

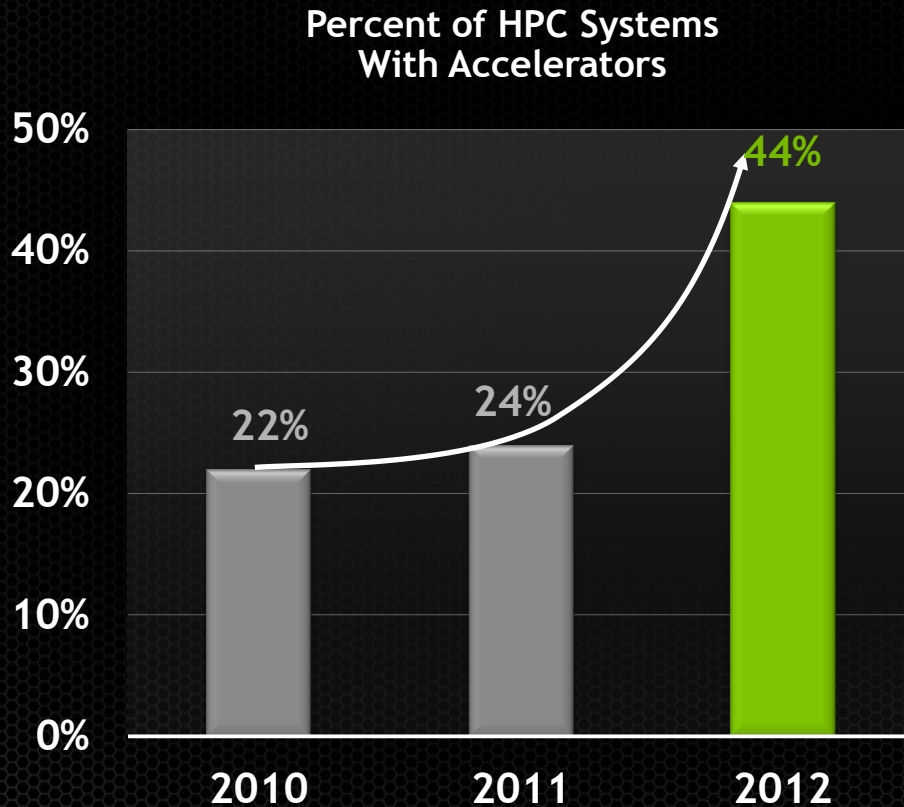


nVIDIA®

SUPERCOMPUTING
NOVEMBER 2013

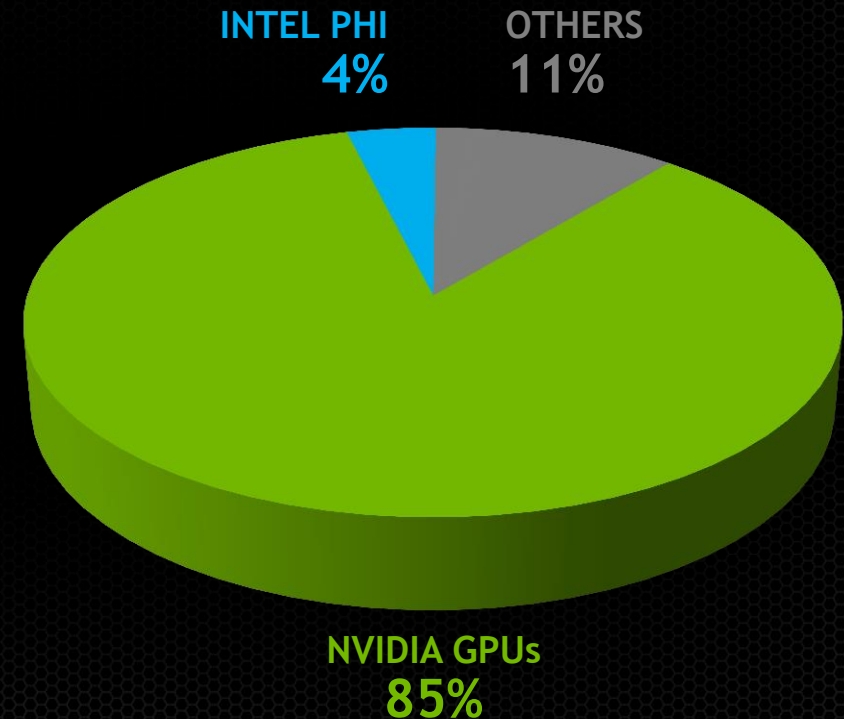
Accelerated Computing Growing Fast

2x Growth in One Year



Intersect360 Research
HPC User Site Census: Systems, July 2013

NVIDIA GPU is Accelerator of Choice



Intersect360 Research
HPC User Site Census: Systems, July 2013



POPULAR GPU-ACCELERATED APPLICATIONS

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Research: Higher Education and Supercomputing

COMPUTATIONAL CHEMISTRY AND BIOLOGY

Bioinformatics

Application	Description	Supported Devices	Corrected Speed Up	Supported GPUs	Multi-GPU Support	Release Status
BarraCUDA	Sequence mapping software	Alignment of short sequencing reads	8-10x	T 2075, 2090, K10, K20, K20X	Yes	Available now Version 0.6.2
CUDASW++	Open source software for Smith-Waterman protein database searches on GPUs	Parallel search of Smith-Waterman database	10-50x	T 2075, 2090, K10, K20, K20X	Yes	Available now Version 2.0.8
CUSHAW	Parallelized short read aligner	Parallel, accurate long read aligner - gapped alignments for large genomes	10x	T 2075, 2090, K10, K20, K20X	Yes	Available now Version 1.0.40
GPU-BLAST	Local search with fast k-tuple heuristic	Protein alignment according to blastp, multi cpu threads	3-4x	T 2075, 2090, K10, K20, K20X	Single only	Available now Version 2.2.26
GPU-HMMER	Parallelized local and global search with profile Hidden Markov models	Parallel local and global search of Hidden Markov Models	40-100x	T 2075, 2090, K10, K20, K20X	Yes	Available now Version 2.3.2
mCUDA-MEME	Ultrafast scalable motif discovery algorithm based on MEME	Scalable motif discovery algorithm based on MEME	4-10x	T 2075, 2090, K10, K20, K20X	Yes	Available now Version 3.0.13
SeqNFind	A GPU Accelerated Sequence Analysis Toolset	Reference assembly, blast, smith-waterman, hmm, de novo assembly	40x	T 2075, 2090, K10, K20, K20X	Yes	Available now Version 3.0.13
UGENE	OpenSource Smith-Waterman for SSE/CUDA. Suffix array based repeats finder and dotplot	Fast short read alignment	10x	T 2075, 2090, K10, K20, K20X	Yes	Available now Version 3.0.13
WideLM	Fits numerous linear models to a fixed design and response	Parallel linear regression on multiple similarly-shaped models	10x	T 2075, 2090, K10, K20, K20X	Yes	Available now Version 3.0.13

Molecular Dynamics

Application	Description	Supported Devices
Abalone	Models molecular dynamics of biopolymers for simulations of proteins, DNA and ligands	Simulations (on 1060 GPU)
ACEMD	GPU simulation of molecular mechanics force fields, implicit and explicit solvent	Written for use on GPUs
AMBER	Suite of programs to simulate molecular dynamics on biomolecule	PMEMD: explicit and implicit solvent
DL-POLY	Simulate macromolecules, polymers, ionic systems, etc on a distributed memory parallel computer	Two-body forces, Link-cell pairs, Ewald SPME forces, Shake W
CHARMM	MD package to simulate molecular dynamics on biomolecule	Implicit (Sx), Explicit (2x) Solvent via OpenMM
GROMACS	Simulation of biochemical molecules with complicated bond interactions	Implicit (Sx), Explicit(2x) solvent
HOOMD-Blue	Particle dynamics package written grounds up for GPUs	Written for GPUs
LAMMPS	Classical molecular dynamics package	Lennard-Jones, Morse, Buckingham, CHARMM, Tabulated, Course grain SDK, Anisotropic Gay-Bern, RE-squared, "Hybrid" combinations
AMD	Designed for high-performance simulation of large molecular systems	100M atom capable
OpenMM	Library and application for molecular dynamics for HPC with GPUs	Implicit and explicit solvent, custom forces

242 GPU-Accelerated Applications

www.nvidia.com/appscatalog

of Apps

300

250

200

150

100

50

0

113

182

242

2011

2012

2013

IBM Using GPUs to Accelerate Enterprise & Data Analytics Applications

Application
Infrastructure



Business Intelligence



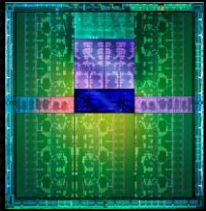
Predictive Analytics



Risk Analytics



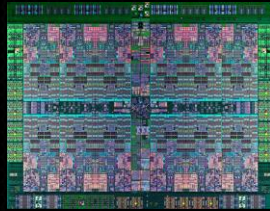
IBM Partners with NVIDIA to Build Next-Generation Supercomputers



Tesla
GPU



+



POWER 8
CPU



GPU-Accelerated POWER-Based Systems Available in 2014

Linux GCC Compiler to Support GPU Accelerators

Open Source

GCC Efforts by Samsung & Mentor Graphics

Pervasive Impact

Free to all Linux users

Mainstream

Most Widely Used HPC Compiler



“*Incorporating OpenACC into GCC is an excellent example of open source and open standards working together to make accelerated computing broadly accessible to all Linux developers.* **”**

Oscar Hernandez
Oak Ridge National Laboratories



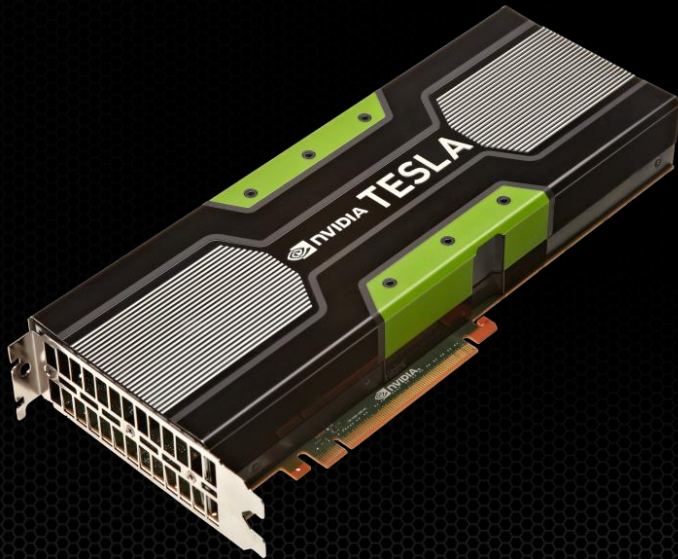
SC13

1 Growing Momentum of Accelerators

2 Product Announcements and Roadmap

3 New Supercomputing Announcements

ANNOUNCING Tesla K40 GPU Accelerator



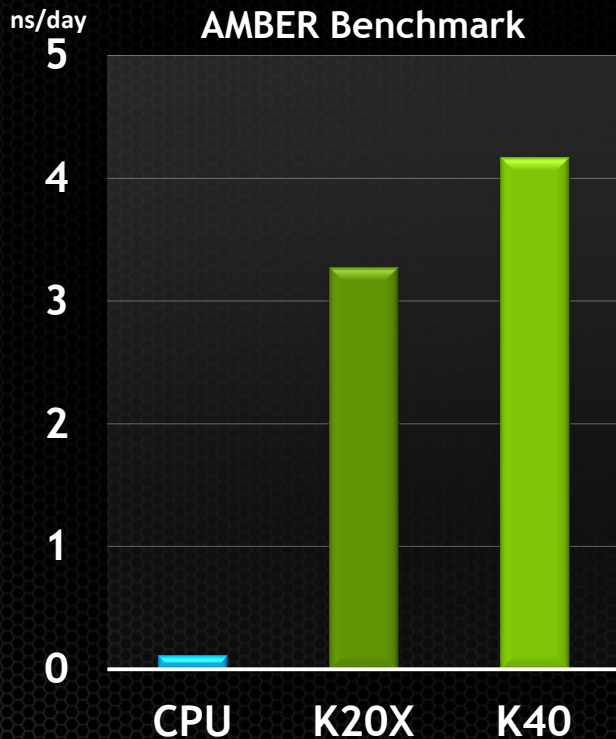
World's Fastest Accelerator for
Supercomputing and
Big Data Analytics

Tesla K40

World's Fastest Accelerator

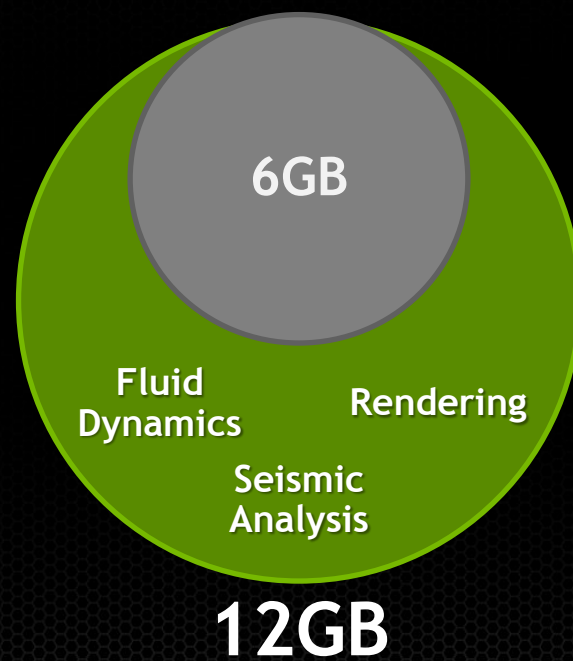
FASTER

1.4 TF | 2880 Cores | 288 GB/s



LARGER

2x Memory Enables More Apps



SMARTER

Unlock Extra Performance
Using Power Headroom



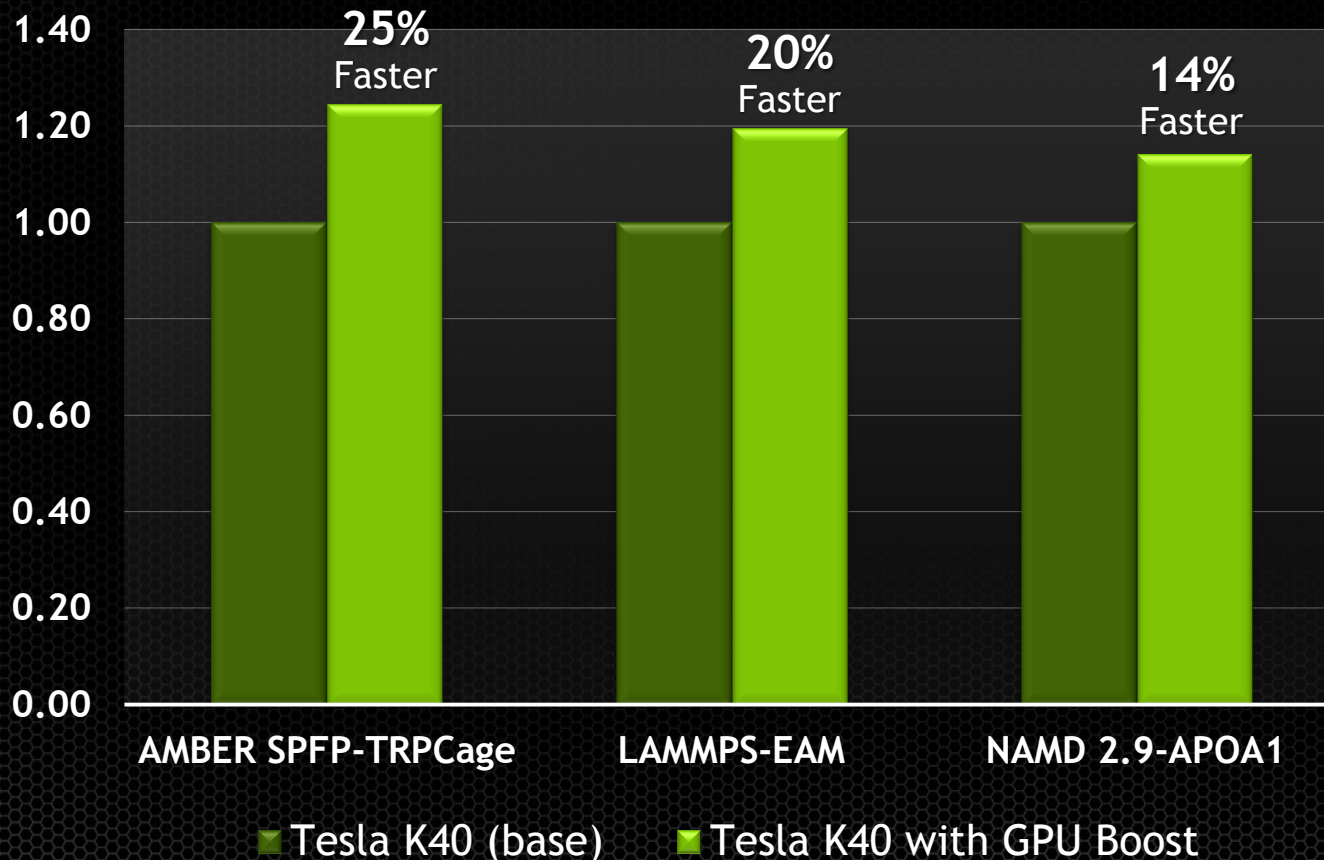
GPU Boost

AMBER Benchmark: SPFP-Nucleosome
CPU: Dual E5-2687W @ 3.10GHz, 64GB System Memory, CentOS 6.2, GPU systems: Single Tesla K20X or Single Tesla K40

GPU Boost

Up to 25% Extra Performance on Applications

Use Power Headroom to Run at Higher Clocks



 **Paradigm®** 17% Faster

 **OpenEye** 13% Faster

ANSYS® 11% Faster

Tesla K40

20-40% Faster than K20X

Structural Mechanics
ANSYS

Physics
CHROMA

Molecular Dynamics
AMBER

Material Science
QMCPACK

Earth Science
SPECFEM3D



0.0x

2.0x

4.0x

6.0x

8.0x

10.0x

12.0x

CUDA: World's Most Pervasive Parallel Programming Model

14,000

Institutions with CUDA Developers

2,000,000

CUDA Downloads

487,000,000

CUDA GPUs Shipped

700+ University Courses In 62 Countries



ANNOUNCING CUDA 6

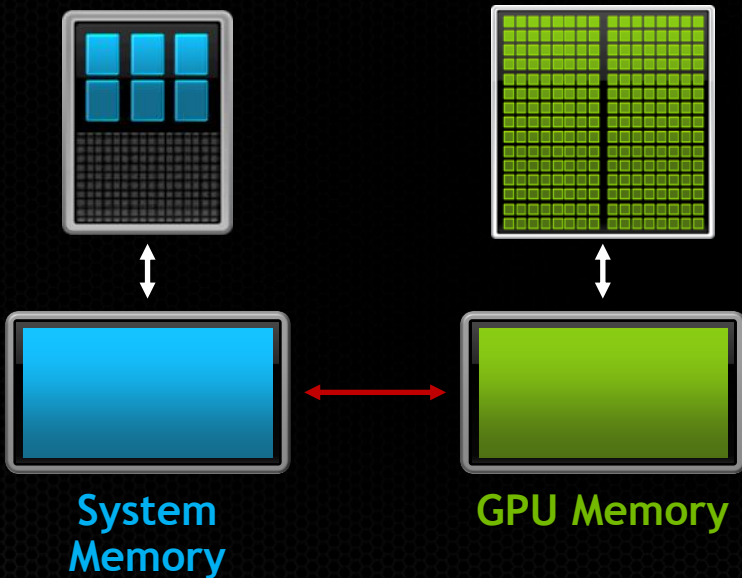


Dramatically Simplifies
Parallel Programming with
Unified Memory

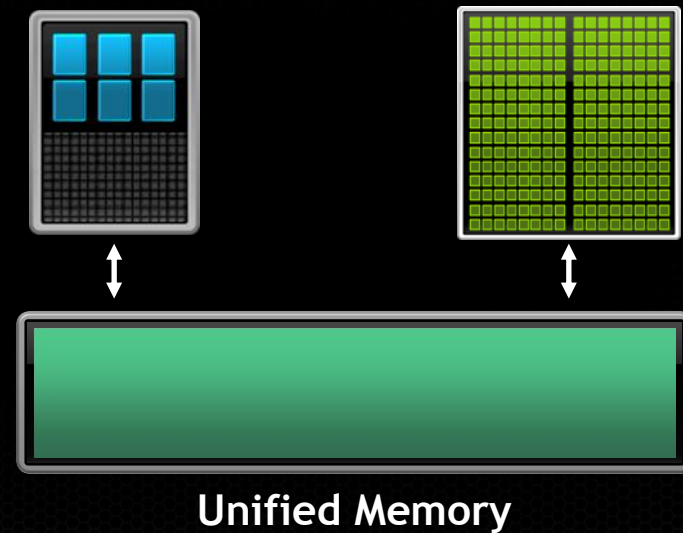
Unified Memory

Dramatically Lower Developer Effort

Developer View Today



Developer View With Unified Memory



Super Simplified Memory Management Code

CPU Code

```
void sortfile(FILE *fp, int N) {  
    char *data;  
    data = (char *)malloc(N);  
  
    fread(data, 1, N, fp);  
  
    qsort(data, N, 1, compare);  
  
    use_data(data);  
  
    free(data);  
}
```

CUDA 6 Code with Unified Memory

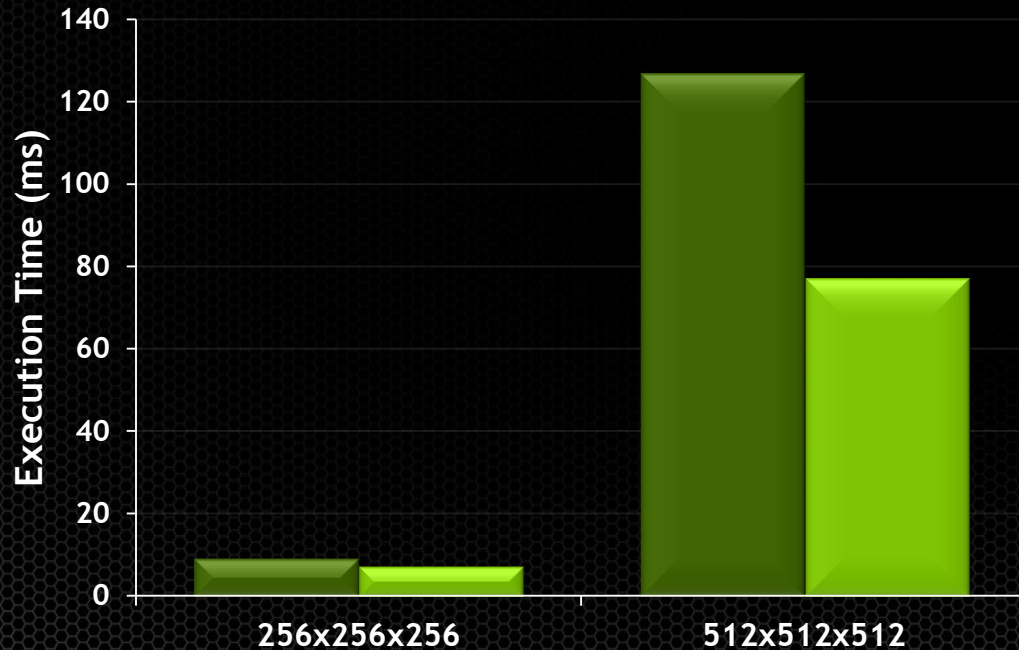
```
void sortfile(FILE *fp, int N) {  
    char *data;  
    cudaMallocManaged(&data, N);  
  
    fread(data, 1, N, fp);  
  
    qsort<<<...>>>(data, N, 1, compare);  
    cudaDeviceSynchronize();  
  
    use_data(data);  
  
    cudaFree(data);  
}
```


Popular Libraries Now Multi-GPU Enabled

cuFFT

3D Performance on 2 GPUs

■ K10: Single GPU ■ K10: Dual GPU



cuBLAS

ZGEMM Performance on 2 GPUS

— 1 K20c — 2 K20c



SC13

1 Growing Momentum of Accelerators

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Fastest Supercomputer In Europe

6.27 PetaFLOPS | 80% Linpack Efficiency

Piz Daint



Greenest Petascale System
3110 MFLOPS/W

#2: JUQUEEN: 2176 MFLOPS/W

Production-Grade
Weather Forecasts: COSMO

7 National Weather Agencies
Germany | Greece | Italy | Poland | Russia |
Romania | Switzerland

Greenest Supercomputer in the World

Tokyo Tech KFC System



4000+ MFLOPS per Watt

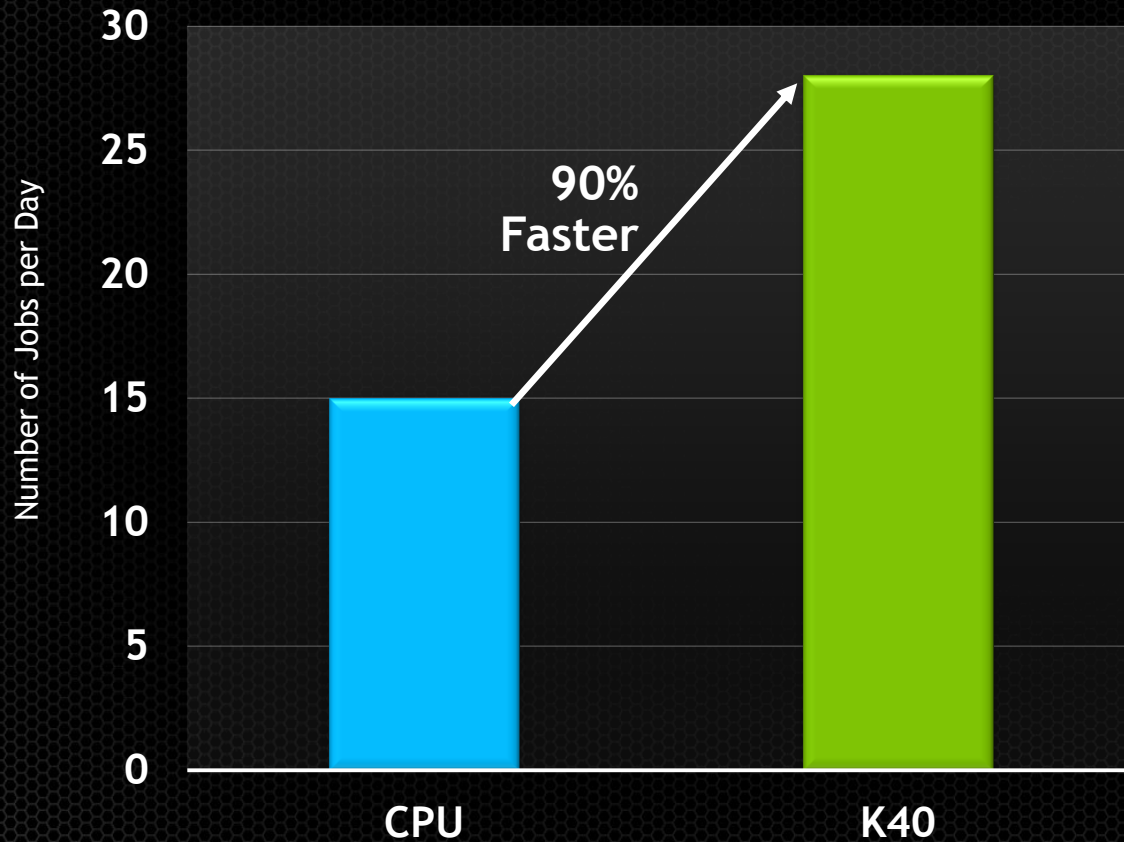
25% Higher than #1 Green500 System

160 Tesla K20X GPUs

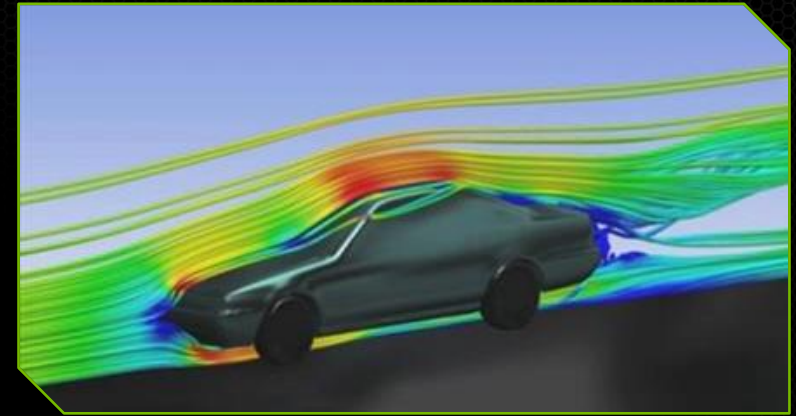
Oil Immersion Technology

ANSYS Fluent Doubles Performance with GPUs

Automobile Drag Simulation Throughput



2 x E5-2680 CPUs 8 cores used; 2 Tesla K40s
Sedan Geometry, 3.6M mixed cells
Steady, turbulent, external aerodynamics- Coupled PBNS, DP Solver



2x Better Insight for Low Drag Design

2% Less Drag

1.5B Gal. of Fuel Saved/Year