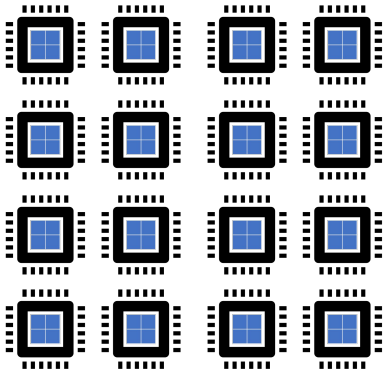
GPUs
bottlenecks in accelerated codes

l.bellentani@cineca.it
Tutorial on Profiling @ MHPC - ICTP

A new paradigm in parallel programming

A new paradigm in parallel programming

90s advent of MPI → distributed programming



Increasing density and frequency
of conventional CPU architecture

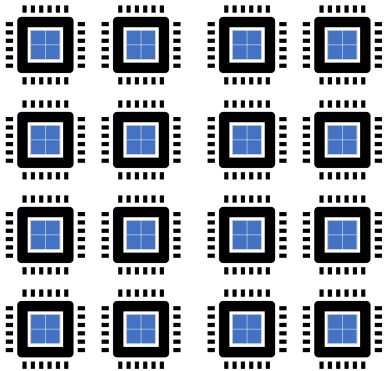
A new paradigm in parallel programming

2008

PETASCALE

Roadrunner supercomputer
Los Alamos National Laboratory (US)

10^{15} FLOP/s



Increasing density and frequency
of conventional CPU architecture

A new paradigm in parallel programming

2008

PETASCALE

Roadrunner supercomputer
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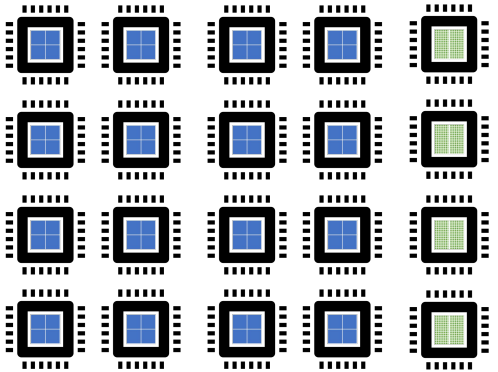
10^{15} FLOP/s

2022

EXASCALE

Frontier supercomputer
Oak Ridge National Laboratory (US)

10^{18} FLOP/s

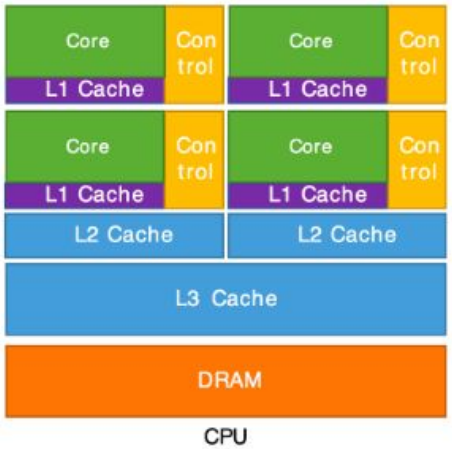


New hardware!
Graphic Processing Units (GPUs)

GPU vs CPU architecture

several strong cores

specialized processing



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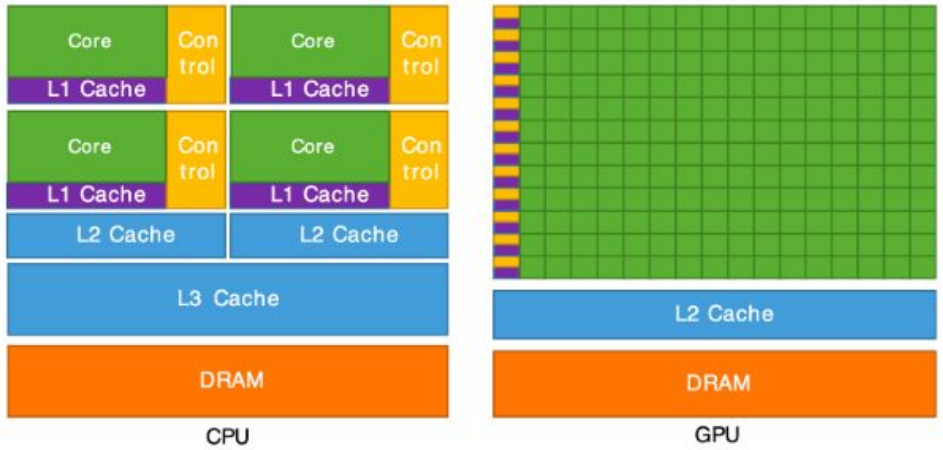


thousands of cores

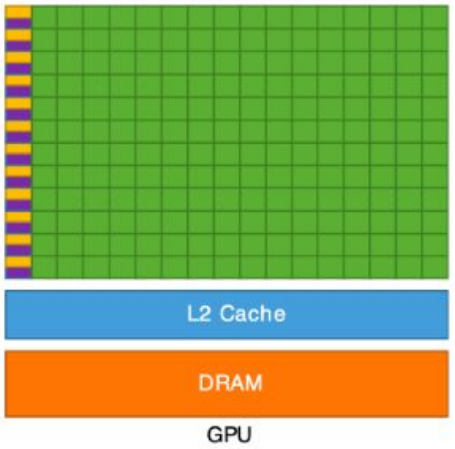
embarrassingly parallel processing

GPU vs CPU architecture

```
for(int i = 0; i < N; i++){
    a[i] = 2 * a[i];
```

a[0]	a[1]	a[2]	a[3]	...	a[N]
↑	↑	↑	↑	↑	↑
th0	th1	th2	th3	...	thN

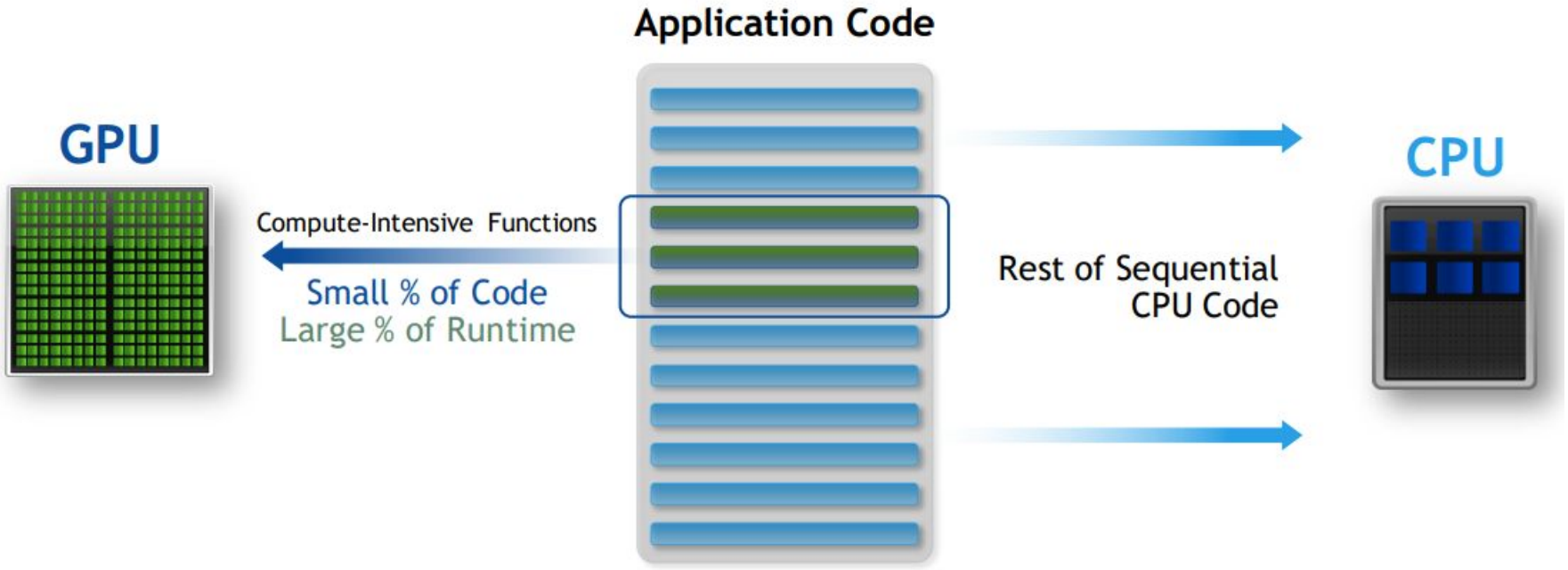
supports very large amount of parallelism



thousands of cores

embarrassingly parallel processing

Heterogeneous programming



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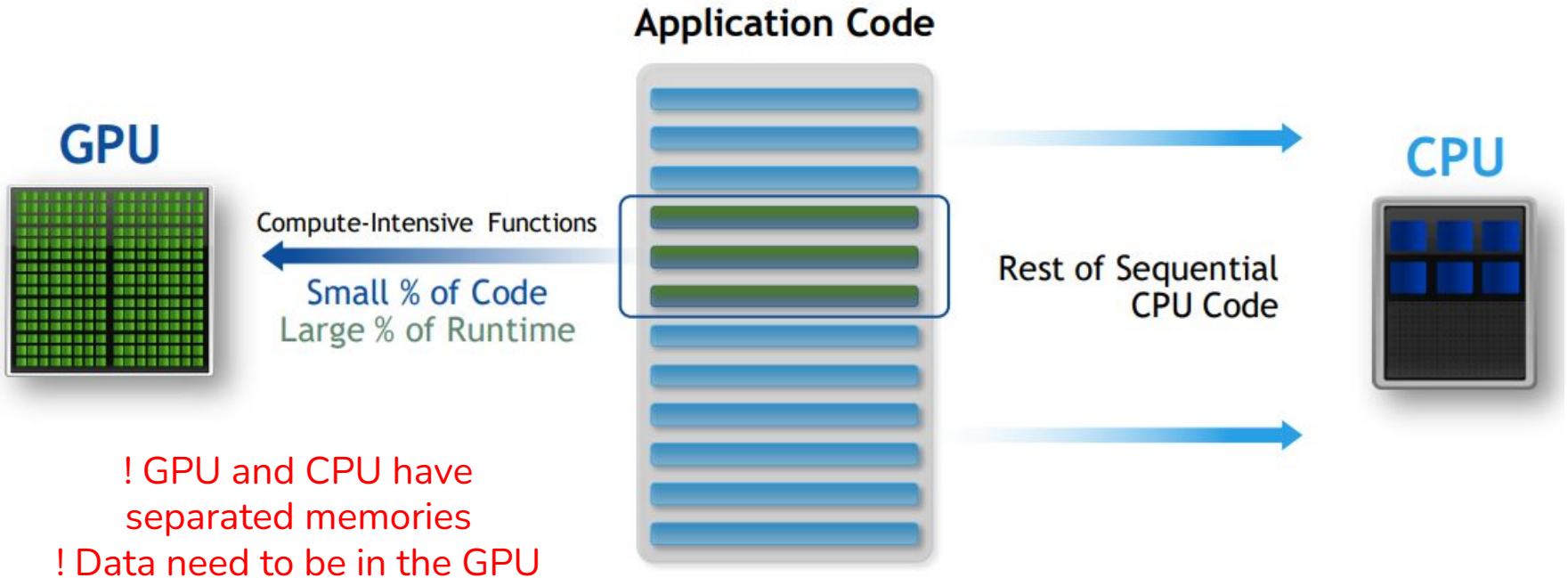
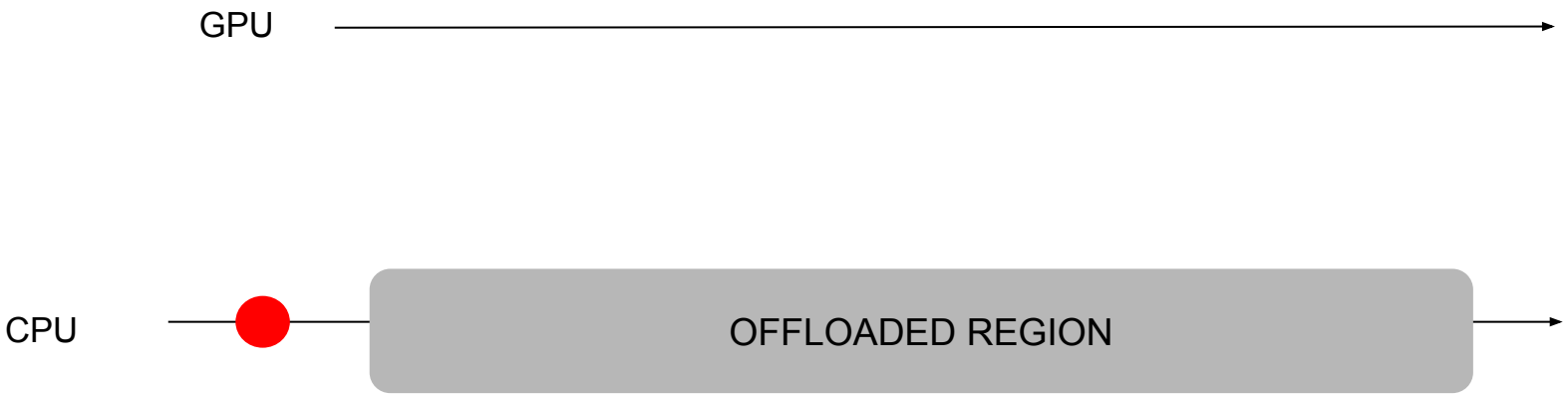


! GPU and CPU have separated memories

! Data need to be in the GPU memory

Traces in heterogeneous programs



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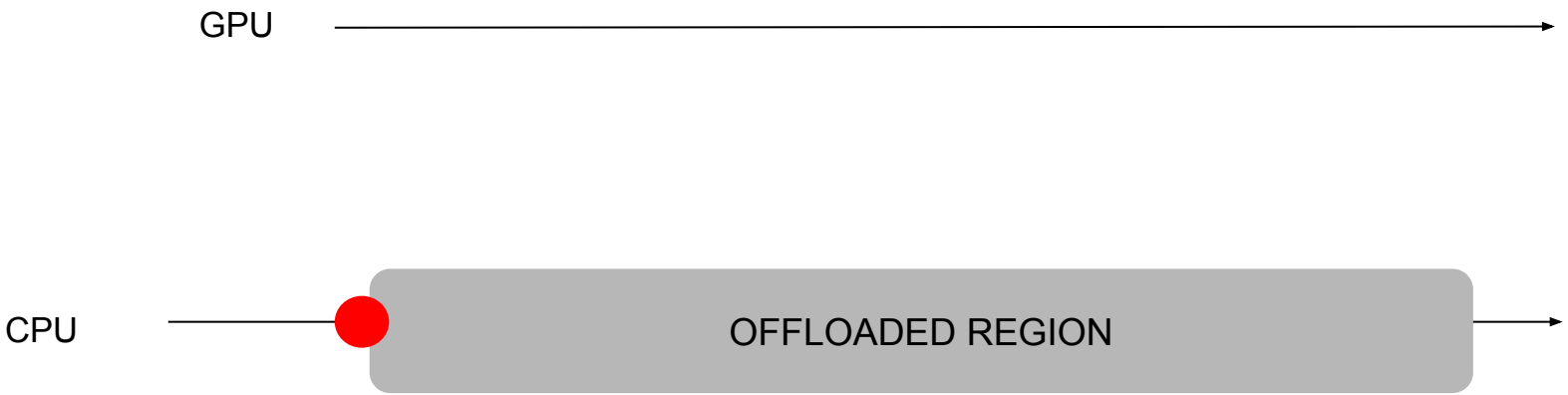

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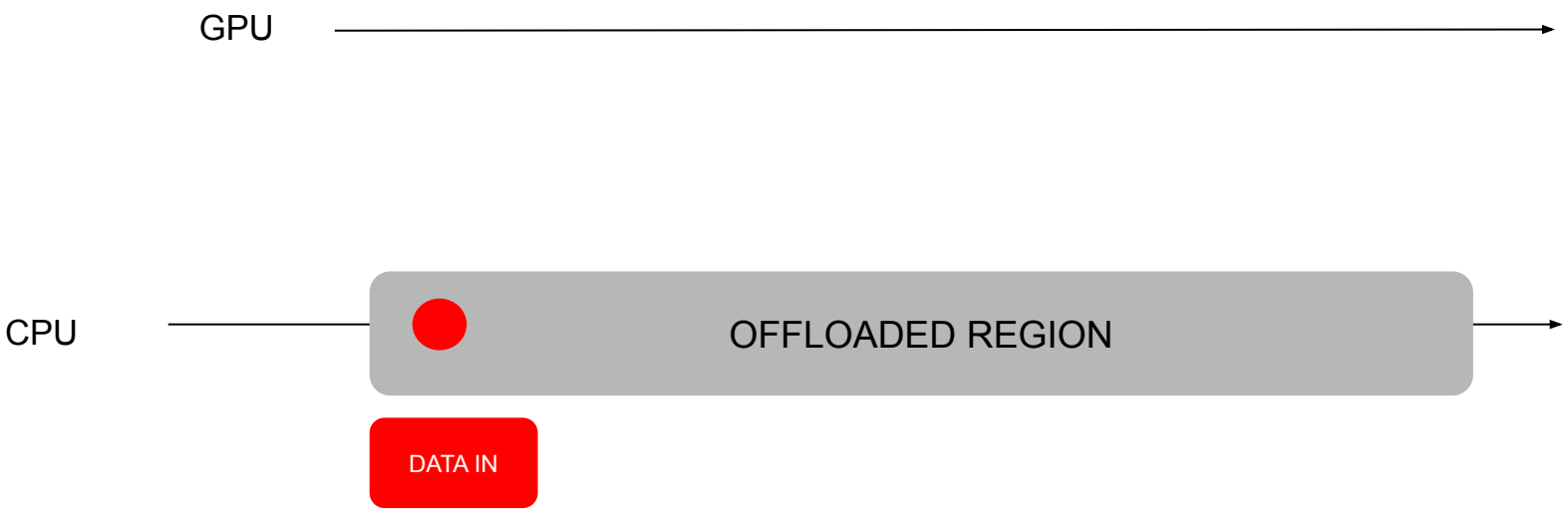

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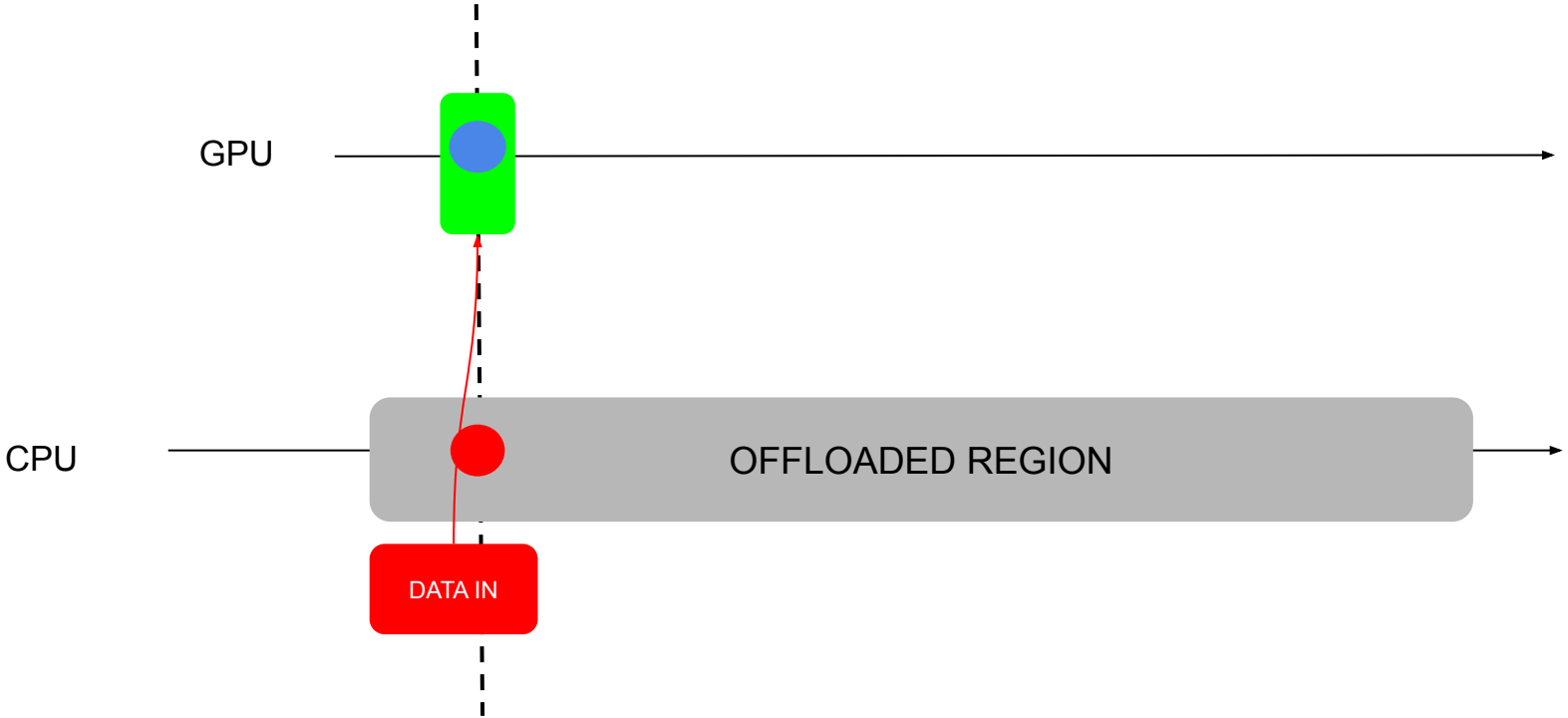

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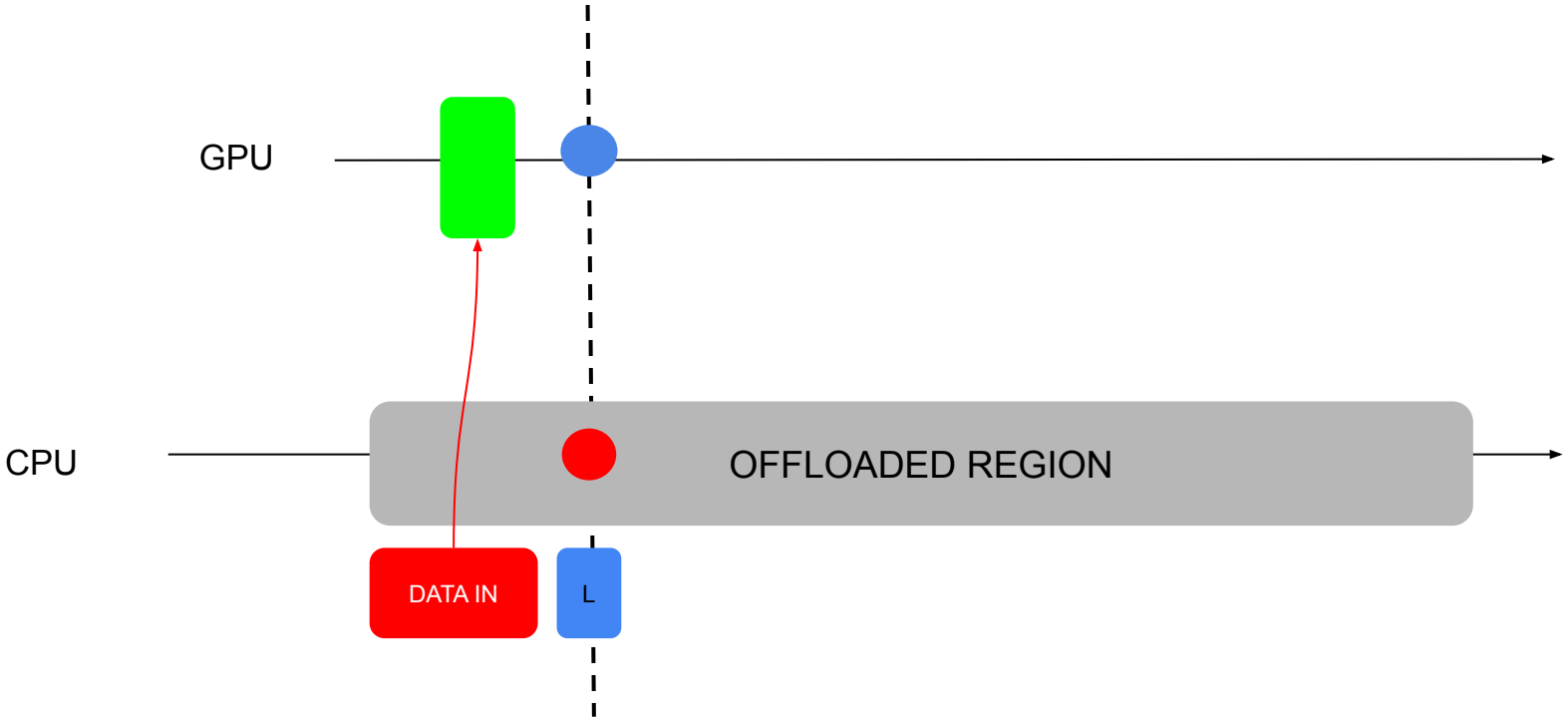

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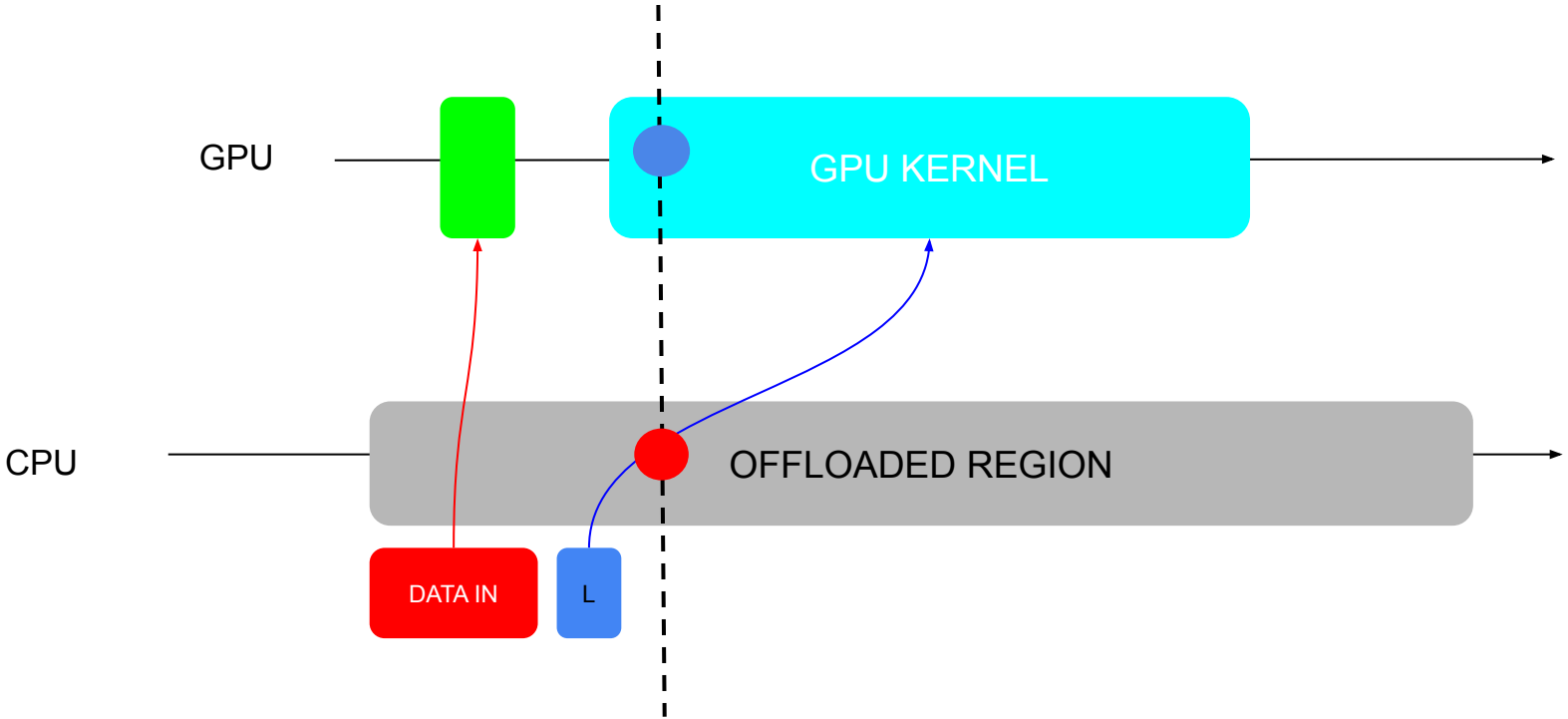

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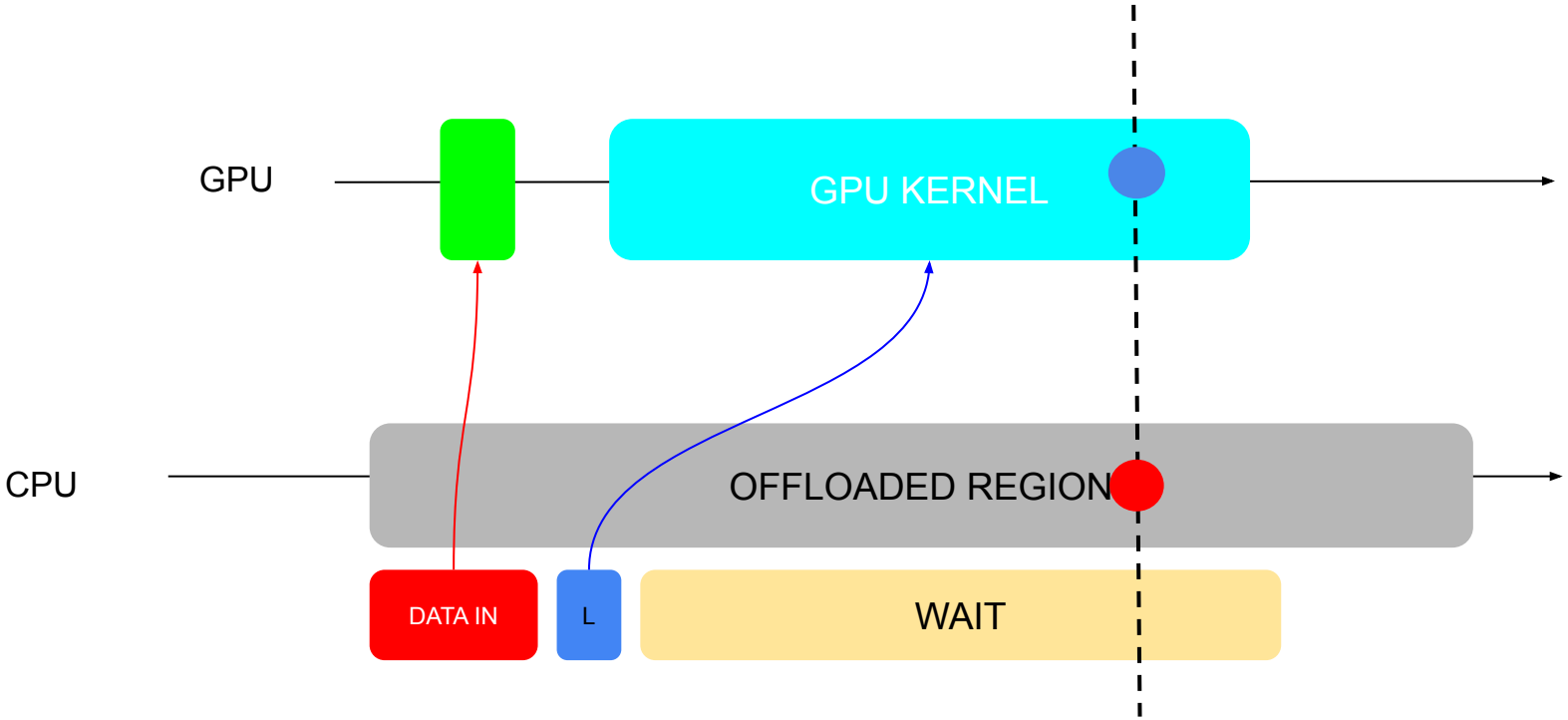

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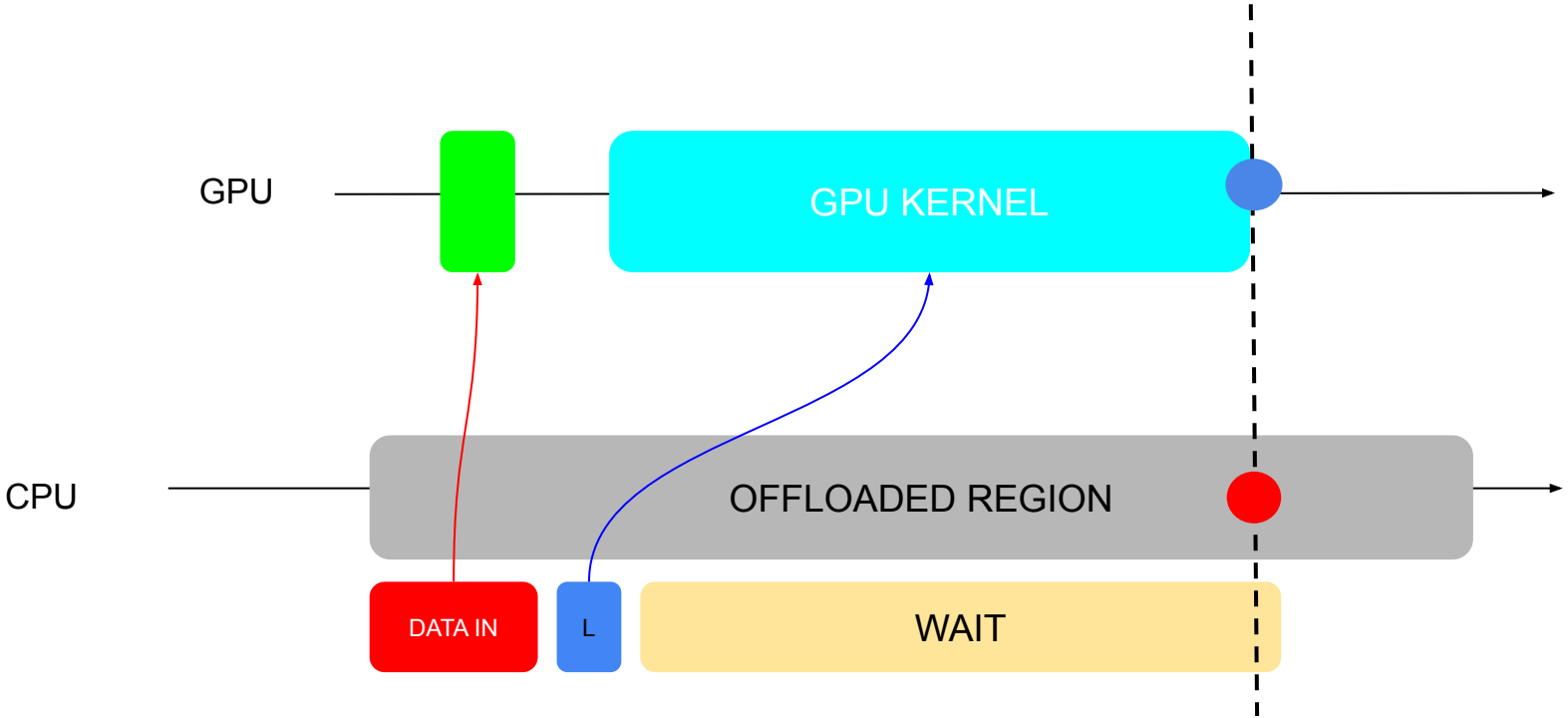

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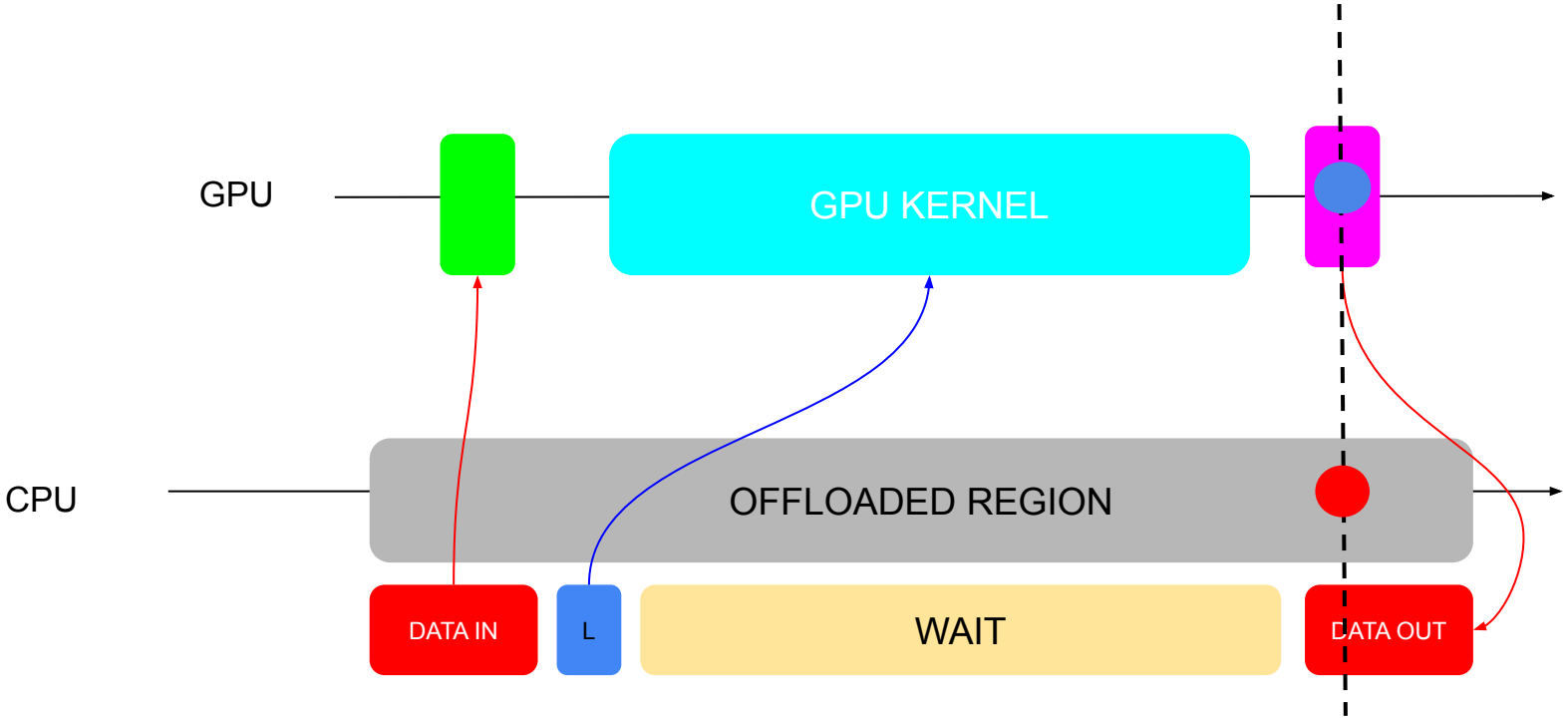

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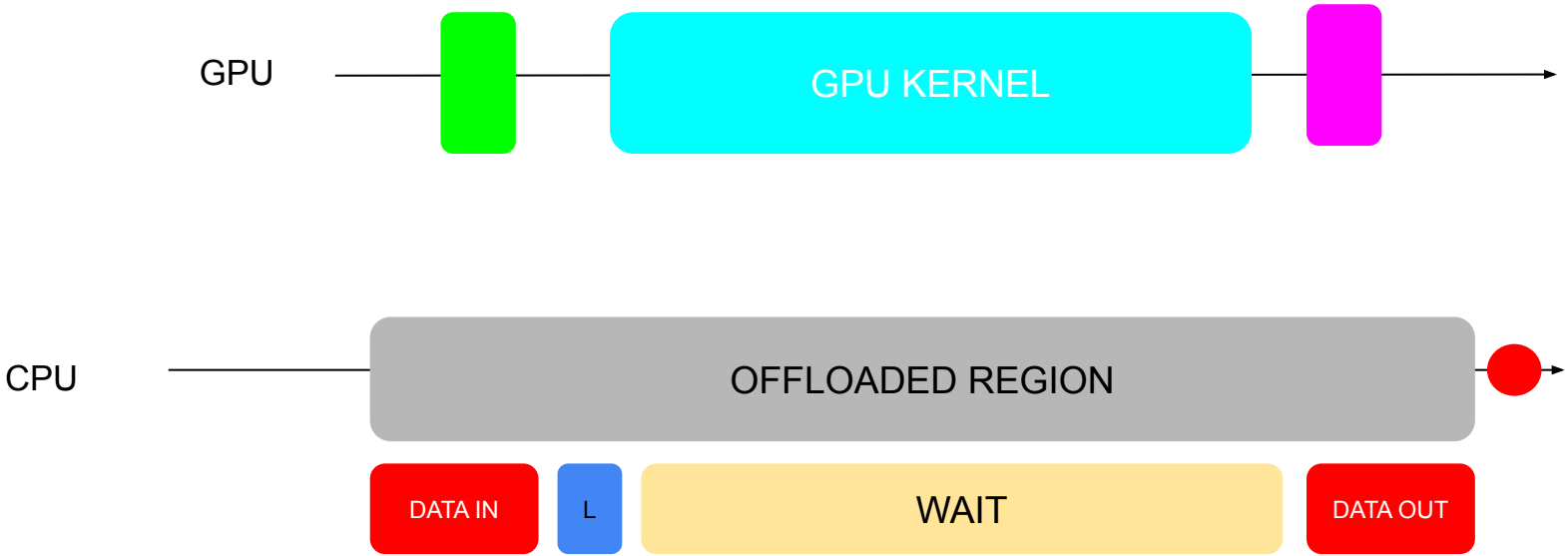

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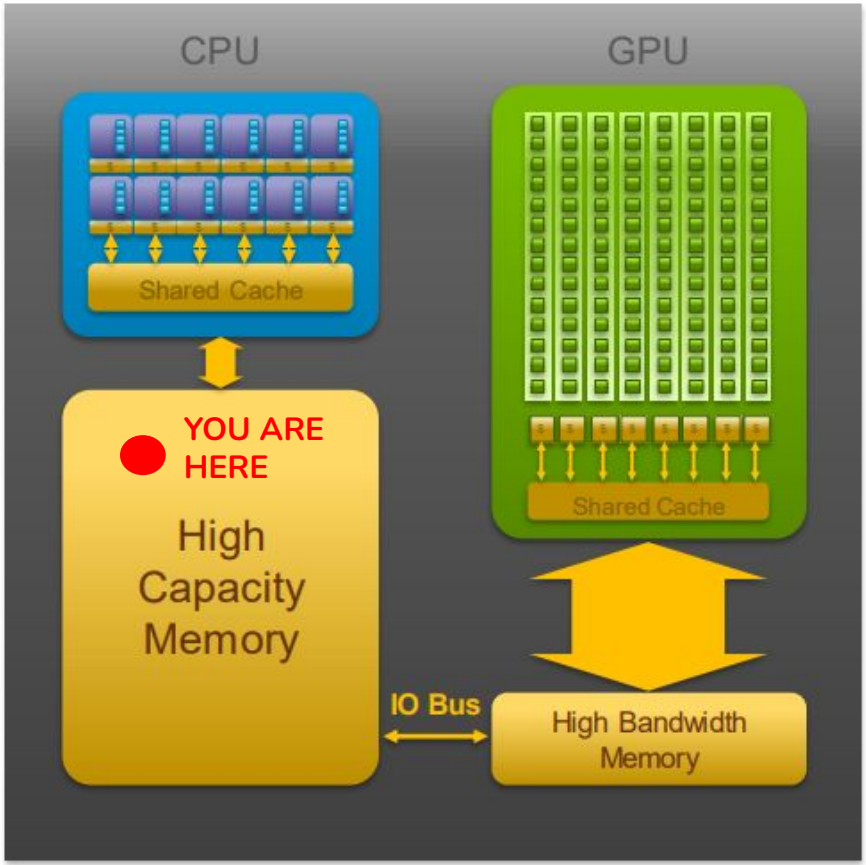

- The program starts on the CPU

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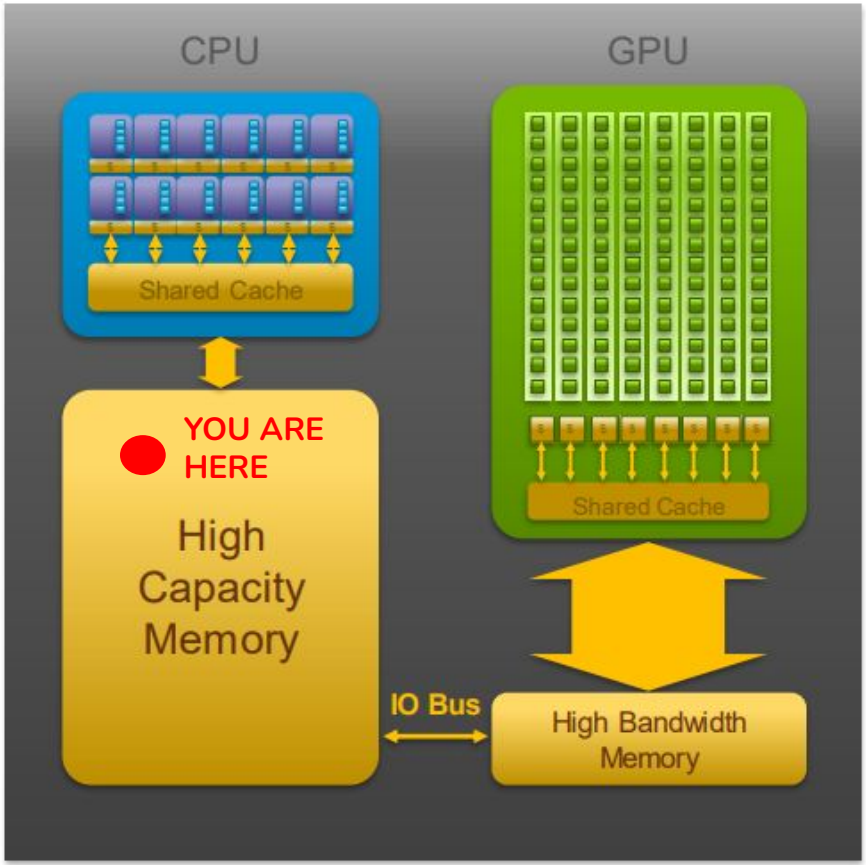

- The program starts on the CPU
- GPUs and CPUs have separated memories

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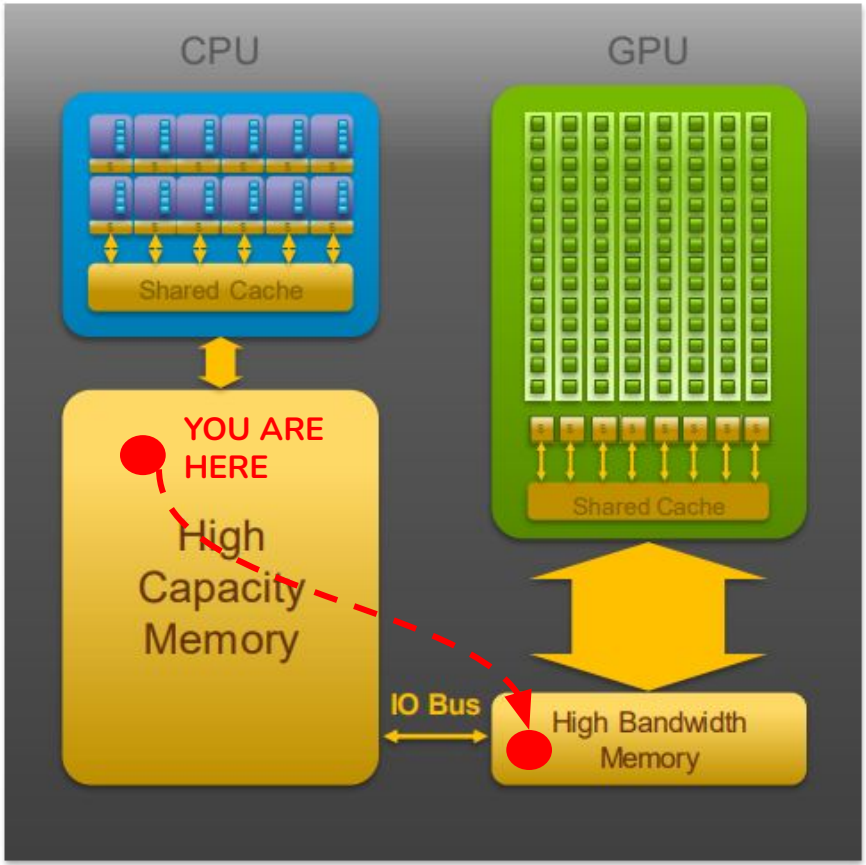

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- GPUs need data in their own memory

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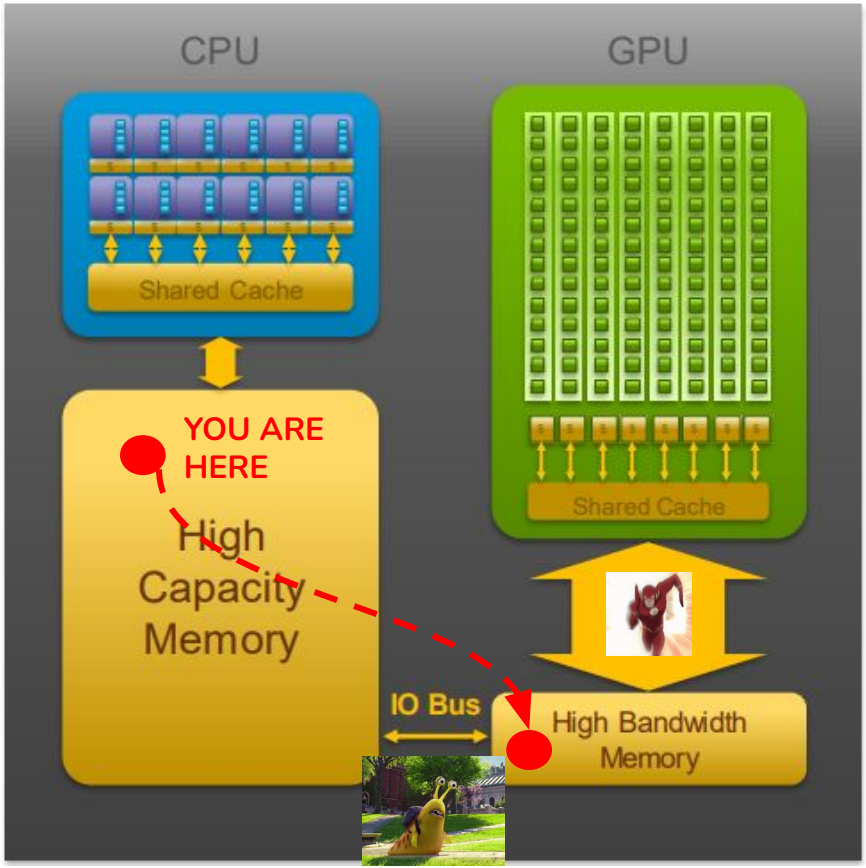

- The program starts on the CPU
- GPUs and CPUs have separated memories
- GPUs need data in their own memory
- IO bus is slow compared to GPU BW

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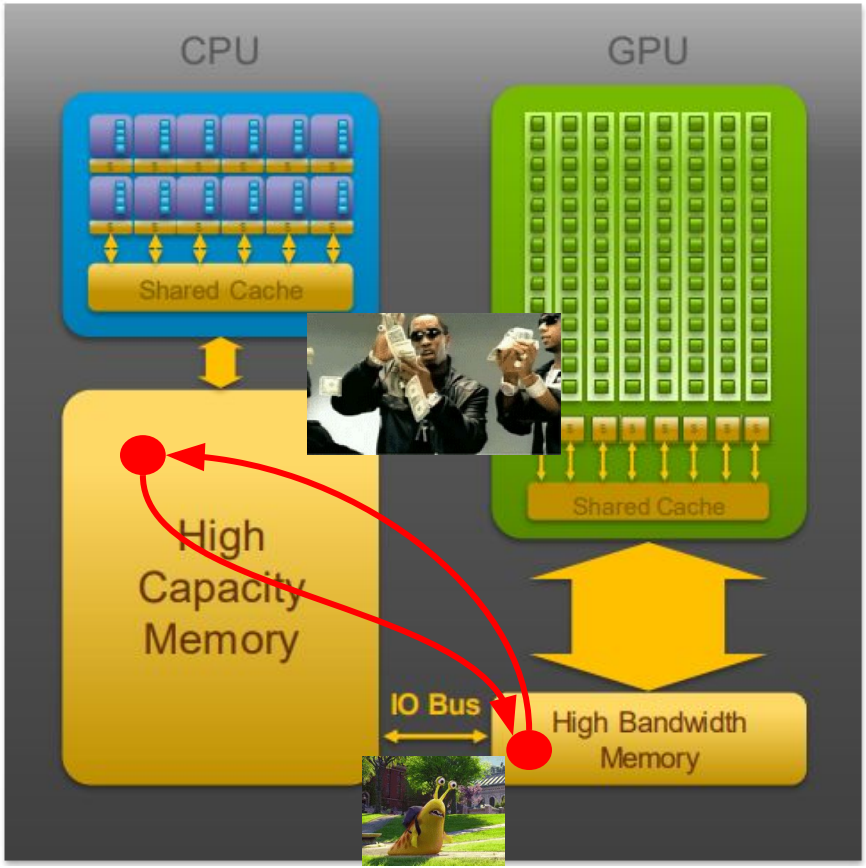

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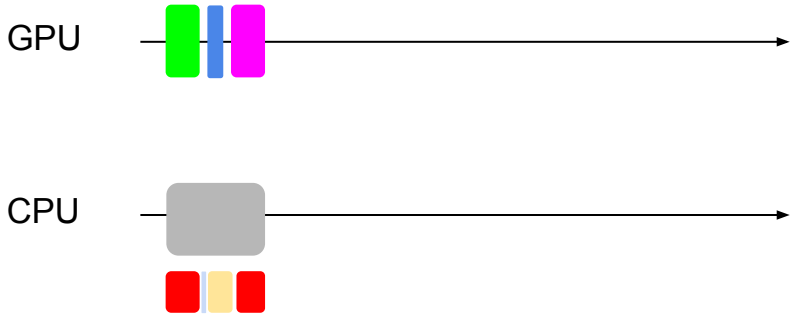
MOVING DATA IS EXPENSIVE



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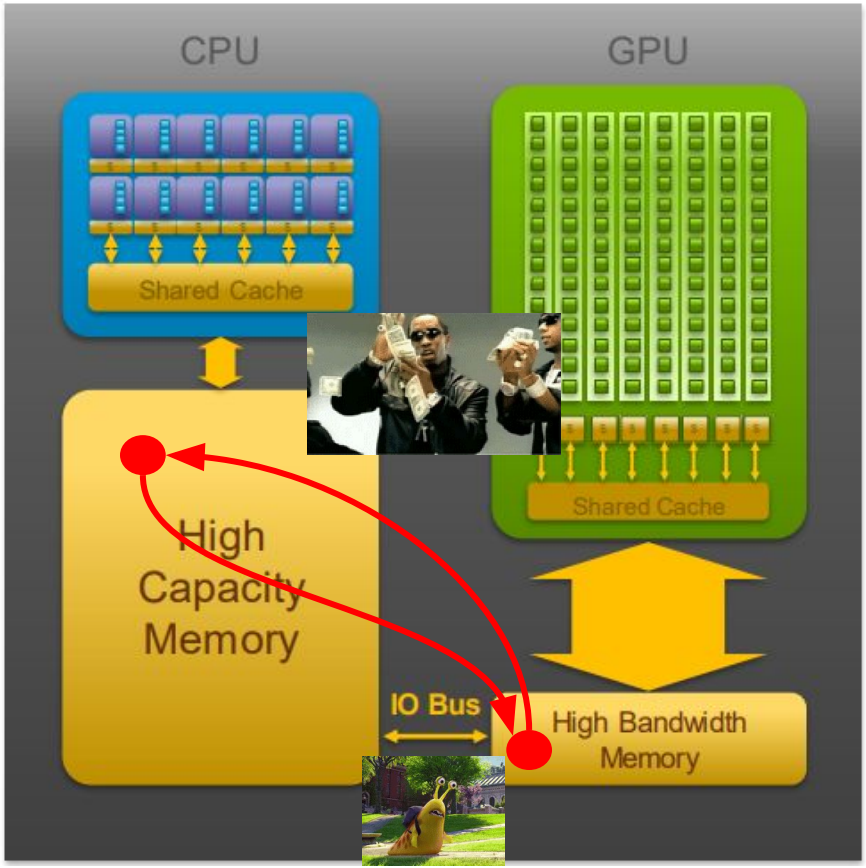

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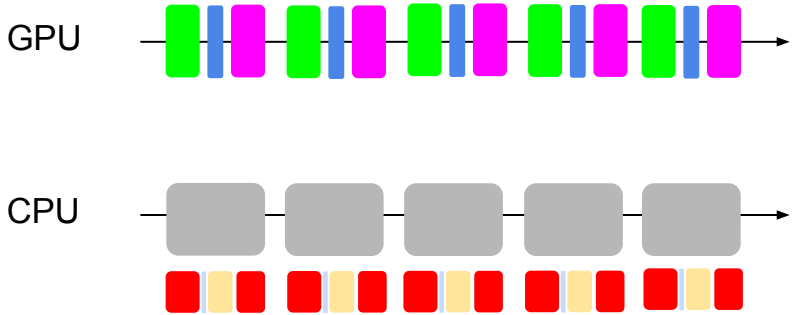

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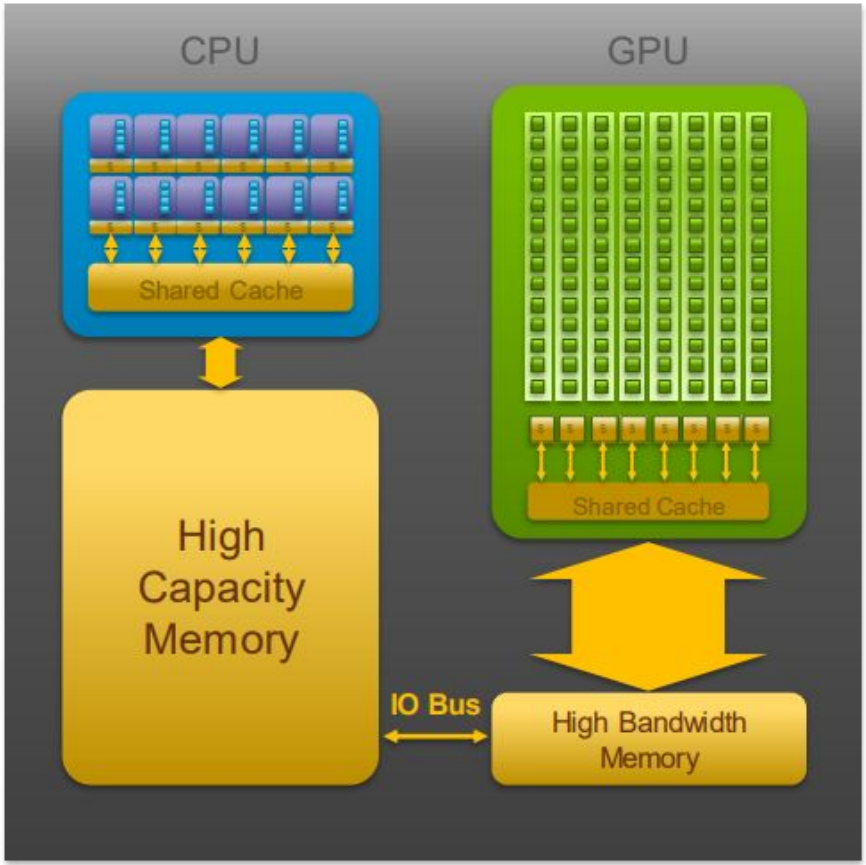

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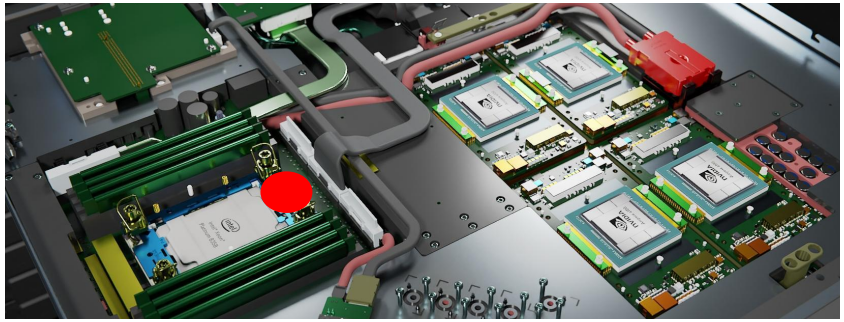
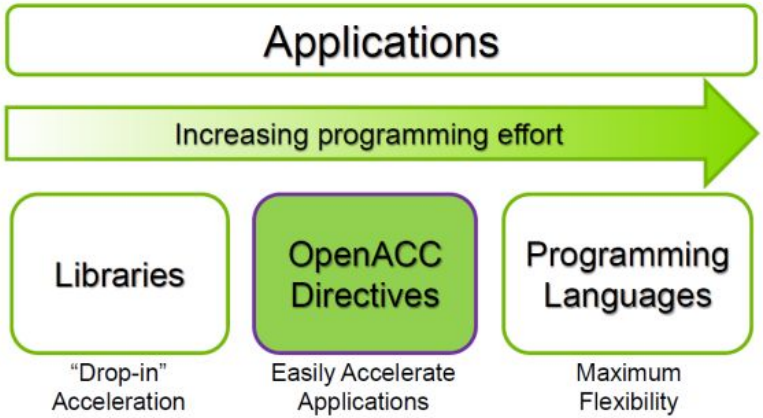
MOVING DATA IS EXPENSIVE

IMPROVE DATA LOCALITY

Heterogeneous programming





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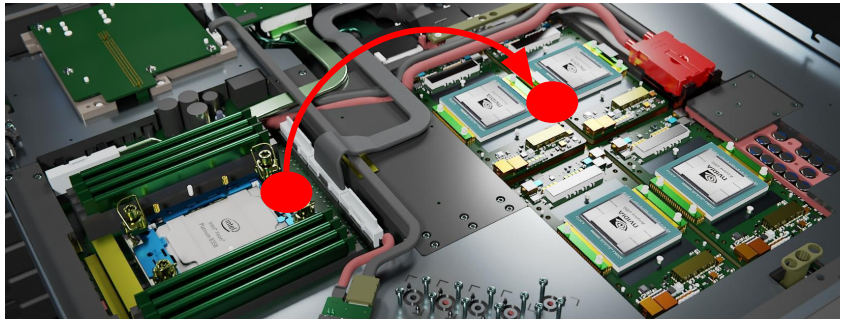
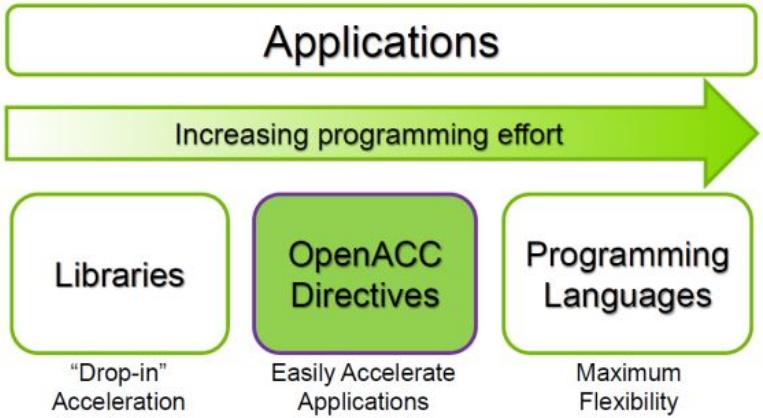


- The program starts on the CPU
- Many ways to offload kernels to GPUs



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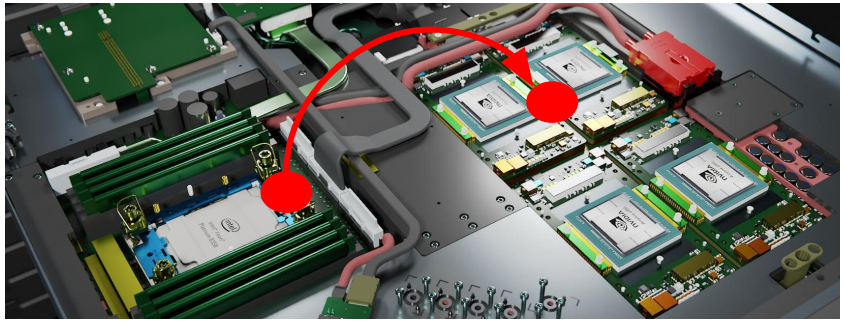

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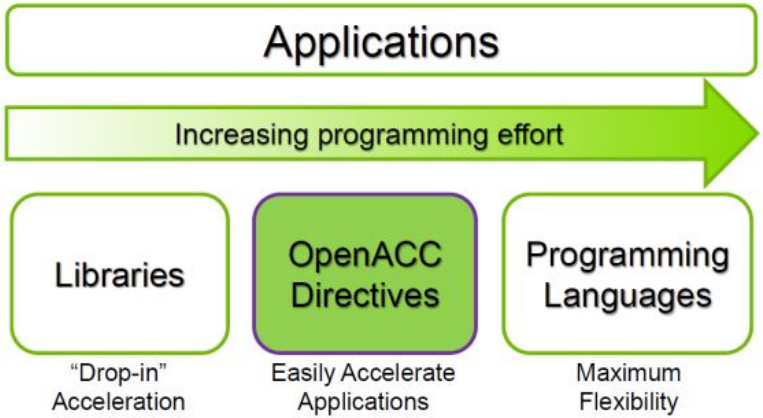

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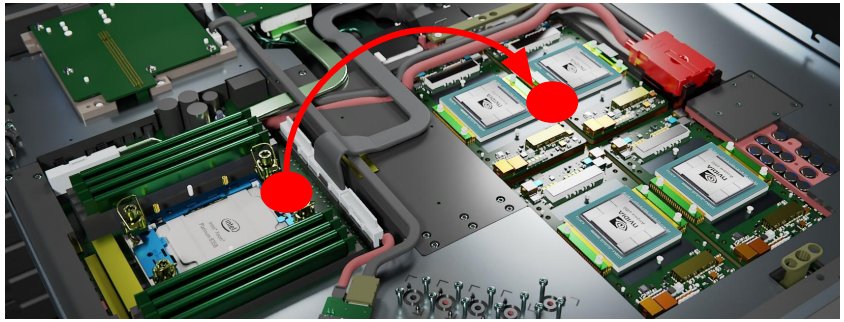

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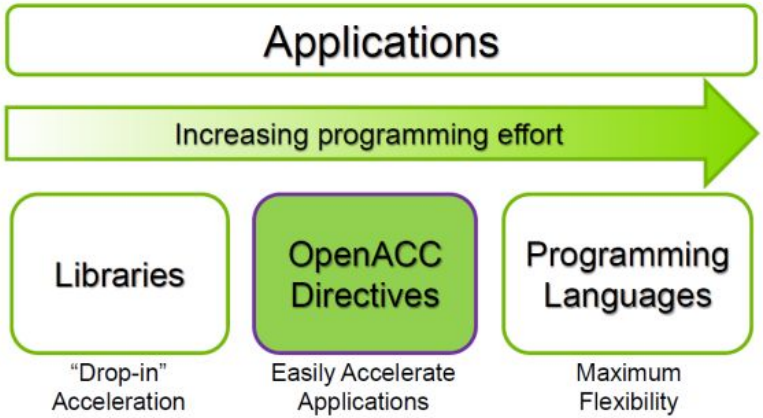

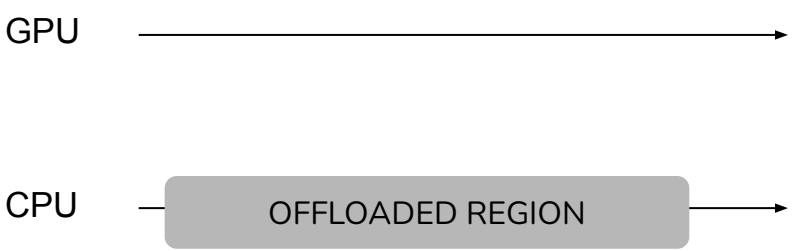

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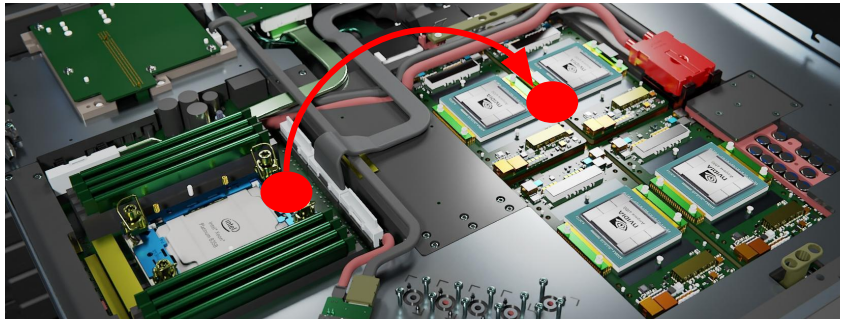

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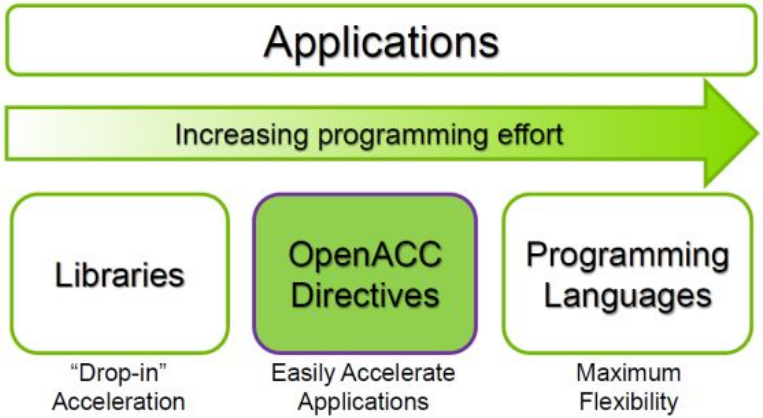

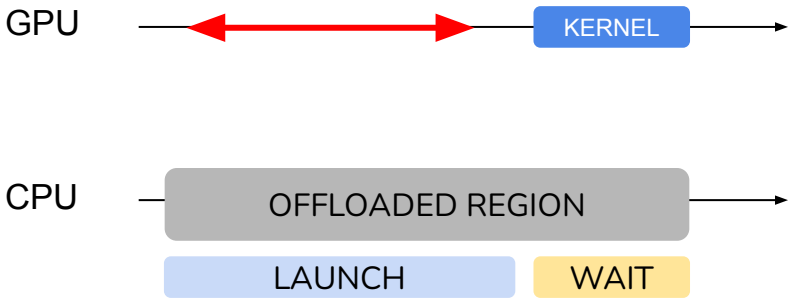

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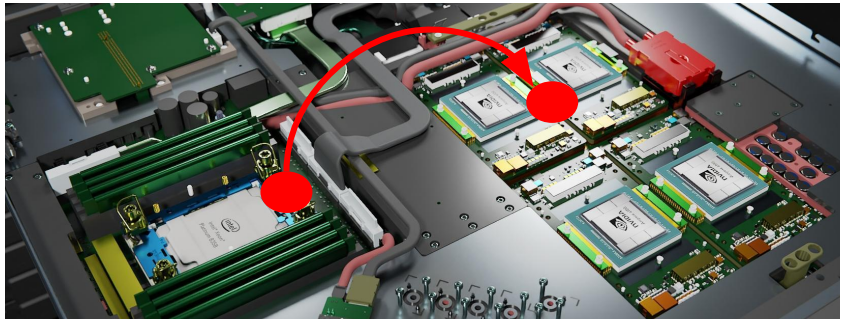

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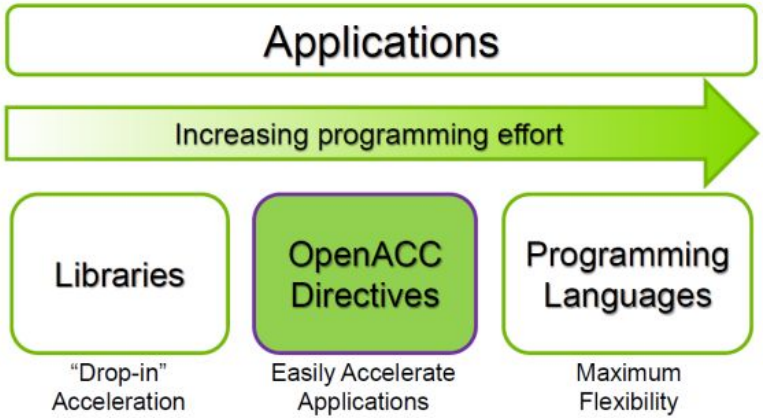

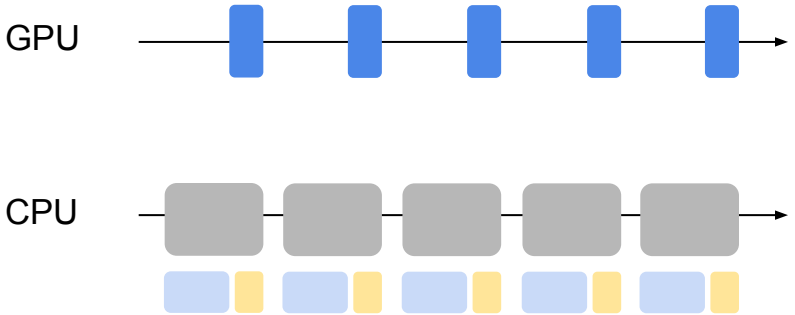

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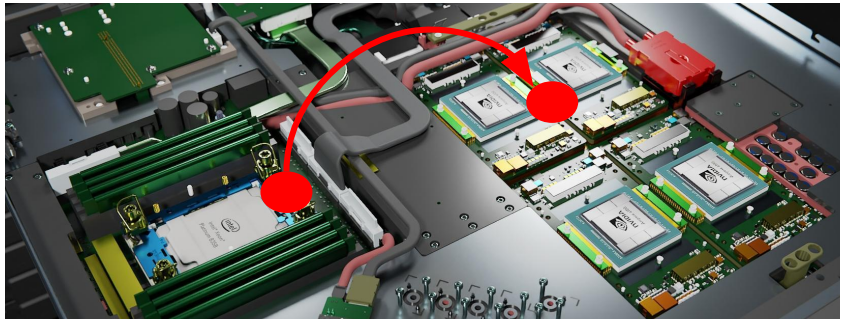

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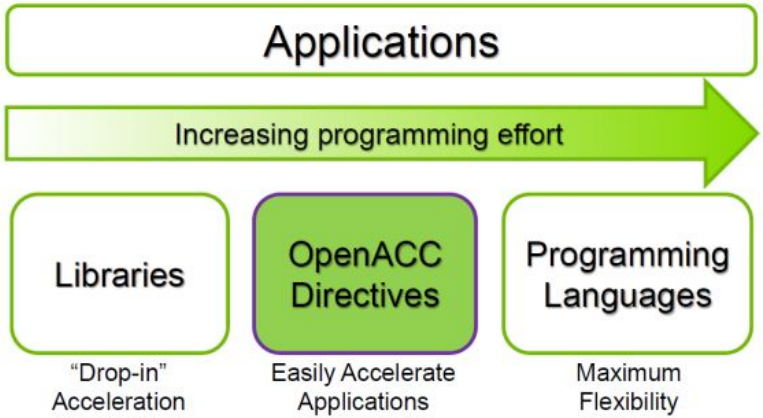
KERNEL LAUNCH ADDS OVERHEAD

EXPOSE AS MUCH PARALLELISM AS POSSIBLE



NSight Systems
Tracing GPUs and CPUs

l.bellentani@cineca.it
Tutorial on Profiling @ MHPC - ICTP

NVIDIA profiling and tracing tools

MEASUREMENT

SAMPLING	GPU	TRACES
INSTRUMENTATION	CPU	SUMMARIES

- Instrument CUDA APIs
- Instrument OpenACC regions
- Instrument MPI, OpenMP for the CPU
- Instrument GPU kernels, GPU metrics
- Sample the CPU (usr routines, libraries)
- Network metrics (H2D, D2D, NIC metrics)

NVIDIA profiling and tracing tools

```
nsys [command_switch][optional command_switch_options][application] [optional application_options]
```

Command switches

- **profile**	All-in-one , needed for concurrent profiling sessions
- start - launch - cancel - shutdown - stop	Interactive mode
- export - stats - analyze	Postprocessing to export / textual summaries

Command switch options

- **--trace=**[nvtx,cuda,osrt],mpi,openmp,openacc,cublas,cusolver,...	Events to trace
- --cuda-memory-usage	Collect GPU memory usage
- --mpi-impl	Select mpi implementation (openmpi, mpich)
- --nic-metrics	Network bandwidth

NVIDIA profiling and tracing tools

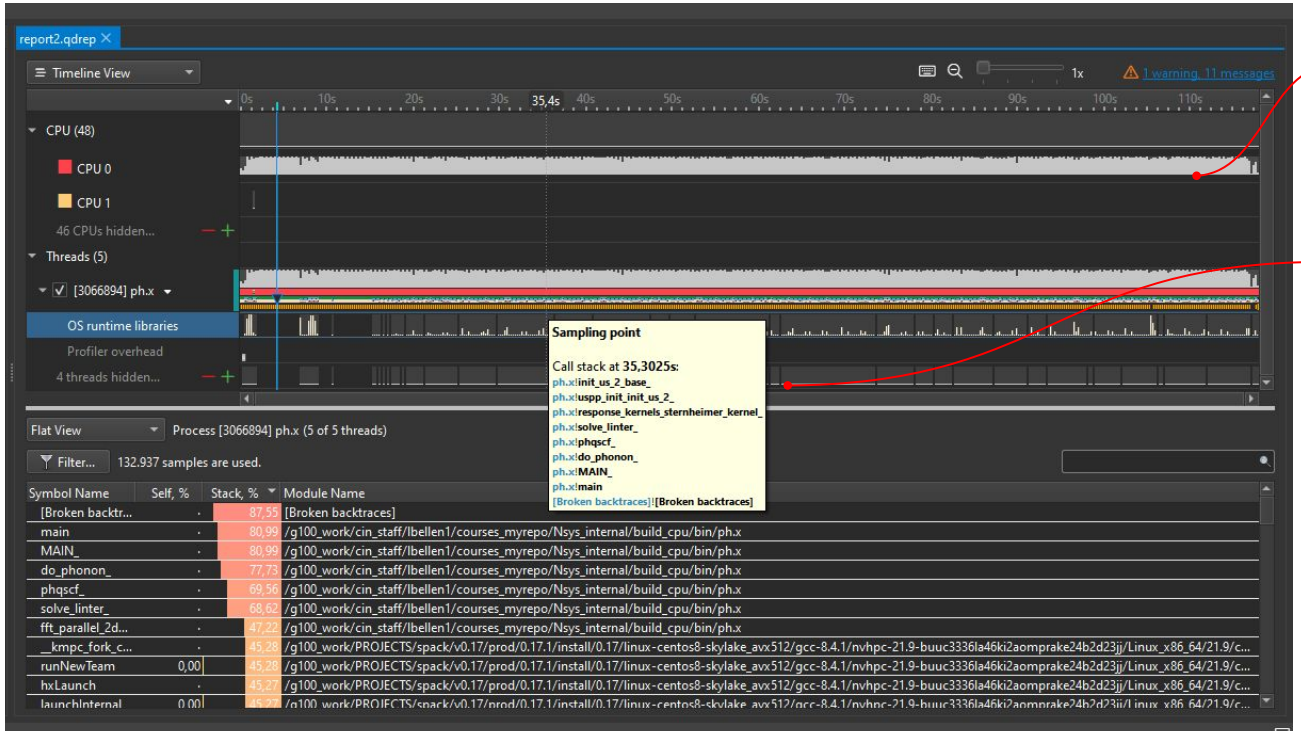
@CINECA cluster : to avoid /tmp/ saturation, do not forget wrapping nsys command with

```
rm -rf /tmp/nvidia
ln -s $TMPDIR /tmp/nvidia
nsys <...>
rm -rf /tmp/nvidia
```

https://wiki.u-gov.it/confluence/display/SCAIUS/UG3.2%3A+MARCONI100+UserGuide#UG3.2:MARCONI100UserGuide-GPUprofilers(NvidiaNsightSystem)

FLAT PROFILES (sampling)

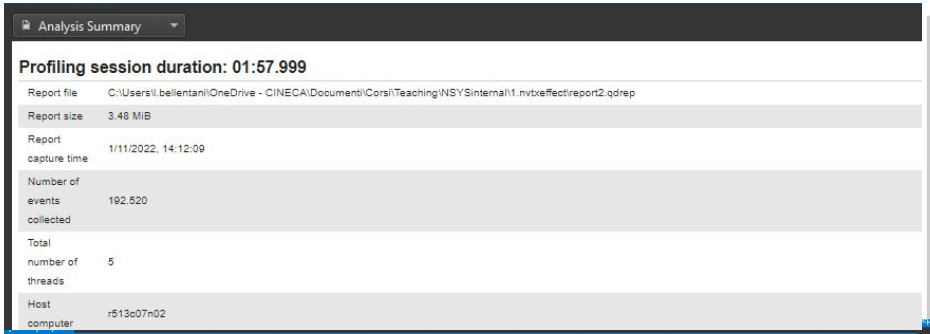
```
nsys profile --sample=cpu --backtrace=fp
```

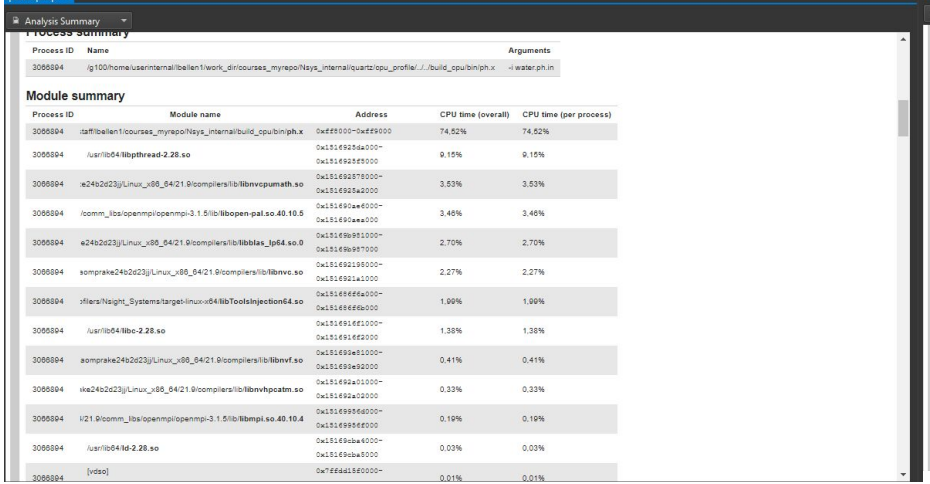


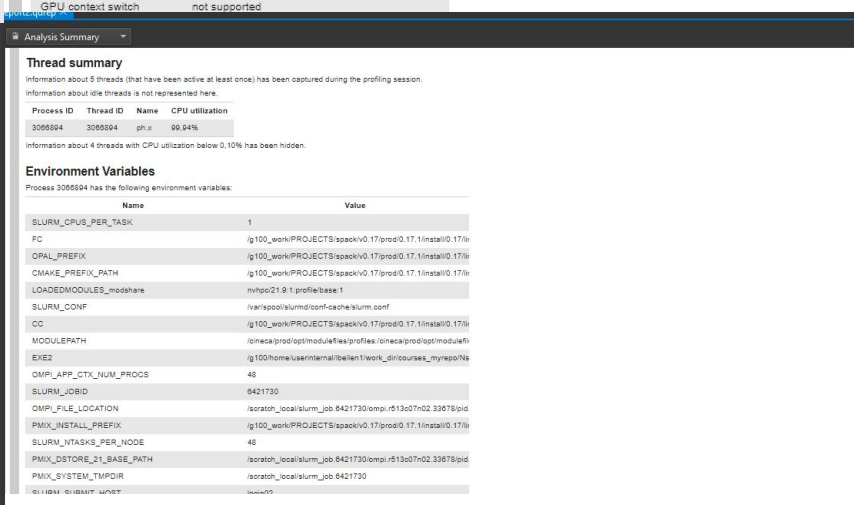
CPU bindling

Debug symbols are needed for backtraces!

Analysis summaries

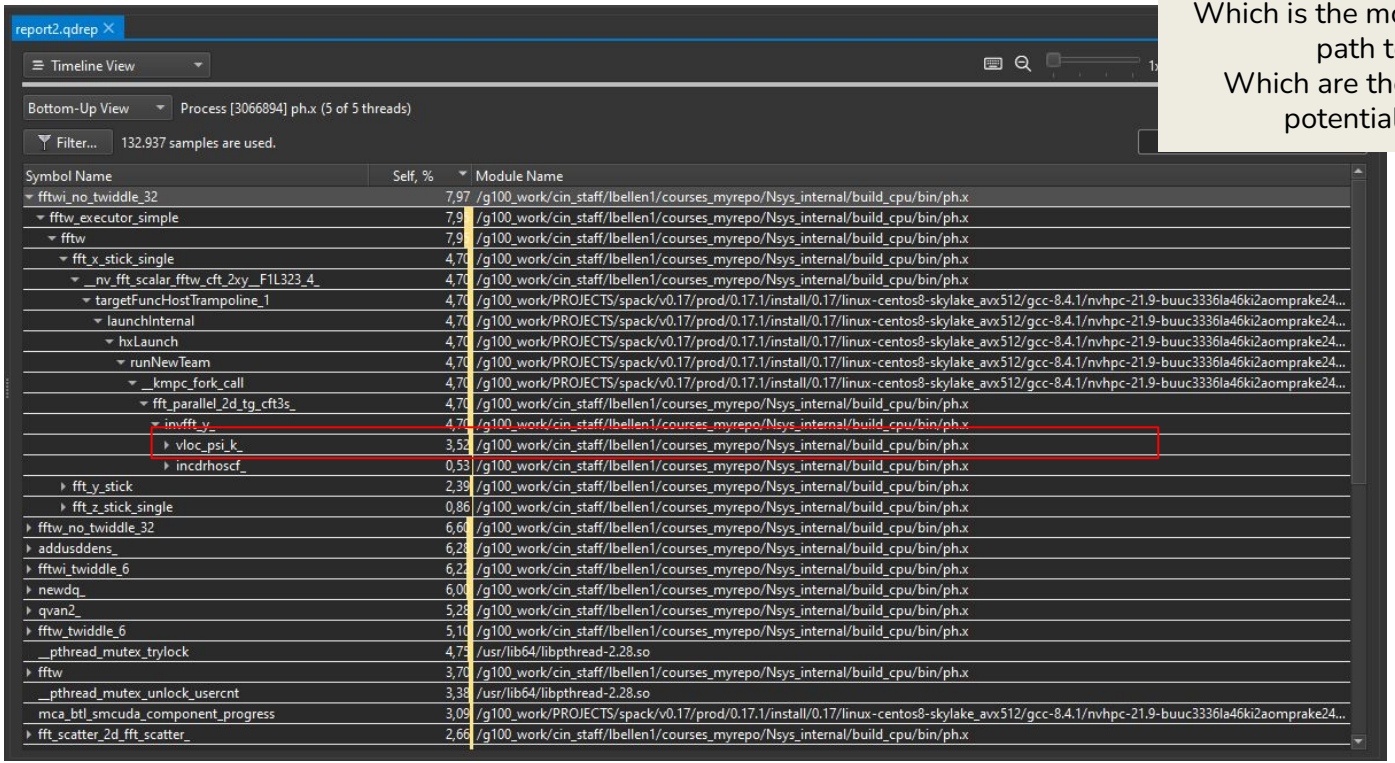






Top-down/bottom-up profiles

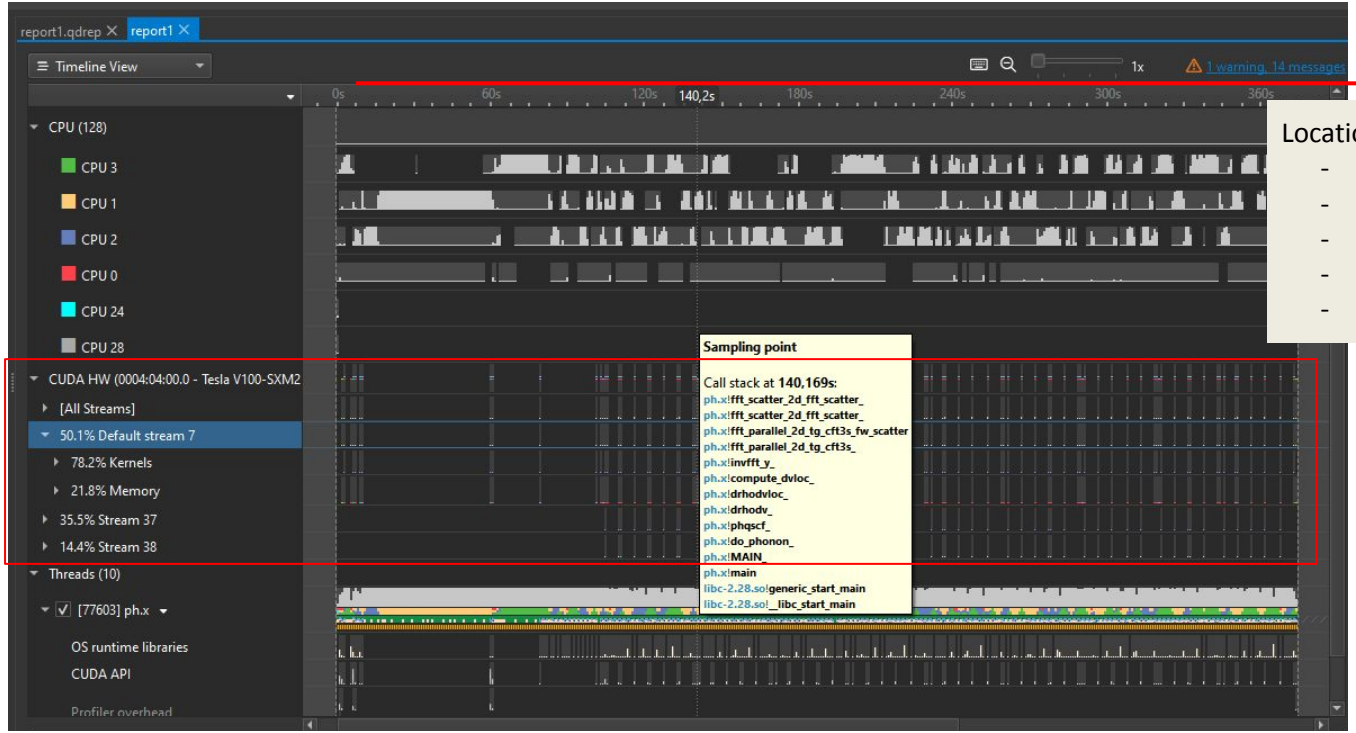
Identify the most time consuming calling path



Which is the most time consuming path to offload?
Which are the parent routines potentially involved?

Timeline view

```
nsys profile  --trace=osrt,cuda --sample=cpu --backtrace=fp
```

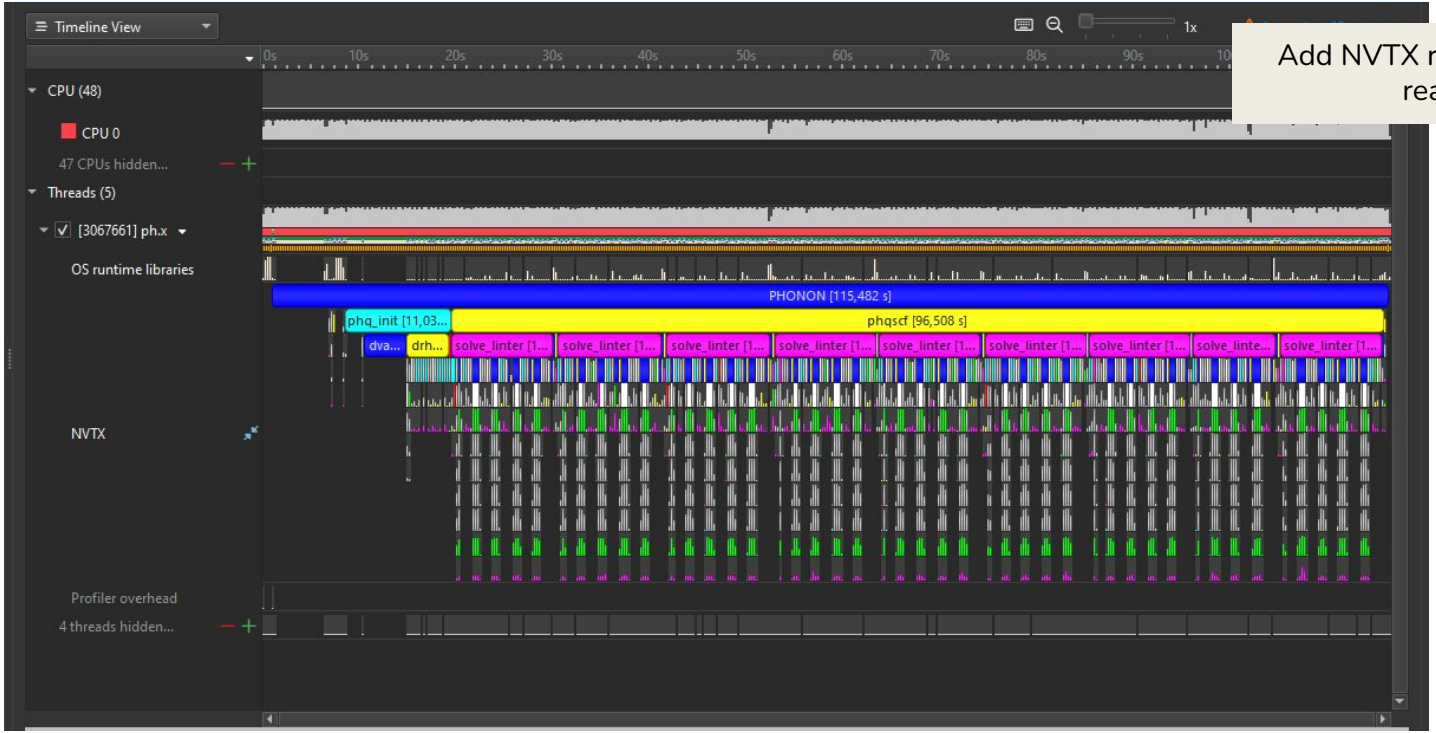


Location can be

- architecture (CPU/PU)
- stream
- thread
- library (CUDA, CUPTI)
- runtime (OpenACC)

NVTX ranges

```
nsys profile  --trace=osrt,nvtx --sample=cpu --backtrace=fp
```



Add NVTX ranges to increase readability

NVTX ranges

Source code is not automatically instrumented. NVTX library (`nvToolsExt.h`) can be used to enhance trace readability:

- C-based API to annotate events and code ranges, to be visualized in the Nsight System timeline
- Limited overhead when the tool is not attached to the application

Functionalities

- **NVTX Markers** → annotate events occurring at a specific time
- **NVTX Ranges** → annotate timespan of code regions

Events

- associated to message (ASCII, Unicode) → **A, W** variant of function calls
- associated to structure with attributes → **Ex** variant of function calls

```
//Set to default

nvtxEventAttributes_t eventAttrib = {0};

//Declare version and size

eventAttrib.version = NVTX_VERSION;
eventAttrib.size = NVTX_EVENT_ATTRIB_STRUCT_SIZE;

// Message type and message
// // ASCII

eventAttrib.messageType = NVTX_MESSAGE_TYPE_ASCII;
eventAttrib.message.ascii = __FUNCTION__ ":ascii";
// //UNICODE

eventAttrib2.messageType = NVTX_MESSAGE_TYPE_UNICODE;
eventAttrib2.message.unicode = __FUNCTIONW__ L
":unicode \u2603 snowman";

// Color type and color

eventAttrib.colorType = NVTX_COLOR_ARGB;
eventAttrib.color = COLOR_YELLOW;
```

NVTX ranges

Source code is not automatically instrumented. NVTX library (`nvToolsExt.h`) can be used to enhance trace readability:

- C-based API to annotate events and code ranges, to be visualized in the Nsight System timeline
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Functionalities

- **NVTX Markers** → annotate events occurring at a specific time
- **NVTX ranges** → annotate timespan of code regions

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- associated to message (ASCII, Unicode) → **A, W** variant of function calls
- associated to structure with attributes → **Ex** variant of function calls

```
//Set to default

nvtxEventAttributes_t eventAttrib = {0};

//Declare version and size

eventAttrib.version = NVTX_VERSION;
eventAttrib.size = NVTX_EVENT_ATTRIB_STRUCT_SIZE;

// Message type and message
// // ASCII

eventAttrib.messageType = NVTX_MESSAGE_TYPE_ASCII;
eventAttrib.message.ascii = __FUNCTION__ ":ascii";
// //UNICODE

eventAttrib2.messageType = NVTX_MESSAGE_TYPE_UNICODE;
eventAttrib2.message.unicode = __FUNCTIONW__ L
":unicode \u2603 snowman";

// Color type and color

eventAttrib.colorType = NVTX_COLOR_ARGB;
eventAttrib.color = COLOR_YELLOW;
```

NVTX ranges

Markers (events at a specific time)

```
nvtxMarkA(__FUNCTION__ ":nvtxMarkA");
nvtxMarkW(__FUNCTIONW__ L":nvtxMarkW");
nvtxMarkEx(&eventAttrib);
```

Ranges (nested time ranges occurring on a CPU thread)

```
start:  nvtxRangePushEx
        nvtxRangePushA
        nvtxRangePushW
end :  nvtxRangePop
```

```
// for message-only events

nvtxRangePushA(__FUNCTION__ ":nvtxRangePushA");
[... code here ...]
nvtxRangePop();

nvtxRangePushW(__FUNCTIONW__
L":nvtxRangePushW");
[... code here ...]
nvtxRangePop();

// for structured events

nvtxRangePushEx(&eventAttrib);
[... code here ...]
nvtxRangePop();
```

NVTX ranges

Markers (events at a specific time)

```
nvtxMarkA(__FUNCTION__ ":nvtxMarkA");
nvtxMarkW(__FUNCTIONW__ L":nvtxMarkW");
nvtxMarkEx(&eventAttrib);
```

Ranges (nested time ranges occurring on a CPU thread)

start: `nvtxRangePushEx`
`nvtxRangePushA`
`nvtxRangePushW`

end : `nvtxRangePop`

```
// for message-only events

nvtxRangePushA(__FUNCTION__ ":nvtxRangePushA");
[... code here ...]
nvtxRangePop();

nvtxRangePushW(__FUNCTIONW__
L":nvtxRangePushW");
[... code here ...]
nvtxRangePop();

// for structured events

nvtxRangePushEx(&eventAttrib);
[... code here ...]
nvtxRangePop();
```

NVTX ranges

Fortran module

Wrapper to NVTX APIs available at https://github.com/maxcuda/NVTX_example

```
subroutine nvtxStartRange(name,id)
  character(kind=c_char,len=*) :: name
  integer, optional:: id
  type(nvtxEventAttributes):: event
  character(kind=c_char,len=256) :: trimmed_name
  integer:: i

  trimmed_name=trim(name)//c_null_char

  ! move scalar trimmed_name into character array tempName
  do i=1,LEN(trim(name)) + 1
     tempName(i) = trimmed_name(i:i)
  enddo

  if ( .not. present(id)) then
    call nvtxRangePush(tempName)
  else
    event%color=col(mod(id,7)+1)
    event%message=c_loc(tempName)
    call nvtxRangePushEx(event)
  end if
end subroutine

subroutine nvtxEndRange
  call nvtxRangePop
end subroutine

end module nvtx
```

```
type, bind(C):: nvtxEventAttributes
  integer(C_INT16_T):: version=1
  integer(C_INT16_T):: size=48 !
  integer(C_INT):: category=0
  integer(C_INT):: colorType=1 ! NVTX_COLOR_ARGB = 1
  integer(C_INT):: color
  integer(C_INT):: payloadType=0 ! NVTX_PAYLOAD_UNKNOWN = 0
  integer(C_INT):: reserved0
  integer(C_INT64_T):: payload   ! union uint,int,double
  integer(C_INT):: messageType=1  ! NVTX_MESSAGE_TYPE_ASCII     = 1
  type(C_PTR):: message  ! ascii char
end type
```

```
interface nvtxRangePush
  ! push range with custom label and standard color
  subroutine nvtxRangePushA(name) bind(C, name='nvtxRangePushA')
  use iso_c_binding
  character(kind=C_CHAR) :: name(256)
  end subroutine

  ! push range with custom label and custom color
  subroutine nvtxRangePushEx(event) bind(C, name='nvtxRangePushEx')
  use iso_c_binding
  import:: nvtxEventAttributes
  type(nvtxEventAttributes):: event
  end subroutine
end interface

interface nvtxRangePop
  subroutine nvtxRangePop() bind(C, name='nvtxRangePop')
  end subroutine
end interface
```

Defines a derived type for the event

Fills color and message attribute according to the presence or not of the optional ID parameter

Resolves the calling routine in *Ex or *A API according to input

Summaries

nsys stats report.nsys-rep

Different kind of metrics can be summarized: nvtxsum, cudaapisum, gpukernsum, gpumemtimesum, etc.

```
nsys stats -r openaccsum report_acc_data1.nsys-rep
Generating SQLite file report_acc_data1.sqlite from report_acc_data1.nsys-rep
Exporting 63118 events: [==================================================100%]
Processing [report_acc_data1.sqlite] with
[/leonardo/prod/spack/03/install/0.19/linux-rhel8-icelake/gcc-8.5.0/nvhpc-23.1-x5lw6edfmfuot2ipna3wseallzl4oolm/Linux_x86_64/23.1/profilers/Nsight_Systems/host-linux-x64/reports/openaccsum.py]...

** OpenACC Summary (openaccsum):

Time(%)  Total Time (ns)  Num Calls    Avg (ns)      Med (ns)     Min (ns)    Max (ns)    StdDev (ns)               Name
-------  ---------------  ---------  ------------  ------------  ----------  -----------  ------------  ------------------------------
   27.9    2,422,224,252         50  48,444,485.0  45,729,730.5  45,576,626  176,454,147  18,476,396.7  Exit Data@jacobi.f90:14
   26.4    2,292,084,948         50  45,841,699.0  45,729,495.0  45,514,774   47,135,248     366,299.5  Exit Data@cfd.f90:144
   20.5    1,779,791,765         50  35,595,835.3  35,474,408.0  35,253,494   36,959,563     390,115.3  Enter Data@cfd.f90:144
   19.8    1,719,850,039         50  34,397,000.8  33,854,316.0  33,666,671   55,305,149   3,046,996.4  Enter Data@jacobi.f90:14
    1.4      123,216,371         50   2,464,327.4   2,328,897.0   2,309,384    8,864,364     923,773.8  Wait@jacobi.f90:21
    1.3      115,610,293         50   2,312,205.9   2,307,225.0   2,283,833    2,386,689      21,258.0  Wait@cfd.f90:150
    0.7       58,974,491        100     589,744.9     584,813.0     497,833      684,812      88,260.9  Wait@cfd.f90:144
    0.7       58,777,669        100     587,776.7     513,375.0      48,488      683,116     100,939.1  Wait@jacobi.f90:14
    0.3       27,516,377          1  27,516,377.0  27,516,377.0  27,516,377   27,516,377           0.0  Device Init@jacobi.f90:14
    0.3       26,569,915         50     531,398.3     530,716.0     523,898      548,907       3,876.9  Compute Construct@jacobi.f90:14
    0.3       26,165,316         50     523,306.3     522,872.0     519,415      530,353       2,344.2  Compute Construct@cfd.f90:144
    0.1        8,457,818      1,000       8,457.8       7,139.5       5,890       72,950       3,862.6  Enqueue Upload@cfd.f90:144
```

CFD code

```
do iter = 1, numiter

   call jacobistep_acc(psitmp, psi, m, n)

!  Compute current error value if required

   if (checkerr .or. iter == numiter) then
      error = deltasq(psitmp, psi, m, n)
      error = sqrt(error)
      error = error / bnorm
   end if

!  Quit early if we have reached required tolerance

   if (checkerr) then
      if (error .lt. tolerance) then
         write(*,*) 'CONVERGED iteration ', iter, ': terminating'
         exit
      end if
   end if

!  Copy back
   do j=1,m
      do i=1,n
        psi(i,j) = psitmp(i,j)
      end do
   end do

!  End iterative Jacobi loop

   if (mod(iter,printfreq) == 0) then

      if (.not. checkerr) then
         write(*,*) 'completed iteration ', iter
      else
         write(*,*) 'completed iteration ', iter, ', error = ', error
      end if

   end if

end do
```

```
subroutine jacobistep_acc(psinew, psi, m, n)
  integer :: m, n
  integer :: i, j

  double precision, dimension(0:m+1, 0:n+1) :: psinew, psi

   do j = 1, n
      do i = 1, m
          psinew(i, j) = 0.25d0*(psi(i+1, j) + psi(i-1, j) + &
                                 psi(i, j+1) + psi(i, j-1)     )
      end do
  end do

end subroutine jacobistep_acc

double precision function deltasq(new, old, m, n)

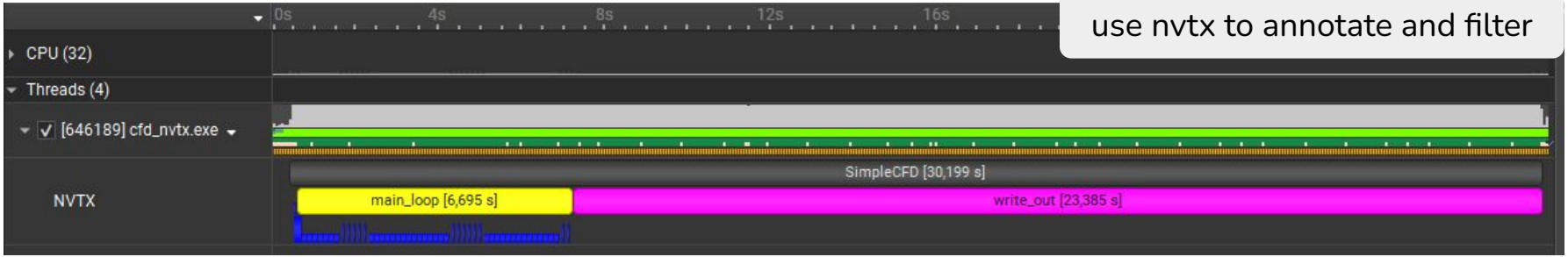
  integer :: m, n, i, j
  double precision, dimension(0:m+1, 0:n+1) :: new, old
  double precision :: deltasq

  integer :: ierr

   deltasq = 0.d0
     do j = 1, n
      do i = 1, m
      deltasq = deltasq + (new(i,j)-old(i,j))**2
     end do
    end do

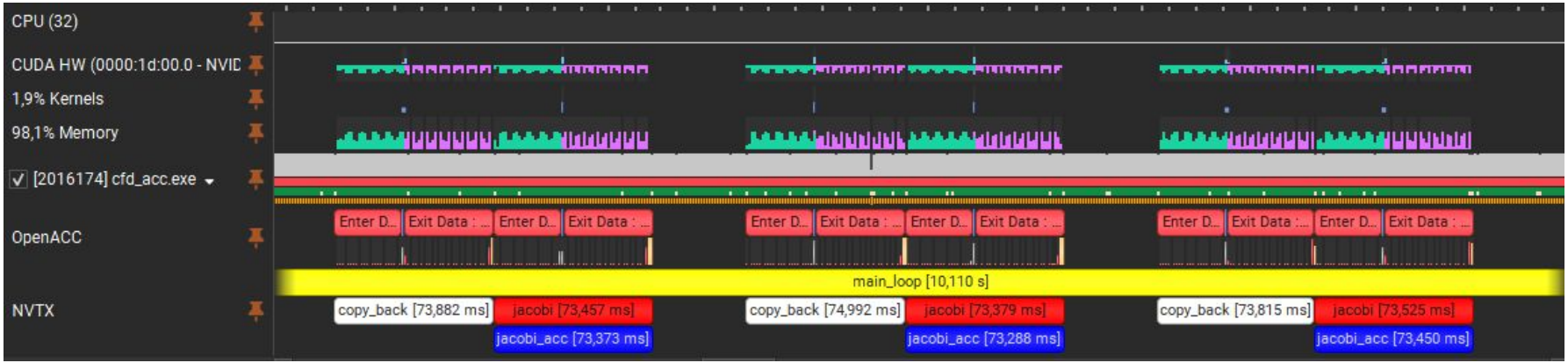
end function deltasq
```

CFD code



use nvtx to annotate and filter

```
--trace=nvtx  --capture-range=nvtx --nvtx-capture='main_loop' --env-var=NSYS_NVTX_PROFILER_REGISTER_ONLY=0
```

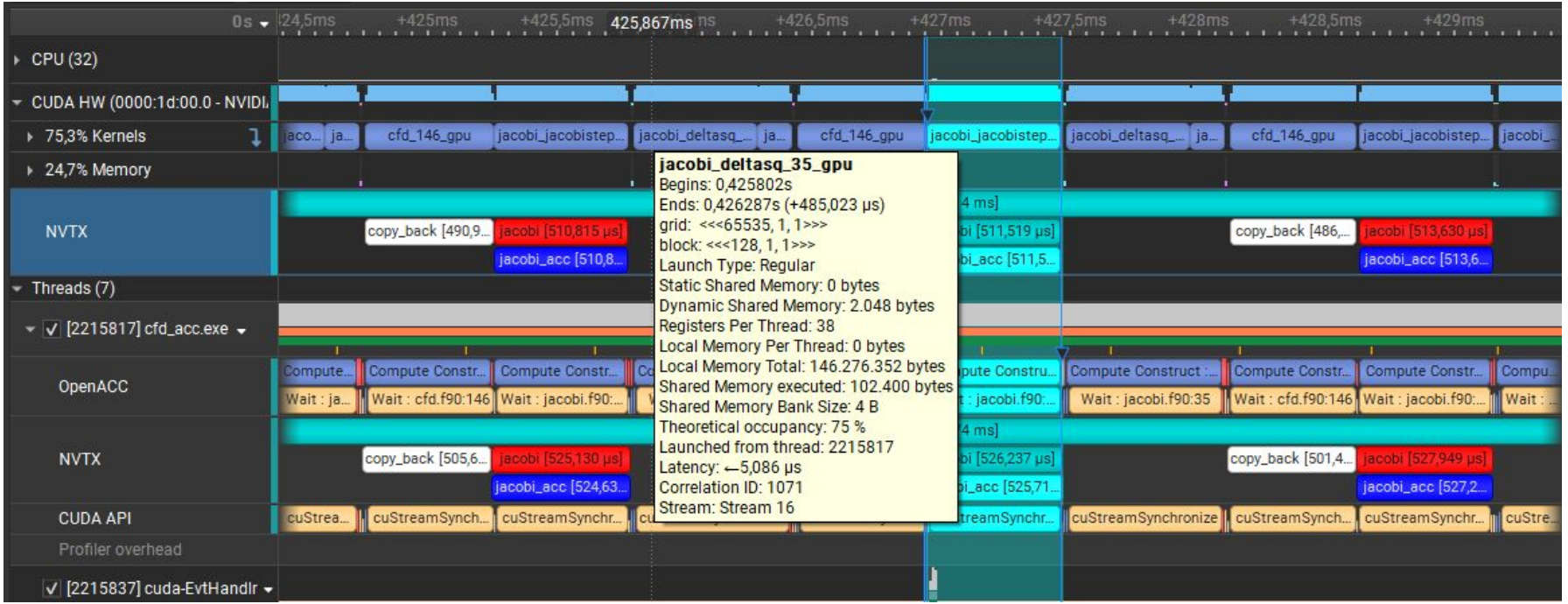


CFD code

check for expensive data movements

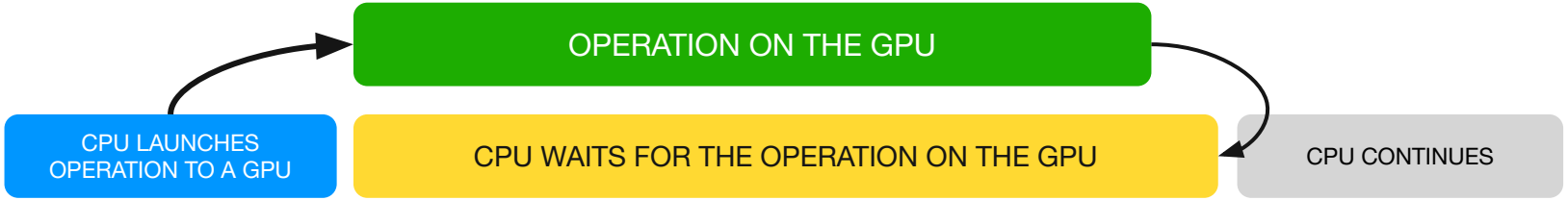
CFD code

analyze how kernels are mapped to GPU hardware

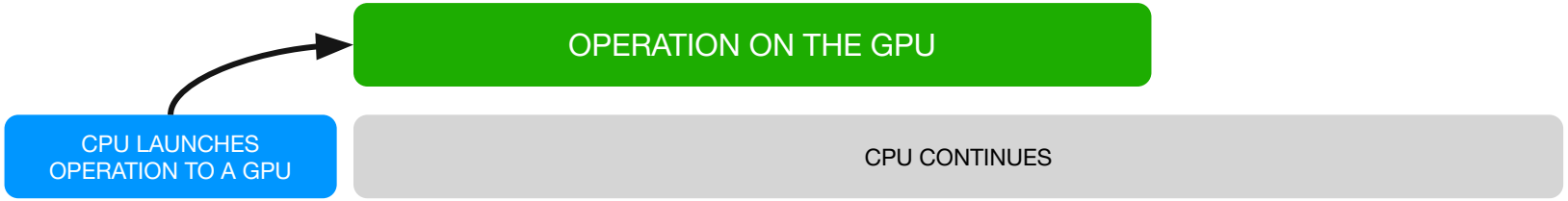


Asynchronous operations

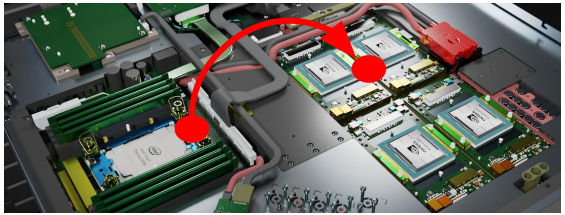
SYNC : CPU waits for the operation on the GPU to be over



ASYNC : CPU does not wait for the operation on the GPU to be over



Asynchronous operations

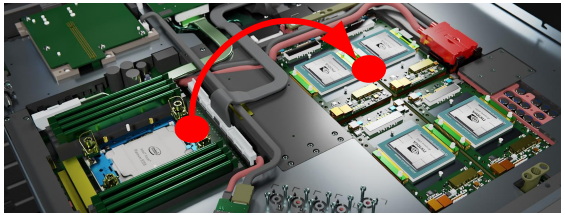


```
for (i = 0; i<n: i++)
 a[i] = 1

for (i = 0; i<n: i++)
 b[i] = 1

for (i = 0; i<n: i++)
c[i] = a[i] + b[i]
```

Asynchronous operations



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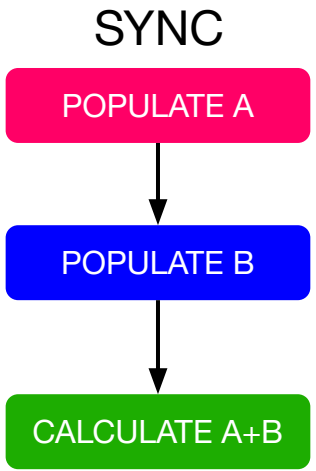
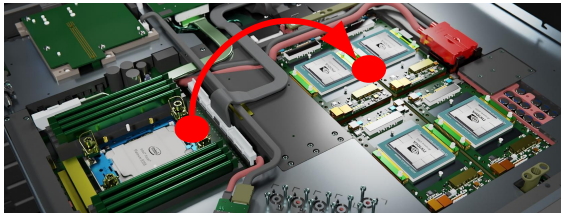


Asynchronous operations



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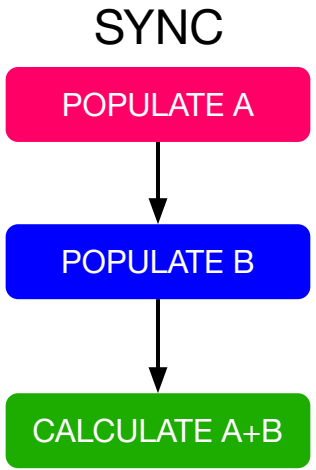
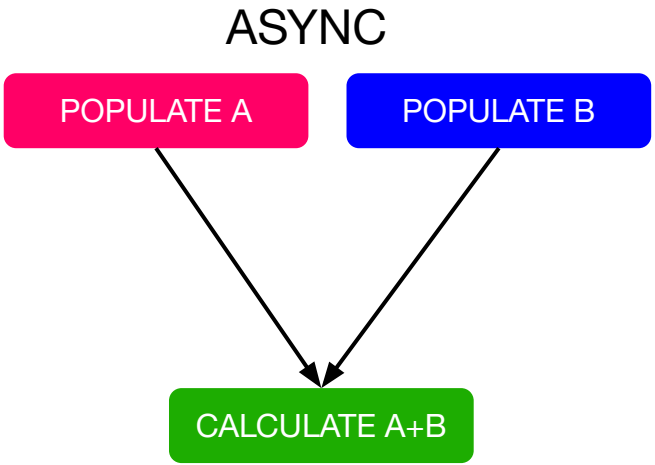
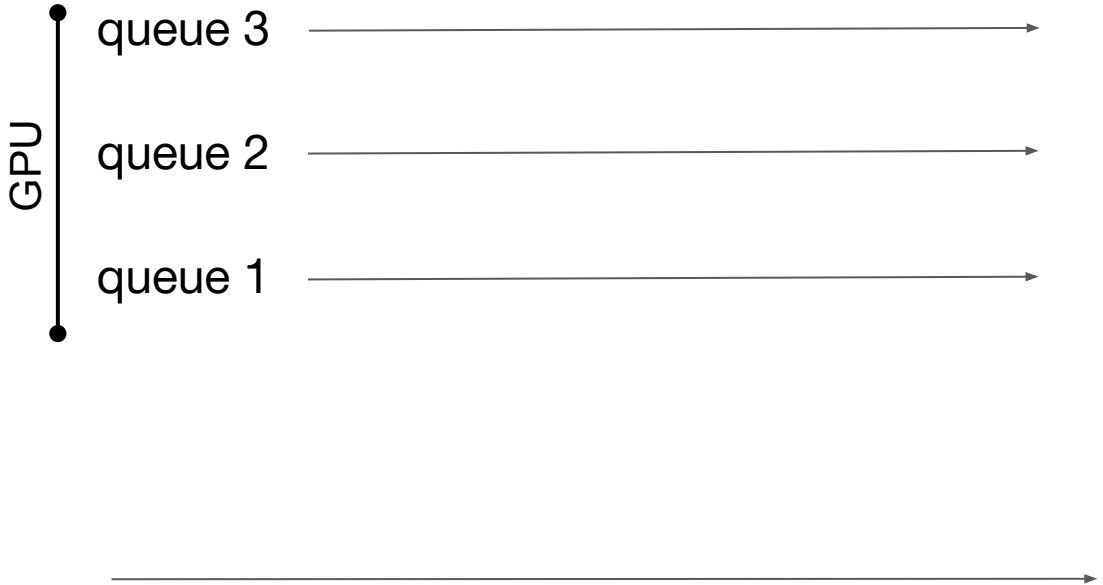
```





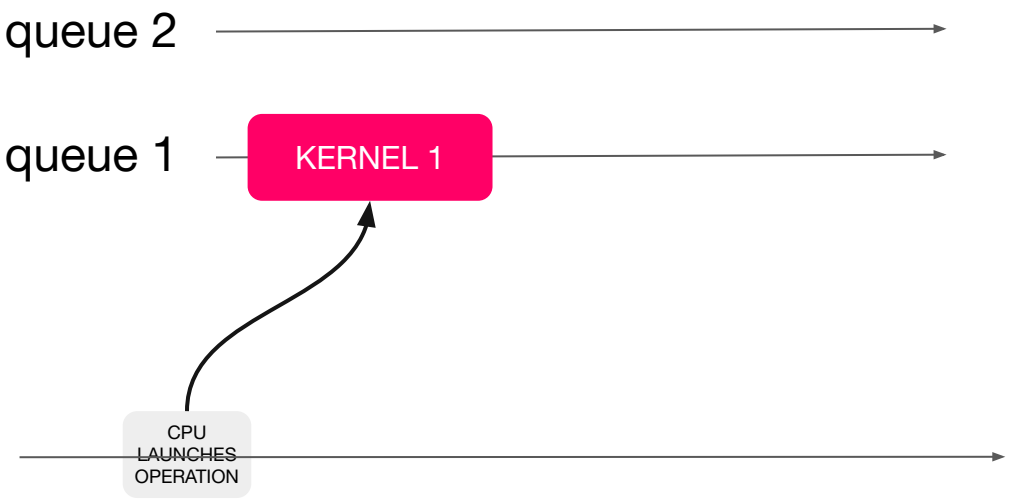
Asynchronous operations & multistream



Asynchronous operations & multistream

```
#pragma acc parallel loop async(1)
for (i = 0; i<n: i++)
 a[i] = 1
```

THIS KERNEL IS COMPUTED ON “STREAM” 1

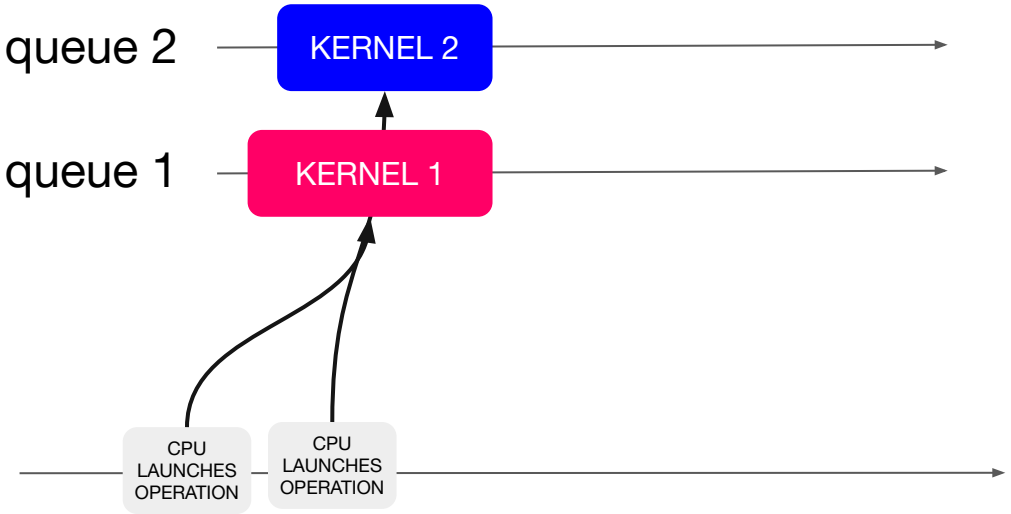


Asynchronous operations & multistream

```
#pragma acc parallel loop async(1)
for (i = 0; i<n: i++)
 a[i] = 1
#pragma acc parallel loop async(2)
for (i = 0; i<n: i++)
 b[i] = 1
```

THIS KERNEL IS COMPUTED ON “STREAM” 1

THIS KERNEL IS COMPUTED ON “STREAM” 2



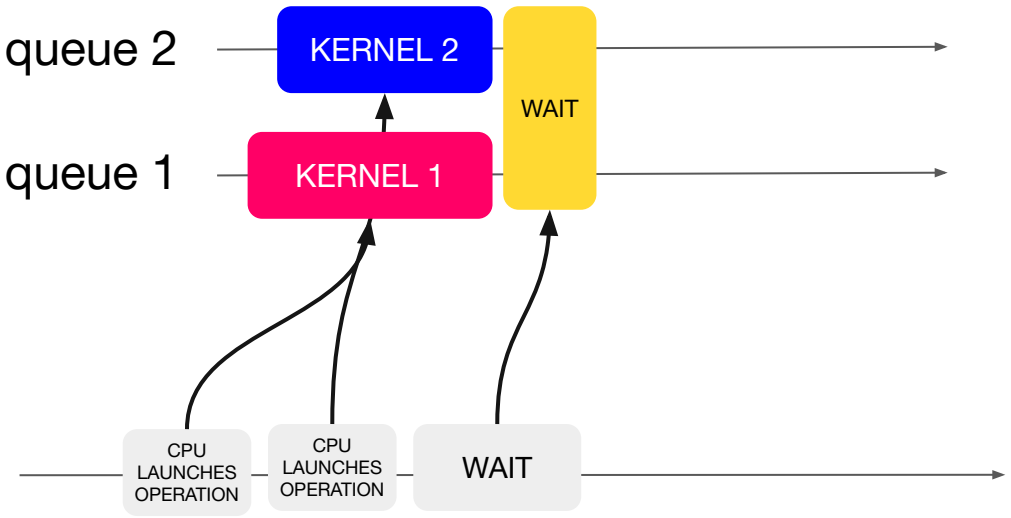
Asynchronous operations & multistream

```
#pragma acc parallel loop async(1)
for (i = 0; i<n: i++)
 a[i] = 1
#pragma acc parallel loop async(2)
for (i = 0; i<n: i++)
 b[i] = 1
#pragma acc wait(1) async(2)
```

THIS KERNEL IS COMPUTED ON “STREAM” 1

THIS KERNEL IS COMPUTED ON “STREAM” 2

THIS KERNEL WAITS FOR OPERATION IN 1 TO BE COMPLETED AND THEN IS PUT IN THE QUEUE OF STREAM 2



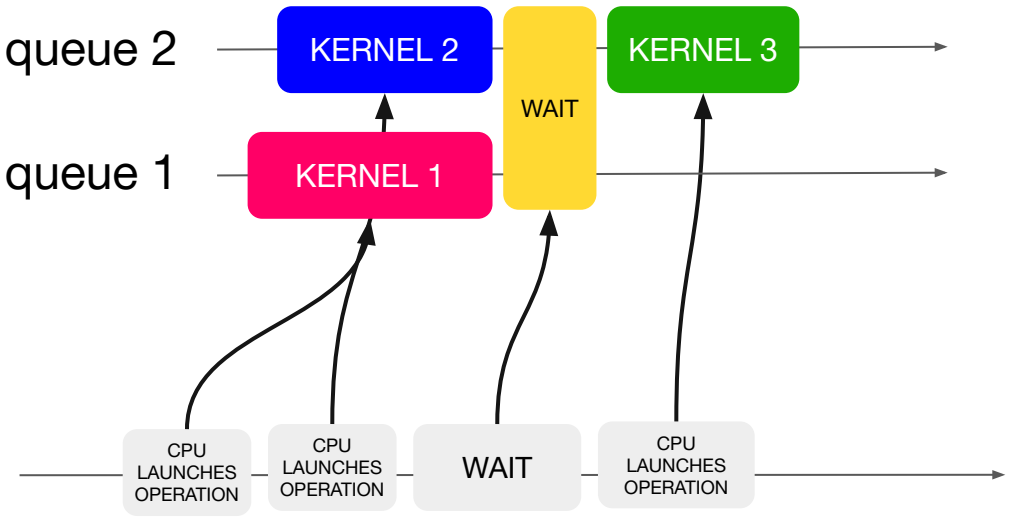
Asynchronous operations & multistream

```
#pragma acc parallel loop async(1)
for (i = 0; i<n: i++)
 a[i] = 1
#pragma acc parallel loop async(2)
for (i = 0; i<n: i++)
 b[i] = 1
#pragma acc wait(1) async(2)
#pragma acc loop async(2)
for (i = 0; i<n: i++)
c[i] = a[i] + b[i]
```

THIS KERNEL IS COMPUTED ON “STREAM” 1

THIS KERNEL IS COMPUTED ON “STREAM” 2

THIS KERNEL WAITS FOR OPERATION IN 1 TO BE COMPLETED AND THEN IS PUT IN THE QUEUE OF STREAM 2



Asynchronous operations & multistream

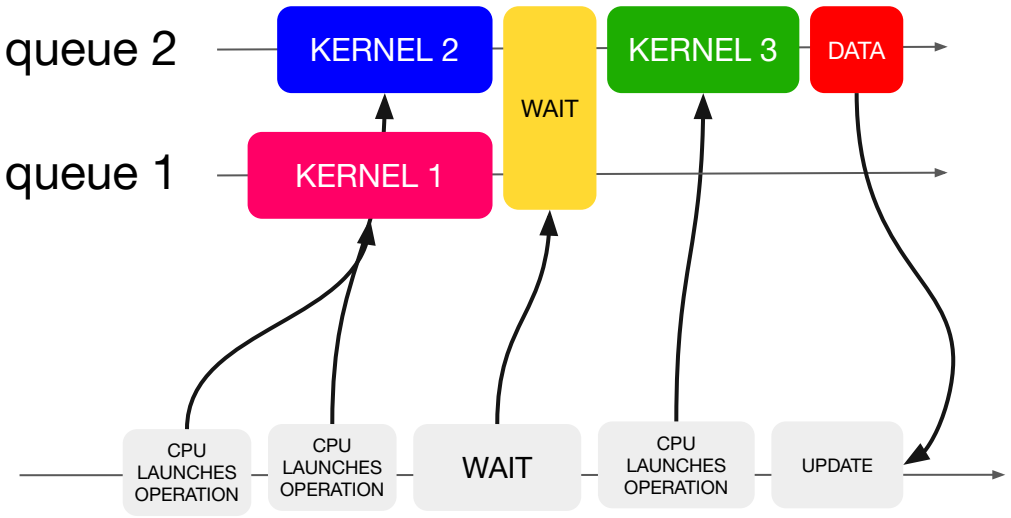
```
#pragma acc parallel loop async(1)
for (i = 0; i<n: i++)
 a[i] = 1
#pragma acc parallel loop async(2)
for (i = 0; i<n: i++)
 b[i] = 1
#pragma acc wait(1) async(2)
#pragma acc loop async(2)
for (i = 0; i<n: i++)
c[i] = a[i] + b[i]
#pragma acc update self[c[0:N]] async(2)
#pragma acc wait
```

THIS KERNEL IS COMPUTED ON “STREAM” 1

THIS KERNEL IS COMPUTED ON “STREAM” 2

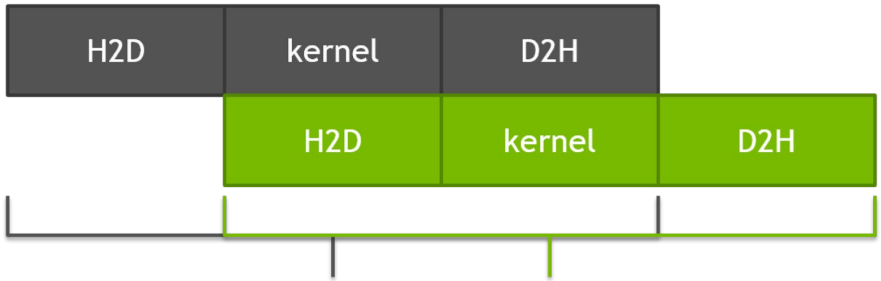
THIS KERNEL WAITS FOR OPERATION IN 1 TO BE COMPLETED AND THEN IS PUT IN THE QUEUE OF STREAM 2

WHEN STREAM2 HAS COMPLETED THE OPERATION, THE HOST IS UPDATED



Asynchronous operations & multistream

Two Independent Operations Serialized



Overlapping Copying and Computation

NOTE: In real applications, your boxes will not be so evenly sized.

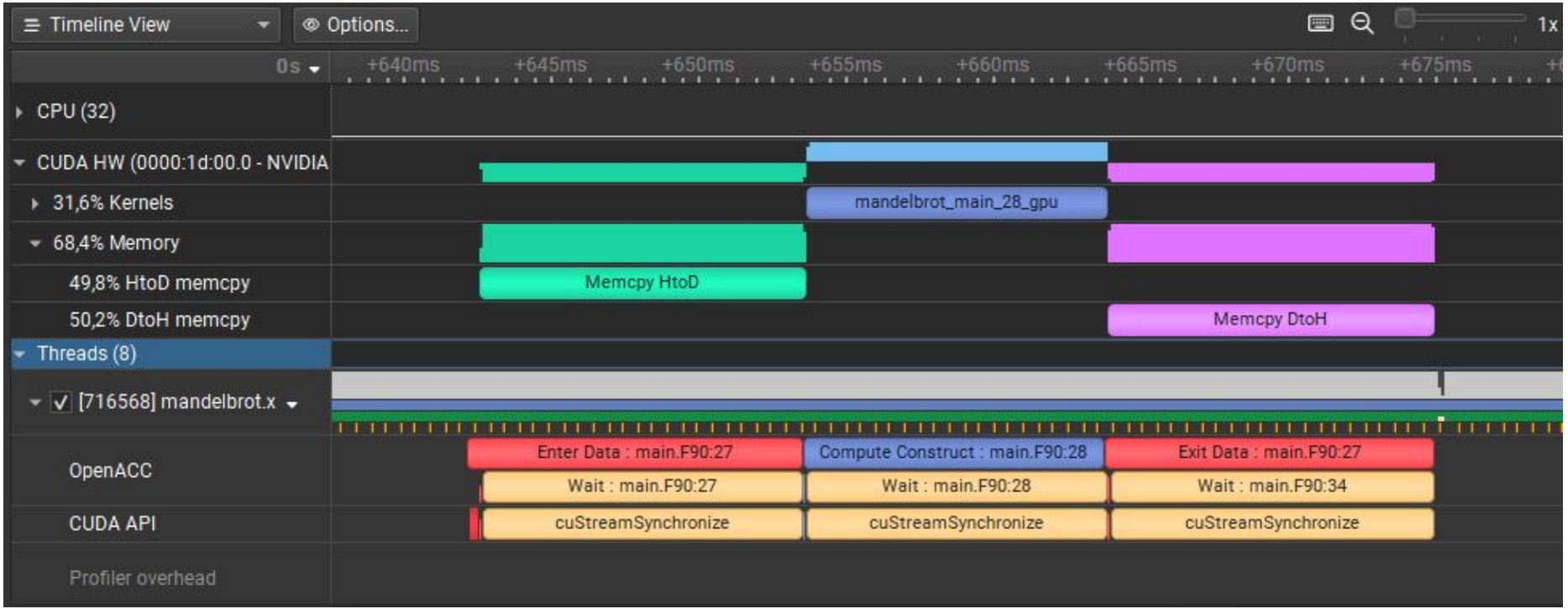
Mandelbrot example

```
!$acc data copy(image(1:HEIGHT, 1:WIDTH))
do block=0,(num_blocks-1)
  starty = block  * (WIDTH/NUM_BLOCKS) + 1
  endy   = min(starty + (WIDTH/NUM_BLOCKS), WIDTH)
  !$acc parallel loop
  do iy=starty,endy
    do ix=1,HEIGHT
      image(ix,iy) = min(max(int(mandelbrot(ix-1,iy-1)),0),MAXCOLORS)
    enddo
  enddo
enddo
!$acc end data
```

```
do while(((x*x+y*y).lt.4.0d0).and.(i.lt.MAX_ITERS))
   xtemp=x*x - y*y + x0
   y=2*x*y + y0
   x=xtemp
   i = i+1
enddo
mandelbrot =  dble(MAXCOLORS)*i/MAX_ITERS
```

- each block is a kernel launched on the GPU
- each unit of work executes and independent “mandelbrot”
- data is already optimized

Mandelbrot example



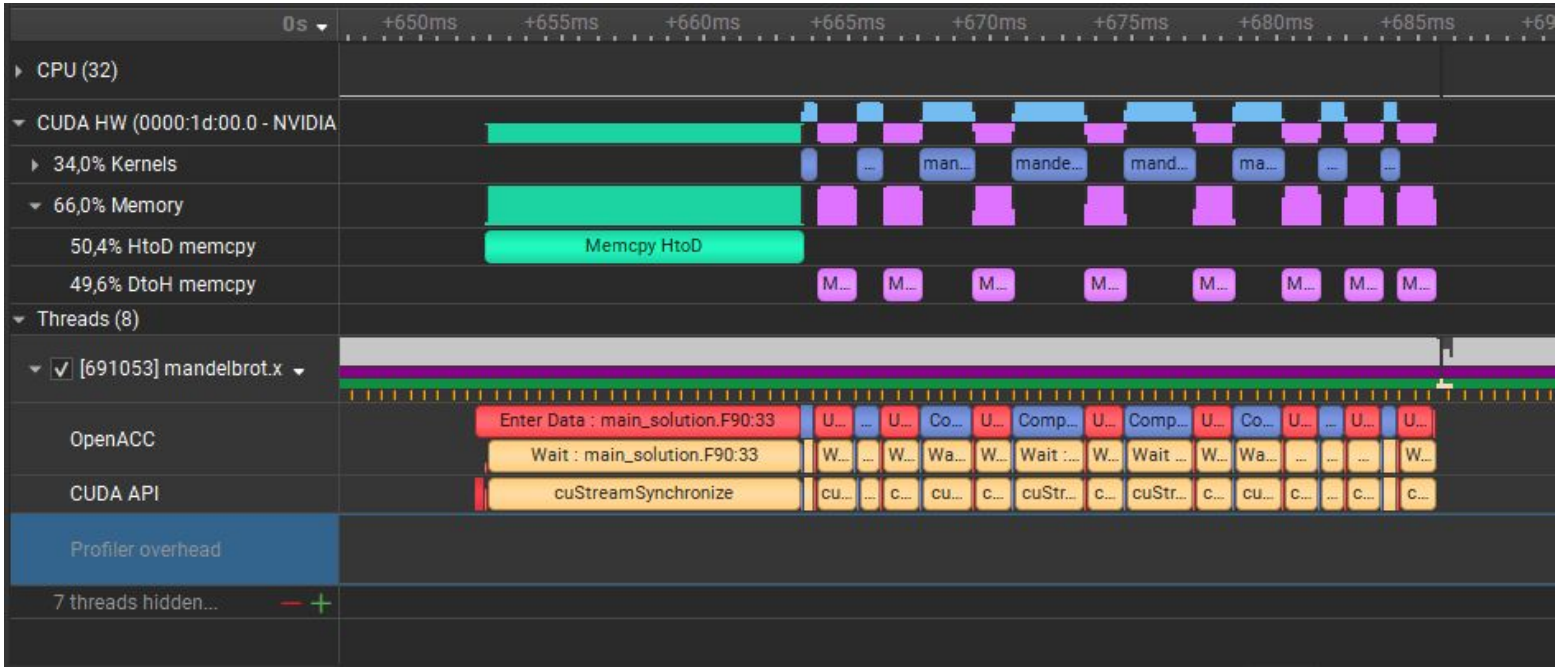
Mandelbrot example

```
!$acc data create(image(1:HEIGHT, 1:WIDTH))
do block=0,(num_blocks-1)
  starty = block  * (WIDTH/NUM_BLOCKS) + 1
  endy   = min(starty + (WIDTH/NUM_BLOCKS), WIDTH)
  !$acc parallel loop
  do iy=starty,endy
    do ix=1,HEIGHT
      image(ix,iy) = min(max(int(mandelbrot(ix-1,iy-1)),0),MAXCOLORS)
    enddo
  enddo
  !$acc update self(image(:,starty:endy))
enddo
!$acc end data
```

```
do while(((x*x+y*y).lt.4.0d0).and.(i.lt.MAX_ITERS))
   xtemp=x*x - y*y + x0
   y=2*x*y + y0
   x=xtemp
   i = i+1
enddo
mandelbrot =  dble(MAXCOLORS)*i/MAX_ITERS
```

- each block is a kernel launched on the GPU
- each unit of work executes and independent “mandelbrot”
- use update instead

Mandelbrot example



about 22 ms for 8 blocks

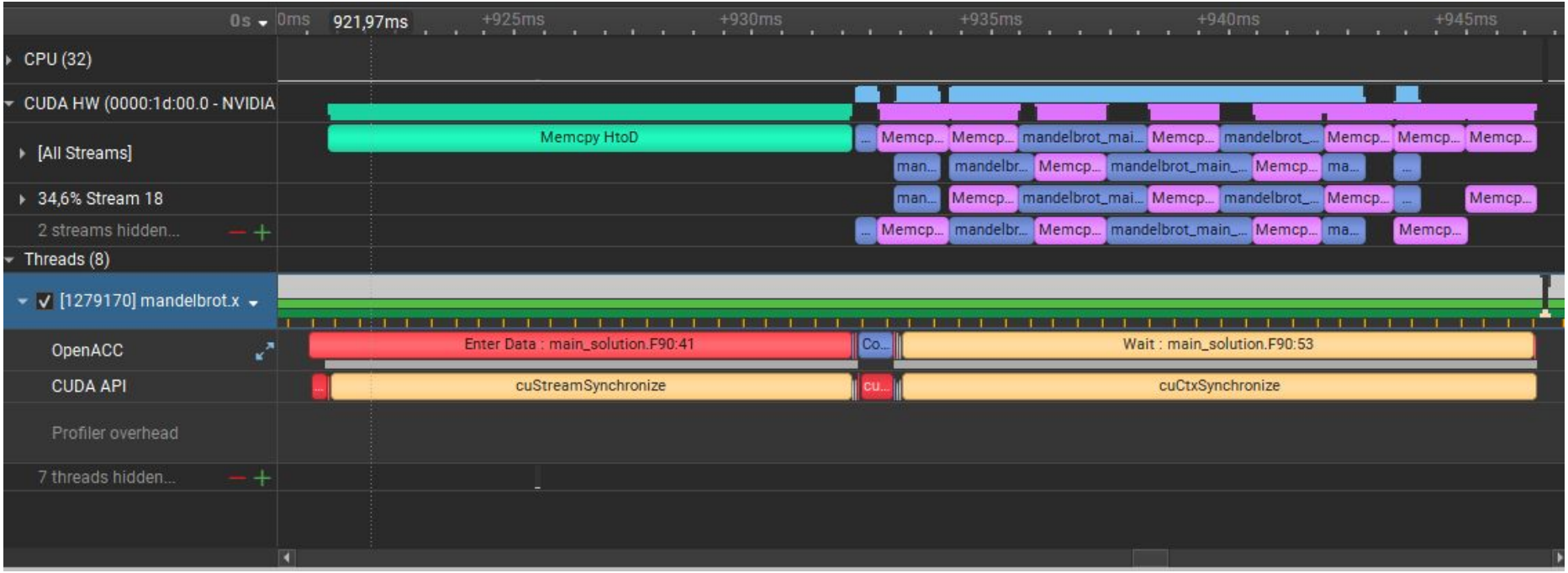
Mandelbrot example

```
!$acc data create(image(1:HEIGHT, 1:WIDTH))
do block=0,(num_blocks-1)
  starty = block  * (WIDTH/num_blocks) + 1
  endy   = min(starty + (WIDTH/num_blocks), WIDTH)
  !$acc parallel loop async(mod(block,2))
  do iy=starty,endy
    do ix=1,HEIGHT
      image(ix,iy) = min(max(int(mandelbrot(ix-1,iy-1)),0),MAXCOLORS)
    enddo
  enddo
  !$acc update self(image(:,starty:endy)) async(mod(block,2))
enddo
!$acc wait
!$acc end data
```

```
do while(((x*x+y*y).lt.4.0d0).and.(i.lt.MAX_ITERS))
   xtemp=x*x - y*y + x0
   y=2*x*y + y0
   x=xtemp
   i = i+1
enddo
mandelbrot =  dble(MAXCOLORS)*i/MAX_ITERS
```

- each block is a kernel launched on the GPU
- it is sent asynchronously to a stream
- each unit of work executes and independent “mandelbrot”
- data update can overlap with computation of the next block on a different stream

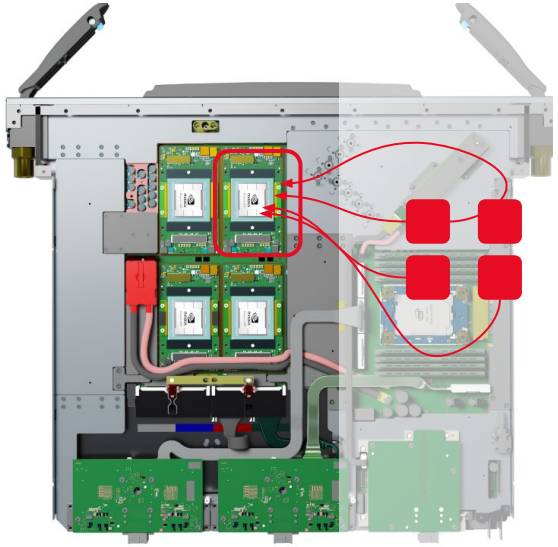
Mandelbrot example



about 14 ms for 8 blocks on 2 streams

Multi process service

Multi process service to enable cooperative multi-process CUDA applications, typically MPI jobs
Uses Hyper-Q to process concurrently CUDA kernels on the same GPU



```
#SLURM -N 1
#SLURM cpus-per-task=1
#SLURM tasks-per-node=8
#SLURM gres=gpu:1

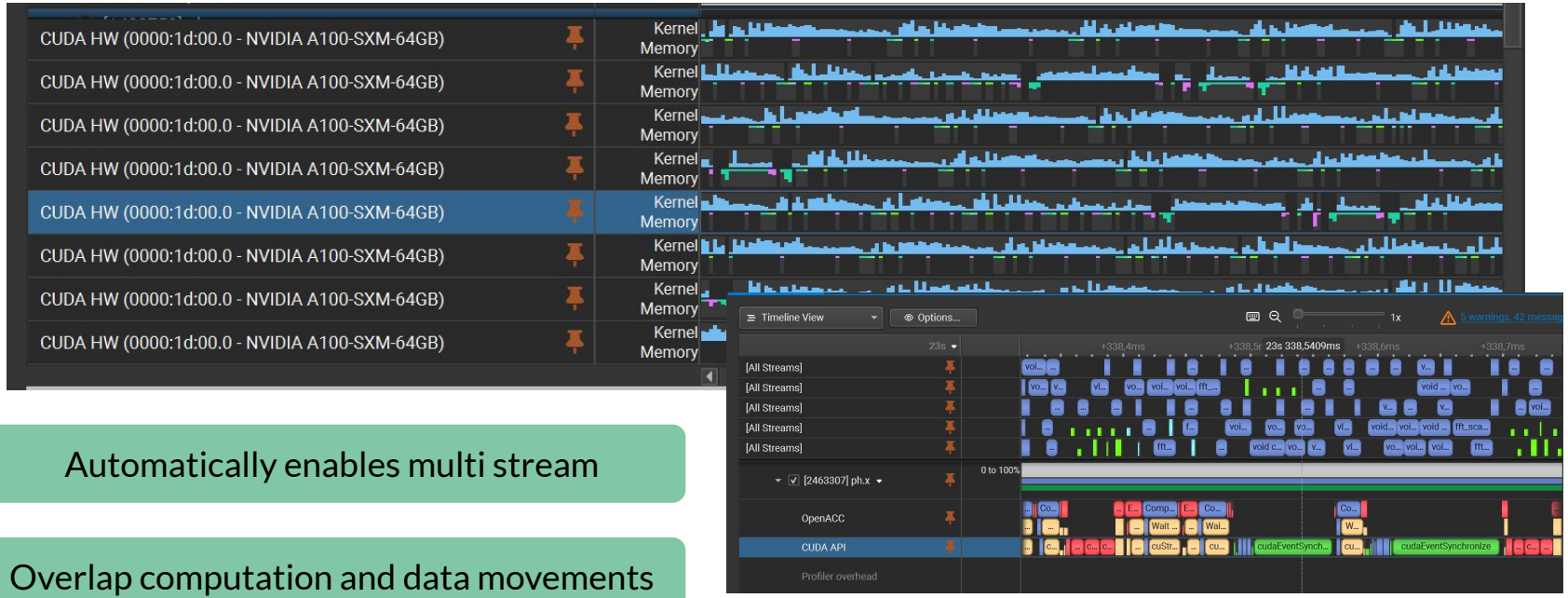
#This must be different for each node
export CUDA_MPS_LOG_DIRECTORY=./pipe0
export CUDA_MPS_PIPE_DIRECTORY=./pipe0

nvidia-cuda-mps-control -d
mpirun -np 8 --map-by node:PE=1 -rank-by core pw.x

echo quit | nvidia-cuda-mps-control
```

Multi process service

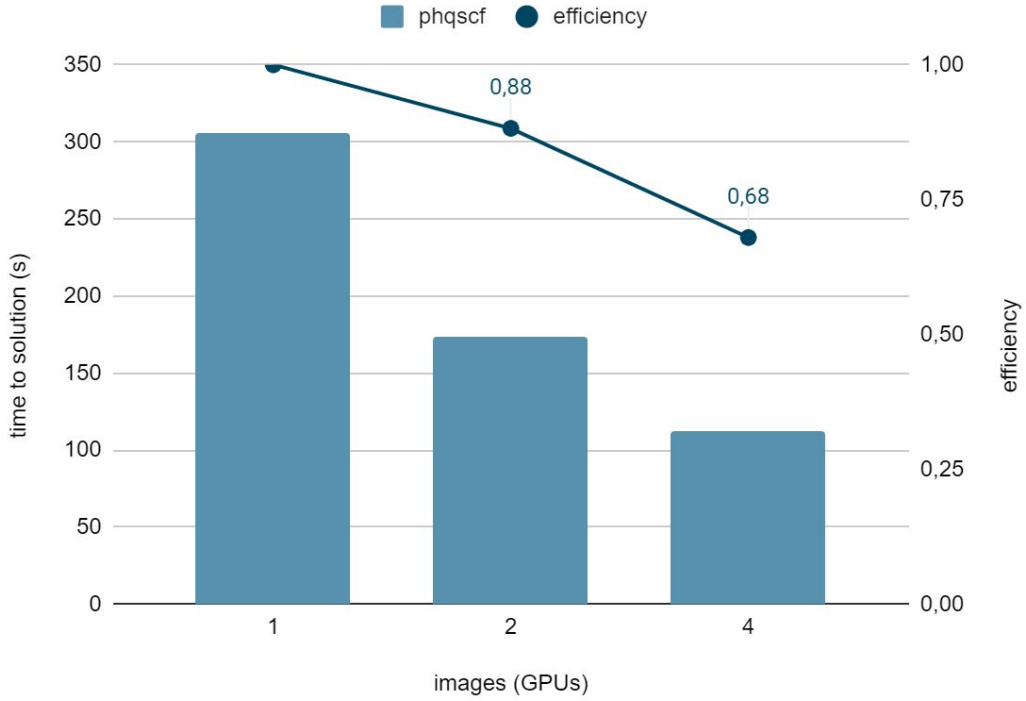
Quartz nat = 9



Automatically enables multi stream

Overlap computation and data movements

Score-P for heterogenous programs



PHonon simulation from QuantumESPRESSO distributed by “images”

- MPI, OpenACC and CUDA
- 1 MPI : 1 GPU
- 1 MPI task per image
- images implement fairly independent computations

Why efficiency is low at 4 GPUs?

Score-P for heterogenous programs

- Code instrumented with Score-P (source-code instrumentation)

```
SCOREP_WRAPPER=off cmake <cmake-options> <source-path>
make SCOREP_WRAPPER_INSTRUMENTER_FLAGS="--mpp=mpi --openacc --cuda" <executable>
```

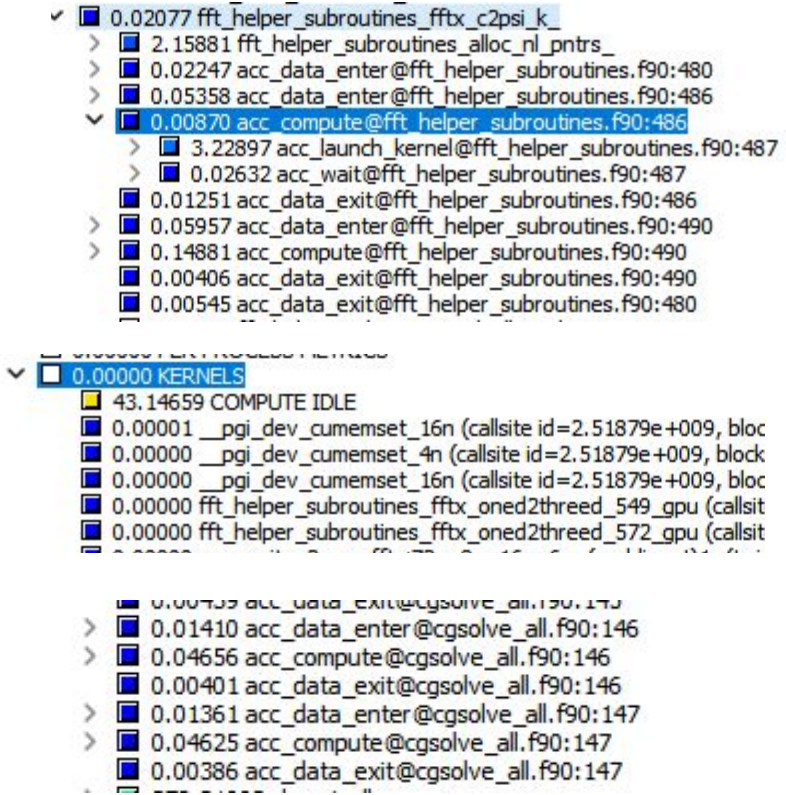
- Measurement at runtime; environment variables to configure it

```
export SCOREP_CUDA_ENABLE=yes
export SCOREP_OPENACC_ENABLE=yes
[. . .]
srun -n <task-number> ./myapp.exe # generates scorep_ folder with profiling data
```

- More at

  https://scorepci.pages.jsc.fz-juelich.de/scorep-pipelines/docs/scorep-6.0/html/scorepmeasurementconfig.html

Score-P workflows



Time spent in OpenACC region

- launching kernels
- waiting for GPU compute
- implicit and explicit data movement

Identify expensive kernel launches

Identify expensive data movements

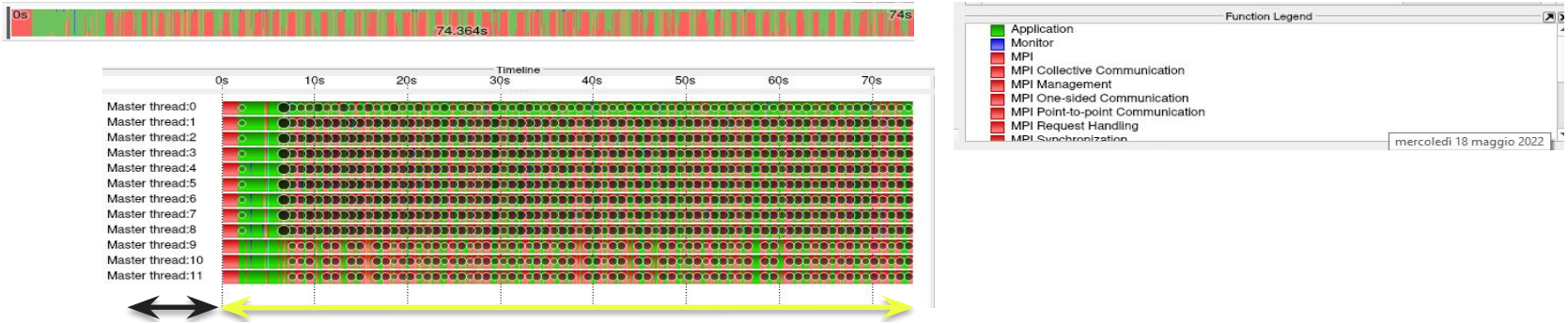
From the GPU perspective

- time spent in GPU kernels
- time spent IDLE state

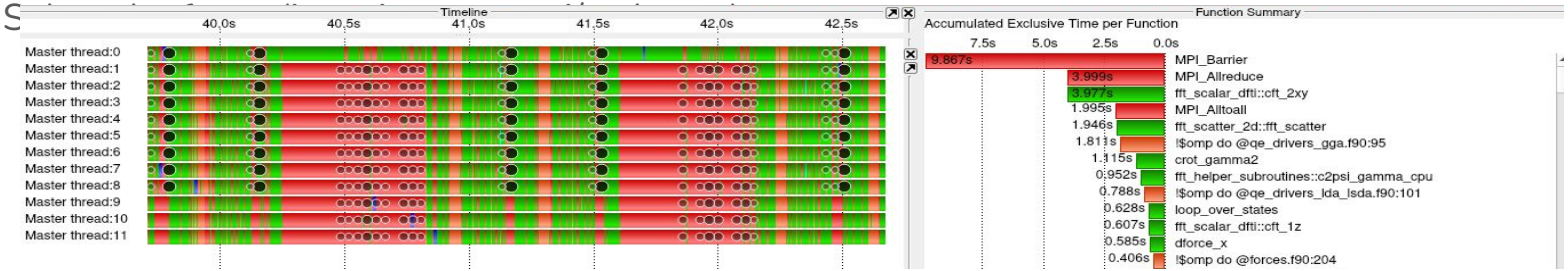
Vampir

```
vampir scorep_12x1_trace/traces.otf2
```

(1) Identify the pattern: initialization, iteration, finalization



(2) S



Vampir

```
vampir scorep_12x1_trace/traces.otf2
```

(3) Visualize communication patterns, durations, data movement (CPU-GPU), CUDA kernels on event timeline