The Era of Accelerated Computing

Denis Gerrer

Sales Manager S.E. HPC

NVIDIA.

Guiding Goals for Tesla Roadmap

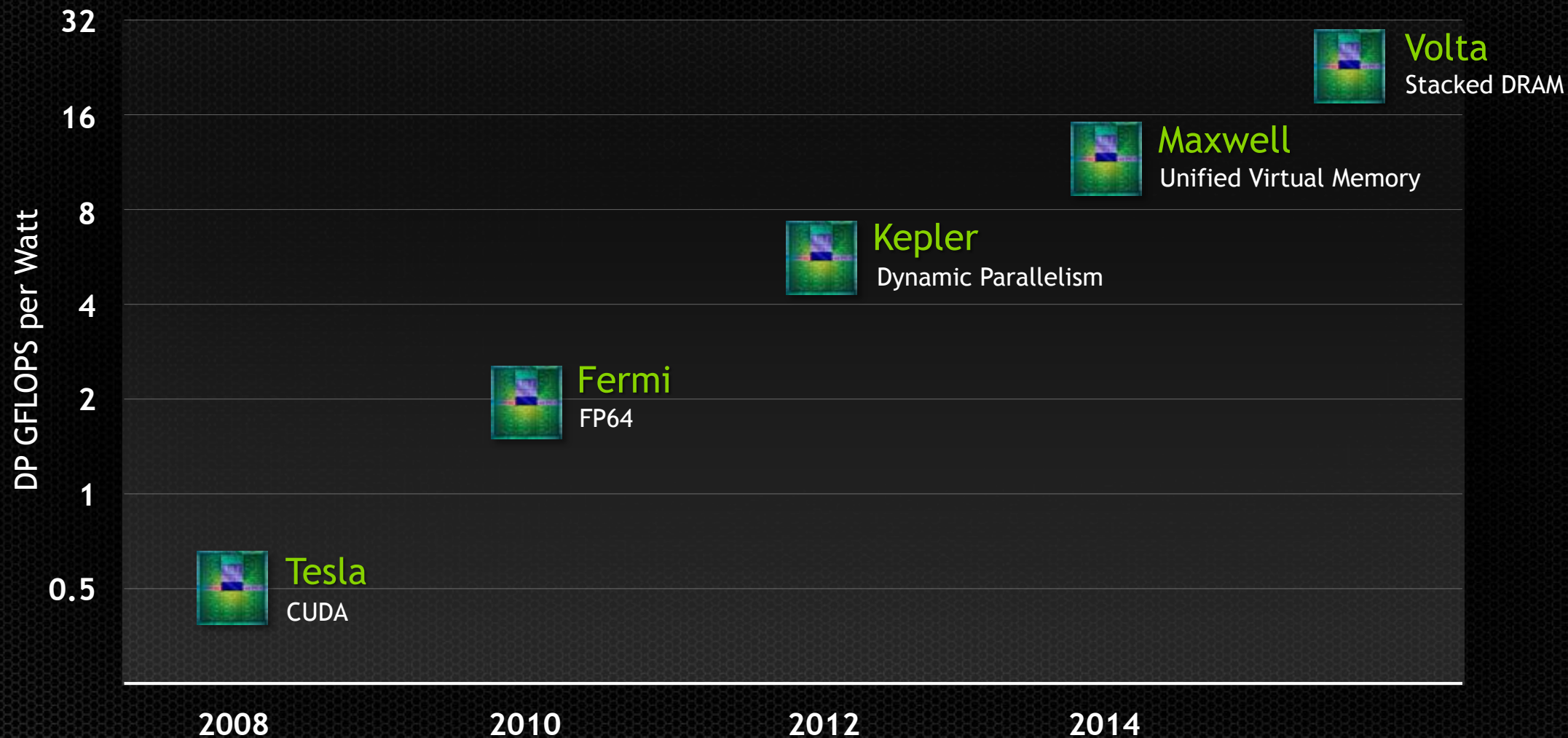Power
Efficiency

Ease of
Programming
And Portability

Application
Space
Coverage

GPU Roadmap

DP GFLOPS per Watt

32 — **Volta**
Stacked DRAM

16 — **Maxwell**
Unified Virtual Memory

8 — **Kepler**
Dynamic Parallelism

4 —

2 — **Fermi**
FP64

1 —

0.5 — **Tesla**
CUDA

2008　2010　2012　2014

Parallel Computing Platform

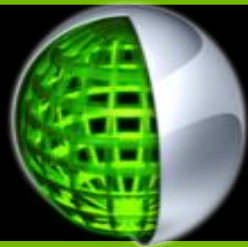|			
Multiple Programming Approaches	**Libraries** "Drop-in" Acceleration	**OpenACC Directives** Easily Accelerate Applications	**Programming Languages** Maximum Flexibility

Development Environment

Parallel Nsight IDE
Linux, Mac and Windows
GPU Debugging and Profiling

CUDA-GDB debugger
NVIDIA Visual Profiler

Third Party Tools
DDT, TotalView, Vampir, ...

Compiler

LLVM COMPILER INFRASTRUCTURE
Open Compiler Tools

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

CRAY THE SUPERCOMPUTER COMPANY **PGI®** **CAPS**
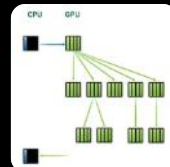OpenACC Compiler

Hardware Capabilities

SMX
CONTROL LOGIC

DynamicParallelism
CPU GPU

HyperQ
KEPLER
32 SIMULTANEOUS MPI TASKS
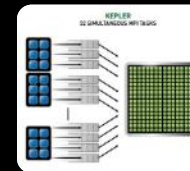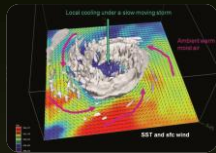
GPUDirect

Wide Adoption of Tesla GPUs

Oil and gas

Reverse Time
Migration
Kirchoff Time
Migration
Reservoir Sim

Edu/Research

Astrophysics
Lattice QCD
Molecular
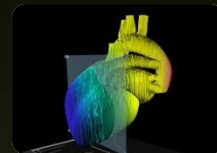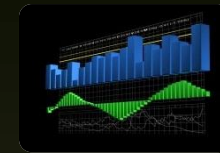Dynamics
Weather / Climate
Modeling

Government

Signal Processing
Satellite Imaging
Video Analytics
Synthetic Aperture
Radar

Life Sciences

Bio-chemistry
Bio-informatics
Material Science
Sequence Analysis
Genomics

Finance

Risk Analytics
Monte Carlo
Options Pricing
Insurance
modeling

Manufacturing

Structural
Mechanics
Computational
Fluid Dynamics
Machine Vision
Electromagnetics

Over 200 GPU-Accelerated Applications

http://www.nvidia.com/object/gpu-applications.html

POPULAR GPU-ACCELERATED APPLICATIONS

Application	Description	Supported Features	Expected	Multi-GPU	Release Status
Molecular Dynamics					
Abalone	Models molecular dynamics of biopol... simulations of proteins, DNA and liga...				
ACEMD	Simulation of mechanics force fields, & explicit solvent on CUDA				
AMBER	Suite of programs to simulate molecu... dynamics on biomolecules				
DL-POLY	Simulate macromolecules, polymers, systems, etc on a distributed memory... parallel computer				
GROMACS	Simulation of biochemical molecules complicated bond interactions				
HOOMD-Blue	Particle dynamics package written gr... up for GPUs				
LAMMPS	Classical molecular dynamics packag...				
NAMD	Designed for high-performance simu... of large molecular systems				
Quantum Chemistry					
GAMESS-US	Computational chemistry suite used t... simulate atomic and molecular electr... structure				
NWChem	Computational chemistry package de... for HPC clusters				
Q-CHEM	Computational chemistry package de... for HPC clusters				
TeraChem	Quantum chemistry software designe... to run on NVIDIA GPU				
Materials Science					
LSMS	Materials code for investigating the e... of temperature on magnetism				
QMCPACK	Solves the many-body Schrodinger e... for electronic structures using a quan... Monte Carlo method				
Quantum-Espresso/PWscf	An integrated suite of computer code... electronic structure calculations and... modeling at the nanoscale				
VASP	First principles materials code that co... electronic structures and quantum-... mechanical molecular dynamics				
Visualization & Docking Software					
Amira 5	A multifaceted software platform for... visualizing, manipulating, and unders... life sciences and bio-medical data				
Core Hopping	Rapid screening of novel cores to imp... drug properties				
FastROCS	3D molecular shape comparison				
VMD	Visualizing and analyzing large bio-m... systems in 3-D graphics				

POPULAR GPU-ACCELERATED APPLICATIONS, Continued

Application	Description	Supported Features	Expected	Multi-GPU	Release Status
Weather & Climate Forecasting					
ASUCA	Weather forecasting model fully optimized for GPUs				
CAM / SE	Community Atmospheric Model is a g... atmosphere model for weather and c... research				
GEOS-5	Weather modeling and forecasting ap... used by NASA				
HIRLAM	Weather forecasting model fully optin... for GPUs				
HOMME	Weather modeling tool for atmospher... scientists				
HYCOM	Weather forecasting model using icos... horizontal grid				
MITgcm	Numerical model designed for study... atmosphere, ocean, and climate				
NIM	Weather forecasting model using icos... horizontal grid				
WRF	Weather and Ocean modeling applica...				
Editing and Effects					
Adobe Premiere Pro	Video editing				
Avid Media Composer	Video editing				
GenArts Sapphire	Effects plug-in for video editing				
Sony Vegas Pro	Video editing				
Animation					
Autodesk 3Ds Max	3D modeling, animation, and rendering				
Autodesk Maya	3D modeling, animation, and rendering				
Defense & Intelligence					
DigitalGlobe Advanced Ortho Series	Geospatial Visualization				
Eternix Blaze Terra	Geospatial Visualization				
Exelis (ITT) ENVI	Geospatial Visualization				
GeoEye Analytics Signature Analyst	Geospatial Visualization				
GeoWeb3d Desktop	Geospatial Visualization				
Incogna GIS	Geospatial Visualization				
Intergraph Motion Video Analyst	Video filters and mosaic'ing — Geo-fu... FMV analytics with intelligence data				
Intuvision Panoptes 3.0	Video Analytics				

POPULAR GPU-ACCELERATED APPLICATIONS, Continued

Application	Description	Supported Features	Expected	Multi-GPU	Release
Electronic Design Automation and CEM					
Agilent Technologies ADS	Simulation tool for design of RF, micr... and high speed digital circuits				
Agilent Technologies EMPro	Modeling and simulation environmen... analyzing 3D EM effects of high speed... RF/Microwave components				
ANSYS Nexxim	Circuit simulation engine for RF/anal... mixed-signal IC design; IBIS-AMI ana... speedup with GPU computing				
CST Microwave Studio (MWS)	High frequency electromagnetic field simulation				
Gauda OPC, OPV	Collection of several software tools fo... computational lithography running on... Gauda hardware platform				
Remcom XFdtd	3D EM modeling and simulation				
Rocketick RocketSim	Verilog simulation				
SPEAG SEMCAD-X	3D EM modeling and simulation				
CAD					
CATIA V6 – Live Rendering	Photorealistic rendering				
Bunkspeed Pro Suite	Easy to use photorealistic rendering s...				
RTT DeltaGen 10.x	Photorealistic rendering used for desi...				
RTT DeltaPix	Photorealistic rendering with integrat... TeamCenter and RTT formats				
Numerical Analysis					
Jacket AccelerEyes	GPU acceleration for MATLAB				
Mathematica Wolfram	Symbolic math analysis				
MATLAB Mathworks	Technical computing language and integrated development environment (MATLAB PCT, MDCS)				

POPULAR GPU-ACCELERATED APPLICATIONS, Continued

Application	Description	Supported Features	Expected	Multi-GPU	Release
Oil&Gas					
Acceleware RTM	Seismic Processing				
CGG/Veritas RTM	Seismic Processing				
ffA SVI Pro	Seismic Interpretation				
Headwave Suite	Seismic Imaging				
Geoteric	Seismic Processing/Interpretation				
Paradigm EarthStudy360	Reservoir Modeling				
Paradigm Echos RTM	Seismic Processing				
Paradigm SKUA	Reservoir Modeling				
Paradigm VoxelGeo	Seismic Interpretation				
Schlumberger WesterGeco Omega2 RTM	Seismic Processing				
Seismic City Prestack Interpretation	Seismic Processing				
SpectraSeis	Seismic Processing / Imaging				
Stoneridge Reservoir Simulation	Reservoir Simulation				
Tsunami RTM	Seismic Processing				
Computational Finance					
Hanweck Associates	Real-time options analytical engine (N...				
MATLAB Mathworks	Data parallel mathematics (MATLAB PCT, MDCS)				
Murex	Risk analytics (MACS)				
Numerical Algorithms Group	Random Number Generators				
SciComp, Inc	Derivative pricing (SciFinance)				
Wolfram Mathematica	Mathematical Development Environm...				

*GPU performance compared against multi-core x86 CPU socket. G... kernel to kernel performance comparison. Performance results...

POPULAR GPU-ACCELERATED APPLICATIONS, Continued

Application	Description	Supported Features	Expected Speed Up*	Multi-GPU Support	Release Status
Physics					
Chroma	General purpose LQCD application	Wilson-clover fermions, Krylov solvers, Domain-decomposition	5-6x	Yes	Available now
MILC	General purpose LQCD application	Staggered fermions, Krylov solvers, Gauge-link fattening	5-6x	Yes	Available now
Computational Fluid Dynamics					
Altair AcuSolve	General purpose CFD flow solver	Linear equation solver	2x	Yes	Available now
Autodesk Moldflow	Optimize design of plastic parts and injection molds	Linear equation solver	2x	Single Only	Available now
FEFLO (GMU-Lohner)	Navier-Stokes flow solver based on unstructured grids for modeling both compressible and incompressible flows	Explicit solver	10x	Yes	In Development
FluiDyna LBultra	Computing physical flows in and around solid bodies	LBM, particle CFD	20x	Yes	Available now
FluiDyna Culises-OpenFOAM	Computing physical flows with Culises — a software library with special algorithms for solving systems of equations	Linear equation solvers	3x Solver	Single Only	Available now
Promotech Particleworks	Fluid simulation for free surface flow like Tsunami, material processing and liquids	MPS, Particle CFD	4x-9x	Yes	Available now
S3D (Sandia NL S3D)	Massively parallel direct numerical solver (DNS) for the full compressible Navier-Stokes	Chemistry kernel	8x SP, 5x DP kernel	Yes	In Development
Turbostream	Ultrafast CFD solver for turbomachines	Explicit solver	19x	Yes	Available now
Vratis SpeedIT-OpenFOAM Solver	Set of accelerated solvers for sparse linear systems of equations	Linear equation solvers	3x Solver	Yes	Available now
Computational Structural Mechanics					
Abaqus/Standard	Simulation and analysis tool for structural mechanics	Linear equation solver	1.5-2.5x	Single Only	Available now
ANSYS Mechanical	Simulation and analysis tool for structural mechanics	Linear equation solver	2x	Single Only	Available now
Impetus Afea	Predicts large deformations of structures and components exposed to extreme loading conditions	Linear equation solver, SPH	10x SPH, 2x Total	Yes	Available now
LS-DYNA Implicit	Multiphysics simulation package used	Linear equation solver	3x	Yes	In Development
MSC Nastran	Simulation and analysis tool for structural mechanics	Linear equation solver	1.4-2x	Yes	Available now
Marc	Simulation and analysis tool for structural mechanics	Linear equation solver	1.5x	Yes	In Development
RADIOSS Implicit	Used to maximize durability, NVH, crash, safety, manufacturability and fluid-structure interaction performance	Linear equation solver	2x	Single Only	In Development

Summary

- NVIDIA provides a powerful development platform for parallel computing
    - Smart compilers, Libraries of common routines , Integrated development environments (IDEs) , Profiling, correctness-checking, and debugging , Open Compiler SDK, 3rd party tools

- Power is the main HPC constraint
    - Vast majority of work must be done by cores designed for efficiency
    - Data movement dominates the power
    - Locality at all levels and reduction of overhead is necessary

- GPU computing has a sustainable model
    - Aligned with technology trends, supported by consumer markets

- GPUs are the path to the tightly-coupled hybrid processor future

Thank You