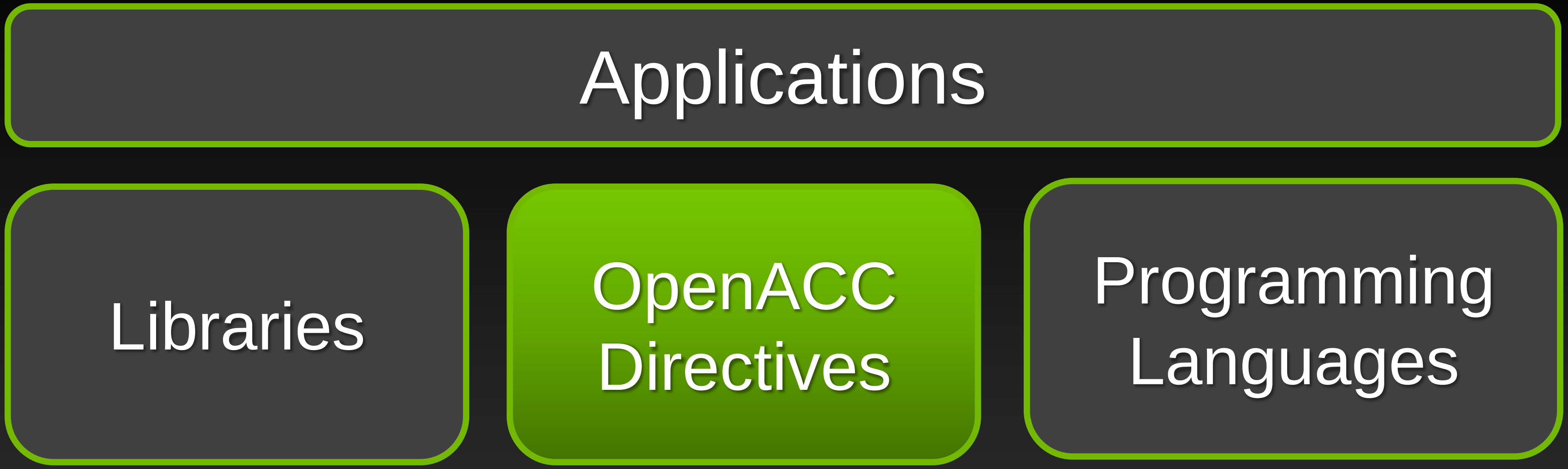
GPU TECHNOLOGY CONFERENCE

Getting Started with OpenACC

Justin Luitjens, NVIDIA

3 Ways to Accelerate Applications



“Drop-in” Acceleration

Easily Accelerate Applications

Maximum Flexibility

OpenACC

The Standard for GPU Directives

- **Simple:** 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

OpenACC®

DIRECTIVES FOR ACCELERATORS

Directives: Easy & Powerful

Real-Time Object Detection

Global Manufacturer of Navigation Systems

5x in 40 Hours

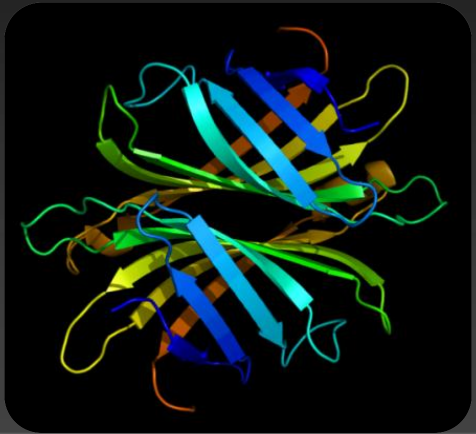
Valuation of Stock Portfolios using Monte Carlo

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.”

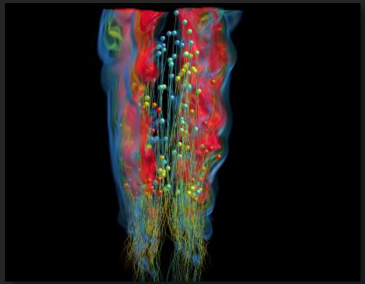
-- Developer at the Global Manufacturer of Navigation Systems

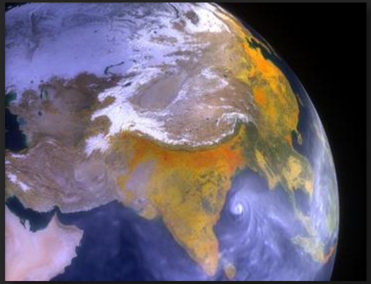
Focus on Expressing Parallelism

With Directives, tuning work focuses on *expressing parallelism*, which makes codes inherently better

Example: Application tuning work using directives for new Titan system at ORNL

S3D
Research more efficient combustion with next-generation fuels





CAM-SE
Answer questions about specific climate change adaptation and mitigation scenarios

- Tuning top 3 kernels (90% of runtime)
- *3 to 6x faster on CPU+GPU vs. CPU+CPU*
- But also improved all-CPU version by 50%

- Tuning top key kernel (50% of runtime)
- 6.5x faster on CPU+GPU vs. CPU+CPU
- Improved performance of CPU version by 100%

OpenACC is not

***GPU Programming*.**

OpenACC is

Expressing Parallelism

in your code.

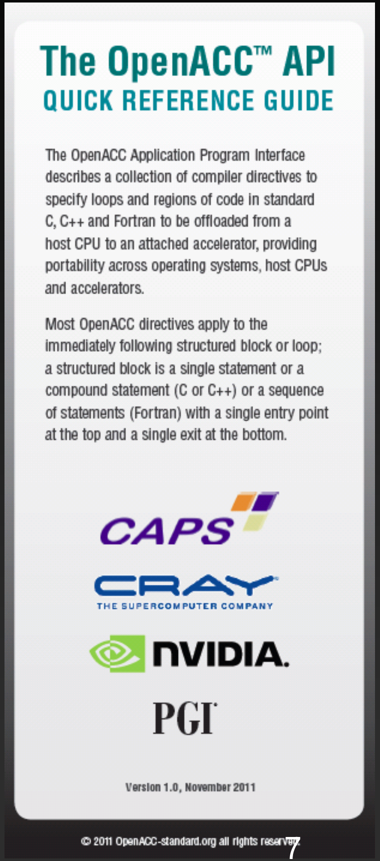
OpenACC Specification and Website

- Full OpenACC 1.0 Specification available online

www.openacc.org

- Quick reference card also available

- Compilers available now from PGI, Cray, and CAPS


The OpenACC™ API
QUICK REFERENCE GUIDE

The OpenACC Application Program Interface describes a collection of compiler directives to specify loops and regions of code in standard C, C++ and Fortran to be offloaded from a host CPU to an attached accelerator, providing portability across operating systems, host CPUs and accelerators.

Most OpenACC directives apply to the immediately following structured block or loop; a structured block is a single statement or a compound statement (C or C++) or a sequence of statements (Fortran) with a single entry point at the top and a single exit at the bottom.

Version 1.0, November 2011

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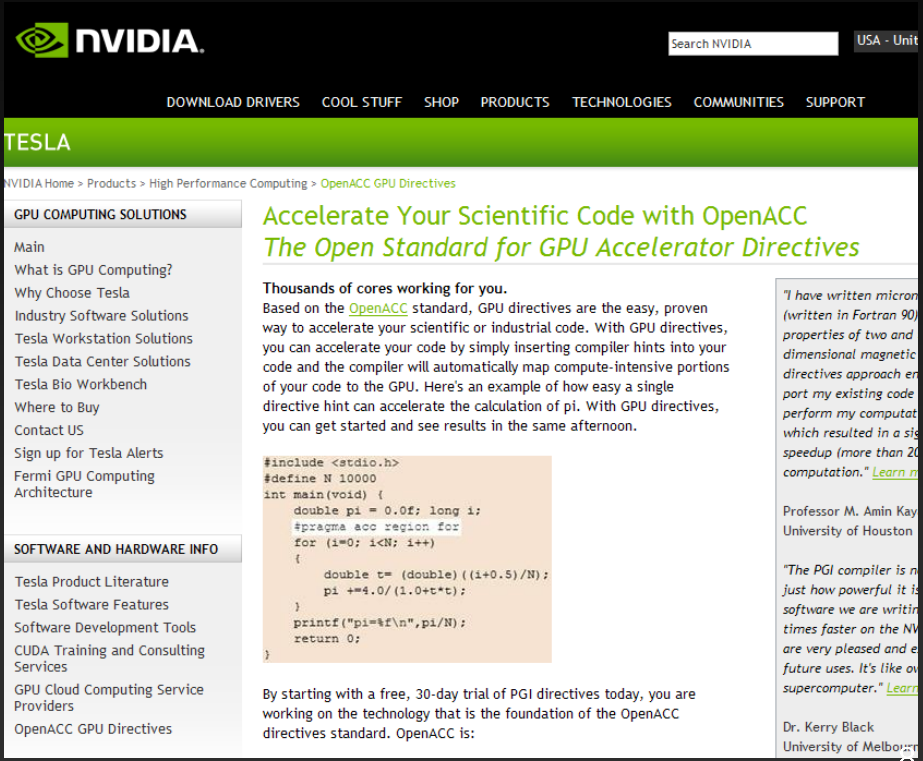
Start Now with OpenACC Directives

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



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Tesla Product Literature
Tesla Software Features
Software Development Tools
CUDA Training and Consulting Services
GPU Cloud Computing Service Providers
OpenACC GPU Directives

Accelerate Your Scientific Code with OpenACC

The Open Standard for GPU Accelerator Directives

Thousands of cores working for you.

Based on the OpenACC standard, GPU directives are the easy, proven way to accelerate your scientific or industrial code. With GPU directives, you can accelerate your code by simply inserting compiler hints into your code and the compiler will automatically map compute-intensive portions of your code to the GPU. Here's an example of how easy a single directive hint can accelerate the calculation of pi. With GPU directives, you can get started and see results in the same afternoon.

```
#include <stdio.h>
#define N 10000
int main(void) {
    double pi = 0.0f; long i;
    #pragma acc region for
    for (i=0; i<N; i++)
    {
        double t= (double)((i+0.5)/N);
        pi +=4.0/(1.0+t*t);
    }
    printf("pi=%f\n",pi/N);
    return 0;
}
```

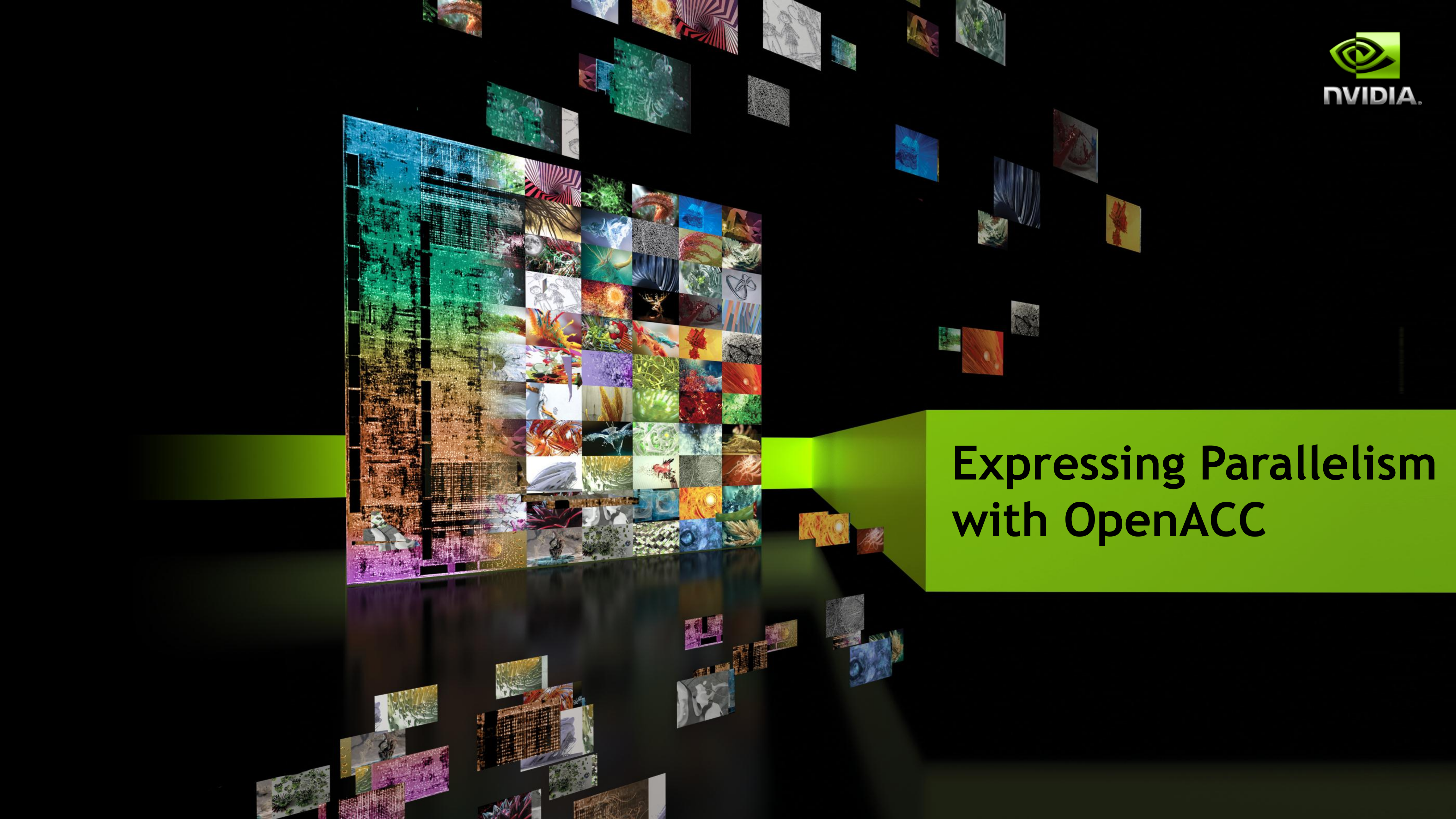
By starting with a free, 30-day trial of PGI directives today, you are working on the technology that is the foundation of the OpenACC directives standard. OpenACC is:

"I have written micron (written in Fortran 90) properties of two and dimensional magnetic directives approach en port my existing code perform my computat which resulted in a sig speedup (more than 20 computation." Learn m

Professor M. Amin Kay
University of Houston

"The PGI compiler is n just how powerful it is software we are writin times faster on the NV are very pleased and e future uses. It's like ov supercomputer." Learn

Dr. Kerry Black
University of Melbourn



Expressing Parallelism with OpenACC

A Very Simple Exercise: SAXPY

SAXPY in C

```c
void saxpy(int n,
           float a,
           float *x,
           float *restrict y)
{

  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);
...
```

SAXPY in Fortran

```fortran
subroutine saxpy(n, a, x, y)
  real :: x(n), y(n), a
  integer :: n, i


  do i=1,n
    y(i) = a*x(i)+y(i)
  enddo

end subroutine saxpy

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

A Very Simple Exercise: SAXPY OpenMP

SAXPY in C

```c
void saxpy(int n,
           float a,
           float *x,
           float *restrict y)
{
#pragma omp parallel for
  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);
...
```

SAXPY in Fortran

```fortran
subroutine saxpy(n, a, x, y)
  real :: x(n), y(n), a
  integer :: n, i

!$omp parallel do
  do i=1,n
    y(i) = a*x(i)+y(i)
  enddo
!$omp end parallel do
end subroutine saxpy

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

A Very Simple Exercise: SAXPY OpenACC

SAXPY in C

```c
void saxpy(int n,
           float a,
           float *x,
           float *restrict y)
{
#pragma acc parallel loop
  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);
...
```

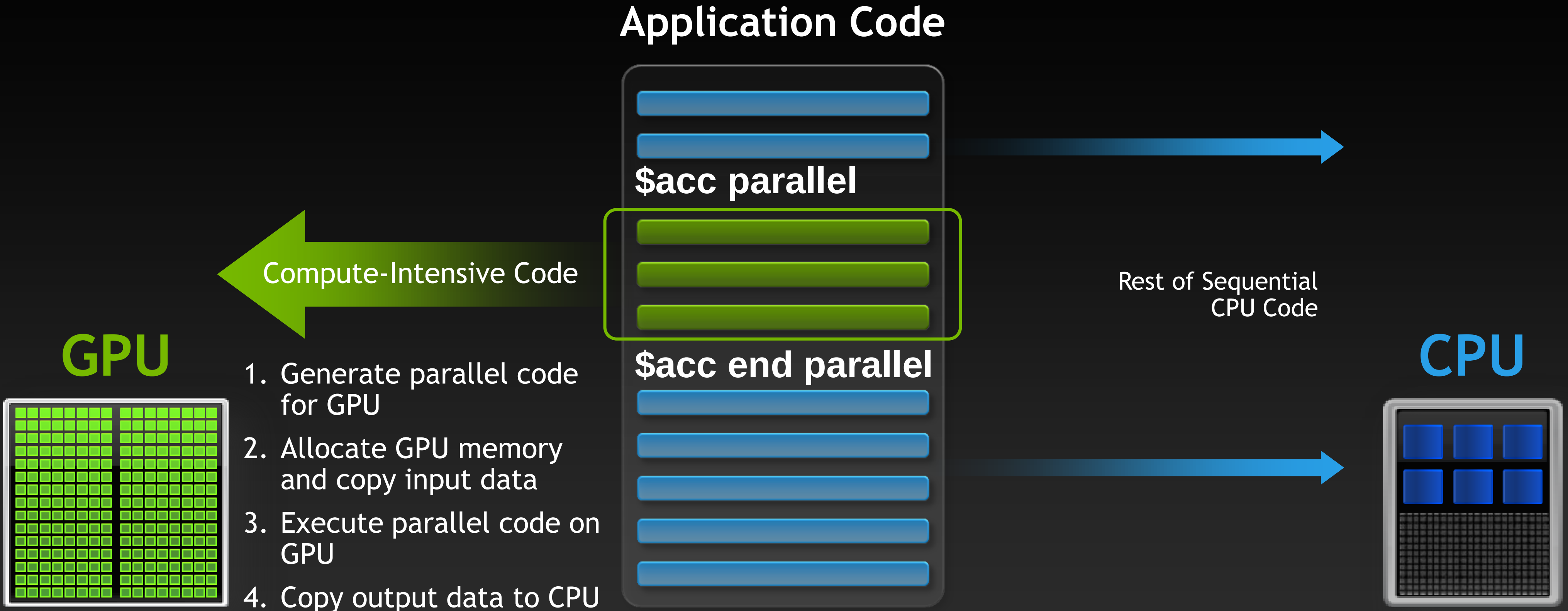
SAXPY in Fortran

```fortran
subroutine saxpy(n, a, x, y)
  real :: x(n), y(n), a
  integer :: n, i

!$acc parallel loop
  do i=1,n
    y(i) = a*x(i)+y(i)
  enddo
!$acc end parallel loop
end subroutine saxpy

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

OpenACC Execution Model



1. Generate parallel code for GPU
2. Allocate GPU memory and copy input data
3. Execute parallel code on GPU
4. Copy output data to CPU and deallocate GPU memory

Directive Syntax

- Fortran

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

  ...often paired with a matching end directive surrounding a structured code block:

  `!$acc end directive`

- C

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

  …often followed by a structured code block

- Common Clauses

  `if(condition), async(handle)`

Complete SAXPY example code

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

```
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;
}
```

Compile (PGI)

- C:

```
pgcc -acc [-Minfo=accel] [-ta=nvidia] -o saxpy_acc saxpy.c
```

- Fortran:

```
pgf90 -acc [-Minfo=accel] [-ta=nvidia] -o saxpy_acc saxpy.f90
```

- Compiler output:

```
pgcc -acc -Minfo=accel -ta=nvidia -o saxpy_acc saxpy.c
saxpy:
     11, Accelerator kernel generated
         13, #pragma acc loop gang, vector(256) /* blockIdx.x threadIdx.x */
     11, Generating present_or_copyin(x[0:n])
         Generating present_or_copy(y[0:n])
         Generating NVIDIA code
         Generating compute capability 1.0 binary
         Generating compute capability 2.0 binary
         Generating compute capability 3.0 binary
```

Run

- The PGI compiler provides automatic instrumentation when `PGI_ACC_TIME=1` at runtime

```
Accelerator Kernel Timing data
/home/jlarkin/kernels/saxpy/saxpy.c
  saxpy  NVIDIA  devicenum=0
        time(us): 3,256
        11: data copyin reached 2 times
             device time(us): total=1,619 max=892 min=727 avg=809
        11: kernel launched 1 times
            grid: [4096]  block: [256]
             device time(us): total=714 max=714 min=714 avg=714
            elapsed time(us): total=724 max=724 min=724 avg=724
        15: data copyout reached 1 times
             device time(us): total=923 max=923 min=923 avg=923
```

Another approach: `kernels` construct

- The kernels construct expresses that a region may contain parallelism and the compiler determines what can safely be parallelized.

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

    do i=1,n
        a(i) = b(i) + c(i)  kernel 2
    end do
!$acc end kernels
```

The compiler identifies 2 parallel loops and generates 2 kernels.

OpenACC parallel vs. kernels

PARALLEL

- Requires analysis by programmer to ensure safe parallelism
- Straightforward path from OpenMP

KERNELS

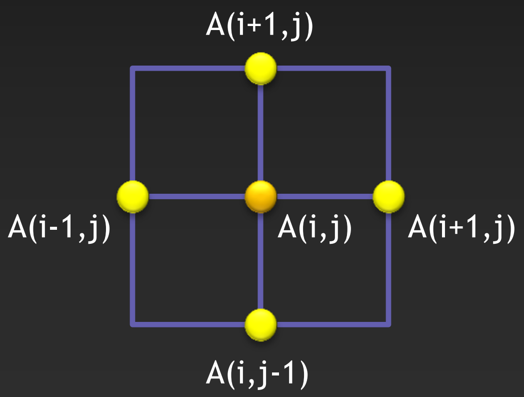
- Compiler performs parallel analysis and parallelizes what it believes safe
- Can cover larger area of code with single directive

Both approaches are equally valid and can perform equally well.

OpenACC by Example

Example: Jacobi Iteration

- Iteratively converges to correct value (e.g. Temperature), by computing new values at each point from the average of neighboring points.
  - Common, useful algorithm
  - Example: Solve Laplace equation in 2D: $\nabla^2 f(x,y) = 0$



$$A_{k+1}(i,j) = \frac{A_k(i-1,j) + A_k(i+1,j) + A_k(i,j-1) + A_k(i,j+1)}{4}$$

Jacobi Iteration: C Code

```c
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++;
}
```

Iterate until converged

Iterate across matrix elements

Calculate new value from neighbors

Compute max error for convergence

Swap input/output arrays

Jacobi Iteration: OpenMP C Code

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

#pragma omp parallel for shared(m, n, Anew, A) 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 omp parallel for shared(m, n, Anew, A)
  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }

  iter++;
}
```

Parallelize loop across CPU threads

Parallelize loop across CPU threads

Jacobi Iteration: OpenACC C Code

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

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

  iter++;
}
```

Parallelize loop nest on GPU

Parallelize loop nest on GPU

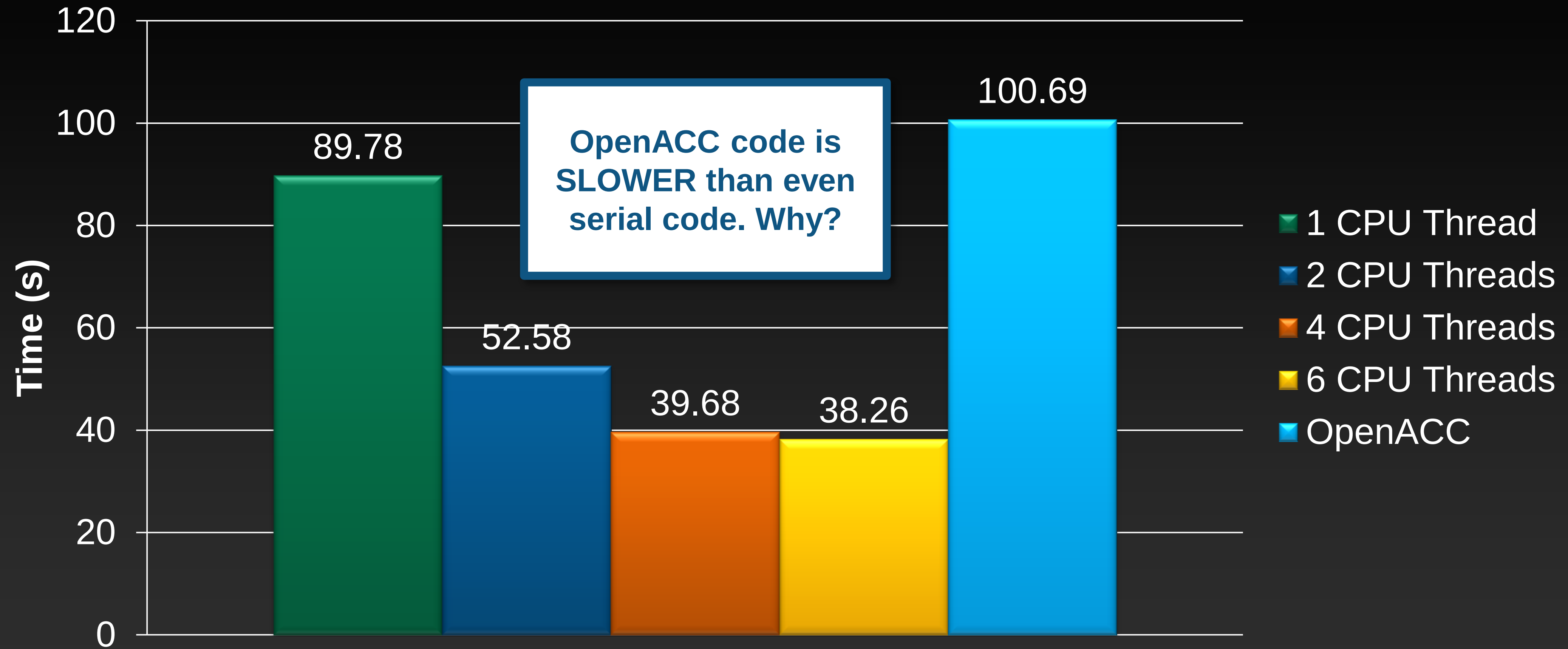
PGI Accelerator Compiler output (C)

```
pgcc -Minfo=all -ta=nvidia:5.0,cc3x -acc -Minfo=accel -o laplace2d_acc laplace2d.c
main:
     56, Accelerator kernel generated
         57, #pragma acc loop gang /* blockIdx.x */
         59, #pragma acc loop vector(256) /* threadIdx.x */
     56, Generating present_or_copyin(A[0:][0:])
         Generating present_or_copyout(Anew[1:4094][1:4094])
         Generating NVIDIA code
         Generating compute capability 3.0 binary
     59, Loop is parallelizable
     68, Accelerator kernel generated
         69, #pragma acc loop gang /* blockIdx.x */
         71, #pragma acc loop vector(256) /* threadIdx.x */
     68, Generating present_or_copyout(A[1:4094][1:4094])
         Generating present_or_copyin(Anew[1:4094][1:4094])
         Generating NVIDIA code
         Generating compute capability 3.0 binary
     71, Loop is parallelizable
```

Execution Time (lower is better)

CPU: Intel i7-3930K
6 Cores @ 3.20GHz

GPU: NVIDIA Tesla K20



OpenACC code is SLOWER than even serial code. Why?

What went wrong?

- Set `PGI_ACC_TIME` environment variable to ‘1’

```
Accelerator Kernel Timing data
/home/jlarkin/openacc-workshop/exercises/001-laplace2D-kernels/laplace2d.c
  main  NVIDIA  devicenum=0
        time(us): 93,201,190
        56: data copyin reached 1000 times
             device time(us): total=23,049,452 max=28,928 min=22,761 avg=23,049
        56: kernel launched 1000 times
            grid: [4094]  block: [256]
             device time(us): total=2,609,928 max=2,812 min=2,593
            elapsed time(us): total=2,872,585 max=3,022 min=2,642
        56: reduction kernel launched 1000 times
            grid: [1]  block: [256]
             device time(us): total=19,218 max=724 min=16 avg=19
            elapsed time(us): total=29,070 max=734 min=26 avg=29
        68: data copyin reached 1000 times
             device time(us): total=23,888,588 max=33,546 min=23,378 avg=23,888
        68: kernel launched 1000 times
            grid: [4094]  block: [256]
             device time(us): total=2,398,101 max=2,961 min=2,137 avg=2,398
            elapsed time(us): total=2,407,481 max=2,971 min=2,146 avg=2,407
        68: data copyout reached 1000 times
             device time(us): total=20,664,362 max=27,788 min=20,511 avg=20,664
        77: data copyout reached 1000 times
             device time(us): total=20,571,541 max=24,837 min=20,521 avg=20,571
```

23 seconds

2.6 seconds

0.19 seconds

23.9 seconds

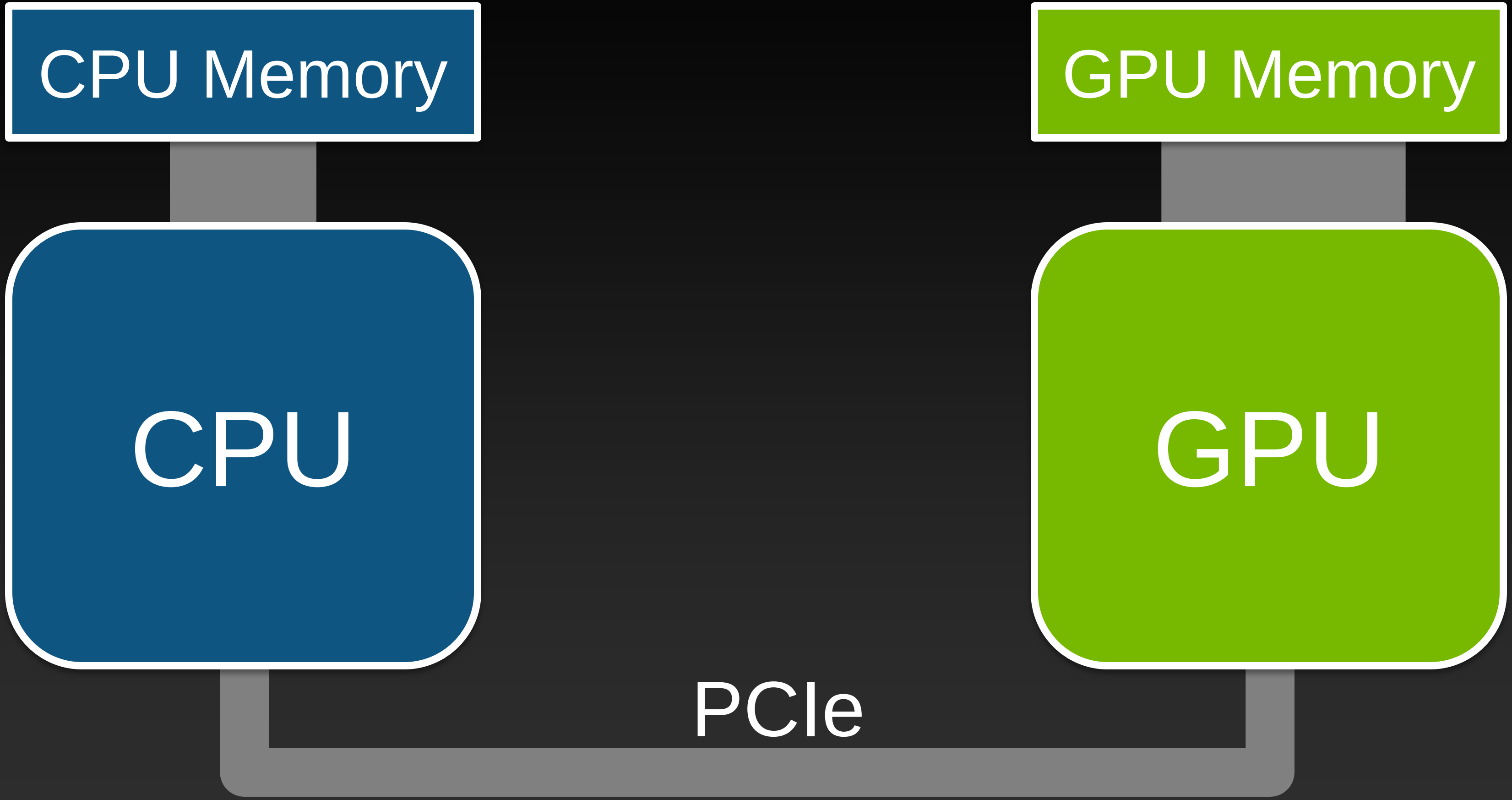
2.4 seconds

27.8 seconds

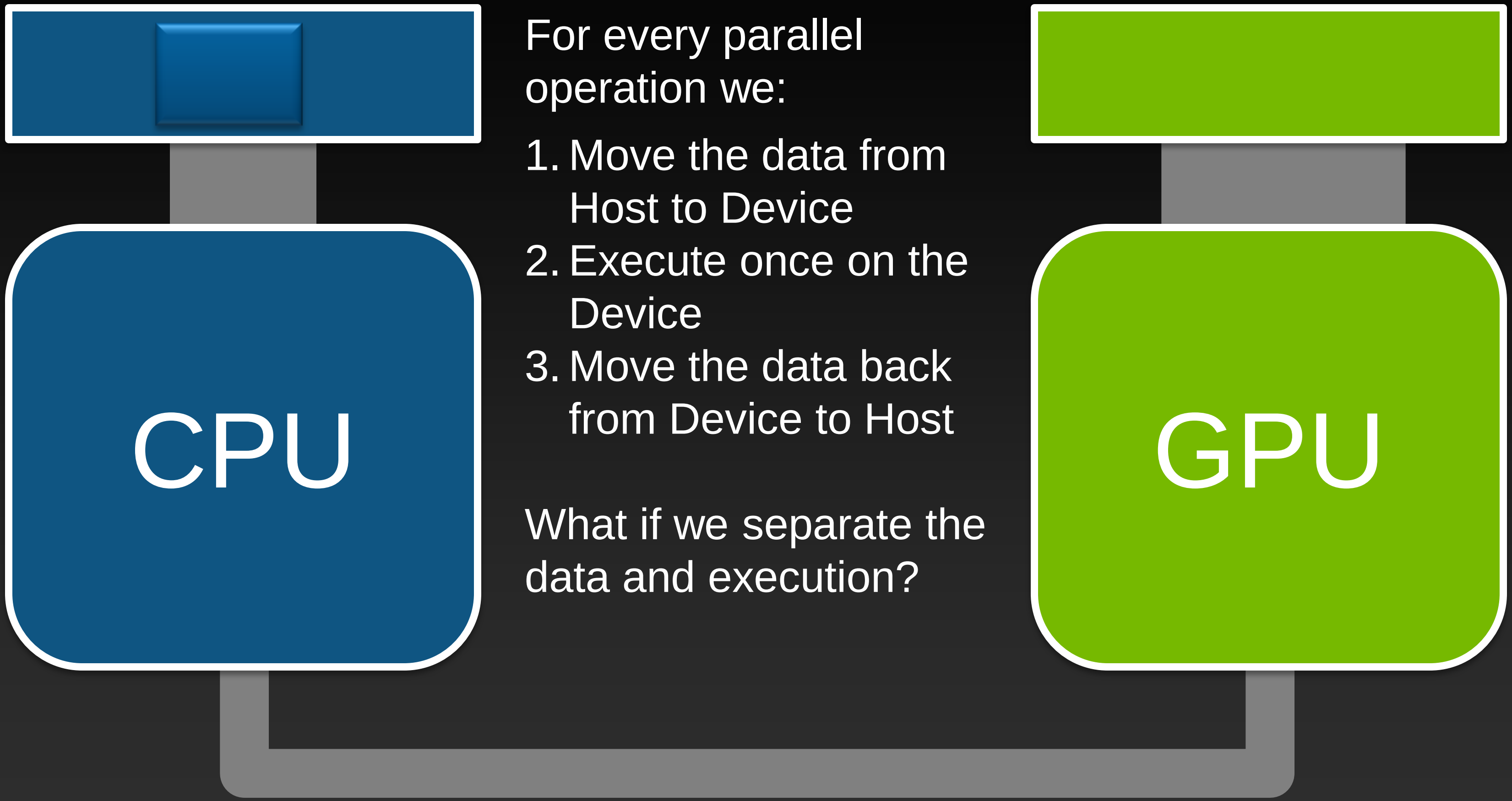
24.8 seconds

Huge Data Transfer Bottleneck!
Computation: 5.19 seconds
Data movement: 74.7 seconds

Offloading a Parallel Kernel



Offloading a Parallel Kernel

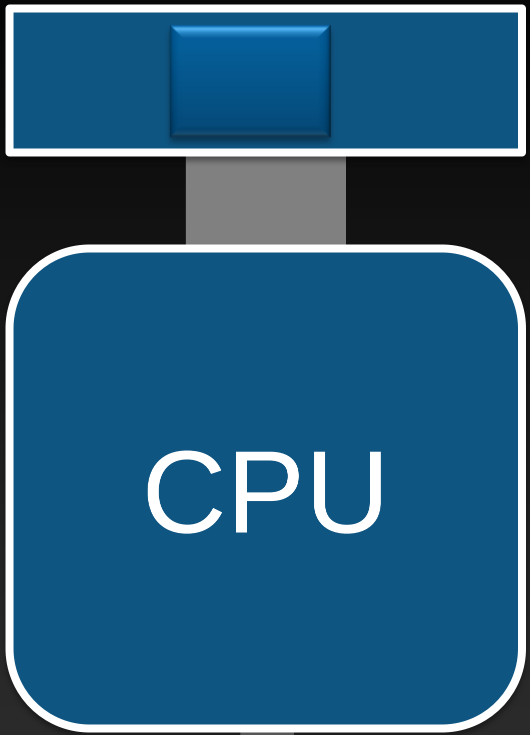


For every parallel operation we:

1. Move the data from Host to Device
2. Execute once on the Device
3. Move the data back from Device to Host

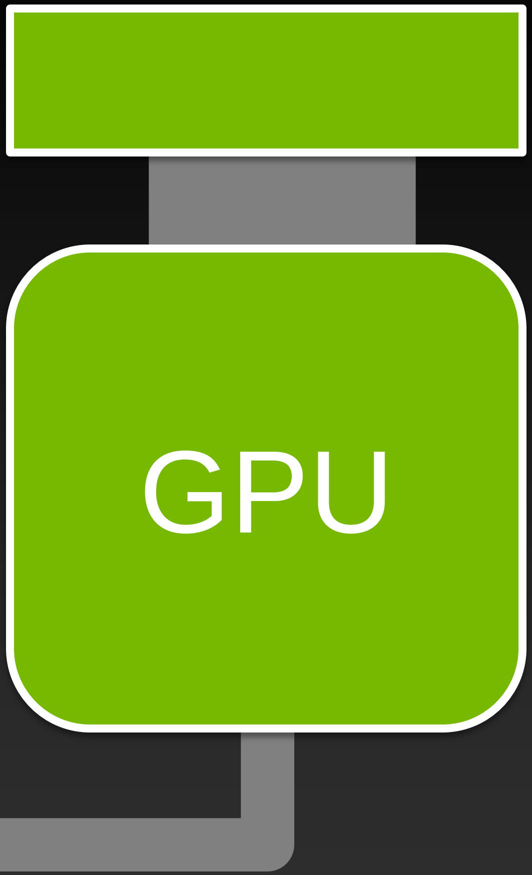
What if we separate the data and execution?

Separating Data from Computation



Now we:

1. Move the data from Host to Device only when needed
2. Execute on the Device multiple times.
3. Move the data back from Device to Host when needed.



Excessive Data Transfers

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

A, Anew resident on host

Copy

```
#pragma acc parallel loop reduction(max:err)
```

A, Anew resident on accelerator

```
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]);
  }
}
```

A, Anew resident on accelerator

Copy

A, Anew resident on host

```
    ...
}
```

These copies happen every iteration of the outer while loop!*

And note that there are two #pragma acc parallel, so there are 4 copies per while loop iteration!

Data Management with OpenACC

Defining data regions

- The data construct defines a region of code in which GPU arrays remain on the GPU and are shared among all kernels in that region.

```
!$acc data
    !$acc parallel loop
    …

    !$acc parallel loop
    …
!$acc end data
```

Data Region

Arrays used within the data region will remain on the GPU until the end of the data region.

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:end)), copyout(b(s/4:3*s/4))
```

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

Jacobi Iteration: Data Directives

- Task: use `acc data` to minimize transfers in the Jacobi example

Jacobi Iteration: OpenACC C Code

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

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

  iter++;
}
```

Copy A in at beginning of loop, out at end. Allocate Anew on accelerator

Did it help?

- Set `PGI_ACC_TIME` environment variable to '1'

```
Accelerator Kernel Timing data
/home/jlarkin/openacc-workshop/exercises/001-laplace2D-kernels/laplace2d.c
  main  NVIDIA  devicenum=0
        time(us): 4,802,950
        51: data copyin reached 1 times
             device time(us): total=22,768 max=22,768 min=22,768 avg=22,768
        57: kernel launched 1000 times
            grid: [4094]  block: [256]
             device time(us): total=2,611,387 max=2,817 min=2,593 avg=2,611
            elapsed time(us): total=2,620,044 max=2,900 min=2,601 avg=2,620
        57: reduction kernel launched 1000 times
            grid: [1]  block: [256]
             device time(us): total=18,083 max=842 min=16 avg=18
            elapsed time(us): total=27,731 max=852 min=25 avg=27
        69: kernel launched 1000 times
            grid: [4094]  block: [256]
             device time(us): total=2,130,162 max=2,599 min=2,112 avg=2,130
            elapsed time(us): total=2,139,919 max=2,712 min=2
        83: data copyout reached 1 times
             device time(us): total=20,550 max=20,550 min=20,550 avg=20,550
```

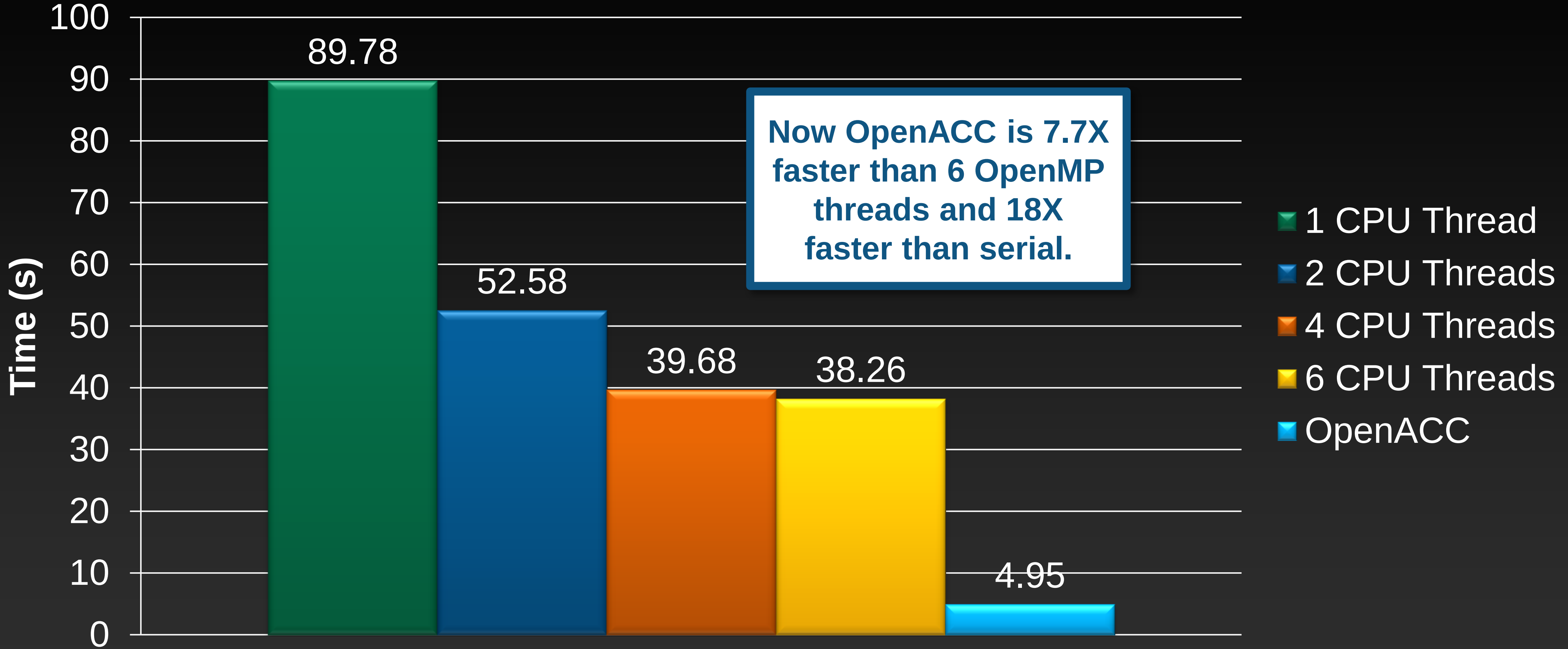
0.23 seconds

0.24 seconds

Execution Time (lower is better)

CPU: Intel i7-3930K
6 Cores @ 3.20GHz

GPU: NVIDIA Tesla K20



Now OpenACC is 7.7X faster than 6 OpenMP threads and 18X faster than serial.

Further speedups

- OpenACC gives us more detailed control over parallelization
  - Via `gang`, `worker`, and `vector` clauses
- By understanding more about the specific GPU on which you’re running, using these clauses may allow better performance.
- By understanding bottlenecks in the code via profiling, we can reorganize the code for even better performance
- More on this in the Optimizing OpenACC session from GTC2013

Communication & IO with OpenACC

Calling MPI with OpenACC (Standard MPI)

```
!$acc data copy(A)
!$acc parallel loop
do i=1,N
 …
enddo
!$acc end parallel loop

call neighbor_exchange(A)

!$acc parallel loop
do i=1,N
 …
enddo
!$acc end parallel loop
!$acc end data
```

Array “A” resides in GPU memory.

Routine contains MPI and requires “A.”

Array “A” returns to CPU here.

OpenACC update Directive

Programmer specifies an array (or partial array) that should be refreshed within a data region.

```
do_something_on_device()

!$acc update host(a)

do_something_on_host()

!$acc update device(a)
```

Copy “a” from GPU to CPU

Copy “a” from CPU to GPU

The programmer may choose to specify only part of the array to update.

Calling MPI with OpenACC (Standard MPI)

```
!$acc data copy(A)
!$acc parallel loop
do i=1,N
 …
enddo
!$acc end parallel loop
!$acc update host(A)
call neighbor_exchange(A)
!$acc update device(A)
!$acc parallel loop
do i=1,N
 …
enddo
!$acc end parallel loop
!$acc end data
```

Copy “A” to CPU for MPI.

Return “A” after MPI to GPU.

OpenACC host_data Directive

Programmer specifies that host arrays should be used within this section, unless specified with use_device. This is useful when calling libraries that expect GPU pointers.

```
!$acc host_data use_device(a)
call MPI_Sendrecv(a,…)
!$acc end host_data
```

Pass the device copy of "a" to subroutine.

```
#pragma host_data use_device(a)
{
cublasDgemm(…,a,…);
}
```

Pass the device copy of "a" to function.

This directive allows interoperability with a variety of other technologies, CUDA, accelerated libraries, OpenGL, etc.

Calling MPI with OpenACC (GPU-aware MPI)

```
!$acc data copy(A)
!$acc parallel loop
do i=1,N
 …
enddo
!$acc end parallel loop
!$acc host_data use_device(A)
call neighbor_exchange(A)
!$acc end host_data
!$acc parallel loop
do i=1,N
 …
enddo
!$acc end parallel loop
!$acc end data
```

Pass device "A" directly to a GPU-aware MPI library called in neighbor_exchange.

*More information about GPU-aware MPI libraries is available in other sessions, please see your agenda.

Thank you