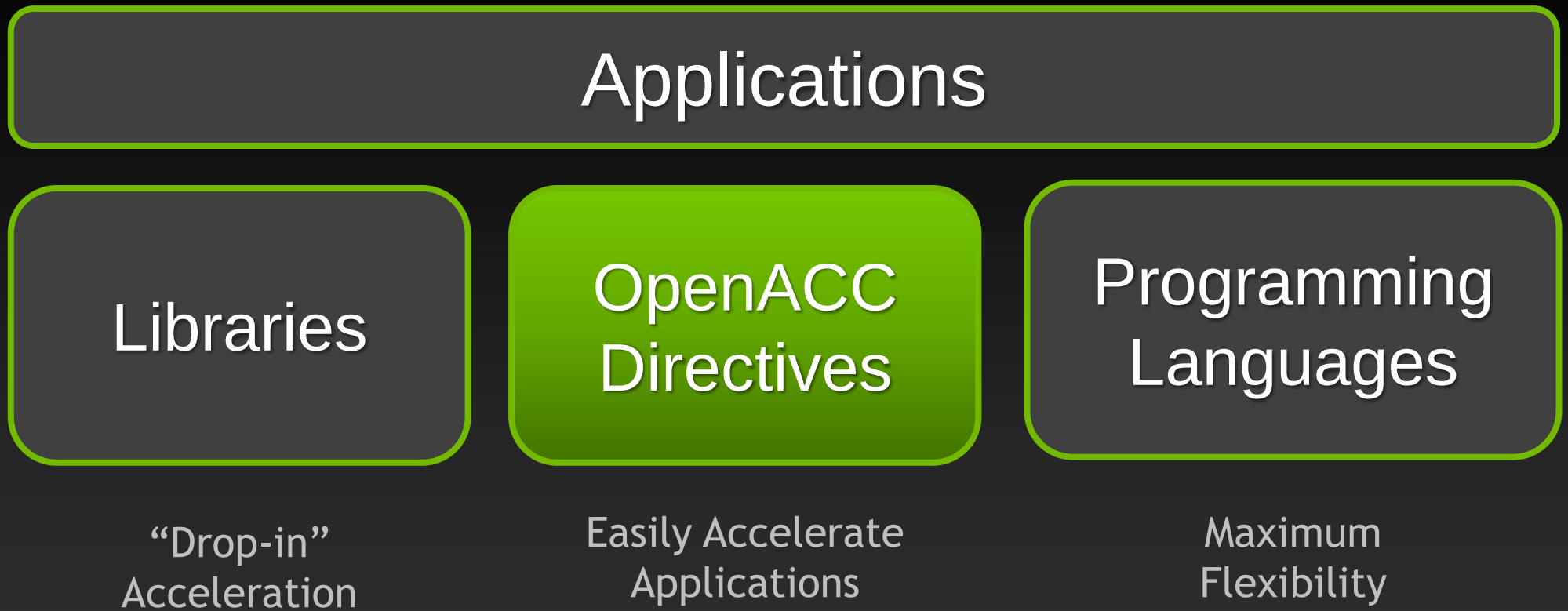

Introduction to
OpenACC
Jeff Larkin, NVIDIA
NVIDIA

3 Ways to Accelerate Applications



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

High-level

- Compiler directives to specify parallel regions in C & Fortran
  - Offload parallel regions
  - Portable across OSes, host CPUs, accelerators, and compilers
- Create high-level heterogeneous programs
  - Without explicit accelerator initialization
  - Without explicit data or program transfers between host and accelerator

High-level… with low-level access

- Programming model allows programmers to start simple
- Compiler gives additional guidance
  - Loop mappings, data location, and other performance details
- Compatible with other GPU languages and libraries
  - Interoperate between CUDA C/Fortran and GPU libraries
  - e.g. CUFFT, CUBLAS, CUSPARSE, etc.

Directives: Easy & Powerful

Real-Time Object Detection

Global Manufacturer of Navigation Systems

5x in 40 Hours

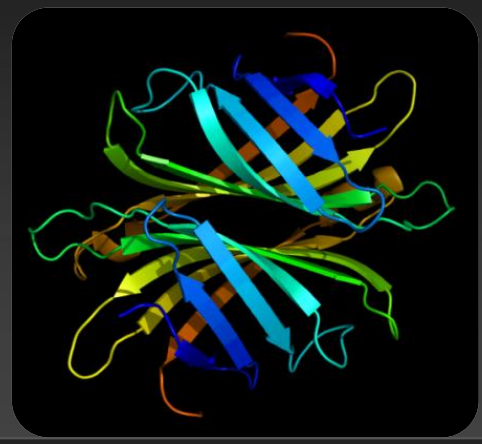
Valuation of Stock Portfolios using Monte Carlo

Global Technology Consulting Company

2x in 4 Hours

Interaction of Solvents and Biomolecules

University of Texas at San Antonio



5x in 8 Hours

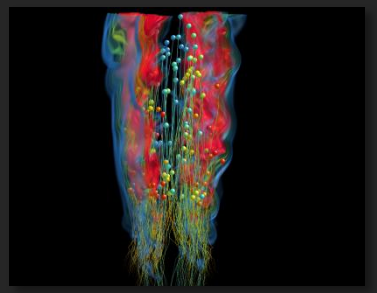
> "Optimizing code with directives is quite easy, especially compared to CPU threads or writing CUDA kernels. The most important thing is avoiding restructuring of existing code for production applications."
>
> *-- Developer at the Global Manufacturer of Navigation Systems*

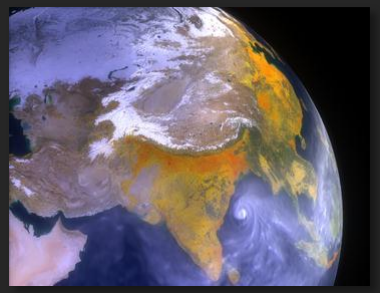
Focus on Exposing Parallelism

With Directives, tuning work focuses on *exposing 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%**

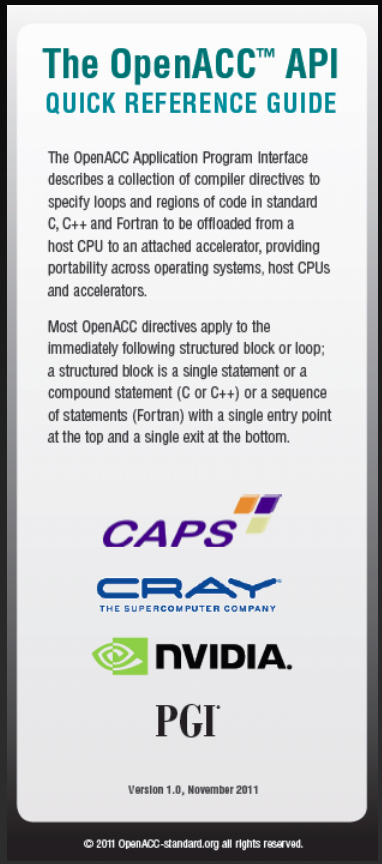
- **Tuning top key kernel (50% of runtime)**
- **6.5x faster on CPU+GPU vs. CPU+CPU**
- **Improved performance of CPU version by 100%**

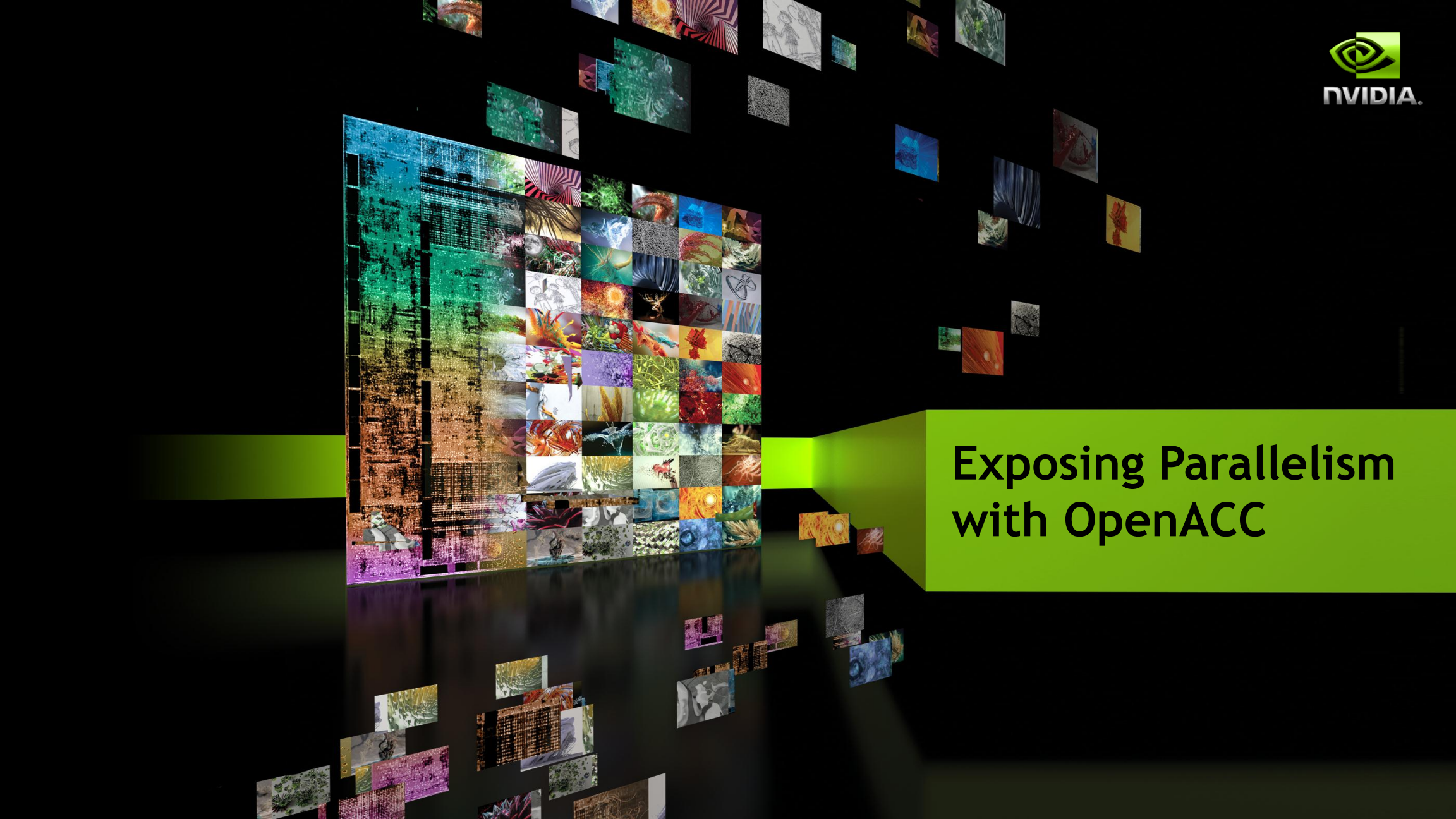
OpenACC Specification and Website

- Full OpenACC 1.0 Specification available online

www.openacc.org

- Quick reference card also available
- Compilers available now from PGI, Cray, and CAPS





Exposing Parallelism with OpenACC

A Very Simple Exercise: SAXPY

SAXPY in 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

```
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

```
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

```
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

```
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);
...
```

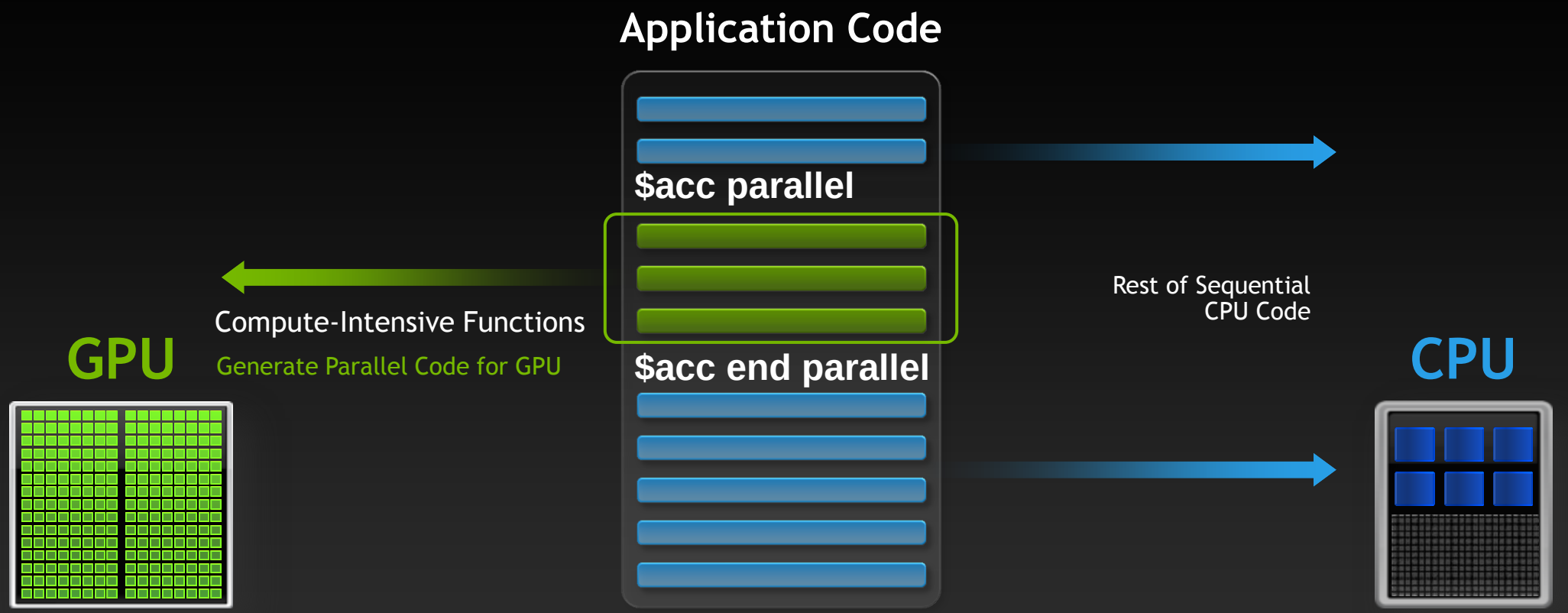
SAXPY in Fortran

```
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 is not *GPU Programming.*

OpenACC is *Exposing Parallelism* in your code.

OpenACC Execution Model



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)
```

OpenACC parallel Directive

Programmer identifies a loop as having parallelism, compiler generates a parallel kernel for that loop.

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

Parallel kernel

Kernel:
A parallel function that runs on the GPU

*Most often `parallel` will be used as `parallel loop`.

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
```

Run

- The Cray compiler provides automatic instrumentation when `CRAY_ACC_DEBUG=<1,2,3>` at runtime

```
ACC: Initialize CUDA
ACC: Get Device 0
ACC: Create Context
ACC: Set Thread Context
ACC: Start transfer 2 items from saxpy.c:17
ACC:       allocate, copy to acc 'x' (4194304 bytes)
ACC:       allocate, copy to acc 'y' (4194304 bytes)
ACC: End transfer (to acc 8388608 bytes, to host 0 bytes)
ACC: Execute kernel saxpy$ck_L17_1 blocks:8192 threads:128 async(auto) from saxpy.c:17
ACC: Wait async(auto) from saxpy.c:18
ACC: Start transfer 2 items from saxpy.c:18
ACC:       free 'x' (4194304 bytes)
ACC:       copy to host, free 'y' (4194304 bytes)
ACC: End transfer (to acc 0 bytes, to host 4194304 bytes)
```

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
       c(i) = 2.0
    end do

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

kernel 1

kernel 2

The compiler identifies 2 parallel loops and generates 2 kernels.

OpenACC parallel vs. kernels

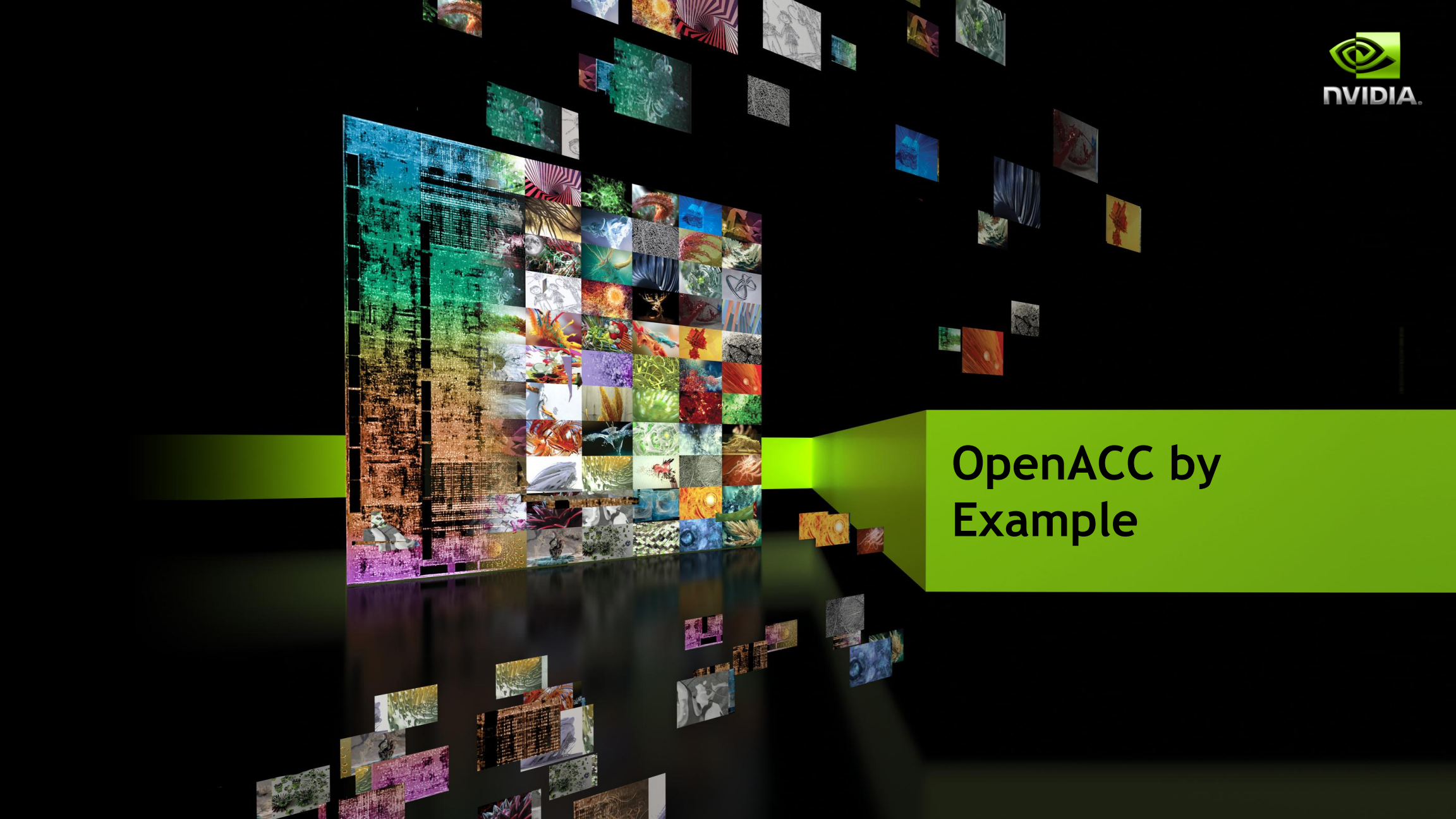
PARALLEL

- 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.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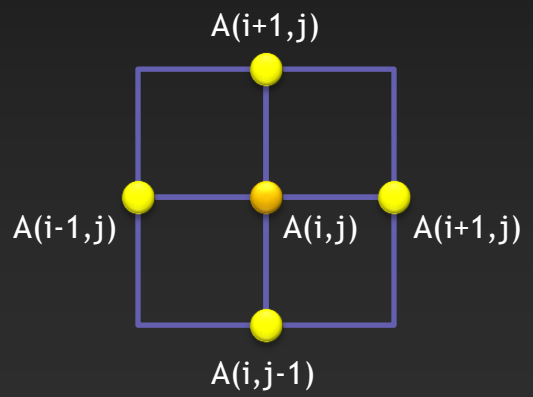
OpenACC by
Example

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

```
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
```

Performance

CPU: AMD IL-16
@ 2.2 GHz

Execution	Time (s)	Speedup
CPU 1 OpenMP thread	109.7	--
CPU 2 OpenMP threads	71.6	1.5x
CPU 4 OpenMP threads	53.7	2.0x
CPU 8 OpenMP threads	65.5	1.7x
CPU 16 OpenMP threads	66.7	1.6x
OpenACC GPU	180.9	0.6x FAIL!

GPU: NVIDIA Tesla K20X

Speedup vs. 1 CPU core

Speedup vs. 4 OpenMP Threads

What went wrong?

- Set `PGI_ACC_TIME` environment variable to '1'

```
Accelerator Kernel Timing data
/lustre/scratch/jlarkin/openacc-workshop/exercises/001-laplace2D-kernels/laplace2d.c
  main
    69: region entered 1000 times
        time(us): total=109,998,808 init=262 region=109,998,546
                  kernels=1,748,221 data=109,554,793
        w/o init: total=109,998,546 max=110,762 min=109,378 avg=109
        69: kernel launched 1000 times
            grid: [4094]  block: [256]
            time(us): total=1,748,221 max=1,820 min=1,727 avg=1,74
/lustre/scratch/jlarkin/openacc-workshop/exercises/001-laplace2D-k
  main
    57: region entered 1000 times
        time(us): total=71,790,531 init=491,553 region=71,298,97
                  kernels=2,369,807 data=68,968,929
        w/o init: total=71,298,978 max=75,603 min=70,486 avg=71,298
        57: kernel launched 1000 times
            grid: [4094]  block: [256]
            time(us): total=2,347,795 max=3,737 min=2,343 avg=2,347
        58: kernel launched 1000 times
            grid: [1]  block: [256]
            time(us): total=22,012 max=1,400 min=19 avg=22
 total: 181.792123 s
```

109.5 seconds

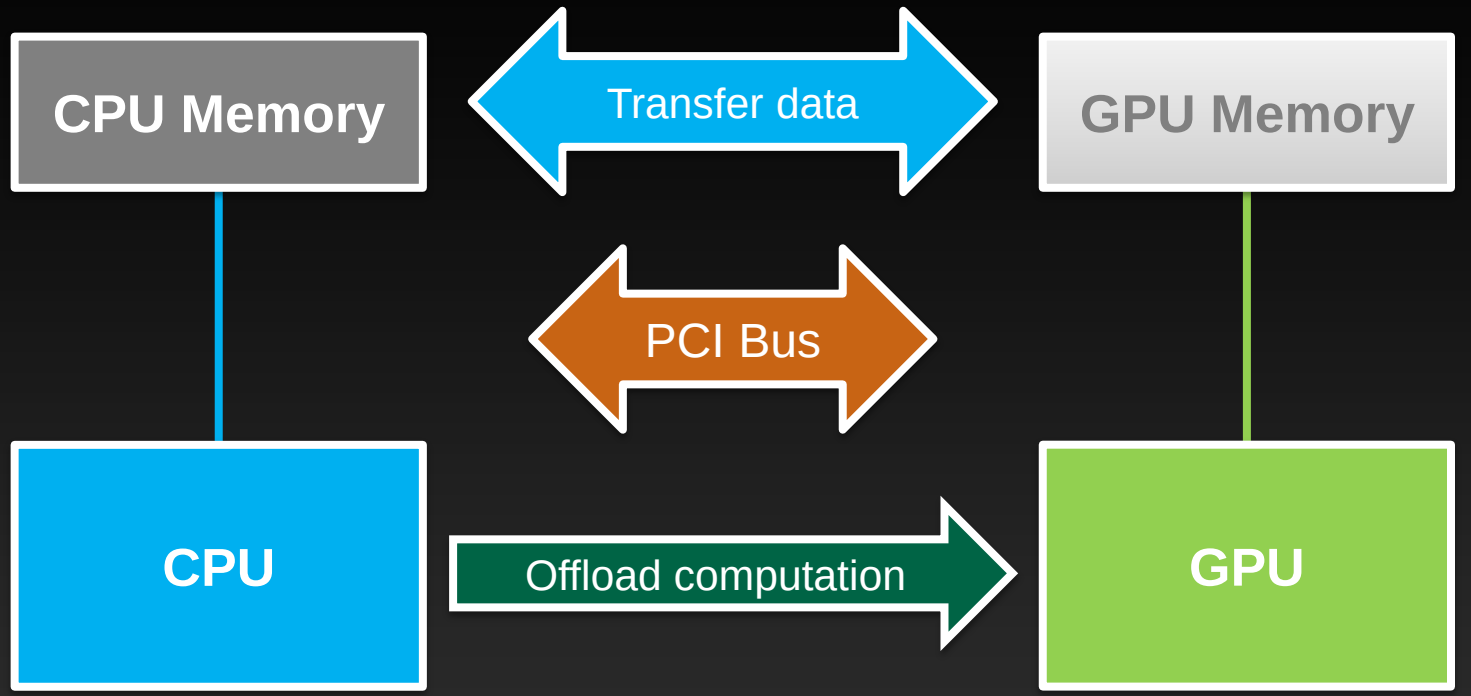
1.7 seconds

Huge Data Transfer Bottleneck!
Computation: 4.1 seconds
Data movement: 178.4 seconds

68.9 seconds

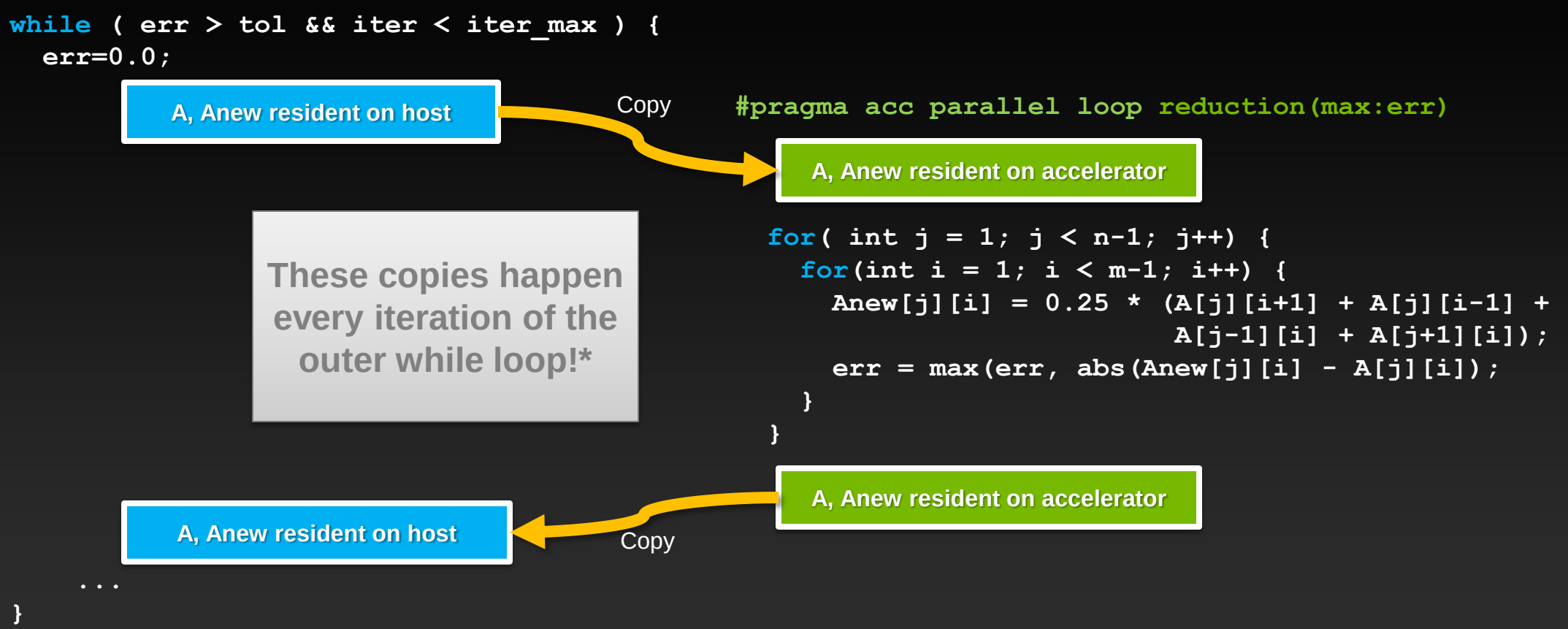
2.4 seconds

Basic Concepts

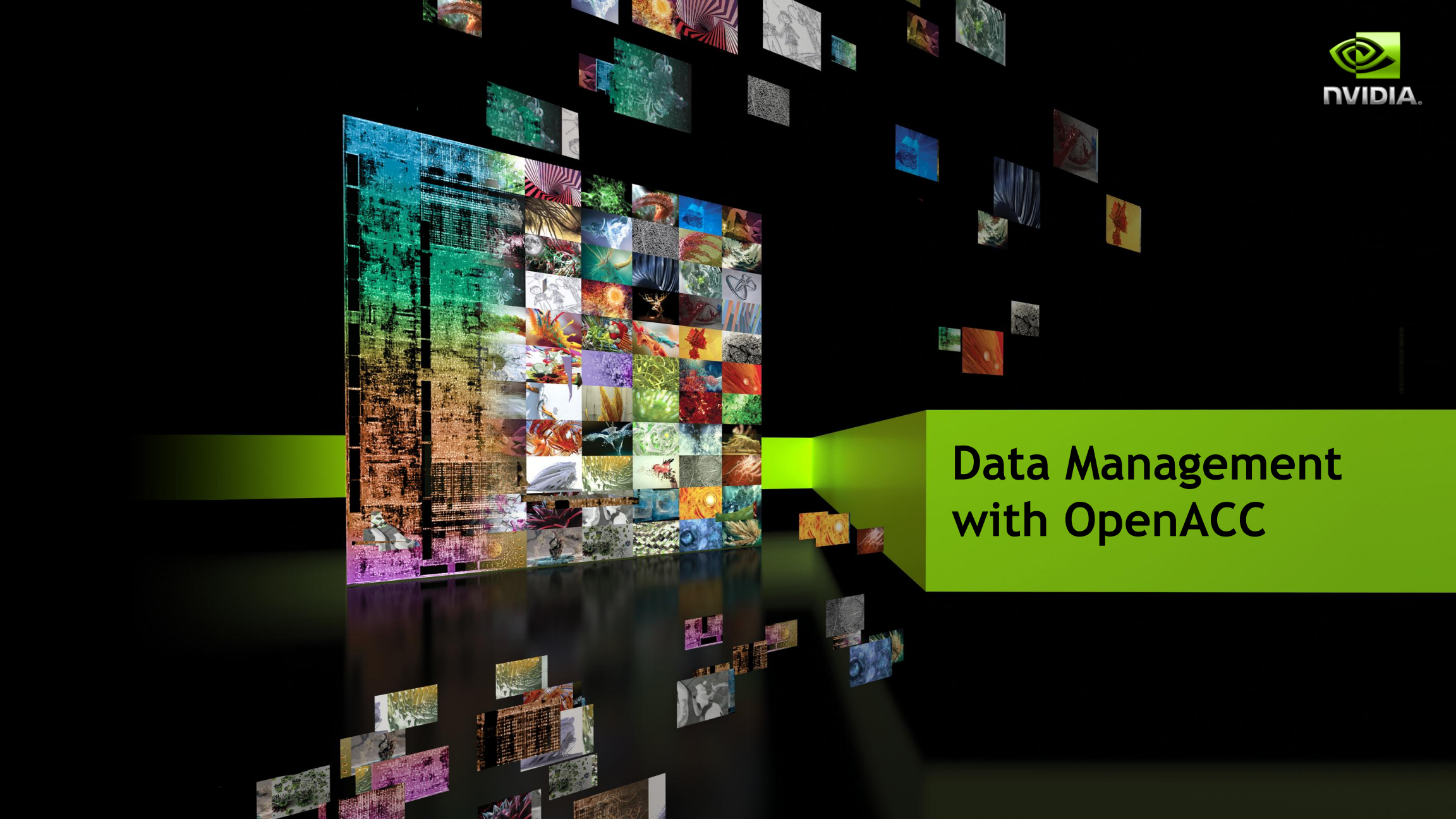


For efficiency, decouple data movement and compute off-load

Excessive Data Transfers



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

Data Region

Arrays a, b, and c 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?

```
Accelerator Kernel Timing data
/lustre/scratch/jlarkin/openacc-workshop/exercises/001-laplace2D-kernels/laplace2d.c
  main
    69: region entered 1000 times
        time(us): total=1,791,050 init=217 region=1,790,833
                  kernels=1,742,066
        w/o init: total=1,790,833 max=1,950 min=1,773 avg=1,790
        69: kernel launched 1000 times
            grid: [4094]  block: [256]
            time(us): total=1,742,066 max=1,809 min=1,725 avg=1,742
/lustre/scratch/jlarkin/openacc-workshop/exercises/001-laplace2D-kernels/laplace2d.c
  main
    57: region entered 1000 times
        time(us): total=2,710,902 init=182 region=2,710,720
                  kernels=2,361,193
        w/o init: total=2,710,720 max=4,163 min=2,697 avg=2,710
        57: kernel launched 1000 times
            grid: [4094]  block: [256]
            time(us): total=2,339,800 max=3,709 min=2,334 avg=2,339
        58: kernel launched 1000 times
            grid: [1]  block: [256]
            time(us): total=21,393 max=1,321 min=19 avg=21
/lustre/scratch/jlarkin/openacc-workshop/exercises/001-laplace2D-kernels/laplace2d.c
  main
    51: region entered 1 time
        time(us): total=5,063,688 init=4[illegible] region=4,574,555
                  data=68,993
        w/o init: total=4,574,555 max=4,574,555 min=4,574,555 avg=4,574,555
```

0.69 seconds

Performance

CPU: AMD IL-16
@ 2.2 GHz

Execution	Time (s)	Speedup
CPU 1 OpenMP thread	109.7	--
CPU 2 OpenMP threads	71.6	1.5x
CPU 4 OpenMP threads	53.7	2.0x
CPU 8 OpenMP threads	65.5	1.7x
CPU 16 OpenMP threads	66.7	1.6x
OpenACC GPU	4.96	10.8x

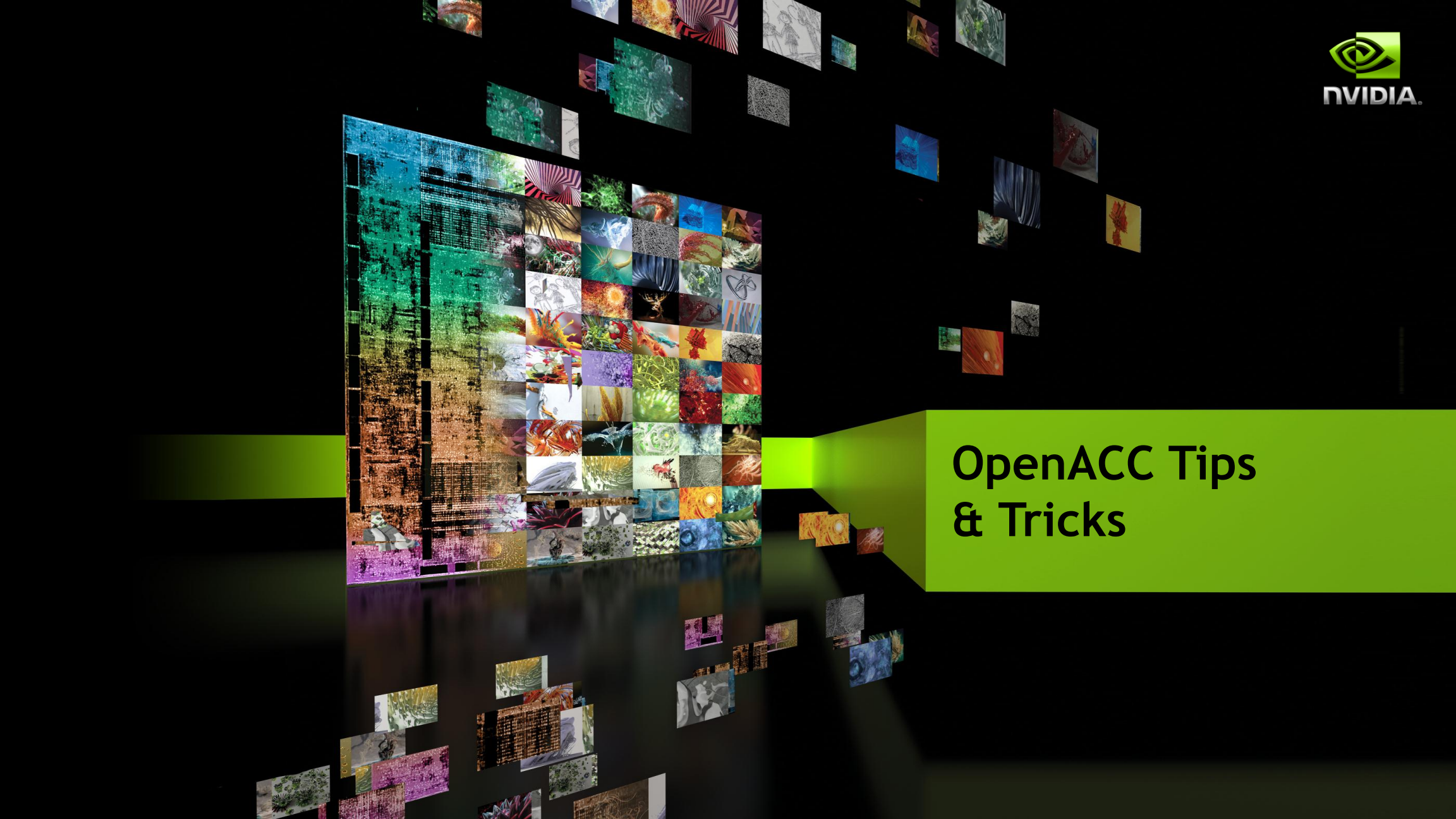
GPU: NVIDIA Tesla K20X

Speedup vs. 1 CPU core

Speedup vs. 4 OpenMP Threads

Further speedups

- OpenACC gives us more detailed control over parallelization
  - Via `gang`, `worker`, and `vector` clauses
- By understanding more about OpenACC execution model and GPU hardware organization, we can get higher speedups on this code
- By understanding bottlenecks in the code via profiling, we can reorganize the code for higher performance
- More on this in the Advanced OpenACC session this afternoon.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OpenACC Tips
& Tricks

C tip: the `restrict` keyword

- Declaration of intent given by the programmer to the compiler
  - Applied to a pointer, e.g.

    ```
    float *restrict ptr
    ```

  - Meaning: "for the lifetime of `ptr`, only it or a value directly derived from it (such as `ptr + 1`) will be used to access the object to which it points"*
- Limits the effects of pointer aliasing
- Compilers often require `restrict` to determine independence (true for OpenACC, OpenMP, and vectorization)
  - Otherwise the compiler can't parallelize loops that access `ptr`
  - Note: if programmer violates the declaration, behavior is undefined

http://en.wikipedia.org/wiki/Restrict

Tips and Tricks

- Nested loops are best for parallelization
  - Large loop counts (1000s) needed to offset GPU/memcpy overhead
- Iterations of loops must be independent of each other
  - To help compiler: use `restrict` keyword in C
- Compiler must be able to figure out sizes of data regions
  - Can use directives to explicitly control sizes
- Inline function calls in directives regions
  - (PGI): `-Minline` or `-Minline=levels:<N>`
  - (Cray): `-hpl=<dir/>`
  - This has been improved in OpenACC 2.0

Tips and Tricks (cont.)

- Use time option to learn where time is being spent
  - (PGI) `PGI_ACC_TIME=1` (runtime environment variable)
  - (Cray) `CRAY_ACC_DEBUG=<1,2,3>` (runtime environment variable)
  - (CAPS) `HMPPRT_LOG_LEVEL=info` (runtime environment variable)
- Pointer arithmetic should be avoided if possible
  - Use subscripted arrays, rather than pointer-indexed arrays.
- Use contiguous memory for multi-dimensional arrays
- Use data regions to avoid excessive memory transfers
- Conditional compilation with `_OPENACC` macro


Thank you
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