



Uni.lu HPC School 2021

PS10a: Introduction to GPU programming with OpenACC

High Performance
Computing &
Big Data Services



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<http://hpc.uni.lu>



Latest versions available on Github:



UL HPC tutorials:

<https://github.com/ULHPC/tutorials>

UL HPC School:

hpc.uni.lu/education/hpcschool

PS10a tutorial sources:

ulhpc-tutorials.rtf.d.io/en/latest/openacc/





Summary

- 1 **Introduction to OpenACC**
- 2 Difference between CPU and GPU
- 3 Basics of OpenACC
- 4 Compute directives in OpenACC
- 5 Loop directive in OpenACC
- 6 Other directives in OpenACC

Objectives

- Understanding the **OpenACC programming model**
- How to use some of the directives from OpenACC to parallelize the code
 - ↪ compute constructs, loop constructs, data clauses
- Implementing OpenACC parallel strategy in **C/C++** and **FORTTRAN** programming languages
- Simple **mathematical examples** to support and understand the OpenACC programming model
- Finally to show how to run these examples using **Iris cluster (ULHPC)** - both **interactively** and using a **batch job script**

Prerequisite

- C/C++ and/or FORTRAN languages
- OpenMP or some basic parallel programming concept (advantage but not necessary)

NOTE: *this lecture is limited to just 45 min, it only covers very basic tutorial about OpenACC. To know more about (from basic to advanced) CUDA programming and OpenACC programming model, please refer to **PRACE MOOC GPU Programming for Scientific Computing and Beyond - Dr. Ezhilmathi Krishnasamy***



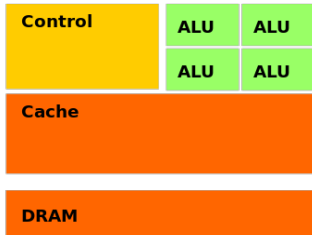
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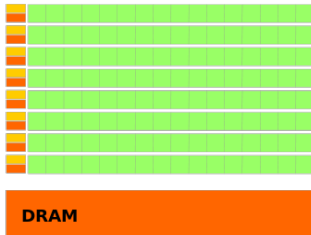
CPU vs GPU

- CPU frequency is higher compared to GPU
- But GPU can run many threads in parallel compared to CPU
- On the GPU, the cores are grouped and called “Streaming Multiprocessor - SM”
- Even on the Nvidia GPU, it has a “Tensor Process Unit - TPU” to handle the AI/ML computations in an optimized way
- GPU are based on the “Single Instruction Multiple Threads”
- Threads are executed in a group on the GPU, typically they have 32 threads. This is called “warps” on the Nvidia GPU and “wavefronts” on the AMD GPU.

CPU vs GPU

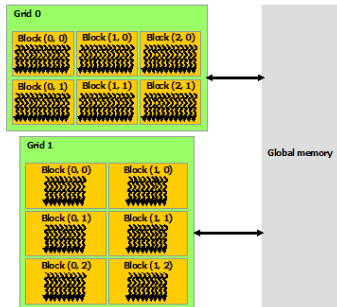
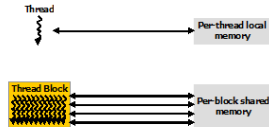
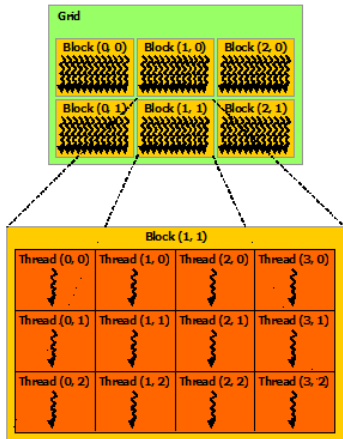


CPU



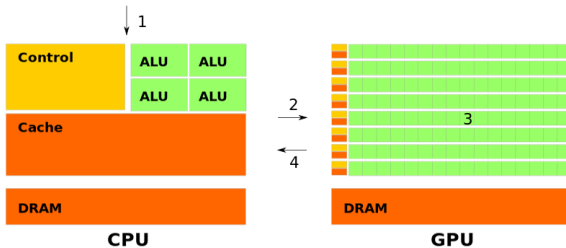
GPU

Thread Hierarchy



How GPUs are used for computations

- Step 1: application preparation, initialize the memories on both CPU and GPU
- Step 2: transfer the data to GPU
- Step 3: do the computation on the GPU
- Step 4: transfer the data back to CPU
- Step 5: finalize the application and delete the memories on both CPU and GPU





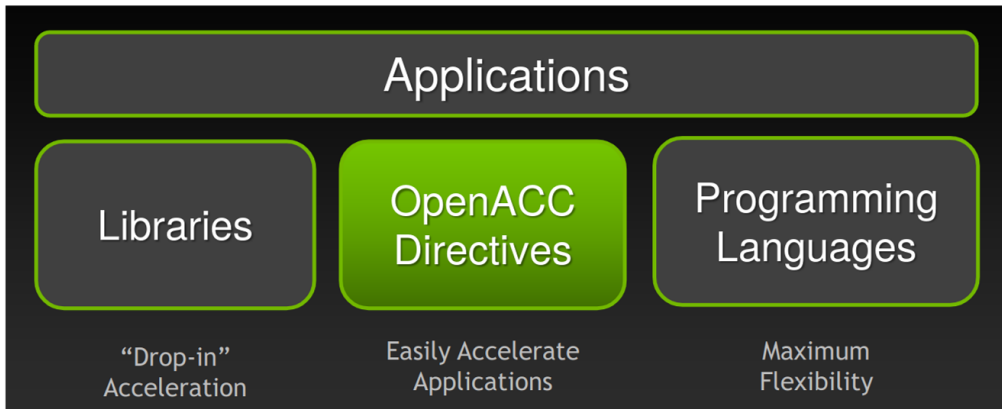
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Few points about OpenACC

- OpenACC is not GPU programming
- OpenACC is expressing the parallelism in your code
- OpenACC can be used in both Nvidia and AMD GPUs
- “OpenACC will enable programmers to easily develop portable applications that maximize the performance and power efficiency benefits of the hybrid CPU/GPU architecture of Titan.”
 - ↪ Buddy Bland, Titan Project Director, Oak Ridge National Lab
- “OpenACC is a technically impressive initiative brought together by members of the OpenMP Working Group on Accelerators, as well as many others. We look forward to releasing a version of this proposal in the next release of OpenMP.”
 - ↪ Michael Wong, CEO OpenMP Directives Board

Ways to accelerate applications on the GPU



Ways to accelerate applications on the GPU

- Libraries: easy to use with very limited knowledge with GPU programming
 - ↪ cuBLAS, cuFFT, CUDA Math Library, etc.,
- Directive based programming model: will accelerate the application with using directives in the existing code
 - ↪ OpenACC and OpenMP (might be applicable in the future)
- Programming languages: low level programming languages that will further optimize the application on the accelerator
 - ↪ CUDA, OpenCL, etc.,



Compilers and directives (only few of them listed in here)

- OpenACC is supported by the Nvidia, PGI, GCC, and HPE Gray (only for FORTRAN) compilers
 - ↪ Now PGI is part of Nvidia, and it is available through Nvidia HPC SDK
- Compute directives:
 - ↪ parallel and kernel
- Loop directive:
 - ↪ loop
- Data management directives:
 - ↪ copyin and copyout
- Others:
 - ↪ reduction

Basic programming structure

```
// C/C++  
#include "openacc.h"  
#pragma acc <directive> [clauses [[,] clause] . . .] new-line  
<code>
```

```
!! Fortran  
use openacc  
!$acc <directive> [clauses [[,] clause] . . .]  
<code>
```




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kernels in C/C++

```
// Hello_World.c                                | // Hello_World_OpenACC.c
void Print_Hello_World()                         | void Print_Hello_World()
{                                                 | {
    for(int i = 0; i < 5; i++)                   | #pragma acc kernels
    {                                             |     for(int i = 0; i < 5; i++)
        printf("Hello World!\n");               |     {
    }                                             |         printf("Hello World!\n");
}                                                 | }
| }
| }
```

- compilation: `pgcc -fast -Minfo=all -ta=tesla -acc Hello_World.c`
↪ Compiler will give already much info, what do you see?

kernels in FORTRAN

```

!! Hello_World.f90
subroutine Print_Hello_World()
  integer :: i

  do i = 1, 5
    print *, "hello world"
  end do

end subroutine Print_Hello_World

| !! Hello_World_OpenACC.f90
| subroutine Print_Hello_World()
|   integer :: i
|   !$acc kernels
|   do i = 1, 5
|     print *, "hello world"
|   end do
|   !$acc end kernels
| end subroutine Print_Hello_World

```

- compilation: `pgfortran -fast -Minfo=all -ta=tesla -acc Hello_World_OpenACC.f90`
 ↳ `-ta` refers to target architecture, here is it Nvidia Tesla and `-acc` compiler flag instructing to target accelerators



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loop and data directive in vector addition in C/C++

```
// Vector_Addition.c
float * Vector_Addition
(float *a, float *b, float *c, int n)
{
    for(int i = 0; i < n; i ++)
    {
        c[i] = a[i] + b[i];
    }
    return c;
}

| // Vector_Addition_OpenACC.c
| float * Vector_Addition
| (float *a, float *b, float *c, int n)
| {
| #pragma acc kernels loop
| copyin(a[:n], b[0:n]) copyout(c[0:n])
|   for(int i = 0; i < n; i ++)
|   {
|       c[i] = a[i] + b[i];
|   }
| }
```

loop and data directive in vector addition in FORTRAN

```
!! Vector_Addition.f90
module Vector_Addition_Mod
  implicit none
  contains
  subroutine Vector_Addition(a, b, c, n)
    !! Input vectors
    real(8), intent(in), dimension(:) :: a
    real(8), intent(in), dimension(:) :: b
    real(8), intent(out), dimension(:) :: c
    integer :: i, n

    do i = 1, n
      c(i) = a(i) + b(i)
    end do

  end subroutine Vector_Addition
end module Vector_Addition_Mod
```

```
/ !! Vector_Addition_OpenACC.f90
| module Vector_Addition_Mod
|   implicit none
| / contains
|   subroutine Vector_Addition(a, b, c, n)
|     !! Input vectors
|     real(8), intent(in), dimension(:) :: a
|     real(8), intent(in), dimension(:) :: b
|     real(8), intent(out), dimension(:) :: c
|     integer :: i, n
|     !$acc kernels loop copyin(a(1:n), b(1:n))
|       copyout(c(1:n))
|       do i = 1, n
|         c(i) = a(i) + b(i)
|       end do
|     !$acc end kernels
|   end subroutine Vector_Addition
| end module Vector_Addition_Mod
```



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reduction directive in vector addition in C/C++

```
// Vector_Addition.c
float * Vector_Addition
(float *a, float *b, float *c, int n)
{
    for(int i = 0; i < n; i ++)
    {
        c[i] = a[i] + b[i];
    }
    return c;
}

/ // Vector_Addition_OpenACC.c
| float * Vector_Addition
| (float *a, float *b, float *c, int n)
| { float sum=0;
| #pragma acc kernels loop
| reduction(+:sum) copyin(a[:n], b[0:n]) copyout(c[0:n])
|   for(int i = 0; i < n; i ++)
|   {
|       c[i] = a[i] + b[i];
|       sum+=c[i];
|   }
| }
```


reduction directive in vector addition in FORTRAN

```
!! Vector_Addition.f90
module Vector_Addition_Mod
  implicit none
  contains
  subroutine Vector_Addition(a, b, c, n)
    !! Input vectors
    real(8), intent(in), dimension(:) :: a
    real(8), intent(in), dimension(:) :: b
    real(8), intent(out), dimension(:) :: c
    integer :: i, n

    do i = 1, n
      c(i) = a(i) + b(i)
    end do

  end subroutine Vector_Addition
end module Vector_Addition_Mod
```

```
/ !! Vector_Addition_OpenACC.f90
| module Vector_Addition_Mod
|   implicit none
|   contains
|   subroutine Vector_Addition(a, b, c, n)
|     !! Input vectors
|     real(8), intent(in), dimension(:) :: a, b
|     real(8):: sum
|     real(8), intent(out), dimension(:) :: c
|     integer :: i, n
|     !$acc kernels loop reduction(+:sum)
|       copyin(a(1:n), b(1:n)) copyout(c(1:n))
|     do i = 1, n
|       c(i) = a(i) + b(i)
|       sum = c(i)
|     end do
|     !$acc end kernels
|   end subroutine Vector_Addition
end module Vector_Addition_Mod
```



Thank you for your attention...

Questions?

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