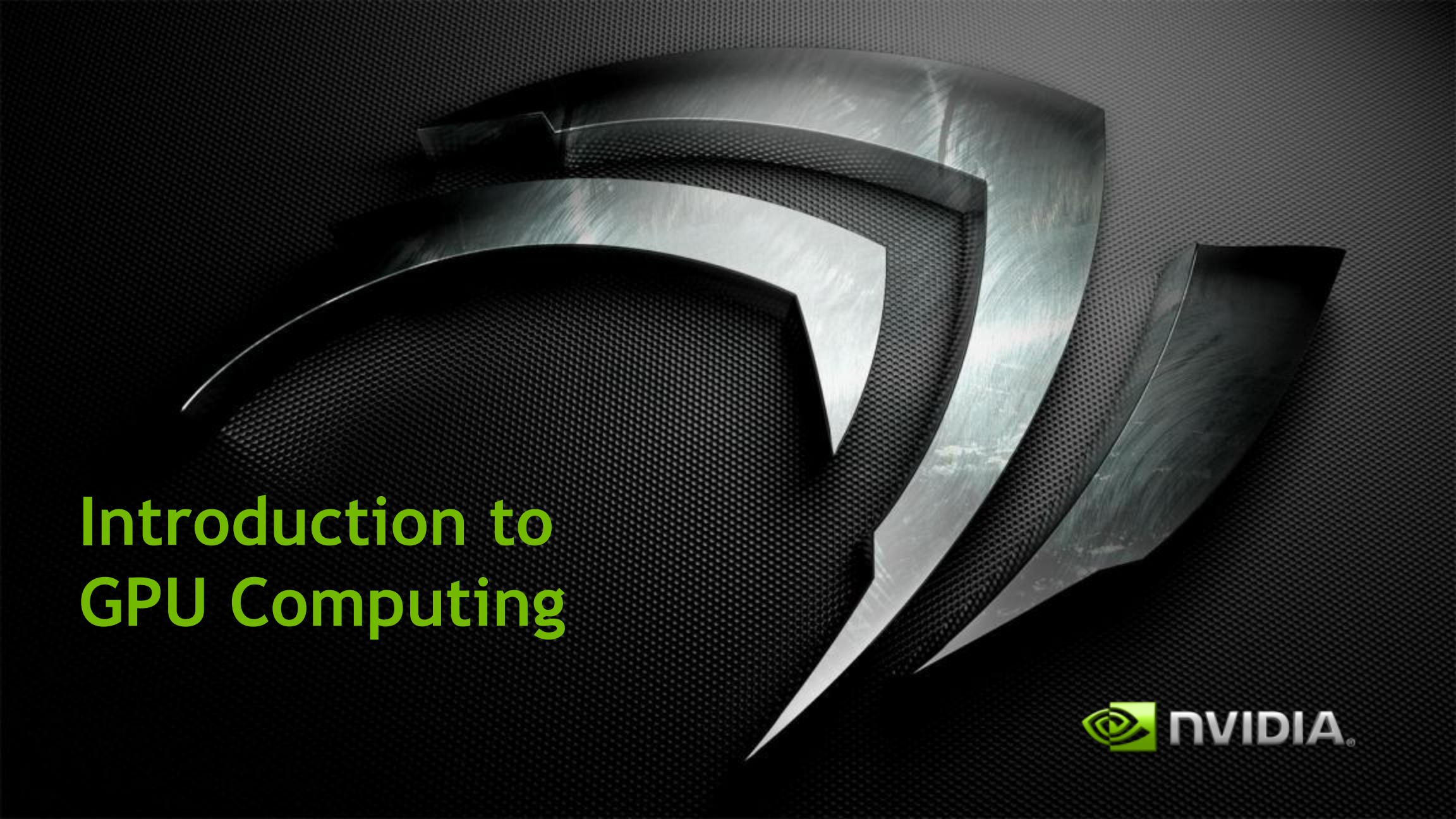
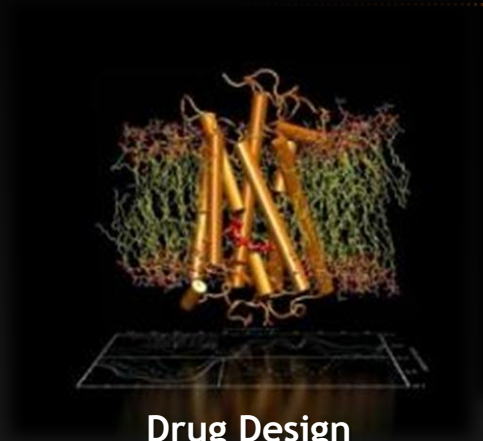
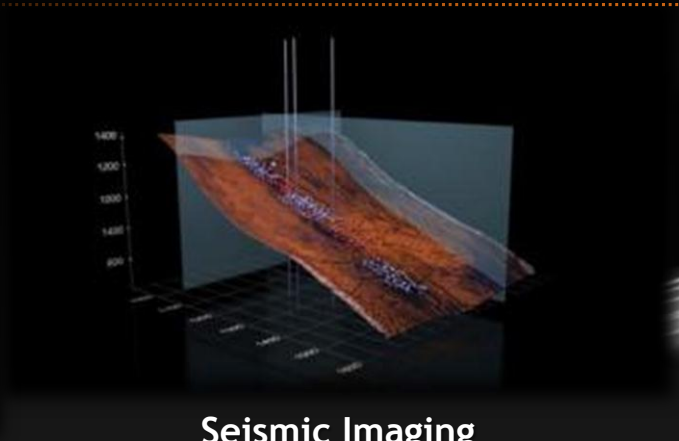

Introduction to
GPU Computing
NVIDIA

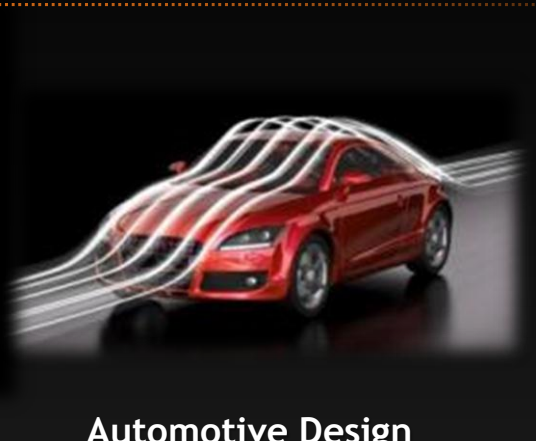
Computing is Integral to Science



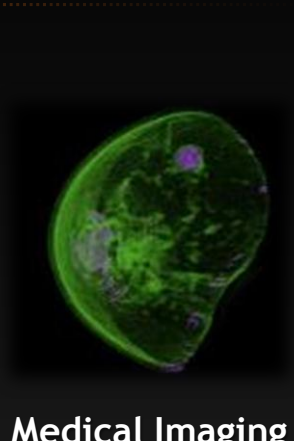
Drug Design
Molecular Dynamics



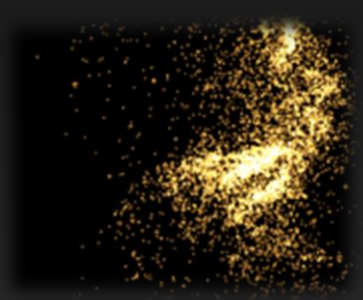
Seismic Imaging
Reverse Time Migration



Automotive Design
Computational Fluid Dynamics

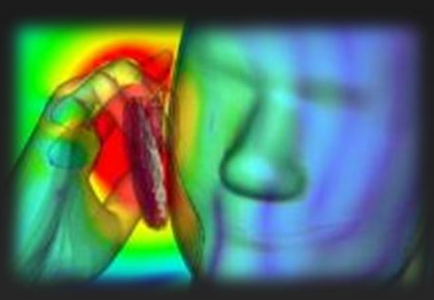


Medical Imaging
Computed Tomography

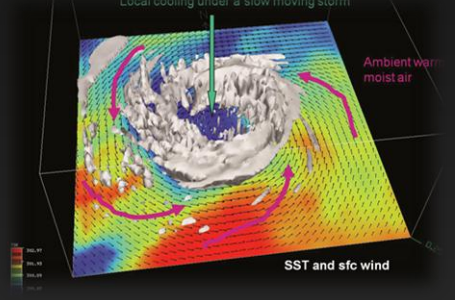


Astrophysics
n-body

Options Pricing
Monte Carlo



Product Development
Finite Difference Time Domain



Weather Forecasting
Atmospheric Physics

GPUs Accelerate Computing

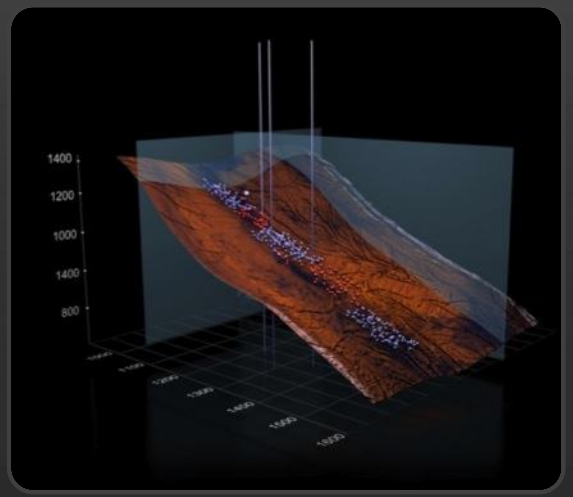
Understand Risk Faster than Competition

Calculate risk in minutes instead of overnight

JPMorgan

Discovering Oil with More Accuracy

From one to four jobs per month for deeper insight



Schlumberger

Understand Effects of Global Warming

From three months to one year of simulation per computing day

NCAR

If Computing is Integral to Science

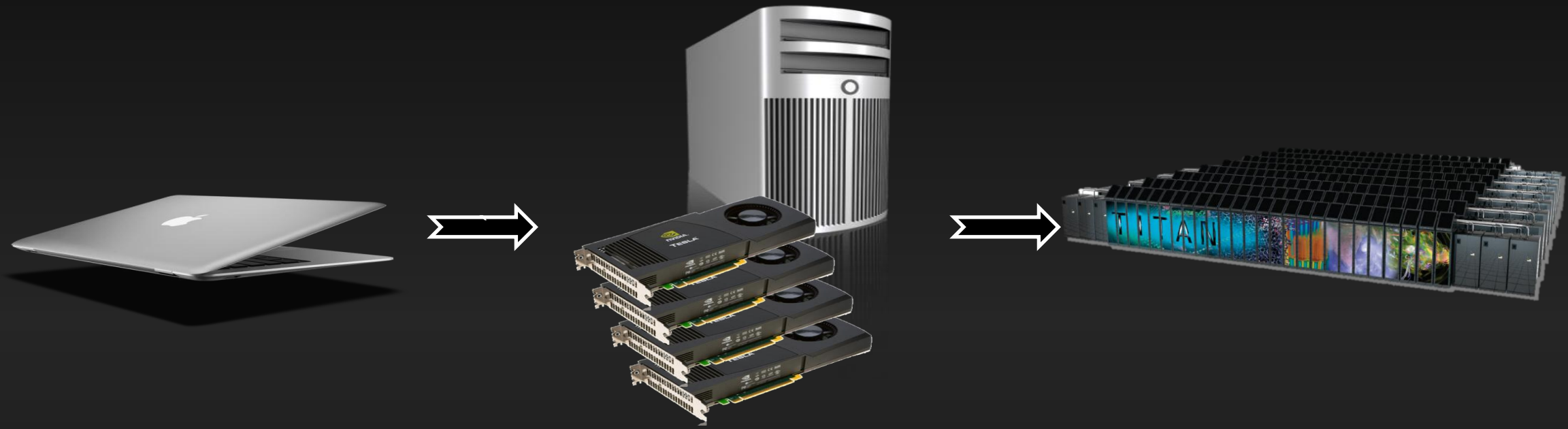
… And GPUs accelerate Computing.

… Then GPUs accelerate Science!

But GPUs are niche! WRONG!

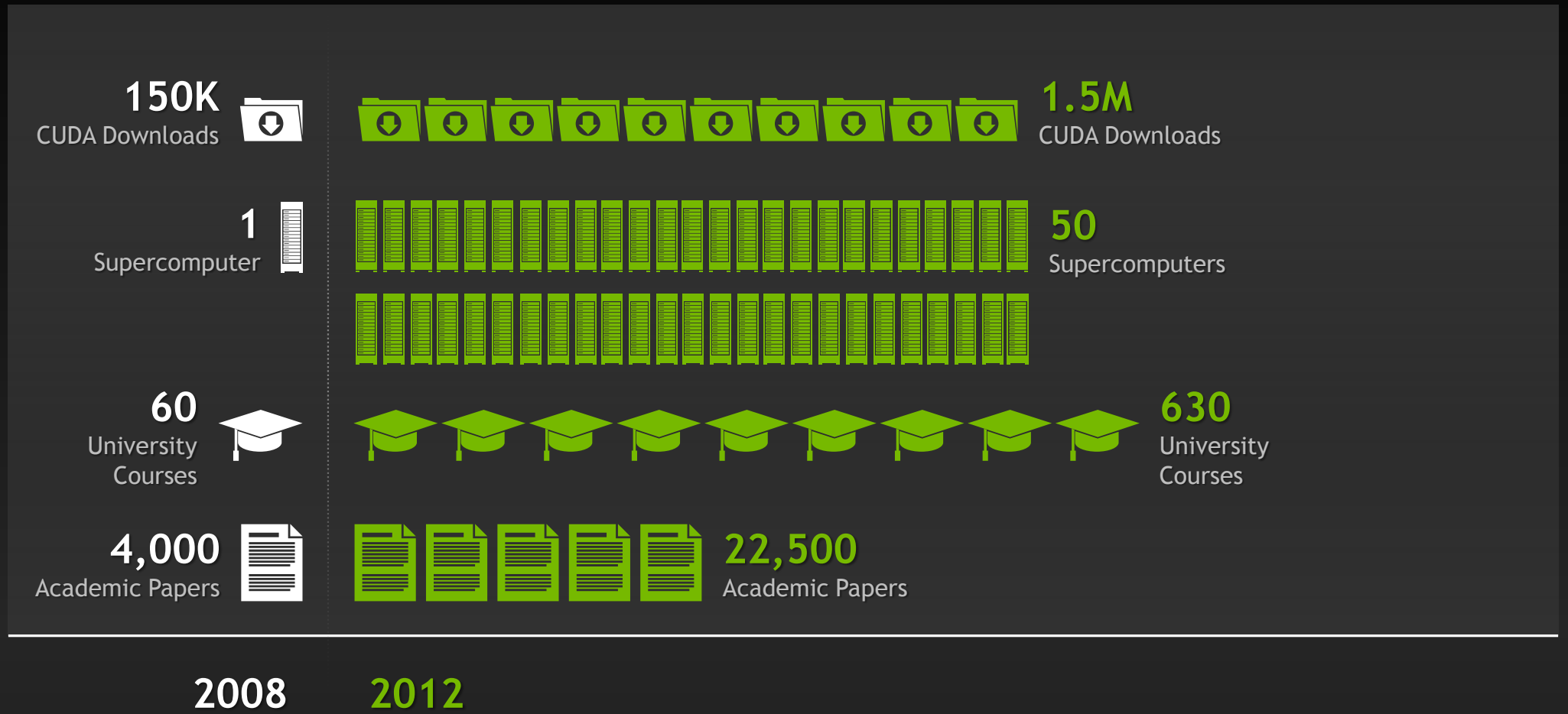
GPUs are Everywhere!

- Over 375,000,000 CUDA-capable GPUs have been shipped in products from laptops, to workstations, to supercomputers.



GPU-Computing is Taught Everywhere!

Explosive Growth of GPU Computing



GPUs are Mainstream

NVIDIA

Oil & Gas	Edu/Research	Government	Life Sciences	Finance	Manufacturing

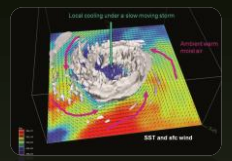
Schlumberger

BR PETROBRAS

TOTAL

Chevron

Paradigm



Chinese Academy of Sciences

Georgia Tech

HARVARD School of Engineering and Applied Sciences

OAK RIDGE National Laboratory

Air Force Research Laboratory

NASA

Naval Research Laboratory

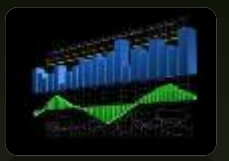
BAE SYSTEMS

Boston Scientific

MGH 1811 Mass General Hospital

Max Planck Institute

BECKMAN COULTER



Bloomberg

BNP PARIBAS

STANDARD LIFE

J.P.Morgan

NumeriX

Agilent

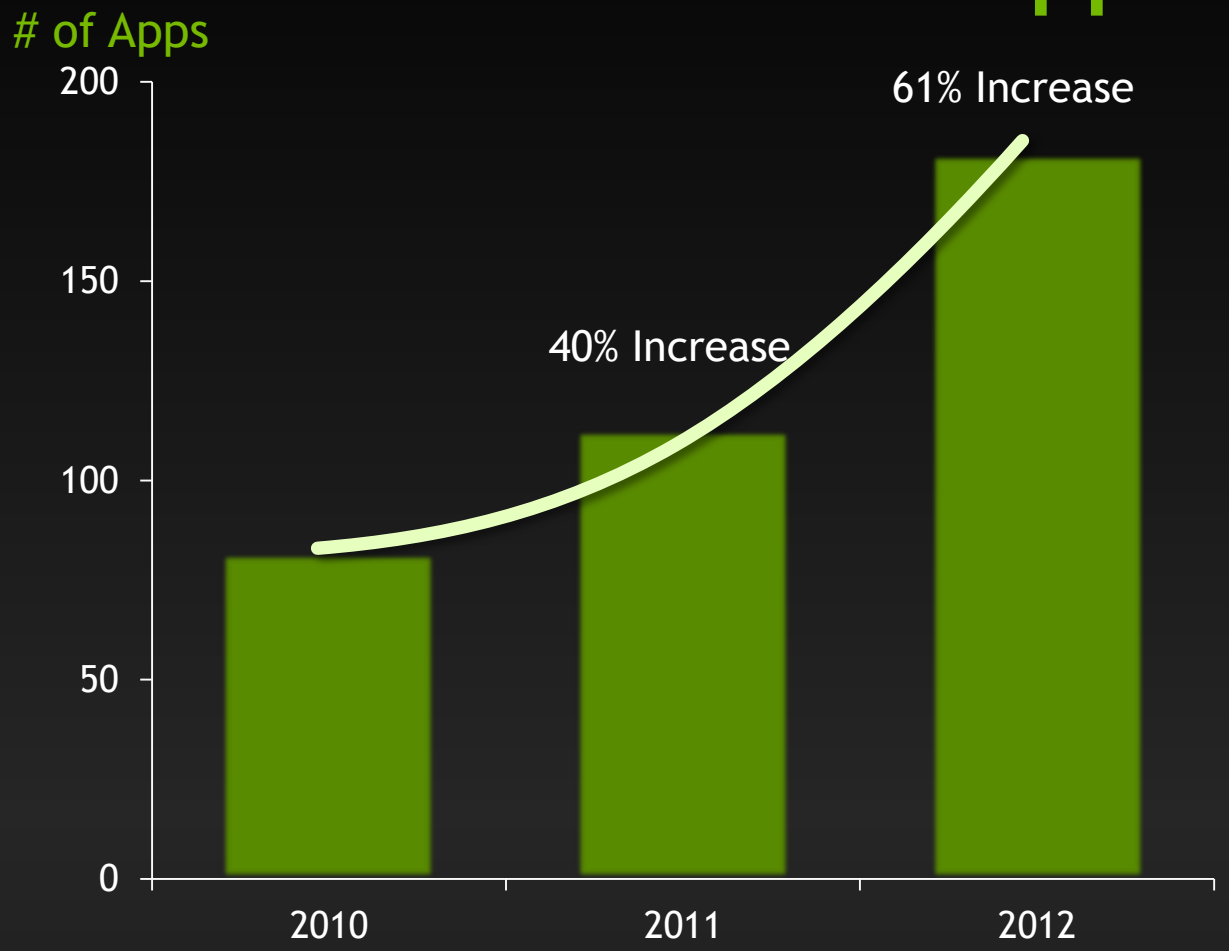
ANSYS

Autodesk

SIMULIA

ACUSIM SOFTWARE

CUDA Apps Grows 60%, Accelerating Key Apps



Top Supercomputing Apps

Computational Chemistry	AMBER CHARMM GROMACS	LAMMPS NAMD DL_POLY
Material Science	QMCPACK Quantum Espresso GAMESS	Gaussian NWChem VASP
Climate & Weather	COSMO GEOS-5	CAM-SE NIM WRF
Physics	Chroma Denovo GTC	GTS ENZO MILC
CAE	ANSYS Mechanical MSC Nastran SIMULIA Abaqus	ANSYS Fluent OpenFOAM LS-DYNA

Accelerated, In Development


NVIDIA
POPULAR GPU-ACCELERATED APPLICATIONS
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COMPUTATIONAL FLUID DYNAMICS
COMPUTATIONAL STRUCTURAL MECHANICS
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10 Media and Entertainment
ANIMATION, MODELING AND RENDERING
COLOR CORRECTION AND GRAIN MANAGEMENT
COMPOSITING, FINISHING AND EFFECTS
EDITING
ENCODING AND DIGITAL DISTRIBUTION
ON-AIR GRAPHICS
ON-SET, REVIEW AND STEREO TOOLS
SIMULATION
WEATHER GRAPHICS
14 Oil and Gas
Research: Higher Education and Supercomputing
COMPUTATIONAL CHEMISTRY AND BIOLOGY
Bioinformatics
BarraCUDA Sequence mapping software Alignment of short sequencing reads 6-10x 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 to 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 60-100x 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 3.0.12
SeqNFind A GPU Accelerated Sequence Analysis Toolset Reference assembly, blast, smith-waterman, hmm, de novo assembly 400x T 2075, 2090, K10, K20, K20X Yes Available now
UGENE Opensource Smith-Waterman for SSE/CUDA, Suffix array based repeats finder and dotplot Fast short read alignment 6-8x T 2075, 2090, K10, K20, K20X Yes Available now Version 1.11
WideLM Fits numerous linear models to a fixed design and response Parallel linear regression on multiple similarly-shaped models 150x T 2075, 2090, K10, K20, K20X Yes Available now Version 0.1-1
Molecular Dynamics
Abalone Models molecular dynamics of biopolymers for simulations of proteins, DNA and ligands Simulations (on 1060 GPU) 4-29x T 2075, 2090, K10, K20, K20X Single Only Available now Version 1.8.48
ACEMD GPU simulation of molecular mechanics force fields, implicit and explicit solvent Written for use on GPUs 160 ns/day GPU version only T 2075, 2090, K10, K20, K20X Yes Available now
AMBER Suite of programs to simulate molecular dynamics on biomolecule PMEMD: explicit and implicit solvent 89.44 ns/day JAC NVE T 2075, 2090, K10, K20, K20X Yes Available now Version 12 + bugfix9
DL-POLY Simulate macromolecules, polymers, ionic systems, etc on a distributed memory parallel computer Two-body forces, Link-cell pairs, Ewald SPME forces, Shake VV 4x T 2075, 2090, K10, K20, K20X Yes Available now, Version4.0 Source only
CHARMM MD package to simulate molecular dynamics on biomolecule. Implicit (5x), Explicit (2x) Solvent via OpenMM TBD T 2075, 2090, K10, K20, K20X Yes In Development 04/12
GROMACS Simulation of biochemical molecules with complicated bond interactions Implicit (5x), Explicit(2x) solvent 165 ns/Day DHFR T 2075, 2090, K10, K20, K20X Single only Available now Version 4.6 in Q4/12
HOOMD-Blue Particle dynamics package written grounds up for GPUs Written for GPUs 2x T 2075, 2090, K10, K20, K20X Yes Available now
LAMMPS Classical molecular dynamics package Lennard-Jones, Morse, Buckingham, CHARMM, Tabulated, Course grain SDK, Anisotropic Gay-Bern, RE-squared, "Hybrid"combinations 3-18x T 2075, 2090, K10, K20, K20X Yes Available now
AMD Designed for high-performance simulation of large molecular systems 100M atom capable 6.44 ns/days STMV 585x 2050s T 2075, 2090, K10, K20, K20X Yes Available now, Version 2.9
enMM Library and application for molecular dynamics for HPC with GPUs Implicit and explicit solvent, custom forces Implicit: 127-213 ns/day; Explic 18-55 ns/ DHFR T 2075, 2090, K10, K20, K20X Yes Available now Version 4.1.1
207 GPU-Accelerated Applications
www.nvidia.com/appscatalog

It's Not Just About CUDA

Applications

Libraries

OpenACC Directives

Programming Languages

"Drop-in" Acceleration

Easily Accelerate Applications

Maximum Performance

GPU Accelerated Libraries

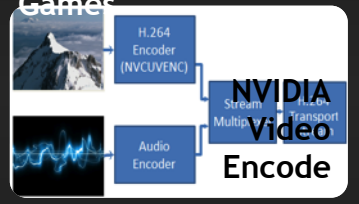
"Drop-in" Acceleration for your Applications

Linear Algebra
FFT, BLAS,
SPARSE, Matrix

Numerical & Math
RAND, Statistics

Data Struct. & AI
Sort, Scan, Zero Sum

Visual Processing
Image & Video



OpenACC

Open Programming Standard for Parallel Computing

"OpenACC will enable programmers to easily develop portable applications that maximize the performance and power efficiency benefits of the hybrid CPU/GPU architecture of Titan."

--Buddy Bland, Titan Project Director, Oak Ridge National Lab

"OpenACC is a technically impressive initiative brought together by members of the OpenMP Working Group on Accelerators, as well as many others. We look forward to releasing a version of this proposal in the next release of OpenMP."

--Michael Wong, CEO OpenMP Directives Board

OpenACC Standard

NVIDIA

CRAY THE SUPERCOMPUTER COMPANY

PGI

CAPS

OIL & GAS

Schlumberger

Chevron

EDU/RESEARCH

OAK RIDGE National Laboratory

Chinese Academy Of Sciences

GOVERNMENT

Air Force Research Laboratory

NASA

MANUFACTURING

ANSYS

SIMULIA

GPUs

Central To Computing

DATA ANALYTICS

synerscope

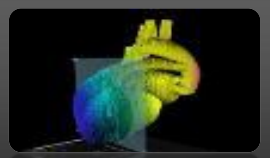
FUZZY LOGIX

MEDIA & ENTMNT.

SONY PICTURES

FOX

LIFE SCIENCES



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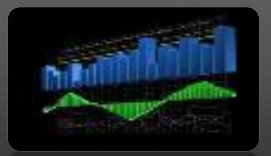
life technologies™

FINANCE



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