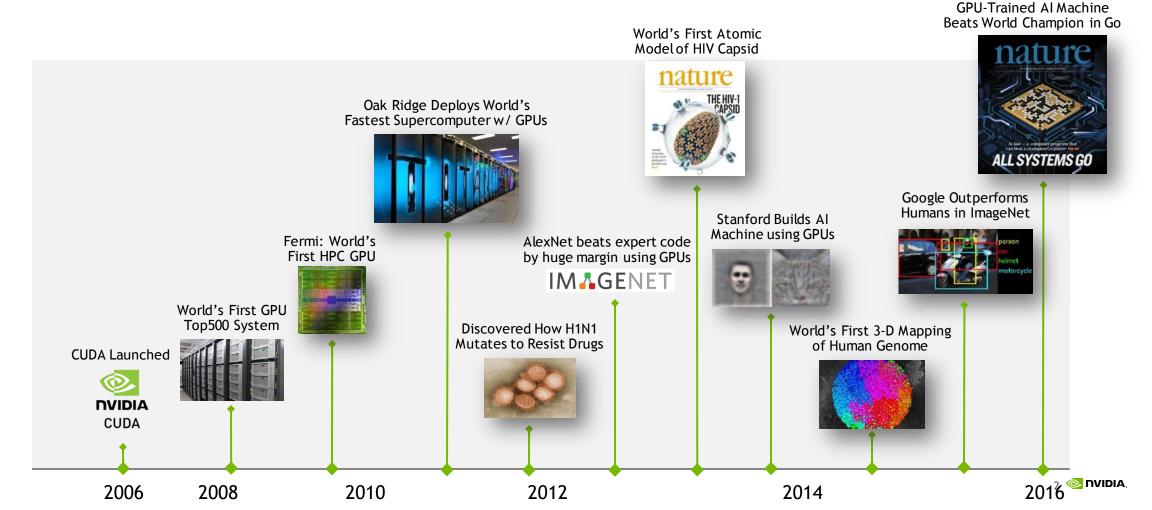
NVIDIA IN HPC AND AI

April 2017, OSC SUG

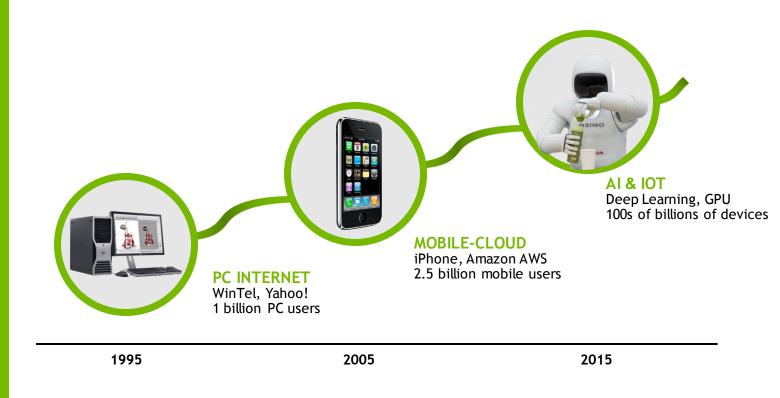


TEN YEARS OF GPU COMPUTING



A NEW ERA OF COMPUTING

 It's clear we're moving from a mobile first to an Al-first world "
 Sundar Pichai, Google CEO



TOUCHING OUR LIVES



Bringing grandmother closer to family by bridging language barrier Predicting sick baby's vitals like heart rate, blood pressure, survival rate Enabling the blind to "see" their surrounding, read emotions on faces

FUELING ALL INDUSTRIES



Increasing public safety with smart video surveillance at airports & malls

Providing intelligent services in hotels, banks and stores

Separating weeds as it harvests, reduces chemical usage by 90%

WHAT DOES HPC HAVE TO DO WITH AI?

EVERYTHING!!!

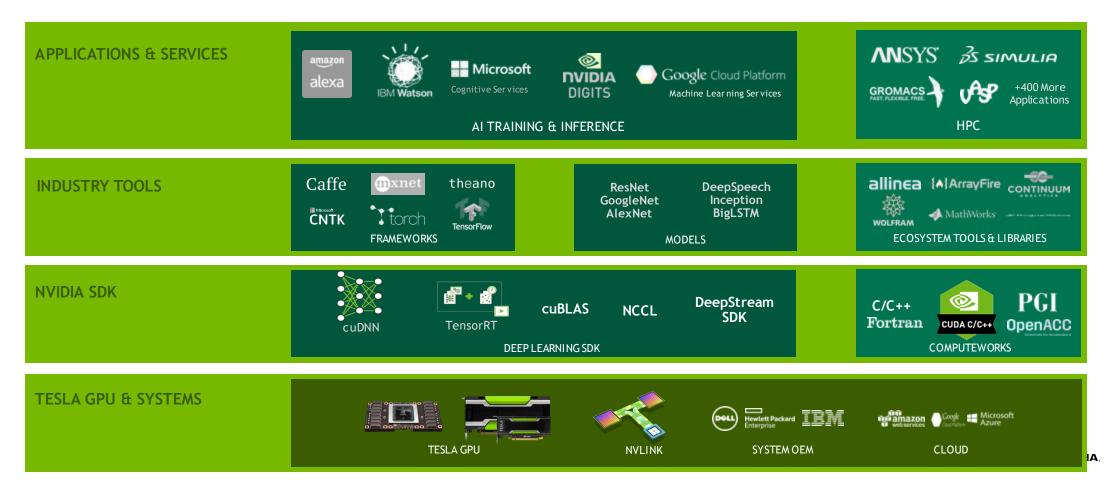


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Code	And	roid	iOS V	Veb	Backend	Hardware
Engi	ne	erir	ng a	at I	ace	book



TESLA PLATFORM

Leading Data Center Platform for HPC and AI



NVIDIA POWERS WORLD'S LEADING DATA CENTERS FOR HPC AND AI





NVIDIA ONE ARCHITECTURE FOR ALL PRODUCTS



GPU Computing

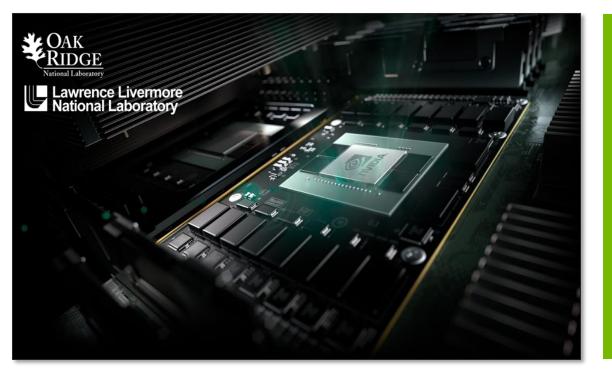
Computer Graphics

Artificial Intelligence



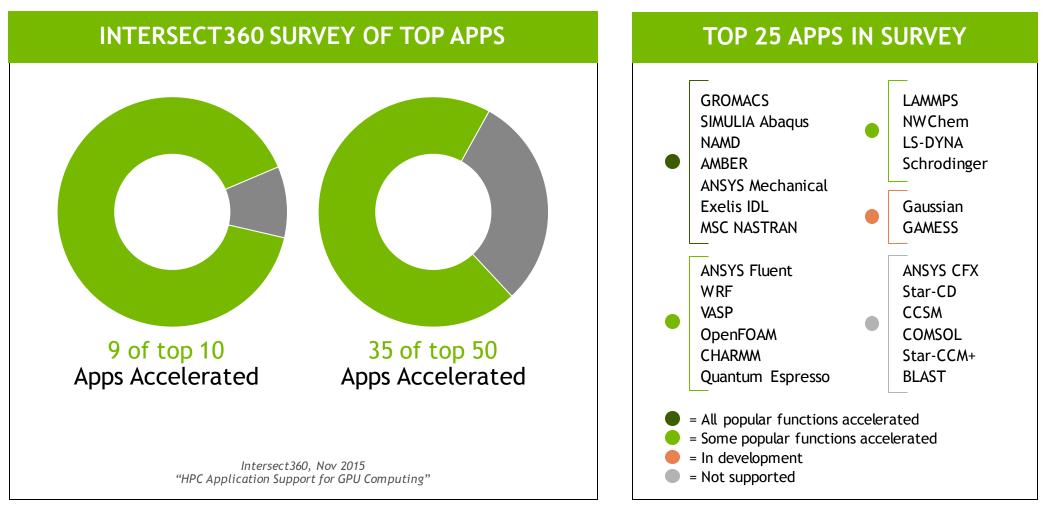
U.S. TO BUILD TWO FLAGSHIP SUPERCOMPUTERS

Pre-Exascale Systems Powered by the Tesla Platform



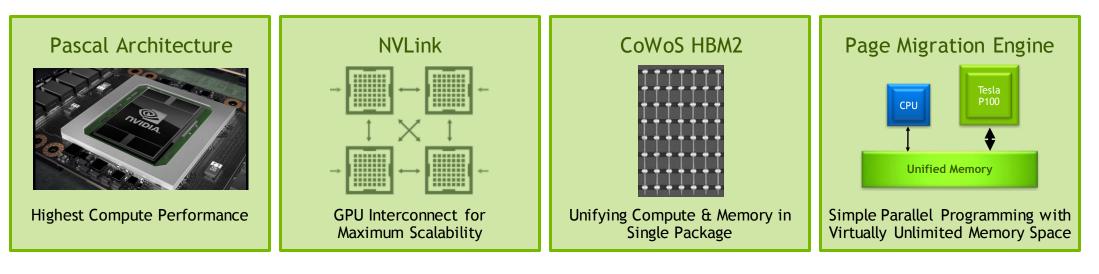
Summit & Sierra Supercomputers 100-300 PFLOPS Peak IBM POWER9 CPU + NVIDIA Volta GPU NVLink High Speed Interconnect 40 TFLOPS per Node, >3,400 Nodes 2017

70% OF TOP HPC APPS ACCELERATED



INTRODUCING TESLA P100

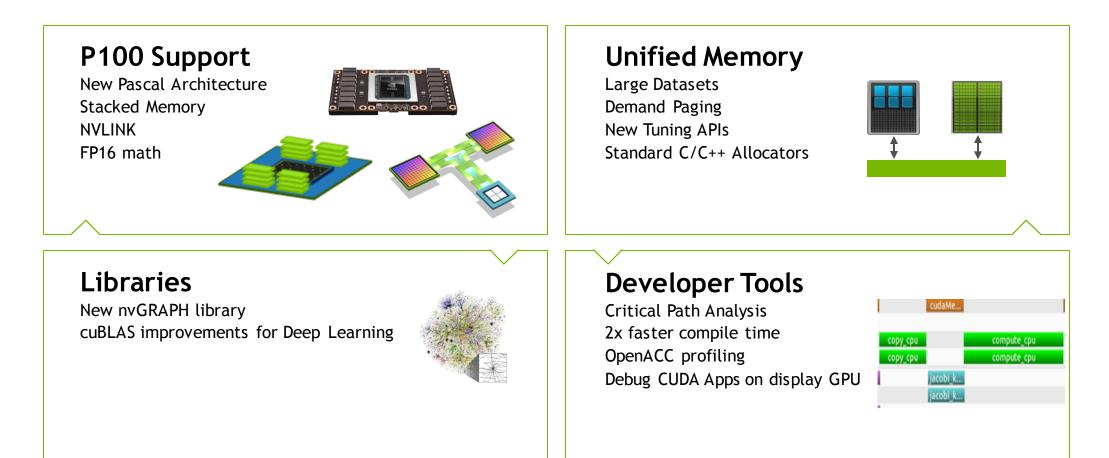
New GPU Architecture to Enable the World's Fastest Compute Node





CONFIDENTIAL. DO NOT DISTRIBUTE.

CUDA 8 - WHAT'S NEW

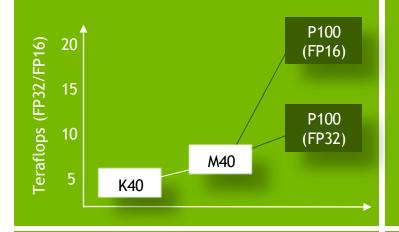


GIANT LEAPS

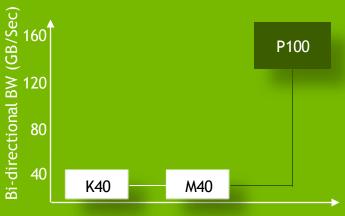
IN EVERYTHING

PASCAL ARCHITECTURE

21 Teraflops of FP16 for Deep Learning

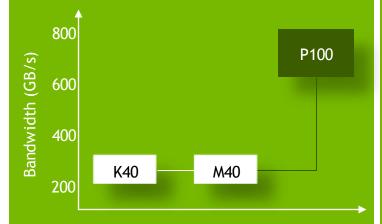


NVLINK 5x GPU-GPU Bandwidth



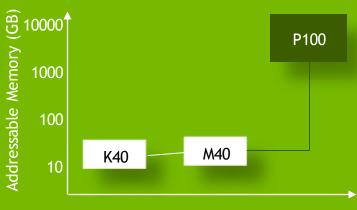
CoWoS HBM2 Stacked Mem

3x Higher for Massive Data Workloads



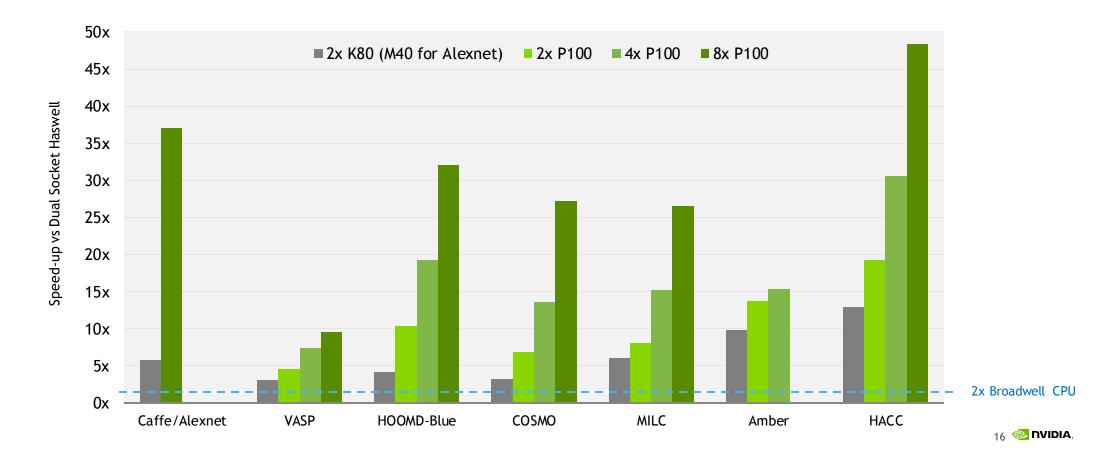
PAGE MIGRATION ENGINE

Virtually Unlimited Memory Space



HIGHEST ABSOLUTE PERFORMANCE DELIVERED

NVLink for Max Scalability, More than 45x Faster with 8x P100



PASCAL ARCHITECTURE

TESLA P100 ACCELERATOR

Compute	5.3 TF DP \cdot 10.6 TF SP \cdot 21.2 TF HP
Memory	HBM2: 720 GB/s · 16 GB
Interconnect	NVLink (up to 8 way) + PCIe Gen3
Programmability	Page Migration Engine Unified Memory
Availability	DGX-1: Order Now Cray, Dell, HP, IBM: Q1 2017

GPU PERFORMANCE COMPARISON

	P100	M40	K40
Double Precision TFlop/s	5.3	0.2	1.4
Single Precision TFlop/s	10.6	7.0	4.3
Half Precision Tflop/s	21.2	NA	NA
Memory Bandwidth (GB/s)	720	288	288
Memory Size	16GB	12GB, 24GB	12GB

IEEE 754 FLOATING POINT ON GP100

3 sizes, 3 speeds, all fast

	MIL		
Feature 🛃	New Half precision	Single precision	Double precision
Layout	s5.10	s8.23	s11.52
Issue rate	pair every clock	1 every clock	1 every 2 clocks
Subnormal support	Yes	Yes	Yes
Atomic Addition	Yes	Yes	New Yes
			MW .

HALF-PRECISION FLOATING POINT (FP16)

• 16 bits



- 1 sign bit, 5 exponent bits, 10 fraction bits
- 2⁴⁰ Dynamic range
 - Normalized values: 1024 values for each power of 2, from 2⁻¹⁴ to 2¹⁵
 - Subnormals at full speed: 1024 values from 2⁻²⁴ to 2⁻¹⁵
- Special values
 - +- Infinity, Not-a-number

USE CASES

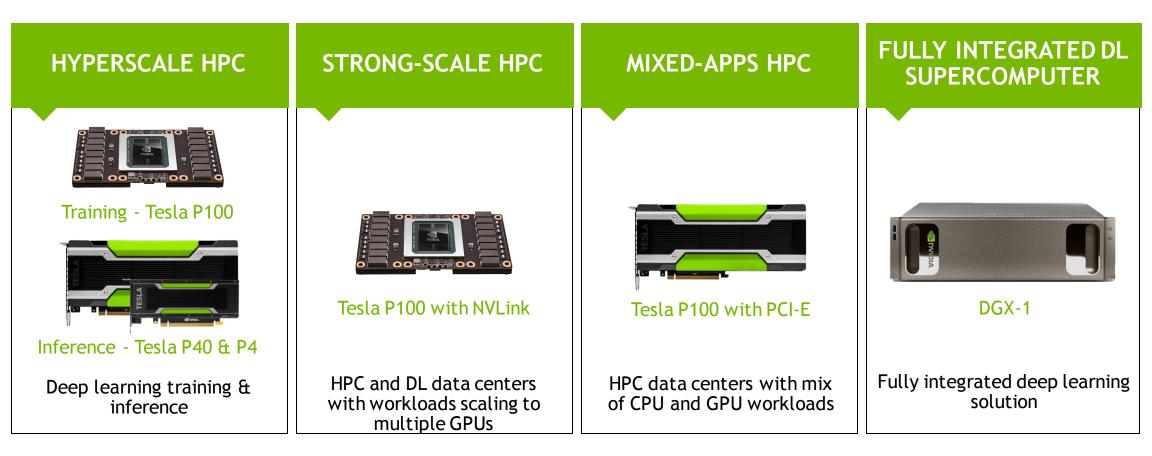
Deep Learning Training

Radio Astronomy

Sensor Data

Image Processing

END-TO-END PRODUCT FAMILY





NVLINK - GPU CLUSTER

Two fully connected quads, connected at corners

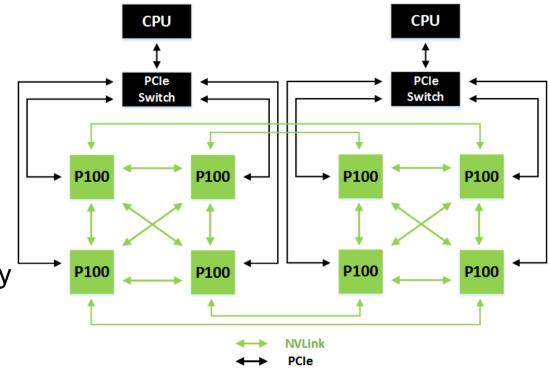
160GB/s per GPU bidirectional to Peers

Load/store access to Peer Memory

Full atomics to Peer GPUs

High speed copy engines for bulk data copy

PCIe to/from CPU



UNIFIED MEMORY

4.5.2017 г.

PAGE MIGRATION ENGINE

Support Virtual Memory Demand Paging

49-bit Virtual Addresses

Sufficient to cover 48-bit CPU address + all GPU memory

GPU page faulting capability

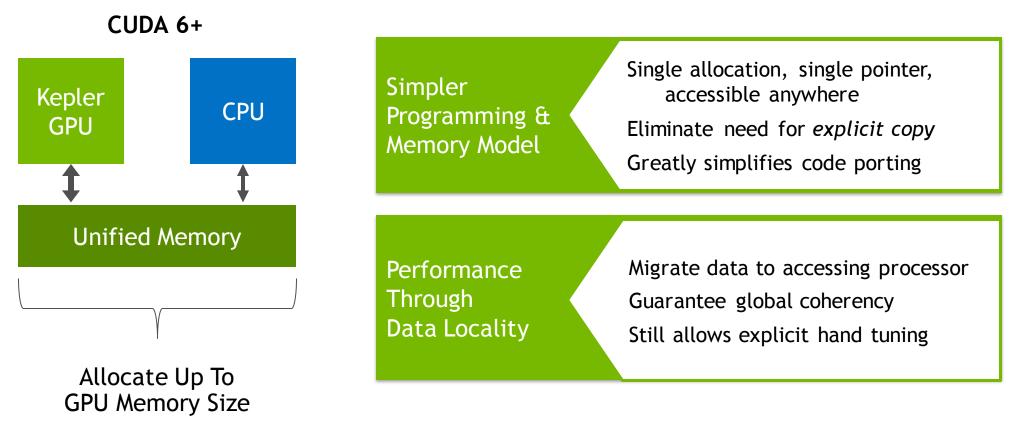
Can handle thousands of simultaneous page faults

Up to 2 MB page size

Better TLB coverage of GPU memory

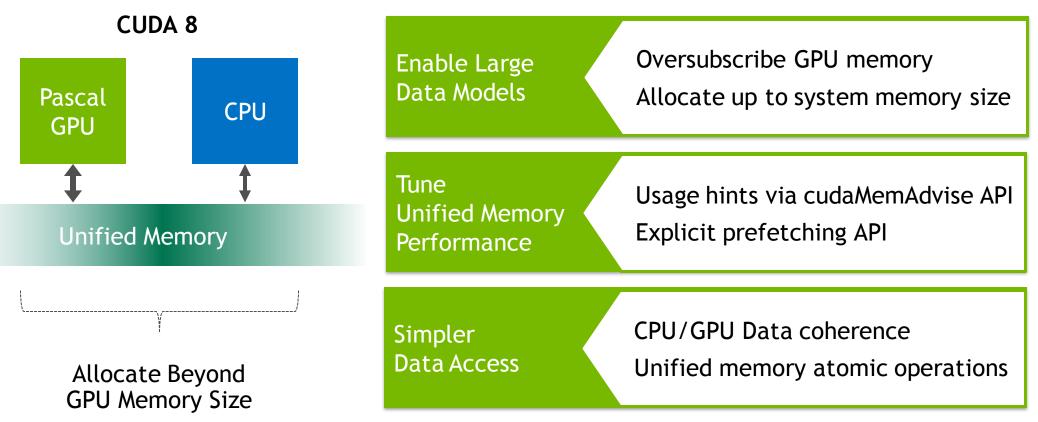


KEPLER/MAXWELL UNIFIED MEMORY



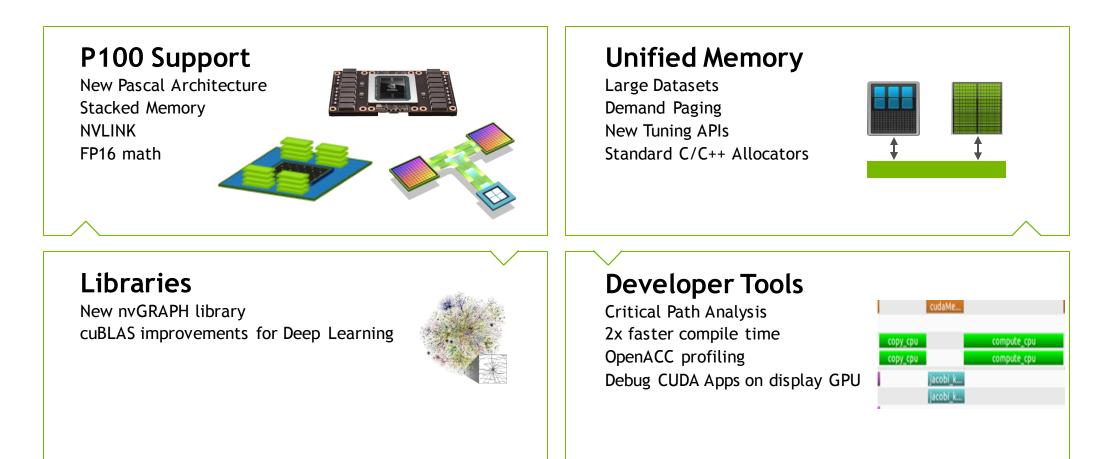
PASCAL UNIFIED MEMORY

Large datasets, simple programming, High Performance





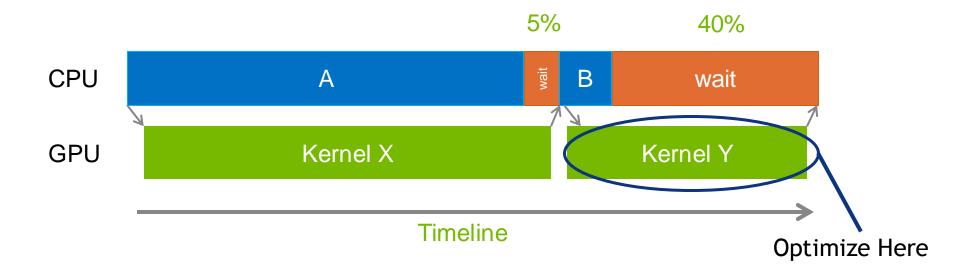
CUDA 8 - WHAT'S NEW



ENHANCED PROFILING

DEPENDENCY ANALYSIS

Easily Find the Critical Kernel To Optimize



The longest running kernel is not always the most critical optimization target

DEPENDENCY ANALYSIS

Visual Profiler

Unguided Analysis

Generating critical path

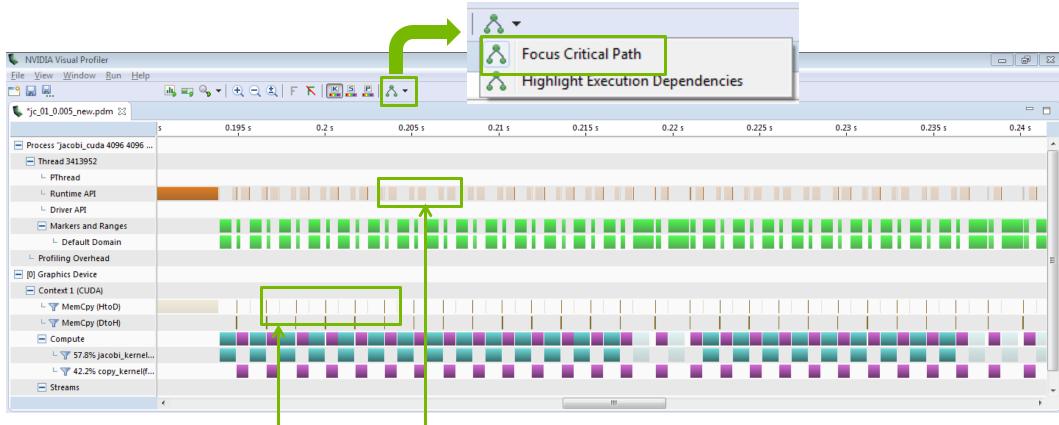
🔚 🚹 🧰 Reset All 🛺 Ar	alyze All	Results					
o enable kernel analysis stages select a host-launched imeline. pplication	I kernel instance in the	i Dependency Analysis The following table shows metrics collected from a c Analysis" menu on the main toolbar to visualize anal		gram execution. The da	ta is summarized per fu	nction type. Use the "Dependency	More
Data Movement And Concurrency	O	Function Name	Time on Critical Path (%)	Time on Critical Path	Waiting time		
		cudaMalloc	32.72 %	127.392 ms	0 ns		
Compute Utilization	🖪 📀 🗌	jacobi_kernel(float const *, float*, int, int, float*)	20.61 %	80.248 ms	0 ns		
		copy_kernel(float*, float const *, int, int)	17.46 %	68.004 ms	0 ns		
Kernel Performance		<other></other>	12.61 %	49.113 ms	0 ns		
		cudaMemcpy	10.75 %	41.844 ms	20.181 ms		
Dependency Analysis	S	[CUDA memcpy DtoH]	5.18 %	20.181 ms	0 ns		
		cudaSetupArgument	0.14 %	534.684 µs	0 ns		
NVLink	🖳 📀	cudaFree	0.11 %	424.883 µs	0 ns		
		[CUDA memcpy HtoD]	0.10 %	400.25 μs	0 ns		
		cuDeviceGetAttribute	0.09 %	336.781 µs	0 ns		
		cudaGetDeviceProperties	0.08 %	319.677 µs	0 ns		
		cudaLaunch	0.05 %	192.598 µs	0 ns		
		cudaConfigureCall	0.05 %	186.452 µs	0 ns		
		cuDeviceTotalMem_v2	0.05 %	182.833 µs	0 ns		
		cuDeviceGetName	0.00 %	18.022 µs	0 ns		
		cudaSetDevice	0.00 %	12.933 µs	0 ns		

Dependency Analysis

Functions on critical path

DEPENDENCY ANALYSIS

Visual Profiler



APIs, GPU activities not in critical path are greyed out

MORE CUDA 8 PROFILER FEATURES

💺 *NewSession1 🛙							Properties X	- 0
	ns	655.875 ms	655.9 ms	655.925 ms	655.95 ms		GPU Page Fault	
Process "UnifiedMemoryStre						6	Start	655.873 ms (655,87
Thread 2580887296							End	655.881 ms (655,88
- Runtime API							Duration	7.855 µs
🛨 Thread 2564101888							Virtual Address	0x700365000
🛨 Thread 2992064448							Process	10032
Thread 2572494592								
- Runtime API								
Profiling Overhead								
[0] Graphics Device								
Unified Memory								
🗆 🍸 GPU Page Fault		GPU P				-		
- 🍸 Data Migration (HtoD))							
- 🍸 Data Migration (DtoH))					0		
Context 1 (CUDA)								
- 🍸 MemCpy (HtoD)								
	AC				()	Ð	(*()))

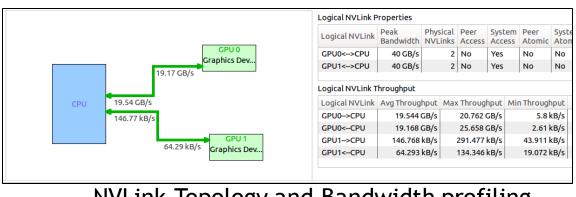
🗔 Analysis 📠 GPU Details 語 CPU Details 🕱 💷	Console 🗔 Se	ttings
TOTAL		
Event	%	Time
 bench_staggeredleapfrog2_ 	95.833%	689.695 ms
CCTKi_BindingsFortranWrapperBenchADM	95.833%	689.695 ms
CCTK_CallFunction	95.833%	689.695 ms
open_nocancel	1.389%	9.996 ms
InitialFlat	1.389%	9.996 ms
¢c_mcopy8	1.389%	9.996 ms

CPU Profiling

Unified Memory Profiling

- 🝸 M	emCpy (DtoH)				
🖃 Com	pute	xpyiiiPfS	_Z	8runSaxpyiiiPfS	. Z8runSaxpy
L 7	100.0% _Z8runSax	xpyiiiPfS	_Z	8runSaxpyiiiPfS	_Z8runSaxpy
Street	ams				
- D	efault	xpyiiiPfS	_Z	8runSaxpyiiiPfS	. Z8runSaxpy
		(4(
analysis	🔤 GPU Details 📃	Console 🗔 S	ettings	acc_openmp.cpp	22
	<pre>float *sub_x = x + (i * N); float *sub_y = y + (i * N); if (loop == 0 && omp_get_thread_num() == 0) { printf("%d OMP_threads\n", omp_get_num_threads()); fflush(NULL); }</pre>				
	acc kernels	No. 1993 F			
<pre>for (j = 0; j < N; ++j) { sub_y[j] = a*sub_x[j]; } return 0; } /* test main */</pre>					

OpenACC Profiling



NVLink Topology and Bandwidth profiling



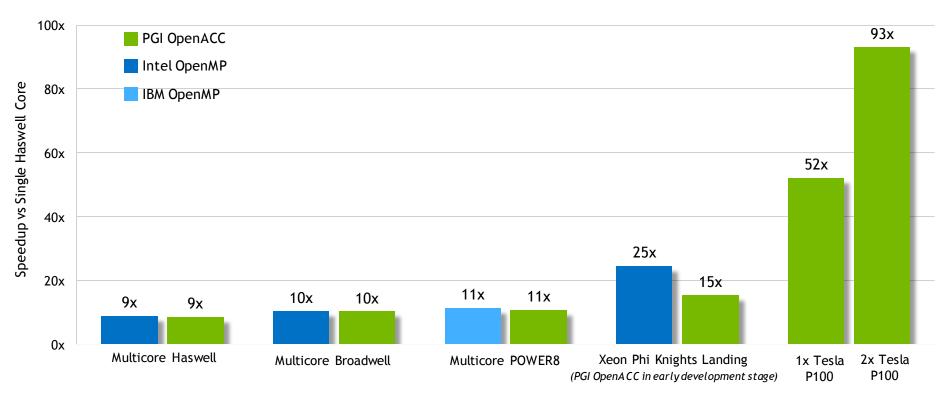
OPENACC

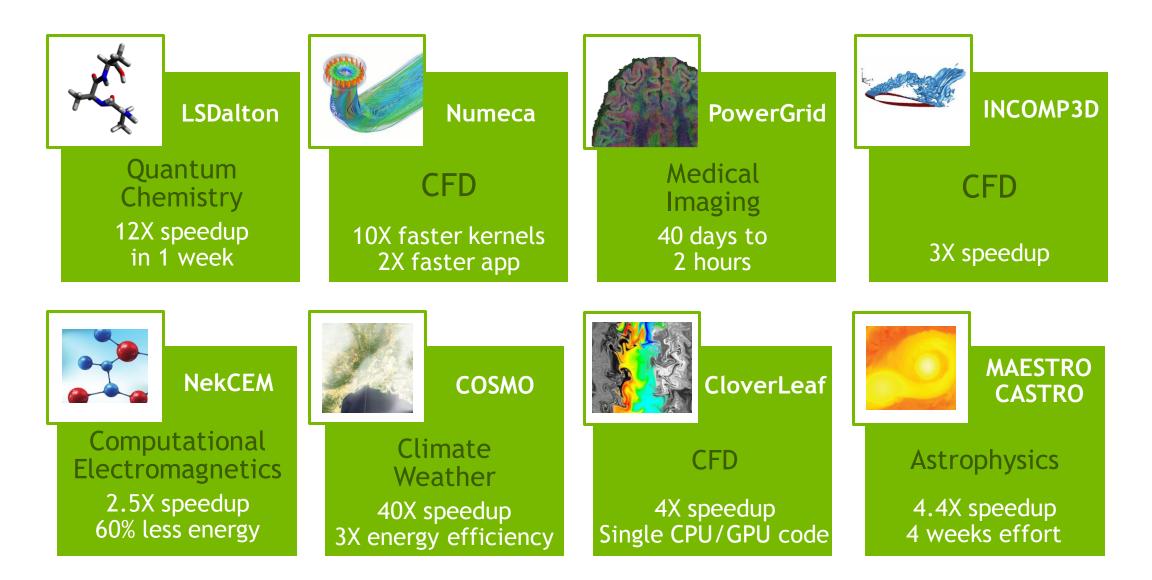
World's Only Performance Portable Programming Model for HPC

Add Simple Compiler Hint	ARM PEZY	LSDALTON Simulation of molecular energies
{ <serial code=""></serial>	POWER	Quicker Development Big Performance CCSD(T) Module, Alanine-3
<pre>#pragma acc kernels</pre>	Sunway	Lines of Code Modified
{ <parallel code=""></parallel>	x86 CPU	
}	x86 Xeon Phi	# of Weeks Required 1.0x
}	NVIDIA GPU	1 Week
Simple	Portable	Powerful

SINGLE OPENACC CODE RUNS ON ALL CPU & GPU PLATFORMS

CloverLeaf- Hydrodynamics Mini-Application





OPENACC FOR EVERYONE

New PGI Community Edition Now Available

FRE	Community EDITION	Professional EDITION	PGI Enterprise EDITION
PROGRAMMING MODELS OpenACC, CUDA Fortran, OpenMP, C/C++/Fortran Compilers and Tools			
PLATFORMS x86, OpenPOWER, NVIDIA GPU		\checkmark	
UPDATES	1-2 times a year	6-9 times a year	6-9 times a year
SUPPORT	User Forums	PGI Support	PGI Enterprise Services
LICENSE	Annual	Perpetual	Volume/Site

PERFORMANCE

MOLECULAR DYNAMICS

AMBER Performance Equivalency

Single GPU Server vs Multiple CPU-Only Servers



CPU Server: Dual Xeon E5-2690 v4@2.6GHz, GPU Servers: same CPU server w/ P100s PCIe (12GB or 16GB) CUDA Version: CUDA 8.0.42, Dataset: GB-Myoglobin

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.

AMBER Molecular Dynamics

Suite of programs to simulate molecular dynamics on biomolecule

VERSION 16.3

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

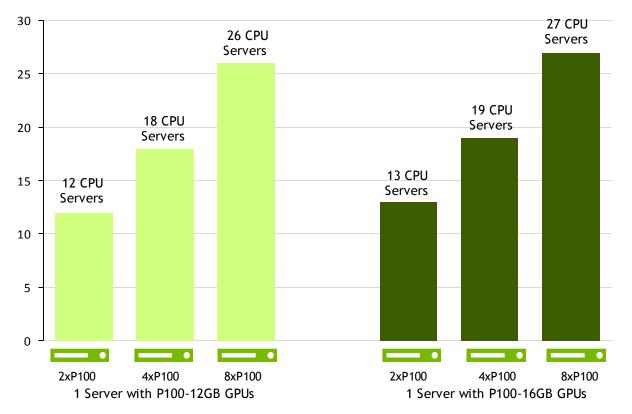
SCALABILITY Multi-GPU and Single-Node

More Information http://ambermd.org/gpus

HOOMD-Blue Performance Equivalency

Single GPU Server vs Multiple CPU-Only Servers

of CPU Only Servers



CPU Server: Dual Xeon E5-2690 v4@2.6GHz, GPU Servers: same CPU server w/ P100s PCIe (12GB or 16GB) CUDA Version: CUDA 8.0.42, DataseT: microsphere

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.

HOOMD-Blue Molecular Dynamics

Particle dynamics package written grounds up for GPUs

VERSION 1.3.3

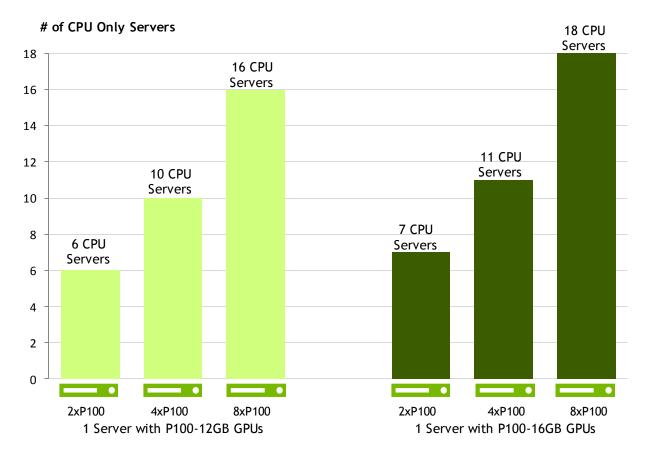
ACCELERATED FEATURES CPU & GPU versions available

SCALABILITY Multi-GPU and Multi-Node

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

LAMMPS Performance Equivalency

Single GPU Server vs Multiple CPU-Only Servers



CPU Server: Dual Xeon E5-2690 v4@2.6GHz, GPU Servers: same CPU server w/ P100s PCIe (12GB or 16GB) CUDA Version: CUDA 8.0.42, Dataset: EAM

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.

LAMMPS Molecular Dynamics

Classical molecular dynamics package

VERSION 2016

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

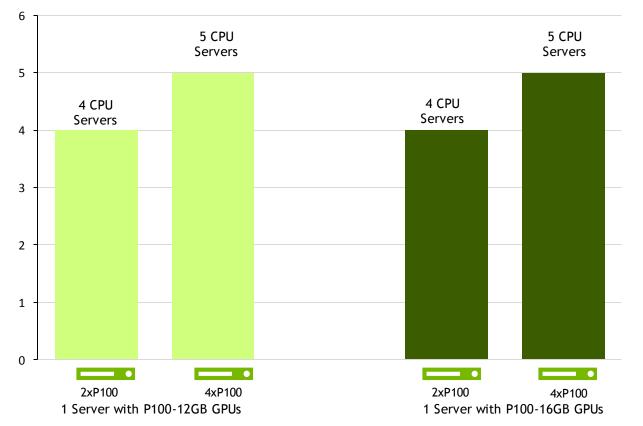
SCALABILITY Multi-GPU and Multi-Node

More Information http://lammps.sandia.gov/index.html

GROMACS Performance Equivalency

Single GPU Server vs Multiple CPU-Only Servers

of CPU Only Servers



CPU Server: Dual Xeon E5-2690 v4@2.6GHz, GPU Servers: same CPU server w/ P100s PCIe (12GB or 16GB) CUDA Version: CUDA 8.0.42, Dataset: Water 3M

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.

GROMACS Molecular Dynamics

Simulation of biochemical molecules with complicated bond interactions

VERSION 5.1.2

ACCELERATED FEATURES PME, Explicit & Implicit Solvent

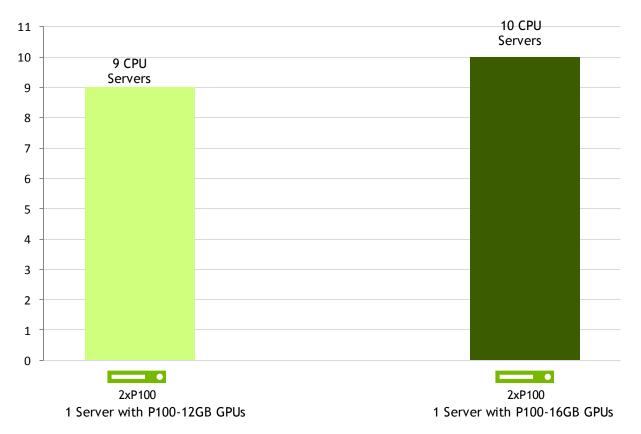
SCALABILITY Multi-GPU and Multi-Node Scales to 4xP100

More Information http://www.gromacs.org_l

NAMD Performance Equivalency

Single GPU Server vs Multiple CPU-Only Servers

of CPU Only Servers



CPU Server: Dual Xeon E5-2690 v4@2.6GHz, GPU Servers: same CPU server w/ P100s PCIe (12GB or 16GB) CUDA Version: CUDA 8.0.42, 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 Geoscience (Oil & Gas)

Designed for high-performance simulation of large molecular systems

VERSION 2.11

ACCELERATED FEATURES Full electrostatics with PME and most simulation features

SCALABILITY

Up to 100M atom capable, multi-GPU, Scale Scales to 2xP100

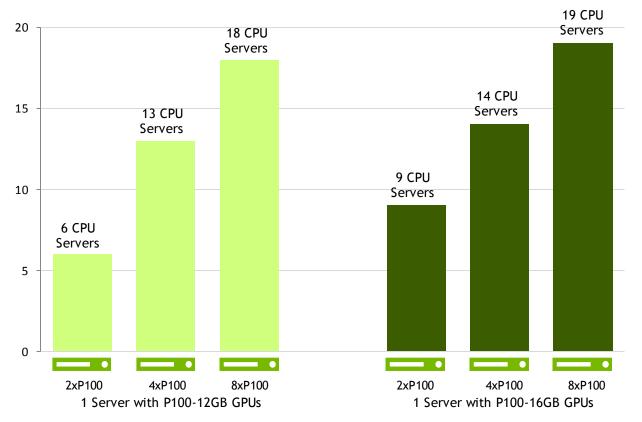
More Information http://www.ks.uiuc.edu/Research/namd/

MATERIALS SCIENCE

VASP Performance Equivalency

Single GPU Server vs Multiple CPU-Only Servers

of CPU Only Servers



CPU Server: Dual Xeon E5-2690 v4@2.6GHz, GPU Servers: same CPU server w/ P100s PCIe (12GB or 16GB) CUDA Version: CUDA 8.0.42, 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 Material Science (Quantum Chemistry)

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

VERSION 5.4.1

ACCELERATED FEATURES RMM-DIIS, Blocked Davidson, K-points and <u>exact-exchange</u>

SCALABILITY Multi-GPU and Multi-Node

More Information

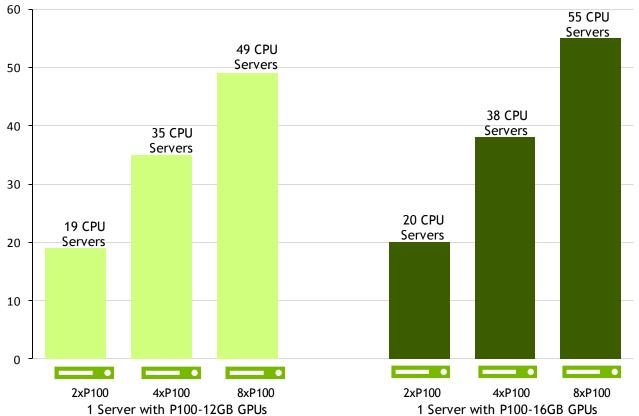
http://www.vasp.at/index.php/news/44-administrative/115new-release-vasp-5-4-1-with-gpu-support

BENCHMARKS

Linpack Performance Equivalency

Single GPU Server vs Multiple CPU-Only Servers

of CPU Only Servers



CPU Server: Dual Xeon E5-2690 v4@2.6GHz, GPU Servers: same CPU server w/ P100s PCIe (12GB or 16GB) CUDA Version: CUDA 8.0.42, Dataset: HPL.dat

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

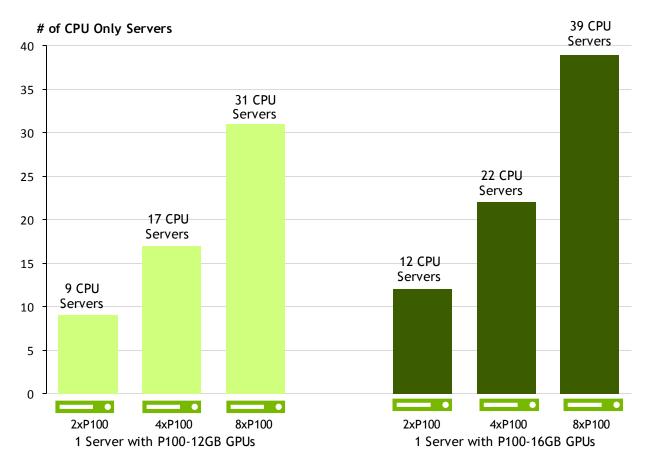
ACCELERATED FEATURES All

SCALABILITY Multi-GPU and Multi-Node

More Information https://www.top500.org/project/linpack/

HPCG Performance Equivalency

Single GPU Server vs Multiple CPU-Only Servers



CPU Server: Dual Xeon E5-2690 v4@2.6GHz, GPU Servers: same CPU server w/ P100s PCIe (12GB or 16GB) CUDA Version: CUDA 8.0.42, Dataset: 256x256 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.

HPCG Benchmark

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

VERSION 3.0

ACCELERATED FEATURES

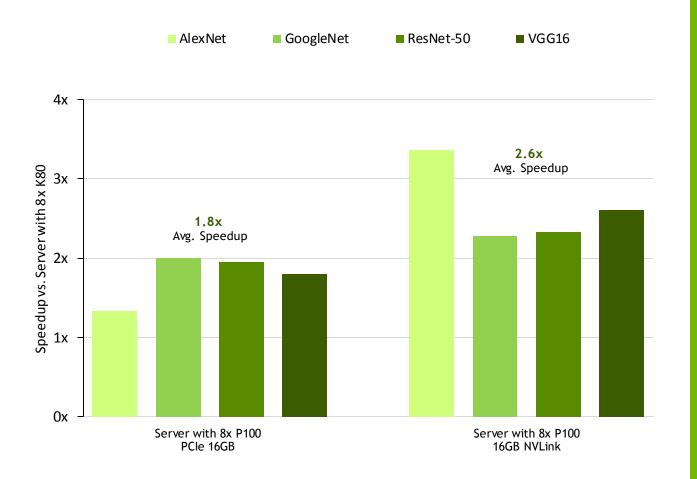
SCALABILITY Multi-GPU and Multi-Node

More Information http://www.hpcg-benchmark.org/index.html

DEEP LEARNING

CAFFE Deep Learning Framework

Training on 8x P100 GPU Server vs 8 x K80 GPU Server



CAFFE Deep Learning

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

VERSION 1.0

ACCELERATED FEATURES Full framework accelerated

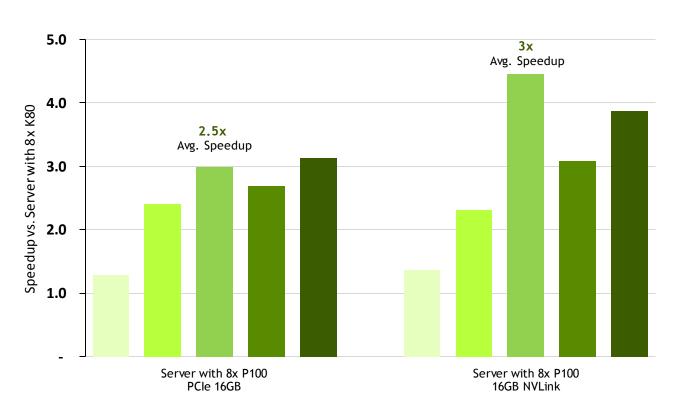
SCALABILITY Multi-GPU

More Information http://caffe.berkeleyvision.org/

TensorFlow Deep Learning Framework

Training on 8x P100 GPU Server vs 8 x K80 GPU Server

■ AlexNet ■ GoogleNet ■ ResNet-50 ■ ResNet-152 ■ VGG16



TensorFlow Deep Learning Training

An open-source software library for numerical computation using data flow graphs.

VERSION 1.0

ACCELERATED FEATURES Full framework accelerated

SCALABILITY Multi-GPU and multi-node

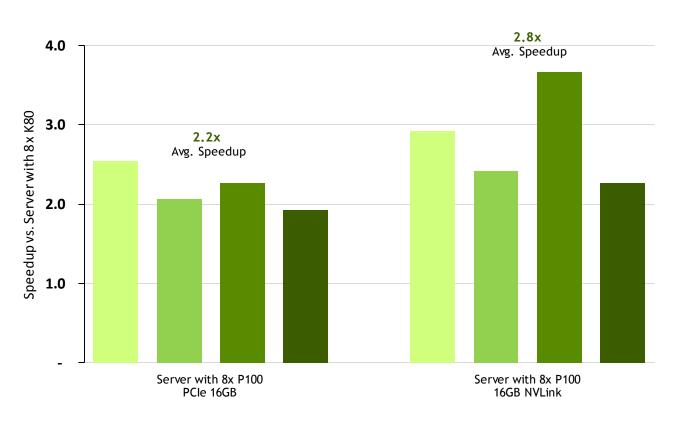
More Information https://www.tensorflow.org/

GPU Servers: Single Xeon E5-2690 v4@2.6GHz with GPUs configs as shown Ubuntu 14.04.5, CUDA 8.0.42, cuDNN 6.0.5; NCCL 1.6.1, data set: ImageNet; batch sizes: AlexNet (128), GoogleNet (256), ResNet-50 (64), ResNet-152 (32), VGG-16 (32)

Torch Deep Learning Framework

Training on 8x P100 GPU Server vs 8 x K80 GPU Server

■ AlexNet ■ InceptionV3 ■ ResNet-50 ■ VGG16



Torch Deep Learning Training

A scientific computing framework with wide support for machine learning algorithms that puts GPUs first.

VERSION 7.0

ACCELERATED FEATURES Full framework accelerated

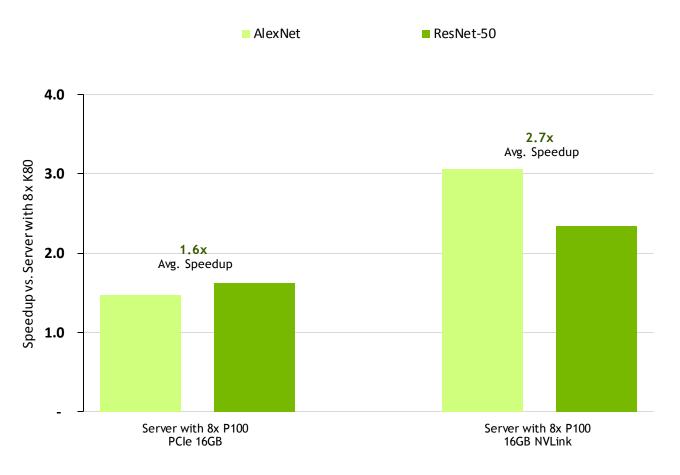
SCALABILITY Multi-GPU

More Information https://www.torch.ch

GPU Servers: Single Xeon E5-2690 v4@2.6GHz with GPUs configs as shown Ubuntu 14.04.5, CUDA 8.0.42, cuDNN 6.0.5; NCCL 1.6.1, data set: ImageNet; batch sizes: AlexNet (128), InceptionV3 (64), ResNet-50 (64), VGG-16 (32)

CNTK Deep Learning Framework

Training on 8x P100 GPU Server vs 8 x K80 GPU Server



GPU Servers: Single Xeon E5-2690 v4@2.6GHz with GPUs configs as shown Ubuntu 14.04.5, CUDA 8.0.42, cuDNN 6.0.5; NCCL 1.6.1, data set: ImageNet; batch sizes: AlexNet (128), ResNet-50 (64)

CNTK Deep Learning Training

A free, easy-to-use, open-source, commercialgrade toolkit that trains deep learning algorithms to learn like the human brain.

VERSION 1.0

ACCELERATED FEATURES Full framework accelerated

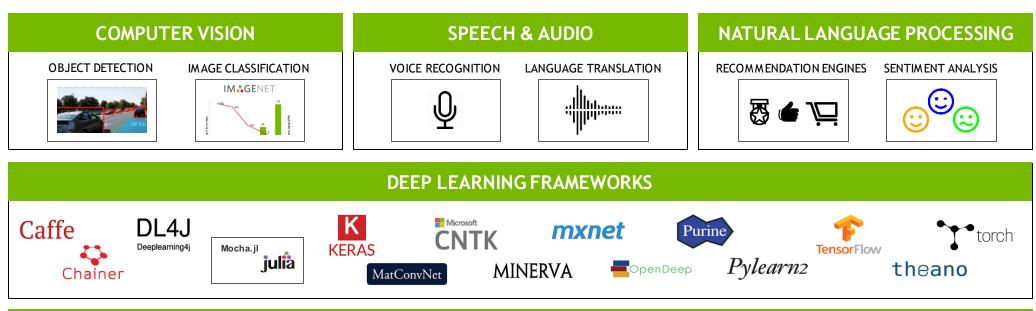
SCALABILITY Multi-GPU and multi-node

More Information www.microsoft.com/enus/research/product/cognitive-toolkit/

DEEP LEARNING SOFTWARE

POWERING THE DEEP LEARNING ECOSYSTEM

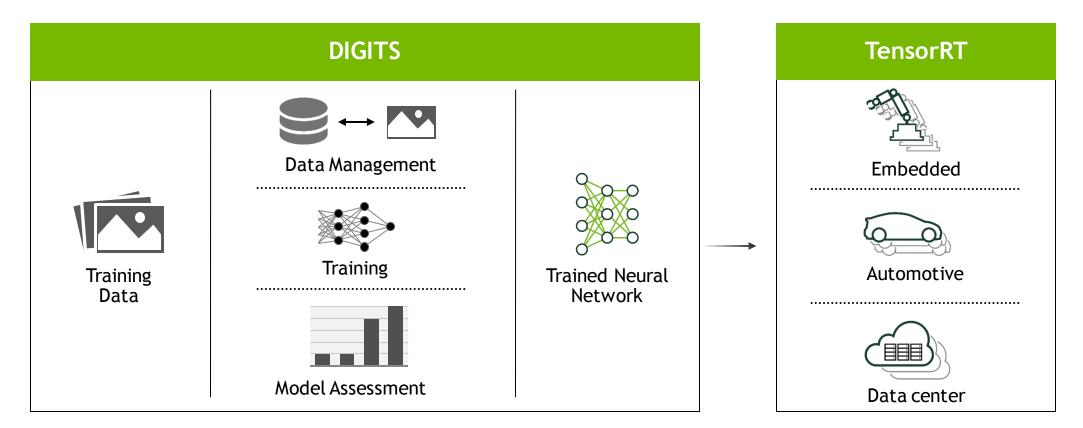
NVIDIA SDK accelerates every major framework





developer.nvidia.com/deep-learning-software

NVIDIA DEEP LEARNING SOFTWARE PLATFORM



NVIDIA DEEP LEARNING SDK

developer.nvidia.com/deep-learning-software

NVIDIA DIGITS

Interactive Deep Learning GPU Training System

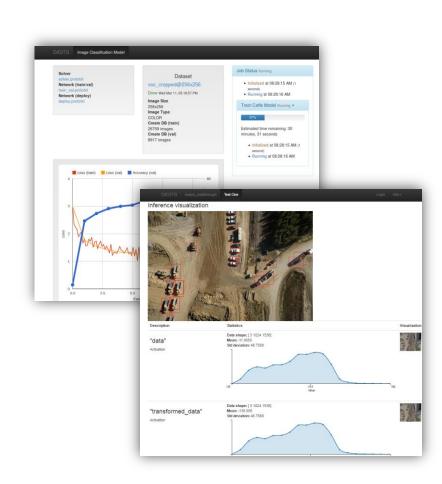
Interactive deep neural network development environment for image classification and object detection

Schedule, monitor, and manage neural network training jobs

Analyze accuracy and loss in real time

Track datasets, results, and trained neural networks

Scale training jobs across multiple GPUs automatically



NVIDIA cuDNN

Accelerating Deep Learning

High performance building blocks for deep learning frameworks

Drop-in acceleration for widely used deep learning frameworks such as Caffe, CNTK, Tensorflow, Theano, Torch and others

Accelerates industry vetted deep learning algorithms, such as convolutions, LSTM, fully connected, and pooling layers

Fast deep learning training performance tuned for NVIDIA GPUs

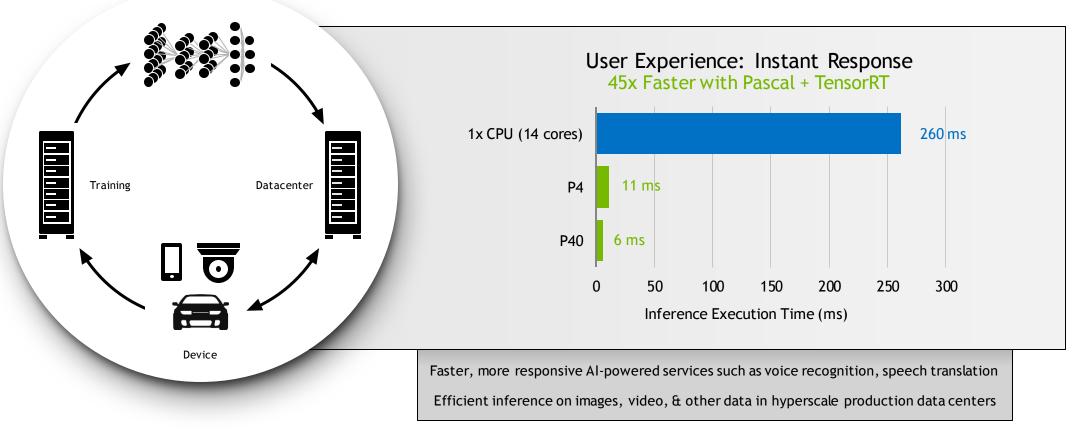
Deep Learning Training Performance Caffe AlexNet 80x Speed-up of Images/Sec vs K40 in 2013 70x 60x 50x 40x 30x 20x 10x 0x K80 + M40 + P100 + K40 cuDN... cuDNN5 cuDNN4

AlexNet training throughput on CPU: 1x E5-2680v3 12 Core 2.5GHz. 128GB System Memory, Ubuntu 14.04 M40 bar: 8x M40 GPUs in a node, P100: 8x P100 NVLink-enabled

"NVIDIA has improved the speed of cuDNN with each release while extending the interface to more operations and devices at the same time."

INTRODUCING NVIDIA TensorRT

High Performance Inference Engine



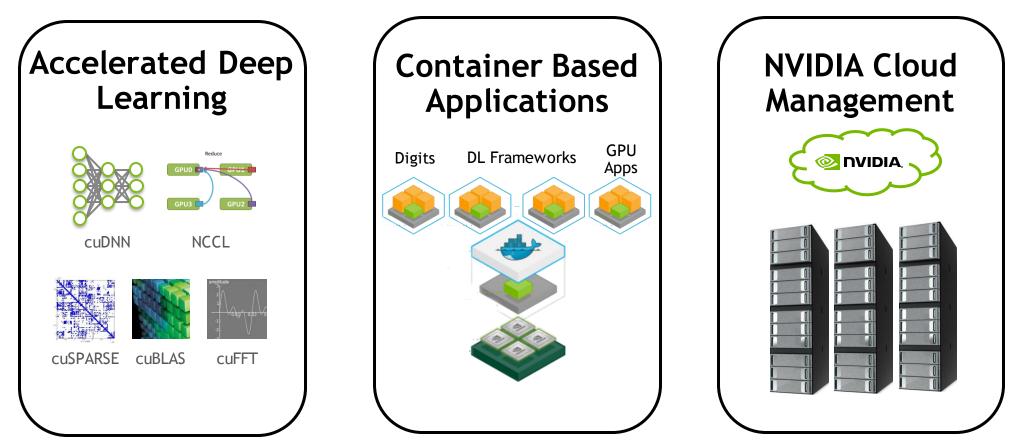
NVIDIA DGX-1 WORLD'S FIRST DEEP LEARNING SUPERCOMPUTER



170 TFLOPS 8x Tesla P100 16GB NVLink Hybrid Cube Mesh Optimized Deep Learning Software Dual Xeon 7 TB SSD Deep Learning Cache Dual 10GbE, Quad IB 100Gb 3RU - 3200W

NVIDIA DGX-1 SOFTWARE STACK

Optimized for Deep Learning Performance

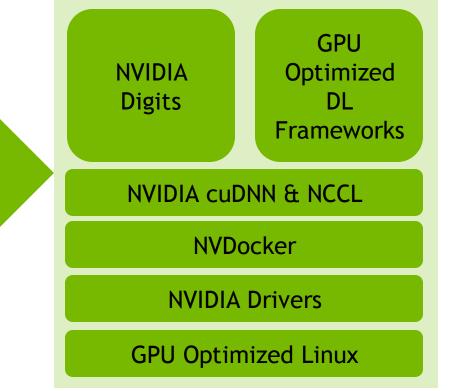


NVIDIA DGX-1 SOFTWARE STACK

Optimized for Deep Learning Performance

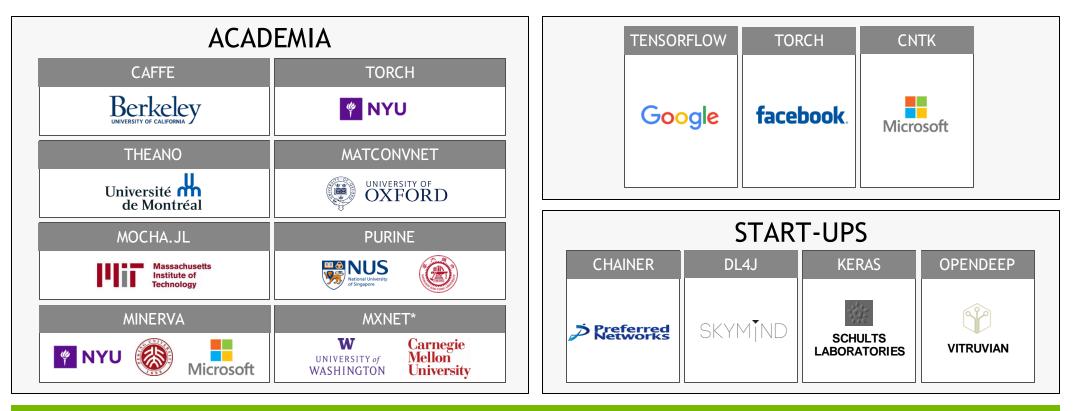


- Container creation & deployment
- Multi DGX-1 cluster manager
- Deep Learning job scheduler
- Application repository
- System telemetry & performance monitoring
- Software update system



NVIDIA DGX-1 76 SINUDIA

ACCELERATE EVERY FRAMEWORK

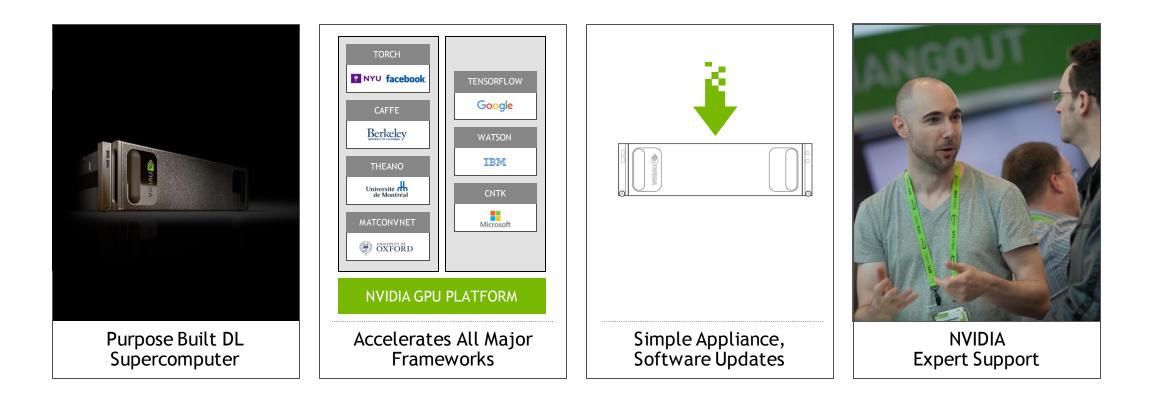


NVIDIA DGX-1

BENEFITS FOR AI RESEARCHERS



BENEFITS FOR INDUSTRY DATA SCIENTISTS



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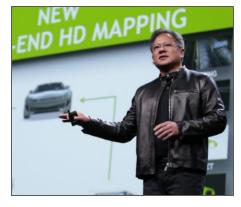
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