Deep Learning and HPC Applications



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 resulting in faster insights and dramatically lower costs. Improved performance and timeto-solution can also have significant favorable impacts on revenue and productivity.

Every HPC data center can benefit from the Tesla platform. Over 500 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.

DEP LEARNINGImage: Constant of the second secon

RESEARCH DOMAINS WITH GPU-ACCELERATED APPLICATIONS INCLUDE:

Over 500 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



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 up to 85% in server and infrastructure acquisition costs.

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

- Caffe, TensorFlow, and CNTK are up to 3x faster with Tesla V100 compared to P100
- > 100% of the top deep learning frameworks are GPU-accelerated
- > Up to 125 TFLOPS of TensorFlow operations
- > Up to 16 GB of memory capacity with up to 900 GB/s memory bandwidth

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





CAFFE

A popular, GPU-accelerated Deep Learning framework developed at UC Berkeley

version 1.0

ACCELERATED FEATURES Full framework accelerated

SCALABILITY

Multi-GPU

MORE INFORMATION caffe.berkeleyvision.org





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 up to 80% in server and infrastructure acquisition costs.

KEY FEATURES OF THE TESLA PLATFORM AND V100 FOR MD

- Servers with V100 replace up to 54 CPU servers for applications such as H00MD-Blue and Amber
- > 100% of the top MD applications are GPU-accelerated
- > Key math libraries like FFT and BLAS
- > Up to 15.7 TFLOPS per second of single precision performance per GPU
- > Up to 900 GB per second of memory bandwidth per GPU

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



HOOMD-BLUE

Particle dynamics package is written from the ground up for GPUs

VERSION

2.1.6

ACCELERATED FEATURES CPU & GPU versions available

SCALABILITY

Multi-GPU and Multi-Node

MORE INFORMATION

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

AMBER Performance Equivalence Single GPU Server vs Multiple CPU-Only Servers

beyond 8 nodes.





AMBER

Suite of programs to simulate molecular dynamics on biomolecule

VERSION 16.8

ACCELERATED FEATURES

PMEMD Explicit Solvent & GB; Explicit & Implicit Solvent, REMD, aMD

scalability Multi-GPU and Single-Node

MORE INFORMATION http://ambermd.org/gpus



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 30% in server and infrastructure acquisition costs.

KEY FEATURES OF THE TESLA PLATFORM AND V100 FOR QC

- Servers with V100 replace up to 5 CPU servers for applications such as 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 16 GB of memory capacity for large datasets

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



VASP

Package for performing ab-initio quantum-mechanical molecular dynamics (MD) simulations

version 5.4.4

ACCELERATED FEATURES

RMM-DIIS, Blocked Davidson, K-points, and exact-exchange

SCALABILITY

Multi-GPU and Multi-Node

MORE INFORMATION

www.nvidia.com/vasp



From fusion energy to high energy particles, physics simulations span a wide range of applications in the HPC data center. Many of the top physics applications are GPU-accelerated, enabling insights previously not possible. A data center with Tesla V100 GPUs can save up to 75% 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 75 CPU servers for applications such as GTC-P, QUDA, and MILC
- > Most of the top physics applications are GPU-accelerated
- > Up to 7.8 TFLOPS of double precision floating point performance
- > Up to 16 GB of memory capacity with up to 900 GB/s memory bandwidth

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





CPU Server: Dual Xeon E5-2690 v4 @ 2.6 GHz, GPU Servers: Same as CPU server with NVIDIA® Tesla® V100 for PCIe | 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.

GTC-P

A development code for optimization of plasma physics

version 2017

ACCELERATED FEATURES Push, shift, and collision

SCALABILITY Multi-GPU

MORE INFORMATION www.nvidia.com/gtc-p

ουσΔ

A library for Lattice Quantum Chromo Dynamics on GPUs

VERSION 2017

ACCELERATED FEATURES

SCALABILITY Multi-GPU and Multi-Node

MORE INFORMATION www.nvidia.com/guda



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 2017

ACCELERATED FEATURES

Staggered fermions, Krylov solvers, Gauge-link fattening

SCALABILITY Multi-GPU and Multi-Node

MORE INFORMATION www.nvidia.com/milc



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 up to 70% in server and infrastructure acquisition costs.

KEY FEATURES OF THE TESLA PLATFORM AND V100 FOR GEOSCIENCE

- Servers with V100 replace up to 82 CPU servers for applications such as RTM and SPECFEM 3D
- > Top Oil and Gas applications are GPU-accelerated
- > Up to 15.7 TFLOPS of single precision floating point performance
- > Up to 16 GB of memory capacity with up to 900 GB/s memory bandwidth

View all related applications at: www.nvidia.com/oil-and-gas-apps





CPU Server: Dual Xeon E5-2690 v4 @ 2.6 GHz, GPU Servers: Same as CPU server with NVIDIA® Tesla® V100 for PCIe | NVIDIA CUDA® Version: 9.0.103 | Dataset: 288x64, 100 mins | To arrive at CPU node equivalence, we use linear scaling to scale beyond 1 nodes.

RTM

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

VERSION

2017

ACCELERATED FEATURES Batch algorithm

SCALABILITY Multi-GPU and Multi-Node

SPECFEM 3D

Simulates Seismic wave propagation

version 7.0.0

SCALABILITY Multi-GPU and Multi-Node

MORE INFORMATION

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



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 20% in server and infrastructure acquisition costs and over 50% in software licensing costs.

KEY FEATURES OF THE TESLA PLATFORM AND V100 FOR ENGINEERING

- Servers with Tesla V100 replace up to 4 CPU servers for applications such as SIMULIA Abaqus and ANSYS FLUENT
- > The top engineering applications are GPU-accelerated
- > Up to 16 GB of memory capacity
- > Up to 900 GB/s memory bandwidth
- > Up to 7.8 TFLOPS of double precision floating point



to scale beyond 8 nodes.

SIMULIA ABAQUS

Simulation tool for analysis of structures

VERSION

2017

ACCELERATED FEATURES

Direct Sparse Solver AMS Eigen Solver Steady-state Dynamics Solver

SCALABILITY Multi-GPU and Multi-Node

MORE INFORMATION

www.nvidia.com/simulia-abaqus

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



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 67 CPU servers for benchmarks such as Cloverleaf, MiniFE, Linpack, and HPCG
- > The top benchmarks are GPU-accelerated
- > Up to 7.8 TFLOPS of double precision floating point up to 16 GB of memory capacity
- > Up to 900 GB/s memory bandwidth





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

MINIFE

Benchmark – Mini-App Finite Element Analysis

VERSION 0.3

ACCELERATED FEATURES All

SCALABILITY Multi-GPU

MORE INFORMATION

https://mantevo.org/about/applications



HPCG Performance Equivalence Single GPU Server vs Multiple CPU-Only Servers 80 67 70 60 **CPU-Only Servers** 50 37 40 . . . 30 19 20 . . . 10 0 = = ٥ 0 2X V100 4X V100 8X V100 1 Server with V100 GPUs

CPU Server: Dual Xeon E5-2690 v4 @ 2.6GHz, GPU Servers: Same as CPU server with NVIDIA® Tesla® V100 for PCIe | NVIDIA CUDA® Version: 9.0.103 | Dataset: 256x256x256 local size | 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.

LINPACK

Benchmark – Measures floating point computing power

VERSION

2.1

ACCELERATED FEATURES

SCALABILITY Multi-Node and Multi-Node

MORE INFORMATION

www.top500.org/project/linpack

HPCG

Benchmark – 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

www.hpcg-benchmark.org/index.html

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	16 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. For example, the Molecular Dynamics application HOOMD-Blue has a GPU Node application speed-up of 37.9X. When scaling CPU nodes to an 8 node cluster, the total system output is 7.1X. So the scaling factor is 8 divided by 7.1 (or 1.13). To calculate the number of CPU nodes required to match the performance of a single GPU node, you multiply 37.9 (GPU Node application speed-up) by 1.13 (CPU node scaling factor) which gives you 43 nodes.

