Heterogeneous Computing & Architectures: OpenACC model

NRIS

Norwegian research infrastructure services

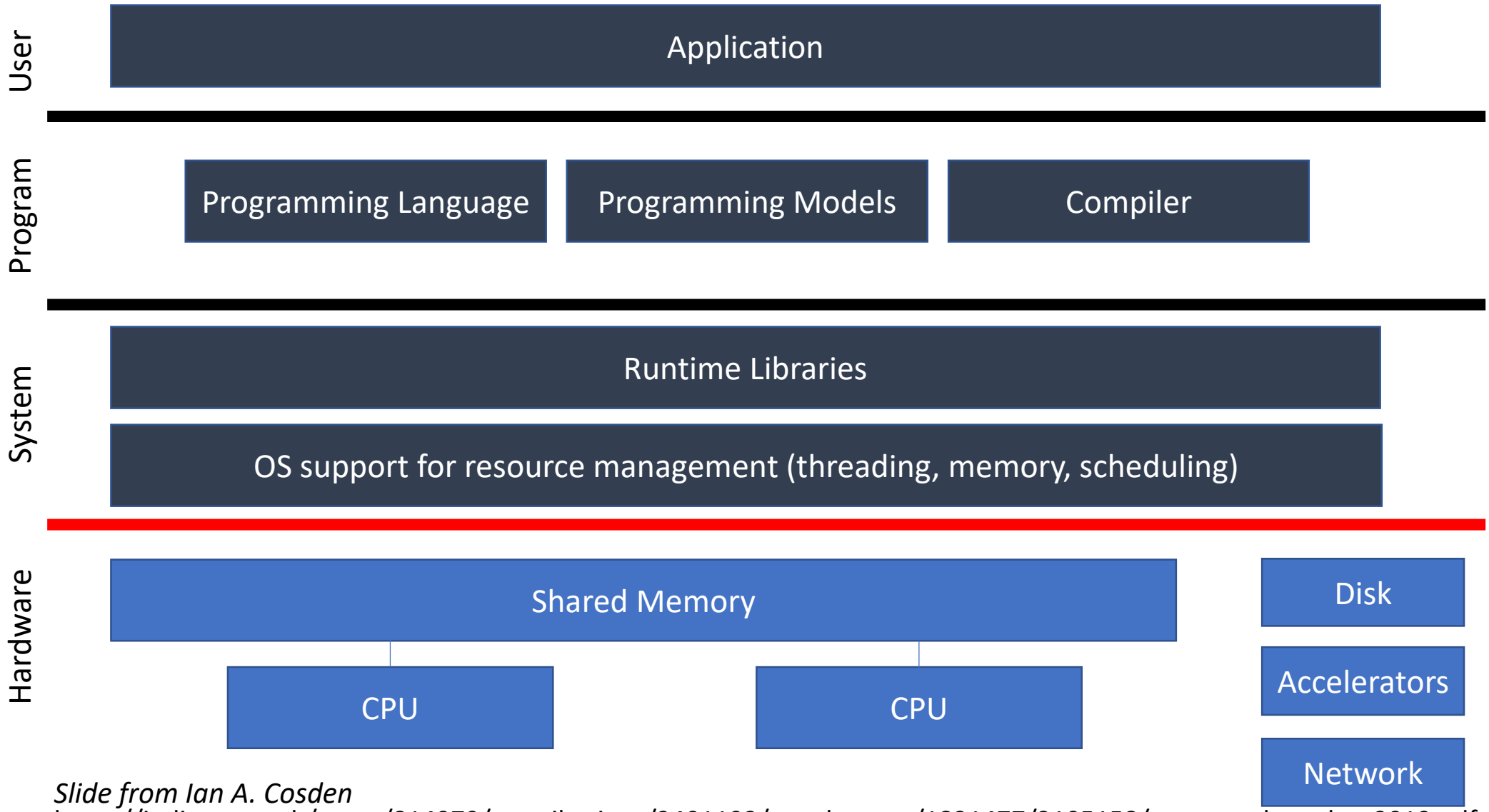
Hicham Agueny, PhD
Scientific Computing Group
IT-department, UiB

Overview

- **Part I**
  - **CPU- & GPU-architectures**
  - **Programming models and supports**
  - **Functionality of OpenACC**
- **Part II**
  - **Synchronous OpenACC**
  - **Combining OpenACC with other models**
  - **Asynchronous OpenACC**
  - **Code-profiling**

Part I

Hardware-architecture

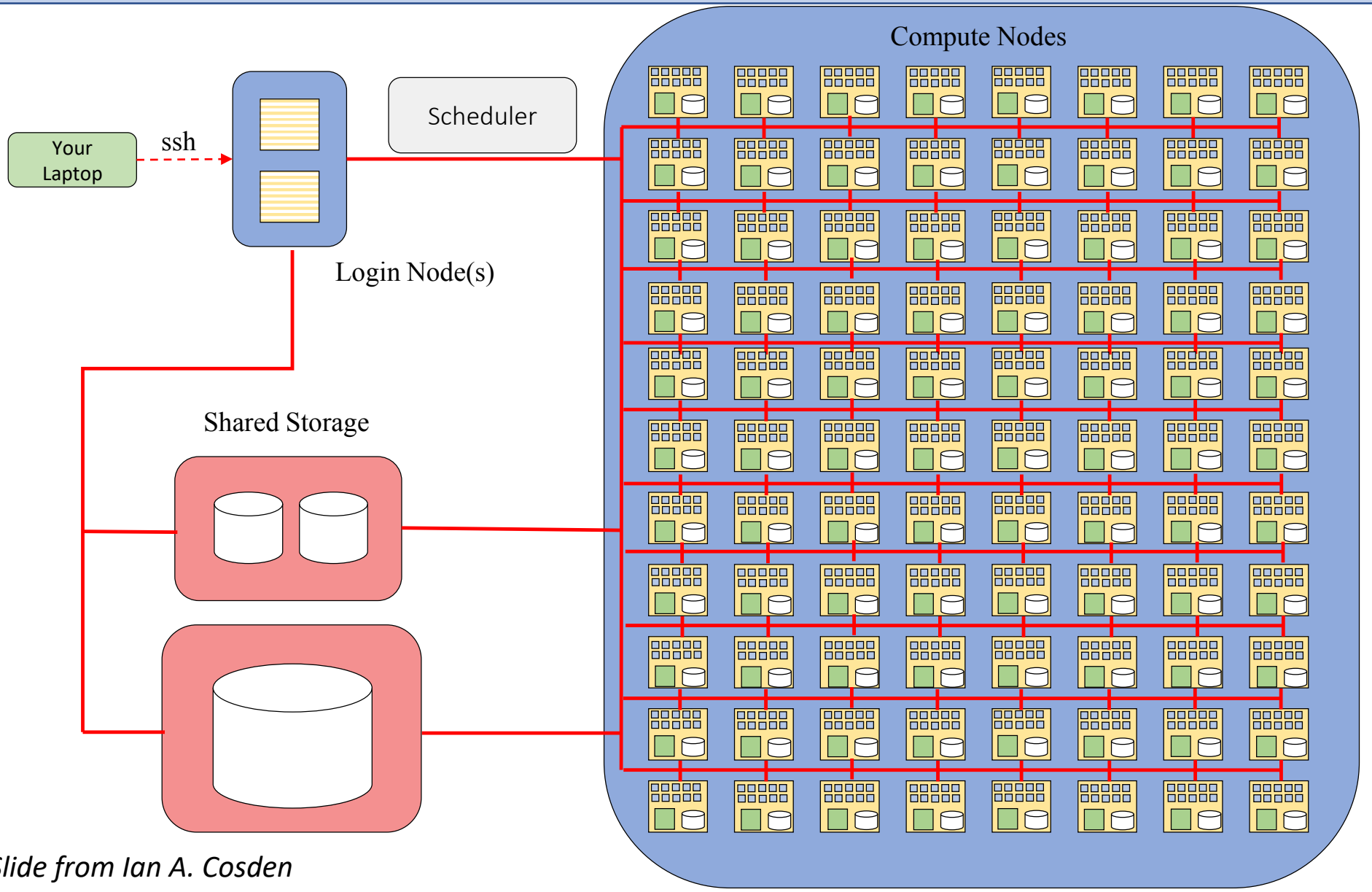


Slide from Ian A. Cosden
https://indico.cern.ch/event/814979/contributions/3401193/attachments/1831477/3105158/comp_arch_codas_2019.pdf

CPU-architecture

CPU: Central Processing Unit

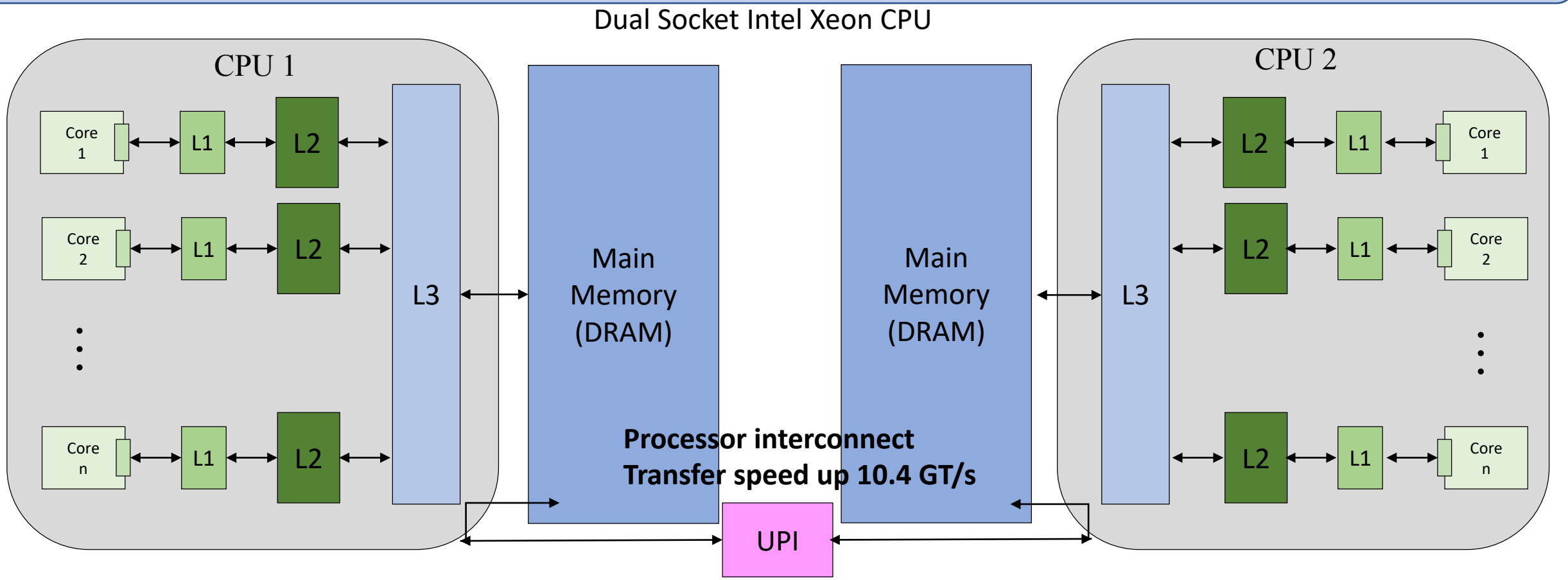
Architecture of Cluster



Slide from Ian A. Cosden

https://indico.cern.ch/event/814979/contributions/3401193/attachments/1831477/3105158/comp_arch_codas_2019.pdf

CPU-Architecture: ex. Betzy 128 cores



Access L1 Memory is Faster than L2

	Registers	L1 Cache	L2 Cache	L3 Cache	DRAM	Disk
Speed	1 cycle	~4 cycles	~10 cycles	~30 cycles	~200 cycles	10ms
Size	< KB per core	~32 KB per core	~256 KB per core	~35 MB per socket	~100 GB per socket	TB

https://indico.cern.ch/event/814979/contributions/3401193/attachments/1831477/3105158/comp_arch_codas_2019.pdf

GPU-architecture

GPU: Graphics Processing Unit

Architecture of NVIDIA GPU devices

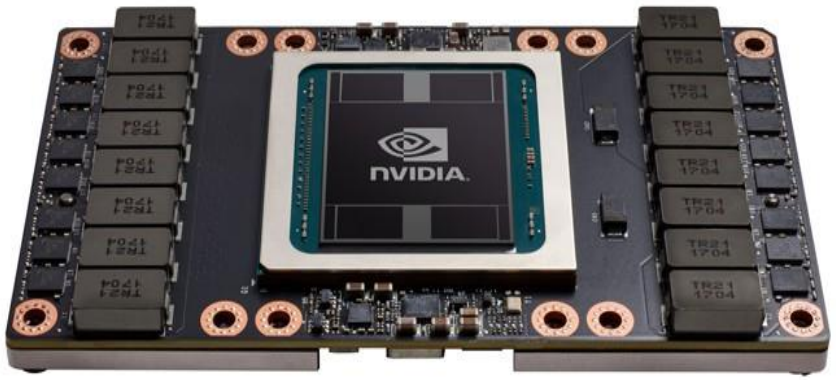


Figure 1. NVIDIA Tesla V100 SXM2 Module with Volta GV100 GPU

Figure 2. Volta GV100 full GPU with 84 SM Units

https://images.nvidia.com/content/volta-architecture/pdf/volta-architecture-whitepaper.pdf

Architecture of NVIDIA GPU devices

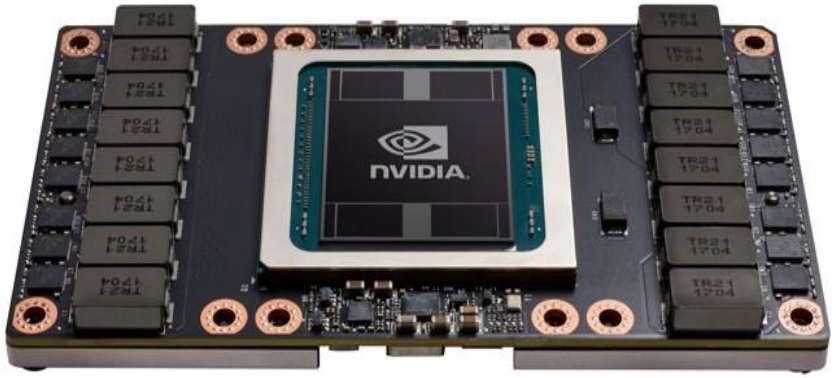


Figure 1. NVIDIA Tesla V100 SXM2 Module with Volta GV100 GPU

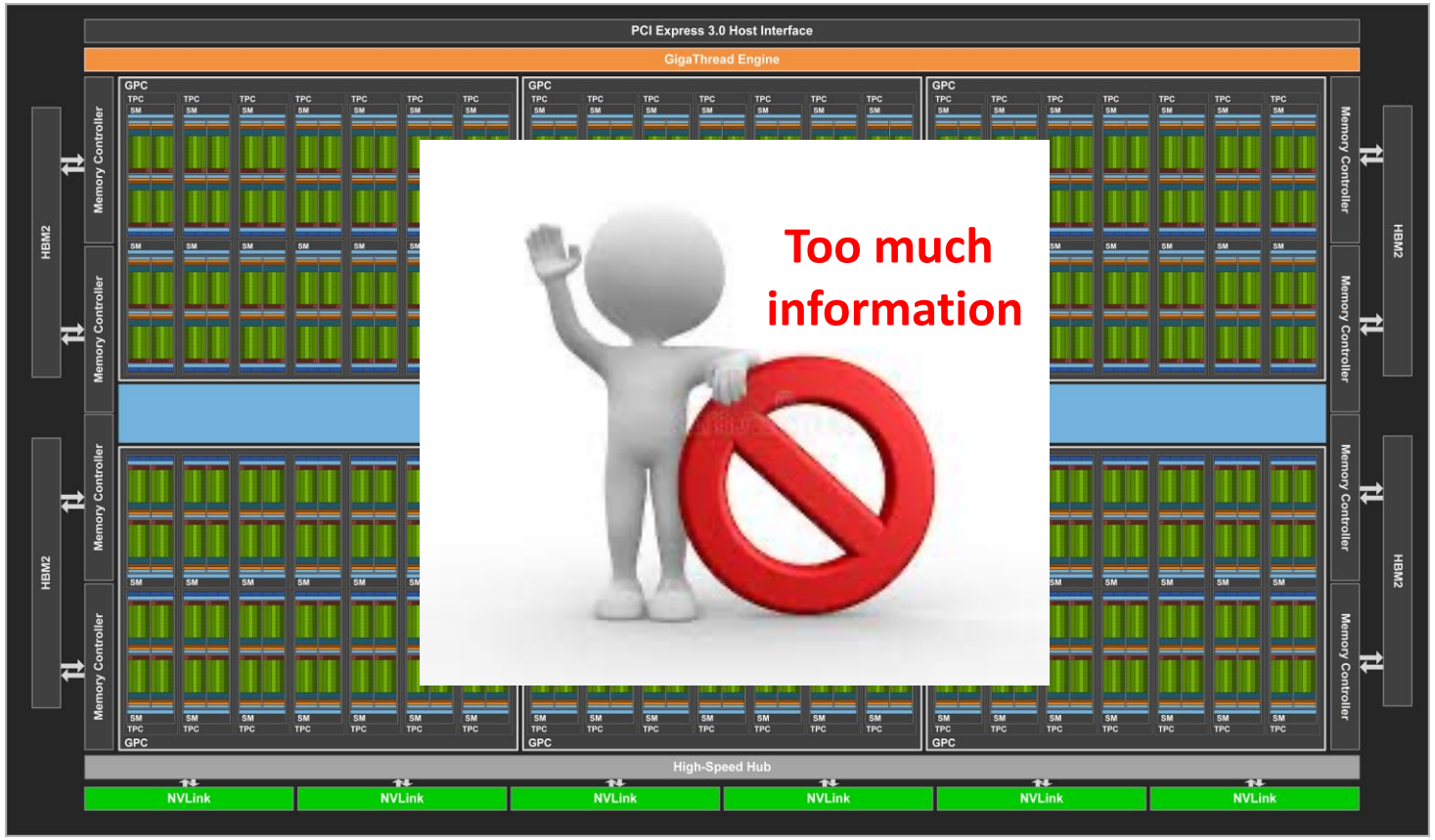
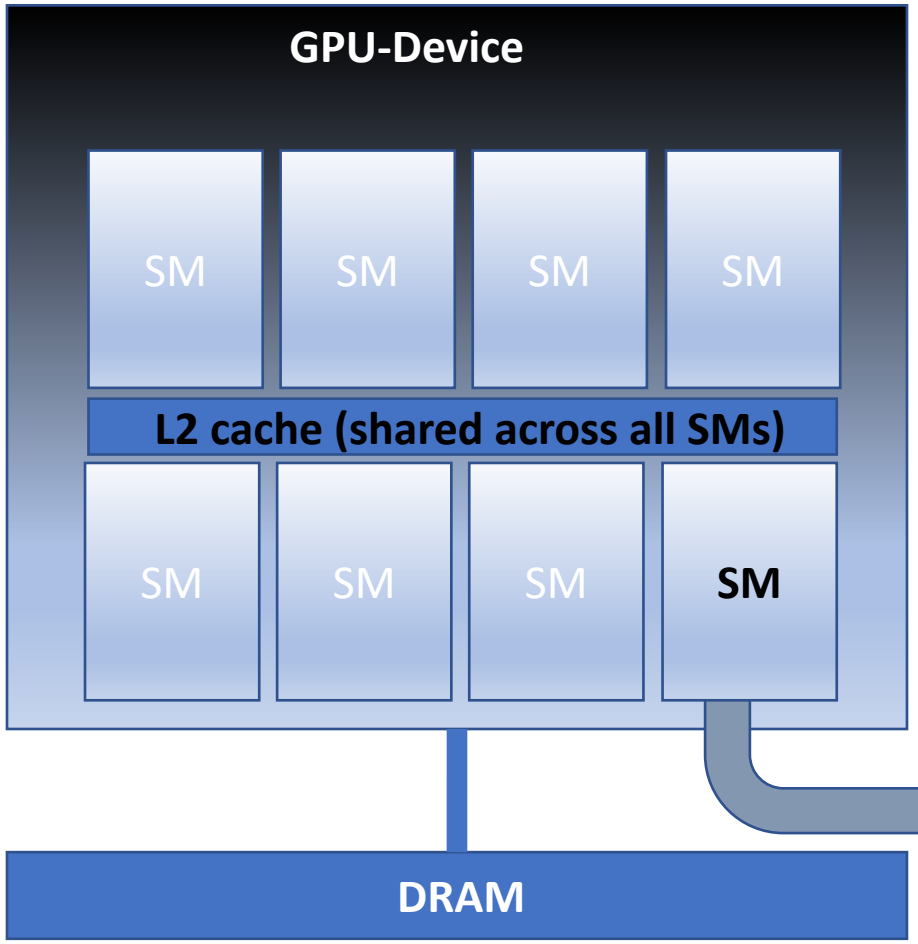


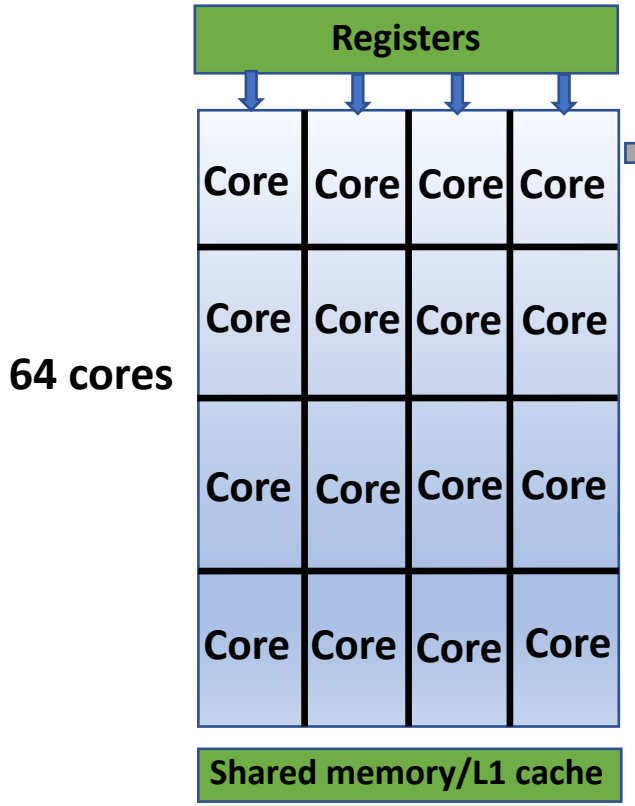
Figure 2. Volta GV100 full GPU with 84 SM Units

https://images.nvidia.com/content/volta-architecture/pdf/volta-architecture-whitepaper.pdf

Architecture of NVIDIA-GPU devices (simplified version)

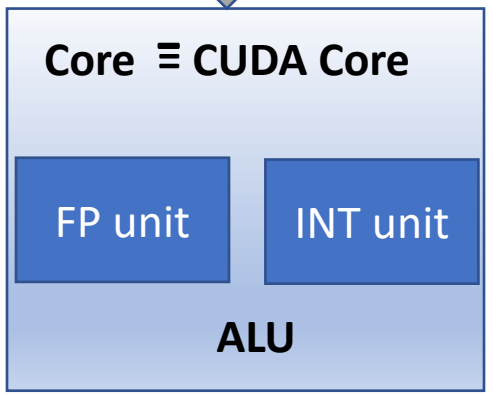


Streaming Multiprocessor (SM)



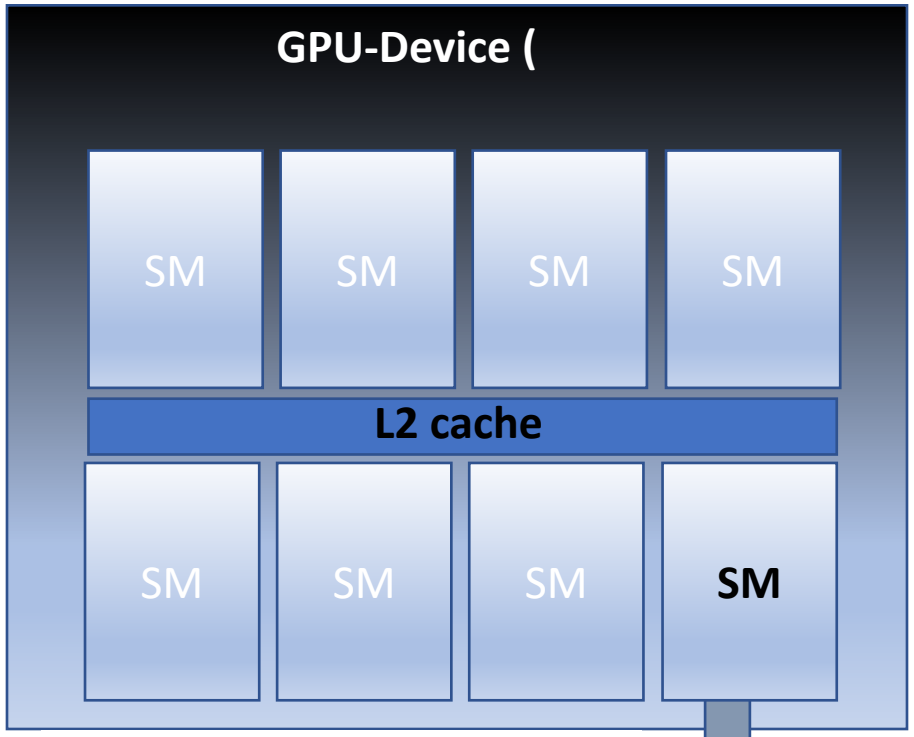
Data are stored temporarily. Registers are private to each thread.

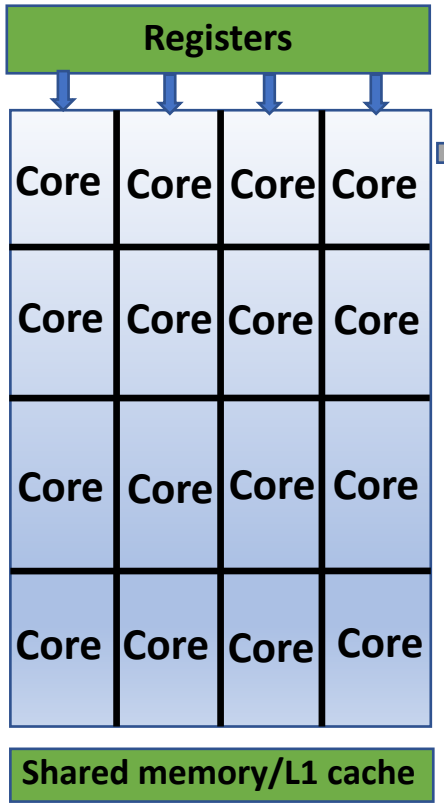
All threads share L1 cache.

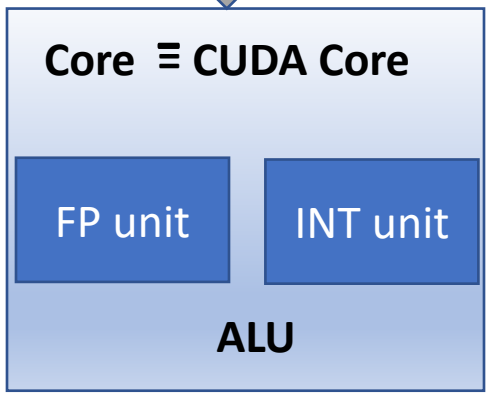


- Core includes ALU. Various logical operations for computations (FP32, FP64,) e.g. addition, multiplication and …
- ALU executes SIMD instructions. (processing multiple data with the same operation concurently (in parallel))

Architecture of NVIDIA-GPU devices (simplified version)





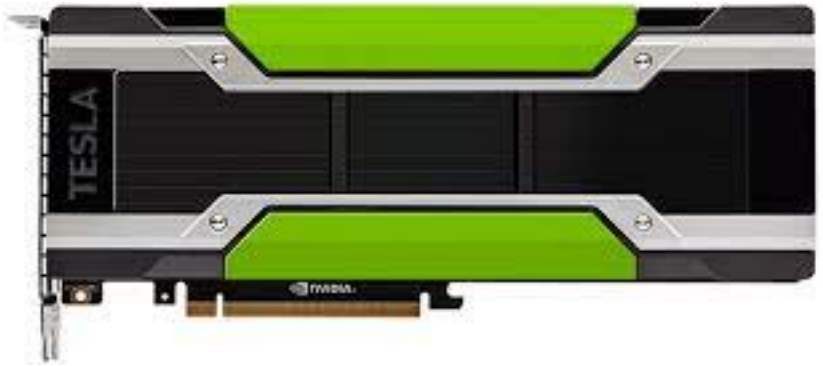


Streaming Multiprocessor (SM)

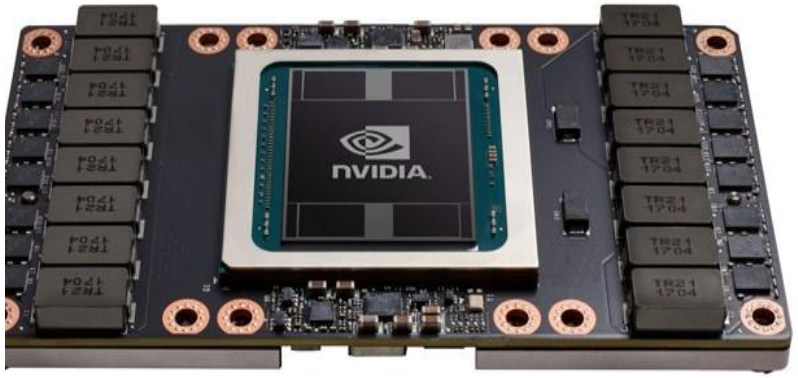
NVIDIA Tesla A100

For Tesla A100 GPU: 108 SMs, each SM has:

64 FP32 cores ===== A total of 6912 FP32 CUDA cores
64 INT32 cores ===== A total of 6912 INT32 CUDA cores.



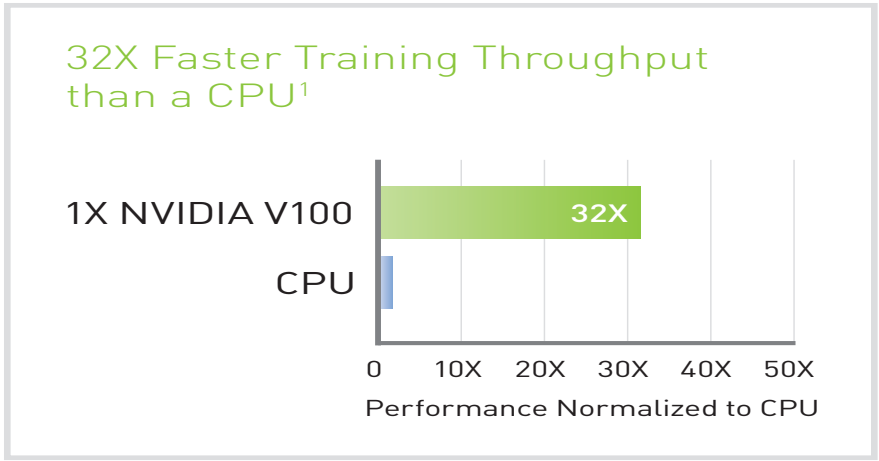
NVIDIA Tesla P100



NVIDIA Tesla V100

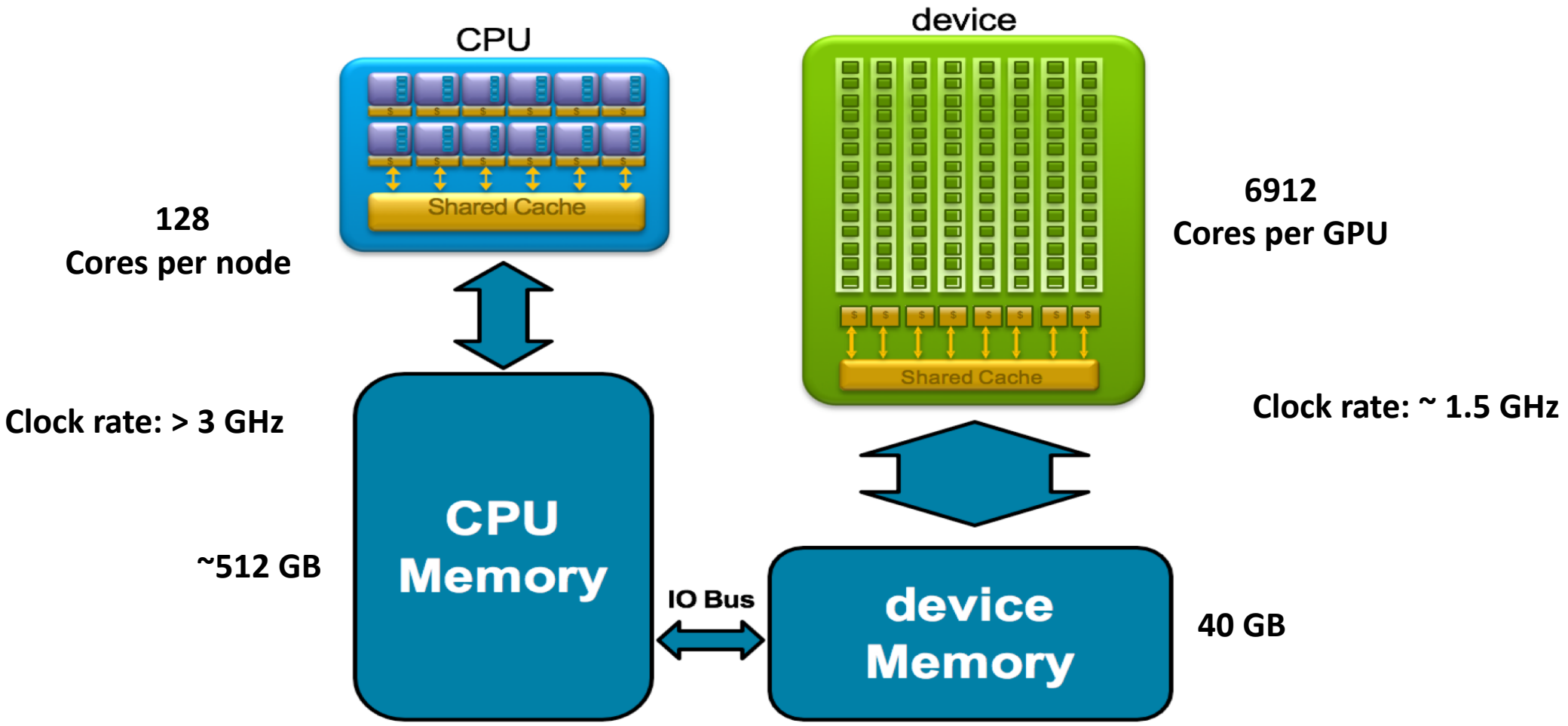
NVIDIA Tesla A100

Architecture	Tesla P100 (Pascal)	Tesla GV100 (Volta)	Tesla A100
SMs	56	84	108
NVIDIA CUDA cores	3584	5376	6912
Tensor cores/GPU	NA	672	432
Peak performance	9.3 TFLOPS	15.7 TFLOPS	39 TFLOPS
Transistors	15.3 billion	21.1 billion	54.2 billion
GPU die size	610 mm2	815 mm2	826 mm2



GPU-Dimension (cm)
26.7x11x4

Conclusion: CPU vs GPU



Taken from NVIDIA

Heterogenous programming models

Heterogenous programming models

Programming models can be hardware-dependent or hardware-independent

Directive based models:

High-level models

OpenACC

OpenMP

Compiler supports

NVHPC | GCC | Cray (only acc .2.0 F) | Clang | Cray | GCC | Icx (Intel)

Hardware

NVIDIA | NVIDIA | NVIDIA | AMD | AMD | AMD | Intel

AMD

Low level offload models:

CUDA

Only on NVIDIA

OpenCL

HIP

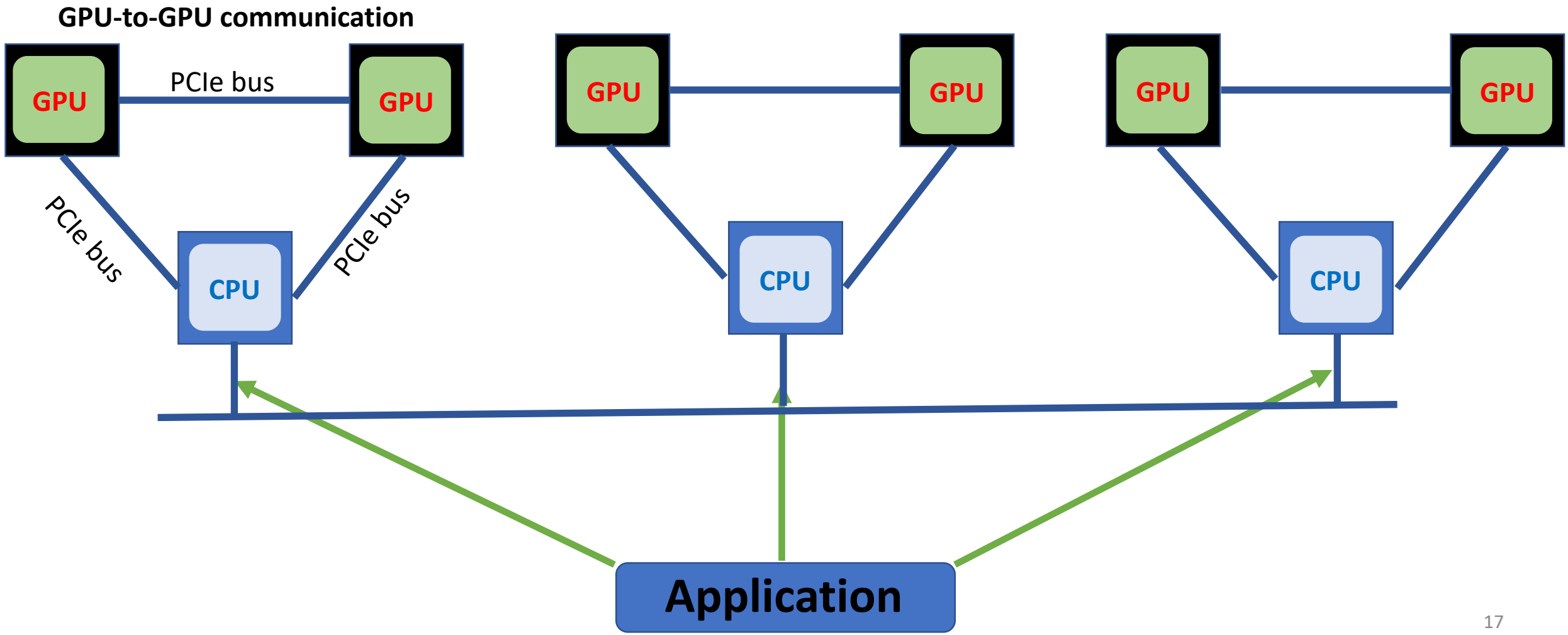
Only on AMD

Intel GPU:OpenCL can be migrated via SYCL API migrating from CUDA to DPC++. DPC++ tool is part of the Intel OneAPI Toolkit.

Hybrid multi-GPU programming: Combining MPI/OpenMP threading & OpenACC/OpenMP offloading

Multi-GPU programming

MPI+GPU programming model



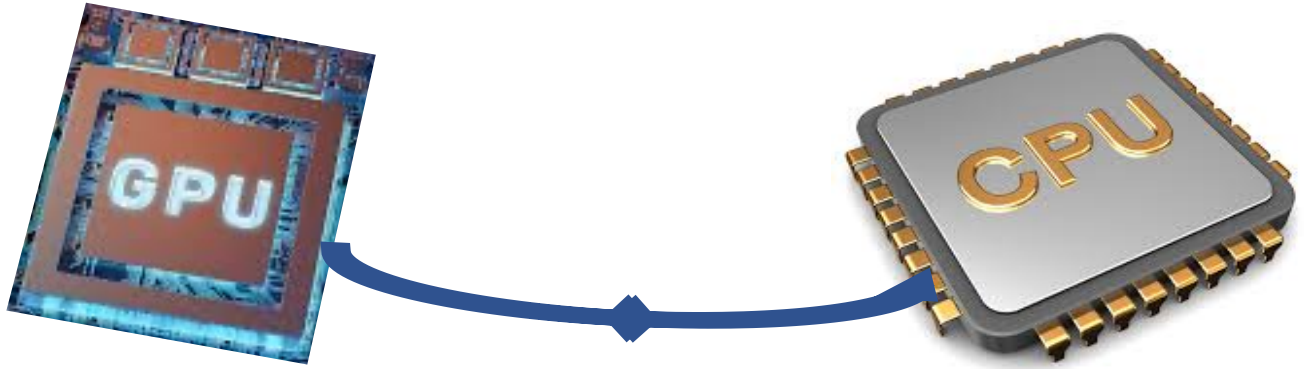
Functionality of OpenACC

What is OpenACC?

OpenACC is a directive-based approach similar to OpenMP.
It is designed to simplify parallel programming between heterogenous systems CPU/GPU.
It is API (Application Programming Interface) to communicate between CPU and GPU.

Parallelism in OpenACC

Heterogenous computing



GPU-Device

Thousands of cores

Programming model
To offload a code region to a GPU-device

CPU-Host

Multiple cores

```
do i=1,n
   do j=1,m
  A(i,j) = B(i,j) + C(i,j)
   enddo
enddo
```

Parallelism in OpenACC

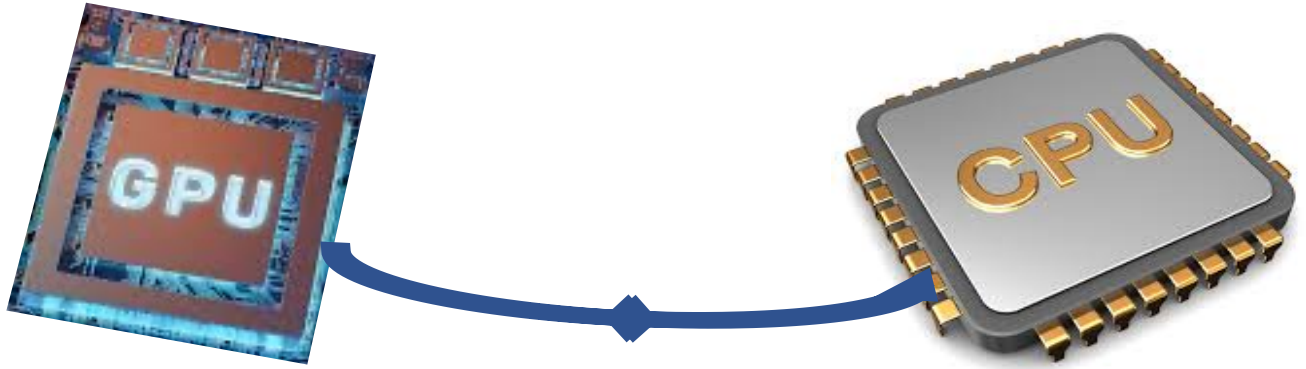
It uses CUDA to exploit parallelism.

Focus on how parallelism is done.

Message from the compiler

```
10, Generating Tesla code
11, !$acc loop gang, vector(32), worker(4)
! blockidx%x threadidx%x threadidx%y
12, !$acc loop seq
10, Generating implicit copyin(B(:,:),C(:,:))
[if not already present]
Generating implicit copyout(A(:,:))
[if not already present]
12, Loop is parallelizable
```

Heterogenous computing



GPU-Device

Thousands of cores

Incorporate directives that the compiler recognises. It tells the compiler to parallelize the loop.

CPU-Host

Multiple cores

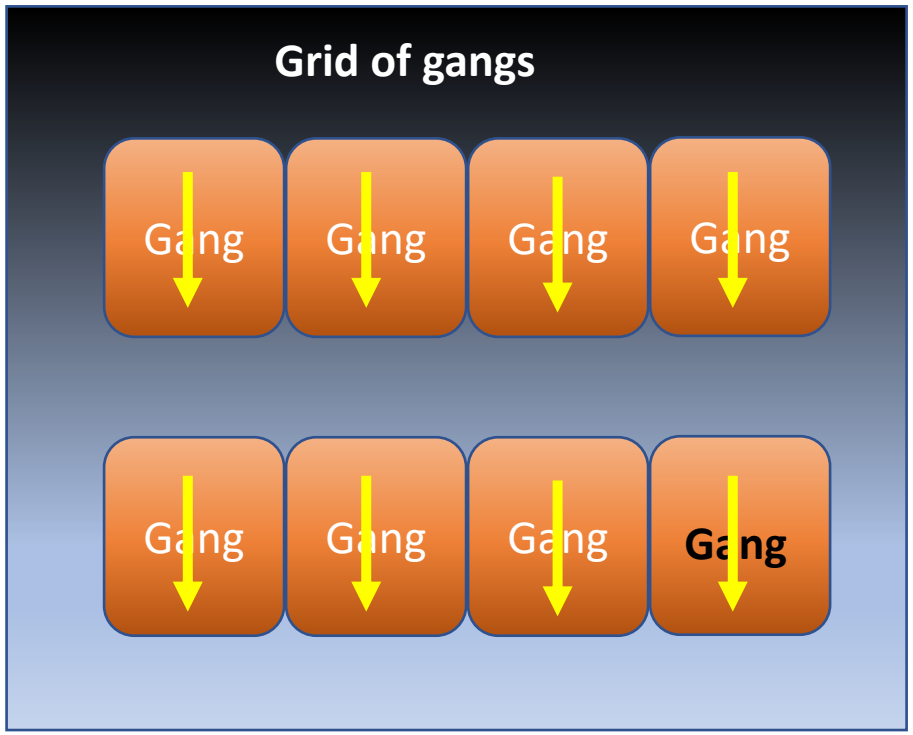
Programming model
To offload a code region to a GPU-device

```
!$acc parallel loop
do i=1,n
   do j=1,m
  A(i,j) = B(i,j) + C(i,j)
   enddo
Enddo
!$acc end parallel
```

Parallelism in OpenACC

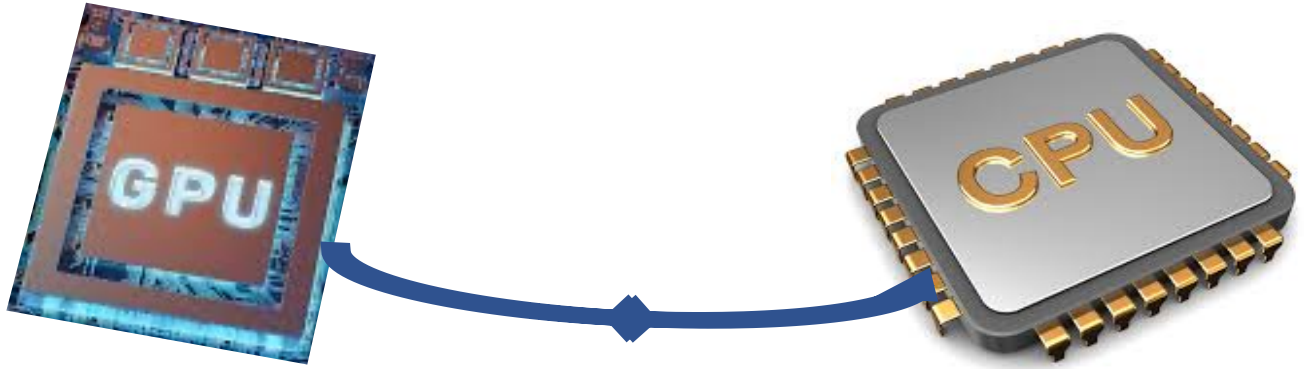
Software scheme

Only the "parallel" construct



Step 1: The compiler generates one or more gangs.
Step 2: The offloaded loop gets executed redundantly on each gang (get duplicated).

Heterogenous computing



GPU-Device

Thousands of cores

Incorporate directives that the compiler recognises. It tells the compiler to parallelize the loop.

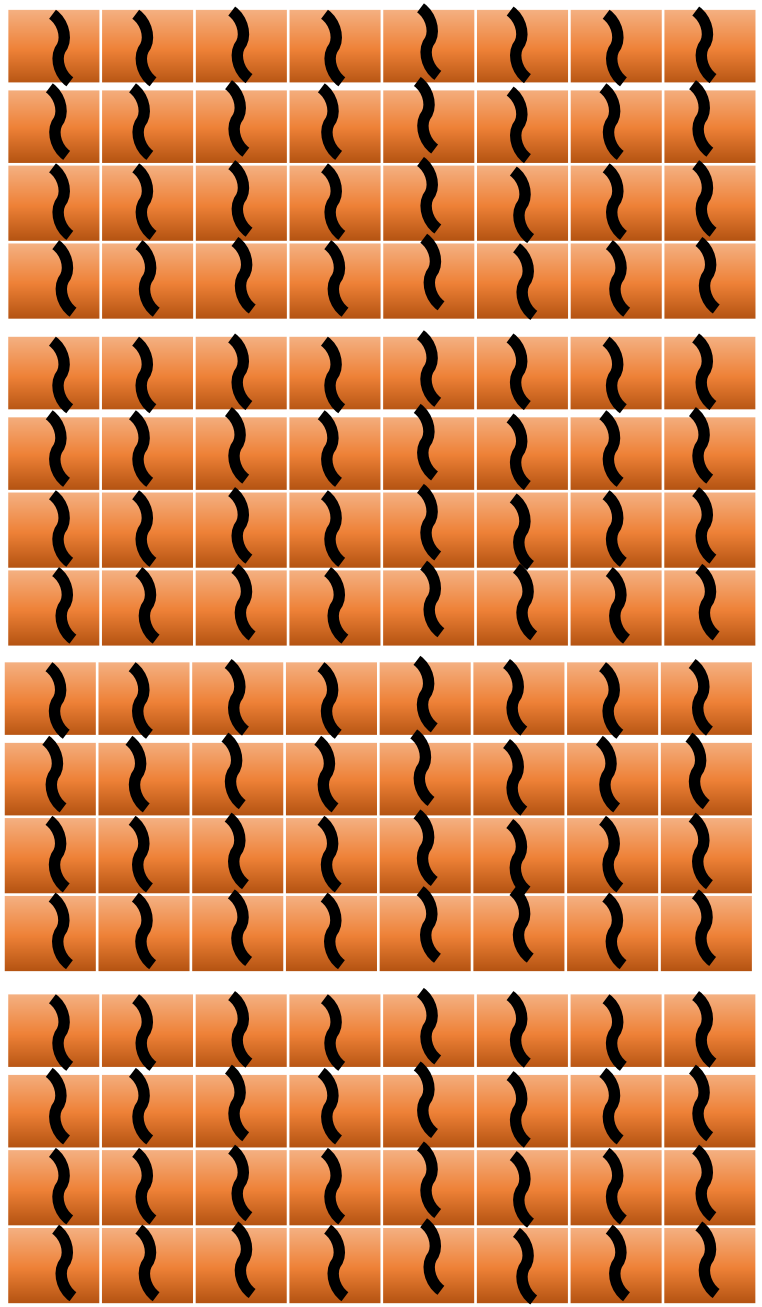
CPU-Host

Multiple cores

Programming model
To offload a code region to a GPU-device

```
!$acc parallel loop
do i=1,n
   do j=1,m
  A(i,j) = B(i,j) + C(i,j)
   enddo
Enddo
!$acc end parallel
```

Parallelism in OpenACC

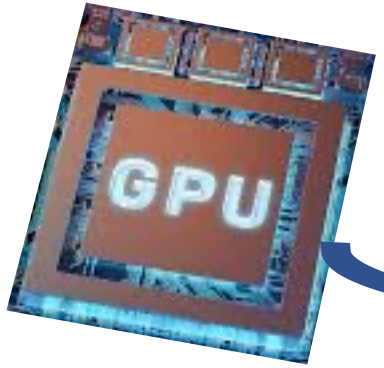


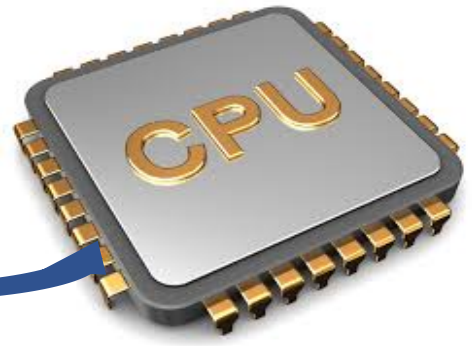
Workers
(Block of Threads)

Each piece of the loop runs by a thread at the same time.

Gang

Heterogenous computing





GPU-Device

Thousands of cores

CPU-Host

Multiple cores

Incorporate directives that the compiler recognises. It tells the compiler to parallelize the loop.

Programming model
To offload a code region to a GPU-device

```
!$acc parallel loop
do i=1,n
   do j=1,m
  A(i,j) = B(i,j) + C(i,j)
   enddo
Enddo
!$acc end parallel
```

Parallelism in OpenACC (it uses CUDA to exploit the parallelism)

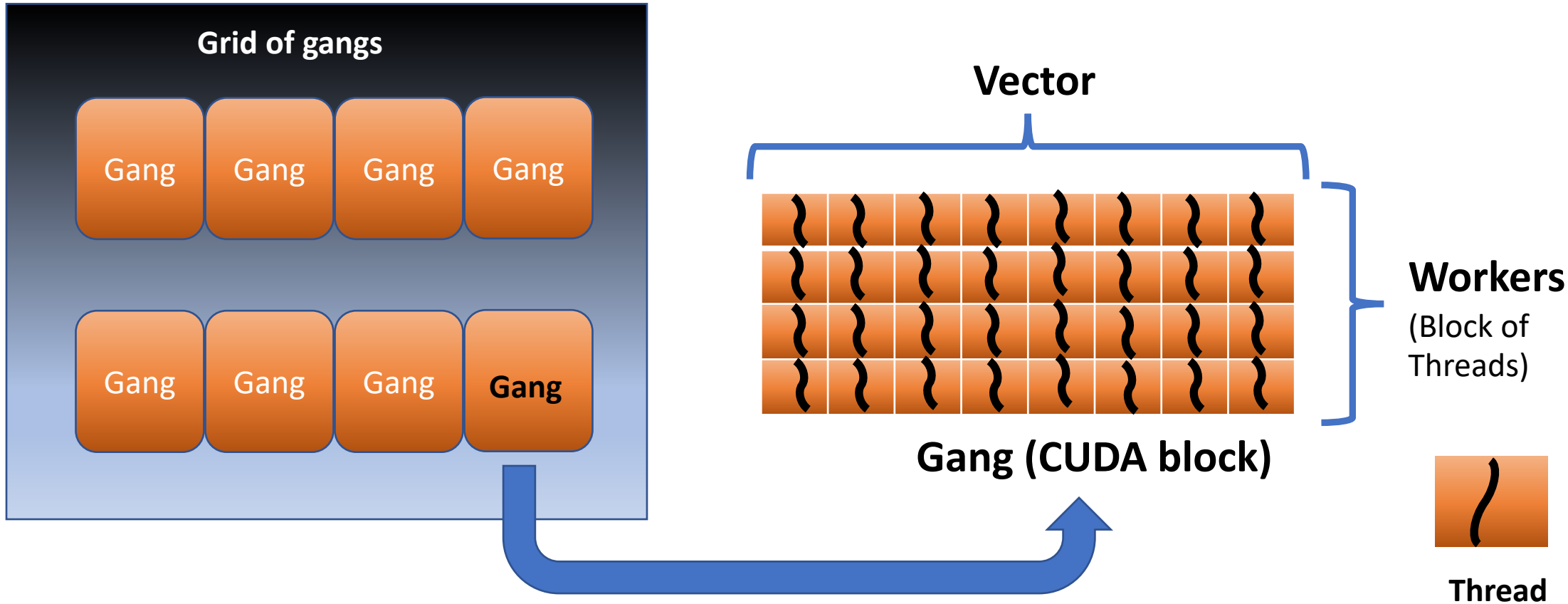
The parallelism in OpenACC is based on three concepts:

- **Gang :** Consists of a set of workers (block of thread)
- **Worker:** threads.
- **Vector: It** tells the OpenACC that it can exploit *vector parallelism*

Each thread has an index: it is used for calculating memory address locations.

vectorization naturally occurs in hardware across a **group of threads** referred to as a warp (**32 threads**) at the **same time**.

Software scheme



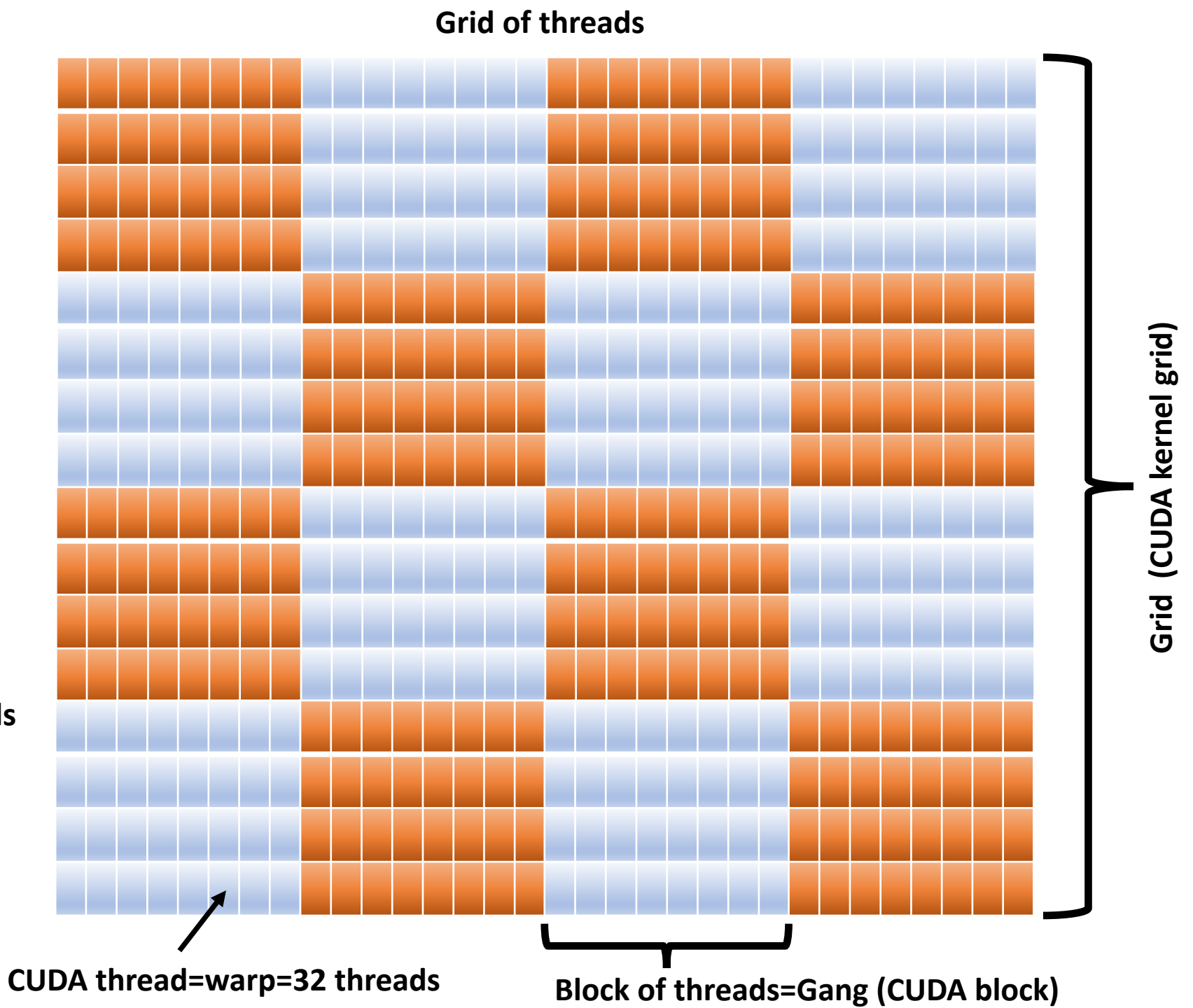
Mapping a matrix into a device

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}$$

Each thread executes a different piece
Of data item (data parallelism).

Each CUDA block has 1024 threads
(32 warps. A warp=collection of 32 threads
are executed simultaneously by a SM)

Execution on hardware
CUDA thread
CUDA block
CUDA grid



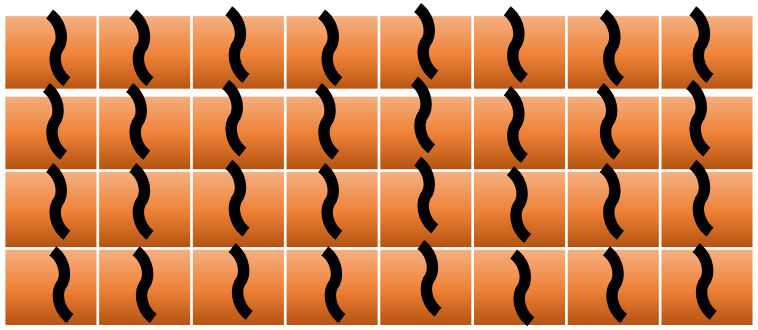
Execution on GPU

Software scheme

Hardware scheme

CUDA thread
(a full warp)

CUDA core



CUDA thread block

is executed on

core core core
core core core

Streaming Multiprocessor (SM)

Grid of gangs
(CUDA kernel grid)

Gang Gang Gang Gang

Gang Gang Gang Gang

GPU-Device

SM SM SM SM

SM SM SM SM

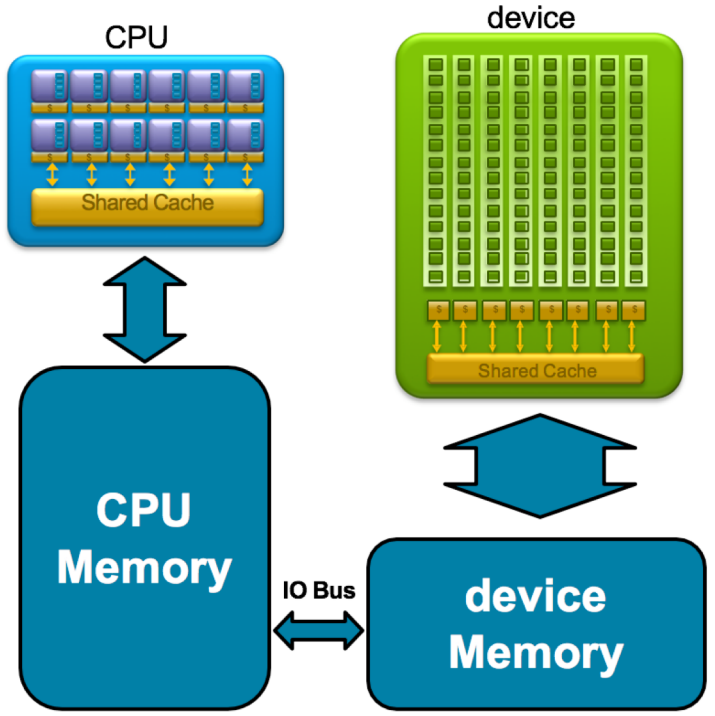
Conclusion

The parallelism in OpenACC is based on introducing three basic steps:

- **Step 1: The compiler generates one or more gangs.**
- **Step 2: The offloaded loop gets executed redundantly on each gang (get duplicated).**
- **Step 3: A block of thread will execute different pieces of the offloaded loop.**
- ***vector parallelism:* to perform multiple data-parallel operations at the same time.**
- vectorization naturally occurs in hardware across a group of threads referred to as a warp at the same time.

- **Data transfer between CPU and GPU is time consuming.**
- **The performance of GPU can be slower than CPU in some cases.**

- **Bottelneck in GPU-programming: Portability and hardware limitation.**
- **Converting codes affects the performance.**
- **Knowledge of GPU-architecture is important for GPU-programming.**



Taken from NVIDIA

Part II

Overview

- **Synchronous OpenACC**

  Various directives and clauses:

  -Parallel loop vs kernels

  - gang, worker, vector, num_workers(), vector_length()

  -Kernels, Reduction, collapse, routine clauses

  -Data locality (structured and unstructured data)

  -Update device/self

  -Atomic operations

  -Host_data use_device()

  -Deviceptr()

- **Asynchronous OpenACC**

  -Async, wait

  -Offloading to multiple GPUs

- **Code-profiling (Gprof, Gcov & Nsight Systems)**

Synchronous OpenACC

Parallelism in OpenACC: parallel loop vs kernels

OpenACC uses two different approaches (directives) for exposing parallelism:

Parallel loop construct and **Kernels** construct**.**

The compiler performs the parallelism of a specified loop and maps it into a GPU-device.

Fortran:

```
!$ acc parallel loop

!$ acc kernels
```

C/C++:

```
#pragma acc parallel loop

#pragma acc kernels
```

Ex.

```
!$ acc parallel loop
do j=1,Nx
  do i=1,Ny
     A(i,j) = B(i,j) + C(i,j)
  enddo
enddo
!$ acc end parallel
```

```
!$ acc kernels
do j=1,Nx
  do i=1,Ny
     A(i,j) = B(i,j) + C(i,j)
  enddo
enddo
!$ acc end kernels
```

Differences: parallel loop vs kernels:

Parallel loop construct: The programmer has more control on the parallelism (e.g. adding more clauses).

Kernels construct: The compiler has more flexibility (generation of efficient parallel codes) and responsibility (safety in parallelising loops).

Portability

Ex. combining loops into a single parallel kernel is included in **kernels** construct.

Message from the OpenACC compiler

Parallel loop construct

```
9, Generating Tesla code
     10, !$acc loop gang ! blockidx%x
     11, !$acc loop vector(128) ! threadidx%x
9, Generating implicit copyin(b(:,:),c(:,:)) [if not already present]
   Generating implicit copyout(a(:,:)) [if not already present]
11, Loop is parallelizable
```

4 workers (warps) each with 32 threads

```
9    !$ acc parallel loop
10   do j=1,Nx
11     do i=1,Ny
         A(i,j) = B(i,j) + C(i,j)
       enddo
     enddo
     !$ acc end parallel
```

```
9    !$ acc kernels
10   do j=1,Nx
11     do i=1,Ny
         A(i,j) = B(i,j) + C(i,j)
       enddo
     enddo
     !$ acc end kernels
```

Kernels construct

```
9, Generating implicitcopyin(b(:,:),c(:,:)) [if not already present]
    Generating implicit copyout(a(:,:)) [if not already present]
   10, Loop is parallelizable
   11, Loop is parallelizable
   Generating Tesla code
   10, !$acc loop gang, vector(128) collapse(2) !blockidx%x threadidx%x
        collapsed-innermost
   11, ! blockidx%x threadidx%x auto-collapsed
```

Another way of specifying the parallel loop

- **`Gang:`** Executes loops in parallel across *num_gangs* gangs.
- **`Worker:`** Executes loops in parallel across *num_workers* workers of a single gang.
- **`Vector:`** Executes loops in SIMD or vector mode, with a maximum *vector_length*.

```
!$ acc parallel loop
do j=1,Nx
  do i=1,Ny
     A(i,j) = B(i,j) + C(i,j)
  enddo
enddo
!$ acc end parallel
```

```
!$ acc parallel loop gang worker vector
do j=1,Nx
  do i=1,Ny
     A(i,j) = B(i,j) + C(i,j)
  enddo
enddo
!$ acc end parallel
```

Fig taken from NVIDIA

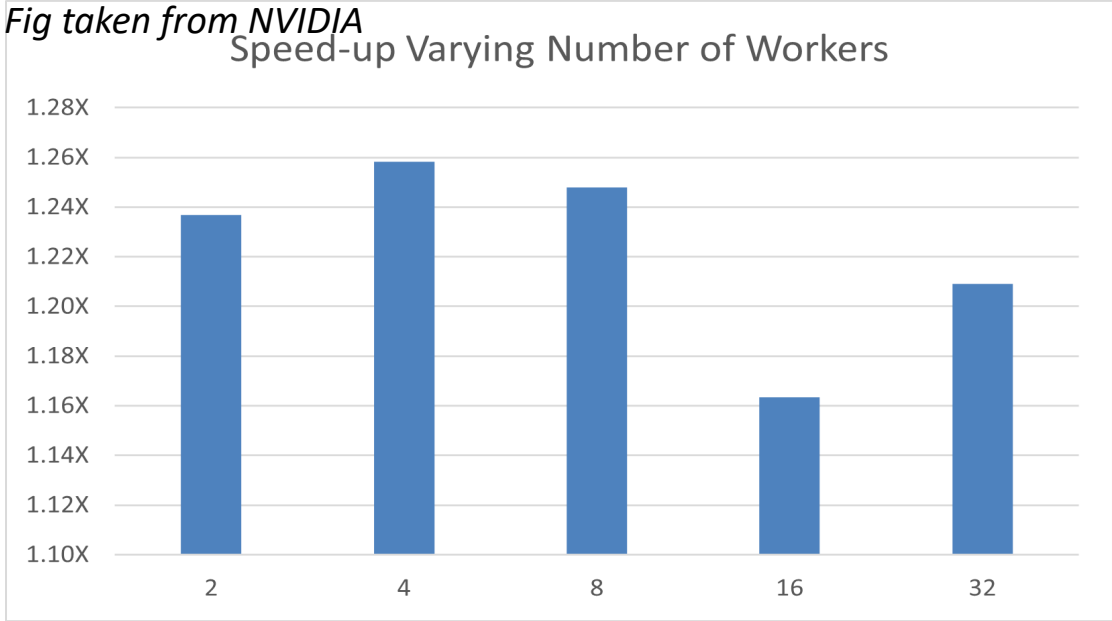


Figure 5.3: Speed-up from varying number of workers for a vector length of 32.

- **num_workers(*N*)**
  Controls how many workers are created in each gang.

- **vector_length(*N*)**

Controls the vector length on each worker.

```
!$ acc parallel loop gang worker num_workers(32) vector_length(32)
do j=1,Nx
  do i=1,Ny
     A(i,j) = B(i,j) + C(i,j)
  enddo
enddo
!$ acc end parallel
```

Reduction clause

Reduction(Operator:Val)

Operator: max,min,+,*… The syntax is valid for C/C++ and fortran.

Val can be a variable or array.

The **reduction** clause implies copying data back and forth between a CPU-host and a GPU-device.

In C/C++: **#pragma acc parallel loop reduction(operator:variable)**

In Fortran: **!$acc parallel loop reduction(operator:variable)**

```
!$acc parallel loop reduction(max:max_err)
      do j=1,ny
        do i=1,nx

          max_err = max(abs(fnew(i,j) - fold(i,j)),max_err)

        enddo
      enddo
!$acc end parallel
```

```
!$acc parallel loop reduction(max:max_err)
      do j=1,ny
!$acc loop reduction(max:max_err)
        do i=1,nx

          max_err = max(abs(fnew(i,j) - fold(i,j)),max_err)

        enddo
      enddo
!$acc end parallel
```

Reduction clause

Reduction(Operator:Val)

Operator: max,min,+,*… The syntaxt is valid for C/C++ and fortran.

Val can be a variable or array.

The **reduction** clause implies copying data back and forth between a CPU-host and a GPU-device.

In C/C++: `#pragma acc parallel loop reduction(operator:variable)`

In Fortran: `!$acc parallel loop reduction(operator:variable)`

max

```
!$acc parallel loop reduction(max:max_err)
      do j=1,ny
        do i=1,nx

          max_err = max(abs(fnew(i,j) - fold(i,j)),max_err)

        enddo
      enddo
!$acc end parallel
```

sum

```
total=0.
!$acc parallel loop reduction(+:total)
      do i=1,nx

          total = total + data(i)

      enddo
!$acc end parallel loop
```

Collapse clause

Collapse(N): transforms N tightly nested loops to a single loop (to improve the performance).

N corresponds to the number of nested loops to be collapsed to a single loop.

The total number of counts or elements involved in the loops remains the same.

In C/C++: `#pragma acc parallel loop collapse(N)`

In Fortran:

```
!$acc parallel loop collapse(N)
```

```
!$acc parallel loop collapse(2)
      do j=1,ny
        do i=1,nx

          ……

        enddo
      enddo
!$acc end parallel
```

```
!$acc parallel loop collapse(2)
      do j=1,ny
        do i=1,nx
!$acc loop collapse(3)
          do k1=1,nz1
            do j1=1,ny1
              do i1=1,nx1
                ……

              enddo
            enddo
          enddo
        enddo
      enddo
!$acc end parallel
```

Combining reduction and collapse clauses

In C/C++: `#pragma acc parallel loop reduction(operator:variable) collapse(N)`

In Fortran: `!$acc parallel loop reduction(operator:variable) collapse(N)`

Parallel loop clause

```
!$acc parallel loop reduction(max:max_err) collapse(2)
      do j=1,ny
        do i=1,nx

          max_err = max(dabs(fnew(i,j) - fold(i,j)),max_err)

        enddo
      enddo
!$acc end parallel
```

Kernels clause

```
!$acc kernels reduction(max:max_err) collapse(2)
      do j=1,ny
        do i=1,nx

          max_err = max(dabs(fnew(i,j) - fold(i,j)),max_err)

        enddo
      enddo
!$acc end kernels
```

Note: The **reduction** and **collapse** clauses are not allowed in the **kernels** clause

Error messages:
NVFORTRAN-S-0533-Clause 'REDUCTION' not allowed in ACC KERNELS

NVFORTRAN-S-0533-Clause 'COLLAPSE' not allowed in ACC KERNELS

Routine directive

The **routine** clause is used for calling functions or subroutines from a region specified by an OpenACC directive.

The **routine** clause must be added to all functions or subroutines underlying a called ones from a parallel loop.

The clause is refered to as **routine seq (i.e. sequential routine)** as it is called by each iteration within a parallel loop.

The clause must be located **below** the corresponding function or subroutine.

In C/C++: `#pragma acc routine seq`

In Fortran: `!$acc routine seq`

```
!$acc parallel loop reduction(max:max_err)
      do j=1,ny
        do i=1,nx
          .......
          call host_fnew(fnew,fold)
           max_err = max(dabs(fnew(i,j) - fold(i,j)),max_err)

        enddo
      enddo
!$acc end parallel
```

```
subroutine host_fnew(fnew,fold)

!$acc routine seq

implicit none
......
......
end subroutine
```

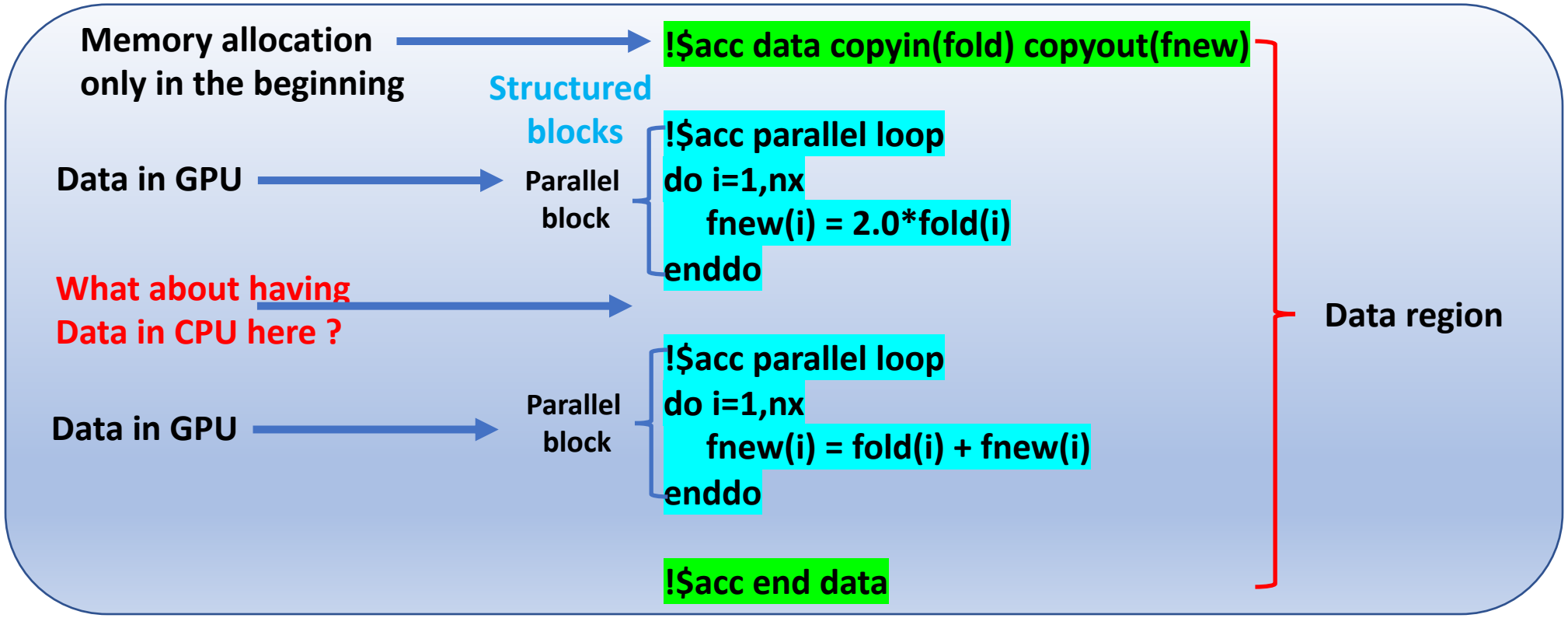
Data management (data locality): Data directive

Data movement between a **CPU-host** and a **GPU-device**.
The **data** directive permits to control and **optimize** memory placement between a host and a device.
The **data** directive permits sharing data between multiple **parallel blocks of loops** within a **data region**.
Two types of data: **structured** and **unstsructed** data.

Structured data: Data remain in a device during the dynamics within a data region. **Offloading ONLY in the beginning.**

In C/C++: `#pragma acc data copy(array[0:n])`

In Fortran:
```
!$acc data copy(array)
!$acc end data
```



Data management: Update directive

The **update** directive permits to synchronizing the change of data between CPU-host and GPU-device.
Two classes of the **update** directives can be distinguished.

The **update device** directive permits to update the change of data in a device by **copying them from a CPU-host to a GPU-device**.
The **update self** directive permits to update data in a host by **copying them from a GPU-device to a CPU-host**.

In C/C++: `#pragma acc update device(array[0:N])` `#pragma acc update self(array[0:N])`

In Fortran: `!$acc update device (array)` `!$acc update self(array)`

```
!$acc data copyin(fold) copyout(fnew)

      Compute the array fnew from GPU-device

 !$acc update self(fnew)   ! GPU → CPU

      Now fnew can be used from the host
      ex. Print fnew in a file or call a subroutine

 call host_fnew(fnew)

!$acc update device(fnew)  !CPU → GPU
!$acc end data
```

```
subroutine host_fnew(fnew)


!$acc parallel loop
do i=1,nx
    do j=1,ny
        fnew(i,j) = 3*fold(i,j)
    enddo
enddo

end subroutine
```

Data management: Data clauses

Data clauses:

copy(array) -- allocates space on a device and copy data to a device and back to a host at the end of a data region.

copyin(array) -- allocates space on a device and copy data to a device at the beginning of a data region.

copyout(array) -- allocates space on a device and copy data back to the host at the end of a data region.

create(array) -- allocates space in a device, no copy to or from the device/host.

present(array) – tells the compiler that no data movement is required.

delete(array) –removes data from a device. It is only used with **exit data** clause.

Note: No data movement will take place if the data are already present in a device.

Data management: Enter Data directive

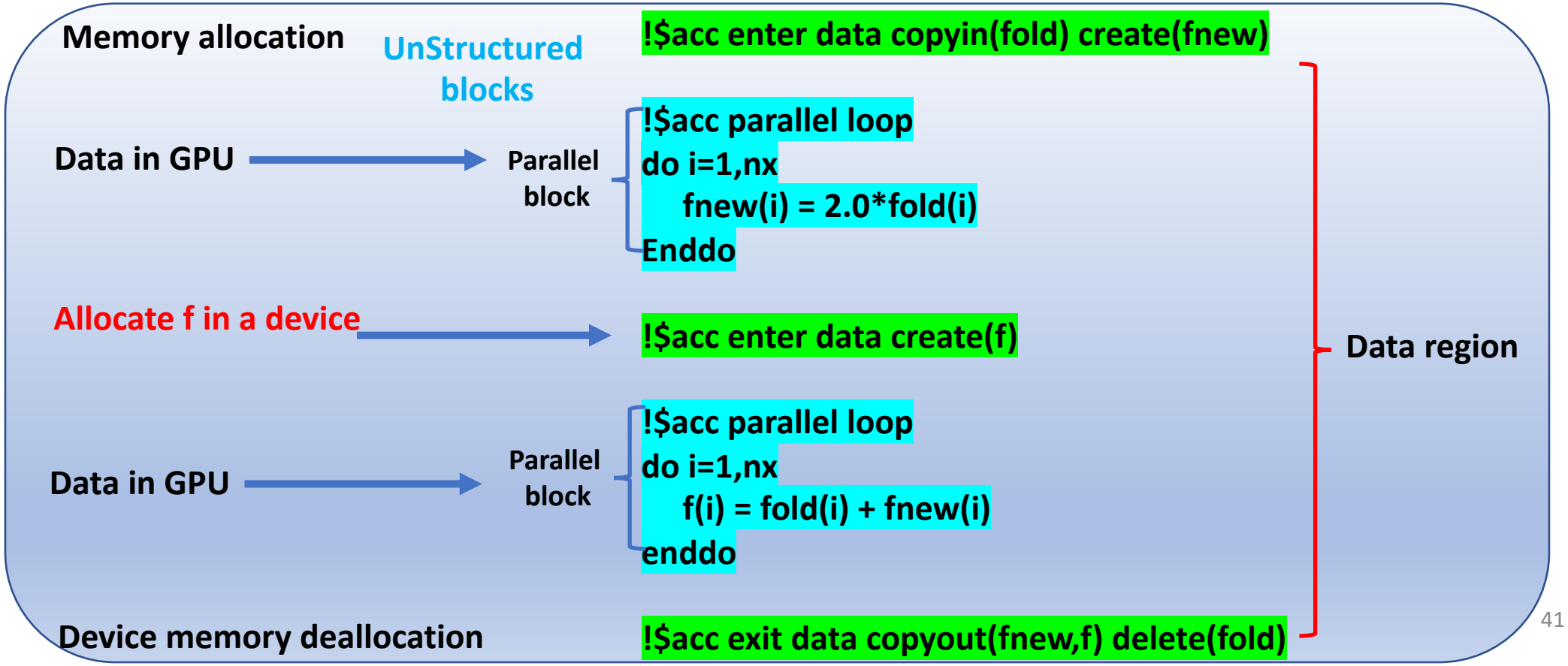
Unstructured data: The use of **structured data** is not always possible. Ex. When **allocating and deallocating** arrays within a **data region**.

In C/C++:

```
#pragma acc enter data copyin(array[0:n]) create(u[0:n])
.....
#pragma acc exit data copyout(u[0:n]) delete(array)
```

In Fortran:

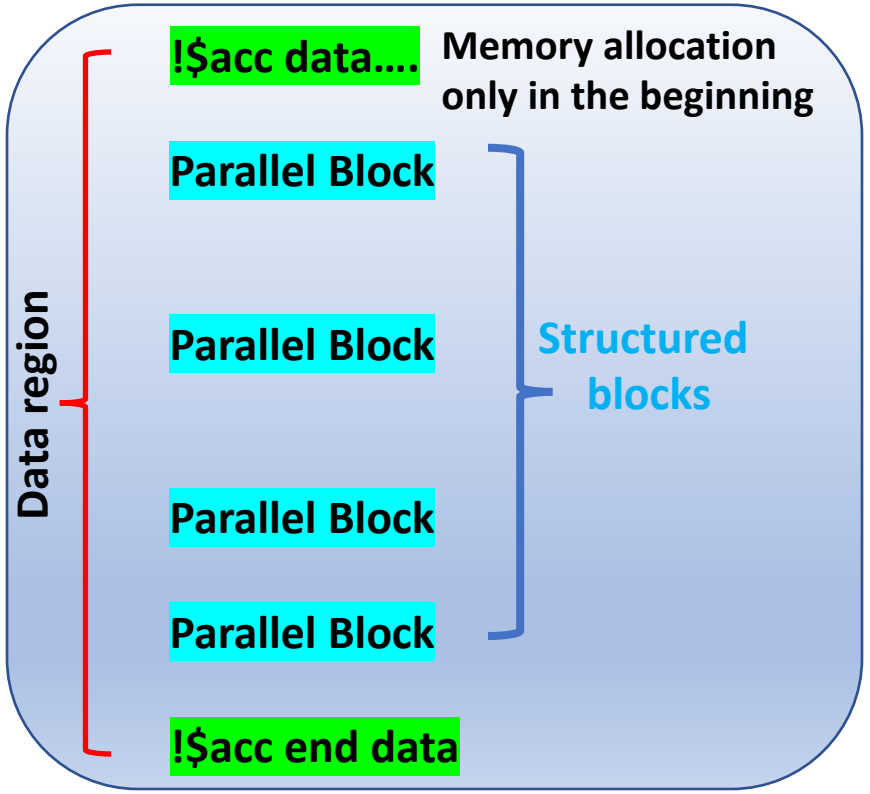
```
!$acc enter data copyin(array) create(u)
.....
!$acc exit data copyout(u) delete(array)
```



Data management: Structured data vs UnStructured data

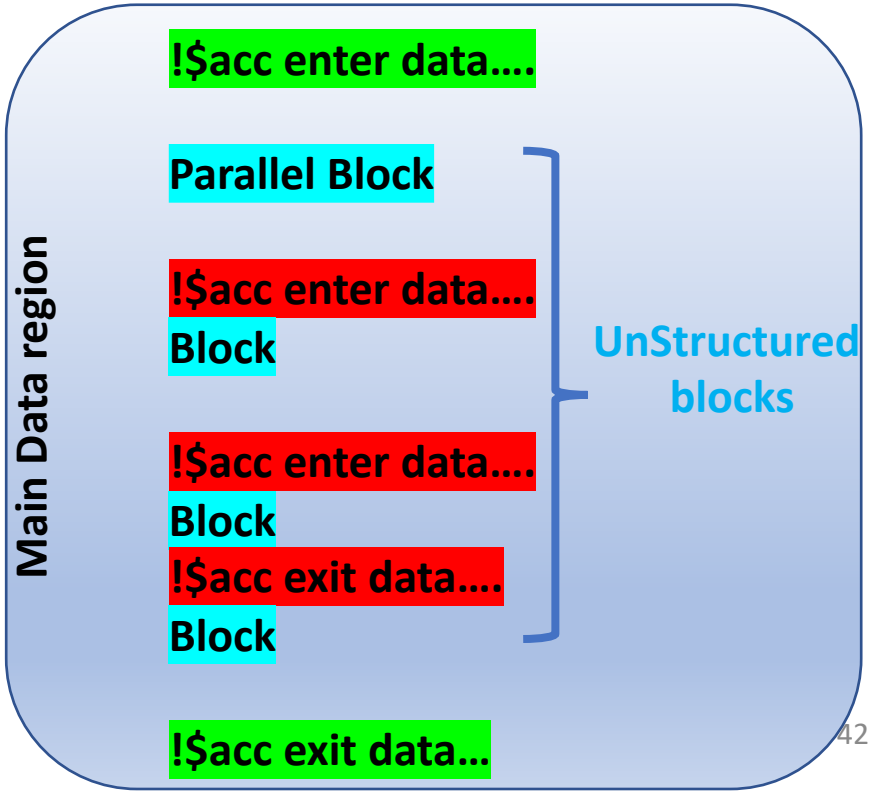
Structured data

- The concept of a data region is well defined: it starts with **!$acc data** and ends with **!$acc end data.**
- The device memory allocation is specified only in the beginning of a data region.



UnStructured data

- Create multiple enter/exit data directives within the main data region .
- Ability of multiple memory allocation/deallocation within the main data region



Atomic operations

Data dependency

When multiple threads access the same variable simultaneously, causing incorrectness of the obtained results (**race conditions**).

Ex. When one loop modifies a variable and a second loop reads the same variable in parallel: **Data dependencies.**
This is not the case in sequential programs.
Ex. Computing a sum. The **reduction directive** ensures the correctness.

The use of the **atomic directive** protects against race conditions.

In C/C++: **#pragma acc atomic update**

In Fortran: **!$acc atomic update**

```
Sum=0.
!$acc parallel loop reduction(+:sum)
      do i=1,n
         sum = sum + v(i)   Data dependency
      enddo
!$acc end parallel loop
```

```
!$acc parallel loop copyin(v) copy(u)
      do i=1,n
!$acc atomic update
         u(i) = u(i) + v(i)      Data dependency
      enddo
!$acc end parallel loop
```

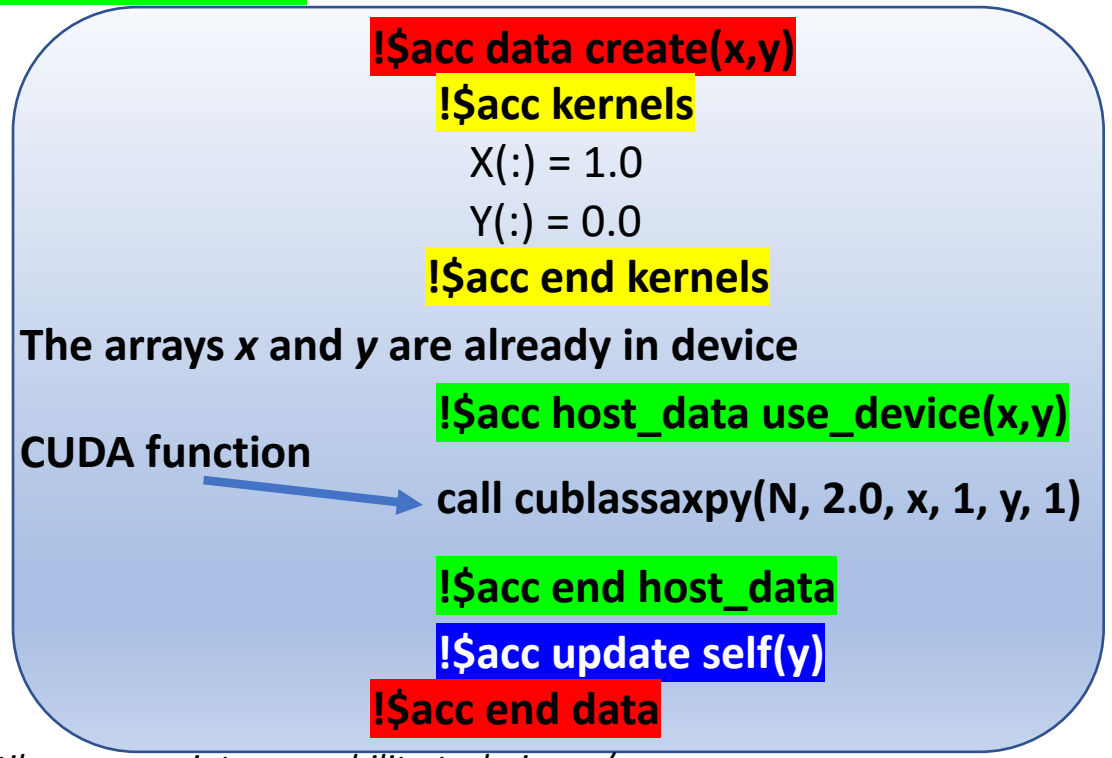
Combining OpenACC with other programming models (e.g.CUDA, OpenCL or accelerated libraries e.g. FFT)

Host_data directive

- The **host_data** directive enables to pass arrays already created in a device to e.g. a CUDA function or to an accelerated library.
- The directive makes the address of the device data available on the host, so that the data can be used by a CUDA function.
- The compiler generates a code to enable copying the arrays created in a device.
- When using the **host_data** directive, a list of the device arrays should be provided using the **use_device** clause.

In C/C++: #pragma acc host_data use_device(list of arrays)

In Fortran:!$acc host_data use_device(list of arrays)



The example is taken from https://developer.nvidia.com/blog/3-versatile-openacc-interoperability-techniques/

Deviceptr clause

- The **deviceptr()** clause is a reverse concept of the **host_data** directive.
- The clause informs the compiler that arrays, which have been allocated using e.g. CUDA, are already present in a device.
- The clause can be used inside a data region with a **parallel** or **kernels** constructs.
- This clause is generally used when OpenACC is combined with another programming model.

In C/C++: #pragma acc kernels deviceptr(list of arrays)

In Fortran:!$acc kernels deviceptr(list of arrays)

```
!$acc kernels deviceptr(x,y)
  y(:) = y(:) + b*x(:)
!$acc end kernels
```

Acc_map_data routine

The routine acc_map_data permits mapping host data to device data.

The routine can be use when sharing memory between CUDA and OpenACC.

The use of the routine requires specifying the header:

In C: **#include <openacc.h>**
In Fortran: **use openacc**

In C/C++

acc_map_data (**host, dev , size**)

In Fortran

subroutine **acc_map_data** (**host, dev**)
or
subroutine **acc_map_data** (**host, dev , size**)

Where ***host*** is a host array (host memory).
dev is a CUDA fortran device array (device memory).
size specifies the length of the array in bytes (integer).

Acc_unmap_data routine

The **acc_unmap_data** routine unmaps the device data from the specified host data.

In C/C++

acc_unmap_data (**host**)

In Fortran

subroutine **acc_unmap_data** (**host**)

Asynchronous OpenACC

Asynchronous features

- Data transfer to a GPU might be time consuming on systems with distinct memories.
- To reduce the computation time, **different parallel regions can be ran asynchronously.**
- The asynchronous process can be done via the following clauses:

```
!$acc data copyin(fold)
copyout(fnew)
!$acc parallel loop
do i=1,nx
    fnew(i) = 2.0*fold(i)
enddo
WAIT
!$acc parallel loop
do i=1,nx
    fnew(i) = fold(i) + fnew(i)
enddo

!$acc end data
```

async(argument) clause:

-It allows to combine multiple tasks (e.g. offloading to GPU and computation).

-While a GPU-device is executing a task, the CPU-host may do computation.

-This is only possible if a block of loops to be treated asynchronously **are independent**.

-The clause can be added to **parallel, kernels** and **update** directives.

-Computation and data transfer can be done concurently.

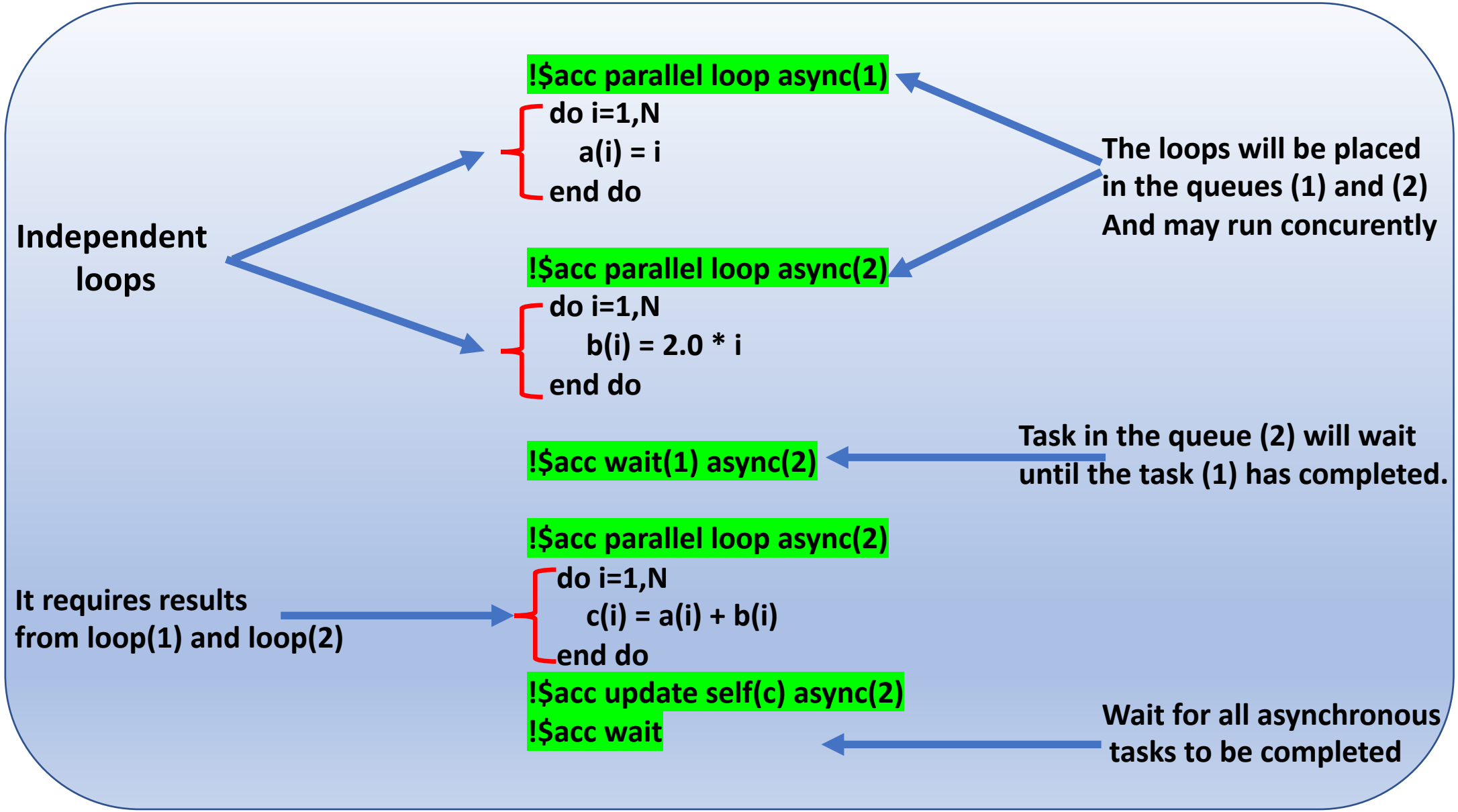
-**argument**: integer number that defines the queue number of a specific task.

wait(argument) clause: No execution will take place until all previous asynchrounous tasks are complete.

In C/C++: `#pragma acc parallel loop async`

In Fortran: `!$ acc parallel loop async`

Asynchronous features



Offloading to Multiple GPU-devices

Copy of data on multiple GPU-devices.

Specifying a device for each unstructured **enter data** directive using the function **acc_set_device_num()** .

Ex. Allocate arrays on multiple devices

Fortran

```
do gpu=0,1
call acc_set_device_num(gpu,acc_device_nvidia)
!$acc enter data create(array)
enddo
```

C

```
for(int gpu=0; gpu<2; gpu ++)
{
acc_set_device_num(gpu,acc_device_nvidia);
#pragma acc enter data create(array[:N])
}
```

Other relevant routines

acc_get_device_type: returns the device type to be used when executing a parallel or kernels region.

acc_get_num_devices: returns the number of devices available for the given type attached to the host.

acc_set_device_num: to set the device number and the device type to be used.

Compilation process

Compilation process

Load NVIDIA HPC environnment.
Find a module:
$ module avail NVHPC
$ load module

Fortran
nvfortran -fast -acc -Minfo=accel -o **executable** myCode.f90
or
nvfortran –acc -gpu=<target> -Minfo=accel -o **executable** myCode.f90

C
nvc -fast -acc -Minfo=accel -o **executable** myCode.c
For **C++**, compile with **nvc++**

- Flags **-acc** and **-gpu=<target>** enables OpenACC directives.
- The option **<target>** reflects the name of the GPU device.
- The latter is set to be **<cc60>** for the device name Tesla **P100** and **<cc70>** for the tesla **V100** device and **<cc80>** for **A100 GPU**. This information can be viewed by running the command \textbf{pgaccelinfo}.
- The flag option **-Minfo** enables the compiler to print out the feedback messages on optimizations and transformations.

Exercice

Ex. Solving the laplace equation

1-Run serial code with gprof

2-Introduce parallel loops

3-Perform profiling with Nsight systems: %kernels (computation) vs %memory (data transfer)

The majority of the computing time is spent in copying data between the host and device.

4-Introduce data locality

5-Perform profiling again: %kernels (computation) vs %memory (data transfer)

Comment on how the data transfer occurs and the time it takes between each iterations.

Code profiling

Code profiling:

Gprof & Gcov: serial codes

Nsight Systems: NVIDIA GPU-based codes

What is code profiling ?

- It is an advanced optimization technique.
- It helps to manage codes/programs.
- Improving the performance of codes/programs.
- Identify regions in which the majority of time is spent.
- It is a dynamical tool (based on gathering statistical data during the running procedure of a code/program).
- There are various source code profiling software.

Gprof (function-by-function analysis)

Gprof is a **GNU** binary tool for performing code profiling.

What do we learn from this tool ?

Gprof provides time information used by functions:

- Computing time used in each function.
- How often a function is called by other functions.
- How often a function called other functions.

The gathered statistical data by the Gprof tool allows us to determine which regions in the code the optimization efforts should be done.

Implementation of Gprof

1-Compilation: include the flag –pg in the compilation syntax.
Ex. (Fortran 90 code) gfortran **-pg –o executable** MyCode.f90
The option **"-pg"** enables the profiling to be performed while compiling.

2-Execution: ./executable
It generates a profile data file "**gmon.out**". The file contains statistical information about the runing time of the code.

3-Running Gprof: this step allows to interpret the "**gmon.out**" file

gprof **executable gmon.out** > **analysis.out**

The results of **Gprof** are thus stored in the **analysis.out** file and can be viewed by any text editor.

Example of profiling with Gprof

Flat profile:

% time	cumulative seconds	self seconds	calls	self s/call	total s/call	name
60.04	13.49	13.49	7	1.93	2.32	deriv_
12.19	16.23	2.74	21	0.13	0.13	aura_
11.57	18.83	2.60	1	2.60	7.24	rot_
5.92	20.16	1.33	1	1.33	1.33	calc_th_
5.03	21.29	1.13	1	1.13	19.96	calc_pv_
1.91	21.72	0.43	1	0.43	0.43	input_levels_
1.87	22.14	0.42	3	0.14	0.14	input_data_
1.42	22.46	0.32	3	0.11	0.11	output_write_
0.04	22.47	0.01	1	0.01	0.01	output_open_
0.00	22.47	0.00	14	0.00	0.00	getind_
0.00	22.47	0.00	2	0.00	0.00	input_close_
0.00	22.47	0.00	2	0.00	0.00	input_open_
0.00	22.47	0.00	1	0.00	22.47	MAIN__
0.00	22.47	0.00	1	0.00	0.00	input_getvars_
0.00	22.47	0.00	1	0.00	0.00	input_grid_
0.00	22.47	0.00	1	0.00	0.00	output_close_

% **time** the percentage of the total running time of the program used by this function.

cumulative seconds a running sum of the number of seconds accounted for by this function and those listed above it.

self seconds the number of seconds accounted for by this function alone. This is the major sort for this listing.

calls the number of times this function was invoked, if this function is profiled, else blank.

self ms/cal the average number of milliseconds spent in this function per call, if this function is profiled, else blank.

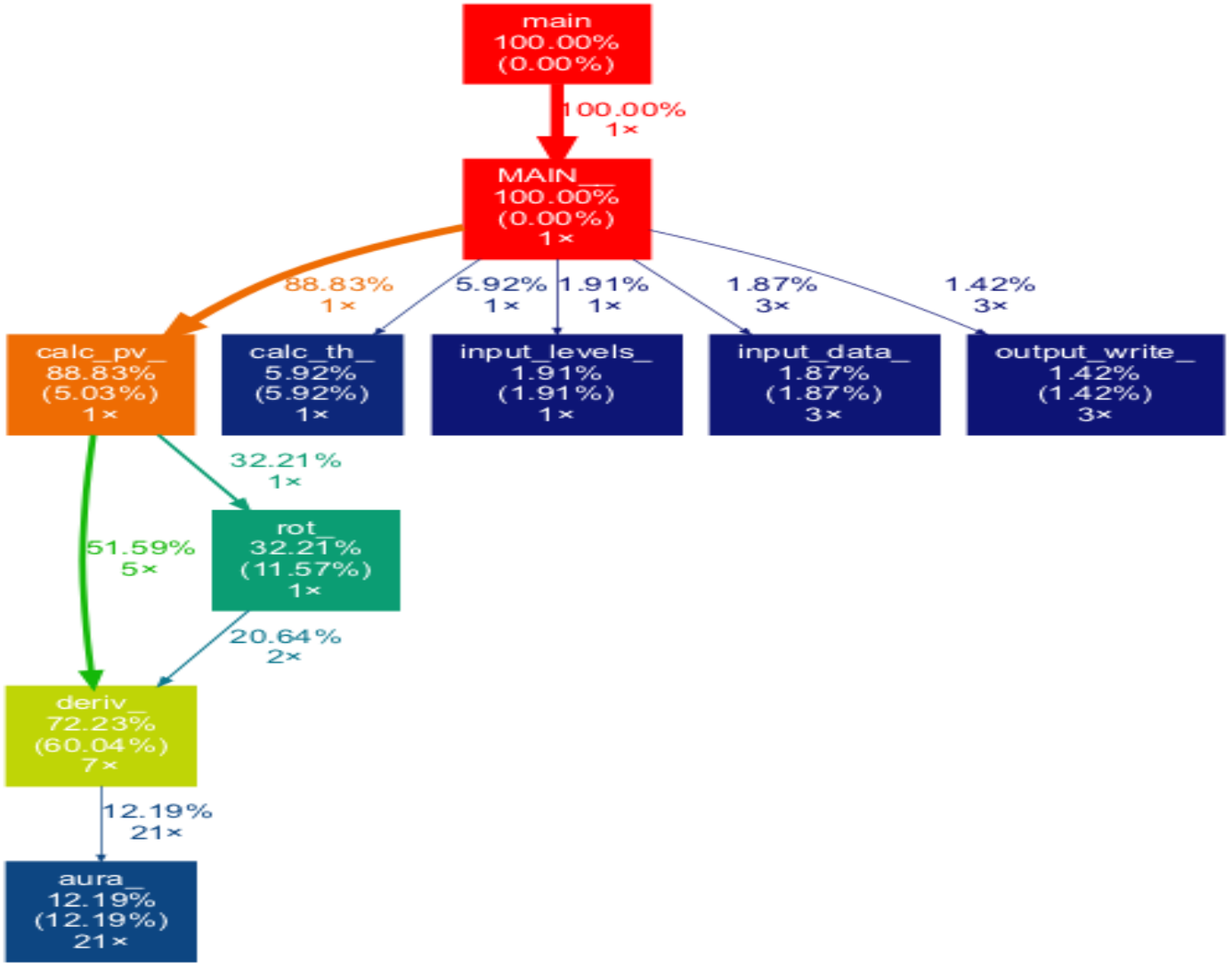
total ms/call the average number of milliseconds spent in this function and its descendents per call, if this function is profiled, else blank.

name the name of the function.

Visualization using Gprof2dot

Converting data to graph: gprof2dot **analysis.out** | dot -Tpng -o **output.png**

Installation: **brew install gprof2dot**



Gcov profiling (line-by-line analysis)

Gcov is a test coverage tool, it defines the % of lines of a code get executed

The **Gcov** tool tells about (**line-by-line**):

- How often each line of a code gets executed.
- What lines of code are actually executed.

1-Compilation: gfortran **-fprofile-arcs -ftest-coverage** subroutine.f90
The option **"- fprofile-arcs**" enables the profiling to be performed while compiling.

2-After executing the code; use: gcov subroutine.f90
It generates a logfile "**subroutine.f90.gcov**". The file contains statistical information about line-by-line execution.

Combining **Gprof** with **Gcov** helps to analyse the code's performance in a more detailed way. **Gprof** provides time information analysis of **function-by-function**, while **Gcov** aids to tune the analysis by performing **line-by-line** investigation.

Example of Gcov profiling

gcov subroutine.f90 creates **subroutine.f90.gcov**

The gcno and gcda files are also generated. These files are required for The visualization using **lcov**

-It can be linked to **Lcov,** which is a Graphical tool for GCC's coverage testing tool (gcov)

-Installation: brew install lcov

-To make lcov generate html reports, use the following commands:

lcov --directory . –zerocounters
lcov --directory . --capture --output-file app.info
genhtml app.info

LCOV - code coverage report

Current view:	top level - Lcov_Analysis		Hit	Total	Coverage
Test:	app.info	Lines:	25	52	48.1 %
Date:	2021-08-24 19:36:59	Functions:	1	1	100.0 %

Filename	Line Coverage		Functions	
fft0.f90	48.1 %	25 / 52	100.0 %	1 / 1

Generated by: LCOV version 1.15

```
        0 :     write(0,'("fft: n is not a power of 2"
        0 :     stop
          :   end if
          :
        0 :   allocate(x(0:n-1),y(0:n-1))
          :
        0 :   x(0:n-1) = real(xy(1:n))
        0 :   y(0:n-1) = imag(xy(1:n))
          :
          :   ! do the bit reversal
        0 :   i2 = n/2
        0 :   j = 0
268439548 :   do i=0,n-2
268308472 :     if (i < j) then
        0 :       tx = x(i)
        0 :       ty = y(i)
        0 :       x(i) = x(j)
        0 :       y(i) = y(j)
        0 :       x(j) = tx
        0 :       y(j) = ty
          :     end if
130090688 :     k = i2
        0 :     do while (k <= j)
        0 :       j = j-k
        0 :       k = k/2
          :     end do
268439548 :     j = j+k
          :   end do
          :
          :   ! compute the FFT
        0 :   c1 = -1d0
        0 :   c2 = 0d0
        0 :   l2 = 1
   720939 :   do l=0,m-1
  1310770 :     l1 = l2
  1310770 :     l2 = l2*2
  1310770 :     u1 = 1d0
  1310770 :     u2 = 0d0
  1310770 :     do j=0,l1-1
1744463814 :       do i=j,n-1,l2
1477466112 :         i1 = i + l1
1477466112 :         t1 = u1 * x(i1) - u2 * y(i1)
1477466112 :         t2 = u1 * y(i1) + u2 * x(i1)
1477466112 :         x(i1) = x(i) - t1
1477466112 :         y(i1) = y(i) - t2
1477466112 :         x(i) = x(i) + t1
1477466112 :         y(i) = y(i) + t2
          :       end do
        0 :       z =  u1 * c1 - u2 * c2
        0 :       u2 = u1 * c2 + u2 * c1
        0 :       u1 = z
```

NVIDIA Nsight Systems

NVIDIA Nsight Systems tool provides timeline information about GPU and CPU activities.
The tool allows to identify issues, such that: *Taken from https://developer.nvidia.com/blog/how-optimize-data-transfers-cuda-cc/*

- GPU starvation
- Unnecessary GPU synchonization
- Expensive computing time during the host-device data transfers.

The tool thus allows to optimize the performance of CUDA, OpenACC and OpenMP applications.

How to measure the computing time during the host-device data transfer without modifying the source code?
It can be done using the command-line **nvprof**

Compile	**For fortran**: nvfortran -fast -acc -Minfo=accel -g -o **executable** Mycode.f90 **For C**: compile with **nvcc**
Run	**nsys** profile -t cuda,openacc -f true -o output **./executable** **nvprof ./executable**

Output of profiling with nvprof

Running **nvprof** generates an output file conatining timeline information about:

- GPU activities
- API calls
- OpenACC

Here is an example of profiling a code based on sloving the laplace quation:

GPU activities

Profiling result:

Type	Time(%)	Time	Calls	Avg	Min	Max	Name
GPU activities:	48.82%	746.66ms	243	3.0727ms	3.0634ms	3.0791ms	**laplace_acc_55_gpu**
	43.84%	670.48ms	243	2.7592ms	2.7041ms	2.8123ms	**laplace_acc_42_gpu**
	2.84%	43.437ms	34	1.2776ms	1.8240us	1.3648ms	**[CUDA memcpy HtoD]**
	2.71%	41.398ms	276	149.99us	1.3120us	1.3360ms	**[CUDA memcpy DtoH]**
	1.76%	26.985ms	243	111.05us	109.95us	117.54us	**laplace_acc_55_gpu__red**
	0.02%	292.80us	243	1.2040us	1.1520us	1.5680us	[CUDA memset]

API calls Information

API: Application Programm Interface

Type	Time(%)	Time	Calls	Avg	Min	Max	Name
API calls:	82.09%	1.44880s	974	1.4875ms	1.6330us	3.1892ms	cuStreamSynchronize
	13.48%	237.88ms	1	237.88ms	237.88ms	237.88ms	cuDevicePrimaryCtxRetain
	2.31%	40.836ms	339	120.46us	1.2510us	1.3429ms	cuEventSynchronize
	1.47%	26.002ms	1	26.002ms	26.002ms	26.002ms	cuMemHostAlloc
	0.20%	3.5720ms	729	4.8990us	3.3450us	32.912us	cuLaunchKernel
	0.14%	2.4206ms	7	345.80us	3.2670us	1.4096ms	cuMemAlloc
	0.10%	1.7416ms	276	6.3100us	3.2380us	24.165us	cuMemcpyDtoHAsync
	0.06%	974.17us	1	974.17us	974.17us	974.17us	cuMemAllocHost
	0.05%	899.70us	341	2.6380us	1.5080us	11.193us	cuEventRecord
	0.05%	884.09us	243	3.6380us	2.3710us	28.147us	cuMemsetD32Async
	0.03%	537.81us	34	15.817us	12.358us	27.082us	cuMemcpyHtoDAsync
	0.02%	314.05us	1	314.05us	314.05us	314.05us	cuModuleLoadDataEx
	0.00%	16.502us	1	16.502us	16.502us	16.502us	cuStreamCreate
	0.00%	11.589us	3	3.8630us	1.9130us	6.5810us	cuPointerGetAttributes
	0.00%	11.249us	4	2.8120us	506ns	4.9420us	cuEventCreate
	0.00%	9.1630us	1	9.1630us	9.1630us	9.1630us	cuDeviceGetPCIBusId
	0.00%	3.4260us	3	1.1420us	280ns	2.5620us	cuModuleGetFunction
	0.00%	3.3130us	2	1.6560us	181ns	3.1320us	cuDeviceGet
	0.00%	3.1270us	3	1.0420us	281ns	2.0310us	cuCtxSetCurrent
	0.00%	1.9530us	5	390ns	133ns	818ns	cuDeviceGetAttribute
	0.00%	1.6750us	3	558ns	203ns	1.2180us	cuDeviceGetCount
	0.00%	1.6540us	1	1.6540us	1.6540us	1.6540us	cuCtxGetCurrent
	0.00%	416ns	1	416ns	416ns	416ns	cuDeviceComputeCapability
	0.00%	176ns	1	176ns	176ns	176ns	cuDriverGetVersion

OpenACC (excl) information

Profiling result:

Type	Time(%)	Time	Calls	Avg	Min	Max	Name
OpenACC (excl):	43.44%	775.36ms	486	1.5954ms	5.8650us	3.1901ms	**acc_wait@laplace_acc.f90:55**
	37.62%	671.56ms	243	2.7636ms	2.7097ms	2.8170ms	**acc_wait@laplace_acc.f90:42**
	11.30%	201.67ms	1	201.67ms	201.67ms	201.67ms	**acc_exit_data@laplace_acc.f90:40**
	6.47%	115.53ms	1	115.53ms	115.53ms	115.53ms	**acc_enter_data@laplace_acc.f90:40**
	0.36%	6.3747ms	1	6.3747ms	6.3747ms	6.3747ms	**acc_wait@laplace_acc.f90:66**
	0.11%	2.0415ms	243	8.4010us	5.8850us	22.482us	acc_enqueue_download@laplace_acc.f90:62
	0.11%	1.9219ms	243	7.9090us	5.1370us	9.9690us	**acc_wait@laplace_acc.f90:62**
	0.09%	1.6290ms	243	6.7030us	5.0930us	38.698us	acc_enqueue_launch@laplace_acc.f90:42 (laplace_acc_42_gpu)
	0.09%	1.5643ms	243	6.4370us	4.8360us	28.268us	acc_enqueue_launch@laplace_acc.f90:55 (laplace_acc_55_gpu)
	0.07%	1.2504ms	243	5.1450us	4.3380us	14.431us	acc_enqueue_launch@laplace_acc.f90:55 (laplace_acc_55_gpu__red)
	0.06%	1.0981ms	243	4.5180us	3.0720us	31.541us	acc_enqueue_upload@laplace_acc.f90:55
	0.05%	977.64us	243	4.0230us	3.1710us	21.249us	**acc_enter_data@laplace_acc.f90:55**
	0.05%	933.82us	243	3.8420us	3.0370us	28.420us	**acc_exit_data@laplace_acc.f90:55**
	0.04%	756.50us	33	22.924us	6.0210us	33.184us	acc_enqueue_download@laplace_acc.f90:66
	0.04%	752.64us	34	22.136us	14.306us	39.348us	acc_enqueue_upload@laplace_acc.f90:40
	0.04%	627.04us	243	2.5800us	2.2000us	7.7770us	**acc_compute_construct@laplace_acc.f90:55**
	0.03%	512.35us	243	2.1080us	1.7520us	19.561us	**acc_compute_construct@laplace_acc.f90:42**
	0.02%	340.94us	1	340.94us	340.94us	340.94us	acc_device_init@laplace_acc.f90:40
	0.00%	8.8790us	1	8.8790us	8.8790us	8.8790us	acc_wait@laplace_acc.f90:40
	0.00%	0ns	243	0ns	0ns	0ns	acc_delete@laplace_acc.f90:62

Guide on the use of NVIDIA Nsight Systems

On local systems

1- Installation guide https://docs.nvidia.com/nsight-systems/InstallationGuide/index.html

2- Download and install from here https://developer.nvidia.com/nsight-systems

3- Launch GUI directly: run nsight-sys executable from the host directory of installation

Or directly from the host desktop where the icon of **NVIDIA Nsight Systems** is located.

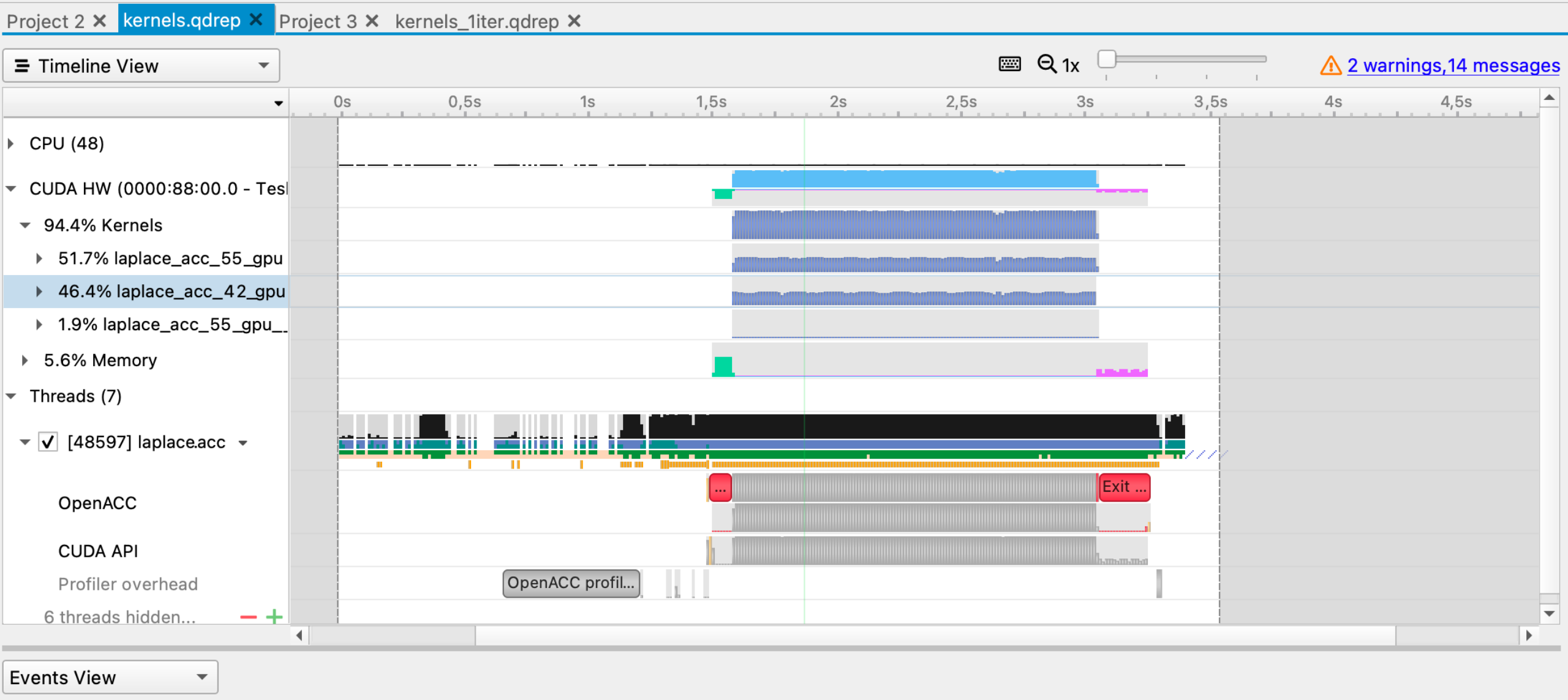
Launching GUI From Saga:

1- Login to Saga with ssh -X

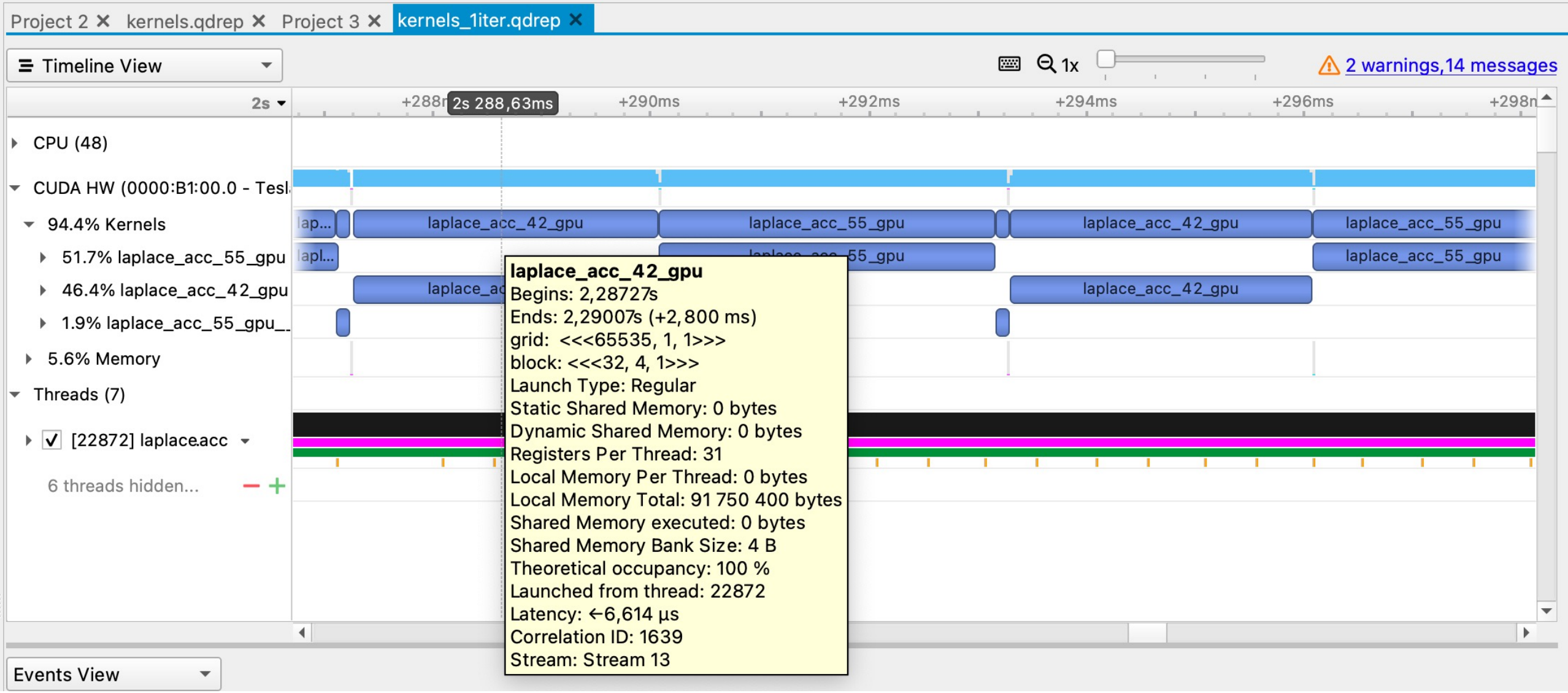
2- Load ml load CUDA/11.4.1 X11/20210802-GCCcore-11.2.0

3- Run **nsight-sys** or **nsys-ui**

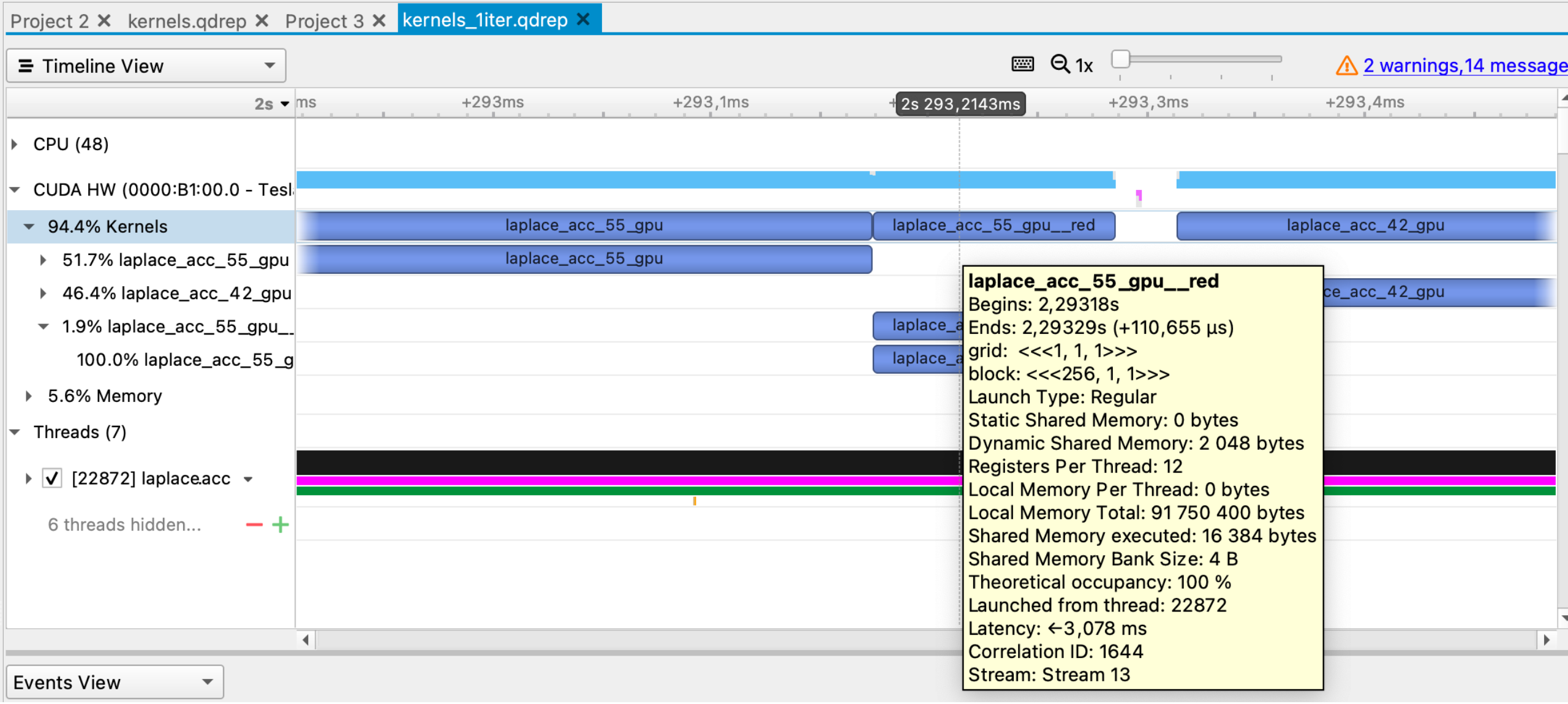
NVIDIA Nsight Systems



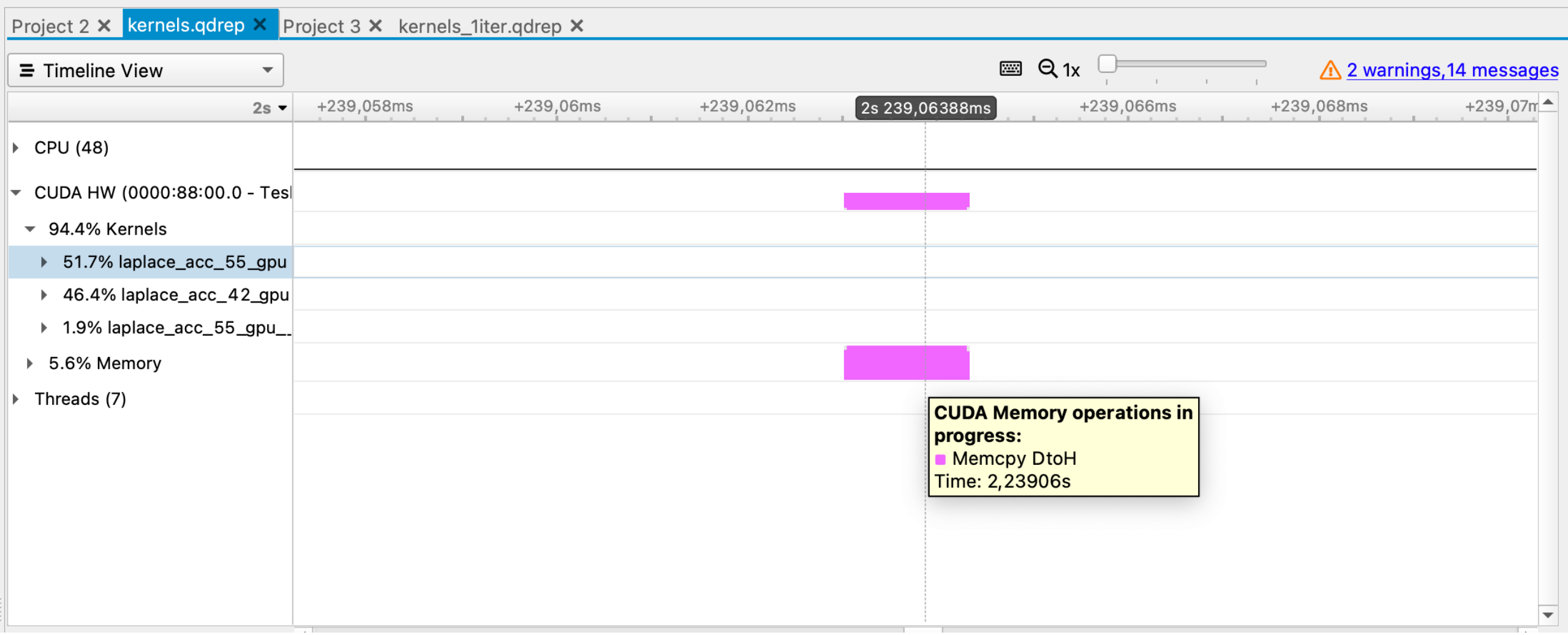
NVIDIA Nsight Systems



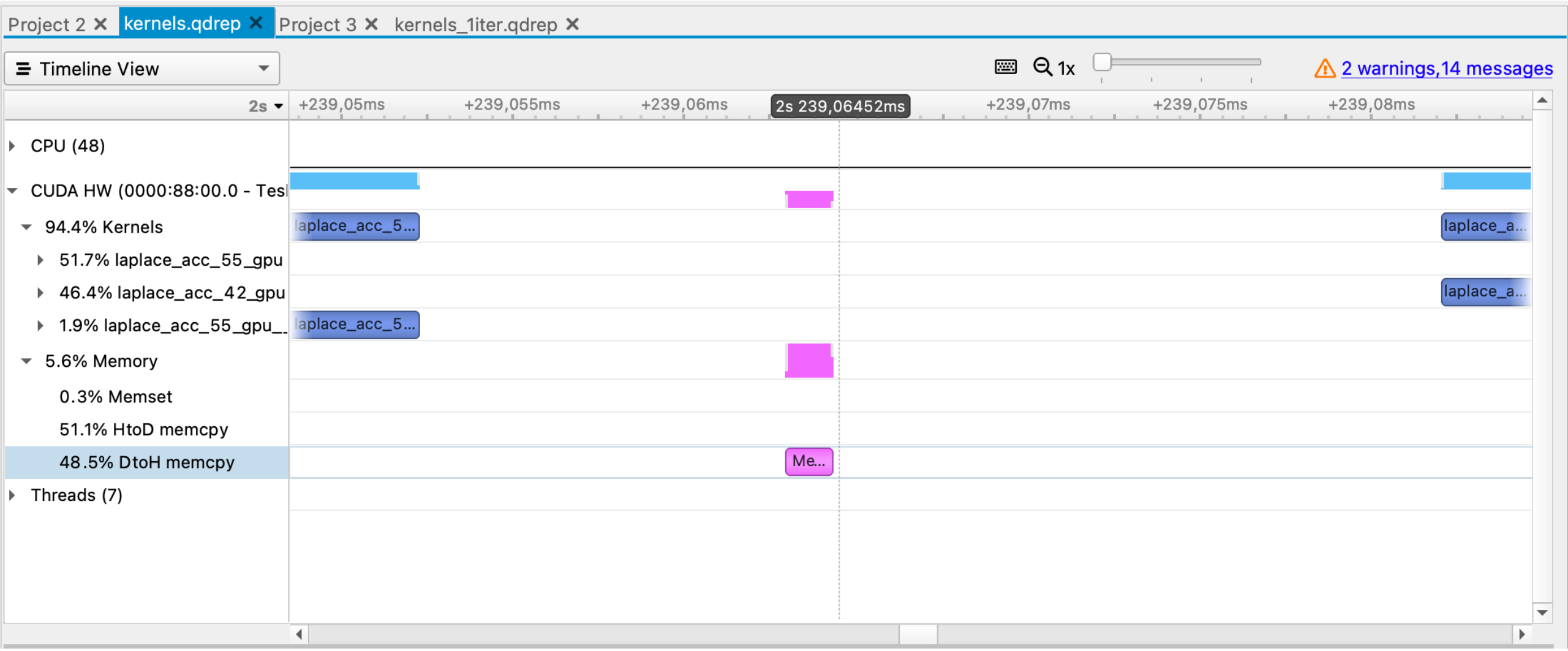
NVIDIA Nsight Systems



NVIDIA Nsight Systems



NVIDIA Nsight Systems



References

- OpenACC programming guide: https://www.openacc.org/sites/default/files/inline-files/OpenACC_Programming_Guide_0_0.pd
- https://docs.nvidia.com/hpc-sdk/pgi-compilers/20.4/x86/openacc-gs/index.htm
- Parallel Programming with OpenACC-Morgan Kaufmann (2016)
- https://developer.nvidia.com/blog/3-versatile-openacc-interoperability-techniques/
- Profiling
- https://ftp.gnu.org/old-gnu/Manuals/gprof-2.9.1/html_node/gprof_1.html
- https://gcc.gnu.org/onlinedocs/gcc/Gcov.html
- https://developer.nvidia.com/nsight-systems
- https://docs.nvidia.com/cuda/profiler-users-guide/index.html