GPU Computing Ecosystem

CUDA 5
Enterprise level GPU Development

GPU Development Paths
Libraries, Directives, Languages

GPU Tools
Tools, libraries and plug-ins for GPU codes
Kepler!

**Tesla K10**
- 3x Single Precision
- 1.8x Memory Bandwidth
- Image, Signal, Seismic
- Available Now

**Tesla K20**
- 3x Double Precision
- Hyper-Q, Dynamic Parallelism
- CFD, FEA, Finance, Physics
- Available Q4 2012
Add GPU Processing Your Way

Start with the PowerEdge C410x

- 3U Rack Mount
- Up to 16 NVIDIA GPUs
- Up to 8 host server connections
- Programmable GPU:host server ratios
- Individual GPU serviceability

Choose your host server

- PowerEdge R620
- PowerEdge R720
- PowerEdge C6220
- PowerEdge C6105
- PowerEdge C6145

Can also take 2 Tesla GPU Internal

Choose your GPU:host ratio

- 2:1
  - Two GPUs per server
  - 8 servers per C410x

- 4:1
  - Four GPUs per server
  - 4 servers per C410x

Intel
- 2S

AMD
- 2S
- 4S
Introducing CUDA 5
CUDA By the Numbers:

- >375,000,000 CUDA-Capable GPUs
- >1,000,000 Toolkit Downloads
- >120,000 Active Developers
- >500 Universities Teaching CUDA
Dynamic Parallelism

CPU

Fermi GPU

Kepler GPU
Dynamic Work Generation

- Coarse grid: Higher Performance, Lower Accuracy
- Fine grid: Lower Performance, Higher Accuracy
- Dynamic grid: Target performance where accuracy is required

Supported on GK110 GPUs
Simpler Code: LU Example

LU decomposition (Fermi)

```c
void dgetrf(N, N) {
    for j=1 to N
        for i=1 to 64
            idamax<<<>>>();
            dswap<<<>>>();
            dscal<<<>>>();
            dger<<<>>>();
            next i
    memcpy;
    dlaswap<<<>>>();
    dtrsm<<<>>>();
    dgemm<<<>>>();
    next j
}
```

LU decomposition (Kepler)

```c
void dgetrf(N, N) {
    dgetrf<<<>>>();
    synchronize();
}

void dgetrf(N, N) {
    for j=1 to N
        for i=1 to 64
            idamax<<<>>>();
            dswap<<<>>>();
            dscal<<<>>>();
            dger<<<>>>();
            next i
    dlaswap<<<>>>();
    dtrsm<<<>>>();
    dgemm<<<>>>();
    next j
}
```

CPU Code

GPU Code

CPU is Free

GPU Code
Easy Speed-up for MPI Codes with Hyper-Q

CP2K Success Story

- M2090 GPU shows no performance improvement over CPUs
- Like most HPC codes, MPI jobs are too small for GPUs
- Hyper-Q provides $2.5\times$ speed-up without major code rewrite

GPU Development Paths
GPUs have evolved to the point where many real-world applications are easily implemented on them and run significantly faster than on multi-core systems.

Future computing architectures will be hybrid systems with parallel-core GPUs working in tandem with multi-core CPUs.

Jack Dongarra
Professor, University of Tennessee
Director of the Innovative Computing Laboratory
Author of LINPACK
Small Changes, Big Speed-up

Application Code

Rest of Sequential CPU Code

GPU

Use GPU to Parallelize Compute-Intensive Functions

CPU
Commercial Apps Accelerated by GPUs

- **Molecular Dynamics**
  - AMBER
  - CHARMM
  - DL_POLY
  - GAMESS-US
  - GROMACS
  - LAMMPS
  - NAMD

- **Fluid Dynamics**
  - Altair Acusolve
  - Autodesk Moldflow
  - OpenFOAM
  - Prometech
  - Particlework
  - Turbostream

- **Earth Sciences**
  - ASUCA
  - HOMME
  - NASA GEOS-5
  - NOAA NIM
  - WRF

- **Engineering Simulation**
  - Agilent EMPro
  - ANSYS Mechanical
  - ANSYS Nexxim
  - CST Microwave Studio
  - Impetus AFEA
  - Remcom XFdtd
  - SIMULIA Abaqus

- **Others**
  - GADGET2
  - MATLAB
  - Mathematica
  - NBODY
  - Paradigm VoxelGeo
  - PARATEC
  - Schlumberger Petrel
Rapidly Growing GPU-Accelerated Application Catalog

POPULAR GPU-ACCELERATED APPLICATIONS

<table>
<thead>
<tr>
<th>Application</th>
<th>Description</th>
<th>Supported Features</th>
<th>Expected Speedup</th>
<th>Multi-GPU Support</th>
<th>Release Status</th>
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<tr>
<td>QMIX</td>
<td>Computational chemistry package for HPC clusters</td>
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<tr>
<td>Q-BEAM</td>
<td>Computational chemistry package for HPC clusters</td>
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<td>Q-Tech</td>
<td>Quantum chemistry software package</td>
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<td>Materials Science</td>
<td>Scientific code for investigating the effect of temperature on materials</td>
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<td>GEMS</td>
<td>Materials code for investigating the effect of temperature on materials</td>
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<td>GEMMICK</td>
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<tr>
<td>Visualization &amp; Data Mining</td>
<td>A visualization software for visualizing, manipulating, and analyzing medical images</td>
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<tr>
<td>MDMiner</td>
<td>Data mining software for drug discovery</td>
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<td>SPOC</td>
<td>Visualization software for 3D structural models</td>
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<tr>
<td>VDS</td>
<td>Visualization and rendering software for 3D graphics</td>
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</tbody>
</table>
3 Ways to Accelerate Applications

- **Libraries**: "Drop-in" Acceleration
- **OpenACC Directives**: Easily Accelerate Applications
- **Programming Languages**: Maximum Flexibility
GPU Accelerated Libraries
“Drop-in” Acceleration for your Applications

NVIDIA cuFFT
NVIDIA cuBLAS
NVIDIA cuSPARSE
NVIDIA cuRAND
Matrix Algebra on GPU and Multicore
GPU Accelerated Linear Algebra
IMSL Library
Sparse Linear Algebra
Building-block Algorithms
C++ Templated Parallel Algorithms
GPU-Aware MPI Libraries
Integrated Support for GPU Computing

OpenMPI
MVAPICH
Platform MPI

GPU0 Memory
GPU1 Memory

CUDA Memcpy()

GPU0
GPU1
PCI-e

Peer-to-Peer Transfers

InfiniBand

Accelerated Communication

developer.nvidia.com/gpudirect
3 Ways to Accelerate Applications

Applications

Libraries

“Drop-in” Acceleration

OpenACC Directives

Easily Accelerate Applications

Programming Languages

Maximum Flexibility
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
PGI
CAPS
OpenACC Directives

Program myscience
... serial code ...
!$acc kernels
do k = 1,n1
do i = 1,n2
... parallel code ...
enddo
enddo
!$acc end kernels
... End Program myscience

Your original Fortran or C code

Simple Compiler hints
Compiler Parallelizes code
Works on many-core GPUs & multicore CPUs

www.nvidia.com/gpudirectives
Directives: Easy & Powerful

Real-Time Object Detection
Global Manufacturer of Navigation Systems

Valuation of Stock Portfolios using Monte Carlo
Global Technology Consulting Company

Interaction of Solvents and Biomolecules
University of Texas at San Antonio

5x in 40 Hours
2x in 4 Hours
5x in 8 Hours

"Optimizing code with directives is quite easy, especially compared to CPU threads or writing CUDA kernels. The most important thing is avoiding restructuring of existing code for production applications."

-- Developer at the Global Manufacturer of Navigation Systems
3 Ways to Accelerate Applications

- **Libraries**: “Drop-in” Acceleration
- **OpenACC Directives**: Easily Accelerate Applications
- **Programming Languages**: Maximum Flexibility
Opening the CUDA Platform with LLVM

CUDA compiler source contributed to open source LLVM compiler project

SDK includes specification documentation, examples, and verifier

Provides ability for anyone to add CUDA to new languages and processors

Learn more at developer.nvidia.com/cuda-source
<table>
<thead>
<tr>
<th>Category</th>
<th>Languages</th>
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</thead>
<tbody>
<tr>
<td>Numerical analytics</td>
<td>MATLAB, Mathematica, LabVIEW</td>
</tr>
<tr>
<td>Fortran</td>
<td>OpenACC, CUDA Fortran</td>
</tr>
<tr>
<td>C</td>
<td>OpenACC, CUDA C</td>
</tr>
<tr>
<td>C++</td>
<td>Thrust, CUDA C++</td>
</tr>
<tr>
<td>Python</td>
<td>PyCUDA, Copperhead</td>
</tr>
<tr>
<td>C#</td>
<td>GPU.NET</td>
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</tbody>
</table>
NVIDIA® Nsight™ Eclipse Edition
for Linux and MacOS

CUDA-Aware Editor
- Automated CPU to GPU code refactoring
- Semantic highlighting of CUDA code
- Integrated code samples & docs

Nsight Debugger
- Simultaneously debug CPU and GPU
- Inspect variables across CUDA threads
- Use breakpoints & single-step debugging

Nsight Profiler
- Quickly identifies performance issues
- Integrated expert system
- Source line correlation

developer.nvidia.com/nsight
Performance Analysis Tools
Single Node to Hybrid Cluster Solutions

NVIDIA Nsight
Eclipse & Visual Studio Editions

NVIDIA Visual Profiler

Vampir Trace Collector

TAU Performance System

PAPI CUDA Component

Under Development

developer.nvidia.com/performance-analysis-tools
Job Scheduling & Cluster Management

- Platform Computing: LSF, HPC, Cluster Manager
- Bright Computing: Bright Cluster Manager
- Adaptive Computing
- PBS Works: PBS Professional
- Ganglia: NVML Plugin for GPUs
- UNIVA: Univa Grid Engine

developer.nvidia.com/cuda-tools-ecosystem
GPU Test Drive
Experience the Acceleration

**What**
Program that provides free access to a remote/cloud GPU cluster

**Who**
For academic researchers

**Why**
To experience how applications accelerate with GPUs

**Benefit to Researchers**
FREE & EASY way to start with GPUs
No GPU programming expertise needed
Access to a remote, pre-configured GPU cluster for evaluation

www.nvidia.com/GPUTestDrive
GPU Technology Conference 2013
March 18-21 | San Jose, CA

Reasons to attend GTC

- Learn about leading-edge advances in GPU computing
- Explore the research as well as the commercial applications
- Discover advances in computational visualization
- Take a deep dive into parallel programming

Ways to participate

- Submit a Research Poster - share your work and gain exposure as a thought leader
- Register - learn from the experts and network with your peers
- Exhibit/Sponsor - promote your organization as a key player in the GPU ecosystem

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Thank you