

*GPUs and the Future of Accelerated
Computing*
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University of Manchester

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Disclaimers



- **These are my views, not NVIDIA's (although I do hope you all will agree by the time I'm done!) , and where I've quoted others, any misrepresentation of their views is mine and mine alone.**
- **There are "forward looking statements" in here. You are warned that my crystal ball is no better than anyone else's, even if I'm speaking about things like NVIDIA roadmaps, etc. It's a lawyer thing.**
- **Trademarks of other firms are their own, etc.**

Agenda



- **Who is NVIDIA?**
- **Why should I care about accelerated computing?**
- **What sort of difference can CUDA make?**
- **Where is NVIDIA going?**

Who is NVIDIA?



NVIDIA products span the power-performance spectrum

GPUs Power World's 10 Greenest Supercomputers



Green500 Rank	MFLOPS/W	Site
1	4,503.17	GSIC Center, Tokyo Tech
2	3,631.86	Cambridge University
3	3,517.84	University of Tsukuba
4	3,185.91	Swiss National Supercomputing (CSCS)
5	3,130.95	ROMEO HPC Center
6	3,068.71	GSIC Center, Tokyo Tech
7	2,702.16	University of Arizona
8	2,629.10	Max-Planck
9	2,629.10	(Financial Institution)
10	2,358.69	CSIRO
37	1959.90	Intel Endeavor (top Xeon Phi cluster)
49	1247.57	Météo France (top CPU cluster)

GPUs are becoming...



100M

CUDA -Capable
GPUs



150K

CUDA Downloads



77

Supercomputing
Teraflops



60

University
Courses



4,000

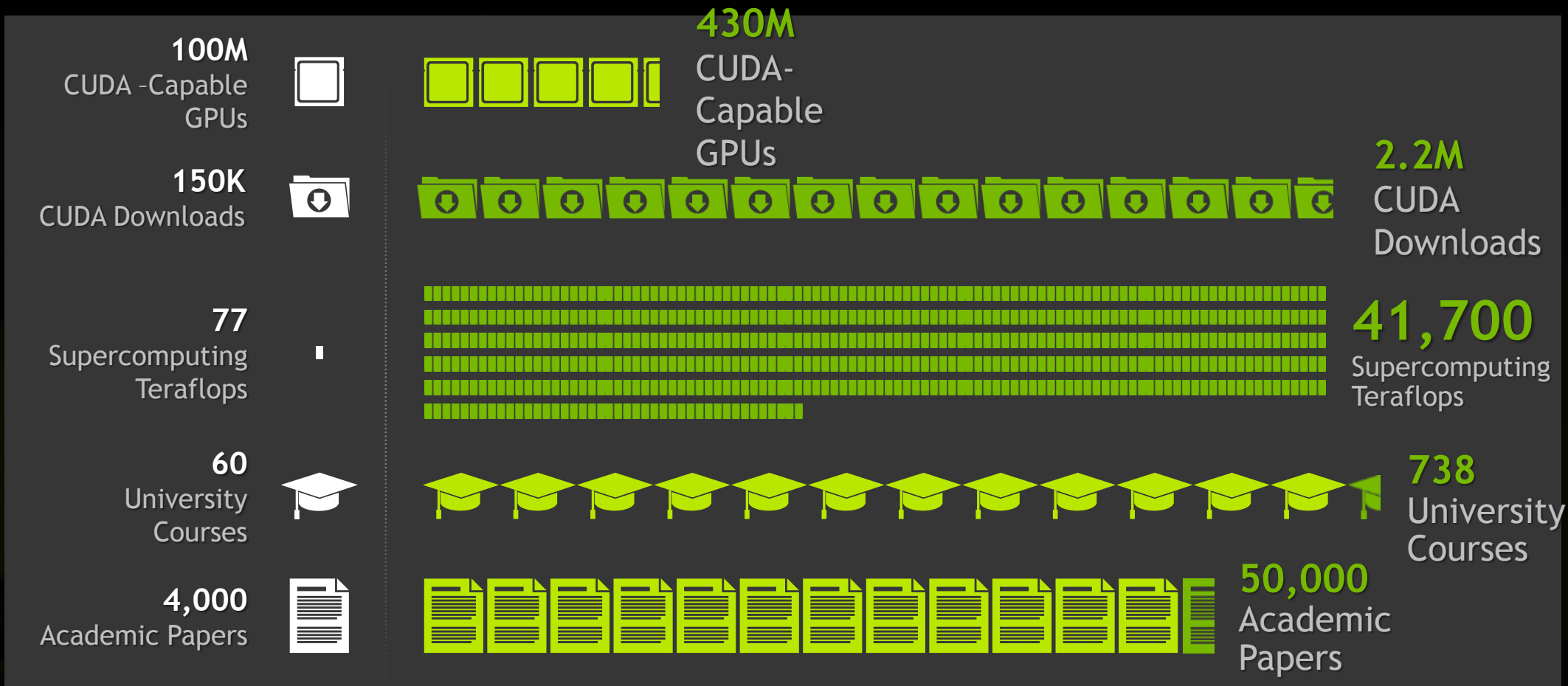
Academic Papers



2008

2014

GPUs are becoming...pervasive

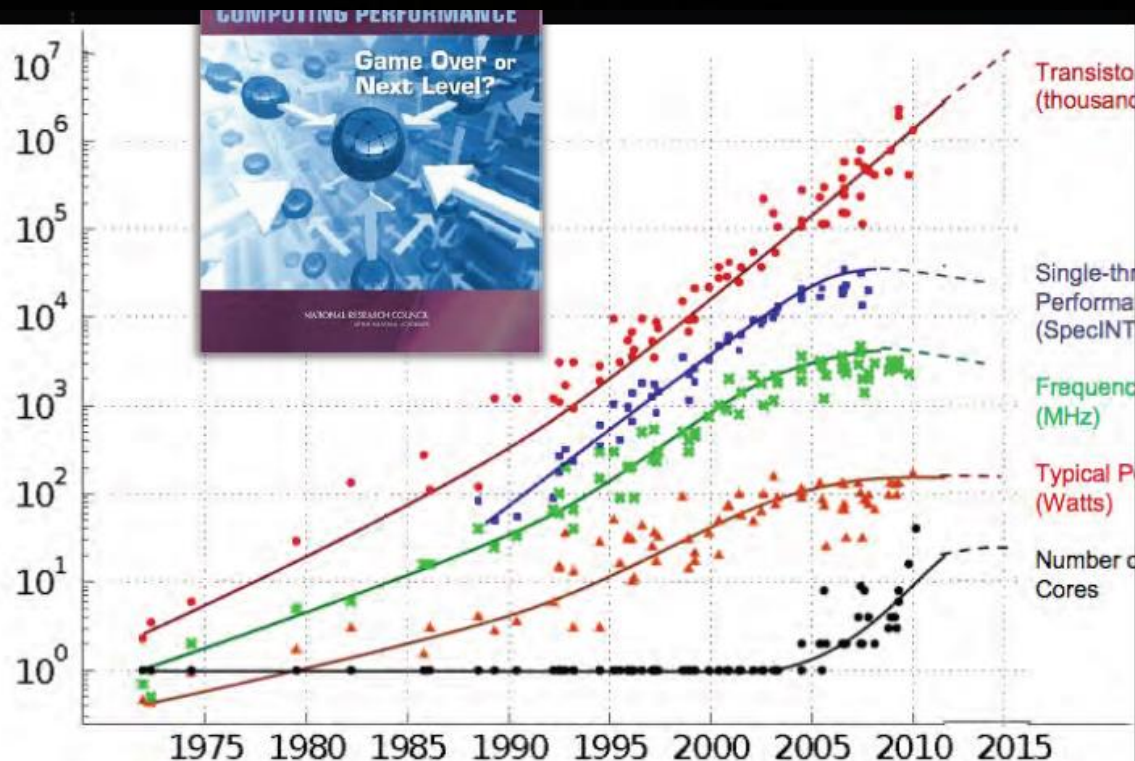


2008

2014

Why should I care about accelerated computing?

Moore's Law isn't what it used to be.



Original data collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond and C. Ball. Dotted line extrapolations by C. Moore

Moore's law is alive and well, but...

Instruction-level parallelism (ILP) was mined out in 2001

Voltage scaling (Dennard scaling) ended in 2005

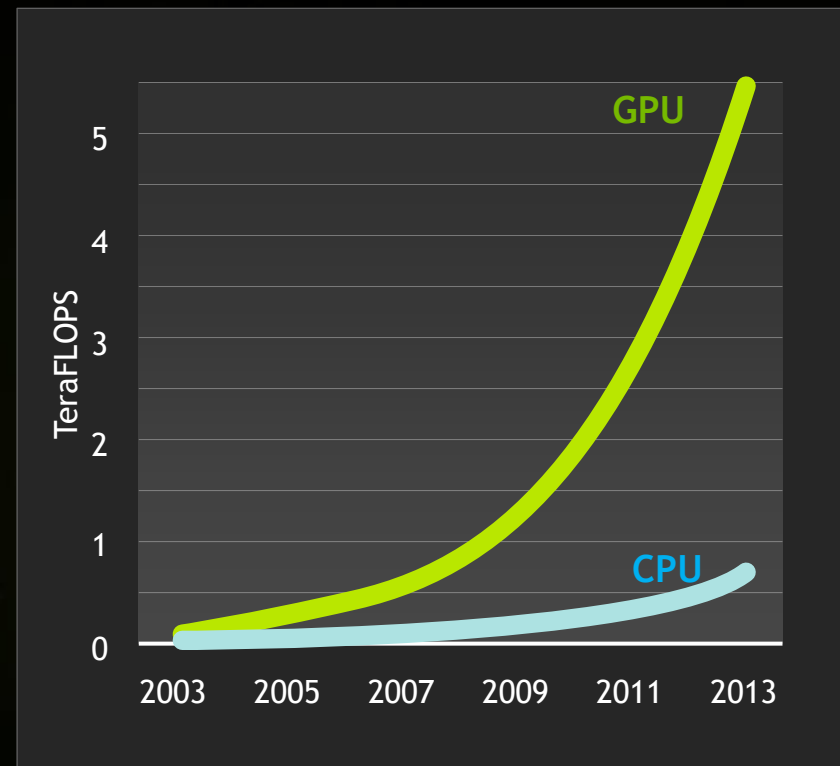
Most power is spent on communication

What does this mean to you?

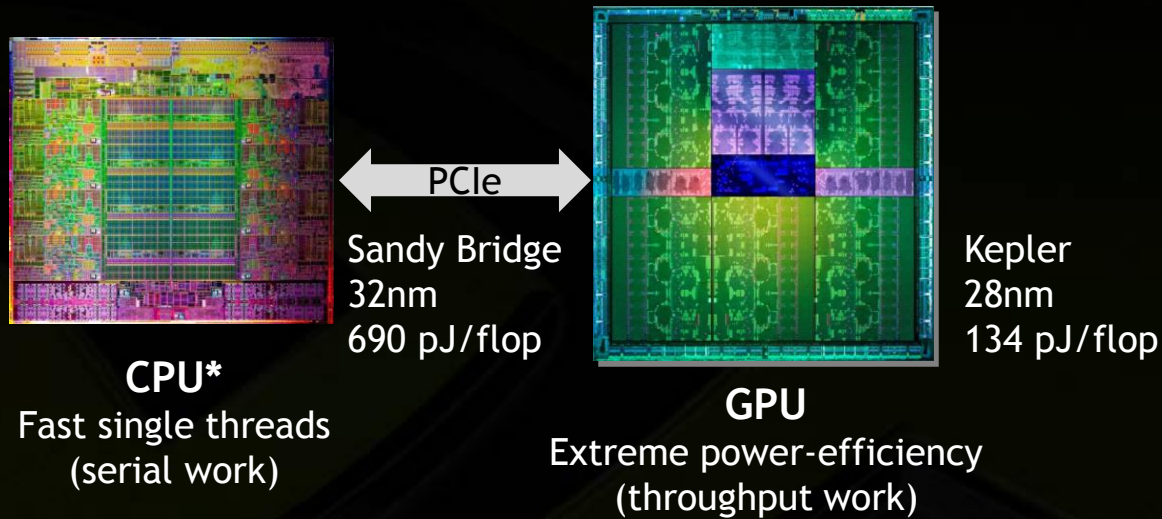
The future is here today ...



- Performance gains come from parallelism
- Systems are power limited (efficiency IS performance)
- Systems are communication limited (locality IS performance)



High Performance Computing is Going Hybrid



- Do most work by many cores optimized for **extreme energy efficiency**
- Still need a few cores optimized for **fast serial work**
- Amdahl's law continues to apply to all architectures

*x86, ARM, Power

What sort of difference can CUDA make?

CUDA Parallel Computing Platform

www.nvidia.com/getcuda



Programming
Approaches

Libraries

“Drop-in” Acceleration

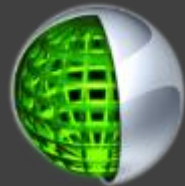
Directives

Easily Accelerate Apps

Programming
Languages

Maximum Flexibility

Development
Environment



Nsight IDE

Linux, Mac and Windows
GPU Debugging and Profiling

CUDA-GDB debugger
NVIDIA Visual Profiler

Open Compiler
Tool Chain



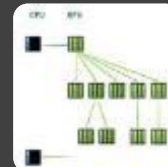
Enables compiling new languages to CUDA platform, and
CUDA languages to other architectures

Hardware
Capabilities

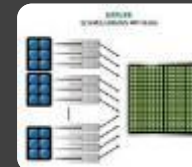
SMX



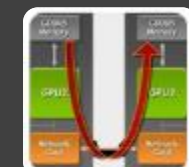
Dynamic Parallelism



HyperQ



GPUDirect




Artificial Neural Network at a Fraction of the Cost with GPUs

*“Now You Can Build Google’s
\$1M Artificial Brain on the Cheap”*

-Wired




GOOGLE BRAIN



1,000 CPU Servers
2,000 CPUs • 16,000 cores

600 kWatts
\$5,000,000

STANFORD AI LAB



3 GPU-Accelerated Servers
12 GPUs • 18,432 cores

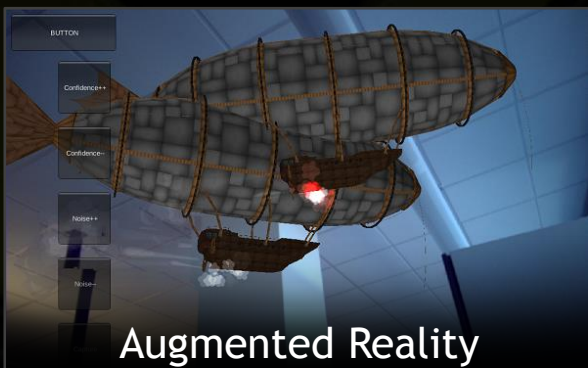
4 kWatts
\$33,000



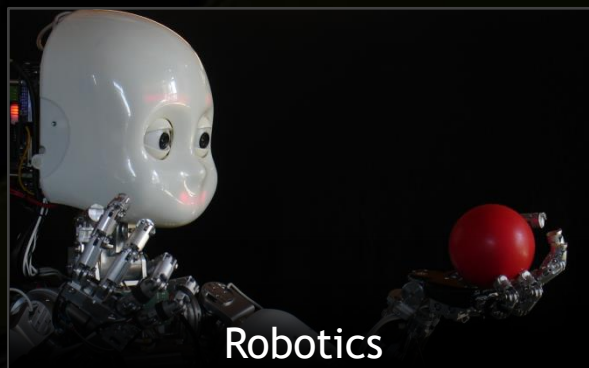
Driver Assistance



Computational Photography



Augmented Reality



Robotics

Your Code

Sample Pipelines

Object Detection /
Tracking

Structure from Motion ...

VisionWorks Primitives

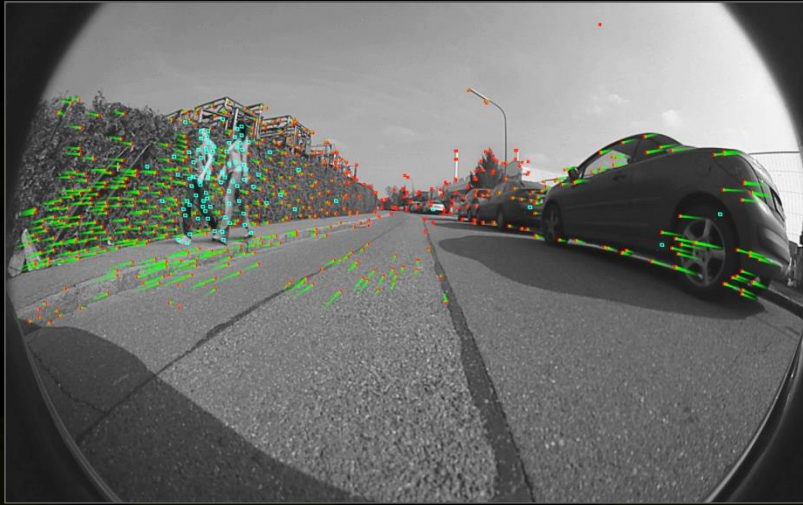
Classifier

Corner Detection ...

CUDA

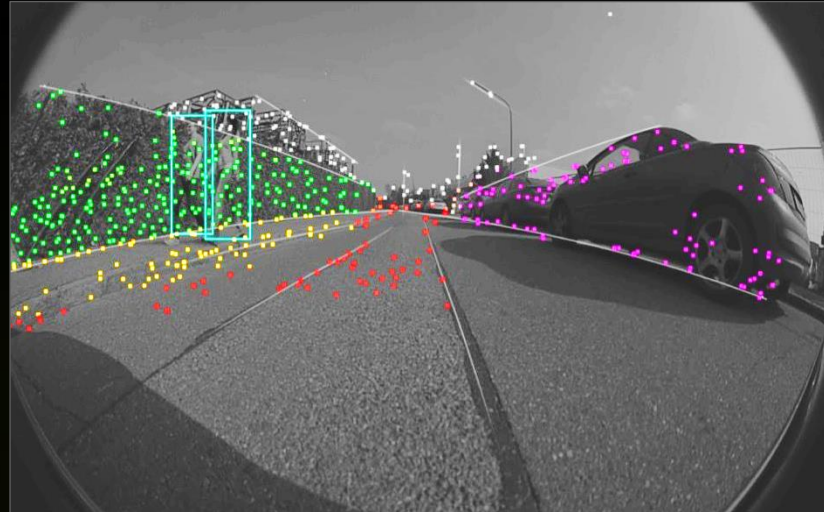
Jetson TK1

Computer Vision on CUDA



Feature Detection / Tracking

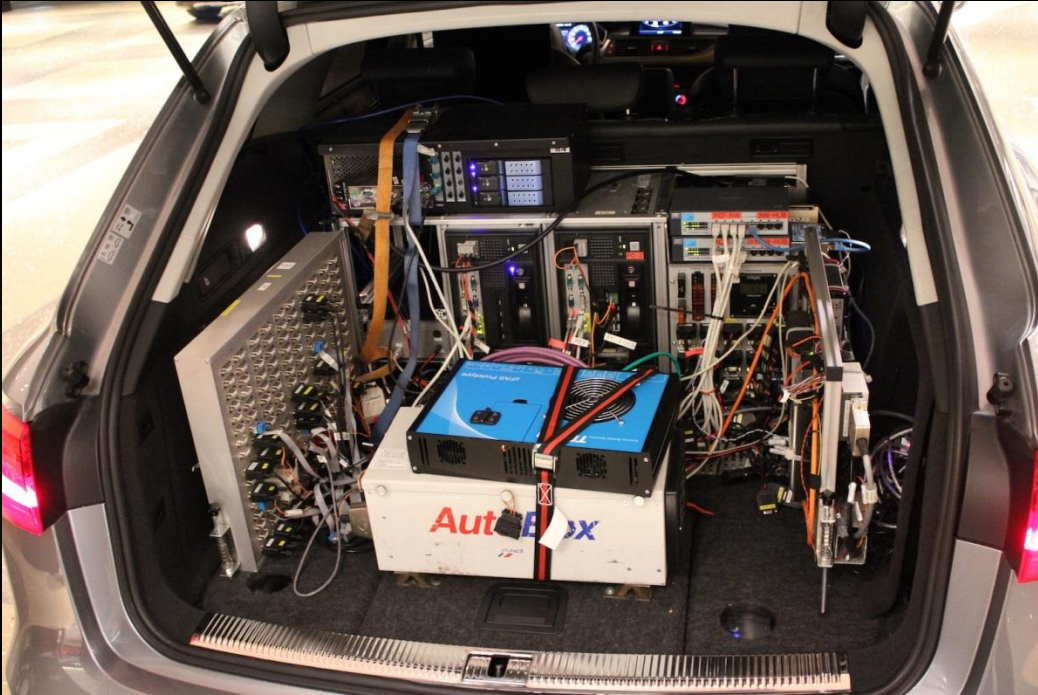
~30 GFLOPS @ 30 Hz



3D Scene Interpretation

~280 GFLOPS @ 30 Hz

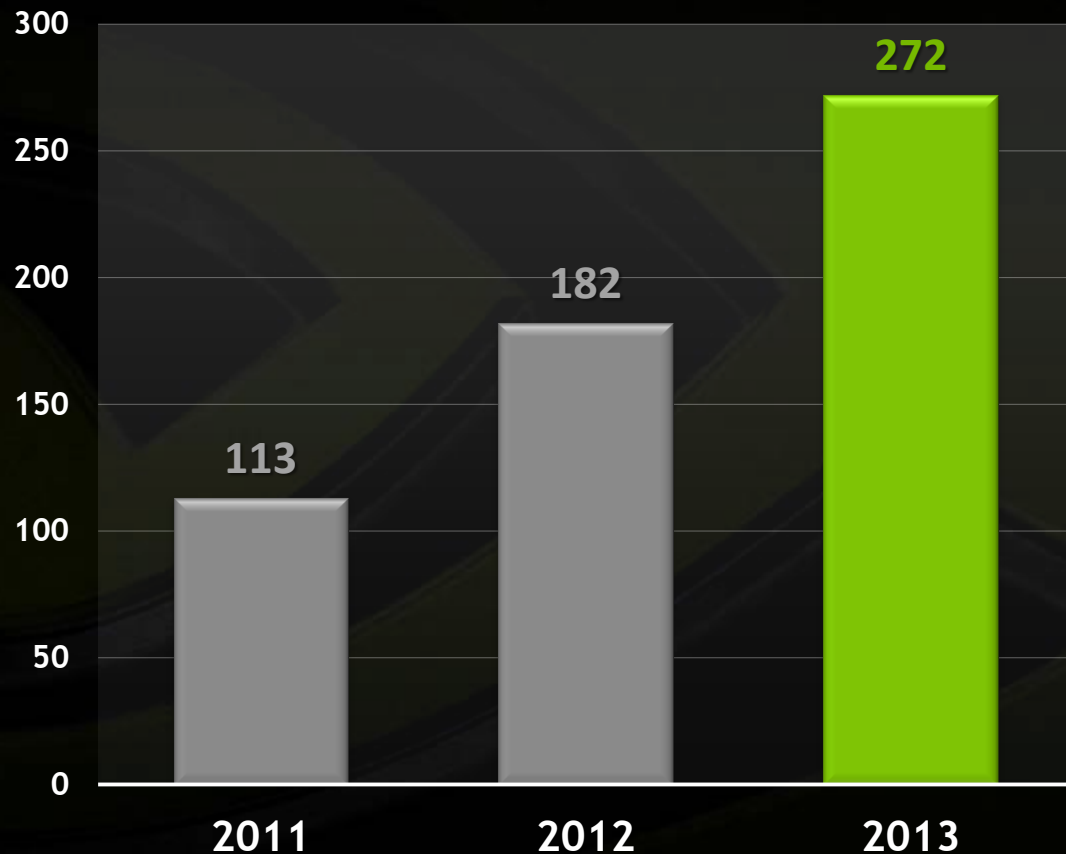
Audi Self Driving Car Before & After CUDA



Solid Growth of GPU Accelerated Apps



of GPU-Accelerated Apps



Top HPC Applications

Molecular Dynamics	AMBER	GROMACS
	CHARMM	LAMMPS
	DESMOND	NAMD
Quantum Chemistry	Abinit	GAMESS
	Gaussian	NWChem
Material Science	CP2K	Quantum Espresso
	QMCPACK	VASP
Weather & Climate	COSMO	CAM-SE
	GEOS-5	NEMO
	HOMME	NIM
		WRF
Lattice QCD	Chroma	MILC
Plasma Physics	GTC	GTS
Structural Mechanics	ANSYS Mechanical	OptiStruct
	LS-DYNA Implicit	Abaqus/Standard
	MSC Nastran	
Fluid Dynamics	ANSYS Fluent	Culises
		(OpenFOAM)



POPULAR GPU-ACCELERATED APPLICATIONS

- 02 Research: Higher Education and Supercomputing**
COMPUTATIONAL CHEMISTRY AND BIOLOGY
PHYSICS
WEATHER AND CLIMATE FORECASTING
- 06 Defense and Intelligence**
- 07 Computational Finance**
- 08 Manufacturing: CAD and CAE**
COMPUTER AIDED DESIGN
COMPUTATIONAL FLUID DYNAMICS
COMPUTATIONAL STRUCTURAL MECHANICS
ELECTRONIC DESIGN AUTOMATION
- 10 Media and Entertainment**
ANIMATION, MODELING AND RENDERING
COLOR CORRECTION AND GRAIN MANAGEMENT
COMPOSITING, FINISHING AND EFFECTS
EDITING
ENCODING AND DIGITAL DISTRIBUTION
ON-SET GRAPHICS
ON-SET, REVIEW AND STEREO TOOLS
SIMULATION
WEATHER SERVICES
- 14 Oil and Gas**

Research: Higher Education and Supercomputing COMPUTATIONAL CHEMISTRY AND BIOLOGY

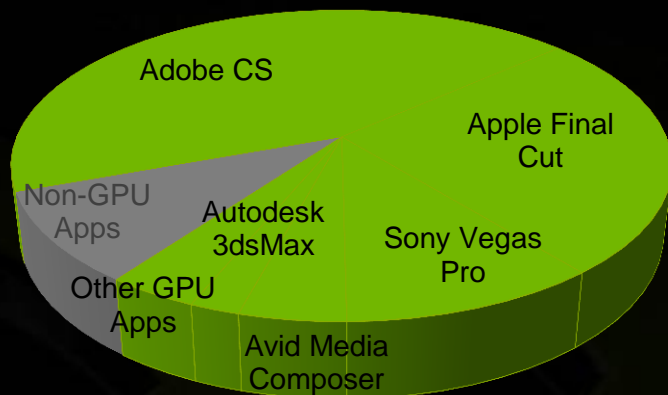
Bioinformatics						
Software	Description	Hardware/Platform	Performance	Architecture	GPU Support	Availability
BernaDBA	Sequence mapping software	alignment of short sequencing reads	4-18s	T.2075, 2090, K10, K20, K20X	Yes	Available now Version 5.4.2
CUSAM++	Open source software for Smith-Waterman protein database searches on GPUs	Parallel search of Smith-Waterman database	10-50s	T.2075, 2090, K10, K20, K20X	Yes	Available now Version 2.0.8
CUSHAM	Parallelized short read aligner	Parallel, accurate long read aligner - gapped alignments to large genomes	10s	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 BLAST, multi-cpu threads	3-4s	T.2075, 2090, K10, K20, K20X	Single only	Available now Version 2.2.34
GPU-HMMER	Parallelized local and global search with profile Hidden Markov models	Parallel local and global search of Hidden Markov Models	60-100s	T.2075, 2090, K10, K20, K20X	Yes	Available now Version 2.2.2
mDADA-MEME	Ultra-fast scalable motif discovery algorithm based on MEME	Scalable motif discovery algorithm based on MEME	4-11s	T.2075, 2090, K10, K20, K20X	Yes	Available now Version 3.0.12
SeqTied	A GPU Accelerated Sequence Analysis Toolkit	Reference assembly, GCAT, protein-expression, terms, de novo assembly	400s	T.2075, 2090, K10, K20, K20X	Yes	Available now
USEN	Open-source Smith-Waterman for SSE/CUDA, suffix array based repeats filter and output	Fast short read alignment	9-3s	T.2075, 2090, K10, K20, K20X	Yes	Available now Version 1.11
WishLM	Fits thousands linear models to a fixed design and response	Parallel linear regression on multiple similarly-shaped matrices	150s	T.2075, 2090, K10, K20, K20X	Yes	Available now Version 0.1-1
Molecular Dynamics						
Software	Description	Hardware/Platform	Performance	Architecture	GPU Support	Availability
Atolene	Models molecular dynamics of biopolymers for simulations of proteins, DNA and ligands	Simulations on 1000 GPUs	4-7hrs	T.2075, 2090, K10, K20, K20X	Single Only	Available now Version 1.0.40
ACEMD	GPU simulation of molecular mechanics force fields, implicit and explicit solvent	Written for use on GPUs	140 ns/day GPU version only	T.2075, 2090, K10, K20, K20X	Yes	Available now
AMBER	Suite of programs to simulate molecular dynamics on biomolecules	PHENIX: explicit and implicit solvent	89-44 ns/day JAC NVE	T.2075, 2090, K10, K20, K20X	Yes	Available now Version 12 + toulg8
DL-POLY	Simulate macromolecules, polymers, ions systems, etc on a distributed memory parallel computer	Two-body forces, Link-cell pairs, Ewald SPME, forces, SHAKE W	4s	T.2075, 2090, K10, K20, K20X	Yes	Available now Version 0.1 Tensor only
CHARMM	MD package to simulate molecular dynamics on biomolecules	Implicit Sol, Explicit Sol, Solvent via OpenMM	700s	T.2075, 2090, K10, K20, K20X	Yes	in Development 04/12
BRIMACS	Simulation of biomolecular molecules with complicated bond interactions	Implicit Sol, Explicit Sol, solvent	145 ns/day D4FR	T.2075, 2090, K10, K20, K20X	Single only	Available now Version 4.5 in 04/12
HOOMD-blue	Particle dynamics package written primarily for GPUs	Written for GPUs	3s	T.2075, 2090, K10, K20, K20X	Yes	Available now
LAMMPS	Classical molecular dynamics package	Lennard-Jones, Morse, Buckingham, CHARMM, Tabulated, Coarse grain, SW, Anisotropic Dipole, RE-squared, Hybrid combination	3-18s	T.2075, 2090, K10, K20, K20X	Yes	Available now
MD	Designed for high-performance simulation of large molecular systems	100M atom-capable	4-44 ns/day 570W 100s 3000s	T.2075, 2090, K10, K20, K20X	Yes	Available now Version 2.9
OpenMM	Library and application for molecular dynamics for xPC with GPUs	Implicit and explicit solvent, custom forces	Implicit: 127-213 ns/day Explicit: 16-10 ns/day D4FR	T.2075, 2090, K10, K20, K20X	Yes	Available now Version 4.1.1

272 GPU-Accelerated Applications
www.nvidia.com/appscatalog

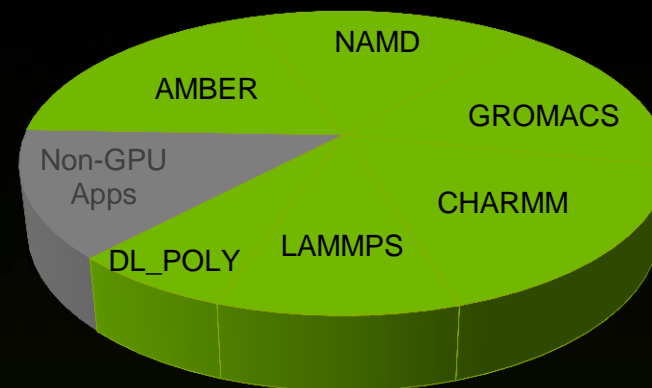
Top Applications Now with Built-in GPU Support



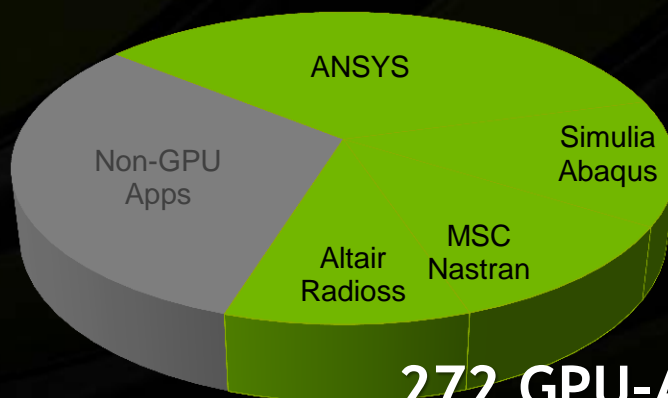
Digital Content Creation



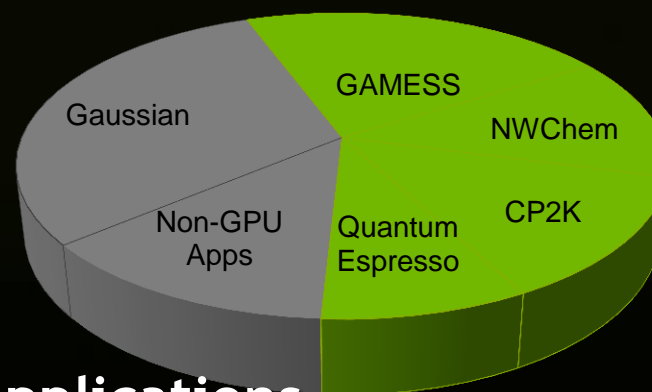
Molecular Dynamics



Computer-Aided Engineering



Quantum Chemistry

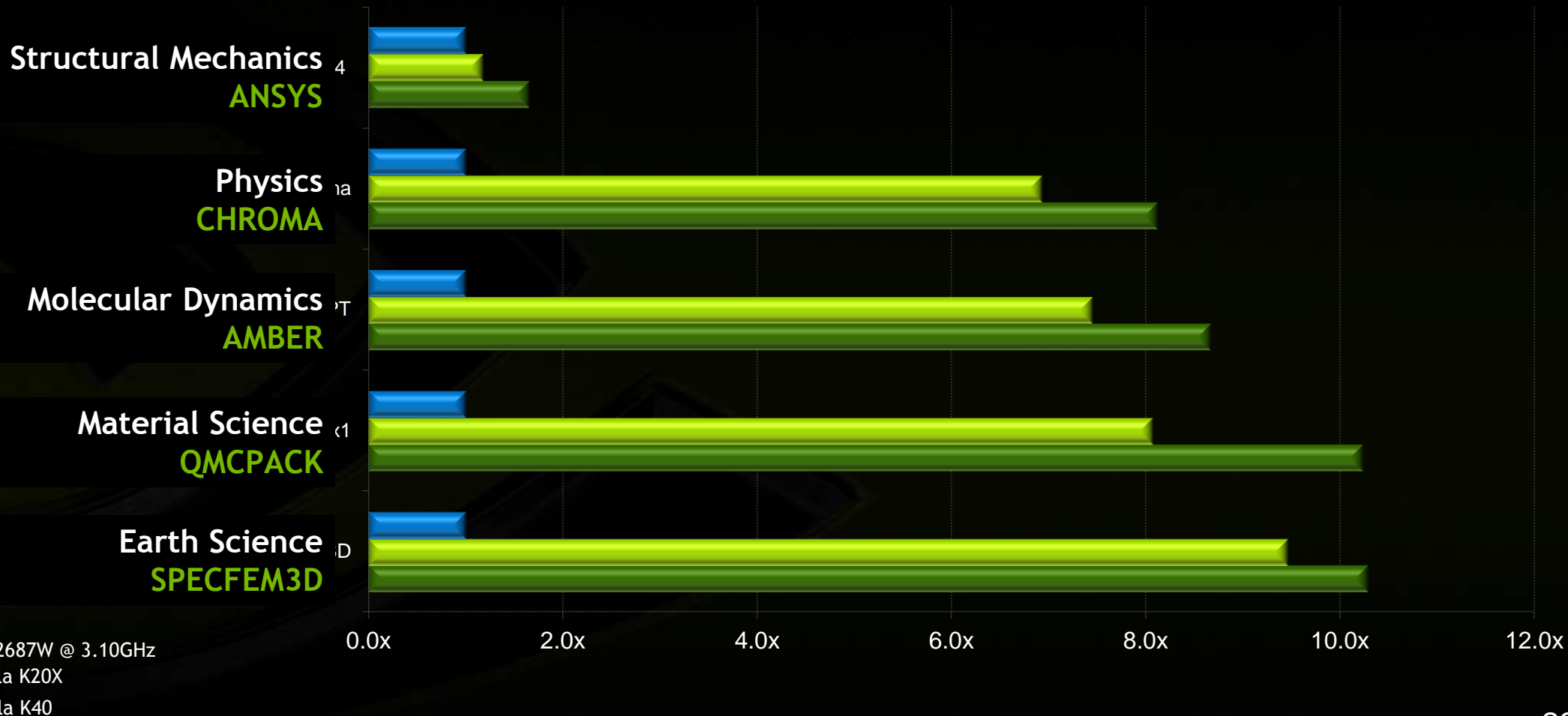


Application
Market Share
by Segment

272 GPU-Accelerated Applications

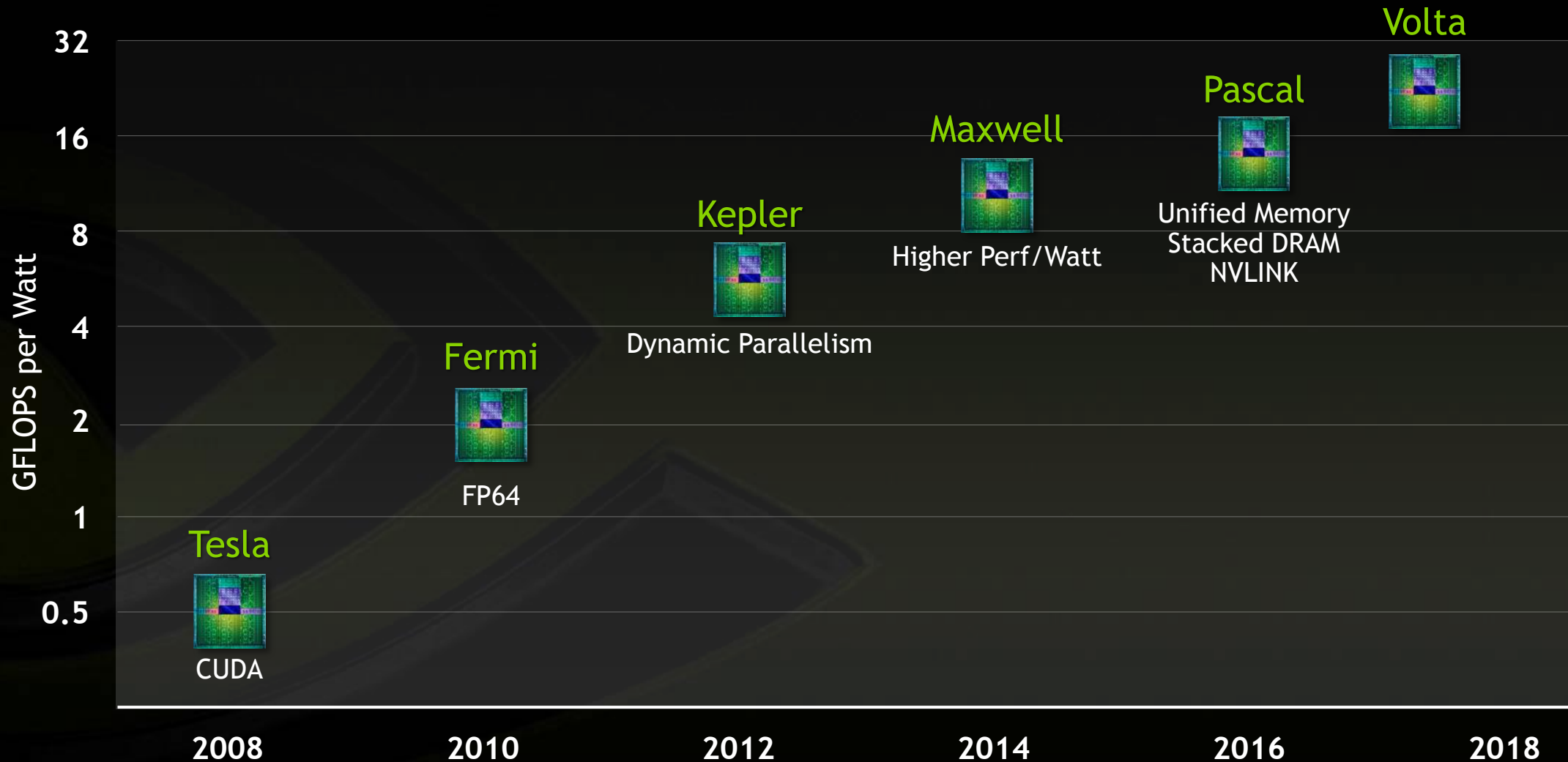
www.nvidia.com/appscatalog

Performance on Leading Scientific Applications



Where is NVIDIA going?

Fast Paced CUDA GPU Roadmap

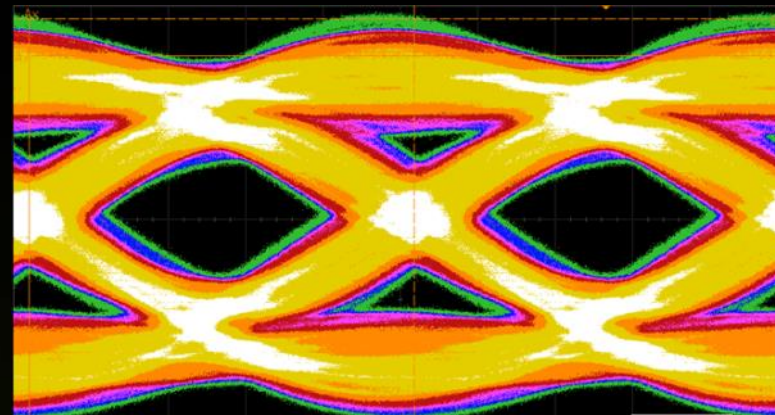


Introducing NVLINK and Stacked Memory



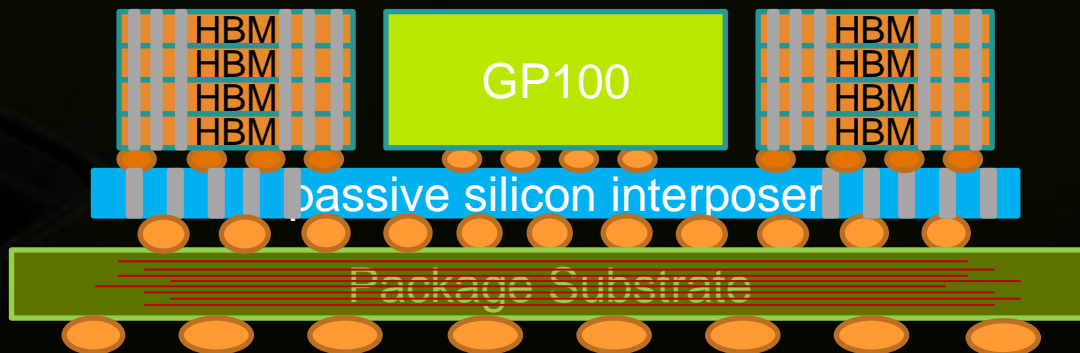
NVLINK

- GPU high speed interconnect
- 5-12x PCIe Gen 3 Bandwidth
- Drastically reduced energy/bit

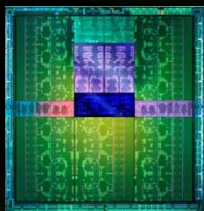


Stacked Memory

- 2-4x Capacity & Bandwidth
- 3-4x More Energy Efficient per bit
- Leaves more power for compute



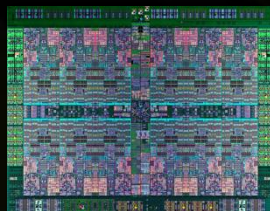
IBM Partners with NVIDIA to Build Next-Generation Supercomputers



Tesla
GPU



+

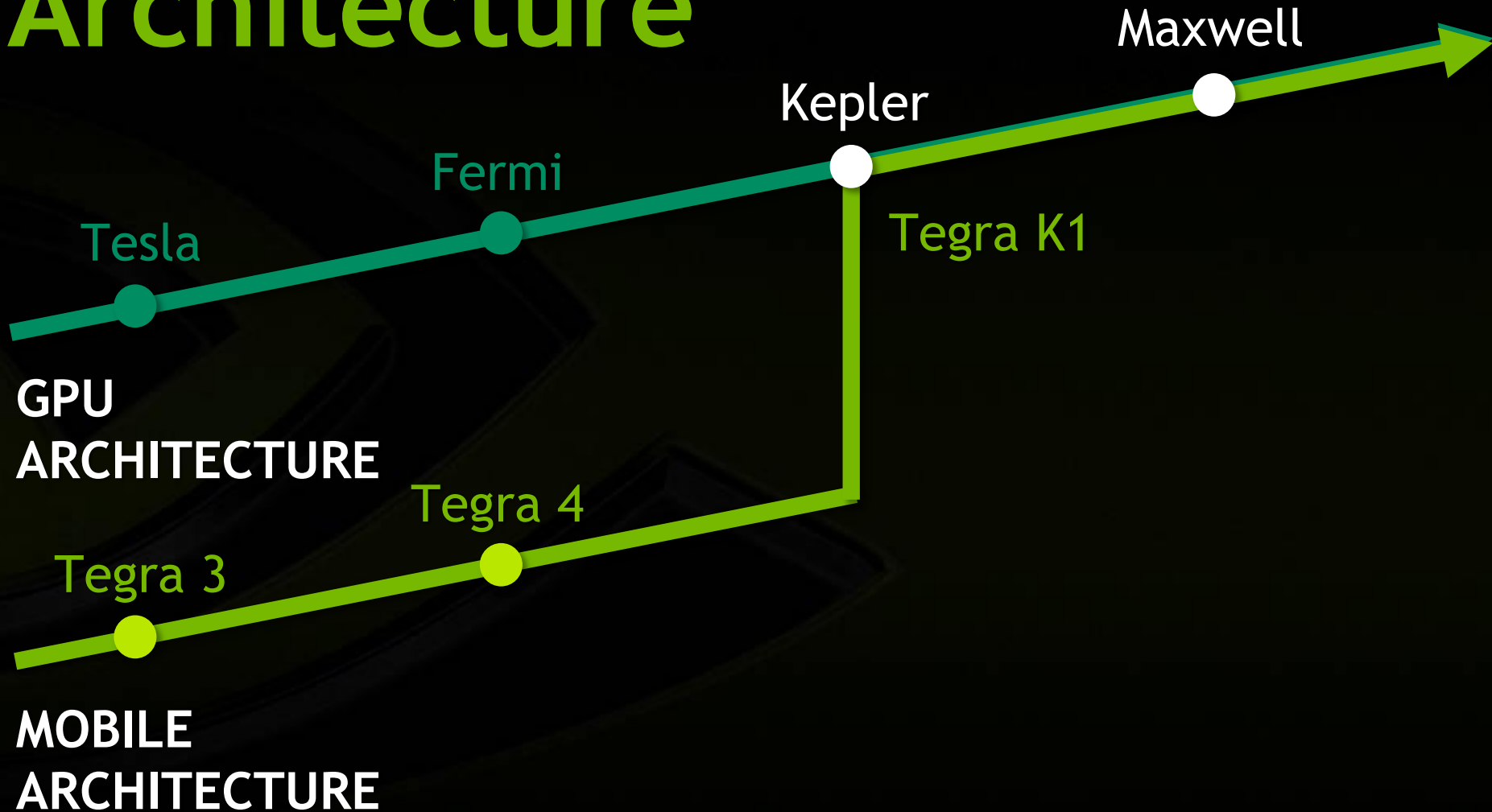


POWER 8
CPU



GPU-Accelerated POWER-Based Systems Available in 2014

Unify GPU and Tegra Architecture



Jetson TK1 Development Kit



- 32 Bit ARM+Kepler SMX SOC
- CUDA capable
- \$192 from US retailers, cost and availability will vary elsewhere
- <https://developer.nvidia.com/jetson-tk1>
- <http://devblogs.nvidia.com/parallelforall/jetson-tk1-mobile-embedded-supercomputer-cuda-everywhere/>



Summary



- **Who is NVIDIA?**

A: The world's leading Visual Computing company, from consumer devices through to world class supercomputers

- **Why should I care about accelerated computing?**

A: Because parallelism and heterogeneous computing is the future of big compute and big data

- **What sort of difference can CUDA make?**

A: Order of magnitude improvements in performance and efficiency are possible with CUDA

- **Where is NVIDIA going?**

A: Relentlessly forward to a CUDA enabled parallel & energy efficient computing future

Questions ?