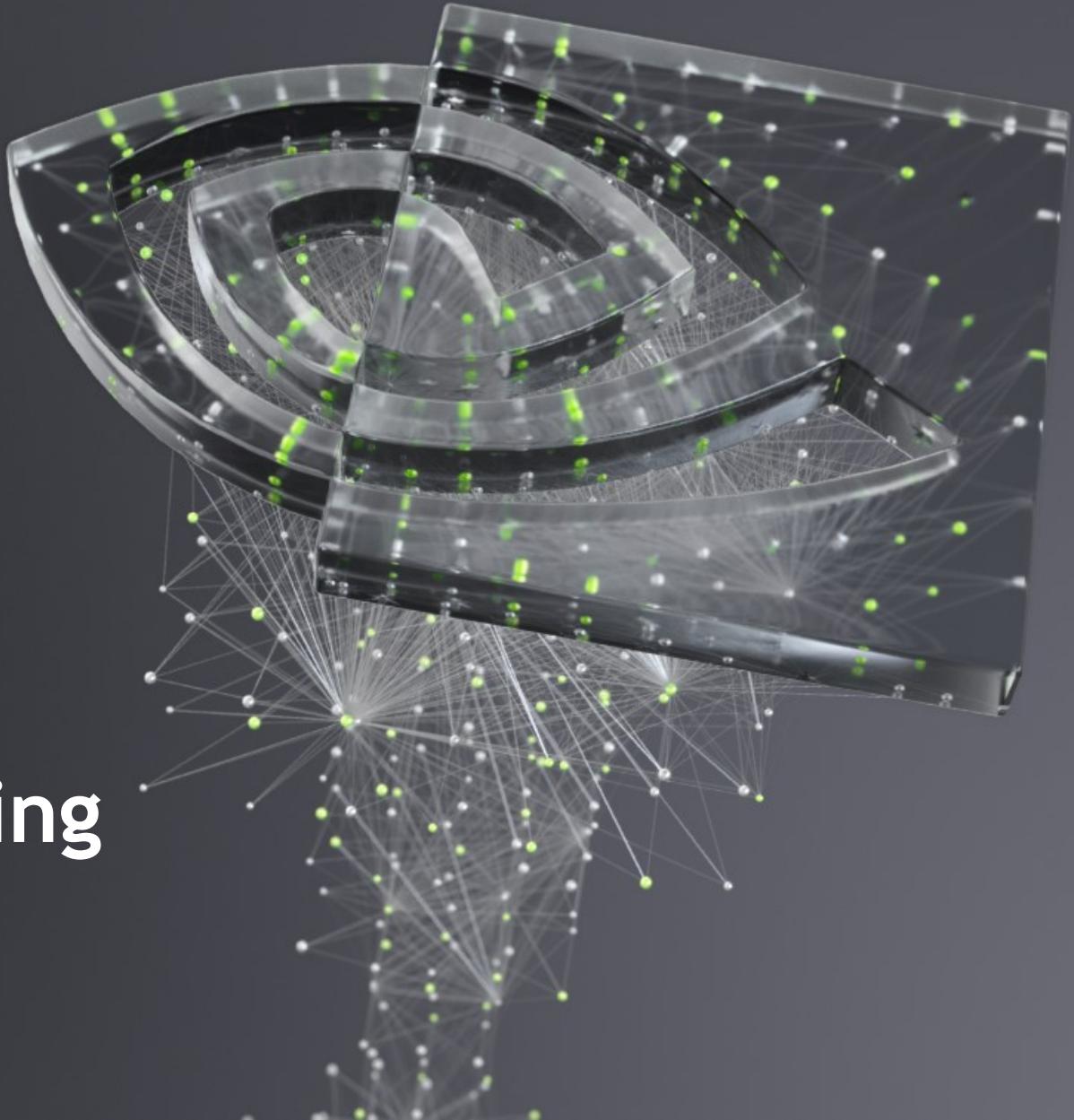




N-WAYS GPU computing

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>
    }
}
```

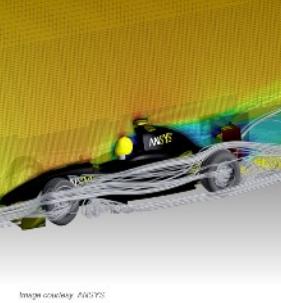


GAUSSIAN 16



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.

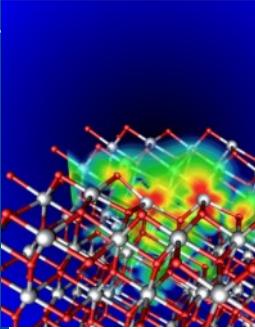


ANSYS FLUENT



Sunil Saha
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 Scientific
Metacodecs

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

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.

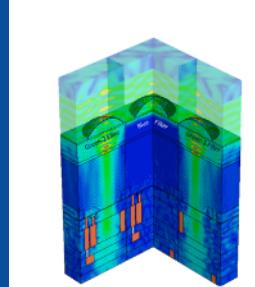


NUMECA FINE/Open



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.



MPAS-A



Richard Loft
Director, Technology Development
NCAR

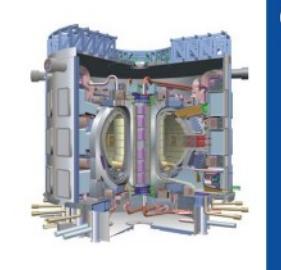
“ Our team has been evaluating OpenACC as a pathway to performance portability for the Model for Prediction (MPAS) atmospheric model. Using this approach on the MPAS dynamical core, we have achieved performance on a single P100 GPU equivalent to 2.7 dual socketed Intel Xeon nodes on our new Cheyenne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

VMD



John Stone
Senior Research Programmer
Beckman 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

PWscf (Quantum ESPRESSO)



Filippo Spiga
Senior Coordinator
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 layout, ISCUF-KERNELS directives give us productivity and source code maintainability. It's the best of both worlds.



GAMERA



Tatsuya Yamaguchi, Kohki Fujita, Etsuyoshi Ichimura, Munenori
Hirai, Genta Watanabe
The University of Tokyo

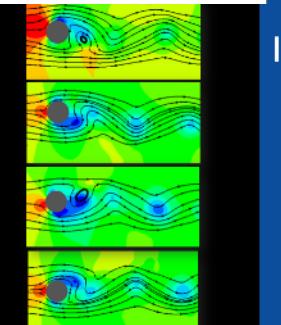
“ With OpenACC and a compute node based on NVIDIA's Tesla P100 GPU, we achieved more than a 14X speed up over a K Computer node running our earthquake disaster simulation code.

SANJEEVINI



Abhilash Jayaram
Project Scientist
Indian Institute of Technology
New Delhi

“ In an academic environment maintenance and porting 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.

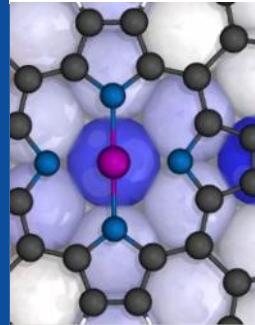


IBM-CFD



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 computation time for the parallel computation of our legacy codes to GPU. Especially the routines involving search algorithm and matrix solvers have been well-parallelized to improve the overall scalability of the code.



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

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

OpenACC
Directives For Accelerators

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 its 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.

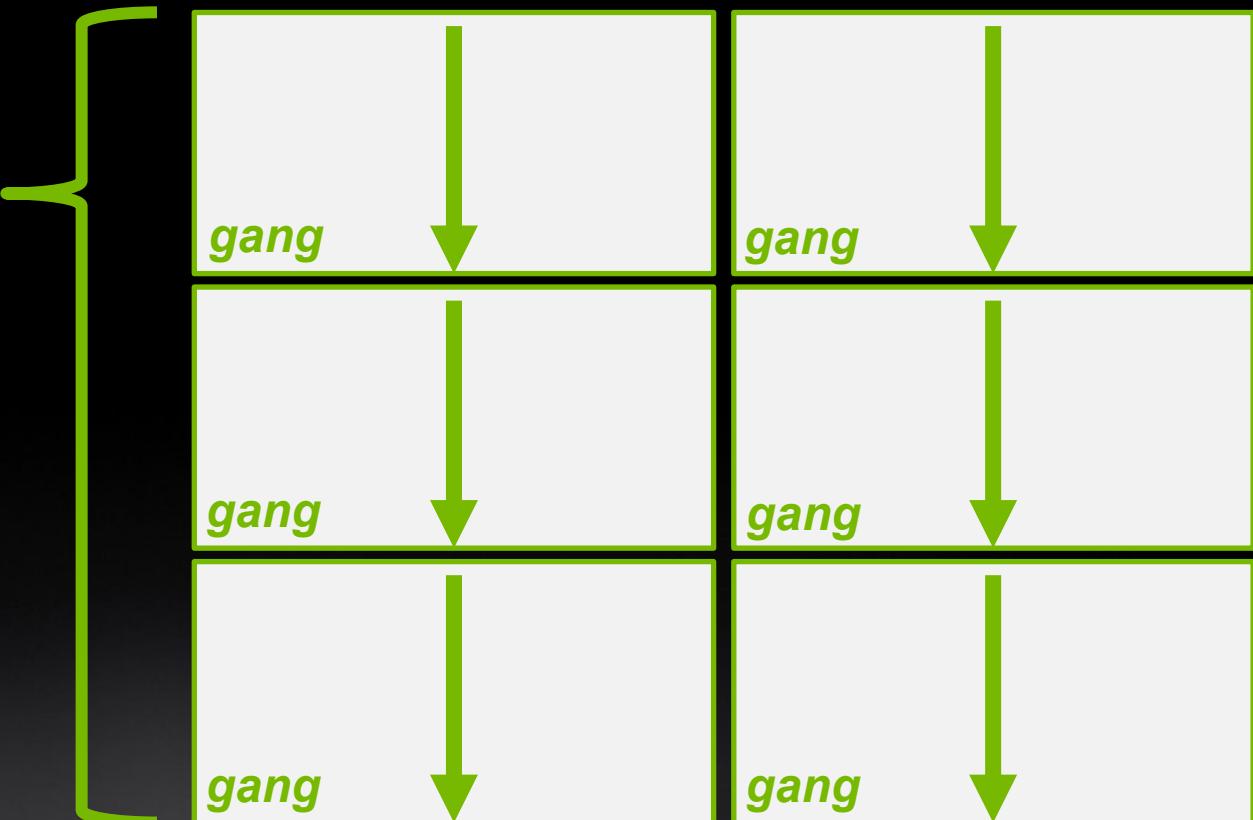
Clauses are specifiers or additions to directives.

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.



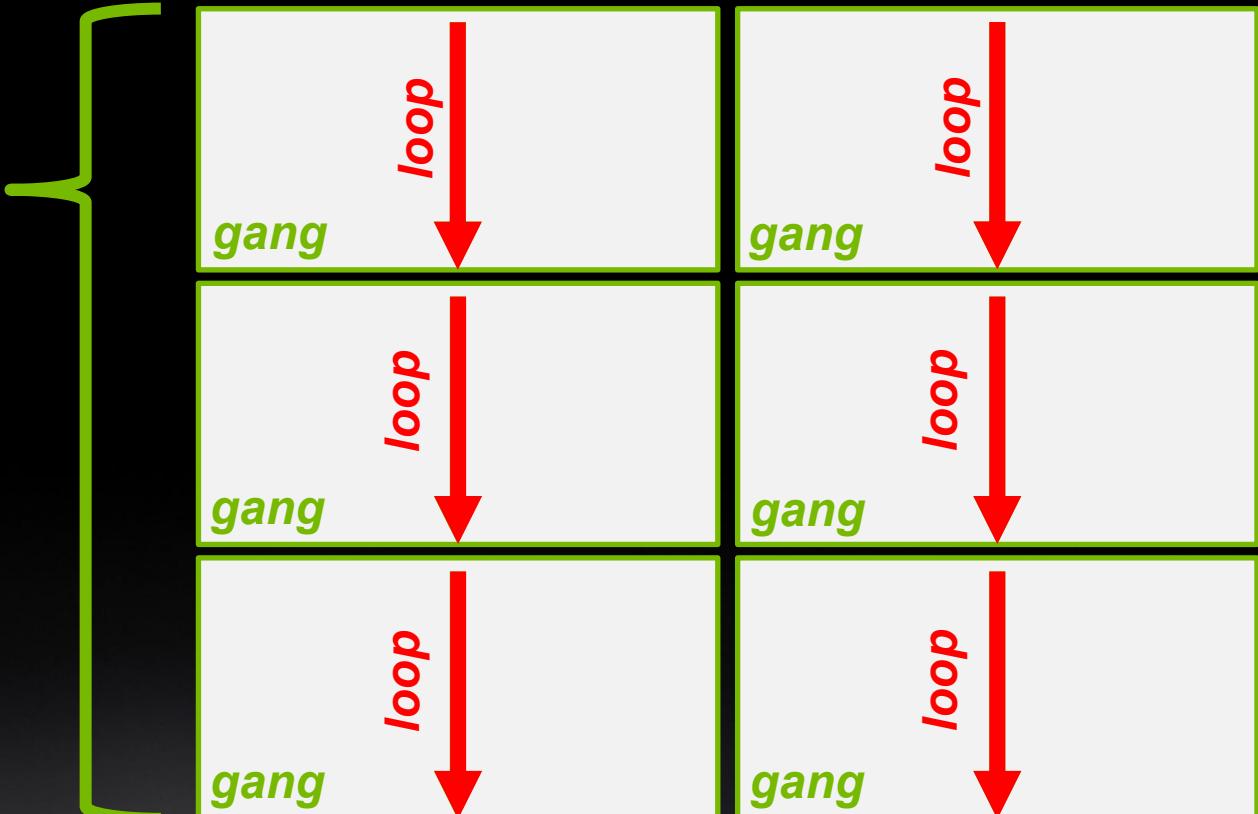
OPENACC PARALLEL DIRECTIVE

Expressing parallelism

```
#pragma acc parallel
```

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

This loop will be
executed redundantly
on each gang

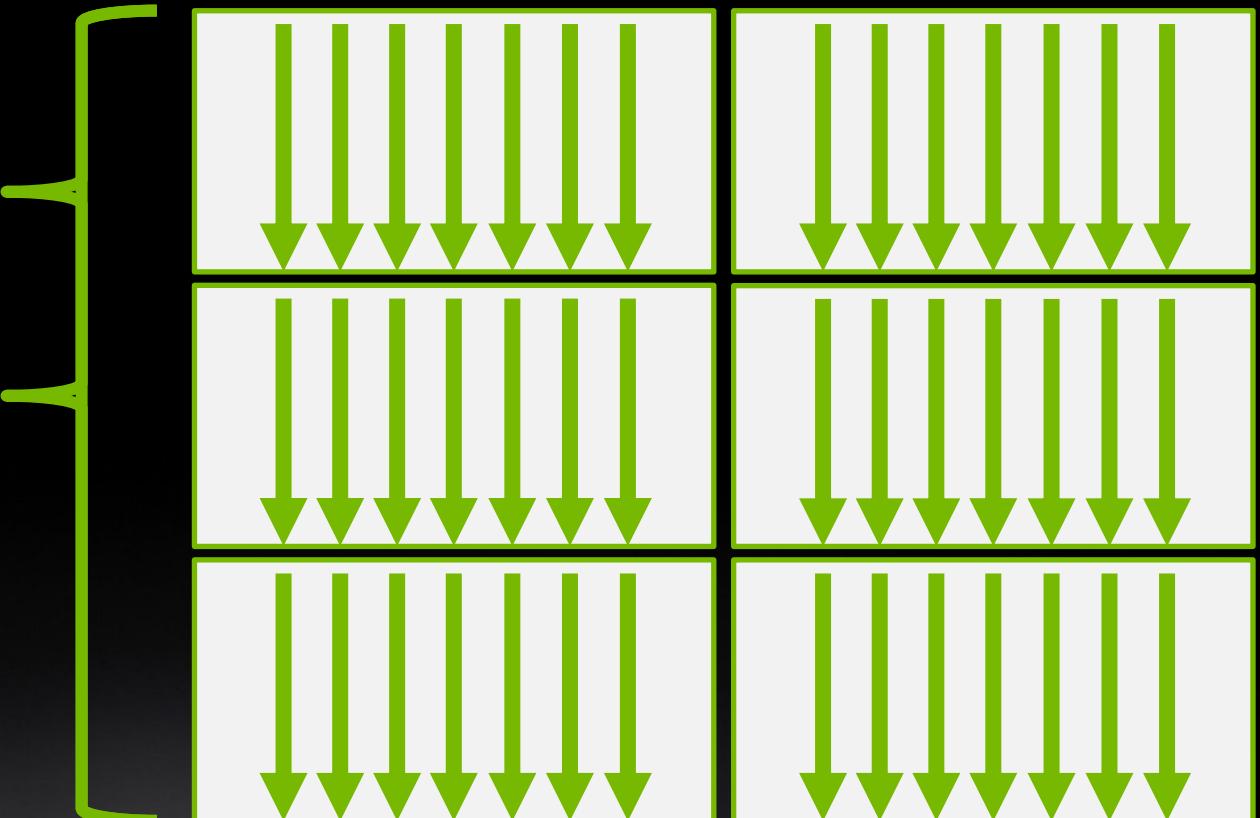


OPENACC PARALLEL DIRECTIVE

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;
}
```

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

Fortran

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

OPENACC PARALLEL DIRECTIVE

Parallelizing a single loop

C/C++

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

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

Fortran

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



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 Tesla 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++) {  
            d_x[];  
            d_y[];  
            d_z[];  
            r=sqrtf(dx*dx+dy*dy+dz*dz);  
            if (r<cut) {  
                jg2=(int)(r/del);
```

- Across Frames

- Find Distance

- Reduction

RDF

Pseudo Code -C

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

- Parallel Loop construct

- Atomic Construct

RDF

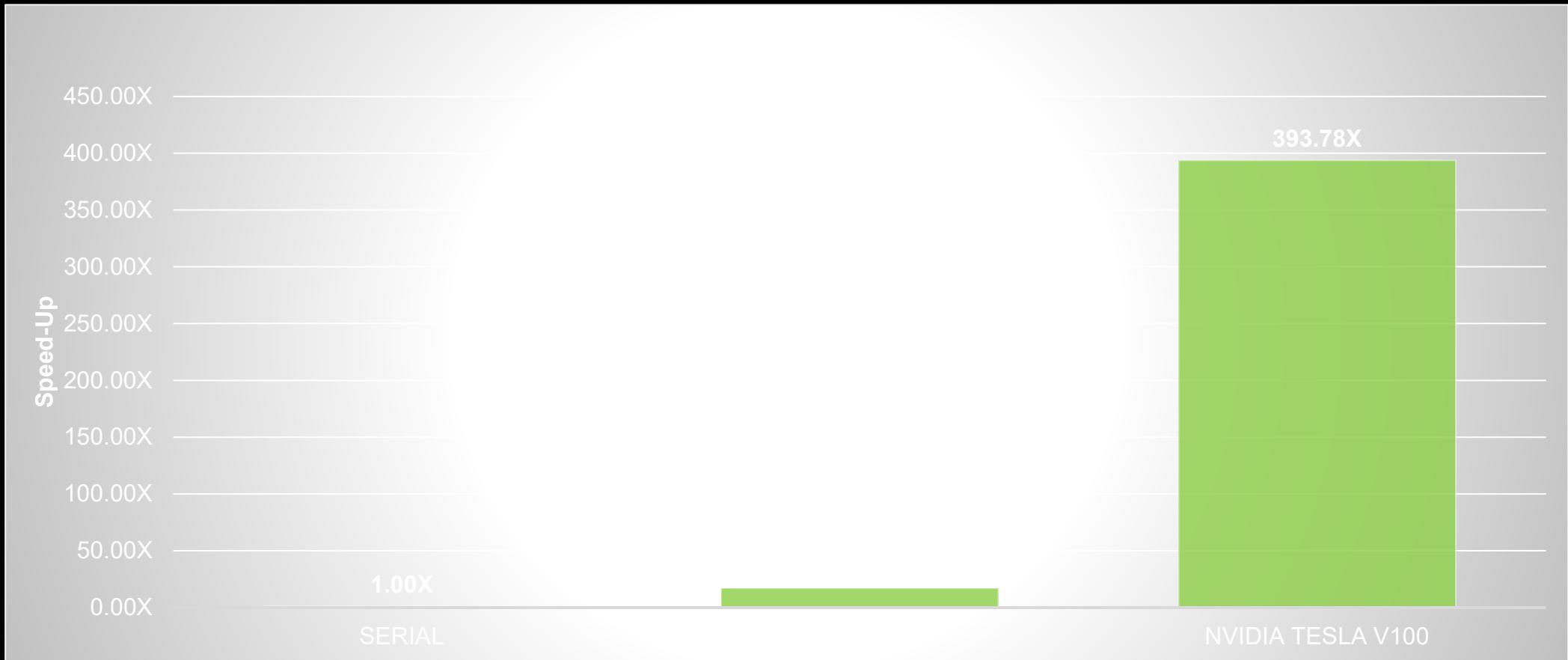
Pseudo Code - Fortran

```
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



REFERENCES

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

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



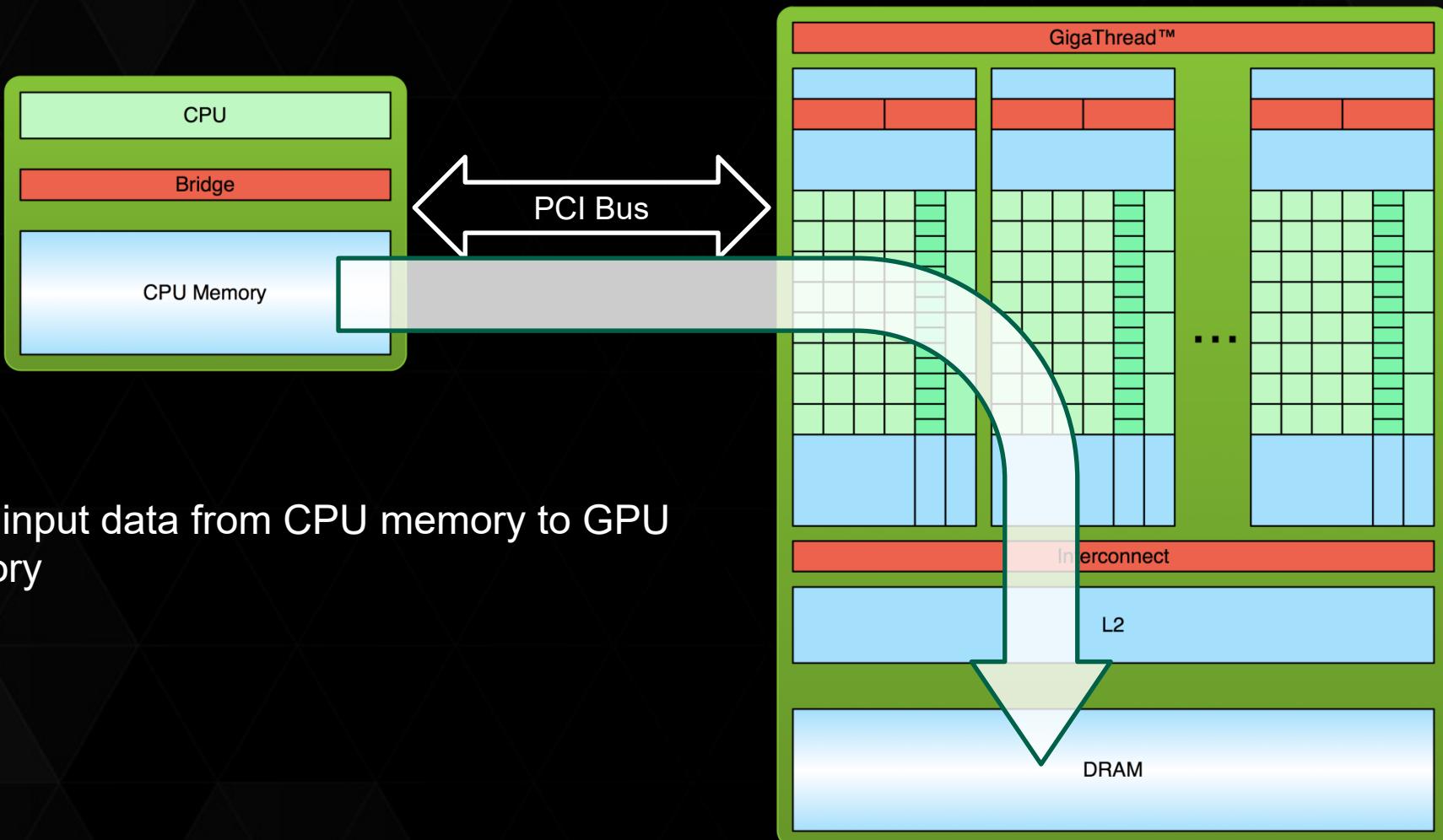
THANK YOU



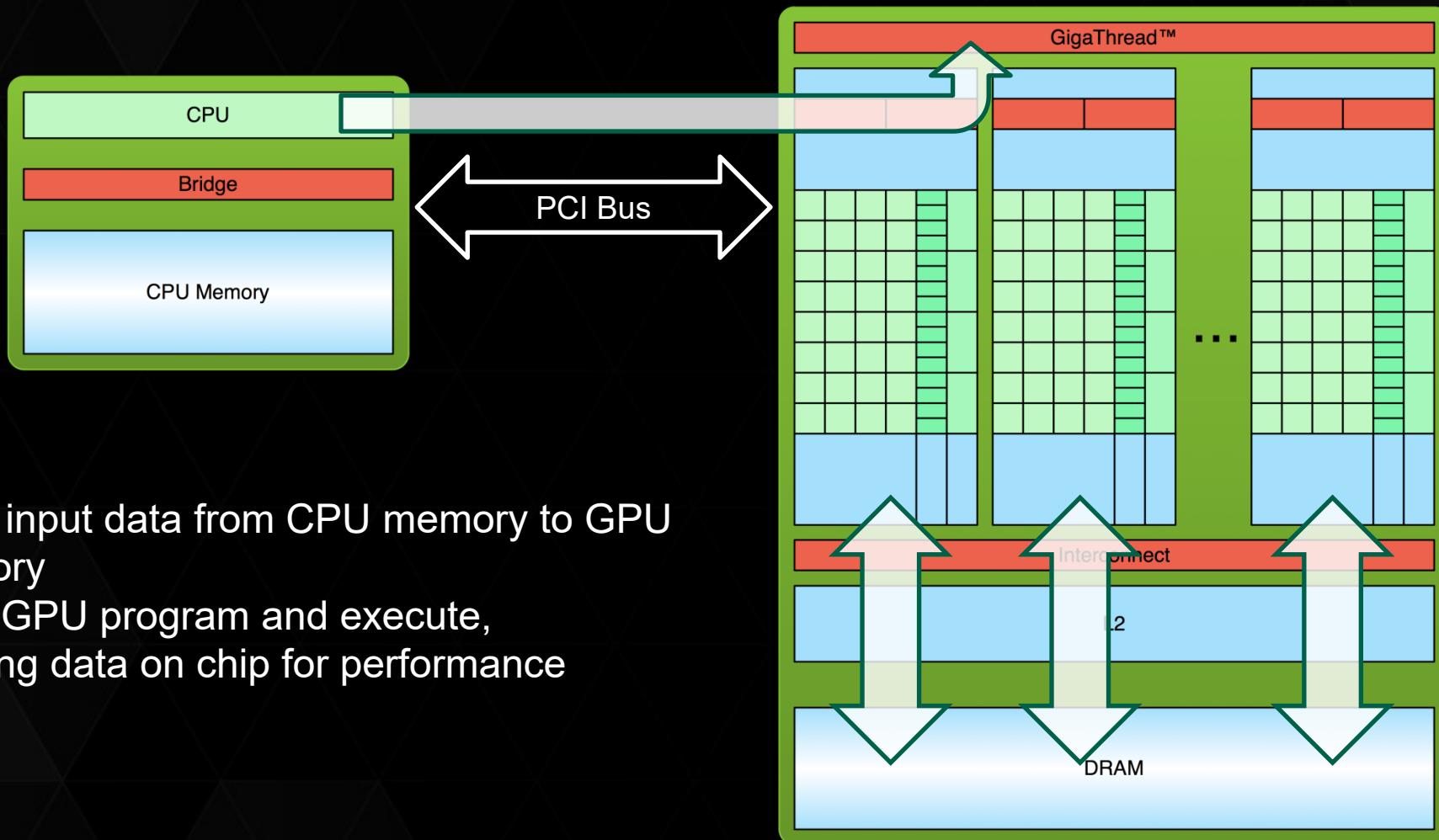


ADDITIONAL EXERCISE
CONTENT

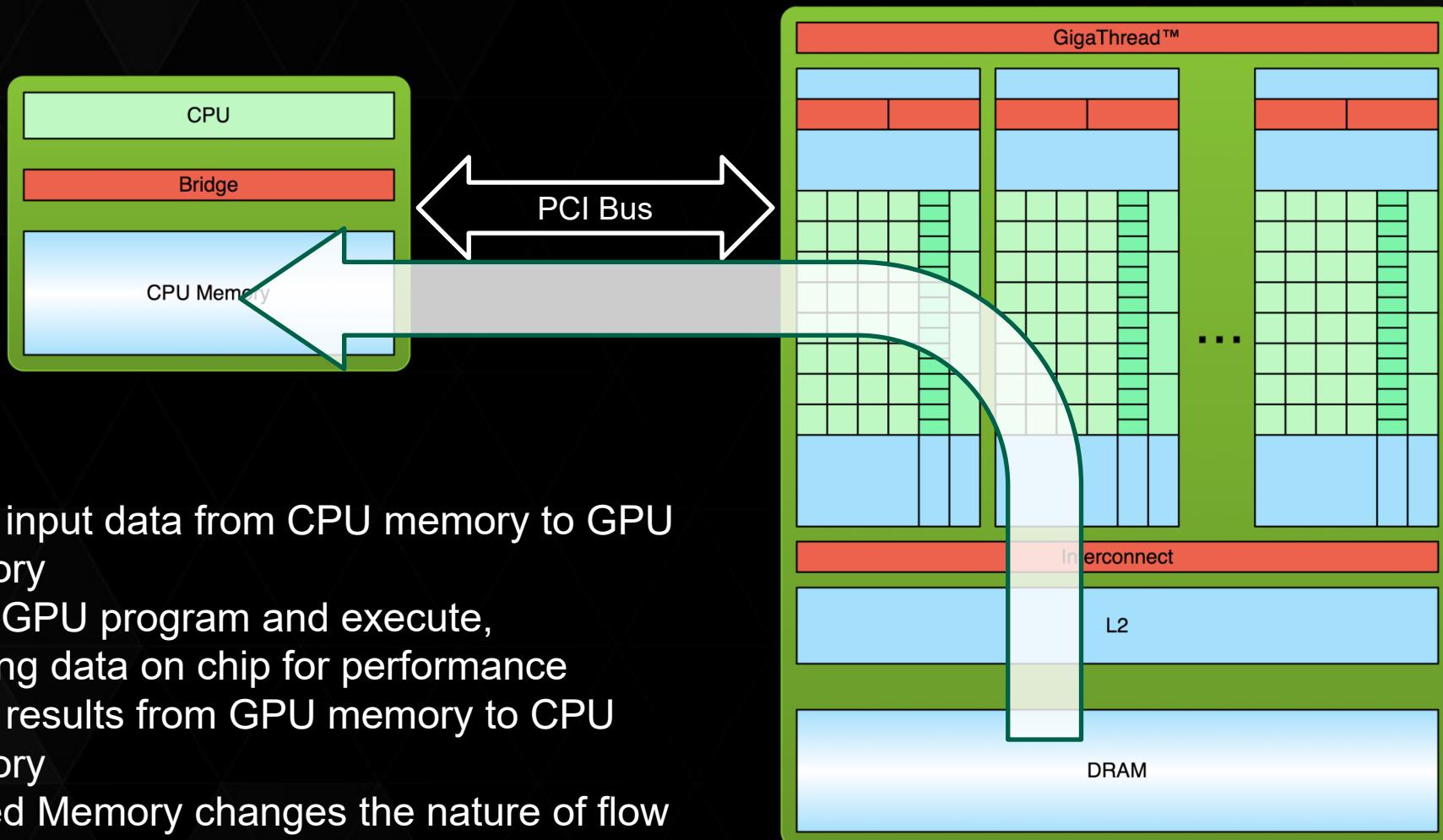
PROCESSING FLOW - STEP 1



PROCESSING FLOW - STEP 2



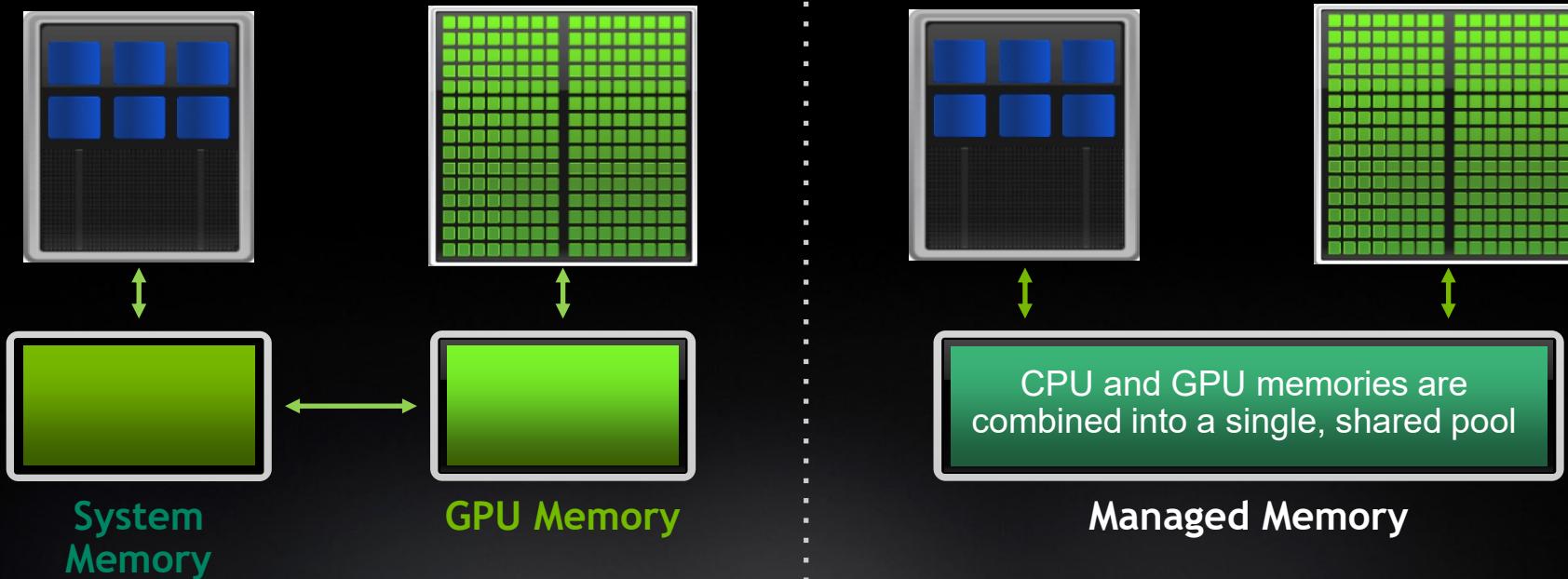
PROCESSING FLOW - STEP 3



CUDA UNIFIED MEMORY

Simplified Developer Effort

Commonly referred to as
“managed memory.”

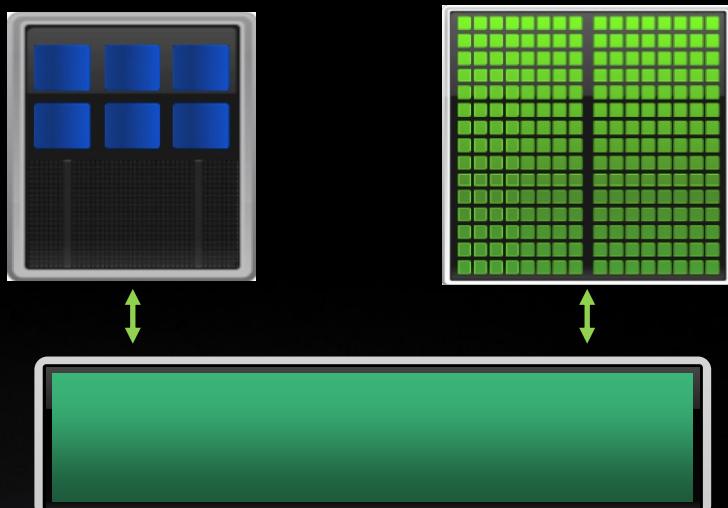


MANAGED MEMORY

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.

With Managed Memory



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

Action

Allocate A
Device
Dependency
Definition
Device Code
device

Host Memory



Device memory

