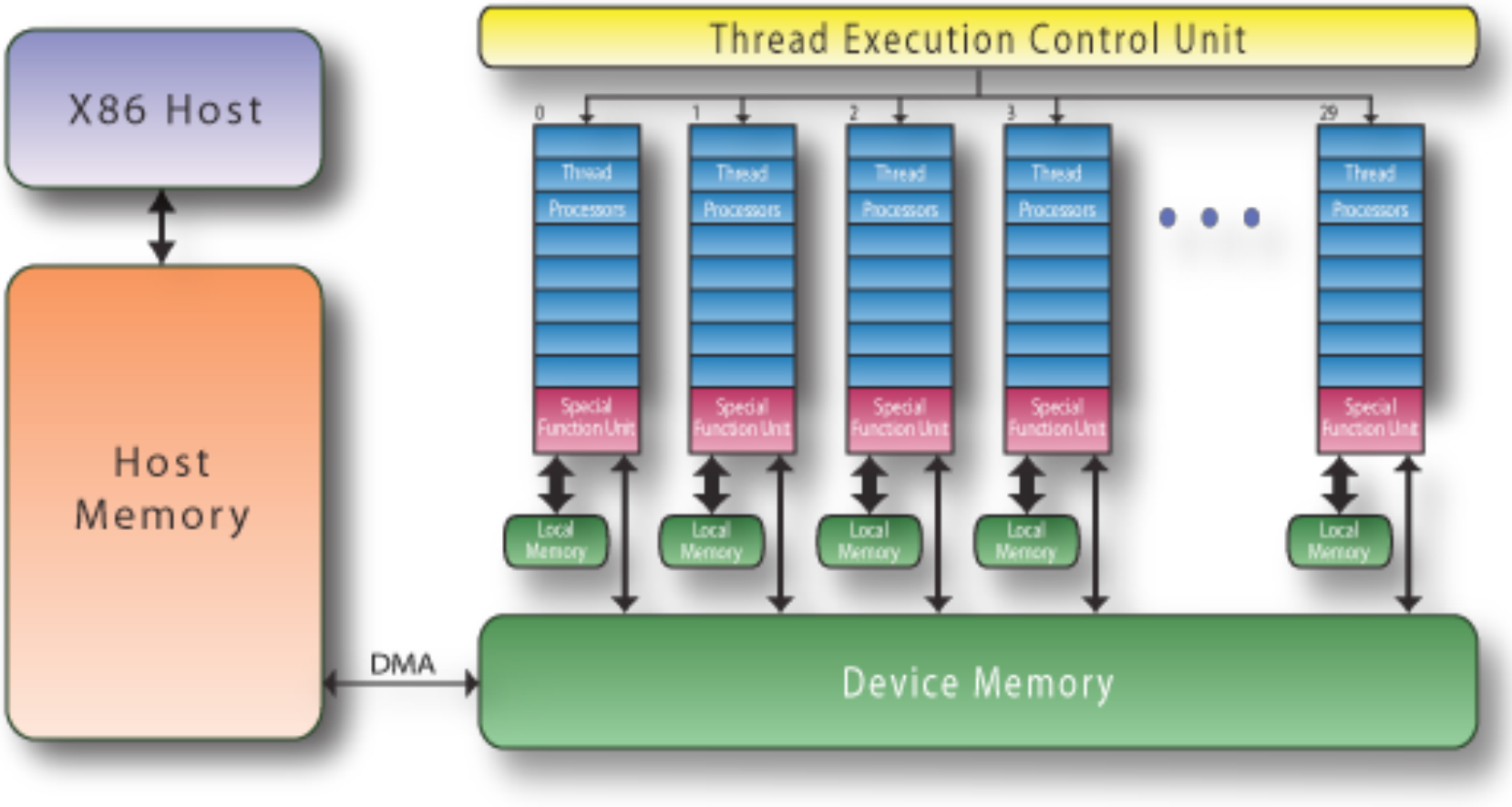
Programming GPUs with OpenACC

Saber Feki
Computational Scientist Lead
Supercomputing Core Laboratory, KAUST
saber.feki@kaust.edu.sa

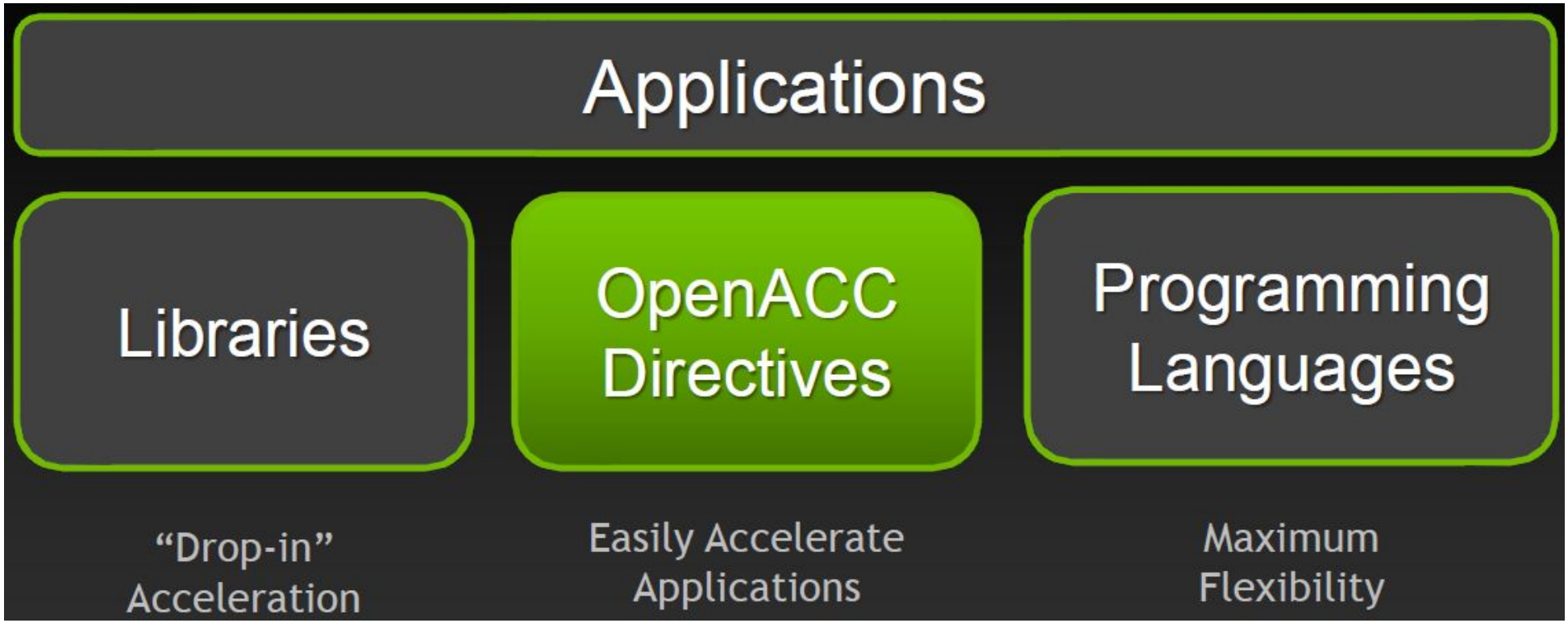
GPU architecture

CPU-GPU memory model



PCIe Interconnect 16X - 8GB/s (gen 2) and 15.75GB/s (gen 3), very thin pipe!
Kepler K40 2,880 cuda cores 1.48 Tflops/s

GPU programming



OpenACC, the standard

- By NVIDIA, CRAY, PGI and CAPS
- The standard was announced in Nov 2011 at SC11 conference
- http://www.openacc-standard.org
- OpenACC 2.0 released in summer 2013
- Now, 20+ partners from academia and industry

OpenACC
DIRECTIVES FOR ACCELERATORS

OpenACC advantages

- **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

PGI and CAPS compilers study (I)

```
#pragma acc kernels
{
for ( l = 0 ;  l < nt; ++l) {  // time loop
#pragma acc loop independent collapse (3)
  for (int i = 0; i < n; ++i){
    for (int j = 0; j < n; ++j){
      for (int k = 0; k < n; ++k){
        B[i][j][k] = B[i]][j][k] + ....
      }
    }
  }

#pragma acc loop independent collapse (3)
  for (int i = 0; i < n; ++i){
    for (int j = 0; j < n; ++j){
      for (int k = 0; k < n; ++k){
        B[i][j][k] = B[i]][j][k] + ....
      }
    }
  }
 } // end time loop
}
```

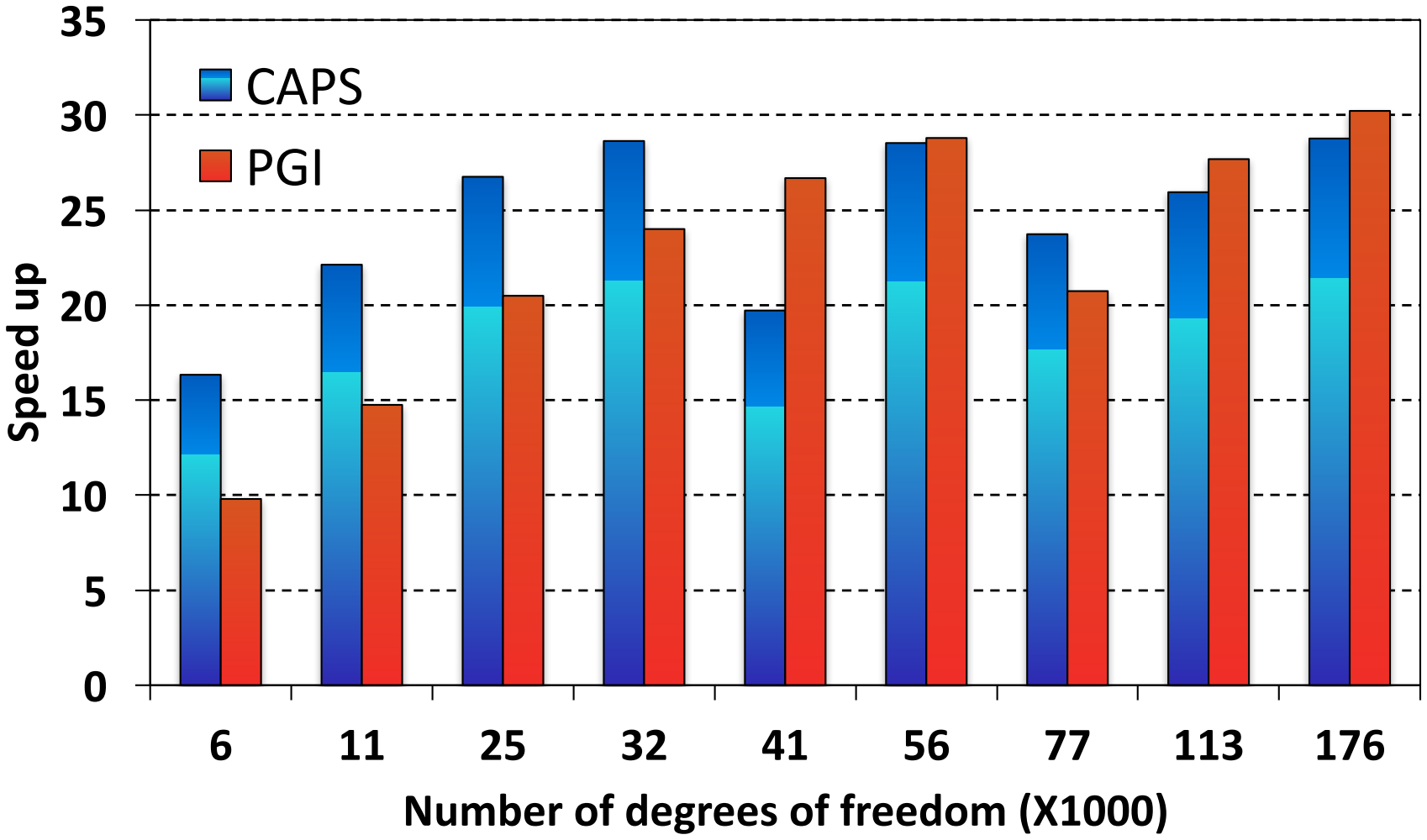
CAPS

```
#pragma acc data
for ( l = 0 ;  l < nt; ++l) {  // time
loop
#pragma acc kernels
#pragma acc loop independent gang
  for (int i = 0; i < n; ++i){
#pragma acc loop independent gang,vector
    for (int j = 0; j < n; ++j){
#pragma acc loop independent gang,vector
      for (int k = 0; k < n; ++k){
        B[i][j][k] = B[i]][j][k] + ....
   } } }
#pragma acc kernels
#pragma acc loop independent gang
  for (int i = 0; i < n; ++i){
#pragma acc loop independent gang,vector
    for (int j = 0; j < n; ++j){
#pragma acc loop independent gang,vector
      for (int k = 0; k < n; ++k){
        B[i][j][k] = B[i]][j][k] + ....
   } } }
 } // end time loop
```

PGI

S. Feki, A. Al-Jarro, H. Bağcı. Porting an Explicit Time Domain Volume Integral Equation Solver on GPUs with OpenACC, IEEE Antennas and Propagation Magazine, July, 2014

PGI and CAPS compilers study (II)



S. Feki, A. Al-Jarro, H. Bağcı. Porting an Explicit Time Domain Volume Integral Equation Solver on GPUs with OpenACC, IEEE Antennas and Propagation Magazine, July, 2014

Directive syntax

- Fortran

!$acc directive [clause [,] clause] …]

… often paired with a matching end directive

!$acc end directive

- C

#pragma acc directive [clause [,] clause] …]

Often followed by a structured code block

kernels: Your first OpenACC Directive

- Each loop executed as a separate ***kernel*** *(a parallel function that runs on the GPU)*

```
!$acc kernels
do i=1,n
   a(i) = 0.0 b(i) = 1.0
   c(i) = 2.0
end do
do i=1,n
  a(i) = b(i) + c(i)
end do
!$acc end kernels
```

Compile and run

- **C:**

pgcc –acc [-Minfo=accel] –o saxpy_acc saxpy.c

- **Fortran:**

pgf90 –acc [-Minfo=accel] –o saxpy_acc saxpy.f90

- **Compiler output:**

```
[sfeki@c4hdn saxpy]$ pgcc -acc -ta=nvidia -Minfo=accel -o saxpy saxpy.c
saxpy:
     5, Generating present_or_copyin(x[0:n])
        Generating present_or_copy(y[0:n])
        Generating compute capability 1.0 binary
        Generating compute capability 2.0 binary
     6, Loop is parallelizable
        Accelerator kernel generated
         6, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
            CC 1.0 : 8 registers; 48 shared, 0 constant, 0 local memory bytes
            CC 2.0 : 12 registers; 0 shared, 64 constant, 0 local memory bytes
```

SAXPY example, revisited

- Trivial first example
  - Apply a loop directive
  - Learn compiler commands

```
#include <stdlib.h>

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

*restrict:
"I promise y does not alias x"

```
int main(int argc, char **argv)
{
  int N = 1<<20; // 1 million floats

  if (argc > 1)
    N = atoi(argv[1]);

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

  for (int i = 0; i < N; ++i) {
    x[i] = 2.0f;
    y[i] = 1.0f;
  }

  saxpy(N, 3.0f, x, y);

  return 0;
}
```

Jacobi Iteration: C code

```
while ( err > tol && iter < iter_max ) {
  err=0.0;

  for( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {

      Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                           A[j-1][i] + A[j+1][i]);

      err = max(err, abs(Anew[j][i] - A[j][i]);
    }
  }

  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }

  iter++;
}
```

Jacobi Iteration: OpenACC code

```
while ( err > tol && iter < iter_max ) {
  err=0.0;

#pragma acc kernels reduction(max:err)
  for( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {

      Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                           A[j-1][i] + A[j+1][i]);

      err = max(err, abs(Anew[j][i] - A[j][i]);
    }
  }

#pragma acc kernels
  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }

  iter++;
}
```

PGI Accelerator Compiler output

```
pgcc  -acc -ta=nvidia -Minfo=accel -o laplace2d_acc laplace2d.c
main:
     57, Generating copyin(A[:4095][:4095])
         Generating copyout(Anew[1:4094][1:4094])
         Generating compute capability 1.3 binary
         Generating compute capability 2.0 binary
     58, Loop is parallelizable
     60, Loop is parallelizable
         Accelerator kernel generated
         58, #pragma acc loop worker, vector(16) /* blockIdx.y threadIdx.y */
         60, #pragma acc loop worker, vector(16) /* blockIdx.x threadIdx.x */
             Cached references to size [18x18] block of 'A'
             CC 1.3 : 17 registers; 2656 shared, 40 constant, 0 local memory bytes; 75% occupancy
             CC 2.0 : 18 registers; 2600 shared, 80 constant, 0 local memory bytes; 100% occupancy
         64, Max reduction generated for err
     69, Generating copyout(A[1:4094][1:4094])
         Generating copyin(Anew[1:4094][1:4094])
         Generating compute capability 1.3 binary
         Generating compute capability 2.0 binary
     70, Loop is parallelizable
     72, Loop is parallelizable
         Accelerator kernel generated
         70, #pragma acc loop worker, vector(16) /* blockIdx.y threadIdx.y */
         72, #pragma acc loop worker, vector(16) /* blockIdx.x threadIdx.x */
             CC 1.3 : 8 registers; 48 shared, 8 constant, 0 local memory bytes; 100% occupancy
             CC 2.0 : 10 registers; 8 shared, 56 constant, 0 local memory bytes; 100% occupancy
```

Performance

Execution	Time (s)	Speedup
CPU 1 OpenMP thread	69.80	--
CPU 2 OpenMP threads	44.76	1.56x
CPU 4 OpenMP threads	39.59	1.76x
CPU 6 OpenMP threads	39.71	1.76x
OpenACC GPU	162.16	0.24x FAIL

CPU: Intel Xeon X568C
6 Cores @ 3.33GHz

GPU: NVIDIA
Tesla M2070

What went wrong ?

- Set PGI_ACC_TIME environment variable to '1'

```
Accelerator Kernel Timing data
./openacc-workshop/solutions/001-laplace2D-kernels/laplace2d.c
  main
    69: region entered 1000 times
        time(us): total=77524918 init=240 region=77524678
                  kernels=4422961 data=66464916
        w/o init: total=77524678 max=83398 min=72025 avg=77524
        72: kernel launched 1000 times
            grid: [256x256]  block: [16x16]
            time(us): total=4422961 max=4543 min=4345 avg=4422
./openacc-workshop/solutions/001-laplace2D-kernels/laplace2d.c
  main
    57: region entered 1000 times
        time(us): total=82135902 init=216 region=82135686
                  kernels=8346306 data=66775717
        w/o init: total=82135686 max=159083 min=76575 avg=82135
        60: kernel launched 1000 times
            grid: [256x256]  block: [16x16]
            time(us): total=8201000 max=8297 min=8187 avg=8201
        64: kernel launched 1000 times
            grid: [1]  block: [256]
            time(us): total=145306 max=242 min=143 avg=145
acc_init.c
  acc_init
    29: region entered 1 time
        time(us): init=158248
```

4.4 seconds

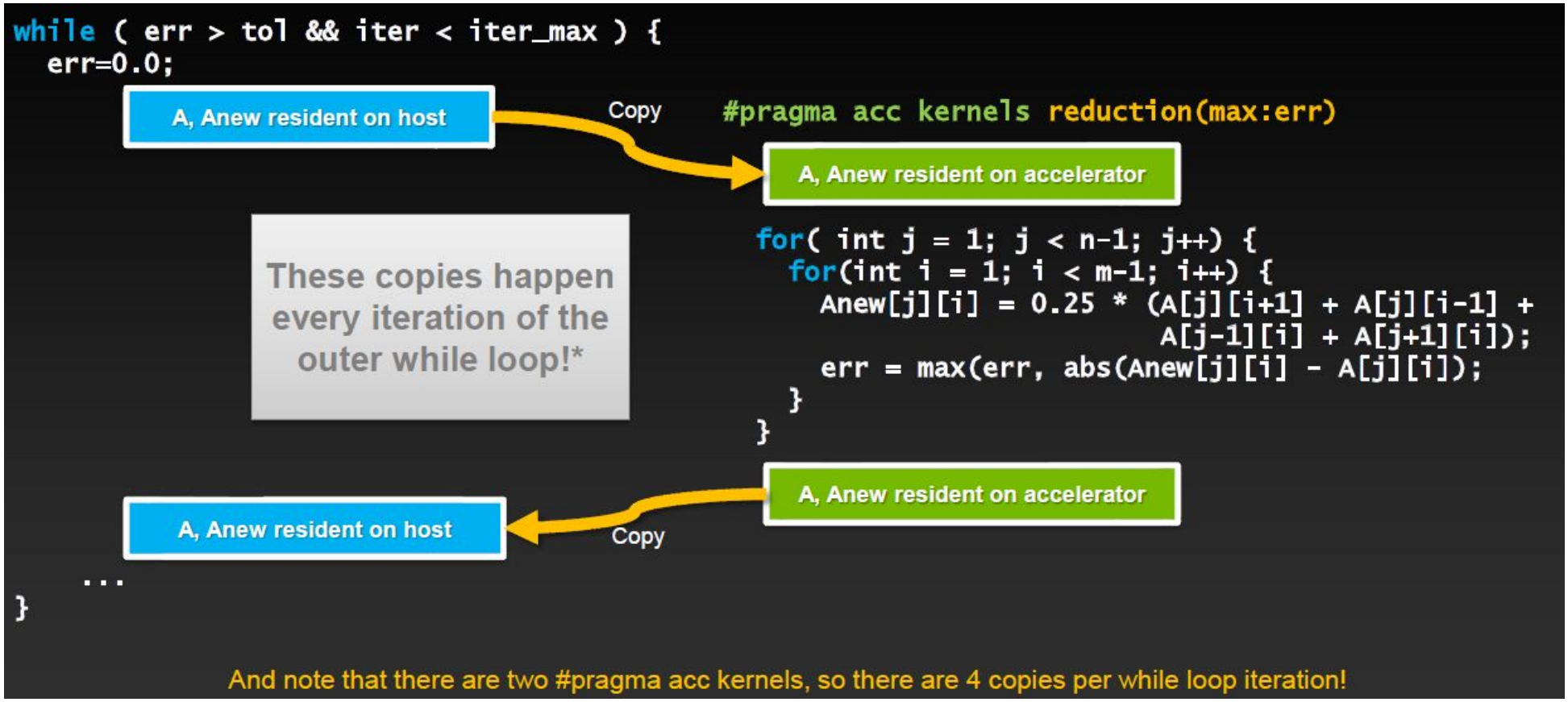
66.5 seconds

8.3 seconds

66.8 seconds

Huge Data Transfer Bottleneck!
Computation: 12.7 seconds
Data movement: 133.3 seconds

Excessive data transfer

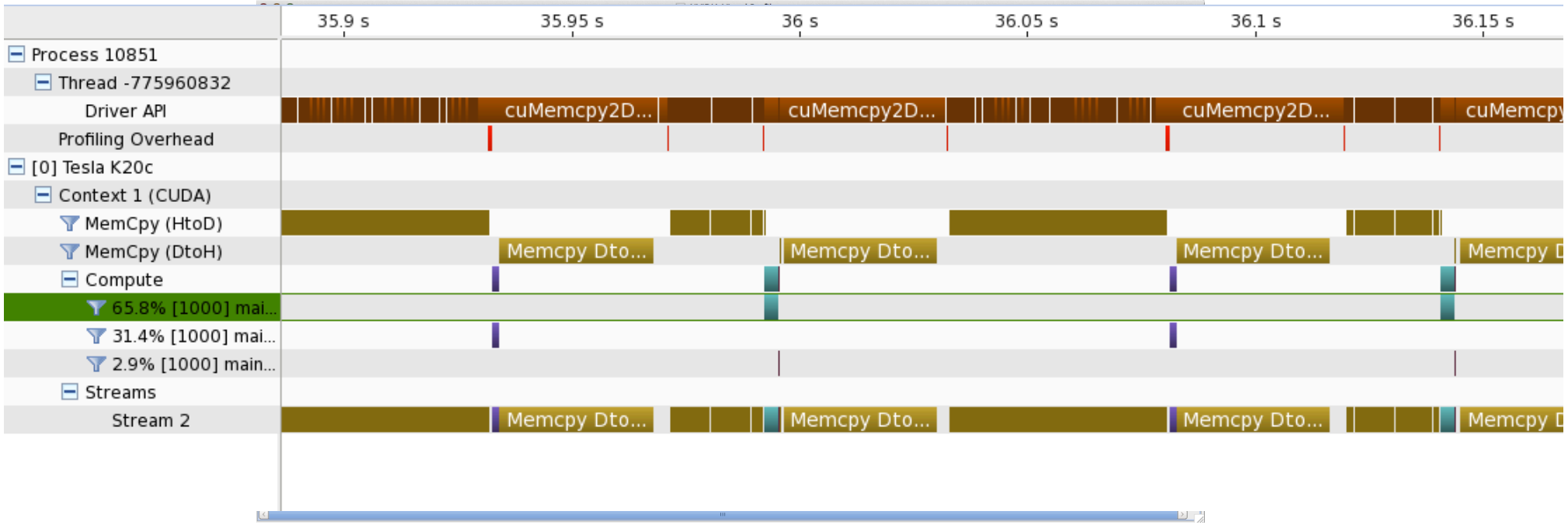


Another way of detecting it: NVIDIA Profiler

- Use nvprof for profiling the GPU application:

```
Time(%)      Time     Calls       Avg       Min       Max  Name
 44.73%  13.0367s      9000  1.4485ms     832ns  1.6954ms  [CUDA memcpy HtoD]
 44.39%  12.9395s      9000  1.4377ms  2.2720us  1.7537ms  [CUDA memcpy DtoH]
  6.76%  1.97137s      1000  1.9714ms  1.9698ms  1.9758ms  main_74_gpu
  3.34%  972.58ms      1000  972.58us  971.59us  973.67us  main_85_gpu
  0.78%  227.16ms      1000  227.16us  226.69us  227.97us  main_78_gpu_red
```

- Use NVVP GUI: NVIDIA Visual Profiler:



Data construct

- **Fortran**

!$acc data *[clause …]*

structured block

!$acc end data

- **C**

#pragma acc data *[clause …] { structured block }*

- Manage data movement. Data regions may be nested
- **General Clauses**

if(*condition*)

async(*expression*)

Data clauses

- **copy** (*list*) Allocates memory on GPU and copies data from host to GPU when entering region and copies data to the host when exiting region.
- **copyin** (*list*) Allocates memory on GPU and copies data from host to GPU when entering region.
- **copyout** (*list*) Allocates memory on GPU and copies data to the host when exiting region.
- **create** (*list*) Allocates memory on GPU but does not copy.
- **present** (*list*) Data is already present on GPU from another containing data region.
- and **present_or_copy[in|out], present_or_create, deviceptr.**

Array shaping

- Compiler sometimes cannot determine size of arrays
- Must specify explicitly using data clauses and array “shape”
- **C**

```
#pragma acc data copyin(a[0:size]), copyout(b[s/4:3*s/4])
```

- **Fortran**

```
!$acc data copyin(a(1:size)), copyout(b(s/4:3*s/4))
```

- **Note: data clauses can be used on** data**,** kernels **or** parallel

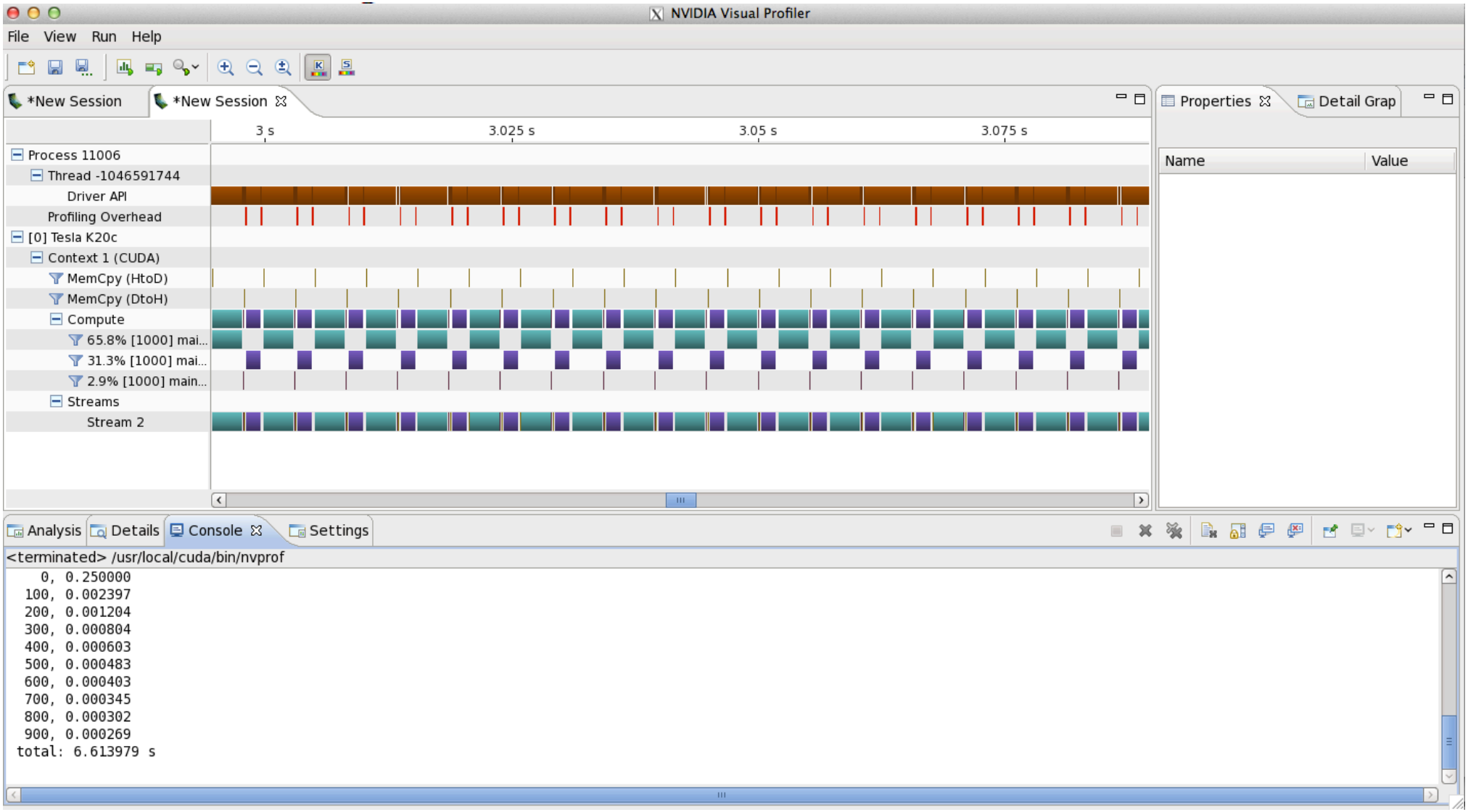
Jacobi Iteration: OpenACC C Code, Revisited

```
#pragma acc data copy(A), create(Anew)
while ( err > tol && iter < iter_max ) {
  err=0.0;

#pragma acc kernels reduction(max:err)
  for( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {

      Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                           A[j-1][i] + A[j+1][i]);

      err = max(err, abs(Anew[j][i] - A[j][i]);
    }
  }

#pragma acc kernels
  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }

  iter++;
}
```

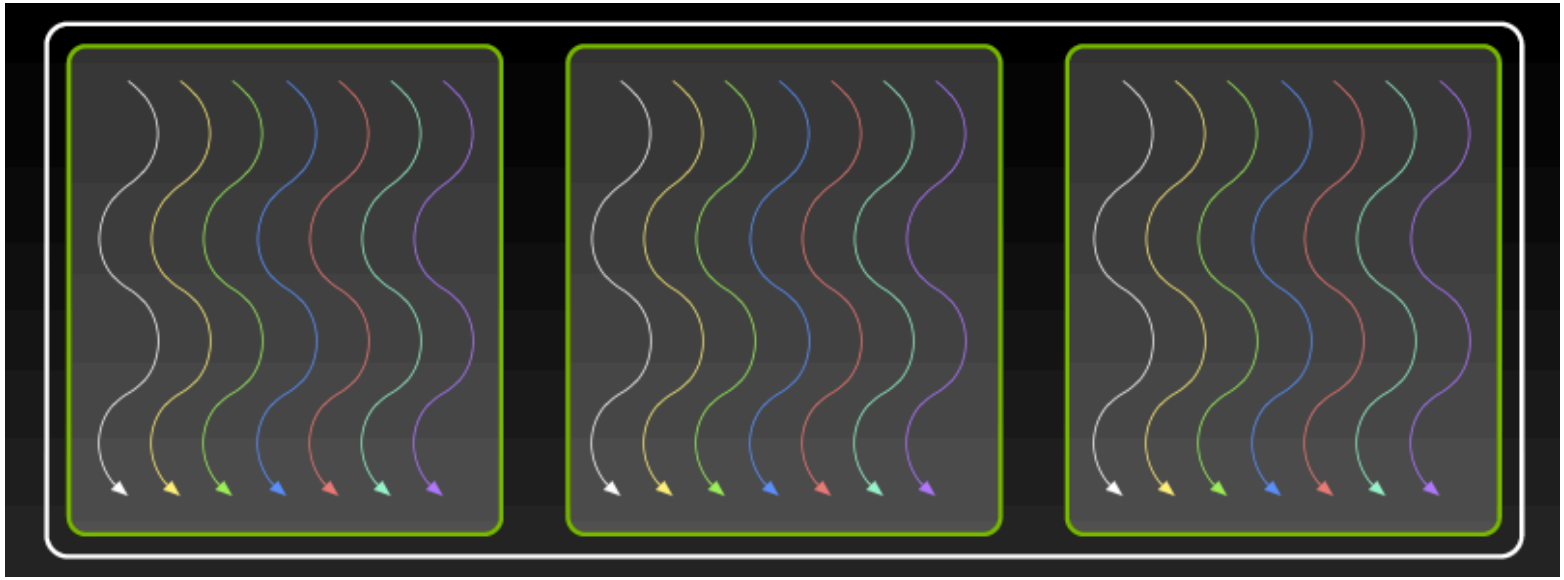
Performance numbers

Execution	Time (s)	Speedup
CPU 1 OpenMP thread	69.80	--
CPU 2 OpenMP threads	44.76	1.56x
CPU 4 OpenMP threads	39.59	1.76x
CPU 6 OpenMP threads	39.71	1.76x
OpenACC GPU	13.65	2.9x

New NVIDIA profiles



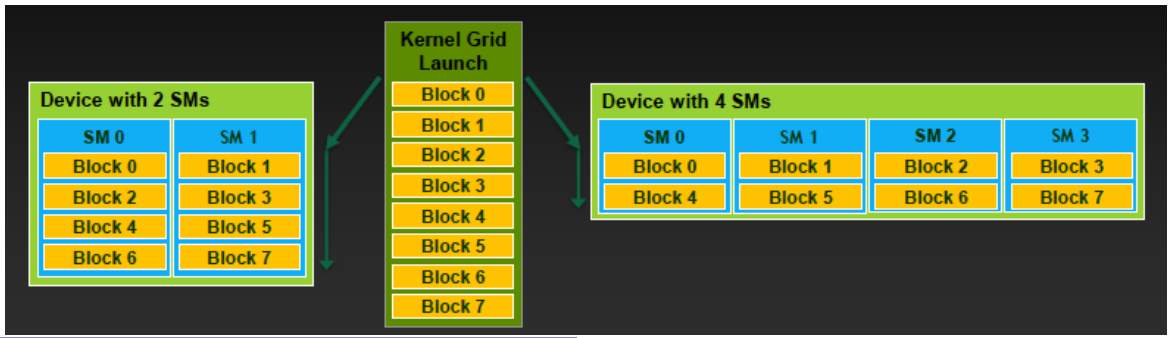
CUDA Kernels



- Threads are grouped into blocks
- Blocks are grouped into a grid
- A kernel is executed as a grid of blocks of threads

Thread blocks

- Thread blocks allow cooperation
  - Cooperatively load/store blocks of memory that they all use
  - Share results with each other or cooperate to produce a single result
  - Synchronize with each other
- Thread blocks allow scalability
  - Blocks can execute in any order, concurrently or sequentially
  - This independence between blocks gives scalability:
    - A kernel scales across any number of SMs



Mapping OpenACC to CUDA I

- The OpenACC execution model has three levels: gang, worker, and vector
- Allows mapping to an architecture that is a collection of Processing Elements (PEs)
- One or more PEs per node
- Each PE is multi-threaded
- Each thread can execute vector instructions

- Tile pragma in OpenACC 2.0

Mapping OpenACC to CUDA II

- For GPUs, the mapping is implementation-dependent. Some possibilities:
  - gang==block, worker==warp, and vector==threads of a warp
  - omit “worker” and just have gang==block, vector==threads of a block
- Depends on what the compiler thinks is the best mapping for the problem
- ...But explicitly specifying that a given loop should map to gangs, workers, and/or vectors is optional anyway
  - Further specifying the *number* of gangs/workers/vectors is also optional
  - So why do it? To tune the code to fit a particular target architecture in a straightforward and easily re-tuned way.

OpenACC loop directive and clauses

```
#pragma acc kernels loop
for( int i = 0; i < n; ++i ) y[i] += a*x[i];
```

Uses whatever mapping to threads and blocks the compiler chooses. Perhaps 16 blocks, 256 threads each

```
#pragma acc kernels loop gang(100), vector(128)
for( int i = 0; i < n; ++i ) y[i] += a*x[i];
```

100 thread blocks, each with 128 threads, each thread executes one iteration of the loop, using kernels

```
#pragma acc parallel num_gangs(100), vector_length(128)
{
  #pragma acc loop gang, vector
  for( int i = 0; i < n; ++i ) y[i] += a*x[i];
}
```

100 thread blocks, each with 128 threads, each thread executes one iteration of the loop, using parallel

Mapping OpenACC to CUDA threads and blocks

- Nested loops generate multi-dimensional blocks and grids:

```
#pragma acc kernels loop gang(100), vector(16)
for( … )
```

100 blocks tall (row/Y direction)

16 thread tall block

```
#pragma acc loop gang(200), vector(32)
for( … )
```

200 blocks wide (column/X direction)

and 32 thread wide

Other clauses for loop directive

#pragma acc loop [cluases]

- independent: for independent loops
- seq: for sequential execution of the loop
- Reduction : for reduction operation such as min,max, etc…

Jacobi example … again

Execution	Time (s)	Speedup
CPU 1 OpenMP thread	69.80	--
CPU 2 OpenMP threads	44.76	1.56x
CPU 4 OpenMP threads	39.59	1.76x
CPU 6 OpenMP threads	39.71	1.76x
OpenACC GPU	13.65	2.9x

Note: same code runs in 9.78s on NVIDIA Tesla M2090 GPU

With Kernels and data directives

Jacobi example … again

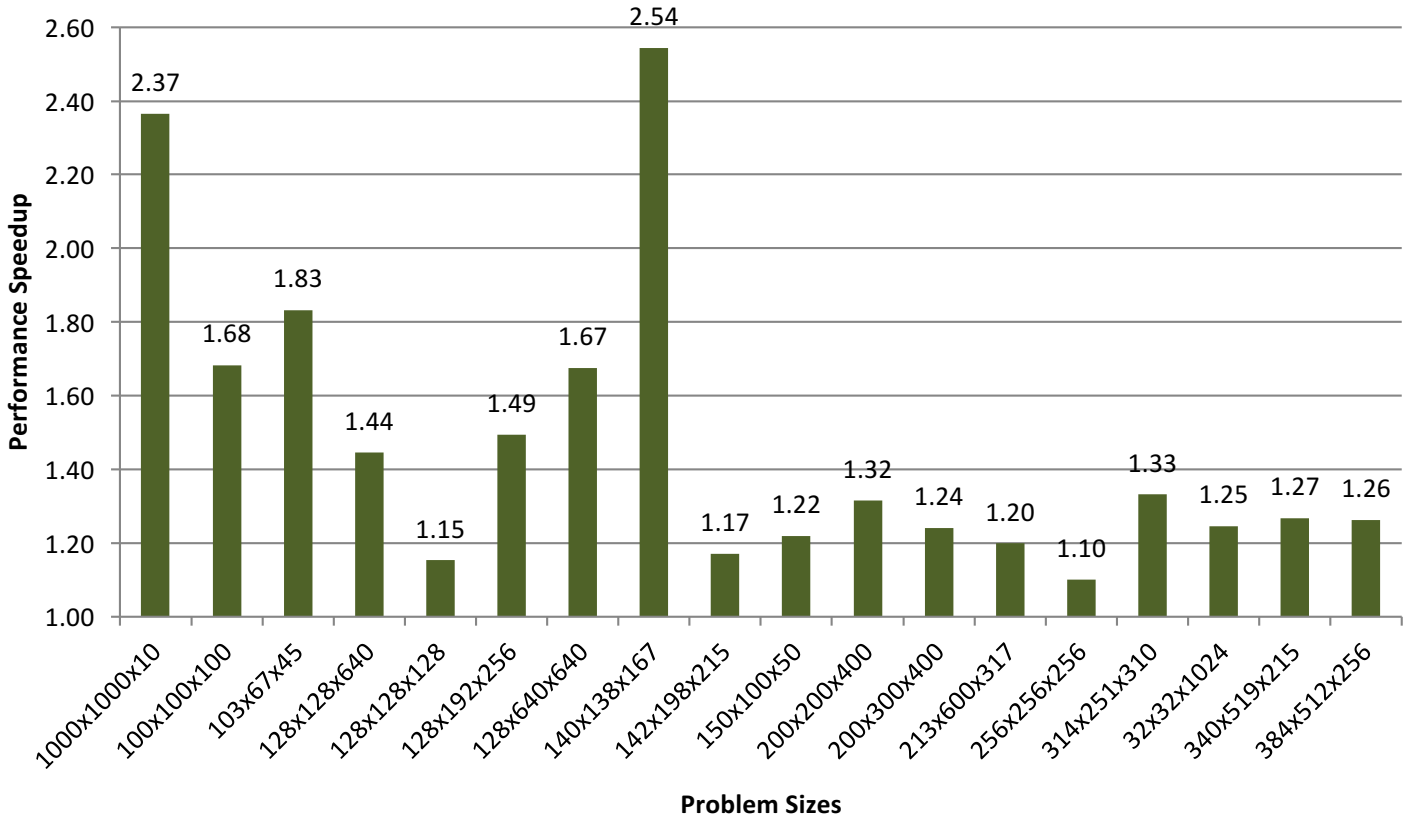
Execution	Time (s)	Speedup
CPU 1 OpenMP thread	69.80	--
CPU 2 OpenMP threads	44.76	1.56x
CPU 4 OpenMP threads	39.59	1.76x
CPU 6 OpenMP threads	39.71	1.76x
OpenACC GPU	10.98	3.62x

Note: same code runs in 7.58s on NVIDIA Tesla M2090 GPU

After adding loop directive with gang and vector clauses

An opportunity for Auto-tuning

- Gang and vector values can be auto-tuned for the application, targeting the available accelerator device



S. Siddiqui, F. Al-Zayer, S. Feki. Historic Learning Approach for Auto-tuning OpenACC Accelerated Scientific Applications, iWAPT 2014, Eugene, Oregon, USA

An opportunity for Auto-tuning

Input code annotated with OpenACC

```
#pragma acc kernels
#pragma acc loop independent
  for (x = 4 ; x < nx-4; x++) {
#pragma acc loop independent
    for (y = 4; y < ny-4; y++) {
#pragma acc loop independent
      for (z = 4; k < nz-4; z++) {
        U[x][y][z] = c1*V[x]][y][z] + ....
      }
    }
  }
```

Accelerator Specification

Automatic code generator

```
#pragma acc kernels
#pragma acc loop independent gang(a),vector(b)
  for (x = 4 ; x < nx-4; x++) {
#pragma acc loop independent gang(c)
    for (y = 4; y < ny-4; y++) {
#pragma acc loop independent vector(d)
      for (z = 4; k < nz-4; z++) {
        U[x][y][z] = c1*V[x]][y][z] + ....
      }
    }
  }
```

```
#pragma acc kernels
#pragma acc loop independent
for (x = 4 ; x < nx-4; x++) {
#pragma acc loop independent gang(a),vector(b)
    for (y = 4; y < ny-4; y++) {
#pragma acc loop independent gang(c),vector(d)
      for (z = 4; k < nz-4; z++) {
        U[x][y][z] = c1*V[x]][y][z] + ....
      }
    }
  }
```

```
#pragma acc kernels
#pragma acc loop independent gang(a)
  for (x = 4 ; x < nx-4; x++) {
#pragma acc loop independent gang(b),vector(c)
    for (y = 4; y < ny-4; y++) {
#pragma acc loop independent vector(d)
      for (z = 4; k < nz-4; z++) {
        U[x][y][z] = c1*V[x]][y][z] + ....
      }
    }
  }
```

```
#pragma acc kernels
#pragma acc loop independent gang(a),vector(b)
  for (x = 4 ; x < nx-4; x++) {
#pragma acc loop independent vector(c)
    for (y = 4; y < ny-4; y++) {
#pragma acc loop independent gang(d),vector(e)
      for (z = 4; k < nz-4; z++) {
        U[x][y][z] = c1*V[x]][y][z] + ....
      }
    }
  }
```

Runtime evaluation and selection

Database

Jacobi example … again

- Which other optimization we can further do ?
  - Restructuring the code will enhance both CPU and GPU version
  - Hint: reduce memory operations

OpenACC Runtime Library

- In C:

```
#include “openacc.h”
```

- In Fortran:

```
#include ‘openacc_lib.h’    or
use openacc
```

- Contains:
  - Prototypes of all routines
  - Definition of datatypes used in these routines including enumeration type describing types of accelerators

OpenACC Runtime Library Definitions

- openacc_version with a value yyyymm (year and month of the openacc version)
- acc_device_t : type of accelerator device
  - acc_device_none
  - acc_device_default
  - acc_device_host
  - acc_device_not_host

OpenACC Runtime Library Routines I

- acc_get_num_devices: returns the number of devices of the given type attached to the host
- acc_set_device_type: tells which type of device to use when executing an accelerator parallel or kernel region.
- acc_get_device_type: tells which type of device to be used for the next accelerated region
- acc_set_device_num: specify which device to use
- acc_get_device_num: returns the device number of the specified device type that will be used to run the next accelerator parallel or kernels region

OpenACC Runtime Library Routines II

- acc_init: initialize the runtime, can be used to isolate the initialization cost from the computation cost
- acc_shutdown: shut down the connection to the device and free any allocated resources
- acc_malloc: allocate memory on the accelerator device
- acc_free: frees memory on the accelerator device

OpenACC Runtime Library Routines: use case

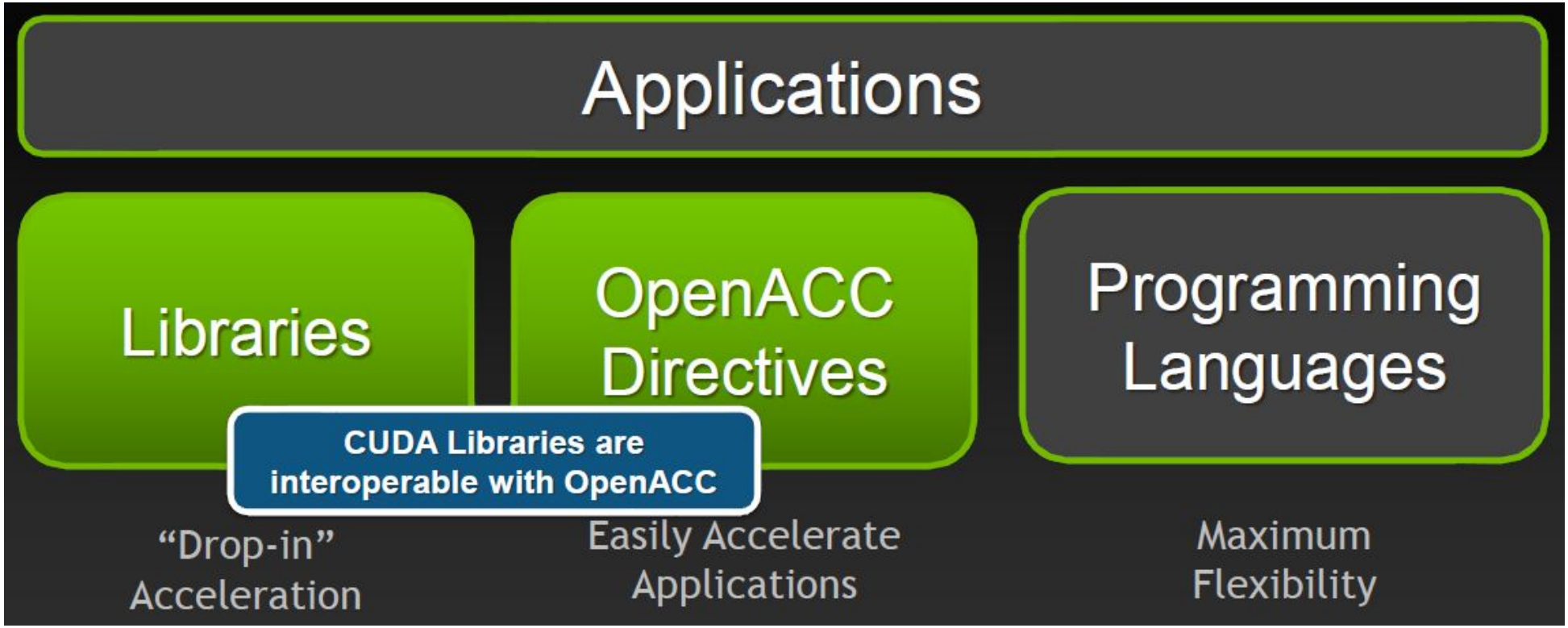
- Porting an MPI code to multiple GPUs.
- Example in running on 8 nodes, with 4 GPUs each, i.e. 32 MPI processes

- acc_init()
- acc_set_device_num(rank%4)

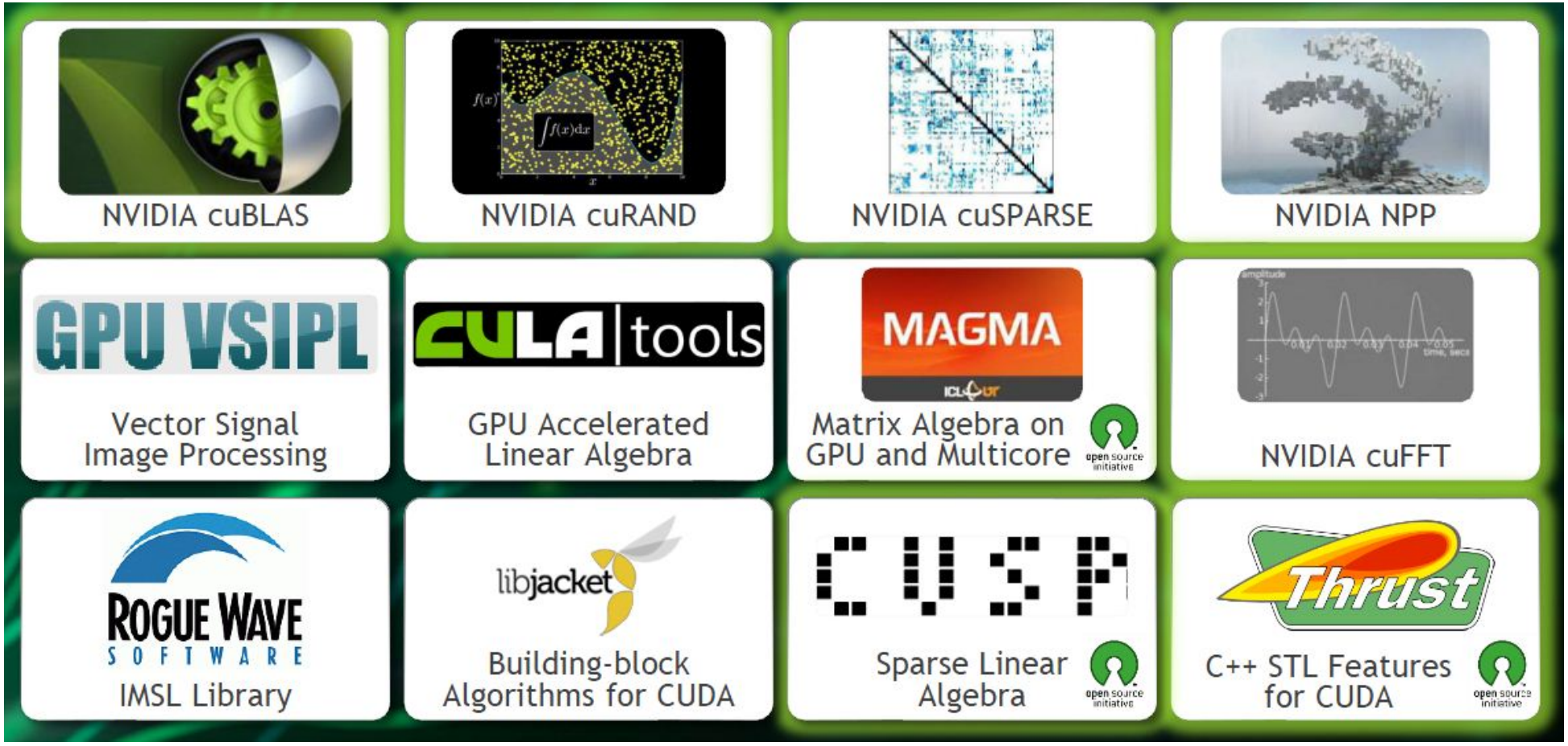
- Each node runs 4 MPI processes, each of them is offloading compute kernels to a separate GPU

S. Feki, A. Al-Jarro, H. Bağcı. Multiple GPUs Electromagnetics Simulations using MPI and OpenACC, Poster in GPU Technology Conference, San Jose, California, USA, March 24-27, 2014

OpenACC and CUDA libraries



GPU accelerated libraries



Sharing data with libraries

- CUDA libraries and OpenACC both operate on device arrays
- OpenACC provides mechanisms for interoperability with library calls
  - deviceptr data clause
  - host_data construct

- Note: same mechanisms useful for interoperability with custom CUDA C/C++/Fortran code

deviceptr Data Clause

deviceptr(*list*) Declares that the pointers in *list* refer to device pointers that need not be allocated or moved between the host and device for this pointer.

Example:

- C

```
#pragma acc data deviceptr(d_input)
```

- Fortran

```
$!acc data deviceptr(d_input)
```

host_data Construct

- Makes the address of device data available on the host.
- deviceptr(*list*) Tells the compiler to use the device address for any variable in *list.* Variables in the list must be present in device memory due to data regions that contain this construct
- Example
- C

```
#pragma acc host_data use_device(d_input)
```

- Fortran

```
$!acc host_data use_device(d_input)
```

Summary on device pointers

- Use deviceptr data clause to pass pre-allocated device data to OpenACC regions and loops
- Use host_data to get device address for pointers inside acc data regions
- The same techniques shown here can be used to share device data between OpenACC loops and
  - Your custom CUDA C/C++/Fortran/etc. device code
  - Any CUDA Library that uses CUDA device pointers

Thanks !