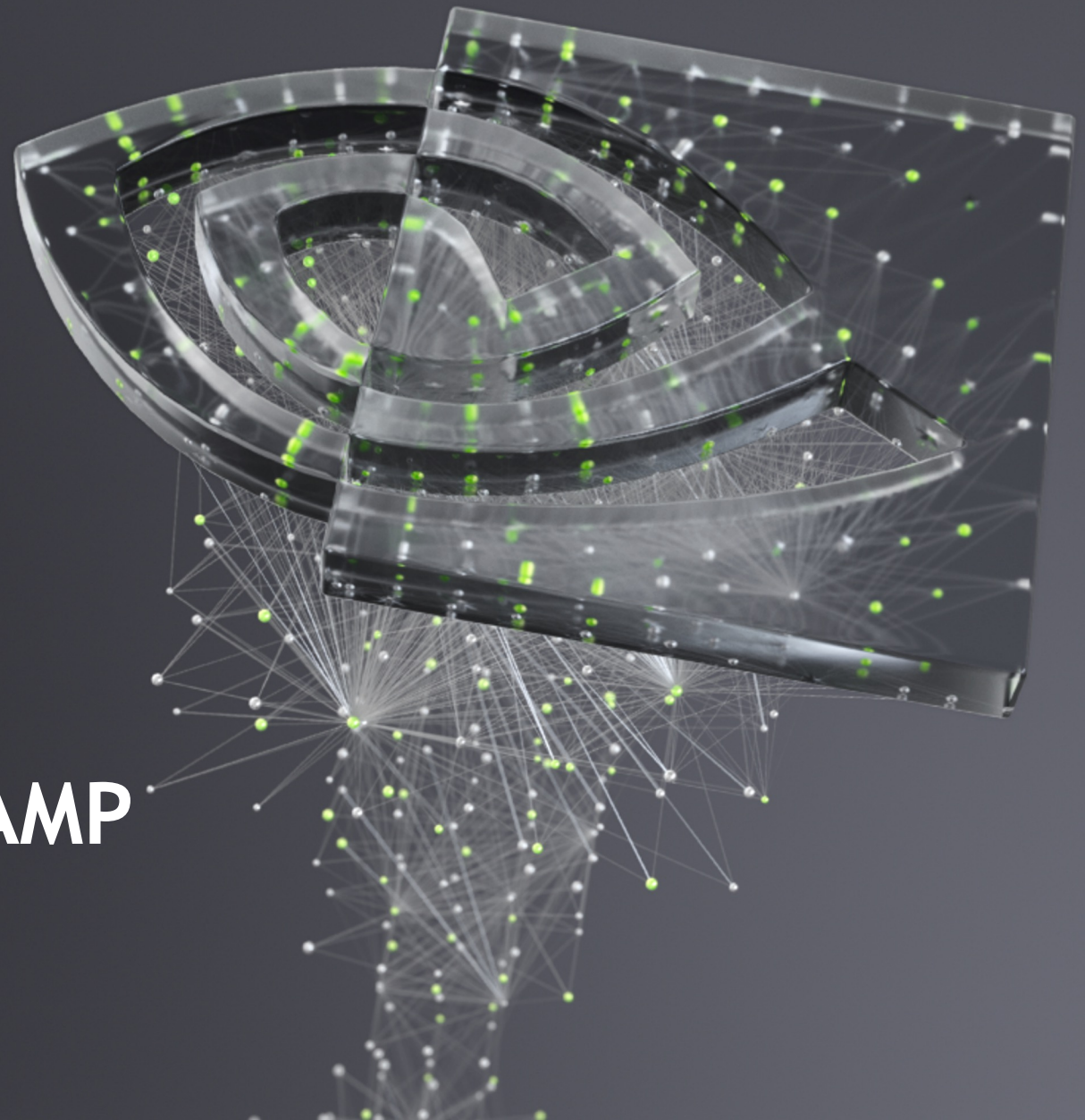


NVIDIA

N-WAYS GPU BOOTCAMP

OPENACC

OPENACC

What to expect?

- Basic introduction to OpenACC directives
- HPC SDK Usage
- Portability across Multicore and GPU

OpenACC is…

a directives-based

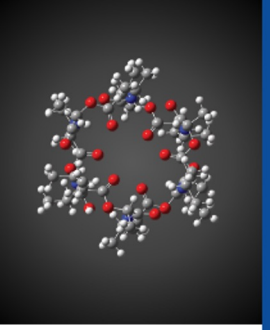
parallel programming model

designed for

performance and **portability**.

Add Simple Compiler Directive

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



GAUSSIAN 16

Mike Frisch, Ph.D.
President and
CEO
Gaussian, Inc.

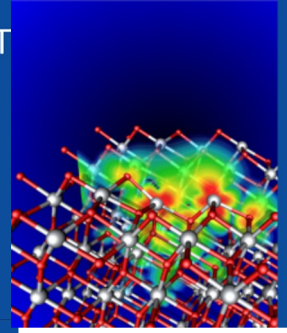
Using OpenACC allowed us to continue development of our fundamental algorithms and software capabilities simultaneously with the GPU-related work. In the end, we could use the same code base for SMP, cluster/network and GPU parallelism. PGI's compilers were essential to the success of our efforts.

Image courtesy ANSYS

ANSYS FLUENT

Sunil Sathe
Lead Software Developer
ANSYS Fluent

We've effectively used OpenACC for heterogeneous computing in ANSYS Fluent with impressive performance. We're now applying this work to more of our models and new platforms.



VASP

Prof. Georg Kresse
Computational Materials Physics
University of Vienna

For VASP, OpenACC is *the* way forward for GPU acceleration. Performance is similar and in some cases better than CUDA C, and OpenACC dramatically decreases GPU development and maintenance efforts. We're excited to collaborate with NVIDIA and PGI as an early adopter of CUDA Unified Memory.

COSMO

Dr. Oliver Fuhrer
Senior Scientist
Meteoswiss

OpenACC made it practical to develop for GPU-based hardware while retaining a single source for almost all the COSMO physics code.

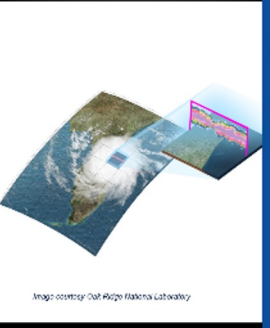


Image courtesy Oak Ridge National Laboratory

E3SM

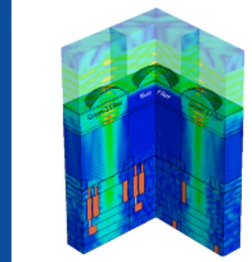
Mark A. Taylor
Multiphysics Applications
Sandia

The CAAR project provided us with early access to Summit hardware and access to PGI compiler experts. Both of these were critical to our success. PGI's OpenACC support remains the best available and is competitive with much more intrusive programming model approaches.

NUMECA FINE/Open

David Gutzwiller
Lead Software Developer
NUMECA

- Porting our unstructured C++ CFD solver FINE/Open to GPUs using OpenACC would have been impossible two or three years ago, but OpenACC has developed enough that we're now getting some really good results.



SYNOPSYS

Dr. Lutz Schneider
Senior R&D Engineer
Synopsys Inc.

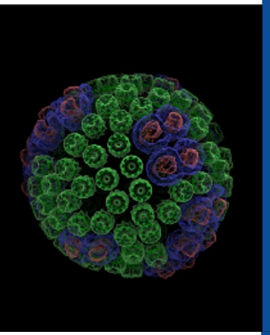
Using OpenACC, we've GPU-accelerated the Synopsys TCAD Sentaurus Device EMW simulator to speed up optical simulations of image sensors. GPUs are key to improving simulation throughput in the design of advanced image sensors.

Image courtesy: NCAR

MPAS-A

Richard Loft
Director, Technology Development
NCAR

Our team has been evaluating OpenACC as a pathway to performance portability for the Model for Prediction (MPAS) atmospheric model. Using this approach on the MPAS dynamical core, we have achieved performance on a single P100 GPU equivalent to 2.7 dual socketed Intel Xeon nodes on our new Cheyenne supercomputer.



VMD

John Stone
Senior Research Programmer
Beckham Institute
University of Illinois

Due to Amdahl's law, we need to port more parts of our code to the GPU if we're going to speed it up. But the sheer number of routines poses a challenge. OpenACC directives give us a low-cost approach to getting at least some speed-up out of these second-tier routines. In many cases it's completely sufficient because with the current algorithms, GPU performance is bandwidth-bound.

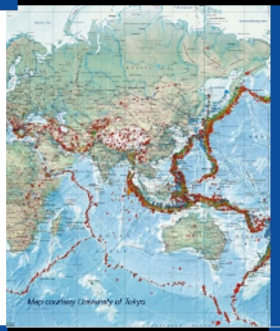
GTC

Zhihong Lin
Professor and Principal Investigator
UC Irvine

Using OpenACC our scientists were able to achieve the acceleration needed for integrated fusion simulation with a minimum investment of time and effort in learning to program GPUs.

OpenACC

More Science, Less Programming

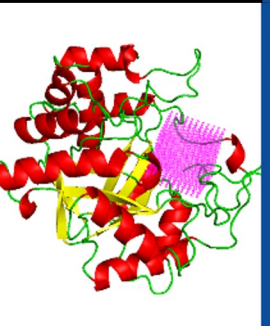


Map courtesy University of Tokyo

GAMERA

Takuma Yamaguchi, Kohei Fujita, Tsuyoshi Ichimura, Muneo Hori, Lalith Wijerathne
The University of Tokyo

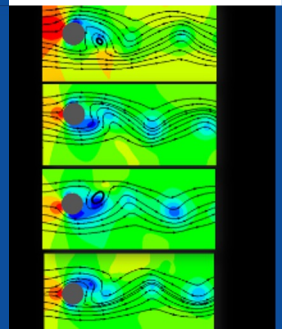
With OpenACC and a compute node based on NVIDIA's Tesla P100 GPU, we achieved more than a 14X speed up over a K Computer node running our earthquake disaster simulation code



SANJEEVINI

Abhilash Jayaraj
Project Scientist
Indian Institute of Technology
New Delhi

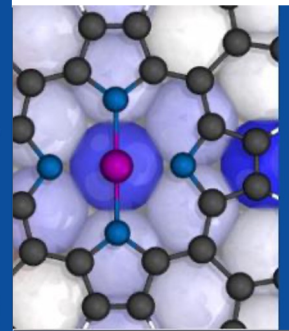
In an academic environment maintenance and speedup of existing codes is a tedious task. OpenACC provides a great platform for computational scientists to accomplish both tasks without involving a lot of efforts or manpower in speeding up the entire computational task.



IBM-CFD

Somnath Roy
Assistant Professor
Mechanical Engineering Department
Indian Institute of Technology Kharagpur

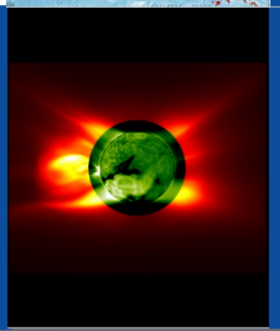
OpenACC can prove to be a handy tool for computational engineers and researchers to obtain fast solution of non-linear dynamics problem. In immersed boundary incompressible CFD, we have obtained order of magnitude reduction in computing time by porting several components of our legacy codes to GPU. Especially the routines involving search algorithm and matrix solvers have been well-accelerated to improve the overall scalability of the code.



PWscf (Quantum ESPRESSO)

Filippo Spiga
Senior Contributor
Quantum ESPRESSO group

- CUDA Fortran gives us the full performance potential of the CUDA programming model and NVIDIA GPUs. While leveraging the potential of explicit data movement, ISCUF KERNELS directives give us productivity and source code maintainability. It's the best of both worlds.



MAS

Ronald M. Caplan
Computational Scientist
Predictive Science Inc.

Adding OpenACC into MAS has given us the ability to migrate medium-sized simulations from a multi node CPU cluster to a single multi-GPU server. The implementation yielded a portable single-source code for both CPU and GPU runs. Future work will add OpenACC to the remaining model features, enabling GPU-accelerated realistic solar storm modeling.

OpenACC Directives

Manage Data Movement

Initiate Parallel Execution

Optimize Loop Mappings

```
#pragma acc data copyin(a,b) copyout(c)
{
  ...
  #pragma acc parallel
  {
  #pragma acc loop gang vector
      for (i = 0; i < n; ++i) {
          c[i] = a[i] + b[i];
          ...
      }
  }
  ...
}
```

OpenACC
Directives for Accelerators

- Incremental
- Single source
- Interoperable
- Performance portable
- CPU, GPU, Manycore

OPENACC SYNTAX

Syntax for using OpenACC directives in code

C/C++

```
#pragma acc directive clauses
<code>
```

Fortran

```
!$acc directive clauses
<code>
```

A *pragma* in C/C++ gives instructions to the compiler on how to compile the code. Compilers that do not understand a particular pragma can freely ignore it.

A *directive* in Fortran is a specially formatted comment that likewise instructions the compiler in it compilation of the code and can be freely ignored.

"*acc*" informs the compiler that what will come is an OpenACC directive

Directives are commands in OpenACC for altering our code.

Clauses are specifiers or additions to directives.

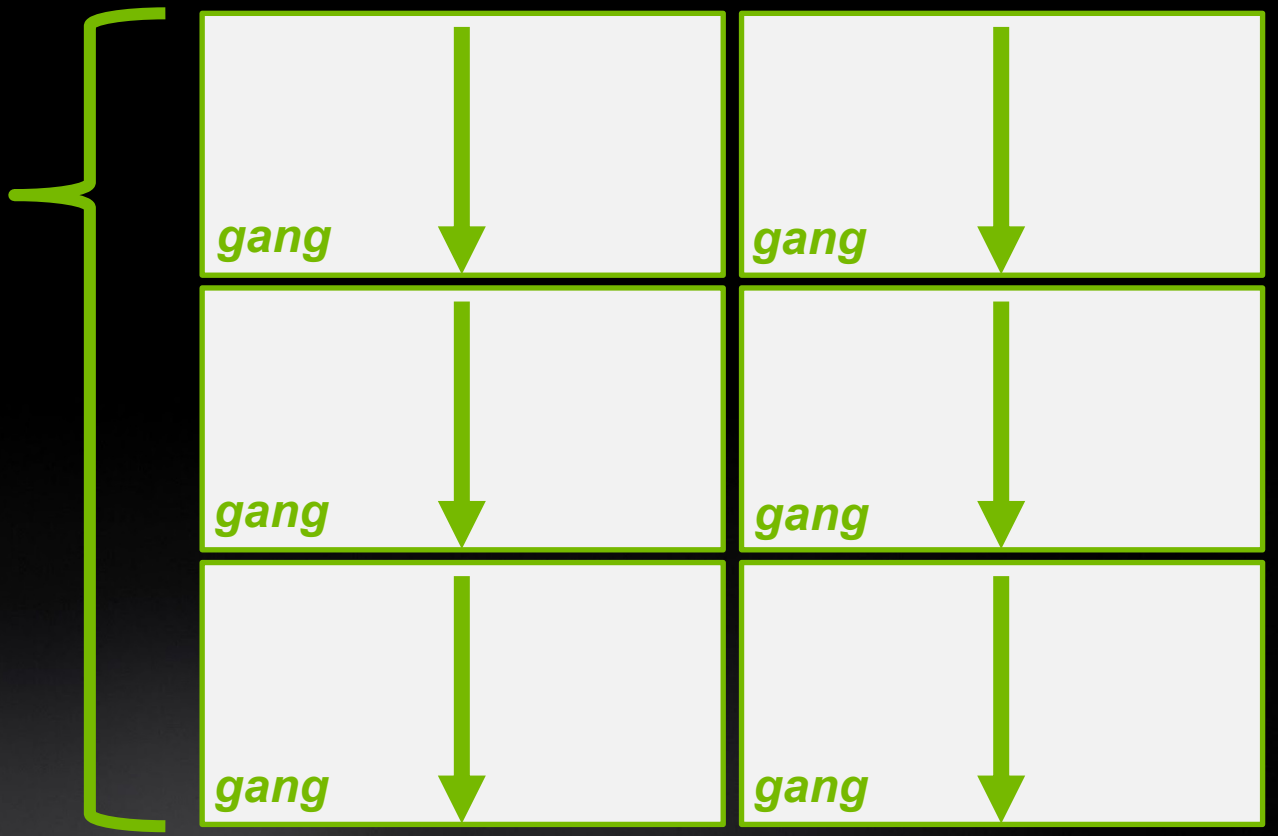
OPENACC PARALLEL DIRECTIVE

Expressing parallelism

```
#pragma acc parallel
{

}
```

When encountering the ***parallel*** directive, the compiler will generate *1 or more parallel* ***gangs***, which execute redundantly.



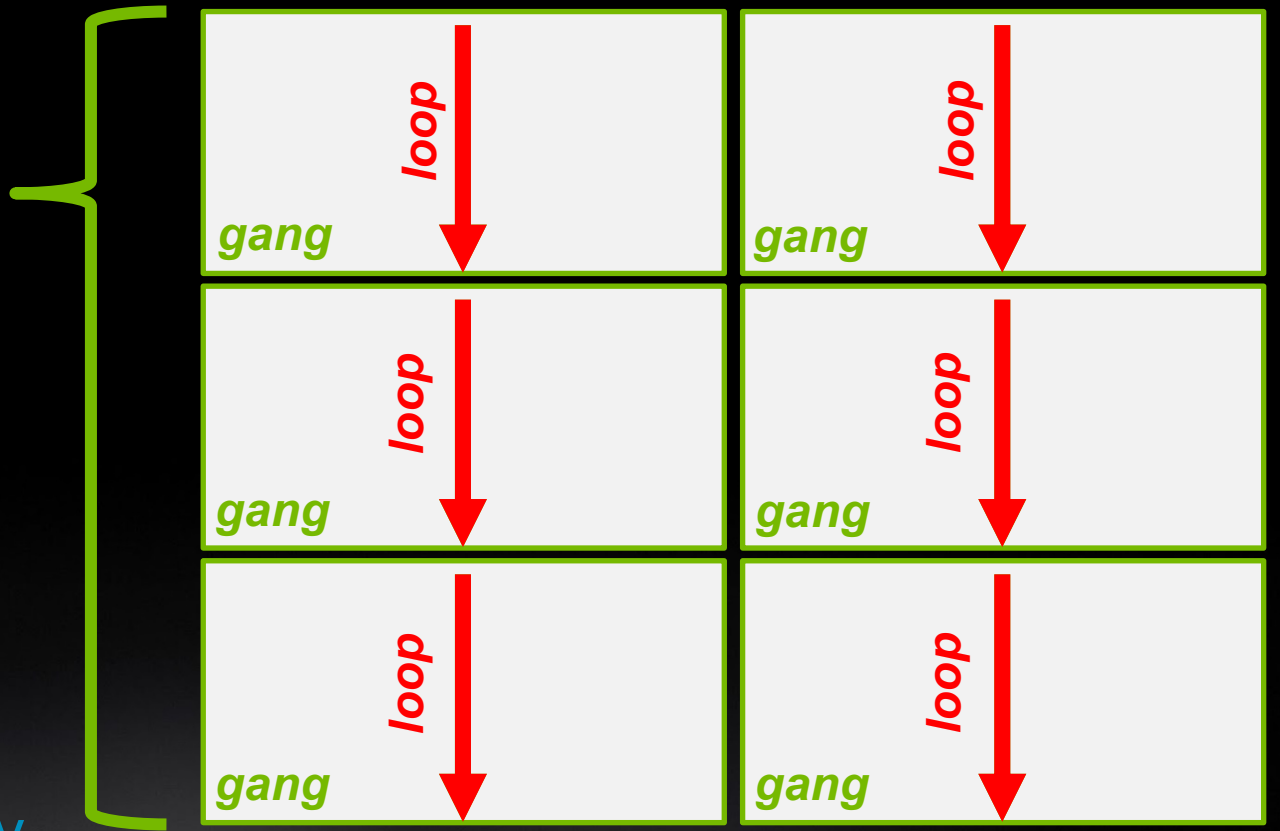
OPENACC PARALLEL DIRECTIVE

Expressing parallelism

```
#pragma acc parallel
{
        for(int i = 0; i < N; i++)
        {
                // Do Something
        }
}
```

loop

This loop will be executed redundantly on each gang



OPENACC PARALLEL DIRECTIVE

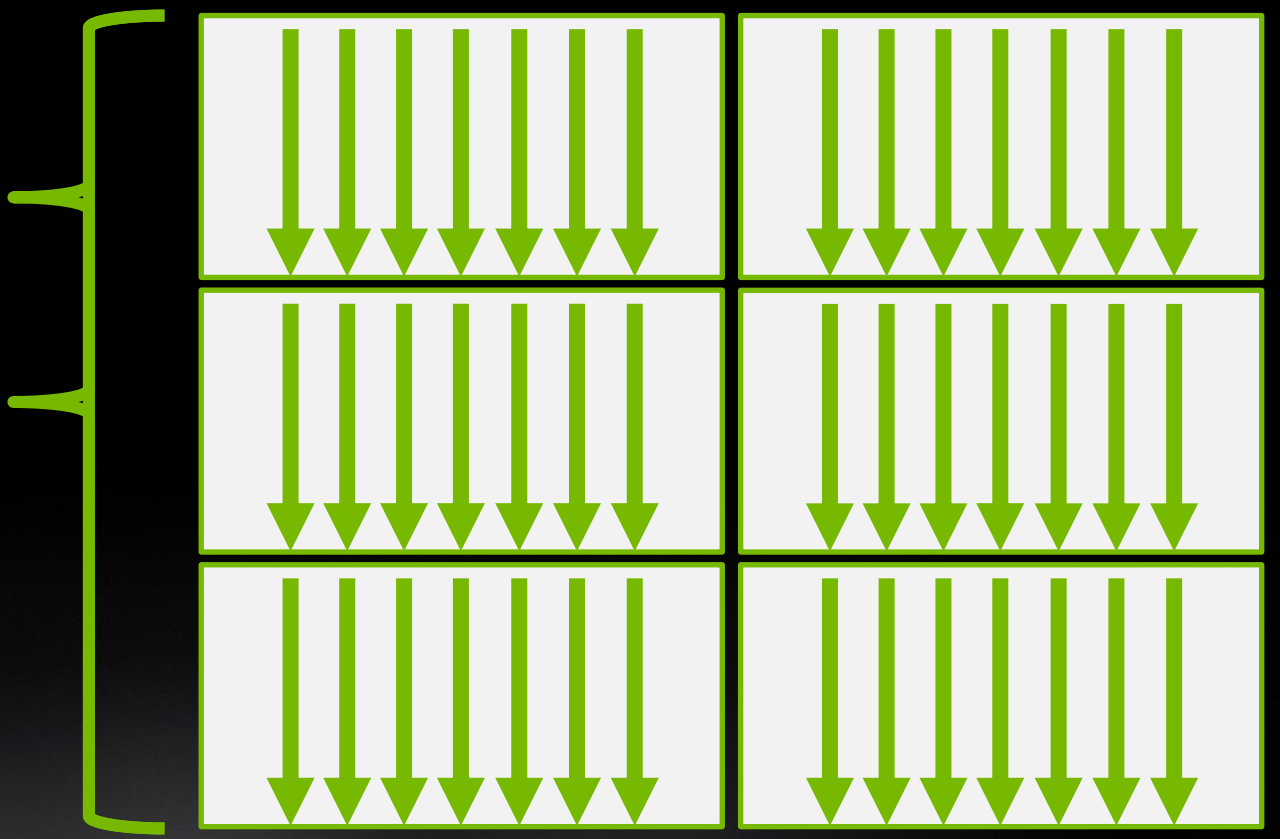
Expressing parallelism

```
#pragma acc parallel
{

        #pragma acc loop
        for(int i = 0; i < N;
i++)
        {
                // Do Something
        }

}
```

The ***loop*** directive informs the compiler which loops to parallelize.



OPENACC PARALLEL DIRECTIVE

Parallelizing a single loop

C/C++

```
#pragma acc parallel
{
        #pragma acc loop
        for(int i = 0; j < N;
i++)
                a[i] = 0;
}
```

Fortran

```
!$acc parallel
        !$acc loop
        do i = 1, N
                a(i) = 0
        end do
!$acc end parallel
```

Use a **parallel** directive to mark a region of code where you want parallel execution to occur

This parallel region is marked by curly braces in C/C++ or a start and end directive in Fortran

The **loop** directive is used to instruct the compiler to parallelize the iterations of the next loop to run across the parallel gangs

OPENACC PARALLEL DIRECTIVE

Parallelizing a single loop

C/C++

```
#pragma acc parallel loop
for(int i = 0; j < N; i++)
        a[i] = 0;
```

Fortran

```
!$acc parallel loop
do i = 1, N
        a(i) = 0
end do
```

This pattern is so common that you can do all of this in a single line of code

In this example, the parallel loop directive applies to the next loop

This directive both marks the region for parallel execution and distributes the iterations of the loop.

When applied to a loop with a data dependency, parallel loop may produce incorrect results. An #pragma acc atomic could make a instruction atomic.


BUILD AND RUN THE CODE

NVIDIA HPC SDK

- Comprehensive suite of compilers, libraries, and tools used to GPU accelerate HPC modeling and simulation application
- The NVIDIA HPC SDK includes the new NVIDIA HPC compiler supporting OpenACC C and Fortran
  - The command to compile C code is ‘nvc’
  - The command to compile C++ code is ‘nvc++’
  - The command to compile Fortran code is ‘nvfortran’

```
nvc –fast –Minfo=accel –ta=tesla:managed main.c
```

```
nvfortran –fast –Minfo=accel –ta=tesla:managed main.f90
```

BUILDING THE CODE

-Minfo shows more details

```
$ nvc -fast -ta=multicore -Minfo=accel laplace2d_uvm.c
main:
     63, Generating Multicore code
         64, #pragma acc loop gang
     64, Accelerator restriction: size of the GPU copy of Anew,A is unknown
         Generating reduction(max:error)
     66, Loop is parallelizable
```

```
$ nvc -fast -ta=tesla:managed -Minfo=accel rdf.c
main:
     63, Accelerator kernel generated
         Generating NVIDIA GPU code
         64, #pragma acc loop gang /* blockIdx.x */
             Generating reduction(max:error)
         66, #pragma acc loop vector(128) /* threadIdx.x */
     63, Generating implicit copyin(A[:])
Generating implicit copy(error)
     66, Loop is parallelizable
```

RDF
Pseudo Code

```
for (int frame=0;frame<nconf;frame++) {
        for(int id1=0;id1<numatm;id1++) {
                for(int id2=0;id2<numatm;id2++) {
                        did1 = frame*numatm+id1
                        did2 = frame*numatm+id2
                        dx=d_x[did1]-d_x[did2];
                        dy=d_y[did1]-d_y[did2];
                        dz=d_z[did1]-d_z[did2];
                        r=sqrtf(dx*dx+dy*dy+dz*dz);

                        if (r<cut) {
                                ig2=(int)(r/del);
                                d_g2[ig2] = d_g2[ig2] +1 ;
                        }
                }
        }
}
```

- Across Frames
- Find Distance
- Reduction

RDF
Pseudo Code -C

```
for (int frame=0;frame<nconf;frame++) {
#pragma acc parallel loop
        for(int id1=0;id1<numatm;id1++) {
                for(int id2=0;id2<numatm;id2++) {
                        did1 = frame*numatm+id1
                        did2 = frame*numatm+id2
                        dx=d_x[did1]-d_x[did2];
                        dy=d_y[did1]-d_y[did2];
                        dz=d_z[did1]-d_z[did2];
                        r=sqrtf(dx*dx+dy*dy+dz*dz);

                        if (r<cut) {
                                ig2=(int)(r/del);
                                #pragma acc atomic
                                d_g2[ig2] = d_g2[ig2] +1 ;
                        }
                }
```

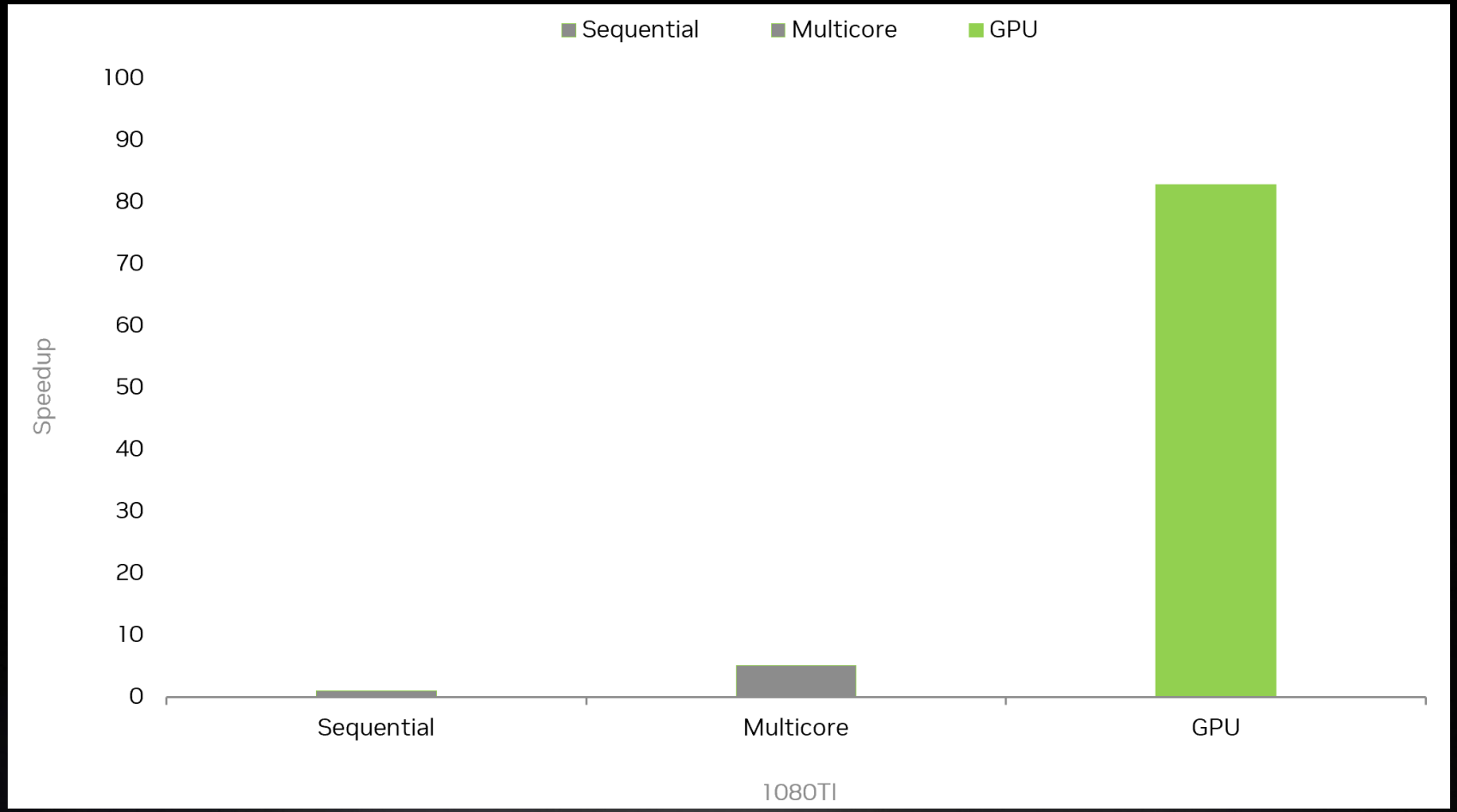
- Parallel Loop construct
- Atomic Construct

RDF
Pseudo Code - Fortran

```
do iconf=1,nframes
      if (mod(iconf,1).eq.0) print*,iconf
      !$acc parallel loop
      do i=1,natoms
        do j=1,natoms
          dx=x(iconf,i)-x(iconf,j)
          dy=y(iconf,i)-y(iconf,j)
          dz=z(iconf,i)-z(iconf,j)
                          ...
              if(r<cut)then
            !$acc atomic
            g(ind)=g(ind)+1.0d0
          endif
        enddo
      enddo
    enddo
```

- Parallel Loop construct
- Atomic Construct

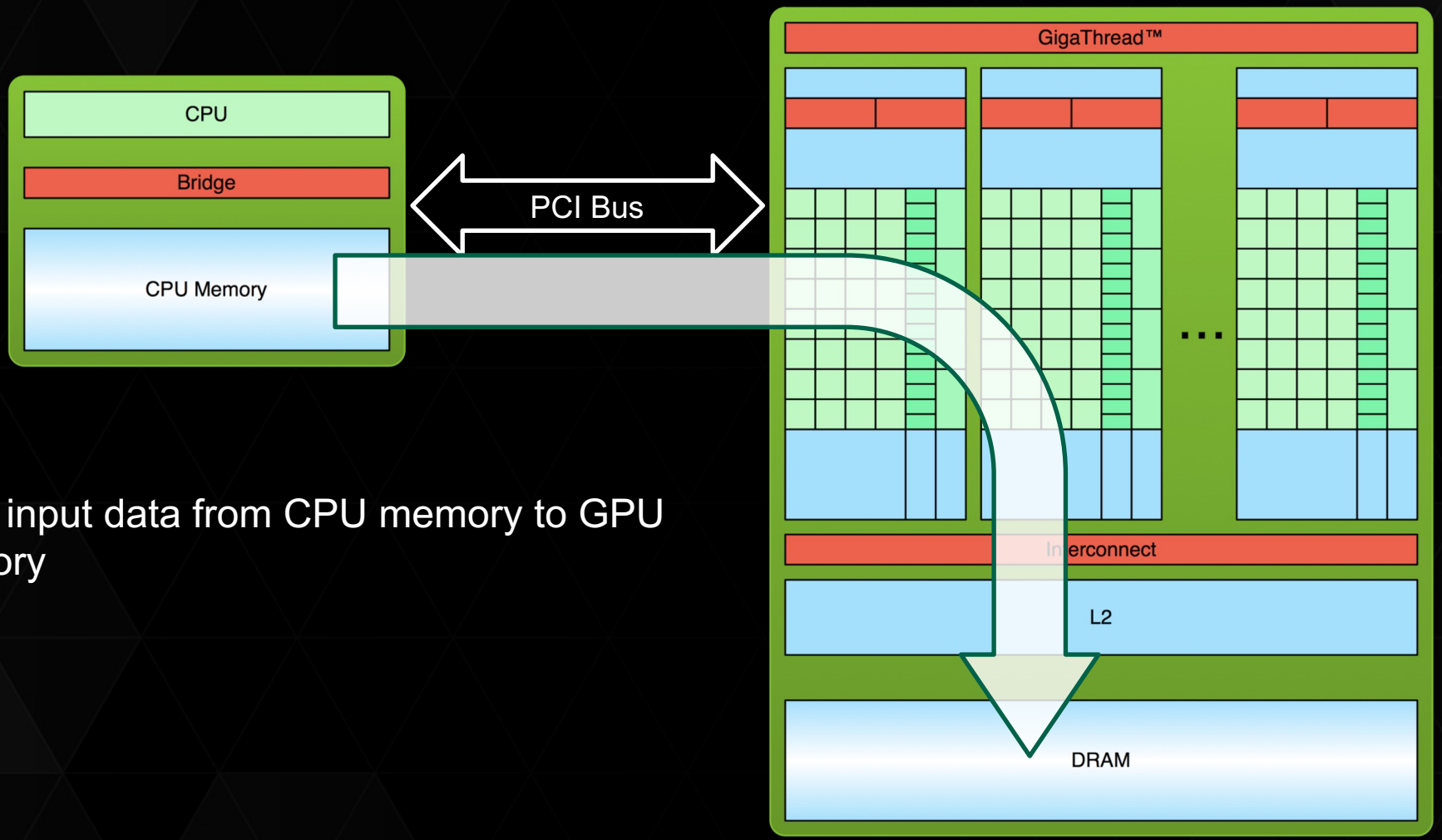
OPENACC SPEEDUP



HPC SDK 20.11, NVIDIA GTX1080TI

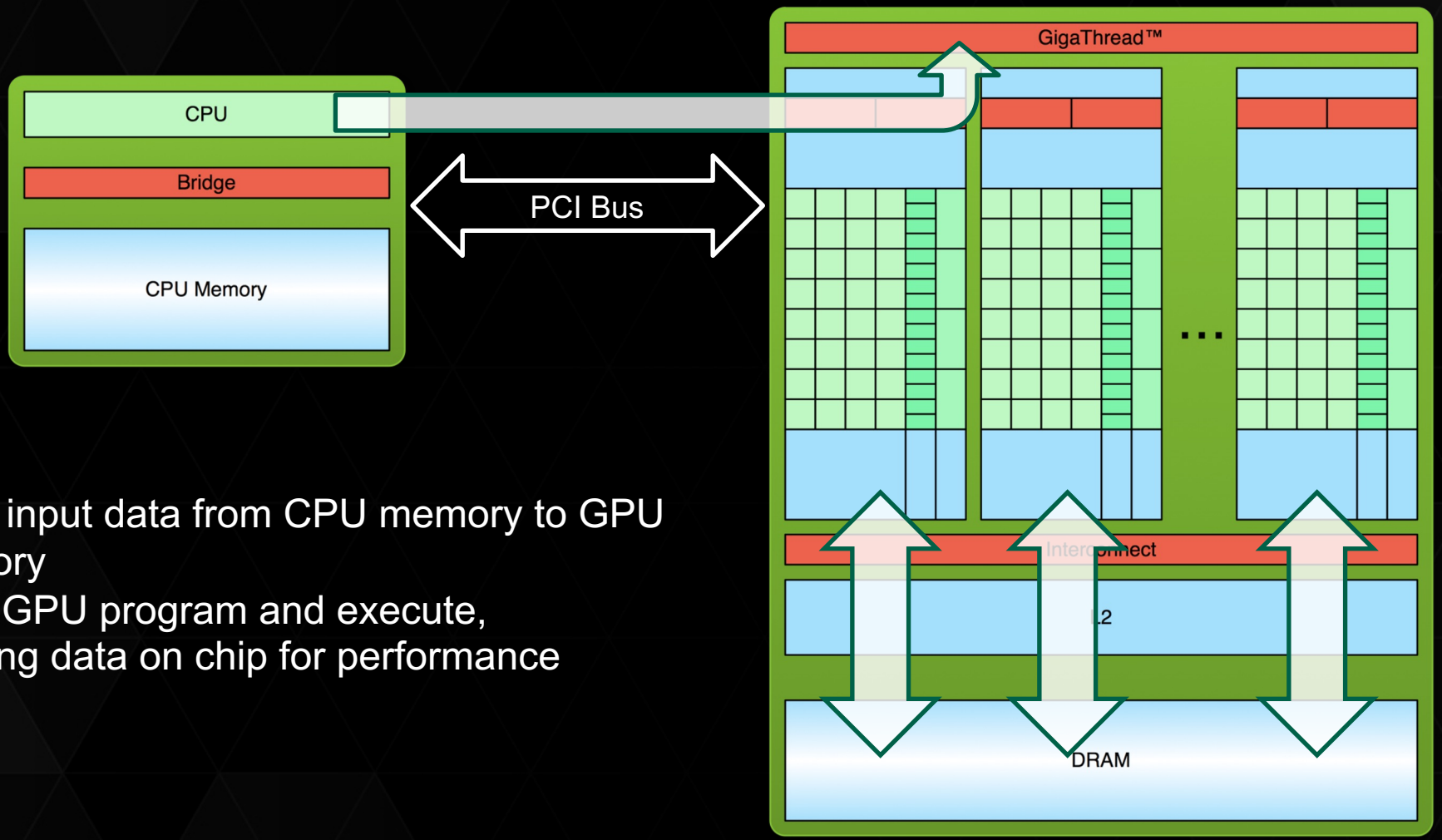
ADDITIONAL EXERCISE CONTENT

PROCESSING FLOW - STEP 1



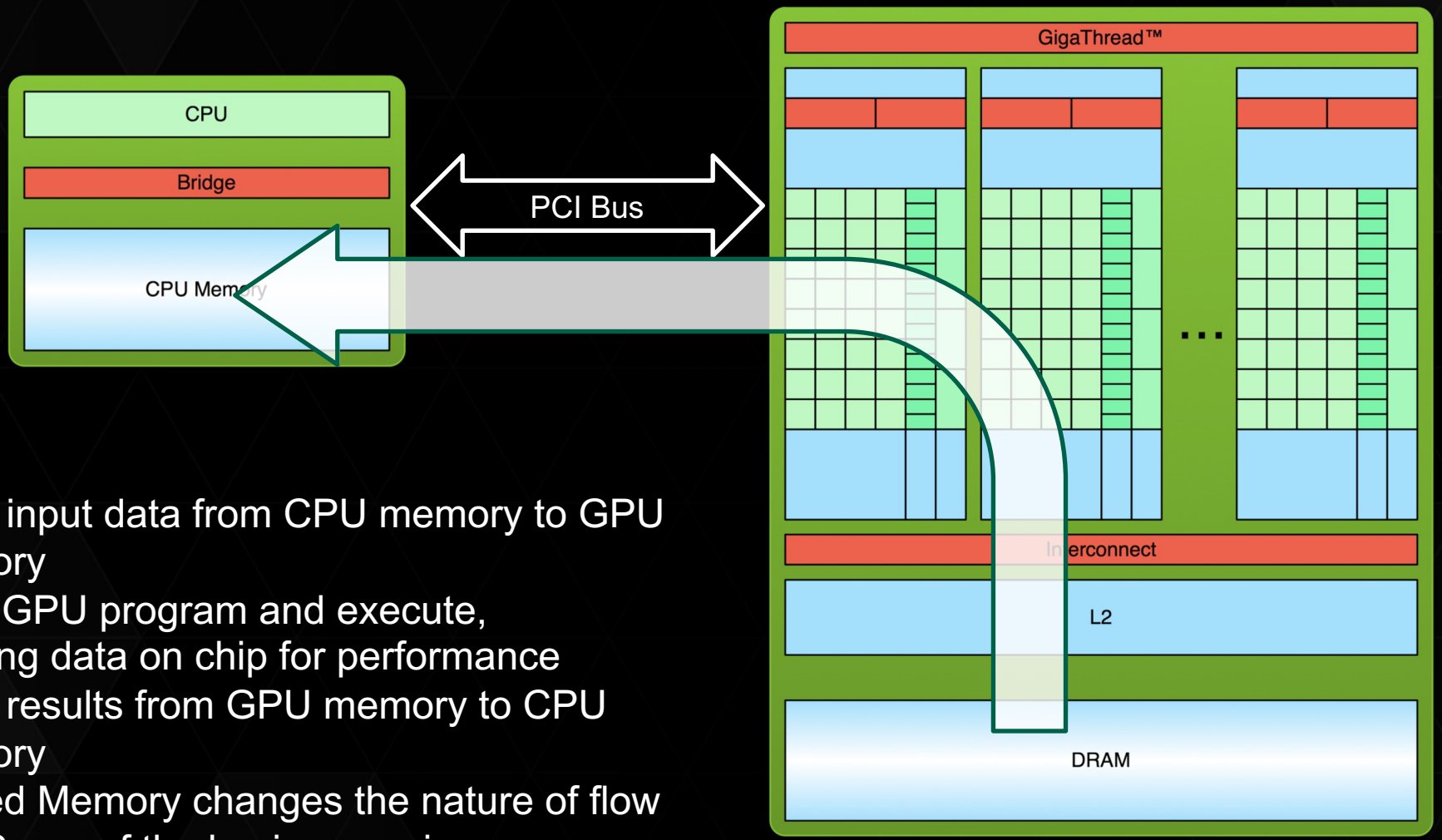
1. Copy input data from CPU memory to GPU memory

PROCESSING FLOW - STEP 2



1. Copy input data from CPU memory to GPU memory
2. Load GPU program and execute, caching data on chip for performance

PROCESSING FLOW - STEP 3

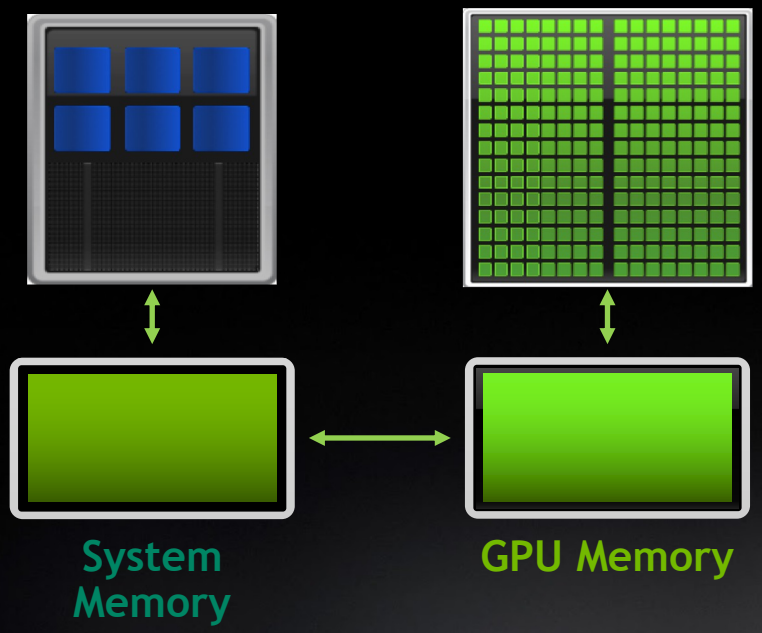


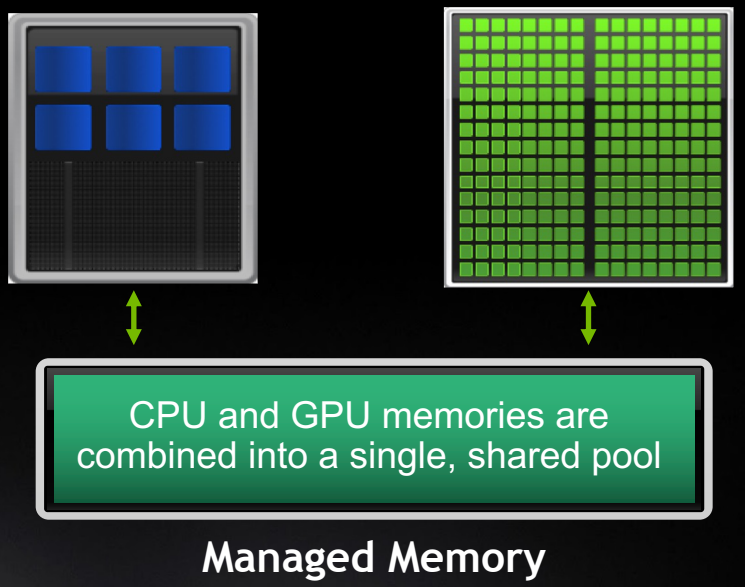
1. Copy input data from CPU memory to GPU memory
2. Load GPU program and execute, caching data on chip for performance
3. Copy results from GPU memory to CPU memory
4. Unified Memory changes the nature of flow
   - Some of the basics remains same

CUDA UNIFIED MEMORY

Simplified Developer Effort

Commonly referred to as
"managed memory."

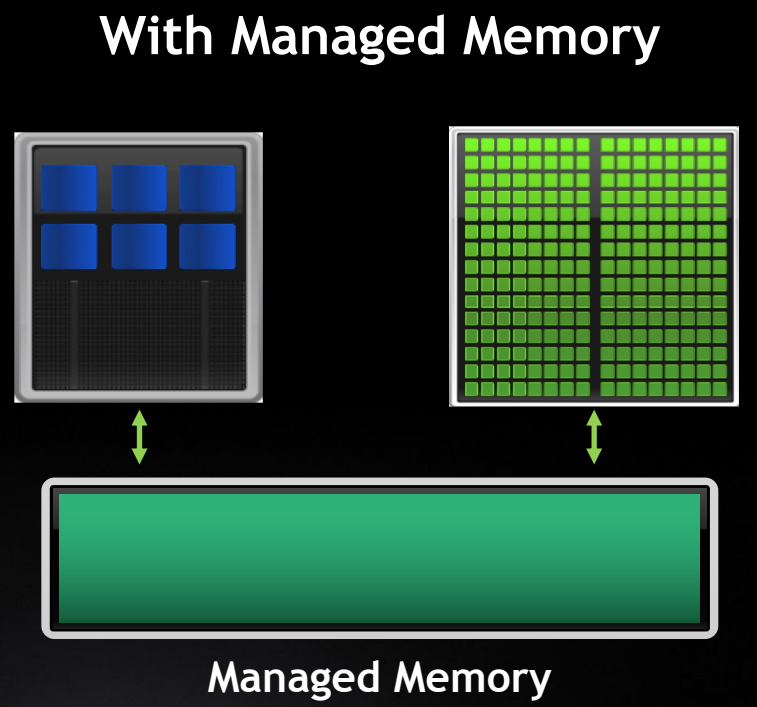




MANAGED MEMORY

Limitations

- The programmer will almost always be able to get better performance by manually handling data transfers
- Memory allocation/deallocation takes longer with managed memory
- Cannot transfer data asynchronously
- Currently only available from PGI on NVIDIA GPUs.



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.**

Principal use: For many important data structures in your code, this is a logical default to input, modify and return the data.

`copyin( list )` — **Allocates memory on GPU and copies data from host to GPU when entering region.**

Principal use: Think of this like an array that you would use as just an input to a subroutine.

`copyout( list )` — **Allocates memory on GPU and copies data to the host when exiting region.**

Principal use: A result that isn't overwriting the input data structure.

`create( list )` — **Allocates memory on GPU but does not copy.**

Principal use: Temporary arrays.

ARRAY SHAPING

Sometimes the compiler needs help understanding the *shape* of an array

The first number is the start index of the array

In C/C++, the second number is how much data is to be transferred

In Fortran, the second number is the ending index

```
copy(array[starting_index:length])
```

C/C++

```
copy(array(starting_index:ending_index))
```

Fortran

ARRAY SHAPING (CONT.)

Multi-dimensional Array shaping

```
copy(array[0:N][0:M])
```

C/C++

Both of these examples copy a 2D array to the device

```
copy(array(1:N, 1:M))
```

Fortran

OPENACC DATA DIRECTIVE

Definition

The data directive defines a lifetime for data on the device beyond individual loops

During the region data is essentially “owned by” the accelerator

Data clauses express shape and data movement for the region

```
#pragma acc data clauses
{
        < Sequential and/or Parallel
code >

}
```

```
!$acc data clauses

        < Sequential and/or Parallel
code >

!$acc end data
```

STRUCTURED DATA DIRECTIVE

Example

```
#pragma acc data copyin(a[0:N],b[0:N]) copyout(c[0:N])
create(t[0:N])
{
        #pragma acc parallel loop
        for(int i = 0; i < N; i++){
                t[i] = a[i] + b[i];
                c[i] = t[i] + 20;
        }
}
```

Action
Allocate A, B on device
Deallocate A, B from device
Copy A, B to device
Copy C from device

COLLAPSE CLAUSE

Parallelizing nested loops

C/C++

```
#pragma acc parallel loop collapse(2)
for(int i = 0; j < N; i++) {
    for (int j = 0; j < N; j++) {
        a[i*N+j] = 0;
}
```

Fortran

```
!$acc parallel loop collapse(2)
do i = 1, N
    do j = 1, N
        a(i*N+j) = 0
    end do
end do
```

The collapse clause allows us to transform a multi-dimensional loop nest into a single-dimensional loop.

This process is helpful for increasing the overall length (which usually increases parallelism) of our loops.

The collapse clause is useful when inner or outer loop has few iterations.

PRIVATE CLAUSE

Make shared variable private

C/C++

```
int d;
#pragma acc parallel loop private(d)
for(int i = 0; j < N; i++) {
    d = a[i] + 1;
    a[i] = a[i] * d;
}
```

Fortran

```
real(rp) :: d
!$acc parallel loop private(d)
do i = 1, N
    d = a(i) + 1
    a(i) = a(i) * d
end do
```

A variable declared outside the loop is shared to all workers.

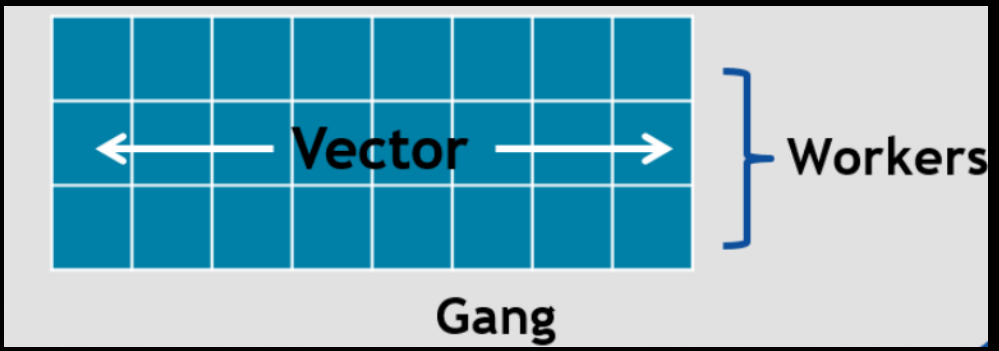
The private clause will make each worker allocate a temporary space for this variable.

Be aware of the OOM if the private variable is a large array!

GANG/VECTOR/WORKER CLAUSE

Gang, Worker, and Vector Syntax

```
#pragma acc parallel
{
    #pragma acc loop gang(8)
    for (int i = 0; i < N; ++i) {
        #pragma acc loop worker
        for (int j = 0; j < M; ++j) {
            #pragma acc loop vector(128)
            for (int k = 0; k < K; ++k) {
                <loop code>
            }
        }
    }
}
```



GANG/VECTOR/WORKER CLAUSE

Preference

The gang clause is mapped to blocks on GPU.

The worker and vector clause is mapped to threads on GPU.

The number of gang should exceed the number of SMs on GPU.

NVIDIA GPUs are optimized to use warps. Warps are groups of 32 threads that are executing the same computer instruction, so vector size should be multiple of 32.

C/C++

REFERENCES

https://www.openacc.org/get-started

https://developer.nvidia.com/hpc-sdk


THANK YOU
NVIDIA