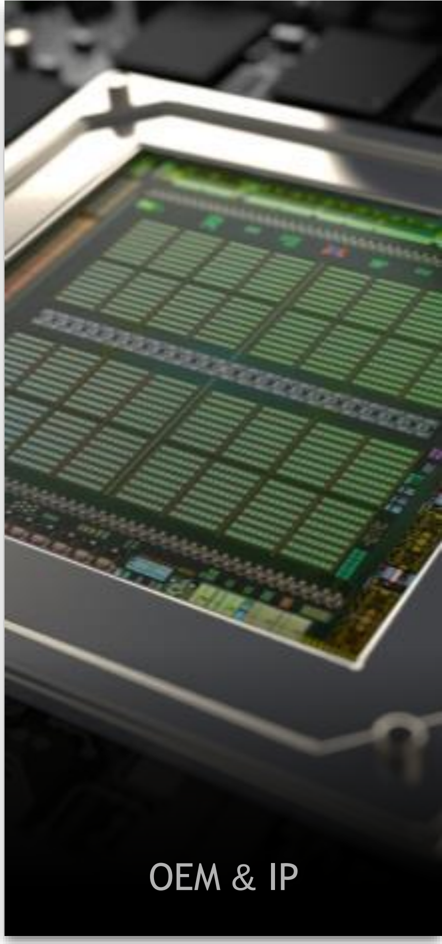
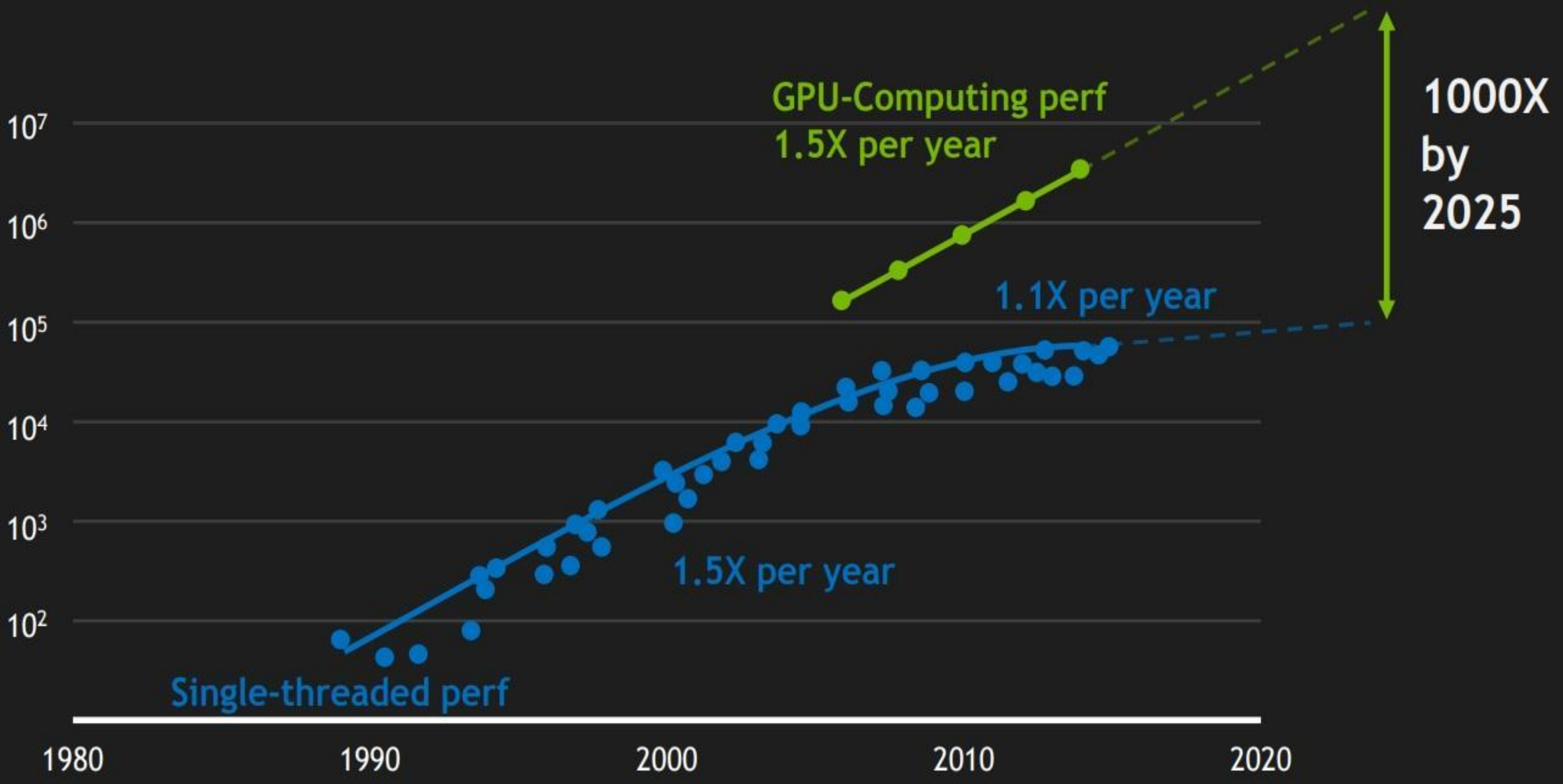
INTRODUCTION TO GPU COMPUTING

Jeff Larkin, June 28, 2018



THE WORLD LEADER IN VISUAL COMPUTING


Power for CPU-only
Exaflop Supercomputer
=
Power for the Bay Area, CA
(San Francisco + San Jose)
HPC's Biggest Challenge: Power



40 Years of Microprocessor Trend Data

CUDA ECOSYSTEM 2018

CUDA DOWNLOADS IN 2017
3,500,000

CUDA REGISTERED DEVELOPERS
800,000

GTC ATTENDEES
8,000+

CUDA APPLICATION ECOSYSTEM

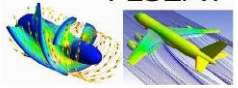
From Ease of Use to Specialized Performance

GROMACS
FAST. FLEXIBLE. FREE.

Vienna Ab-initio Simulation Package

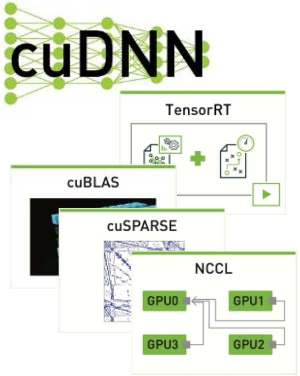
NAMD
Scalable Molecular Dynamics

ANSYS
FLUENT



Applications

Frameworks



Libraries

OpenACC
Directives for Accelerators

C++

Thrust

Directives and Standard Languages

CUDA-C++
CUDA Fortran

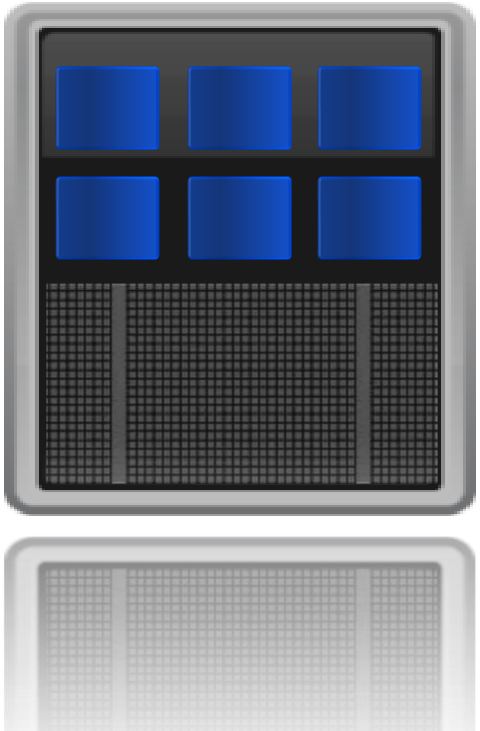
Specialized Languages

FUNDAMENTALS OF GPU COMPUTING

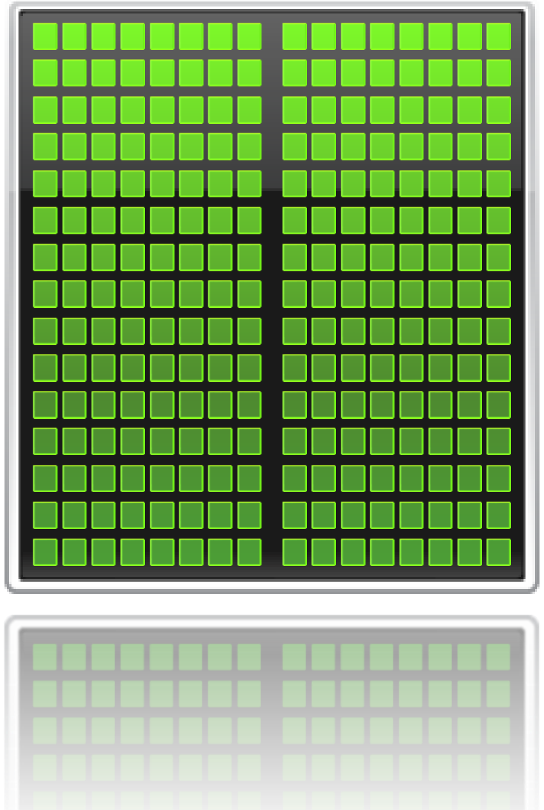
ACCELERATED COMPUTING

10X PERFORMANCE & 5X ENERGY EFFICIENCY FOR HPC

CPU
Optimized for
Serial Tasks



GPU Accelerator
Optimized for
Parallel Tasks

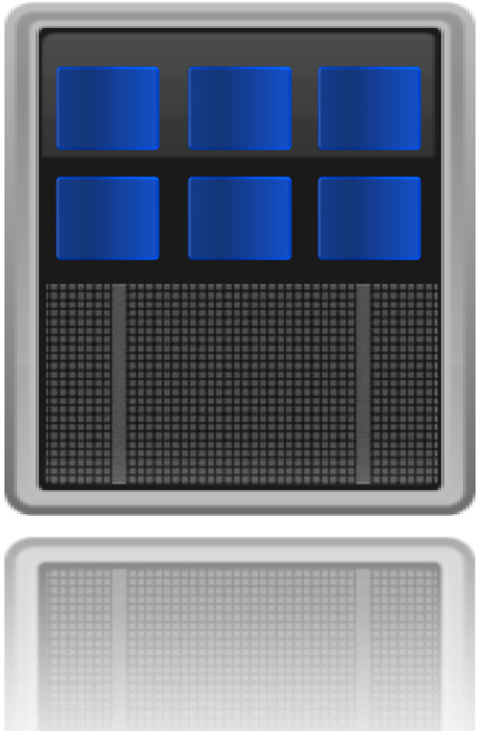


ACCELERATED COMPUTING

10X PERFORMANCE & 5X ENERGY EFFICIENCY FOR HPC

CPU

Optimized for
Serial Tasks



CPU Strengths

- Very large main memory
- Very fast clock speeds
- Latency optimized via large caches
- Small number of threads can run very quickly

CPU Weaknesses

- Relatively low memory bandwidth
- Cache misses very costly
- Low performance/watt

ACCELERATED COMPUTING

10X PERFORMANCE & 5X ENERGY EFFICIENCY FOR HPC

GPU Strengths

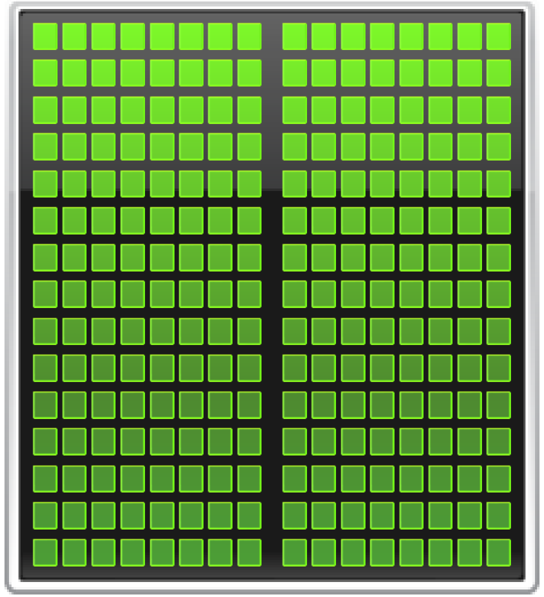
- High bandwidth main memory
- Latency tolerant via parallelism
- Significantly more compute resources
- High throughput
- High performance/watt

GPU Weaknesses

- Relatively low memory capacity
- Low per-thread performance

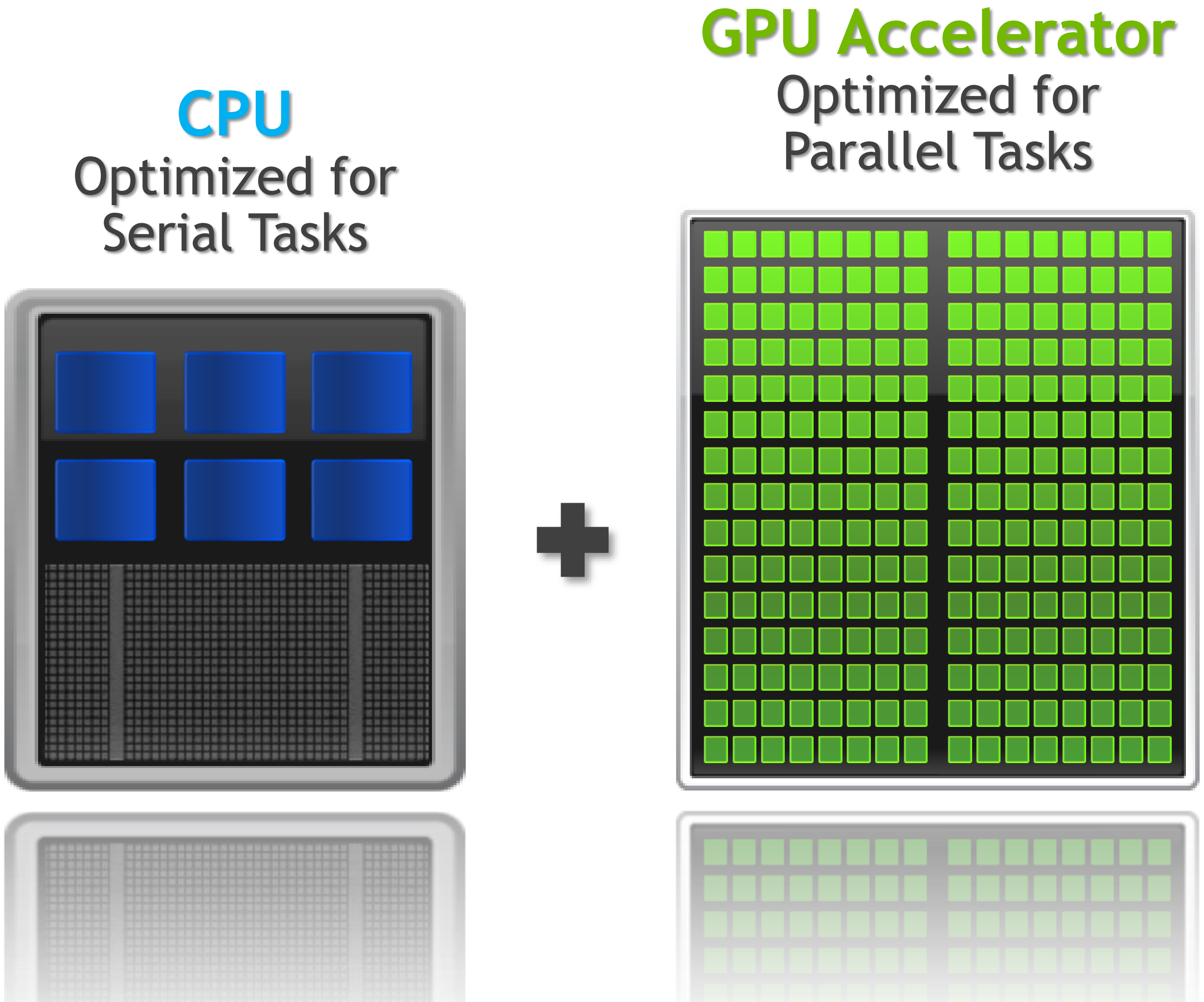
GPU Accelerator

Optimized for Parallel Tasks



ACCELERATED COMPUTING

10X PERFORMANCE & 5X ENERGY EFFICIENCY FOR HPC



Speed v. Throughput

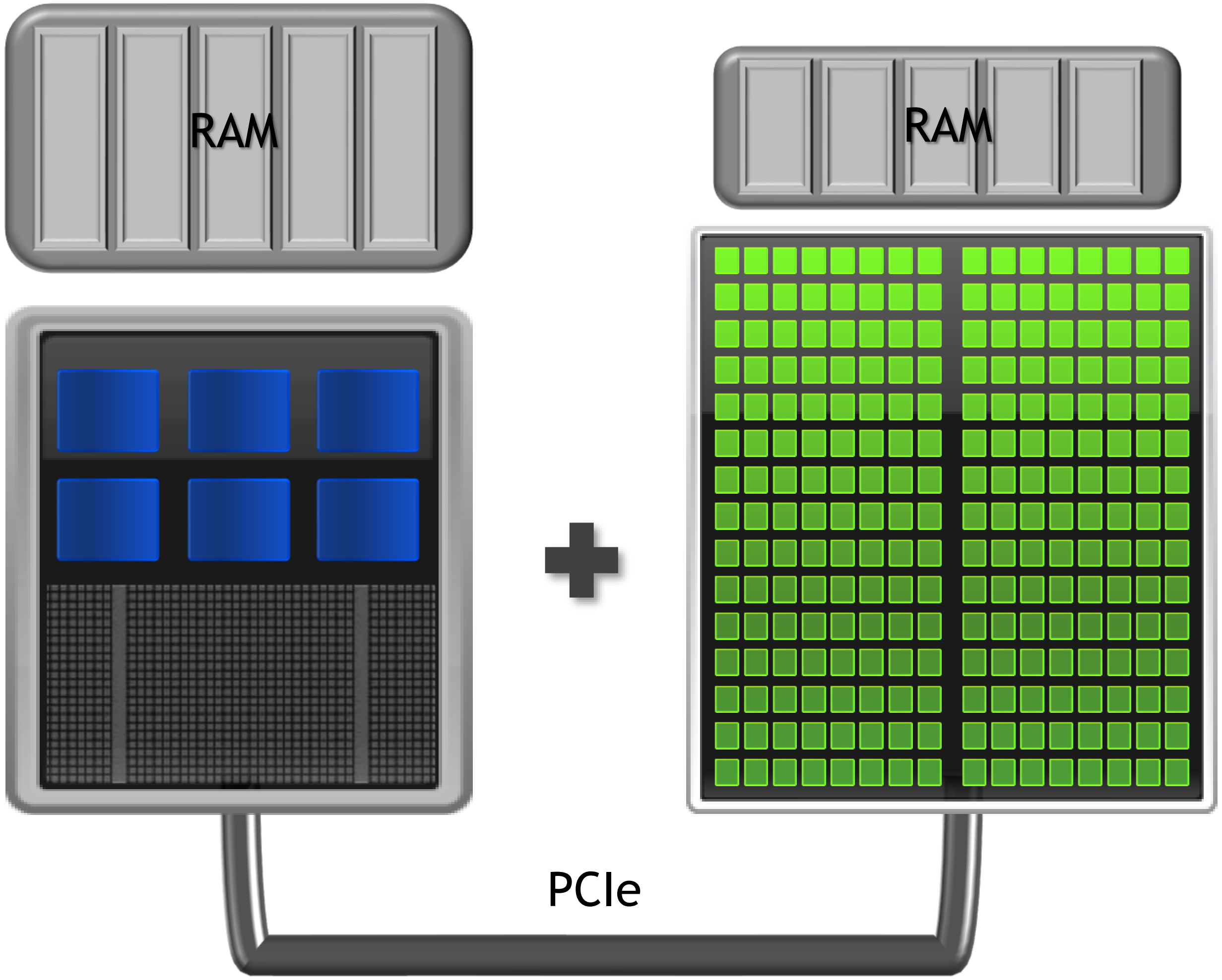
Speed

Throughput

Which is better depends on your needs…

*Images from Wikimedia Commons via Creative Commons

Accelerator Nodes



CPU and GPU have distinct memories

- CPU generally larger and slower
- GPU generally smaller and faster

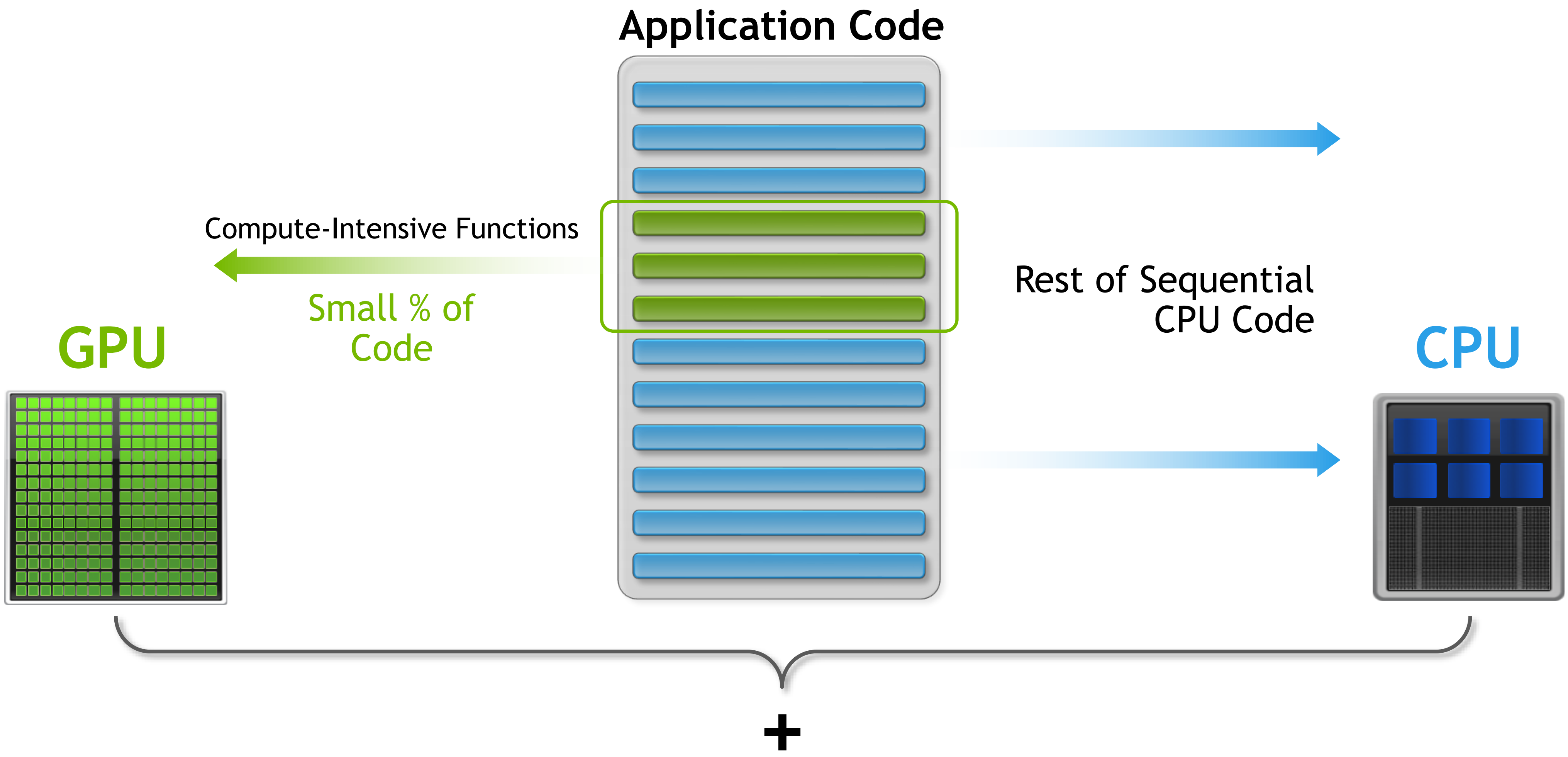
Execution begins on the CPU

- Data and computation are offloaded to the GPU

CPU and GPU communicate via PCIe

- Data must be copied between these memories over PCIe
- PCIe Bandwidth is much lower than either memories

HOW GPU ACCELERATION WORKS

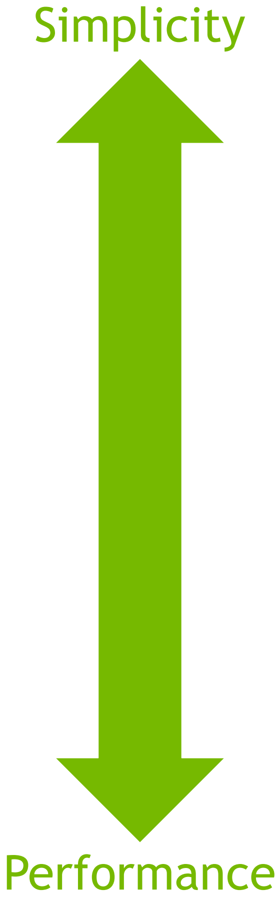


3 WAYS TO PROGRAM GPUS

Applications

Libraries	OpenACC Directives	Programming Languages
"Drop-in" Acceleration	Easily Accelerate Applications	Maximum Flexibility

SIMPLICITY & PERFORMANCE



Accelerated Libraries

- Little or no code change for standard libraries; high performance
- Limited by what libraries are available

Compiler Directives

- High Level: Based on existing languages; simple and familiar
- High Level: Less control over performance

Parallel Language Extensions

- Expose low-level details for maximum performance
- Often more difficult to learn and more time consuming to implement

CODE FOR SIMPLICITY & PERFORMANCE

Libraries

- Implement as much as possible using portable libraries.

Directives

- Use directives to rapidly accelerate your code.

Languages

- Use lower level languages for important kernels.

GPU DEVELOPER ECO-SYSTEM

Numerical Packages
- MATLAB
- Mathematica
- NI LabView
- pyCUDA

Debuggers & Profilers
- cuda-gdb
- NV Visual Profiler
- Parallel Nsight
- Visual Studio
- Allinea
- TotalView

GPU Compilers
- C
- C++
- Fortran
- Java
- Python

Auto-parallelizing & Cluster Tools
- OpenACC
- mCUDA
- OpenMP
- Ocelot

Libraries
- BLAS
- FFT
- LAPACK
- NPP
- Video
- Imaging
- GPULib

Consultants & Training

acceleware, GASS, STONE RIDGE TECHNOLOGY, ANEO, GPU Tech, TECH, ArrayFire, HPC Project, EM Photonics, SCALABLE GRAPHICS, WIPRO

OEM Solution Providers

DELL, hp, IBM, CRAY, ASUS, SUPERMICRO, sgi, FUJITSU, BULL, APPRO, lenovo 联想, NEC

GPU LIBRARIES

LIBRARIES: EASY, HIGH-QUALITY ACCELERATION

EASE OF USE Using libraries enables GPU acceleration without in-depth knowledge of GPU programming

“DROP-IN” Many GPU-accelerated libraries follow standard APIs, thus enabling acceleration with minimal code changes

QUALITY Libraries offer high-quality implementations of functions encountered in a broad range of applications

PERFORMANCE NVIDIA libraries are tuned by experts

GPU ACCELERATED LIBRARIES

"Drop-in" Acceleration for Your Applications

Linear Algebra
FFT, BLAS,
SPARSE, Matrix

NVIDIA cuFFT, cuBLAS, cuSPARSE | CULA tools | MAGMA | CUSP

Numerical & Math
RAND, Statistics

IMSL Fortran Numerical Library | NVIDIA Math Lib | ArrayFire | NVIDIA cuRAND

Data Struct. & AI
Sort, Scan, Zero Sum

Thrust | GPU AI – Board Games | GPU AI – Path Finding

Visual Processing
Image & Video

NVIDIA NPP | NVIDIA Video Encode | Sundog Software

DROP-IN ACCELERATION

In Two Easy Steps

```
int N = 1 << 20;          // 1M elements

x = (float *)malloc(N * sizeof(float));
y = (float *)malloc(N * sizeof(float));
initData(x, y);

// Perform SAXPY on 1M elements: y[]=a*x[]+y[]
saxpy(N, 2.0, x, 1, y, 1);

useResult(y);
```

```
int N = 1 << 20;          // 1M elements

x = (float *)malloc(N * sizeof(float));
y = (float *)malloc(N * sizeof(float));
initData(x, y);

// Perform SAXPY on 1M elements: y[]=a*x[]+y[]
saxpy(N, 2.0, x, 1, y, 1);

useResult(y);
```

DROP-IN ACCELERATION

With Automatic Data Management

```
int N = 1 << 20;          // 1M elements

x = (float *)malloc(N * sizeof(float));
y = (float *)malloc(N * sizeof(float));
initData(x, y);

// Perform SAXPY on 1M elements: y[]=a*x[]+y[]
saxpy(N, 2.0, x, 1, y, 1);

useResult(y);
```

```
int N = 1 << 20;          // 1M elements

cudaMallocManaged(&x, N * sizeof(float));
cudaMallocManaged(&y, N * sizeof(float));
initData(x, y);

// Perform SAXPY on 1M elements: y[]=a*x[]+y[]
saxpy(N, 2.0, x, 1, y, 1);

useResult(y);
```

Step 1: Update memory allocation to be CUDA-aware

Here, we use Unified Memory which automatically migrates
between host (CPU) and device (GPU) as needed by the program

DROP-IN ACCELERATION

With Automatic Data Management

```
int N = 1 << 20;         // 1M elements

x = (float *)malloc(N * sizeof(float));
y = (float *)malloc(N * sizeof(float));
initData(x, y);

// Perform SAXPY on 1M elements: y[]=a*x[]+y[]
saxpy(N, 2.0, x, 1, y, 1);

useResult(y);
```

```
int N = 1 << 20;         // 1M elements

cudaMallocManaged(&x, N * sizeof(float));
cudaMallocManaged(&y, N * sizeof(float));
initData(x, y);

// Perform SAXPY on 1M elements: y[]=a*x[]+y[]
cublasSaxpy(N, 2.0, x, 1, y, 1);

useResult(y);
```

Step 2: Call CUDA library version of API

Many standard libraries (BLAS, FFT, etc) have well-defined interfaces
CUDA will try to match interfaces as far as possible

DROP-IN ACCELERATION

With Explicit Data Management

```
int N = 1 << 20;          // 1M elements

x = (float *)malloc(N * sizeof(float));
y = (float *)malloc(N * sizeof(float));
initData(x, y);

// Perform SAXPY on 1M elements: y[]=a*x[]+y[]
saxpy(N, 2.0, x, 1, y, 1);

useResult(y);
```

Step 3: Manage Data Locality

If not using unified memory, the program moves the data up to the GPU and back

```
int N = 1 << 20;          // 1M elements

x = (float *)malloc(N * sizeof(float));
y = (float *)malloc(N * sizeof(float));
cudaMalloc(&d_x, N * sizeof(float));
cudaMalloc(&d_y, N * sizeof(float));
initData(x, y);

// Copy working data from CPU->GPU
cublasSetVector(N, sizeof(x[0]), x, 1, d_x, 1);
cublasSetVector(N, sizeof(y[0]), y, 1, d_y, 1);

// Perform SAXPY on 1M elements: y[]=a*x[]+y[]
cublasSaxpy(N, 2.0, d_x, 1, d_y, 1);

// Bring the result back to the CPU
cublasGetVector(N, sizeof(y[0]), d_y, 1, y, 1);

useResult(y);
```

EXPLORE CUDA LIBRARIES

developer.nvidia.com/gpu-accelerated-libraries

GPU-Accelerated Libraries for Computing

Home > ComputeWorks > Tools & Ecosystem > GPU-Accelerated Libraries for Computing

GPU-accelerated Libraries for Computing

NVIDIA GPU-accelerated libraries provide highly-optimized functions that perform 2x-10x faster than CPU-only alternatives. Using drop-in interfaces, you can replace CPU-only libraries such as MKL, IPP and FFTW with GPU-accelerated versions with almost no code changes. The libraries can optimally scale your application across multiple GPUs.

With NVIDIA's libraries, you get highly efficient implementations of algorithms that are regularly extended and optimized. Whether you are building a new application or trying to speed up an existing application, NVIDIA's libraries provide the easiest way to get started with GPUs. You can download NVIDIA libraries as part of the CUDA Toolkit.

Download Now >

COMPONENTS

- Deep Learning
- Linear Algebra
- Signal, Image and Video
- Parallel Algorithms

OPENACC DIRECTIVES

OpenACC is a directives-based programming approach to **parallel computing** designed for **performance** and **portability** on CPUs and GPUs for HPC.

Add Simple Compiler Directive

```
main()
 {
  <serial code>
  #pragma acc kernels
  {
    <parallel code>
  }
}
```

OpenACC

Simple | Powerful | Portable

Fueling the Next Wave of Scientific Discoveries in HPC

```
main()
{
  <serial code>
  #pragma acc kernels
  //automatically runs on GPU
  {
    <parallel code>
  }
}
```

University of Illinois
PowerGrid- MRI Reconstruction

70x Speed-Up
2 Days of Effort

RIKEN Japan
NICAM- Climate Modeling

7-8x Speed-Up
5% of Code Modified

8000+

Developers

using OpenACC

http://www.cray.com/sites/default/files/resources/OpenACC_213462.12_OpenACC_Cosmo_CS_FNL.pdf
http://www.hpcwire.com/off-the-wire/first-round-of-2015-hackathons-gets-underway
http://on-demand.gputechconf.com/gtc/2015/presentation/S5297-Hisashi-Yashiro.pdf
http://www.openacc.org/content/experiences-porting-molecular-dynamics-code-gpus-cray-xk7

SINGLE CODE FOR MULTIPLE PLATFORMS

OpenACC - Performance Portable Programming Model for HPC

POWER

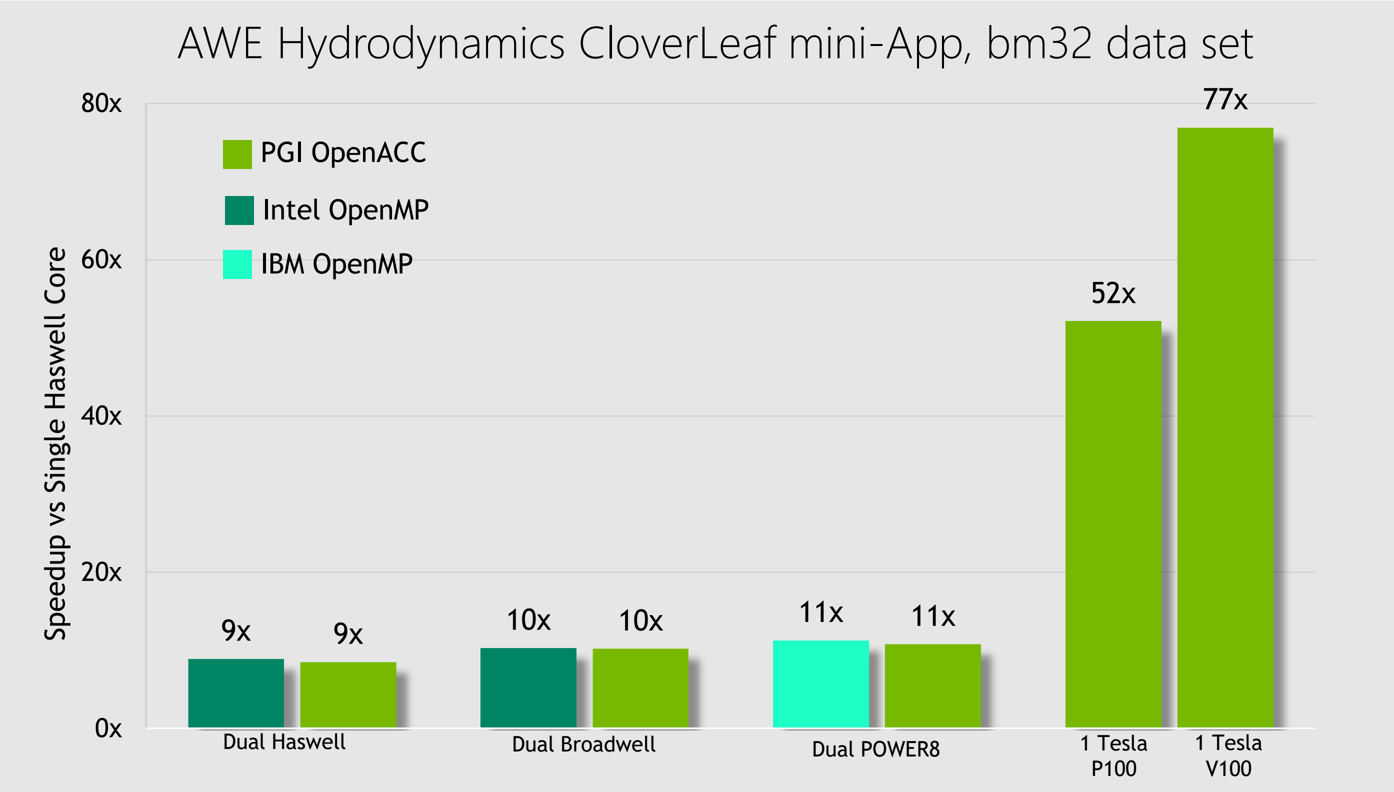
Sunway

x86 CPU

x86 Xeon Phi

NVIDIA GPU

PEZY-SC



Systems: Haswell: 2x16 core Haswell server, four K80s, CentOS 7.2 (perf-hsw10), Broadwell: 2x20 core Broadwell server, eight P100s (dgx1-prd-01), Minsky: POWER8+NVLINK, four P100s, RHEL 7.3 (gsn1).
Compilers: Intel 17.0, IBM XL 13.1.3, PGI 16.10.
Benchmark: CloverLeaf v1.3 downloaded from http://uk-mac.github.io/CloverLeaf the week of November 7 2016; CloverlLeaf_Serial; CloverLeaf_ref (MPI+OpenMP); CloverLeaf_OpenACC (MPI+OpenACC)
Data compiled by PGI November 2016, Volta data collected June 2017

1

OpenACC COMPILER DIRECTIVES

Parallel C Code

```
void saxpy(int n,
           float a,
           float *x,
           float *y)
{
#pragma acc kernels
  for (int i = 0; i < n; ++i)
    y[i] = a*x[i] + y[i];
}

...
// Perform SAXPY on 1M elements
saxpy(1<<20, 2.0, x, y);
...
```

Parallel Fortran Code

```
subroutine saxpy(n, a, x, y)
  real :: x(:), y(:), a
  integer :: n, i
!$acc kernels
  do i=1,n
    y(i) = a*x(i)+y(i)
  enddo
!$acc end kernels
end subroutine saxpy

...
! Perform SAXPY on 1M elements
call saxpy(2**20, 2.0, x_d, y_d)
...
```

http://developer.nvidia.com/openacc or http://openacc.org

PROGRAMMING LANGUAGES

3

CUDA C

```
void saxpy(int n, float a,
           float *x, float *y)
{
    for (int i = 0; i < n; ++i)
        y[i] = a*x[i] + y[i];
}

int N = 1<<20;



// Perform SAXPY on 1M elements
saxpy(N, 2.0, x, y);
```

```
__global__
void saxpy(int n, float a,
           float *x, float *y)
{
    int i = blockIdx.x*blockDim.x + threadIdx.x;
    if (i < n) y[i] = a*x[i] + y[i];
}

int N = 1<<20;
cudaMemcpy(d_x, x, N, cudaMemcpyHostToDevice);
cudaMemcpy(d_y, y, N, cudaMemcpyHostToDevice);

// Perform SAXPY on 1M elements
saxpy<<<4096,256>>>(N, 2.0, d_x, d_y);

cudaMemcpy(y, d_y, N, cudaMemcpyDeviceToHost);
```

http://developer.nvidia.com/cuda-toolkit

4 THRUST C++ TEMPLATE LIBRARY

Serial C++ Code
with STL and Boost

```
int N = 1<<20;
std::vector<float> x(N), y(N);

...




// Perform SAXPY on 1M elements
std::transform(x.begin(), x.end(),
               y.begin(), y.end(),
         2.0f * _1 + _2);
```

www.boost.org/libs/lambda

Parallel C++ Code

```
int N = 1<<20;
thrust::host_vector<float> x(N), y(N);

...

thrust::device_vector<float> d_x = x;
thrust::device_vector<float> d_y = y;

// Perform SAXPY on 1M elements
thrust::transform(d_x.begin(), d_x.end(),
                  d_y.begin(),d_y.begin(),
                  2.0f * _1 + _2)
```

http://thrust.github.com

5

CUDA FORTRAN

Standard Fortran

```
module mymodule contains
  subroutine saxpy(n, a, x, y)
    real :: x(:), y(:), a
    integer :: n, i
    do i=1,n
      y(i) = a*x(i)+y(i)
    enddo
  end subroutine saxpy
end module mymodule

program main
  use mymodule
  real :: x(2**20), y(2**20)
  x = 1.0, y = 2.0
  ! Perform SAXPY on 1M elements
  call saxpy(2**20, 2.0, x, y)
end program main
```

Parallel Fortran

```
module mymodule contains
  attributes(global) subroutine saxpy(n, a, x, y)
    real :: x(:), y(:), a
    integer :: n, i
    attributes(value) :: a, n
    i = threadIdx%x+(blockIdx%x-1)*blockDim%x
    if (i<=n) y(i) = a*x(i)+y(i)
  end subroutine saxpy
end module mymodule

program main
  use cudafor; use mymodule
  real, device :: x_d(2**20), y_d(2**20)
  x_d = 1.0, y_d = 2.0
  ! Perform SAXPY on 1M elements
  call saxpy<<<4096,256>>>(2**20, 2.0, x_d, y_d)
end program main
```

http://developer.nvidia.com/cuda-fortran

6

PYTHON

Standard Python

```
import numpy as np


def saxpy(a, x, y):
  return [a * xi + yi
          for xi, yi in zip(x, y)]

x = np.arange(2**20, dtype=np.float32)
y = np.arange(2**20, dtype=np.float32)



cpu_result = saxpy(2.0, x, y)
```

http://numpy.scipy.org

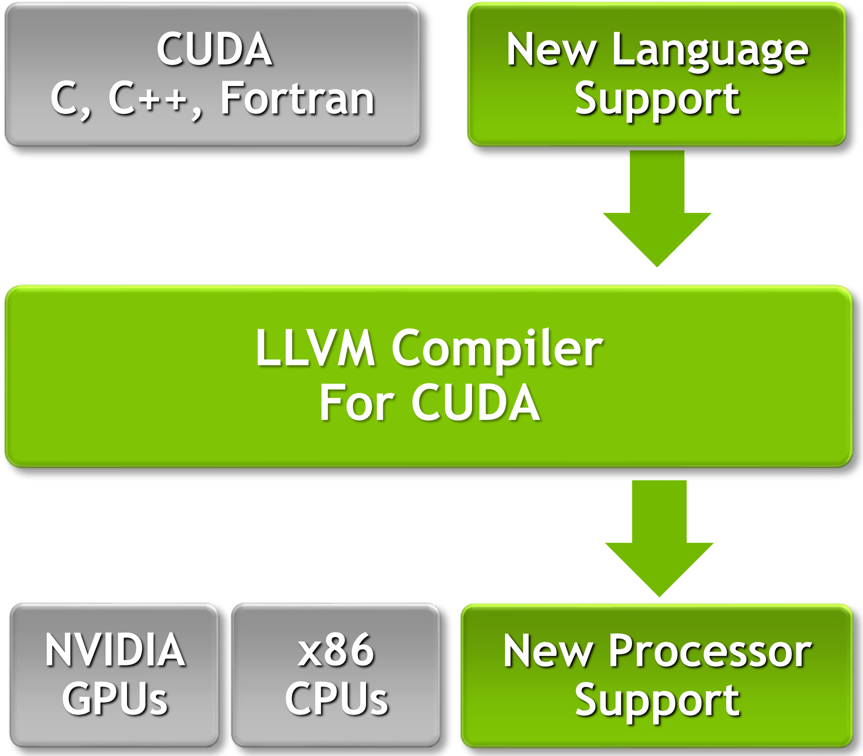
Numba Parallel Python

```
import numpy as np
from numba import vectorize

@vectorize(['float32(float32, float32,
float32)'], target='cuda')
def saxpy(a, x, y):
  return a * x + y

N = 1048576

# Initialize arrays
A = np.ones(N, dtype=np.float32)
B = np.ones(A.shape, dtype=A.dtype)
C = np.empty_like(A, dtype=A.dtype)

# Add arrays onGPU
C = saxpy(2.0, X, Y)
```

https://numba.pydata.org

ENABLING ENDLESS WAYS TO SAXPY

- Build front-ends for Java, Python, R, DSLs
- Target other processors like ARM, FPGA, GPUs, x86



CUDA Compiler Contributed to Open Source LLVM

CUDA TOOLKIT - DOWNLOAD TODAY!

Everything You Need to Accelerate Applications

CUDA DOCUMENTATION

- Installation Guide
- Best Practices Guide
- Programming Guide
- CUDA Tools Guide
- API Reference
- Samples

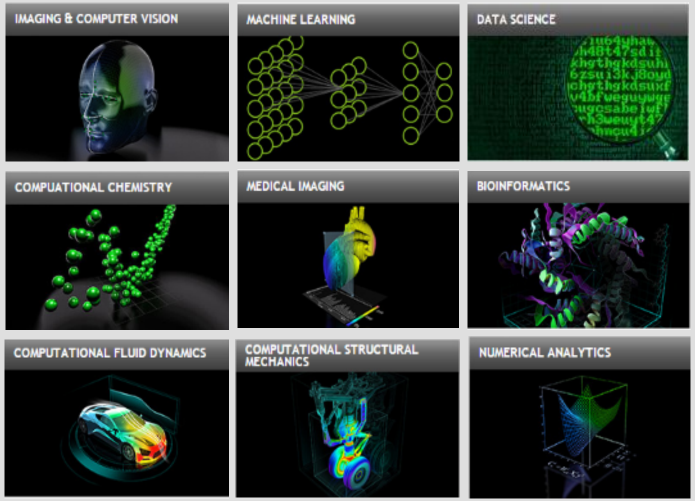
GETTING STARTED RESOURCES

GTC WEBINARS

UDACITY

qwikLABS

INDUSTRY APPLICATIONS



developer.nvidia.com/cuda-toolkit