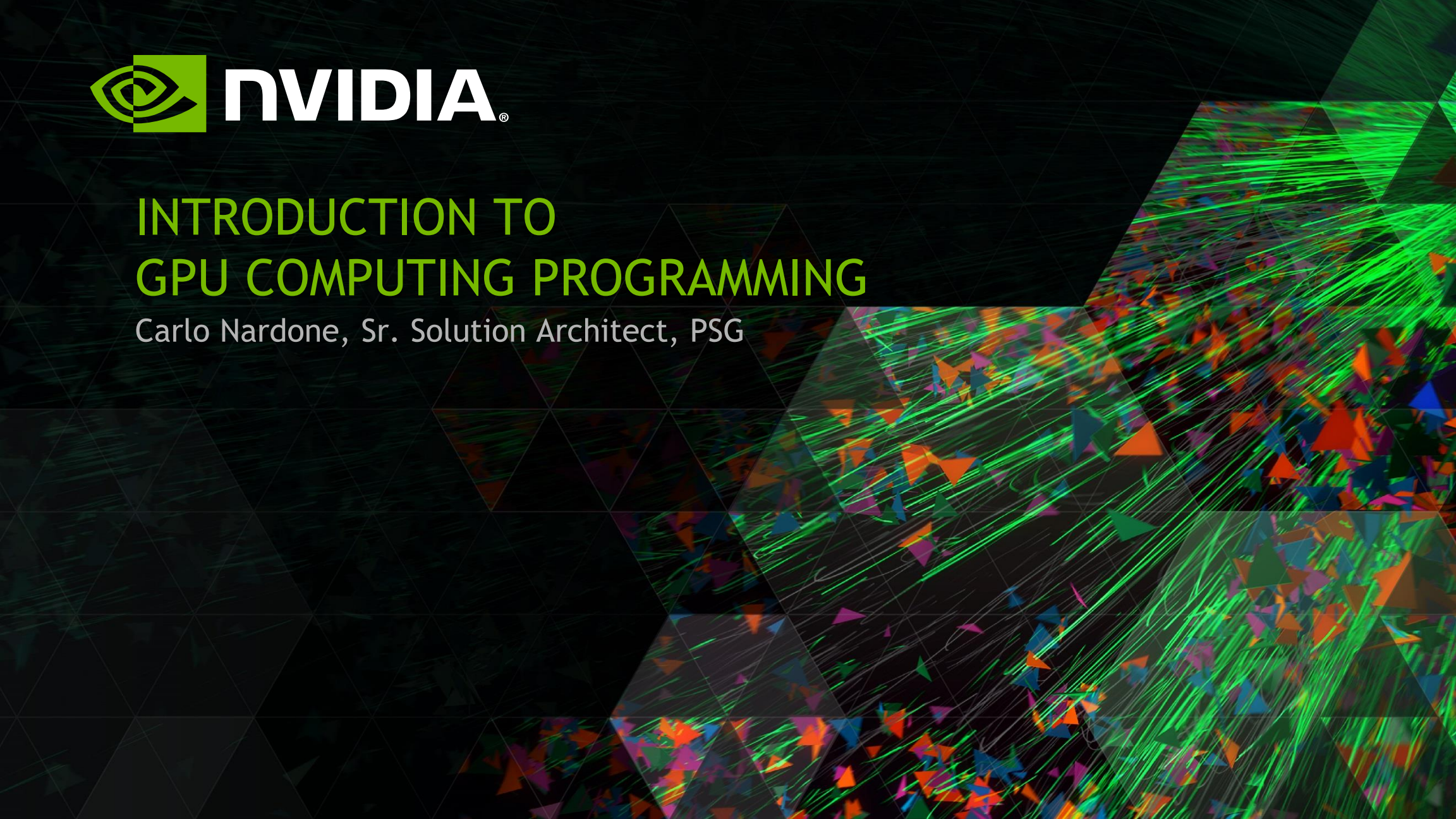


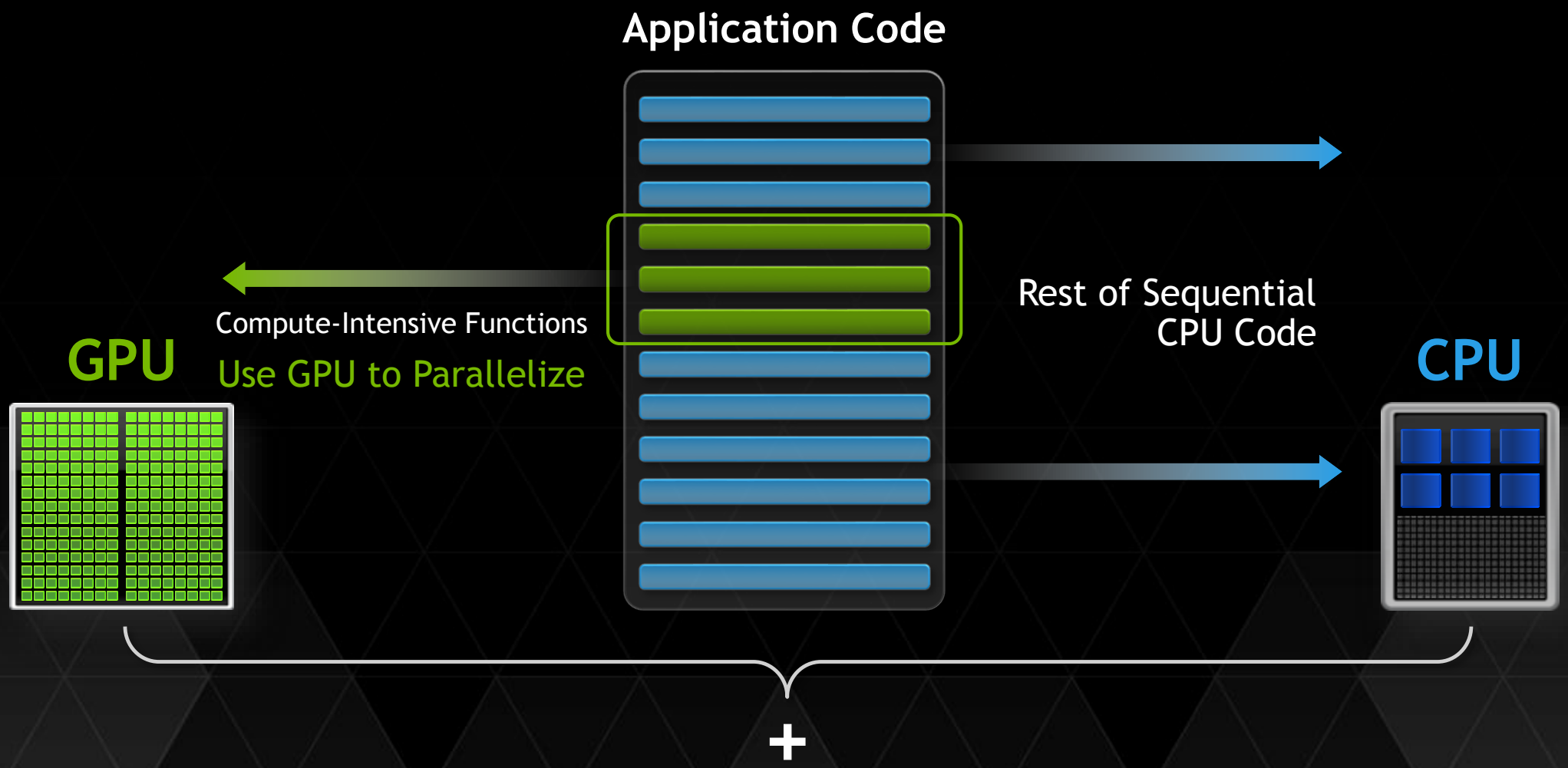
INTRODUCTION TO GPU COMPUTING PROGRAMMING

Carlo Nardone, Sr. Solution Architect, PSG

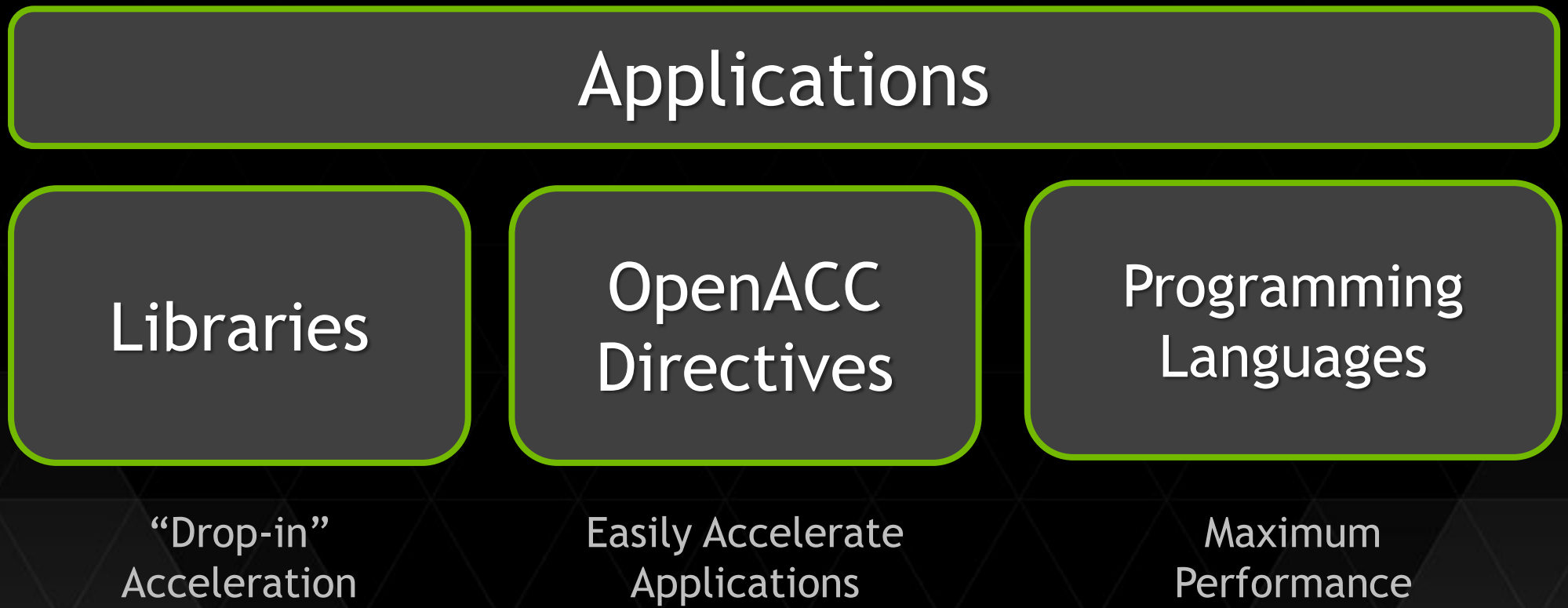
AGENDA

1. Intro
2. Libraries
3. OpenACC
4. Languages
5. An example: 6 ways to SAXPY
6. Software Roadmap

SMALL CHANGES, BIG SPEED-UP



3 WAYS TO ACCELERATE APPLICATIONS



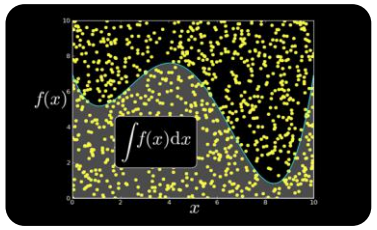
3 WAYS TO ACCELERATE APPLICATIONS

LIBRARIES: EASY, HIGH-QUALITY ACCELERATION

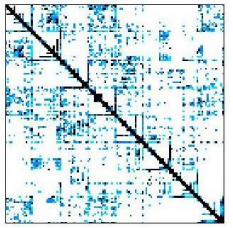
- **Ease of use:** Using libraries enables GPU acceleration without in-depth knowledge of GPU programming
- **"Drop-in":** Many GPU-accelerated libraries follow standard APIs, thus enabling acceleration with minimal code changes
- **Quality:** Libraries offer high-quality implementations of functions encountered in a broad range of applications
- **Performance:** NVIDIA libraries are tuned by experts

SOME GPU-ACCELERATED LIBRARIES

NVIDIA cuBLAS



NVIDIA cuRAND



NVIDIA cuSPARSE

NVIDIA NPP

GPU VSIPL

Vector Signal Image Processing

CULA tools

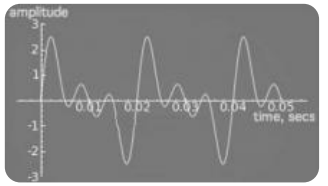
GPU Accelerated Linear Algebra

MAGMA

ICL UT

Matrix Algebra on GPU and Multicore

open source initiative



NVIDIA cuFFT

ROGUE WAVE SOFTWARE

IMSL Library

ArrayFire Matrix Computations

CUSP

Sparse Linear Algebra

open source initiative

Thrust

C++ STL Features for CUDA

open source initiative

NVIDIA

3 STEPS TO CUDA-ACCELERATED APPLICATION

- **Step 1:** Substitute library calls with equivalent CUDA library calls

  `saxpy ( … )` ➔ `cublasSaxpy ( … )`

- **Step 2:** Manage data locality

  - with CUDA: `cudaMalloc(), cudaMemcpy(), etc.`
  - with CUBLAS: `cublasAlloc(), cublasSetVector(), etc.`

- **Step 3:** Rebuild and link the CUDA-accelerated library

  ```
  nvcc myobj.o –l cublas
  ```

DROP-IN ACCELERATION (STEP 1)

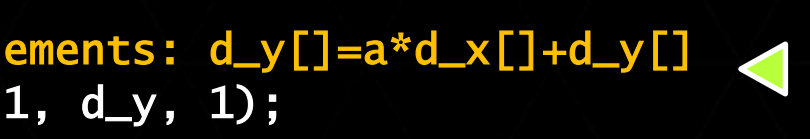
```
int N = 1 << 20;
```

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

DROP-IN ACCELERATION (STEP 1)

```
int N = 1 << 20;
```

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



DROP-IN ACCELERATION (STEP 2)

```
int N = 1 << 20;
cublasInit();
```

Initialize CUBLAS

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

```
cublasShutdown();
```

Shut down CUBLAS

DROP-IN ACCELERATION (STEP 2)

```
int N = 1 << 20;
cublasInit();
cublasAlloc(N, sizeof(float), (void**)&d_x);
cublasAlloc(N, sizeof(float), (void*)&d_y);
```

Allocate device vectors

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

```
cublasFree(d_x);
cublasFree(d_y);
cublasShutdown();
```

Deallocate device vectors

DROP-IN ACCELERATION (STEP 2)

```
int N = 1 << 20;
cublasInit();
cublasAlloc(N, sizeof(float), (void**)&d_x);
cublasAlloc(N, sizeof(float), (void*)&d_y);

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: d_y[]=a*d_x[]+d_y[]
cublasSaxpy(N, 2.0, d_x, 1, d_y, 1);

cublasGetVector(N, sizeof(y[0]), d_y, 1, y, 1);

cublasFree(d_x);
cublasFree(d_y);
cublasShutdown();
```

Transfer data to GPU

Read data back GPU

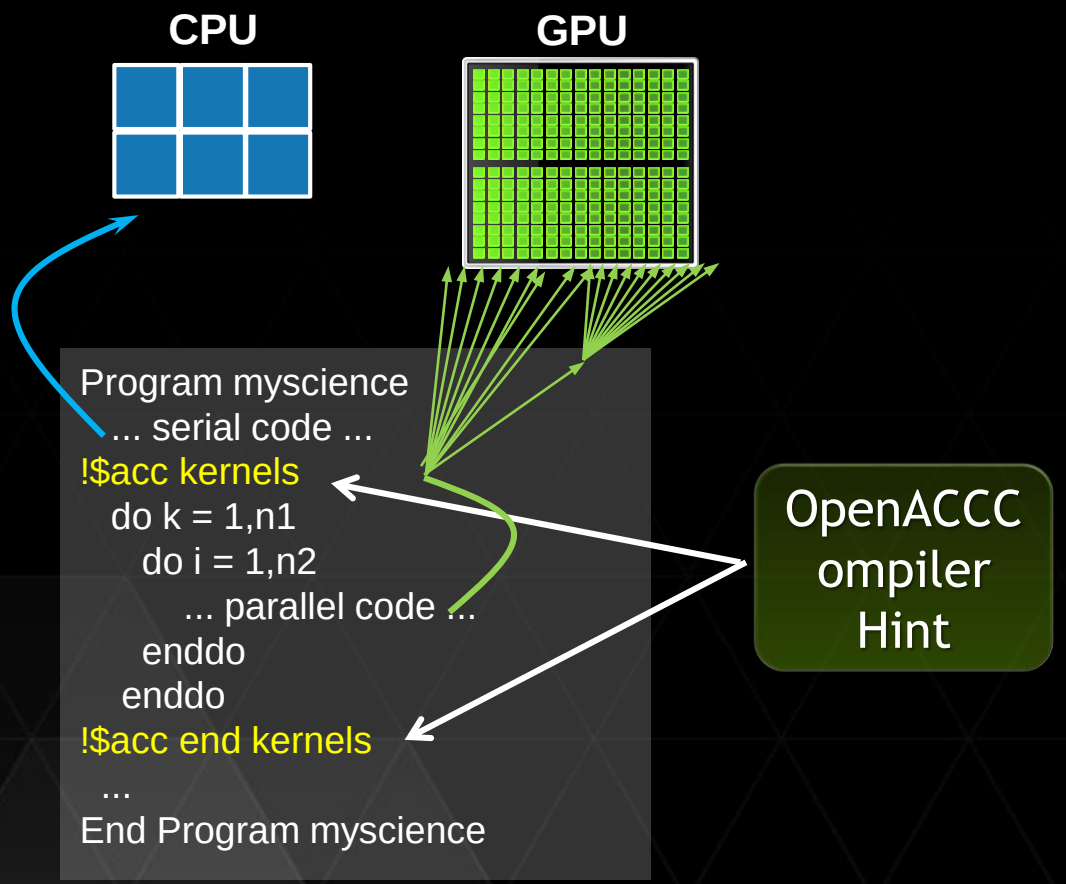
EXPLORE THE CUDA (LIBRARIES) ECOSYSTEM

- CUDA Tools and Ecosystem described in detail on NVIDIA Developer Zone:

developer.nvidia.com/cuda-tools-ecosystem

3 WAYS TO ACCELERATE APPLICATIONS

OPENACC DIRECTIVES



Simple Compiler hints

Compiler Parallelizes code

Works on many-core GPUs & multicore CPUs

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

OpenACC
The Standard for GPU Directives

- **Easy:** Directives are the easy path to accelerate compute intensive applications
- **Open:** OpenACC is an open GPU directives standard, making GPU programming straightforward and portable across parallel and multi-core processors
- **Powerful:** GPU Directives allow complete access to the massive parallel power of a GPU

2 BASIC STEPS TO GET STARTED

- **Step 1:** Annotate source code with directives:

```
!$acc data copy(util1,util2,util3) copyin(ip,scp2,scp2i)
  !$acc parallel loop
  …
  !$acc end parallel
!$acc end data
```

- **Step 2:** Compile & run:

```
pgf90 -ta=nvidia -Minfo=accel file.f
```

OPENACC DIRECTIVES EXAMPLE

```
!$acc data copy(A,Anew)
 iter=0
 do while ( err > tol .and. iter < iter_max )

  iter = iter +1
  err=0._fp_kind

!$acc kernels
   do j=1,m
    do i=1,n
     Anew(i,j) = .25_fp_kind *( A(i+1,j  ) + A(i-1,j  ) &
                               +A(i  ,j-1) + A(i  ,j+1))
     err = max( err, Anew(i,j)-A(i,j))
    end do
   end do
!$acc end kernels
   IF(mod(iter,100)==0 .or. iter == 1)    print *, iter, err
   A= Anew

 end do
!$acc end data
```

Copy arrays into GPU memory within data region

Parallelize code inside region

Close off parallel region

Close off data region, copy data back

Directives: Easy & Powerful

Real-Time Object Detection

Global Manufacturer of Navigation Systems

5x in 40 Hours

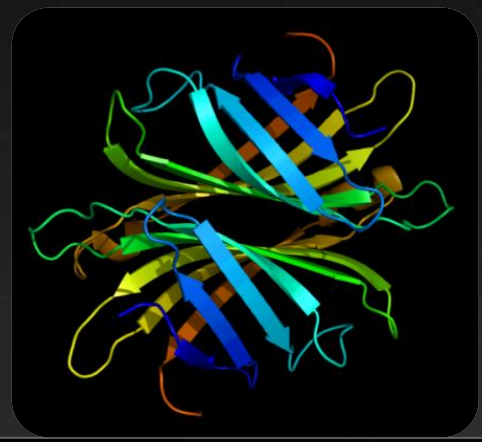
Valuation of Stock Portfolios using Monte Carlo

Global Technology Consulting Company

2x in 4 Hours

Interaction of Solvents and Biomolecules

University of Texas at San Antonio



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

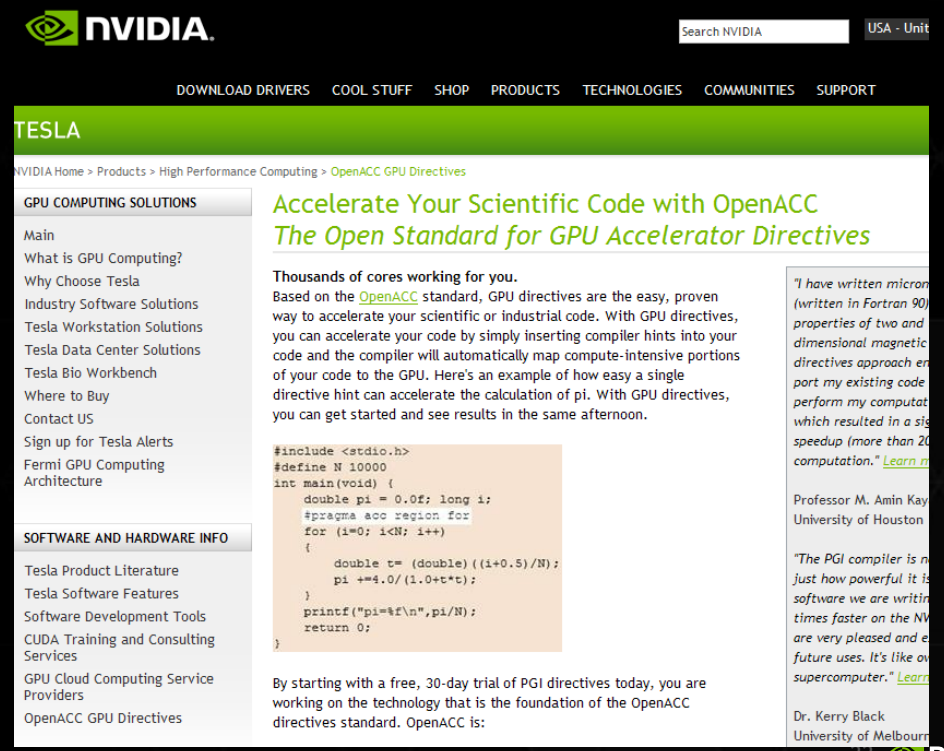
START NOW WITH OPENACC DIRECTIVES

Sign up for a free trial of the directives compiler now!

Free trial license to PGI Accelerator

Tools for quick ramp

www.nvidia.com/gpudirectives



NVIDIA

PGI®

3 WAYS TO ACCELERATE APPLICATIONS

GPU PROGRAMMING LANGUAGES

Numerical analytics	MATLAB, Mathematica, LabVIEW
Fortran	OpenACC, CUDA Fortran
C	OpenACC, CUDA C
C++	Thrust, CUDA C++
Python	PyCUDA, Copperhead
C#	GPU.NET

CUDA C

Standard C Code

```
void saxpy_serial(int n,
                  float a,
                  float *x,
                  float *y)
{

  for (int i = 0; i < n; ++i)
    y[i] = a*x[i] + y[i];
}

// Perform SAXPY on 1M elements
saxpy_serial(4096*256, 2.0, x, y);
```

Parallel C Code

```
__global__
void saxpy_parallel(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];
}

// Perform SAXPY on 1M elements
saxpy_parallel<<<4096,256>>>(n,2.0,x,y);
```

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

CUDA C++: DEVELOP GENERIC PARALLEL CODE

CUDA C++ features enable sophisticated and flexible applications and middleware

- Class hierarchies
- __device__ methods
- Templates
- Operator overloading
- Functors (function objects)
- Device-side new/delete
- More…

```
template <typename T>
struct Functor {
  __device__ Functor(_a) : a(_a) {}
  __device__ T operator(T x) { return a*x; }
  T a;
}

template <typename T, typename Oper>
__global__ void kernel(T *output, int n) {
  Oper op(3.7);
  output = new T[n]; // dynamic allocation
  int i = blockIdx.x*blockDim.x + threadIdx.x;
  if (i < n)
    output[i] = op(i);  // apply functor
}
```

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

RAPID PARALLEL C++ DEVELOPMENT

- Resembles C++ STL
- High-level interface
  - Enhances developer productivity
  - Enables performance portability between GPUs and multicore CPUs
- Flexible
  - CUDA, OpenMP, and TBB backends
  - Extensible and customizable
  - Integrates with existing software
- Open source


```
// generate 32M random numbers on host
thrust::host_vector<int> h_vec(32 << 20);
thrust::generate(h_vec.begin(),
                 h_vec.end(),
                 rand);

// transfer data to device (GPU)
thrust::device_vector<int> d_vec = h_vec;

// sort data on device
thrust::sort(d_vec.begin(), d_vec.end());

// transfer data back to host
thrust::copy(d_vec.begin(),
             d_vec.end(),
             h_vec.begin());
```

http://developer.nvidia.com/thrust or http://thrust.googlecode.com

CUDA FORTRAN

- Program GPU using Fortran
  - Key language for HPC
- Simple language extensions
  - Kernel functions
  - Thread / block IDs
  - Device & data management
  - Parallel loop directives
- Familiar syntax
  - Use allocate, deallocate
  - Copy CPU-to-GPU with assignment (=)

```
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
  call saxpy<<<4096,256>>>(2**20,3.0,x_d,y_d,)
  y = y_d
  write(*,*) 'max error=', maxval(abs(y-5.0))
end program main
```

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

MORE PROGRAMMING LANGUAGES

Python ▶ PyCUDA 

C# .NET ▶ GPU.NET tidepowerd

Numerical Analytics ▶ MATLAB The Language of Technical Computing Wolfram Mathematica 8

GET STARTED TODAY

These languages are supported on all CUDA-capable GPUs.

You might already have a CUDA-capable GPU in your laptop or desktop PC!

CUDA C/C++
http://developer.nvidia.com/cuda-toolkit

Thrust C++ Template Library
http://developer.nvidia.com/thrust

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

PyCUDA (Python)
http://mathema.tician.de/software/pycuda

GPU.NET
http://tidepowerd.com

MATLAB
http://www.mathworks.com/discovery/matlab-gpu.html

Mathematica
http://www.wolfram.com/mathematica/new-in-8/cuda-and-opencl-support/

An Example: 6 Ways to SAXPY

SINGLE PRECISION ALPHA X PLUS Y (SAXPY)

Part of Basic Linear Algebra Subroutines (BLAS) Library

$$z = \alpha x + y$$

x, y, z : vector

α : scalar

GPU SAXPY in multiple languages and libraries

A menagerie* of possibilities, not a tutorial

*technically, a *program chrestomathy*: http://en.wikipedia.org/wiki/Chrestomathy

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

2 CUBLAS LIBRARY

Serial BLAS Code

```
int N = 1<<20;


...

// Use your choice of blas library

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

Parallel cuBLAS Code

```
int N = 1<<20;


cublasInit();
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
cublasSaxpy(N, 2.0, d_x, 1, d_y, 1);

cublasGetVector(N, sizeof(y[0]), d_y, 1, y, 1);

cublasShutdown();
```

You can also call cuBLAS from Fortran, C++, Python, and other languages

http://developer.nvidia.com/cublas

CUDA C

Standard 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);
```

Parallel C

```
__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

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

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

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

Copperhead: Parallel Python

```
from copperhead import *
import numpy as np

@cu
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)

with places.gpu0:
  gpu_result = saxpy(2.0, x, y)

with places.openmp:
  cpu_result = saxpy(2.0, x, y)
```

http://copperhead.github.com

ENABLING ENDLESS WAYS TO SAXPY

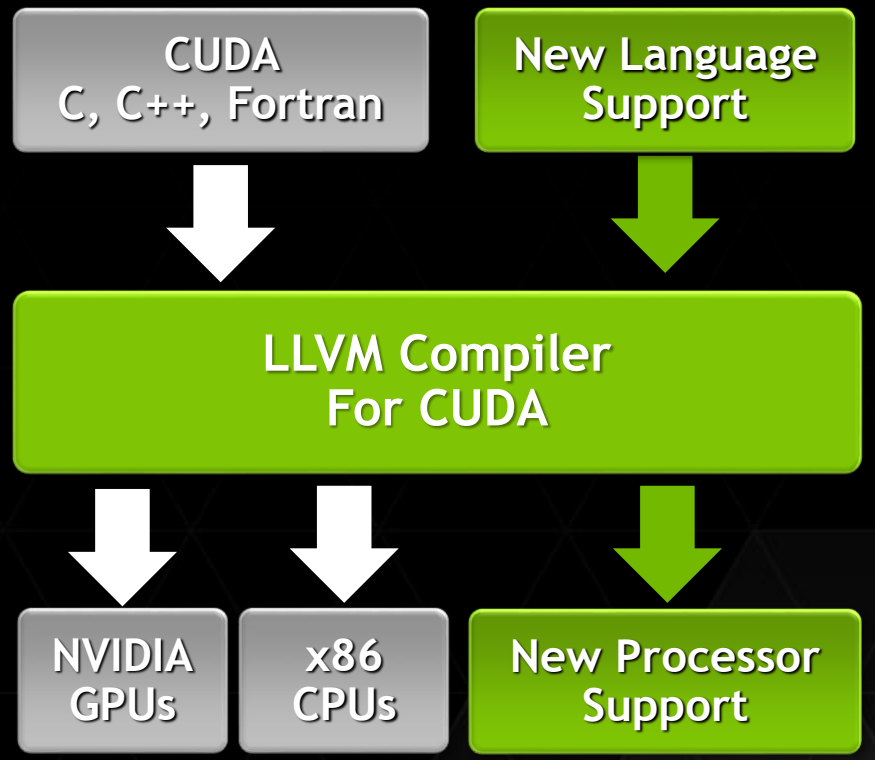
Developers want to build front-ends for

Java, Python, R, DSLs

Target other processors like

ARM, FPGA, GPUs, x86

CUDA Compiler Contributed to Open Source LLVM

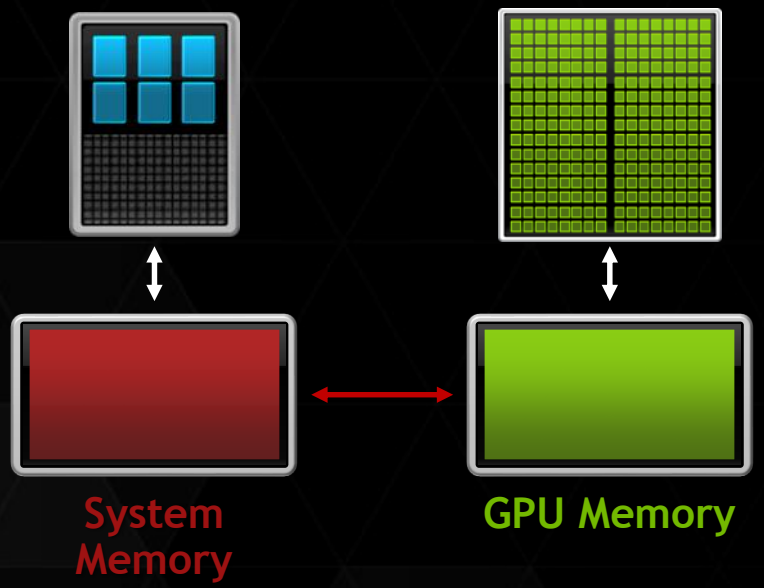


Software Roadmap

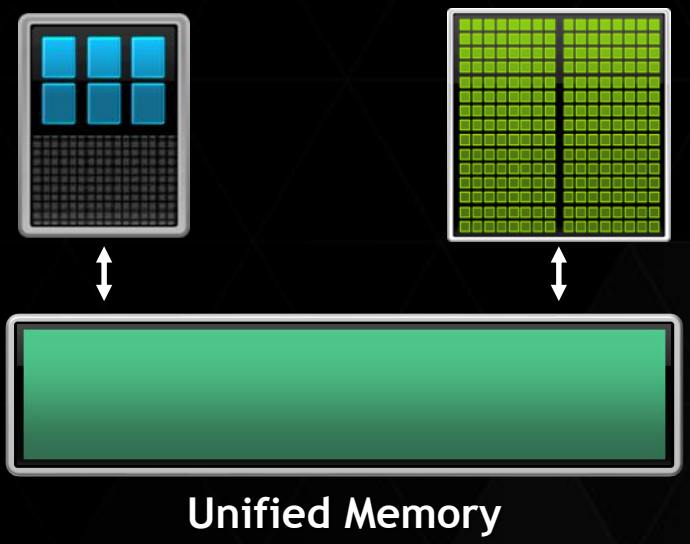
UNIFIED MEMORY

Dramatically Lower Developer Effort

Developer View Today



Developer View With Unified Memory



UNIFIED MEMORY DELIVERS

1. Simpler Programming & Memory Model
   - Single pointer to data, accessible anywhere
   - Tight language integration
   - Greatly simplifies code porting

2. Performance Through Data Locality
   - Migrate data to accessing processor
   - Guarantee global coherency
   - Still allows *cudaMemcpyAsync()* hand tuning

SIMPLIFIED MEMORY MANAGEMENT

CPU Code

```
void sortfile(FILE *fp, int N) {
  char *data;
  data = (char *)malloc(N);

  fread(data, 1, N, fp);

  qsort(data, N, 1, compare);


  use_data(data);

  free(data);
}
```

CUDA 6 Code with Unified Memory

```
void sortfile(FILE *fp, int N) {
  char *data;
  cudaMallocManaged(&data, N);

  fread(data, 1, N, fp);

  qsort<<<...>>>(data,N,1,compare);
  cudaDeviceSynchronize();

  use_data(data);

  cudaFree(data);
}
```

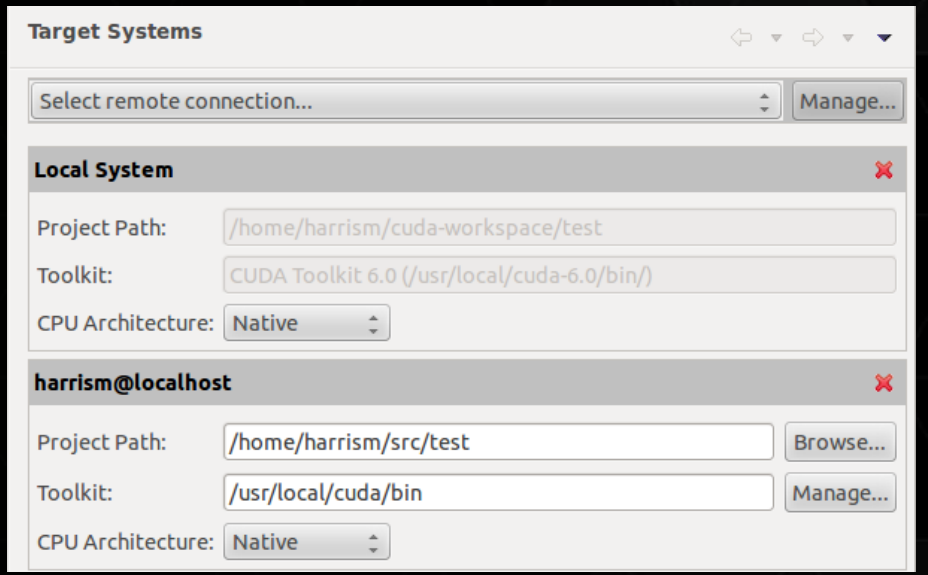
GRAFICAL & CLI PROFILING TOOLS

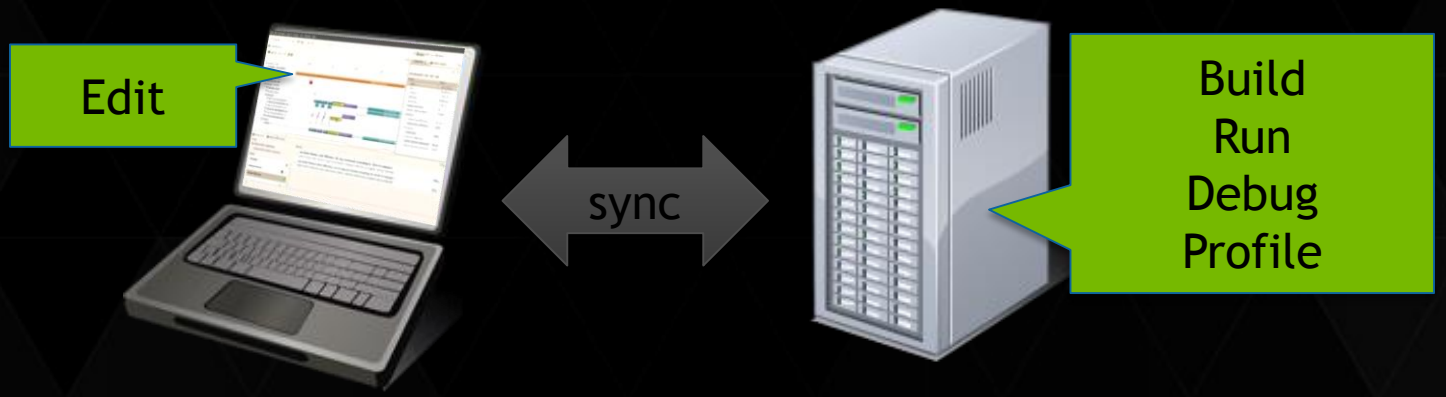
- NVIDIA® Visual Profiler
  - Standalone (nvvp)
  - Integrated into NVIDIA® Nsight™ Eclipse Edition (nsight)
- nvprof *
- NVIDIA® Nsight™ Visual Studio Edition
- Old environment variable based command-line profiler still available *

* Android CUDA APK profiling not supported (yet)

REMOTE DEVELOPMENT TOOLS

- Local IDE, remote application
  - Edit locally, build & run remotely
  - Automatic sync via ssh
  - Cross-compilation to ARM
- Full debugging & profiling via remote connection





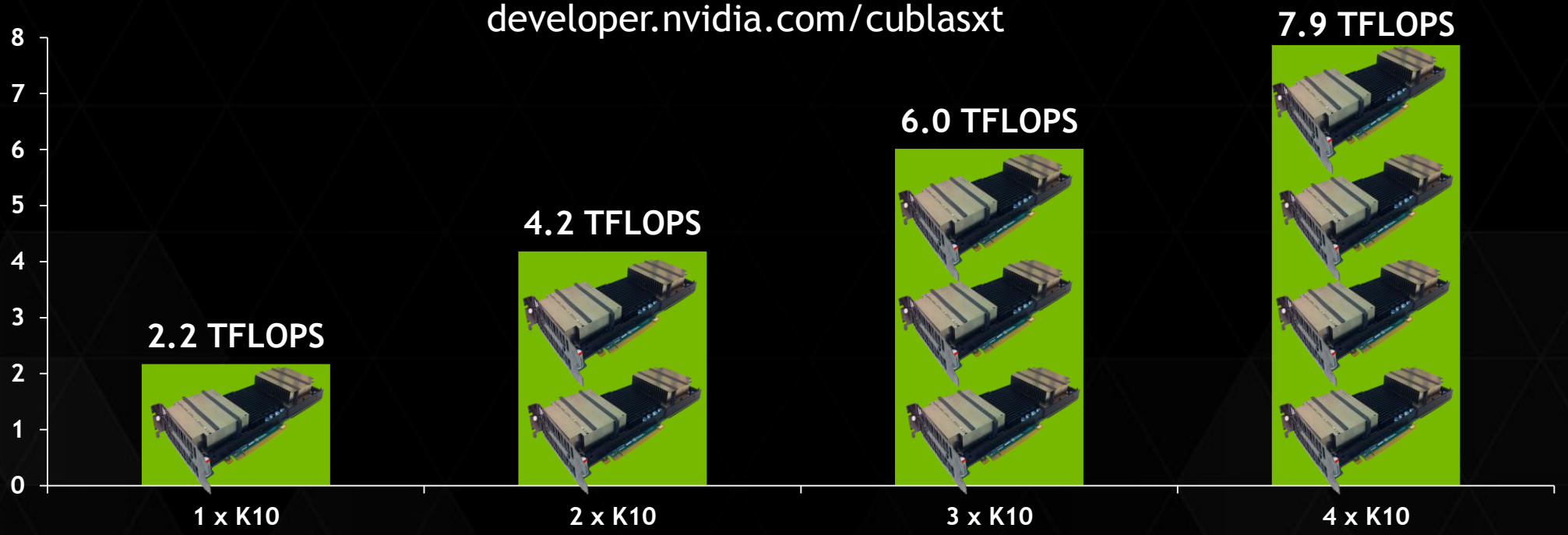
EXTENDED (XT) LIBRARY INTERFACES

Automatic Scaling to multiple GPUs per node

cuFFT 2D/3D & cuBLAS level 3

Operate directly on large datasets that reside in CPU memory

developer.nvidia.com/cublasxt



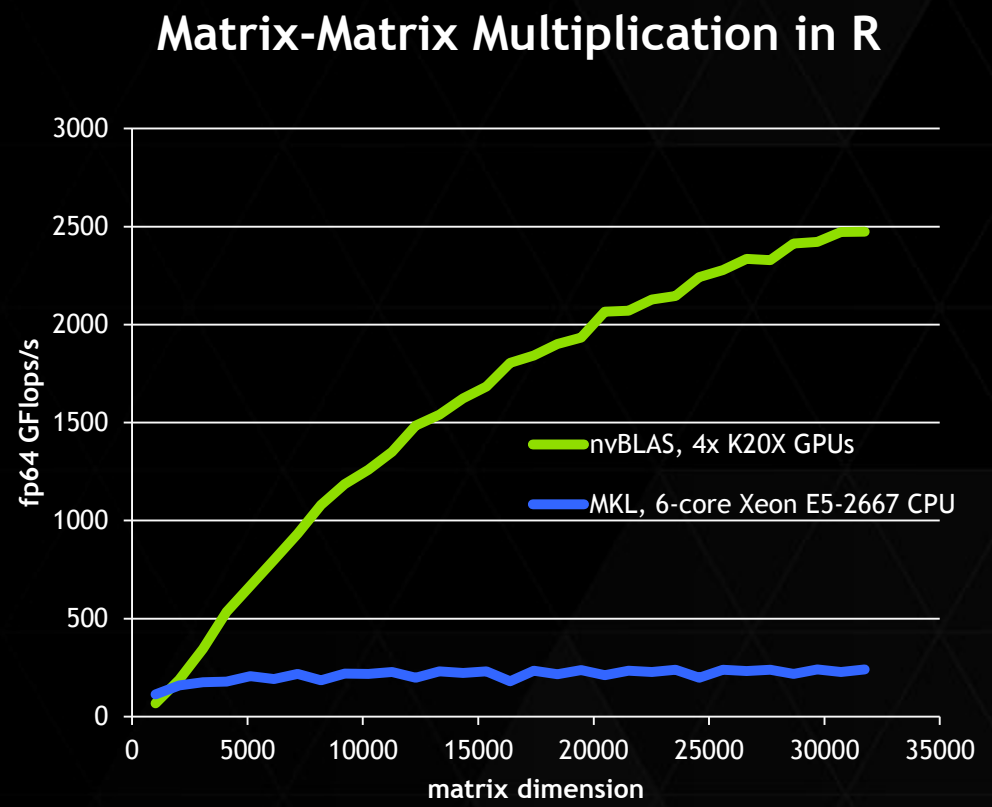
16K x 16K SGEMM on Tesla K10

NEW DROP-IN NVBLAS LIBRARY

- Drop-in replacement for CPU-only BLAS
  - Automatically route BLAS3 calls to cuBLAS
- Example: Drop-in Speedup for R

```
> LD_PRELOAD=/usr/local/cuda/lib64/libnvblas.so R
> A <- matrix(rnorm(4096*4096), nrow=4096, ncol=4096)
> B <- matrix(rnorm(4096*4096), nrow=4096, ncol=4096)
> system.time(C <- A %*% B)
   user  system elapsed
  0.348   0.142   0.289
```

- Use in any app that uses standard BLAS3
  - Octave, Scilab, etc.



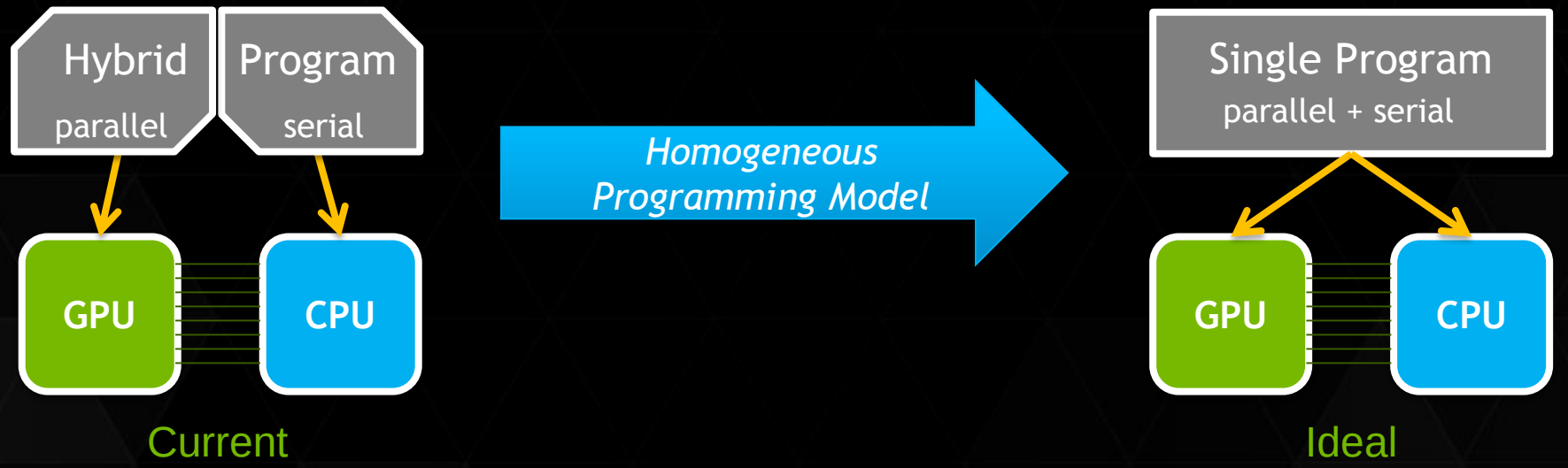
GOALS FOR THE CUDA PLATFORM

Simplicity	• Learn, adopt, & use parallelism with ease
Productivity	• Quickly achieve feature & performance goals
Portability	• Write code that can execute on all targets
Performance	• High absolute performance and scalability

SIMPLER HETEROGENEOUS APPLICATIONS

We want: *homogeneous* programs, *heterogeneous* execution

- Unified programming model includes parallelism in language
- Abstract heterogeneous execution via Runtime or Virtual Machine



PARALLELISM IN MAINSTREAM LANGUAGES

- Enable more programmers to write parallel software
- Give programmers the choice of language to use
- GPU support in key languages

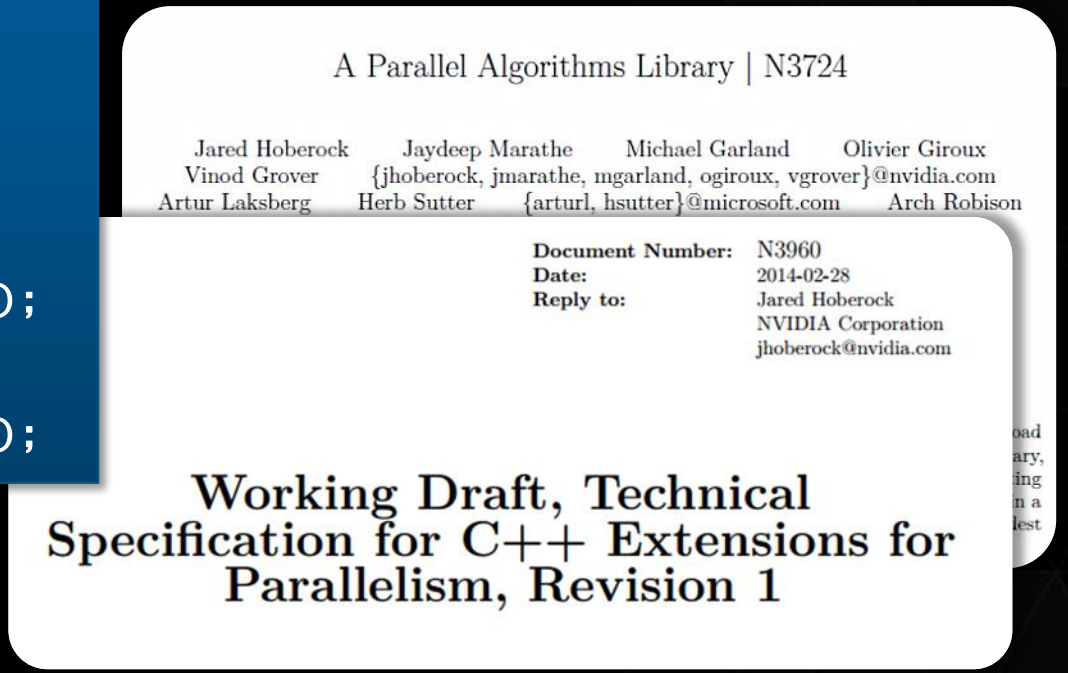
C++ PARALLEL ALGORITHMS LIBRARY

```
std::vector<int> vec = ...

// previous standard sequential loop
std::for_each(vec.begin(), vec.end(), f);

// explicitly sequential loop
std::for_each(std::seq, vec.begin(), vec.end(), f);

// permitting parallel execution
std::for_each(std::par, vec.begin(), vec.end(), f);
```



A Parallel Algorithms Library | N3724

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Document Number: N3960
Date: 2014-02-28
Reply to: Jared Hoberock
NVIDIA Corporation
jhoberock@nvidia.com

Working Draft, Technical Specification for C++ Extensions for Parallelism, Revision 1

- Complete set of parallel primitives: for_each, sort, reduce, scan, etc.
- ISO C++ committee voted unanimously to accept as official tech. specification working draft

N3960 Technical Specification Working Draft:
http://www.open-std.org/jtc1/sc22/wg21/docs/papers/2014/n3960.pdf
Prototype:
https://github.com/n3554/n3554

GNU LINUX GCC TO SUPPORT OPENACC

- **Open Source**
  - GCC Efforts by Samsung & Mentor Graphics
- **Pervasive Impact**
  - Free to all Linux users
- **Mainstream**
  - Most Widely Used HPC Compiler

OpenACC®
DIRECTIVES FOR ACCELERATORS

Incorporating OpenACC into GCC is an excellent example of open source and open standards working together to make accelerated computing broadly accessible to all Linux developers. ”

Oscar Hernandez
Oak Ridge National Laboratories

OAK RIDGE National Laboratory

NUMBA PYTHON COMPILER

- Free and open source compiler for array-oriented Python
- NEW numba.cuda module integrates CUDA directly into Python

```
@cuda.jit("void(float32[:], float32, float32[:], float32[:])")
def saxpy(out, a, x, y):
    i = cuda.grid(1)
    out[i] = a * x[i] + y[i]

# Launch saxpy kernel
saxpy[griddim, blockdim](out, a, x, y)
```

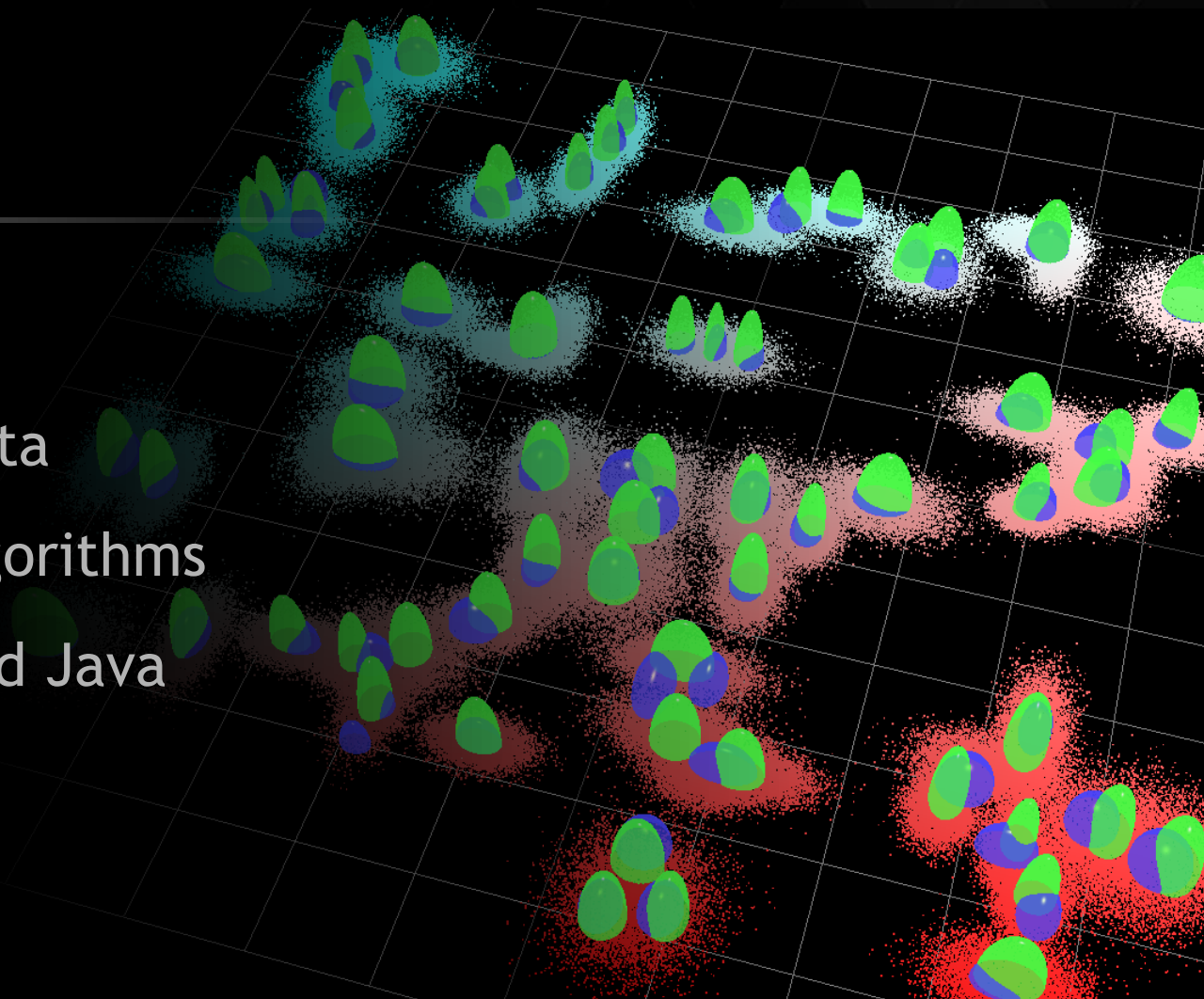
- http://numba.pydata.org/

GPU-ACCELERATED HADOOP

Extract insights from customer data

Data Analytics using clustering algorithms

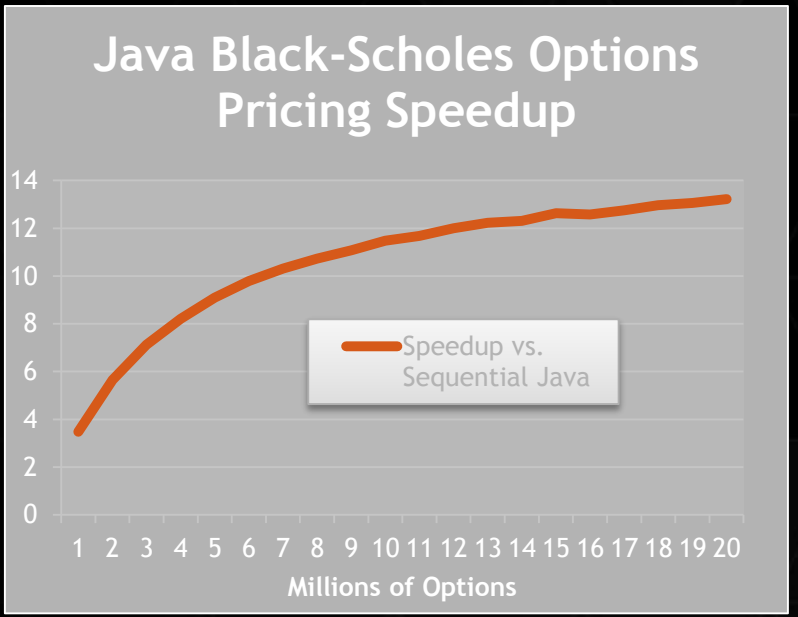
Developed using CUDA-accelerated Java



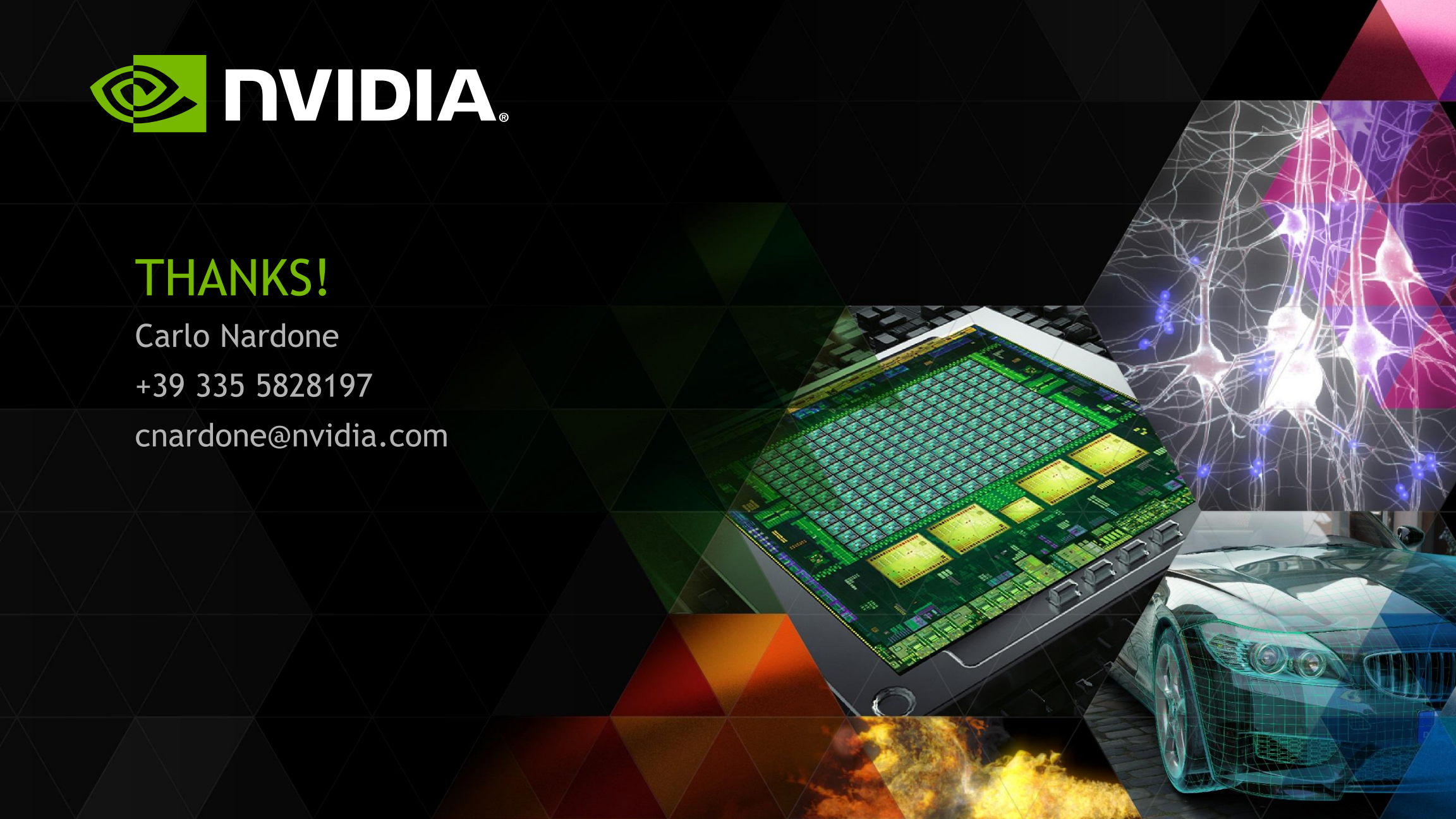
COMPILE JAVA FOR GPUS

- Approach: apply a closure to a set of arrays

```
// vector addition
float[] X = {1.0, 2.0, 3.0, 4.0, … };
float[] Y = {9.0, 8.1, 7.2, 6.3, … };
float[] Z = {0.0, 0.0, 0.0, 0.0, … };
jog.foreach(X, Y, Z, new jogContext(),
  new jogClosureRet<jogContext>() {
    public float execute(float x, float y) {
      return x + y;
    }
  }
);
```



- foreach iterations parallelized over GPU threads
  - Threads run closure `execute()` method



THANKS!

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