





GPU programming using OpenACC

CSCS-USI Summer School 2020 Andreas Jocksch, Vasileios Karakasis, CSCS July 13–24, 2020

Goals of the course

- Part I
 - Basic concepts
 - Execution and memory model
 - Basic directives
 - Hands-on sessions
 - Advanced topics
 - Asynchronous execution and wait queues
 - Interoperability with CUDA and MPI
 - Deep copy
 - Hands-on sessions
- Part II
 - Port the miniapp to GPU using OpenACC
 - Walk away ready to start hacking your own code





Introduction to OpenACC

What is OpenACC?

- Collection of compiler directives for specifying loops and regions to be offloaded from a host CPU to an attached accelerator device
- Host + Accelerator programming model
- High-level representation
- Current specification version: 2.7
- Similarities to classic OpenMP for multicores







Why to use OpenACC?

Because ...

- I don't care about all the little hardware details, I want my science done.
- I want to run on accelerators, but I still need a fast and readable code.
- I need portability across different accelerator vendors, but also to be able to run on the multicore.
- I inhereted a large legacy monolithic codebase, which I don't dare to refactor completely, but I need to get my results faster.
- My code is in Fortran.





OpenACC is not a silver bullet

- A high-level representation is not a panacea.
 - You still need to understand and adapt to the programming model.

- Does not substitute hand-tuning, but can serve as a very good starting point.
 - Some low-level CUDA constructs are not exposed (shared memory, groups etc.)



- User base not yet as large as of classic OpenMP for multicores, but it is expanding.
 - You may run into compiler bugs or specification ambiguities.



Format of directives

- C/C++
 - #pragma acc directive-name [clause-list] new-line
 - Scope is the following block of code
- Fortran
 - !\$acc directive-name [clause-list] new-line
 - Scope is until !\$acc end directive-name





Programming model

- Host-directed execution
- Compute intensive regions are offloaded to attached accelerator devices
- Host orchestrates the execution on the device
 - Allocations on the device
 - Data transfers
 - Kernel launches
 - Wait for events
 - Etc...





- The device executes parallel or kernel regions
- Parallel region
 - Work-sharing loops
- Kernel region
 - Multiple loops to be executed as multiple kernels
- Levels of parallelism
 - 1. Gang
 - 2. Worker
 - 3. Vector
 - Parallelism levels are decided by the compiler but can be fine-tuned by the user



- The device executes parallel or kernel regions
- Parallel region
 - Work-sharing loops
- Kernel region
 - Multiple loops to be executed as multiple kernels
- Levels of parallelism
 - 1. Gang → CUDA block
 - 2. Worker → CUDA warp
 - 3. Vector → CUDA threads
 - Parallelism levels are decided by the compiler but can be fine-tuned by the user
 - Mapping to CUDA blocks/warps/threads is implementation defined

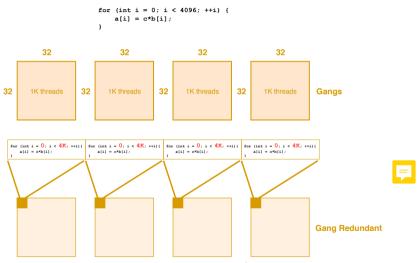




- Gang
 - Gang-redundant (GR)Gang-partioned (GP)
- F

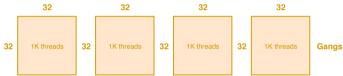
- Worker
 - Worker-single (WS)
 - Worker-partitioned (WP)
- Vector
 - Vector-single (VS)
 - Vector-partitioned (VP)

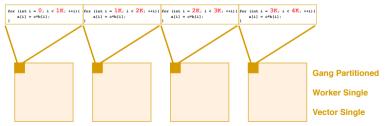




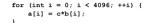




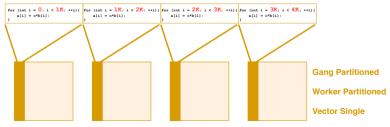




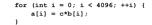




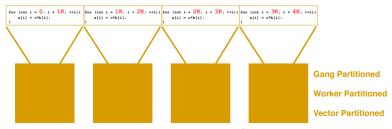














The kernels construct

```
Multiple loops inside ke 50 s construct
! $acc kernels
    IGR model
    y(1) = y(1) + x(1)
    do i = 1. N
        !compiler decides on the partitioning (GP/WP/VP modes)
        y(i) = y(i) + a*x(i)
    enddo
    do i = 1. N
        !compiler decides on the partitioning (GP/WP/VP modes)
        y(i) = b*y(i) + a*x(i)
    enddo
I $acc end kernels
```

- Compiler will try to deduce parallelism
- Loops are launched as different GPU kernels



The parallel construct

```
Parallel construct
!$acc parallel
    y(1) = y(1) + x(1) !GR model
! $acc end parallel
! $acc parallel
    do i = 1, N !loop executed in GR mode
        v(i) = v(i) + a*x(i)
    enddo
! $acc end parallel
!$acc parallel
    !$acc loop
    do i = 1. N !compiler decides on the partitioning (GP/WP/VP modes)
        v(i) = b*v(i) + a*x(i)
    enddo
!$acc end parallel
```

- No automatic parallelism deduction → parallel loops must be specified explicitly
- Implicit gang barrier at the end of parallel

Work-sharing loops

- C/C++: #pragmaacc loop
 - Applies to the immediately following for loop
- Fortran: !\$acc loop
 - Applies to the immediately following do loop
- Loop will be automatically striped and assigned to different threads
 - Use the independent clause to force striping
- Convenience syntax combines parallel/kerne and loop constructs
 - #pragmaacc parallel loop
 - #pragmaacc kernels loop
 - !\$acc parallel loop
 - !\$acc kernels loop





Work-sharing loops - the collapse clause

- OpenACC vs. OpenMP
 - OpenACC: apply the loop directive to the follow N loops and possibly collapse their iteration spaces if independent
 - OpenMP: Collapse the iteration spaces of the following N loops



Controlling parallelism

- Amount of parallelism at the kernels and parallel level
 - num_gangs(...), num_workers(...), vector_length(...)
- At the loop level
 - gang, worker, vector

100 thread blocks with 128 threads each

```
!$acc parallel num_gangs(100), vector_length(128)
  !$acc loop gang, worker, vector
  do i = 1, n
      y(i) = y(i) + a*x(i)
  enddo
!$acc end parallel
```





Variable scoping

- Allowed in the parallel directive only
- private: A copy of the variable is placed in each gang (CUDA block)
- firstprivate: Same as private but initialized from the host value







Variable scoping

- Allowed in the parallel directive only
- private: A copy of the variable is placed in each gang (CUDA block)
- firstprivate: Same as private but initialized from the host value

Implicit scoping:

- (C/C++/Fortran) Scalar variables are firstprivate to the thread that executes the loop, array variables are shared in global memory (different to OpenMP!)
- (C/C++ only) Scope of variables declared inside a parallel block depends on the current execution mode:
 - Vector-partitioned mode → private to the thread
 - Worker-partitioned, Vector-single mode → private to the worker
 - Worker-single mode → private to the gang







Reduction operations

- #pragmaacc parallel reduction(<op>:<var>)
 - e.g., #pragmaacc parallel reduction(+:sum)
- #pragmaacc loop reduction(<op>:<var>)
- var must be scalar
- var is copied and default initialized within each gang
- Intermediate results from each gang are combined and made available outside the parallel region
- Complex numbers are also supported
- Operators: +, *, max, min, &, |, %, &&, | |





Calling functions from parallel regions

- #pragmaacc routine {gang | worker | vector | seq}
 - Just before the function declaration or definition
- !\$acc routine {gang | worker | vector | seq}
 - In the specification part of the subroutine
- Parallelism level of the routine
 - gang: must be called from GR context
 - worker: must be called from WS context
 - vector: must be called from VS context
 - seq: must be called from sequential context





Where is my data?

- The host and the device have separate address spaces
 - Data management between the host and the device is the programmer's responsibility
 - You must make sure that all the necessary data for a computation is available on the accelerator before entering the compute region
 - You must make sure to transfer the processed data back to the host if needed
 - Internally the address spaces are linked with a so-called present table



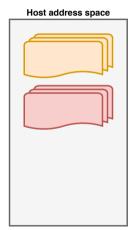


Where is my data?

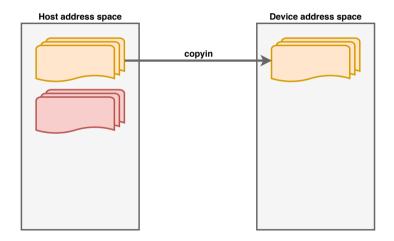
- The host and the device have separate address spaces
 - Data management between the host and the device is the programmer's responsibility
 - You must make sure that all the necessary data for a computation is available on the accelerator before entering the compute region
 - You must make sure to transfer the processed data back to the host if needed
 - Internally the address spaces are linked with a so-called present table
- But there can be some exceptions:
 - The "device" might be the multicore → no need for data management
 - Some compilers may infer automatically the necessary data transfers
 - Nvidia Pascal GPUs provide efficient support for a unified memory view ween the host and the accelerator



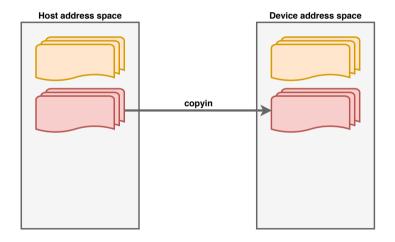




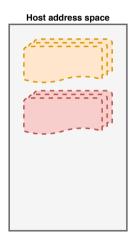


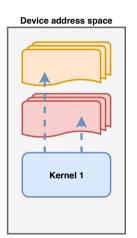


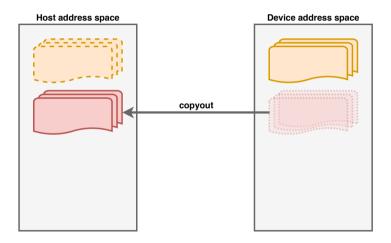




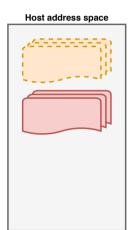


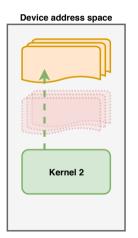


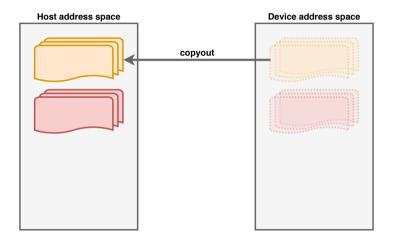






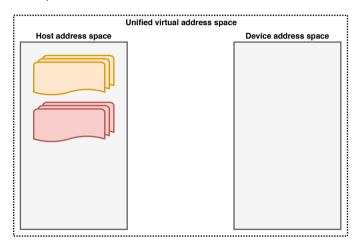






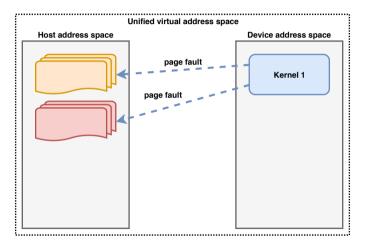


Unified memory address space



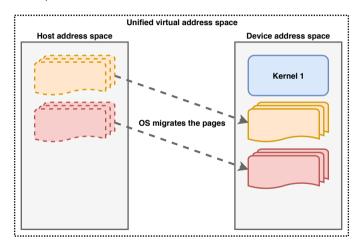


Unified memory address space





Unified memory address space





Directives accepting data clauses

Data clauses may appear in the following directives:

- Compute directives:
 - #pragmaacc kernels
 - #pragmaacc parallel
- Data directives:
 - #pragmaacc data
 - #pragmaacc enter data
 - #pragmaacc exit data
 - #pragmaacc declare
 - #pragmaacc update





Data clauses

- create(a[]): Allocate array a on device
- copyin(a[0:n]): Copy array a to device
- copyout(a[0:n]): Copy array a from device
- copy(a[0:n]): Copy array a to and from device
- present (a): Inform OpenACC runtime that array a is on device
- delete(a): Deallocate array a from device (exit data only)

Not for the acc update directive







The acc data directive

- Defines a scoped data region
 - Data will be copied in at entry of the region and copied out at exit
 - A structural reference count is associated with each memory region that appears in the data clauses
- C/C++: #pragma acc data [data clauses]
 - The next block of code is a data region
- Fortran: !\$acc data [data clauses]
 - Defines a data region until !\$acc end data is encountered





The acc enter/exit data directives

- Defines an unscoped data region
 - Data will be resident on the device till a corresponding exit data directive is found
 - Useful for managing data on the device across compilation units
 - A dynamic reference count is associated with each memory region that appears in the data clauses
- C/C++:
 - #pragmaacc enter data [data clauses]
 - #pragma acc exit data [data clauses]
- Fortran:
 - !\$acc enter data [data clauses]
 - !\$acc exit data [data clauses]



The acc declare directive



- Functions, subroutines and programs define implicit data regions
- The acc declare directive is used in variable declarations for making them available on the device during the lifetime of the implicit data region
- Useful for copying global variables to the device
- C/C++: #pragma acc declare [data clauses]
- Fortran: !\$acc declare [data clauses]
- The variables are not initalized





The acc update directive



 May be used during the lifetime of device data for updating the copies on either host or the device

- #pragmaacc update host(<var-list>)
 - Update host copy with corresponding data from the device

- #pragmaacc update device(<var-list>)
 - Update device copy with corresponding data from the host





Array ranges

Data clauses may accept as arguments:

Whole arrays



- C/C++: You must specify bounds for dynamically allocated arrays
 - #pragmaacc data copyin(a[0:n])
 - But #pragmaacc data present(a) is acceptable: a's bounds can be inferred by the runtime
- Fortran: array shape information is already embedded in the data type
 - !\$acc data copyin(a)
- Array subranges
 - C/C++: start and length
 - #pragmaacc data copyin(a[2:n-2])
 - Fortran: first index and last index
 - !\$acc data copyin(a[3:n])





Synchronization directives

- Atomic operations
 - #pragmaacc atomic [atomic-clause]
 - !\$acc atomic [atomic-clause]
 - Atomic clauses: read, write, update and capture
 - Example of "capturing" a value:
 - v = x++:
- No global barriers → cannot be implemented due to hardware restrictions
- No equivalent of __syncthreads()







Leverage the unified memory

- Virtual address space shared between CPU and GPU
- The CUDA driver and the hardware take care of the page migration
- Introduced with the Kepler architecture and CUDA 6, but is significantly improved with Pascal





Leverage the unified memory

- Virtual address space shared between CPU and GPU
- The CUDA driver and the hardware take care of the page migration
- Introduced with the Kepler architecture and CUDA 6, but is significantly improved with Pascal

- You could completely omit the data management in OpenACC!
- Supported by the PGI compiler using the -ta=tesla:managed option





Hands-on exercises

General information

- Base directory for the OpenACC exercises is topics/openacc:
- practicals/: The hands-on exercises
- solutions/: Where the solutions will appear
- ci/: Continuous integration tests for the exercises (ask me offline if interested)





Hands-on exercises

General information

grep TODO *.{cpp,f90,f03}



PGI compiler is recommended, GNU and Cray compiler are present in make files module load craype-accel-nvidia60 for loading CUDA and set the target architecture to the GPU

make

Exercise 1 - AXPY

- practicals/axpy/axpy_openacc.{cpp,f90}
- Run as: srun --reserv=summer_school -Cgpu ./axpy.openacc [ARRAY_SIZE]
 - ARRAY_SIZE is power of 2, default is 16
- Try with different sizes. Does the GPU outperform the CPU version?



Exercise 2 - Dot product

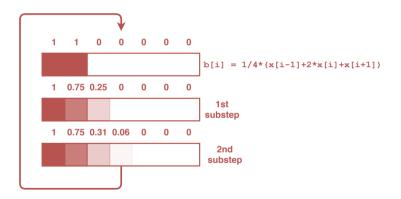
- practicals/basics/dot_openacc.{cpp,f90}
- Run as:

```
srun --reserv=summer_school -Cgpu ./dot.openacc [ARRAY_SIZE]
```

- ARRAY_SIZE is power of 2, default is 2
- Try with different sizes. Does the GPU outperform the CPU version?



Exercise 3 – 1D blur kernel





Exercise 3 - 1D blur kernel

- practicals/basics/blur_openacc.{cpp,f90}
- Run as: srun --reserv=summer_school -Cgpu ./blur.openacc [ARRAY_SIZE]
 - ARRAY_SIZE is multiple of 2, default is 20
- Offload to GPU the loops of the naive kernel; why is it so slow?

Exercise 3 – 1D blur kernel

- practicals/basics/blur_openacc.{cpp,f90}
- Run as: srun --reserv=summer_school -Cgpu ./blur.openacc [ARRAY_SIZE]
 - ARRAY_SIZE is multiple of 2, default is 20
- Offload to GPU the loops of the naive kernel; why is it so slow?
- Moving data to and from the device is slow (≈7–8 GB/s per direction)
- Avoid unnecessary data movement in the nocopies kernel
 - Move the necessary data to GPU early enough and keep it the slong as possible
 - Update host copies using #pragma acc update directive if needed



Exercise 4 – Experiment with the unified memory

- Remove all the data directives and data clauses
- Compile the blur_twice_naive kernel with -ta=tesla:managed
- How does it compare to the manual data management in terms of performance?
- Can you explain the performance difference?





By default, all OpenACC directives are blocking.

- The calling CPU thread must wait for the OpenACC operation (data transfer, kernel etc.) to complete
- All OpenACC operations are enqueued in a single activity queue (CUDA stream)
- All items in an activity queue are executed synchronously, but activity queues are independent from each other





OpenACC allows you to enqueue operations on different activity queues using the async clause and wait for them using the wait directive/clause.

- async (<qno>): push operations to activity queue qno and continue execution on the host
- wait(<qno>): wait for pending operations in activity queue qno to finish before launching next operation on the device
- #pragma acc wait(<qno>): Wait for all events in activity queue qno to finish before continuing execution on the host
 - Wait for all queues to finish if used without an argument





Example of operations pipelining

Operations are executed sequentially





Example of operations pipelining

```
Operations are pipelined
#pragma acc data ...
for (auto p = 0; p < n; ++p) {
    #pragma acc update device(A[p][0:m]) async(p)
    #pragma acc parallel loop async(p)
   for (auto i = 0; i < m; ++i) {
       // work on A[p] array
    #pragma acc update host(A[p][0:m]) asvnc(p)
#pragma acc wait
```

This concept is useful for overlapping computation and data transfers to the device.





Can I use a CUDA pointer inside OpenACC device context?

Can I call a CUDA function from OpenACC host context?

Short answer is yes.





Use CUDA pointers inside OpenACC device context

A scenario:

- Have a CUDA code that needs to call a function that uses OpenACC.
- This function may accept an array that has been allocated already on the GPU by CUDA.

The problem?

OpenACC only knows of pointers that it is managing itself; the present clause won't work. No idea what this pointer is; never seen it before!





Use CUDA pointers inside OpenACC device context

Solution:

- We need to instruct the OpenACC runtime to trust this pointer and that it is a valid device pointer.
- OpenACC runtime will just treat that pointer as known, but it won't check its shape.
- Use the deviceptr(<ptrlist>) clause with parallel, kernels and data directives

Use CUDA pointers inside OpenACC device context - Example

```
void copy(double *dst, const double *src, size_t n) {
  #pragma acc parallel loop deviceptr(dst, src)
  for (size_t i = 0; i < n; ++i) {</pre>
    dst[i] = src[i]:
int main() {
  double *a, *b;
  cudaMalloc(&a, 1024);
  cudaMalloc(&b, 1024);
  copy(b, a, 1024);
  return 0:
```





Register CUDA pointers in the present table with runtime library routine

Another scenario:

You want to call OpenACC code without deviceptr (<ptrlist>) clause, e.g., from OpenACC and CUDA.

The Solution:

You register the CUDA pointer with acc_map_data in the present table.

```
int main() {
   double *a_host, *a_device;
   a_host = new double[1024];
   cudaMalloc(&a_device, 1024);
   acc_map_data(a_host, a_device, sizeof(double)*1024);
   ...
   acc_unmap_data(a_host);
   ...
   return 0;
}
```



Call a CUDA function from OpenACC host context

Scenario:

My code is in OpenACC, but I need to call an optimized library written in CUDA, which accepts device pointers, e.g., cuBLAS.



Call a CUDA function from OpenACC host context

Scenario:

My code is in OpenACC, but I need to call an optimized library written in CUDA, which accepts device pointers, e.g., cuBLAS.

Problem:

I only "see" device pointers while in a parallel region, but I want to get a device pointer, while executing on the host.





Call a CUDA function from OpenACC host context

Scenario:

My code is in OpenACC, but I need to call an optimized library written in CUDA, which accepts device pointers, e.g., cuBLAS.

Problem:

I only "see" device pointers while in a parallel region, but I want to get a device pointer, while executing on the host.

Solution:

- Use a host_data region
 - #pragmaacc host_data use_device(<varlist>)





The host_data directive

- C/C++: #pragma acc host_data use_device(<varlist>)
 - In the next block of code the compiler will make available the device address of any variable in <varlist>.
- Fortran: !\$acc host_data use_device(<varlist>)
 - The compiler will make available the device address of any variable in <varlist>
 until a matching !\$acc end host_data is found.
- Optional clauses:
 - if (condition): Use the device pointer if condition is true.
 - if_present: Use the device pointer if variables in <varlist> are present on the device.

Heads-up: Remember this directive if you want to combine OpenACC and MPI.





Exercise 5 – Calling cuBLAS methods

Source code:

- practicals/gemm/gemm.cpp
- Run as:

```
srun --reserv=summer_school -Cgpu ./axpy.openacc [ARRAY_SIZE]
```

ARRAY_SIZE is power of 2, default is 8

Steps:

- 1. Compile with 'make CPPFLAGS=' to get also the naive implementation → too slow!
- 2. Offload the GEMM method to the GPU using OpenACC
- 3. Make use of cuBLAS GEMM through OpenACC
- 4. Compare the performance of the different versions



Exercise 6.1 – 2D diffusion example

Source code:

- diffusion2d_omp.{cpp,f90}: our baseline code
 - Single node OpenMP version for the CPU
- diffusion2d_openacc.{cpp,f90}
 - Single node OpenACC version
 - Run as:

- ARRAY_SIZE is power of 2, default is 16
- Fill in the parts where OPENACC_DATA is defined.





Exercise 6.2 – 2D diffusion example using CUDA data management

Source code:

- diffusion2d_openacc.{cpp,f90}
 - Single node OpenACC version
 - Single flode OpenACC versionRun as:

```
srun --reserv=summer_school -Cgpu ./diffusion2d.openacc.cuda [ARRA
```

- ARRAY_SIZE is power of 2, default is 16
- Fill in the parts where OPENACC_DATA is undefined.





Deep Copy The concept

True deep copy (ideal)

```
struct foo {
    int *arr;
    size_t len;
};
for (auto i = 0; i < 3; ++i) {
   f[i].len = 10;
   f[i].arr = new int[f[i].len];
#pragma acc enter data copyin(f[0:3])
```

Where will f [i] arr refer to?



Deep Copy

The concept

```
True deep copy (ideal)
struct foo {
    int *arr;
    size t len:
};
for (auto i = 0; i < 3; ++i) {
    f[i].len = 10;
    f[i].arr = new int[f[i].len];
#pragma acc enter data copyin(f[0:3])
```

- Where will f [i] .arr refer to? → They will be host pointers!
- Ideally, we would like everything to be magically copied.
 - Not so easy, especially for C/C++.





Deep Copy

The manual solution - OpenACC 2.6

- The runtime will attach the f[i] arr pointer to the device copy of the data.
- This happens implicitly if the f [i] . arr pointer is present on the device.





Deep Copy

The manual solution - OpenACC 2.6

Manual deep copy (bottom-up approach)

- At the time when f [i] . arr is copied to the device, the pointer is not already present on the device.
- If we copy the struct later, we need to manually attach the pointer to the device copy of the data.





OpenACC vs. OpenMP

- OpenMP 4.0 introduced directives for offloading computation to accelerators
- Similar concepts to OpenACC but OpenMP is a more prescriptive standard
- There is no OpenMP-OpenACC merger envisioned right now
- Compiler support for GPU targets
 - Cray
 - IBM XL
 - GCC (needs to be compiled specially)
 - Clang (under development)





OpenACC and compiler support

PGI

- Latest spec support; drives the OpenACC development
- Twice per year a community release

Cray

- Support up to OpenACC 2.0; no new features or later spec support
- Bug fixes and support for the current implementation only
- From CCE 9.0 onward support will be dropped

GCC

- Support of OpenACC 2.0a from GCC 5.1 onward
- Support of OpenACC 2.5 in development branch





More information and events

- http://www.openacc.org
 - Specification and related documents
 - Tutorials
 - Events
- GPU Hackathons
 - One week+ of intensive development for porting your code to the GPUs
 - 3 developers + 2 mentors per team
 - Several virtual events scheduled for 2020
 - Find the one that fits you and apply!









Porting the miniapp to GPUs using OpenACC

General information

- C++ only
- OpenACC version resides in miniapp/openacc
- MPI+OpenACC version resides in miniapp/mpi/openacc
- Plotting script inside the scripts/ folder
 - Use plot.sh in order not to mess with your environment.
- Interesting files
 - main.cpp: the solver
 - data.h: domain types
 - linalg.cpp: linear algebra kernels
 - operators.cpp: the diffusion kernel + communication routines





Differences to CUDA version

- No need for a separate kernels namespace
- No need for keeping a a copy of the device pointer
 - OpenACC runtime does just that for you
- No need for grid and block dimensions calculations
- The calculations for the interior points and the boundaries are based on the serial version





- There are two C++ abstractions that complicate things:
 - 1. Domain data is encapsulated inside the Field class
 - Allocated and initialized inside the constructor
 - Deallocated inside the destructor





- There are two C++ abstractions that complicate things:
 - 1. Domain data is encapsulated inside the Field class
 - · Allocated and initialized inside the constructor
 - Deallocated inside the destructor

Hint: OpenACC provides the enter data and exit data directives for unscoped data management





- There are two C++ abstractions that complicate things:
 - 1. Domain data is encapsulated inside the Field class
 - Allocated and initialized inside the constructor
 - Deallocated inside the destructor

Hint: OpenACC provides the enter data and exit data directives for unscoped data management

2. Operators for accessing the domain data





- There are two C++ abstractions that complicate things:
 - 1. Domain data is encapsulated inside the Field class
 - Allocated and initialized inside the constructor
 - Deallocated inside the destructor

Hint: OpenACC provides the enter data and exit data directives for unscoped data management

2. Operators for accessing the domain data

Hint: Operators are just another kind of functions; acc routine directive is just for that



Performance tips

- All OpenACC operations are synchronous. Do we really want that?
 - You may just push your operations to an activity queue (note: cuBLAS is pushing to queue 0), but . . .
 - ... you will need to synchronize sometimes!
- Fine tune your parallelism
- Try dropping the C++ operator abstractions
 - Code will become ugly (and error-prone), but you may get some bits of performance; judge if it's worth it.



