High Performance Computing & Big Data Services

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PS10a: Introduction to GPU programming with OpenACC

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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.rtfd.io/en/latest/openacc/

Summary

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 FORTRAN programming languages
- Simple mathematical examples to support and understand the OpenACC programming model
- Finally, show you 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***

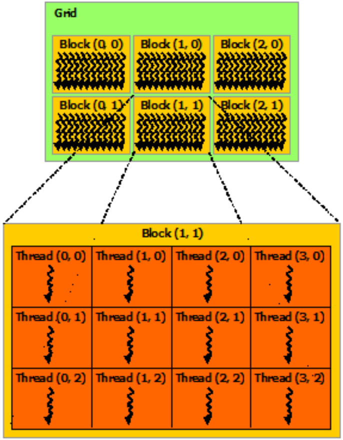
Summary

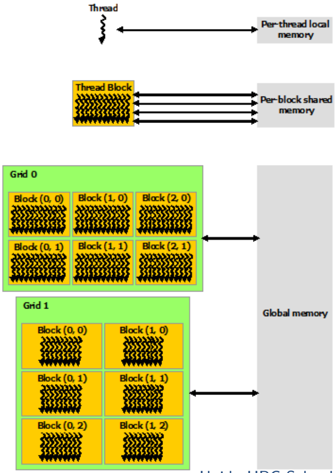
CPU vs GPU

- 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
- GPUs 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 Nividia GPU and “wavefronts” on the AMD GPU

CPU vs GPU

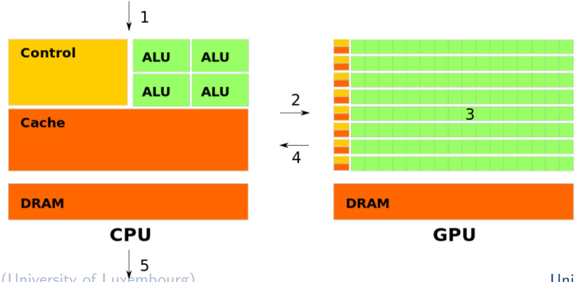
Thread Hierarchy





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 the CPU
- Step 5: finalize the application and delete the memories on both CPU and GPU

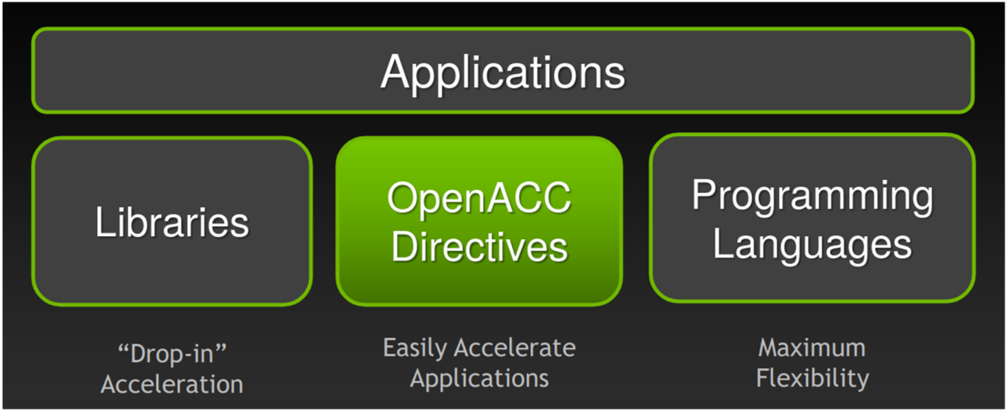


Summary

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 of GPU programming
  - ↪ cuBLAS, cuFFT, CUDA Math Library, etc.
- Directive based programming model: will accelerate the application by 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 constructs:
  - ↪ parallel and kernel
- Loop constructs:
  - ↪ loop, collapse, gang, worker, vector, etc.
- Data management clauses:
  - ↪ copy, create, copyin, copyout, delete and present
- Others:
  - ↪ reduction, atomic, cache, etc.
- More information about the OpenACC directives can be found here

Basic programming structure

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

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

Summary

kernels in C/C++

```
// Hello_World.c                           | // Hello_World_OpenACC.c
void Print_Hello_World()                   | void Print_Hello_World()
{                                          | {
                                           | #pragma acc kernels loop
  for(int i = 0; i < 5; i++)               |    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`
  - ↪ The compiler will already give much info; what do you see?

kernels in FORTRAN

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

Summary

Data management

- copyin(list) - Allocates memory on GPU and copies data from CPU(host) to GPU when entering a region
- copyout(list) - Allocates memory on GPU and copies data to the CPU(host)host when exiting a region
- copy(list) - Allocates memory on GPU and copies data from CPU(host) to GPU when entering region and copies data to the CPU(host) when exiting a region
- create(list) - Allocates memory on GPU but does not copy
- delete(list) - Deallocate memory on the GPU without copying
- present(list) - Data is already present on GPU from another containing data a region

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

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

loop and data clauses in vector addition in FORTRAN

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

Summary

reduction clause in C/C++

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

reduction clause in FORTRAN

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

Thank you for your attention...

Questions?

ulhpc-tutorials.rtfd.io/en/latest/openacc/

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