates Seismic wave propagation

VERSION

github_a2d23d27

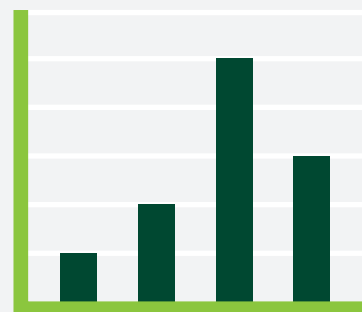
SCALABILITY

Multi-GPU and Single-Node

MORE INFORMATION

https://geodynamics.org/cig/software/specfem3d_globe

HPC BENCHMARKS



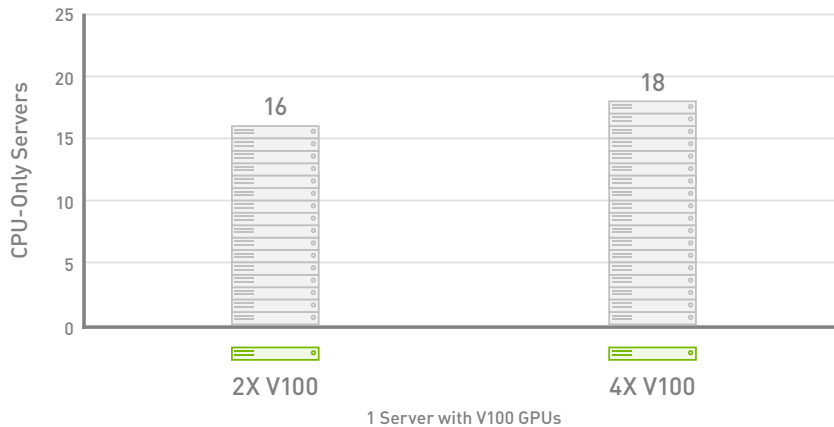
Benchmarks provide an approximation of how a system will perform at production-scale and help to assess the relative performance of different systems. The top benchmarks have GPU-accelerated versions and can help you understand the benefits of running GPUs in your data center.

KEY FEATURES OF THE TESLA PLATFORM AND V100 FOR BENCHMARKING

- > Servers with Tesla V100 replace up to 41 CPU servers for benchmarks such as Cloverleaf, MiniFE, Linpack, and HPCG
- > The top HPC benchmarks are GPU-accelerated
- > Up to 7.8 TFLOPS of double precision floating point performance per GPU
- > Up to 32 GB of memory capacity per GPU
- > Up to 900 GB/s memory bandwidth per GPU

Cloverleaf Performance Equivalency

Single GPU Server vs Multiple Skylake CPU-Only Servers



CPU Server: Dual Xeon Gold 6140 @ 2.30GHz, GPU Servers: Same as CPU server with NVIDIA® Tesla® V100 PCIe | NVIDIA CUDA® Version: 9.0.103 | Dataset: bm32 | To arrive at CPU node equivalence, we use measured benchmark with up to 8 CPU nodes. Then we use linear scaling to scale beyond 8 nodes.

CLOVERLEAF

Benchmark – Mini-App
Hydrodynamics

VERSION

1.3

ACCELERATED FEATURES

Lagrangian-Eulerian
explicit hydrodynamics mini-application

SCALABILITY

Multi-Node (MPI)

MORE INFORMATION

<http://uk-mac.github.io/CloverLeaf>

HPCG Performance Equivalence

Single GPU Server vs Multiple Skylake CPU-Only Servers



CPU Server: Dual Xeon Gold 6140 @ 2.30 GHz, GPU Servers: Same as CPU server with NVIDIA® Tesla® V100 PCIe | NVIDIA CUDA® Version: 9.0.103 | Dataset: 256x256x256 local size | To arrive at CPU node equivalence, we use linear scaling to scale beyond 1 node.

HPCG

Exercises computational and data access patterns that closely match a broad set of important HPC applications

VERSION

3

ACCELERATED FEATURES

All

SCALABILITY

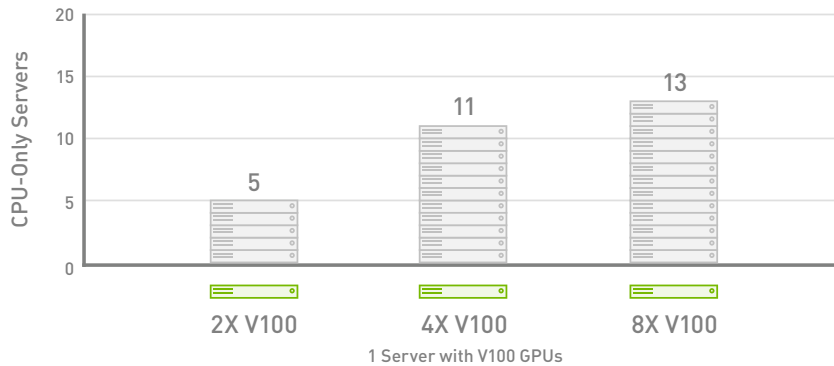
Multi-GPU and Multi-Node

MORE INFORMATION

<http://www.hpcg-benchmark.org/index.html>

Linpack Performance Equivalency

Single GPU Server vs Multiple Skylake CPU-Only Servers



CPU Server: Dual Xeon Gold 6140 @ 2.30 GHz, GPU Servers: Same as CPU server with NVIDIA® Tesla® V100 PCIe | NVIDIA CUDA® Version: 9.0.103 | Dataset: HPL.dat | To arrive at CPU node equivalence, we use a measured benchmark with up to 8 CPU nodes. Then we use linear scaling to scale beyond 8 nodes.

LINPACK

Benchmark – Measures floating point computing power

VERSION

2.1

ACCELERATED FEATURES

All

SCALABILITY

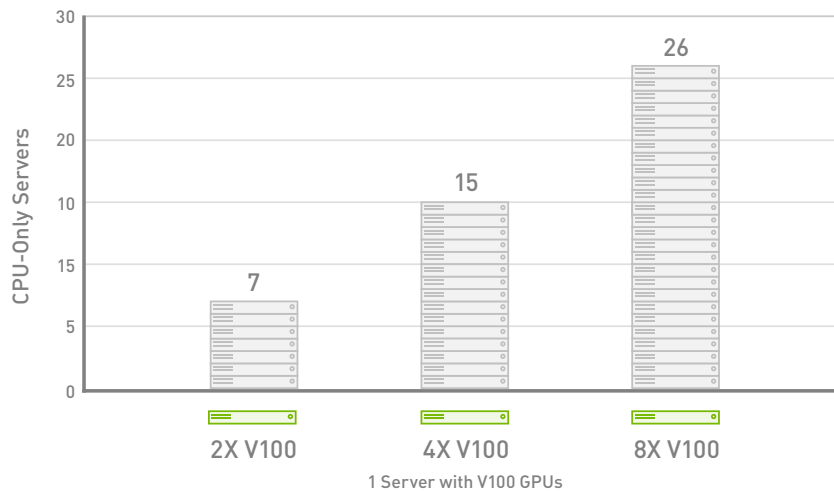
Multi-Node and Multi-Node

MORE INFORMATION

www.top500.org/project/linpack

MiniFE Performance Equivalency

Single GPU Server vs Multiple Skylake CPU-Only Servers



CPU Server: Dual Xeon Gold 6140 @ 2.30 GHz, GPU Servers: Same as CPU server with NVIDIA® Tesla® V100 PCIe | NVIDIA CUDA® Version: 9.0.103 | Dataset: 350x350x350 | To arrive at CPU node equivalence, we use a measured benchmark with up to 8 CPU nodes. Then we use linear scaling to scale beyond 8 nodes.

MINIFE

Benchmark – Mini-App Finite element analysis

VERSION

0.3

ACCELERATED FEATURES

All

SCALABILITY

Multi-GPU

MORE INFORMATION

<https://mantevo.org/about/applications>

MICROSCOPY



Microscopy has many applications in the forensic sciences, requiring significant computing resources to process the images that are produced. Today, GPUs accelerate the top microscopy applications, and data centers running these applications with Tesla V100 GPUs can see a reduction of over 50% in server and infrastructure acquisition costs.

KEY FEATURES OF THE TESLA PLATFORM AND V100 FOR QC

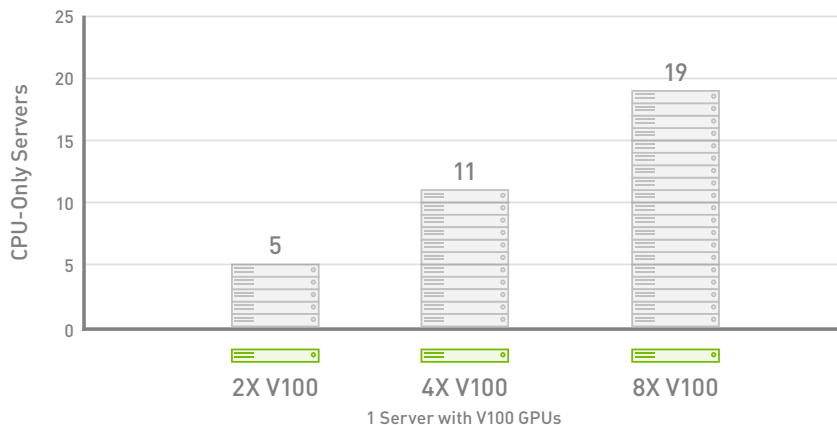
- > A single server with Tesla V100 GPUs replaces up to 19 CPU servers for applications such as Relion
- > Key math libraries like FFT and BLAS
- > Up to 7.8 TFLOPS per second of double precision performance per GPU
- > Up to 32 GB of memory capacity per GPU
- > Up to 900 GB/s of memory bandwidth per GPU

View all related applications at:

www.nvidia.com/teslaapps

Relion Performance Equivalency

Single GPU Server vs Multiple Skylake CPU-Only Servers



CPU Server: Dual Xeon Gold 6140 @ 2.30 GHz, GPU Servers: Same as CPU server with NVIDIA® Tesla® V100 PCIe | NVIDIA CUDA® Version: 9.0.176 | Dataset: Plasmodium Ribosome | To arrive at CPU node equivalence, we use a measured benchmark with up to 8 CPU nodes. Then we use linear scaling to scale beyond 8 nodes.

RELION

Stand-alone computer program that employs an empirical Bayesian approach to refinement of (multiple) 3D reconstructions or 2D class averages in electron cryo-microscopy (cryo-EM)

VERSION

2.0.3

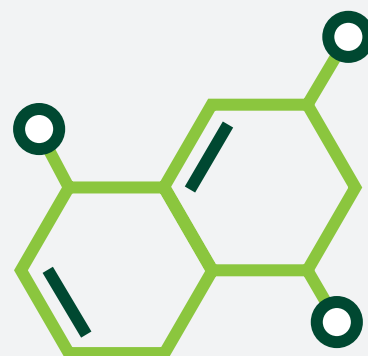
ACCELERATED FEATURES

Image classification, high resolution refinement and template-based particle selection

SCALABILITY

Multi-GPU and Single-Node

MOLECULAR DYNAMICS



Molecular Dynamics (MD) represents a large share of the workload in an HPC data center. 100% of the top MD applications are GPU-accelerated, enabling scientists to run simulations they couldn't perform before with traditional CPU-only versions of these applications. When running MD applications, a data center with Tesla V100 GPUs can save over 90% in server and infrastructure acquisition costs.

KEY FEATURES OF THE TESLA PLATFORM AND V100 FOR MD

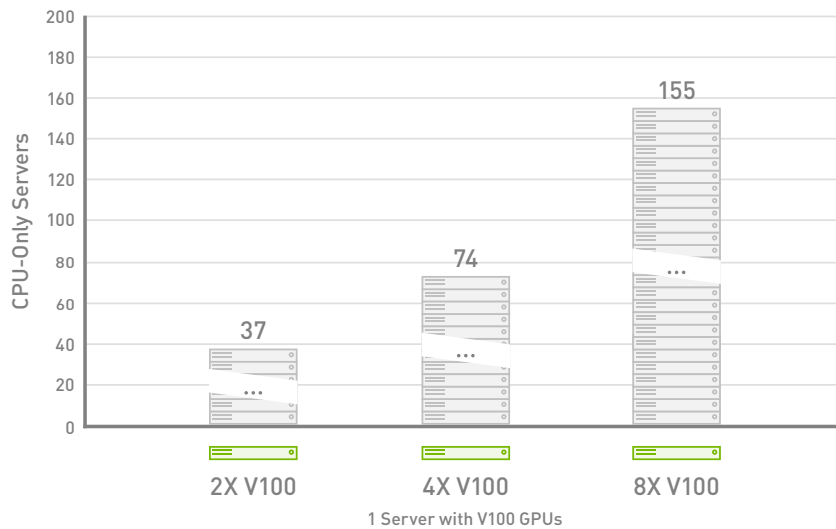
- > Servers with V100 replace over 155 CPU servers for applications such as Amber, HOOMD-blue, LAMMPS, and NAMD
- > 100% of the top MD applications are GPU-accelerated
- > Key math libraries like FFT and BLAS
- > Up to 15.7 TFLOPS of single precision performance per GPU
- > Up to 32 GB of memory capacity per GPU
- > Up to 900 GB/s of memory bandwidth per GPU

View all related applications at:

www.nvidia.com/molecular-dynamics-apps

AMBER Performance Equivalency

Single GPU Server vs Multiple Skylake CPU-Only Servers



CPU server: Dual Xeon Gold 6140 @ 2.30 GHz, GPU servers: same CPU server with NVIDIA® Tesla® V100 PCIe or V100 SXM2 on 8X V100 config | NVIDIA CUDA® version: CUDA 10.0.130 | Dataset: PME-Cellulose_NVE | To arrive at CPU node equivalency, we use a measured benchmark with up to 8 CPU nodes. Then we use linear scaling to scale beyond 8 nodes.

AMBER

Suite of programs to simulate molecular dynamics on biomolecule

VERSION

18.6

ACCELERATED FEATURES

PMEMD Explicit Solvent and GB Implicit Solvent

SCALABILITY

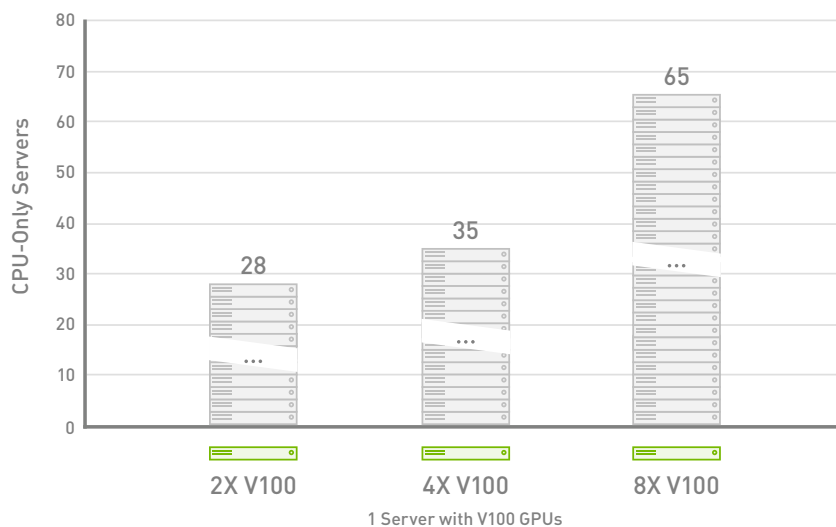
Multi-GPU and Single-Node

MORE INFORMATION

<http://ambermd.org/gpus>

HOOMD-blue Performance Equivalency

Single GPU Server vs Multiple Skylake CPU-Only Servers



CPU Server: Dual Xeon Gold 6140 @ 2.30 GHz, GPU Servers: same CPU server with NVIDIA® Tesla® V100 PCIe or V100 SXM2 on 8X V100 config | NVIDIA CUDA® Version: CUDA 9.0.176; Dataset: microsphere | To arrive at CPU node equivalency, we use measured benchmark with up to 8 CPU nodes. Then we use linear scaling to scale beyond 8 nodes.

HOOMD-BLUE

Particle dynamics package written grounds up for GPUs

VERSION

2.2.2

ACCELERATED FEATURES

CPU and GPU versions available

SCALABILITY

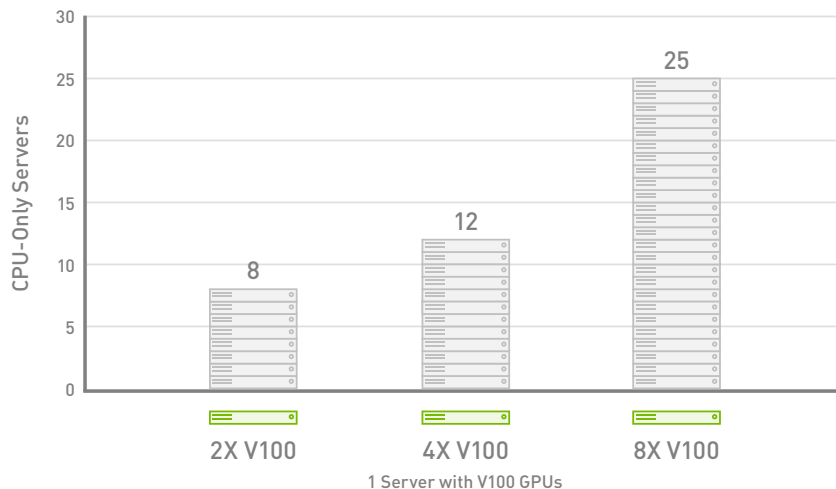
Multi-GPU and Multi-Node

MORE INFORMATION

<http://codeblue.umich.edu/hoomd-blue/index.html>

LAMMPS Performance Equivalency

Single GPU Server vs Multiple Skylake CPU-Only Servers



CPU Server: Dual Gold 6140 @ 2.30 GHz, GPU Servers: Same as CPU server with NVIDIA® Tesla® V100 PCIe or V100 SXM2 on 8X V100 config | NVIDIA CUDA® Version: 10.0.130 | Dataset: Atomic-Fluid Lennard-Jones 2.5 Cutoff | To arrive at CPU node equivalence, we use a measured benchmark with up to 8 CPU nodes. Then we use linear scaling to scale beyond 8 nodes.

LAMMPS

Classical molecular dynamics package

VERSION

2018

ACCELERATED FEATURES

Lennard-Jones, Gay-Berne, Tersoff, many more potentials

SCALABILITY

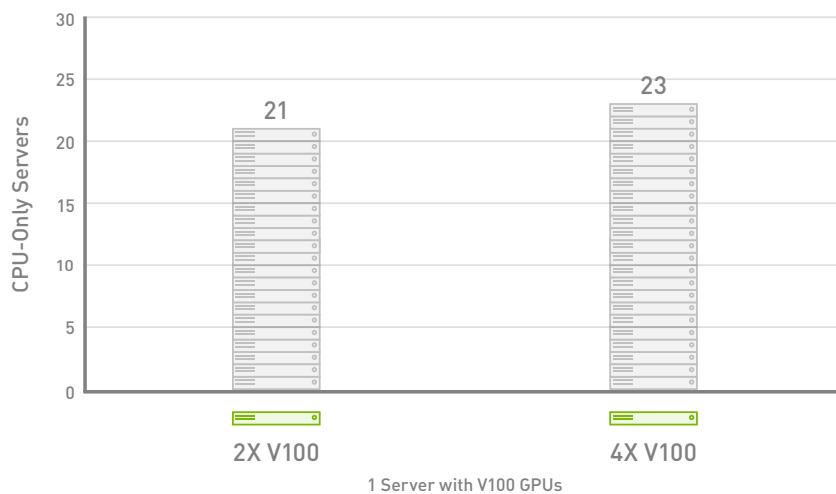
Multi-GPU and Multi-Node

MORE INFORMATION

<http://lammps.sandia.gov/index.html>

NAMD Performance Equivalency

Single GPU Server vs Multiple Skylake CPU-Only Servers



CPU Server: Dual Xeon Gold 6140 @ 2.30GHz, GPU Servers: same CPU server with NVIDIA® Tesla® V100 PCIe | NVIDIA CUDA® Version: CUDA 10.0.130 | Dataset: STMV | To arrive at CPU node equivalence, we use measured benchmark with up to 8 CPU nodes. Then we use linear scaling to scale beyond 8 nodes.

NAMD

Designed for high-performance simulation of large molecular systems

VERSION

2.13

ACCELERATED FEATURES

Full electrostatics with PME and most simulation features

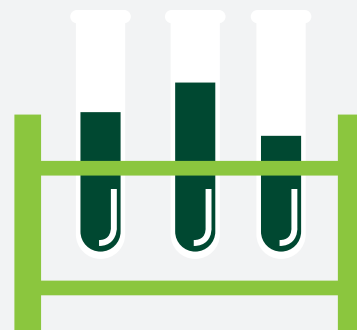
SCALABILITY

Up to 100M atom capable, multi-GPU, single node

MORE INFORMATION

<http://www.ks.uiuc.edu/Research/namd>

QUANTUM CHEMISTRY



Quantum chemistry (QC) simulations are key to the discovery of new drugs and materials and consume a large part of the HPC data center's workload. 60% of the top QC applications are accelerated with GPUs today. When running QC applications, a data center's workload with Tesla V100 GPUs can save over 85% in server and infrastructure acquisition costs.

KEY FEATURES OF THE TESLA PLATFORM AND V100 FOR QC

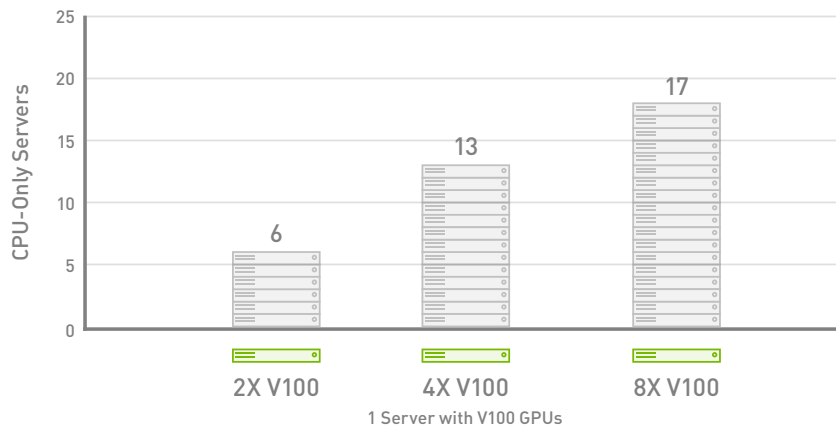
- > Servers with V100 replace up to 37 CPU servers for applications such as Quantum Espresso and VASP
- > 60% of the top QC applications are GPU-accelerated
- > Key math libraries like FFT and BLAS
- > Up to 7.8 TFLOPS per second of double precision performance per GPU
- > Up to 32 GB of memory capacity per GPU
- > Up to 900 GB/s of memory bandwidth per GPU

View all related applications at:

www.nvidia.com/quantum-chemistry-apps

Quantum Espresso Performance Equivalency

Single GPU Server vs Multiple Skylake CPU-Only Servers



CPU Server: Dual Xeon Gold 6140 @ 2.30 GHz, GPU Servers: Same as CPU server with NVIDIA® Tesla® V100 PCIe | NVIDIA CUDA® Version: 9.2.88 | Dataset: AUSURF112-jR | To arrive at CPU node equivalence, we use a measured benchmark with up to 8 CPU nodes. Then we use linear scaling to scale beyond 8 nodes.

QUANTUM ESPRESSO

An open-source suite of computer codes for electronic structure calculations and materials modeling at the nanoscale

VERSION

6.1

ACCELERATED FEATURES

Linear algebra (matrix multiply), explicit computational kernels, 3D FFTs

SCALABILITY

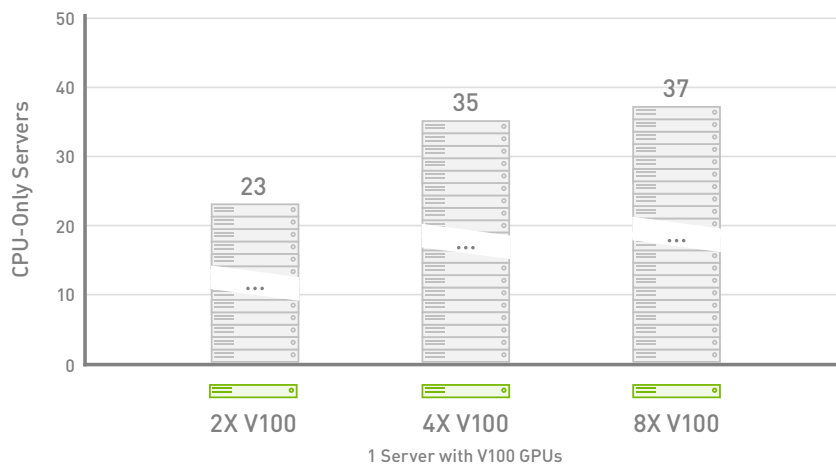
Multi-GPU and Multi-Node

MORE INFORMATION

<http://www.quantum-espresso.org>

VASP Performance Equivalency

Single GPU Server vs Multiple Skylake CPU-Only Servers



CPU server: Dual Xeon Gold 6140 @ 2.30 GHz, GPU servers: same CPU server with NVIDIA® Tesla® V100 PCIe or V100 SXM2 on 8X V100 config | NVIDIA CUDA® version: CUDA 9.0.176 | Dataset: B.hR105 | To arrive at CPU node equivalence, we use measured benchmark with up to 8 CPU nodes. Then we use linear scaling to scale beyond 8 nodes.

VASP

Complex package for performing ab-initio quantum-mechanical molecular dynamics (MD) simulations using pseudopotentials or the projector-augmented wave method and a plane wave basis set

VERSION

5.4.4

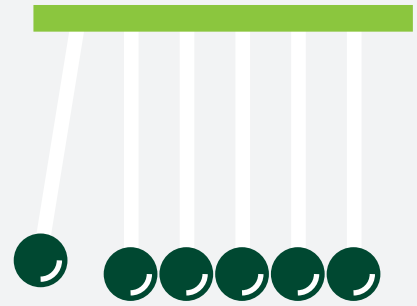
ACCELERATED FEATURES

Blocked Davidson (ALGO = NORMAL & FAST), RMM-DIIS (ALGO = VERYFAST & FAST), K-Points and optimization

SCALABILITY

Multi-GPU and Multi-Node

PHYSICS



From fusion energy to high energy particles, physics simulations span a wide range of applications in the HPC data center. All of the top physics applications are GPU-accelerated, enabling insights previously not possible. A data center with Tesla V100 GPUs can save over 90% in server acquisition cost when running GPU-accelerated physics applications.

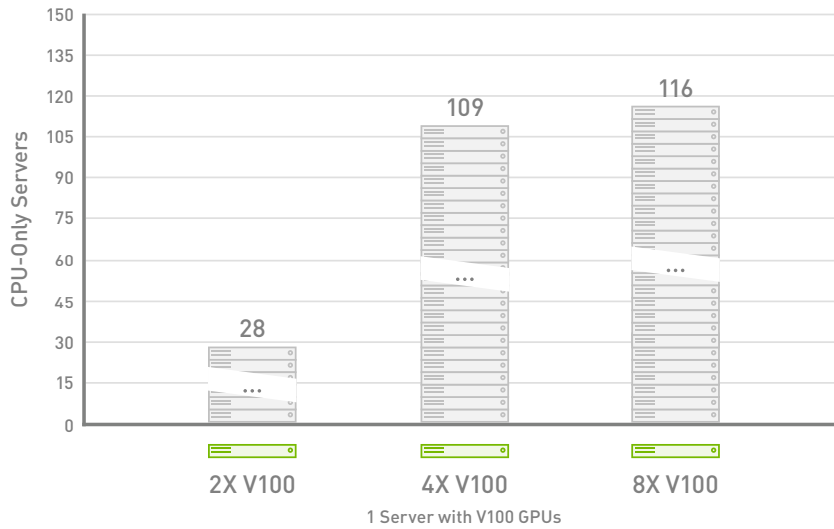
KEY FEATURES OF THE TESLA PLATFORM AND V100 FOR PHYSICS

- > Servers with V100 replace up to 116 CPU servers for applications such as Chroma, GTC, MILC, and QUDA
- > Most of the top physics applications are GPU-accelerated
- > Up to 7.8 TFLOPS of double precision floating point performance per GPU
- > Up to 32 GB of memory capacity per GPU
- > Up to 900 GB/s memory bandwidth per GPU

View all related applications at:
www.nvidia.com/physics-apps

Chroma Performance Equivalency

Single GPU Server vs Multiple Skylake CPU-Only Servers



CPU Server: Dual Xeon Gold 6140 @ 2.30 GHz, GPU Servers: Same as CPU server with NVIDIA® Tesla® V100 PCIe | NVIDIA CUDA® Version: 9.0.176 | Dataset: szscl21_24_128 | To arrive at CPU node equivalence, we use a measured benchmark with up to 8 CPU nodes. Then we use linear scaling to scale beyond 8 nodes.

CHROMA

Lattice quantum chromodynamics (LQCD)

VERSION

2018

ACCELERATED FEATURES

Wilson-clover fermions, Krylov solvers, Domain-decomposition

SCALABILITY

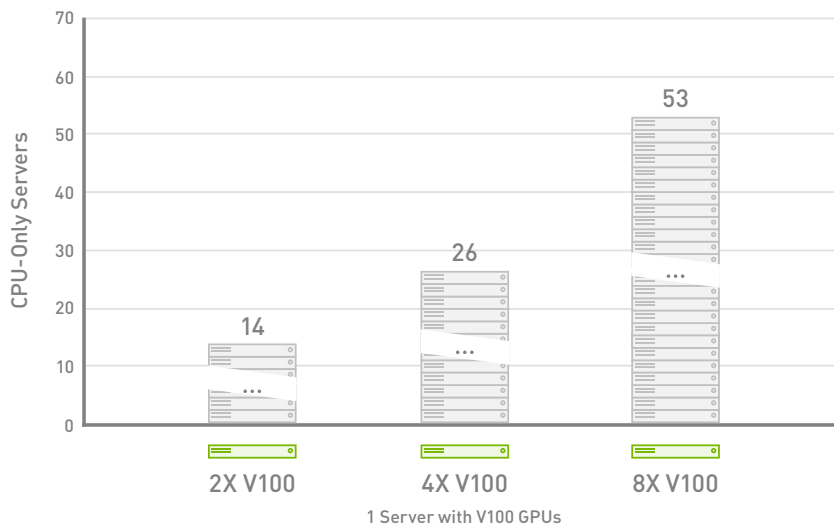
Multi-GPU and Multi-Node

MORE INFORMATION

<http://jeffersonlab.github.io/chroma>

GTC Performance Equivalence

Single GPU Server vs Multiple Skylake CPU-Only Servers



CPU Server: Dual Xeon Gold 6140 @ 2.30 GHz, GPU Servers: Same as CPU server with NVIDIA® Tesla® V100 PCIe | NVIDIA CUDA® Version: 10.0.130 | Dataset: mpi#proc.in | To arrive at CPU node equivalence, we use a measured benchmark with up to 8 CPU nodes. Then we use linear scaling to scale beyond 8 nodes.

GTC

GTC is used for gyrokinetic particle simulation of turbulent transport in burning plasmas

VERSION

4.2

ACCELERATED FEATURES

Push, shift, and collision

SCALABILITY

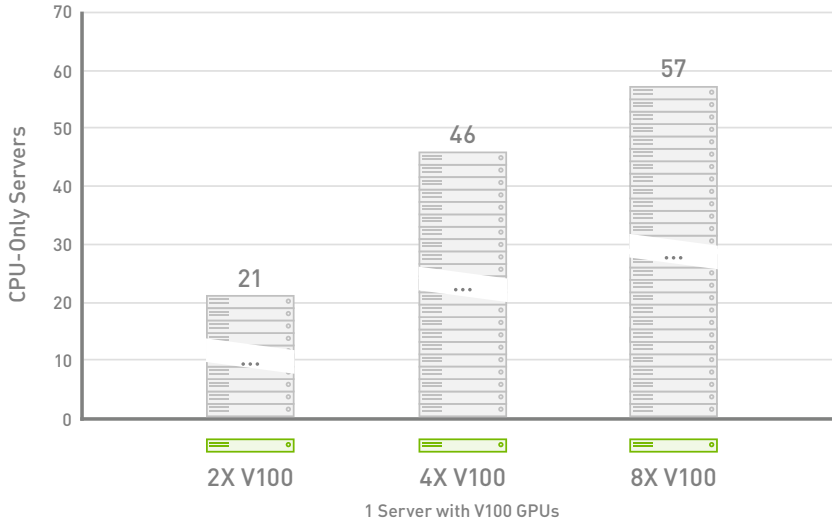
Multi-GPU and Multi-Node

MORE INFORMATION

www.nvidia.com/gtc-p

MILC Performance Equivalence

Single GPU Server vs Multiple Skylake CPU-Only Servers



CPU Server: Dual Xeon Gold 6140 @ 2.30 GHz, GPU Servers: Same as CPU server with NVIDIA® Tesla® V100 PCIe | NVIDIA CUDA® Version: 10.0.130 | Dataset: APEX Medium | To arrive at CPU node equivalence, we use a measured benchmark with up to 8 CPU nodes. Then we use linear scaling to scale beyond 8 nodes.

MILC

Lattice quantum chromodynamics (LQCD) codes simulate how elemental particles are formed and bound by the “strong force” to create larger particles like protons and neutrons.

VERSION
2018

ACCELERATED FEATURES

Staggered fermions, Krylov solvers, gauge-link fattening

SCALABILITY

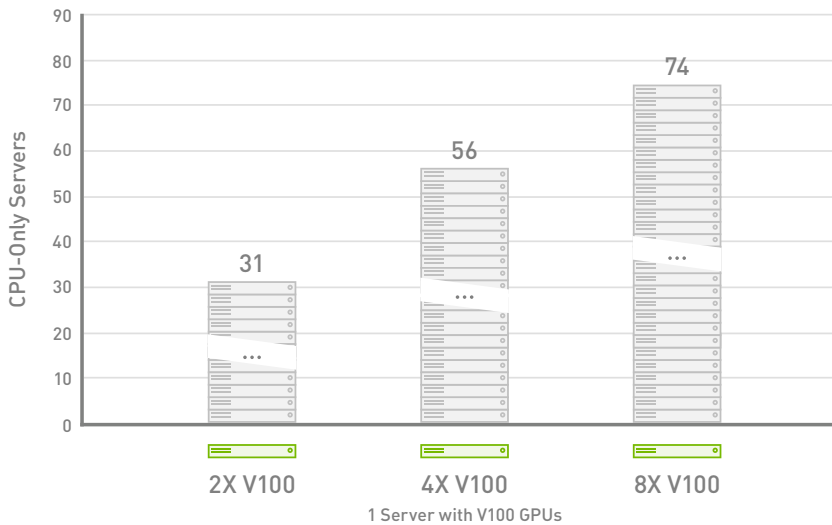
Multi-GPU and Multi-Node

MORE INFORMATION

www.nvidia.com/milc

QUDA Performance Equivalence

Single GPU Server vs Multiple Broadwell CPU-Only Servers



CPU Server: Dual Xeon Gold 6140 @ 2.30GHz, GPU Servers: Same as CPU server with NVIDIA® Tesla® V100 PCIe or V100 SXM2 on 8X V100 config | NVIDIA CUDA® Version: 9.0.103 | Dataset: Dslash Wilson-Clove; Precision: Single; Gauge Compression/Recon: 12; Problem Size 32x32x32x64 | To arrive at CPU node equivalence, we use measured benchmark with up to 8 CPU nodes. Then we use linear scaling to scale beyond 8 nodes.

QUDA

A library for lattice quantum chromodynamics on GPUs

VERSION
2017

ACCELERATED FEATURES

All

SCALABILITY

Multi-GPU and Multi-Node

MORE INFORMATION

www.nvidia.com/quda

WEATHER AND CLIMATE



Numerical weather prediction (NWP) represents a large segment of HPC because reliable weather forecasts help save lives in extreme weather events. NWP also drives economic decisions in industries such as aviation, energy and utilities, insurance, retail, and others. When running weather and climate applications, a data center's workload with Tesla V100 GPUs can reduce infrastructure acquisition costs by over 50%.

KEY FEATURES OF THE TESLA PLATFORM AND V100 FOR WEATHER AND CLIMATE

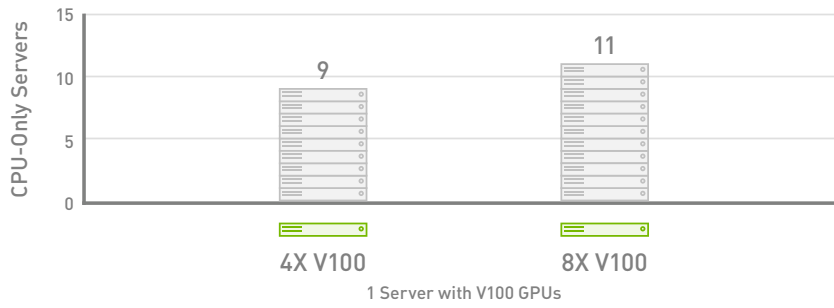
- > Servers with V100 replace up to 11 CPU servers for applications such as Weather Research and Forecasting (WRF)
- > Leading Weather and Climate applications are GPU-accelerated
- > Key math libraries like FFT and BLAS
- > Up to 7.8 TFLOPS per second of double precision performance per GPU
- > Up to 32 GB of memory capacity per GPU
- > Up to 900 GB/s memory bandwidth per GPU

View all related applications at:

www.nvidia.com/teslaapps

WRF Performance Equivalency

Single GPU Server vs Multiple Skylake CPU-Only Servers



CPU Server: Dual Xeon Gold 6140 @ 2.30GHz, GPU Servers: Same as CPU server with NVIDIA® Tesla® V100 PCIe | NVIDIA CUDA® Version: 9.2.148 | Dataset: Conus_2.5k_JA | To arrive at CPU node equivalence, we use measured benchmark with up to 8 CPU nodes. Then we use linear scaling to scale beyond 8 nodes.

WEATHER RESEARCH AND FORECASTING (WRF)
Numerical weather prediction system designed for both atmospheric research and operational forecasting applications

VERSION
WRFg 3.7.1 developed by NVIDIA

ACCELERATED FEATURES
Dynamics and several Physics

SCALABILITY
Multi-GPU and Multi-Node

MORE INFORMATION
<https://www.mmm.ucar.edu/weather-research-and-forecasting-model>

TESLA V100 PRODUCT SPECIFICATIONS



	NVIDIA Tesla V100 for PCIe-Based Servers	NVIDIA Tesla V100 for NVLink-Optimized Servers
Double-Precision Performance	up to 7 TFLOPS	up to 7.8 TFLOPS
Single-Precision Performance	up to 14 TFLOPS	up to 15.7 TFLOPS
Deep Learning	up to 112 TFLOPS	up to 125 TFLOPS
NVIDIA NVLink™ Interconnect Bandwidth	-	300 GB/s
PCIe x 16 Interconnect Bandwidth	32 GB/s	32 GB/s
CoWoS HBM2 Stacked Memory Capacity	32 GB / 16 GB	32 GB / 16 GB
CoWoS HBM2 Stacked Memory Bandwidth	900 GB/s	900 GB/s

Assumptions and Disclaimers

The percentage of top applications that are GPU-accelerated is from top 50 app list in the i360 report: HPC Support for GPU Computing.

Calculation of throughput and cost savings assumes a workload profile where applications benchmarked in the domain take equal compute cycles: <http://www.intersect360.com/industry/reports.php?id=131>

The number of CPU nodes required to match single GPU node is calculated using lab performance results of the GPU node application speed-up and the Multi-CPU node scaling performance.