24th Summer School on PARALLEL COMPUTING

Introduction to Accelerator Computing with OpenACC and OpenMP 4 Directives

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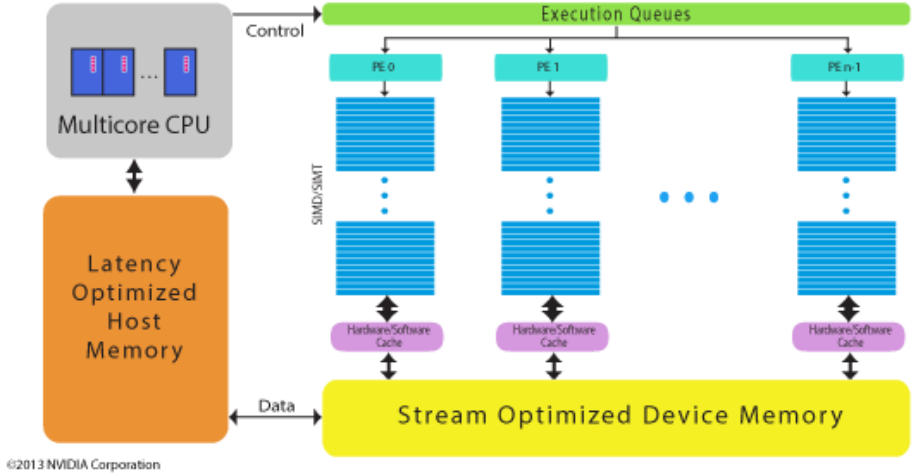
OPENACC: BASICS

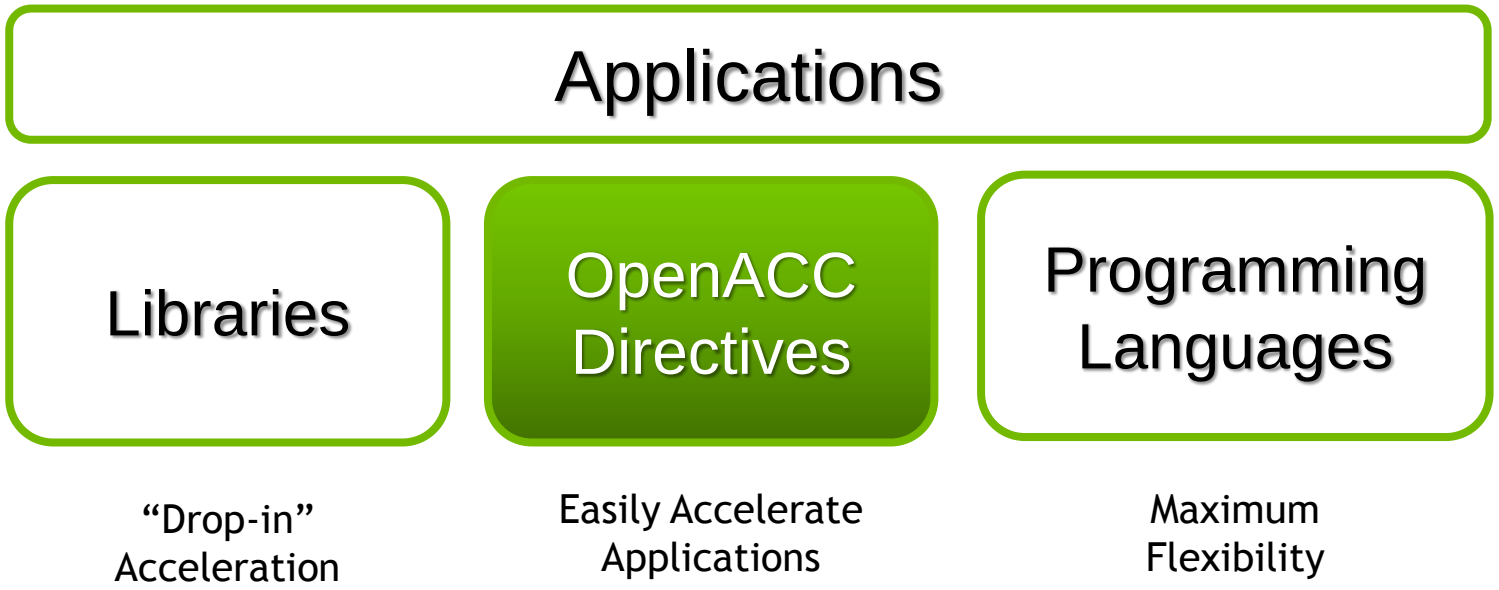
Common Accelerator Architecture Themes

- **NVIDIA GPU**
- **ATI GPU**
- **Intel MIC**

- Separate device memory
- Many-cores
- Multithreading
- Vectors
- In-order instruction issue
- Memory strides matter
- Smaller caches



3 Ways to Accelerate Applications



OpenACC friendly Disclaimer

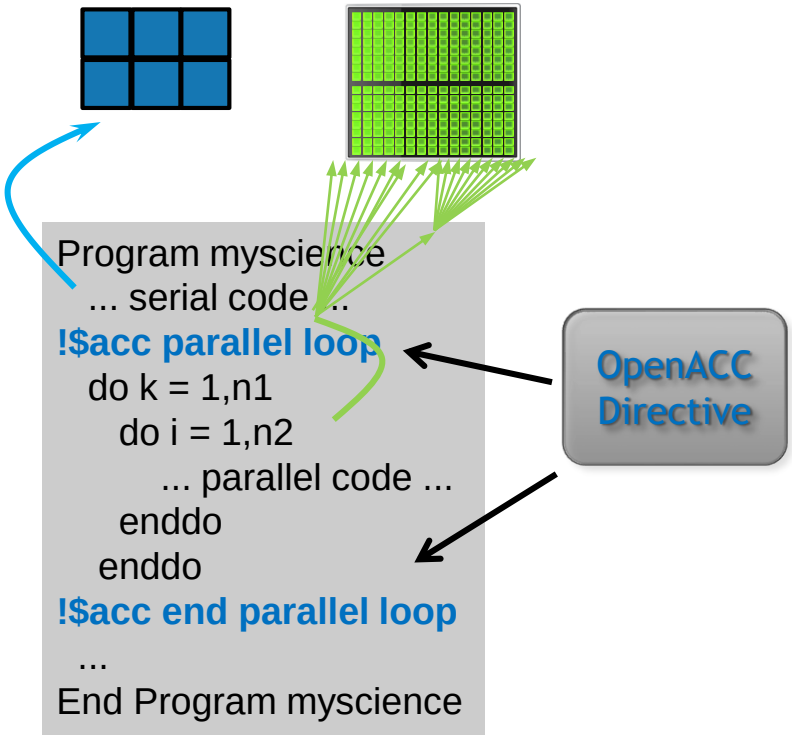
OpenACC Directives

Easily Accelerate Applications

OpenACC does not make GPU programming easy.
(...)
GPU programming and parallel programming is not easy. It cannot be made easy. However, GPU programming need not be difficult, and certainly can be made straightforward, once you know how to program and know enough about the GPU architecture to optimize your algorithms and data structures to make effective use of the GPU for computing. OpenACC is designed to fill that role.

(Michael Wolfe, The Portland Group)

OpenACC Directives



Simple Compiler directives

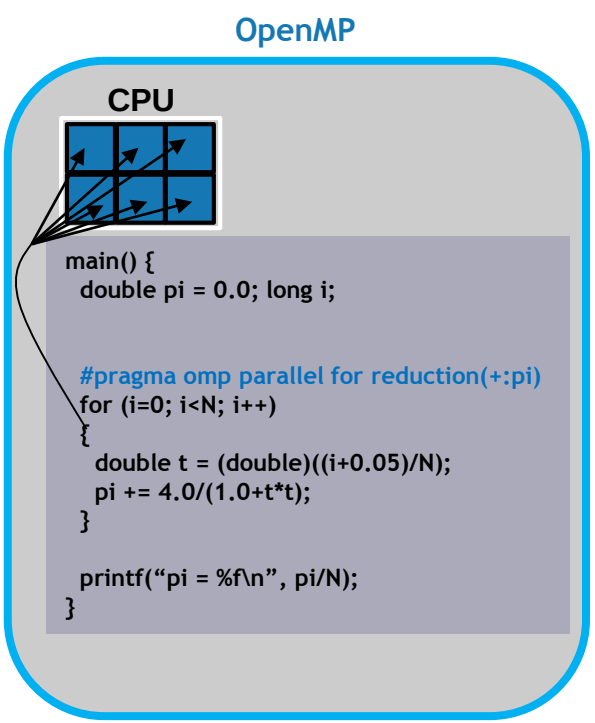
Compiler Parallelizes code

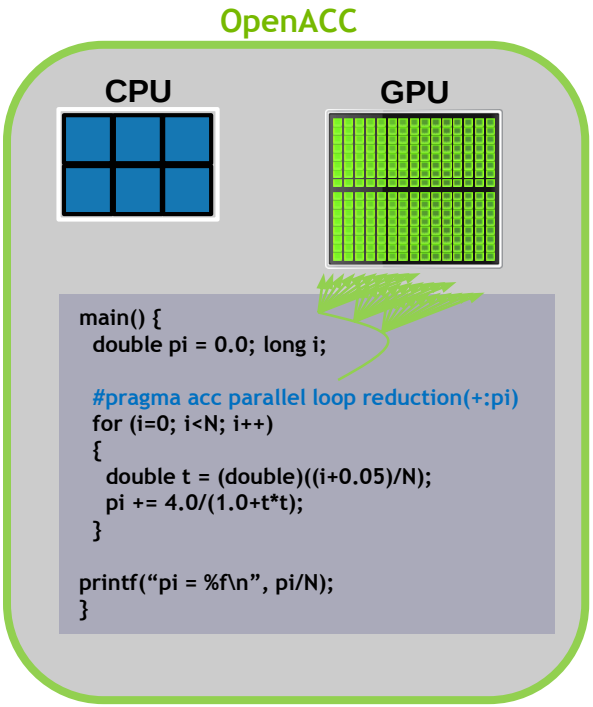
Works on many-core GPUs & multicore CPUs

OpenACC – Directive Based Approach

- Directives are added to serial source code
  - Manage loop parallelization
  - Manage data transfer between CPU and GPU memory
- Works with C, C++, or Fortran
  - Can be combined with explicit CUDA C/Fortran usage
- Directives are formatted as comments
  - They don't interfere with serial execution
- Maintaines portability of original code

Familiar to OpenMP Programmers





OpenACC

The Standard for GPU Directives

- **Easy:** Directives are the easy path to accelerate compute intensive applications
- **Open:** OpenACC is an open GPU directives standard, making GPU programming straightforward and portable across parallel and multi-core processors
- **Powerful:** GPU Directives allow complete access to the massive parallel power of a GPU

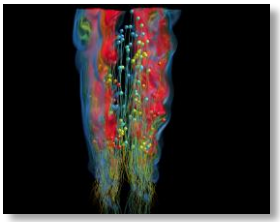
OpenACC®
DIRECTIVES FOR ACCELERATORS

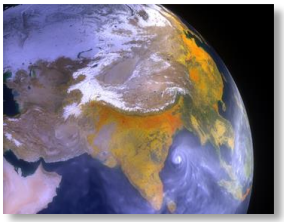
Focus on Exposing Parallelism

With Directives, tuning work focuses on *exposing parallelism*, which makes codes inherently better

Example: Application tuning work using directives for new Titan system at ORNL

S3D
Research more efficient combustion with next-generation fuels





- **Tuning top 3 kernels (90% of runtime)**
- ***3 to 6x faster on CPU+GPU vs. CPU+CPU***
- **But also improved all-CPU version by 50%**

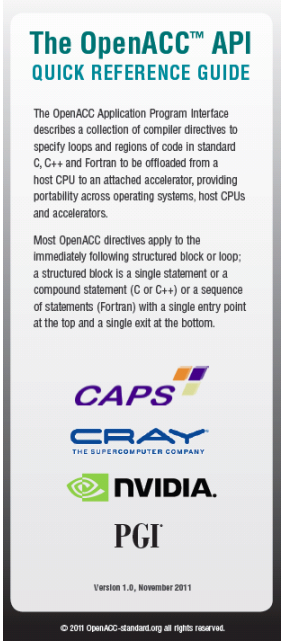
- **Tuning top key kernel (50% of runtime)**
- **6.5x faster on CPU+GPU vs. CPU+CPU**
- **Improved performance of CPU version by 100%**

OpenACC Specification and Website

- Full OpenACC 1.0 Specification available online
- OpenACC 2.0a revised on August 2013

  http://www.openacc-standard.org

- Novelty in OpenACC 2.0 are significant
  - OpenACC 1.0 maybe not very mature...
- Some changes are inspired by the development of CUDA programming model
  - but the standard is not limited to NVIDIA GPUs: one of its pros is the interoperability between platforms

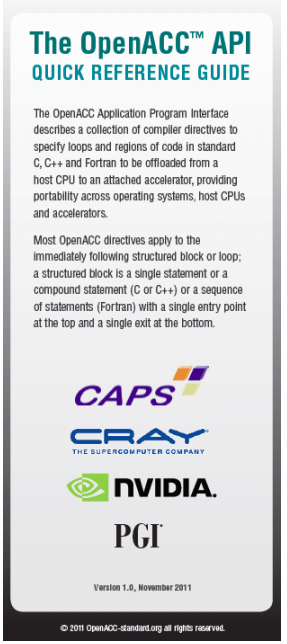


OpenACC: Implementations and Vendors

- Standard implementation
  - CRAY provides full OpenACC 2.0 support in CCE 8.2
  - PGI support to OpenACC 2.0 is almost complete
  - **GNU implementation effort ongoing (there is a partial implementation in the 5.1 release)**

- We will focus on PGI compiler
  - 30 days trial license useful for testing

- PGI:
  - all-in-one compiler, easy usage
  - sometimes the compiler tries to help you...
  - but also a constraint on the compiler to use



PGI compilers

- Check the feature you need!

Feature	Version	Feature	Version
!$acc kernels	12.3	!$acc declare	12.3
clauses:		clauses:	
if()	12.3	copy()/copyin()	12.3
async()	12.3	copyin()/copyout()	12.3
copy()	12.3	create()	12.3
copyin()	12.3	present()	12.3
copyout()	12.3	present_or_copy()	12.3
create()	12.3	present_or_copyin()	12.3
present()	12.3	present_or_copyout()	12.3
present_or_copy()	12.3	present_or_create()	12.3
present_or_copyin()	12.3	device_resident()	12.6
present_or_copyout()	12.3	deviceptr()	12.6
present_or_create()	12.3		
deviceptr()	12.3	!$acc update	12.3
		clauses:	
!$acc parallel	12.5	if()	12.3
clauses:		async()	12.3
if()	12.5		
async()	12.5	!$acc cache	12.6
num_gangs()	12.5		
num_workers()	12.6	!$acc host_data	14.1
vector_length()	12.5		

A Very Simple Exercise: SAXPY

```
void saxpy(int n,
           float a,
           float *x,
           float *restrict y)
{
#pragma acc parallel loop
  for (int i = 0; i < n; ++i)
    y[i] = a*x[i] + y[i];
}

...
// Perform SAXPY on 1M elements
saxpy(1<<20, 2.0, x, y);
...
```

```
subroutine saxpy(n, a, x, y)
  real :: x(:), y(:), a
  integer :: n, i
$!acc parallel loop
  do i=1,n
    y(i) = a*x(i)+y(i)
  enddo
$!acc end parallel loop
end subroutine saxpy


...
! Perform SAXPY on 1M elements
call saxpy(2**20, 2.0, x_d, y_d)
...
```

Directive Syntax

- C

  ```
  #pragma acc directive [clause [,] clause] …]
  ```

  Often followed by a structured code block

- Fortran

  ```
  !$acc directive [clause [,] clause] …]
  ```

  Often paired with a matching end directive surrounding a structured code block

  ```
  !$acc end directive
  ```

OpenACC parallel Construct

- Programmer **identifies** a block of code suitable for parallelization
  - and **guarantees** that no dependency occurs across iterations
- Compiler generates parallel instructions for that loop
  - e.g., a parallel CUDA kernel for a GPU

```
#pragma acc parallel loop
for (int j=1;j<n-1;j++) {
   for (int i=1;i<n-1;i++) {
       A[j][i] = B[j][i] + C[j][i]
   }
}
```

First let us focus on the simplest usage, combining `parallel` and `loop` directives

Another approach: kernels construct

- The `kernels` construct expresses that a region `may` contain parallelism and the compiler determines what can be safely parallelized

```
!$acc kernels
      do i=1,n
         a(i) = 0.0
         b(i) = 1.0
         c(i) = 2.0
      end do

      do i=1,n
         a(i) = b(i) + c(i)
      end do
!$acc end kernels
```

kernel 1

kernel 2

C

```
#pragma acc kernels [clause …]
    { structured block }
```

The compiler identifies 2 parallel loops and generates 2 kernels

OpenACC parallel vs. kernels

parallel

- Requires analysis by programmer to ensure safe parallelism
- Straightforward path from OpenMP
- Mandatory to fully control the different levels of parallelism
- Implicit barrier at the end of the parallel region

kernels

- Compiler performs parallel analysis and parallelizes what it believes safe
- Can cover larger area of code with a single directive
- Please, write clean codes and add directives to help the compiler
- Implicite barrier at the end and between each kernel (e.g. loop)

Which is the best?

C tip: the `restrict` keyword

- Declaration of intent given by the programmer to the compiler

  Applied to a pointer, e.g.

  ```
  float *restrict ptr
  ```

  Meaning: “for the lifetime of `ptr`, only it or a value directly derived from it (such as `ptr + 1`) will be used to access the object to which it points”*
- Limits the effects of pointer aliasing
- OpenACC compilers often require `restrict` to determine independence between the iterations of a loop
  - Crucial when adopting `kernels` directive, but also for other optimizations
  - Note: if the programmer violates the declaration, the behavior is undefined

Complete SAXPY example code

- Use restrict to help the compiler when adopting **kernels**
  - Apply a **loop** directive
- Be careful: restrict is C99 but not C++ standard

```
#include <stdlib.h>

void saxpy(int n,
           float a,
           float *x,
           float *restrict y)
{
#pragma acc kernels
for (int i = 0; i < n; ++i)
    y[i] = a * x[i] + y[i];
}
```

*restrict:
"I promise y does not alias x"

```
int main(int argc, char **argv)
{
  int N = 1<<20; // 1 million floats

  if (argc > 1)
    N = atoi(argv[1]);

  float *x = (float*)malloc(N * sizeof(float));
  float *y = (float*)malloc(N * sizeof(float));

  for (int i = 0; i < N; ++i) {
    x[i] = 2.0f;
    y[i] = 1.0f;
  }

  saxpy(N, 3.0f, x, y);

  return 0;
}
```

Loop Construct

- Applies to a loop which must immediately follow this directive
- Describes:
  - type of parallelism
  - loop-private variables, arrays, and reduction operations
- We already encountered it combined with the parallel directive
  - combining kernels and loop is also possible but limits the capability of kernels construct (i.e. extending to wide regions of code)

C

```
#pragma acc loop [clause …]
    { for block }
```

Fortran

```
!$acc loop [clause …]
    { do block }
```

Independent clause

- In a **kernels** construct, the **independent loop** clause helps the compiler in guaranteeing that the iterations of the loop are independent wrt each other
- E.g., consider m>n

```
#pragma acc kernels
#pragma acc loop independent
    for(int i;i<n;i++)
            c[i] = 2.*c[m+i];
```

- In **parallel** construct the independent clause is implied on all **loop** directives without a **seq** clause

Seq and collapse

- The seq clause specifies that the associated loops have to be executed sequentially on the accelerator
- Beware: the loop directive applies to the immediately following loop

```
#pragma acc parallel
#pragma acc loop collapse(2)      // independent is automatically enforced
for(int i;i<n;i++)
for(int k;k<n;k++)
#pragma acc loop seq
for(int j;j<n;j++)
            c[i][j][k] = 2.*c[i][j+1][k];
```

- collapse(<n_loops>) clause allows for extending loop to tightly nested loops
  - but the compiler may decide to collapse loops anyway, check the report!

Loop reductions

- The **reduction** clause on a loop specifies a reduction operator on one or more scalar variables
  - For each variable, a private copy is created for each thread executing the associated loops
  - At the end of the loop, the values for each thread are combined using the reduction clause

- Reductions may be defined even at **parallel** level (advanced topic)

- Common operators are supported:

+ * max min && || ....

Finding Parallelism in your code

- (Nested) **for** loops are best for parallelization
- Large loop counts needed to offset GPU/memcpy overhead
- Iterations of loops must be independent of each other
  - To help compiler: **restrict** keyword (C), **independent** clause
- Compiler must be able to figure out sizes of data regions
  - You can use directives to explicitly control sizes (see next)
- Pointer arithmetic should be avoided if possible
  - Use subscripted arrays, rather than pointer-indexed arrays.
- Function calls within accelerated regions must be handled with care

Environment and Conditional Compilation

`ACC_DEVICE` *`device`*	Specifies which device type to connect to.
`ACC_DEVICE_NUM num`	Specifies which device number to connect to.
`_OPENACC`	Preprocessor directive for conditional compilation. Set to OpenACC version

Runtime Library Routines

Fortran

```
use openacc
#include "openacc_lib.h"
```

```
acc_get_num_devices
acc_set_device_type
acc_get_device_type
acc_set_device_num
acc_get_device_num
acc_async_test
acc_async_test_all
```

C

```
#include "openacc.h"
```

```
acc_async_wait
acc_async_wait_all
acc_shutdown
acc_on_device
acc_malloc
acc_free
```

Selecting the device

- Device selection can be achieved by OpenACC runtime library routines
  - device type: acc_device_cuda/acc_device_nvidia for PGI
  - GPUs are numbered starting from 0 (PGI)

```
#ifdef _OPENACC
   int mygpu, myrealgpu, num_devices;     acc_device_t my_device_type;
#ifdef CAPS
   my_device_type = acc_device_cuda;
#elif PGI
   my_device_type = acc_device_nvidia;
#endif
   if(argc == 1) mygpu = 0; else mygpu = atoi(argv[1]);
   acc_set_device_type(my_device_type) ;
   num_devices = acc_get_num_devices(my_device_type) ;
   fprintf(stderr,"Number of devices available: %d \n ",num_devices);
   acc_set_device_num(mygpu,my_device_type);
   fprintf(stderr,"Trying to use GPU: %d \n",mygpu);
   myrealgpu = acc_get_device_num(my_device_type);
   fprintf(stderr,"Actually I am using GPU: %d \n",myrealgpu);
  if(mygpu != myrealgpu) {fprintf(stderr,"I cannot use the requested GPU: %d\n",mygpu);exit(1); }
#endif
```

Compiling and running (PGI)

- Example of compilation:

```
pgcc -acc=noautopar -ta=nvidia -Minfo=accel -o saxpy_acc saxpy.c -DPGI
```

noautopar is needed to avoid automatic parallelization of loops

- Compiler output (-Minfo=accel):

```
pgcc -acc -Minfo=accel -ta=nvidia -o saxpy_acc saxpy.c
saxpy:
      8, Generating copyin(x[:n-1])
         Generating copy(y[:n-1])
         Generating compute capability 1.0 binary
         Generating compute capability 2.0 binary
      9, Loop is parallelizable
         Accelerator kernel generated
          9, #pragma acc loop worker, vector(256) /* blockIdx.x threadIdx.x */
             CC 1.0 : 4 registers; 52 shared, 4 constant, 0 local memory bytes; 100% occupancy
             CC 2.0 : 8 registers; 4 shared, 64 constant, 0 local memory bytes; 100% occupancy
```

– For the hands-on, compile using the makefile and run by typing
  - **make pgi**
  - **./laplace2d_acc_pgi N** **(N is the GPU number to use, 0 1 2 ...)**

Submission scripts

Submission scripts

submit_acc.sh – submit_omp.sh – submit_mpiacc.sh

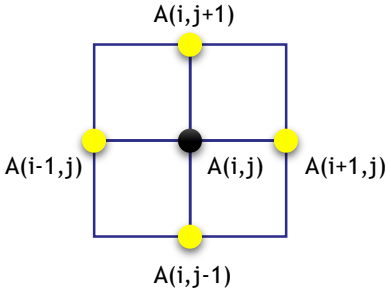
```
#!/bin/bash
#PBS -N laplace_acc
#PBS -o job.out
##PBS -e job.err
#PBS -j oe
#PBS -l walltime=00:10:00
#PBS -l select=1:ncpus=1:ngpus=1:mpiprocs=1
#PBS -q debug
#PBS -A train_scA2014
##PBS -q R426809

module load pgi/14.1
cd $PBS_O_WORKDIR
DIR=001-laplace2D-accparallel
#DIR=002-laplace2D-kernels
#DIR=003-laplace2D-collapse
#DIR=004-laplace2D-data
#DIR=005-laplace2D-declare
#DIR=006-laplace2D-function
#DIR=007-laplace2D-withcuda
#DIR=008-laplace2D-dynamic
#DIR=009-laplace2D-c++
cd $DIR
./laplace2d_acc_pgi
```

Example: Jacobi Iteration

- Iteratively converges to correct value (e.g. Temperature), by computing new values at each point from the average of neighboring points.
  - Common, useful algorithm
  - Example: Solve Laplace equation in 2D:

$$\nabla^2 f(x,y) = 0$$



$$A_{k+1}(i,j) = \frac{A_k(i-1,j) + A_k(i+1,j) + A_k(i,j-1) + A_k(i,j+1)}{4}$$

Jacobi Iteration C Code

```
while ( error > tol && iter < iter_max ) {
  error=0.0;

  for( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {


      Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                           A[j-1][i] + A[j+1][i]);


      error = max(error, abs(Anew[j][i] - A[j][i]);
    }
  }

  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }

  iter++;
}
```

Note! This is an didactic implementation: the second loop could be avoided implementing a 2-step iteration A->Anew ; Anew->A

- Iterate until converged
- Iterate across matrix elements
- Calculate new value from neighbors
- Compute max error for convergence
- Swap input/output arrays

Jacobi Iteration Fortran Code

```
do while ( err > tol .and. iter < iter_max )
  err=0._fp_kind

  do j=1,m
    do i=1,n


      Anew(i,j) = .25_fp_kind * (A(i+1, j  ) + A(i-1, j  ) + &
                                 A(i  , j-1) + A(i  , j+1))


      err = max(err, Anew(i,j) - A(i,j))
    end do
  end do

  do j=1,m-2
    do i=1,n-2
      A(i,j) = Anew(i,j)
    end do
  end do

  iter = iter +1
end do
```

- Iterate until converged
- Iterate across matrix elements
- Calculate new value from neighbors
- Compute max error for convergence
- Swap input/output arrays

Base Exercise 0: OpenMP C Code

```
while ( error > tol && iter < iter_max ) {
  error=0.0;

#pragma omp parallel for shared(m, n, Anew, A) reduction(max:error)
  for( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {

      Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                           A[j-1][i] + A[j+1][i]);

      error = max(error, abs(Anew[j][i] - A[j][i]);
    }
  }

#pragma omp parallel for shared(m, n, Anew, A)
  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }

  iter++;
}
```

Parallelize loop across CPU threads

Parallelize loop across CPU threads

Base Exercise 0: OpenMP Fortran

```
do while ( err > tol .and. iter < iter_max )
  err=0._fp_kind

!$omp parallel do shared(m,n,Anew,A) reduction(max:err)
  do j=1,m
    do i=1,n

      Anew(i,j) = .25_fp_kind * (A(i+1, j  ) + A(i-1, j  ) + &
                                 A(i  , j-1) + A(i  , j+1))

      err = max(err, Anew(i,j) - A(i,j))
    end do
  end do

!$omp parallel do shared(m,n,Anew,A)
  do j=1,m-2
    do i=1,n-2
      A(i,j) = Anew(i,j)
    end do
  end do

  iter = iter +1
end do
```

Parallelize loop across CPU threads

Parallelize loop across CPU threads

Exercises: More Compiling Instructions

- To compile, first load environment variables for the compiler
  `module load pgi/14.10`
- Then, use the provided makefile, e.g.
  `> cd 000-laplace2D-openmp`
  C:
  ➢ `make pgi`

`Take the elapsed times using 1 or more threads`

- setenv OMP_NUM_THREADS 6 if using tcsh
- export OMP_NUM_THREADS=6 if using bash

Exercise 1: Jacobi Acc parallel

- Task: use **acc parallel** to parallelize the Jacobi nested loops
- Edit laplace2d.c
  - In the `001-laplace2D-accparallel` directory
  - Add directives where needed
  - Modify the Makefile to activate the acceleration
    - **PGI compiler**
    - **Figure out the proper compilation commands (similar to SAXPY example)**
  - Compile and run the OpenACC version and compare the performances with that of OpenMP version, in the `000-laplace2D-openmp`
    - **compare the performances using OMP_NUM_THREADS=1 and OMP_NUM_THREADS=4 or more**

Exercise 1 Solution: C Makefile

```
PGCC        = pgcc -acc=noautopar -ta=nvidia,time,cuda5.0,cc35 -Minfo=accel -O3
GCC         = gcc -O3 #-Wall -Wextra

BIN = laplace2d_acc_pgi laplace2d_acc_caps

help:
        @echo "Please specify the make target according to the compiler"
        @echo "make pgi"

pgi: laplace2d.c
        $(PGCC) -o laplace2d_acc_$@ $<

clean:
        $(RM) $(BIN) __hmpp*
```

Exercise 1 Solution: Fortran

```
F90       = pgf90
CCFLAGS   =
ACCFLAGS = -acc=noautopar -ta=nvidia,time,cuda5.0,cc35 -Minfo=accel -O3
OMPFLAGS = -fast -mp -Minfo

BIN =  laplace2d_f90_omp laplace2d_f90_acc

all: $(BIN)

laplace2d_f90_acc: laplace2d.f90
        $(F90) $(CCFLAGS) $(ACCFLAGS) -o $@ $<

laplace2d_f90_omp: laplace2d.f90
        $(F90) $(CCFLAGS) $(OMPFLAGS) -o $@ $<

clean:
        $(RM) $(BIN)
```

Exercise 1: Compiler output (C - PGI)

```
pgcc  -acc -ta=nvidia -Minfo=accel -o laplace2d_acc laplace2d.c
main:
     57, Generating copyin(A[:4095][:4095])
         Generating copyout(Anew[1:4094][1:4094])
         Generating compute capability 1.3 binary
         Generating compute capability 2.0 binary
     58, Loop is parallelizable
     60, Loop is parallelizable
         Accelerator kernel generated
         58, #pragma acc loop worker, vector(16) /* blockIdx.y threadIdx.y */
         60, #pragma acc loop worker, vector(16) /* blockIdx.x threadIdx.x */
             Cached references to size [18x18] block of 'A'
             CC 1.3 : 17 registers; 2656 shared, 40 constant, 0 local memory bytes; 75% occupancy
             CC 2.0 : 18 registers; 2600 shared, 80 constant, 0 local memory bytes; 100% occupancy
         64, Max reduction generated for error
     69, Generating copyout(A[1:4094][1:4094])
         Generating copyin(Anew[1:4094][1:4094])
         Generating compute capability 1.3 binary
         Generating compute capability 2.0 binary
     70, Loop is parallelizable
     72, Loop is parallelizable
         Accelerator kernel generated
         70, #pragma acc loop worker, vector(16) /* blockIdx.y threadIdx.y */
         72, #pragma acc loop worker, vector(16) /* blockIdx.x threadIdx.x */
             CC 1.3 : 8 registers; 48 shared, 8 constant, 0 local memory bytes; 100% occupancy
             CC 2.0 : 10 registers; 8 shared, 56 constant, 0 local memory bytes; 100% occupancy
```

Exercise 1: Performance

2 eight-core Intel(R) Xeon(R) CPU E5-2687W @ 3.10GHz

GPU: Nvidia Tesla K20s

Execution	Time (s) - PGI
CPU 1 OpenMP thread	21.9
CPU 2 OpenMP threads	11.3
CPU 4 OpenMP threads	6.0
CPU 8 OpenMP threads	3.7
CPU 16 OpenMP threads	3.3
OpenACC GPU	**30**

accelerated?
NO!

Exercise 2: Jacobi Acc kernels

- Task: use **acc kernels** to parallelize the Jacobi loops
- For this simple case, no significant difference wrt **acc parallel**
  - but, try to understand the compiler report to be sure about what the compiler is doing
- Edit laplace2d.c in the `002-laplace2D-kernels` directory
  - any change in performances?
  - actually, no significant change...

Exercise 3: Collapsing loops

- Look at the compiler report:
  - GPUs work well when there is a large number of iterations to be parallelized
  - exploiting multiple loop nesting is crucial
- Use loop construct and collapse clause to optimize loops
  - which loop is actually affected? why?
- Edit laplace2d.c in the `003-laplace2D-collapse` directory
  - any change in performances?

Exercise 3: Performance

2 eight-core Intel(R) Xeon(R) CPU E5-2687W @ 3.10GHz

GPU: Nvidia Tesla K20s

Execution	Time (s) - PGI
CPU 1 OpenMP thread	21.9
CPU 8 OpenMP threads	3.7
OpenACC GPU-parallel	**30**
OpenACC GPU-collapse	**27**

Small performance gain. For PGI *noautopar* is crucial, otherwise inner loop is always parallelized

What is going wrong?

- Add `-ta=nvidia,time` to compiler command line

```
Accelerator Kernel Timing data
001-laplace2D-kernels/laplace2d.c
  main
    69: region entered 1000 times
        time(us): total=77524918 init=240 region=77524678
                  kernels=4422961 data=66464916
        w/o init: total=77524678 max=83398 min=72025 avg=77524
        72: kernel launched 1000 times
            grid: [256x256]  block: [16x16]
            time(us): total=4422961 max=4543 min=4345 avg=4422
001-laplace2D-kernels/laplace2d.c
  main
    57: region entered 1000 times
        time(us): total=82135902 init=216 region=82135686
                  kernels=8346306 data=66775717
        w/o init: total=82135686 max=159083 min=76575 avg=82135
        60: kernel launched 1000 times
            grid: [256x256]  block: [16x16]
            time(us): total=8201000 max=8297 min=8187 avg=8201
        64: kernel launched 1000 times
            grid: [1]  block: [256]
            time(us): total=145306 max=242 min=143 avg=145
acc_init.c
  acc_init
    29: region entered 1 time
        time(us): init=158248
```

4.4 seconds

66.5 seconds

8.3 seconds

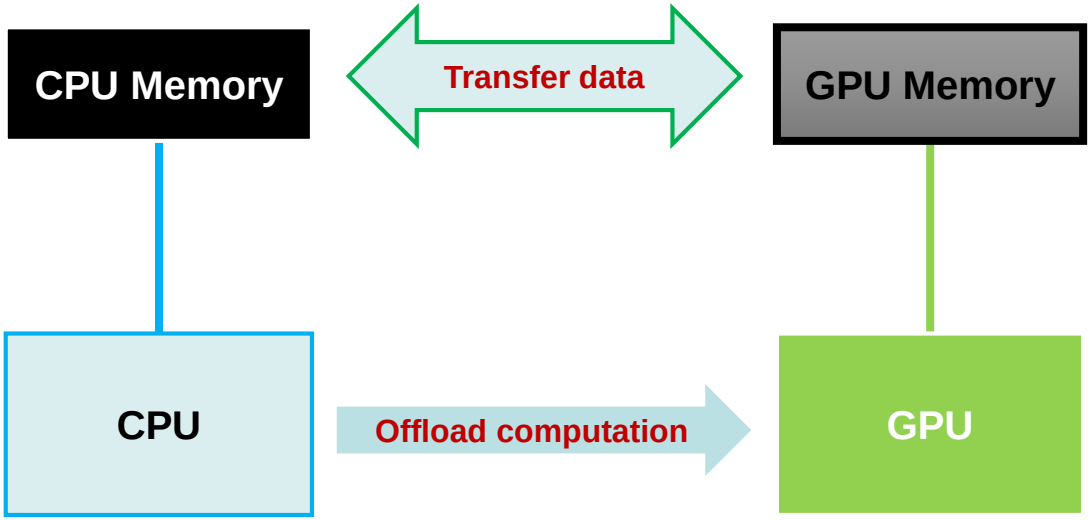
66.8 seconds

Huge Data Transfer Bottleneck!

Computation: 12.7 seconds

Data movement: 133.3 seconds

Basic Concepts



For efficiency, decouple data movement and compute off-load

Excessive Data Transfers

```
while ( error > tol && iter < iter_max ) {
  error=0.0;
```

A, Anew resident on host

Copy

```
#pragma acc parallel loop reduction(max:error)
```

A, Anew resident on accelerator

```
for( int j = 1; j < n-1; j++) {
  for(int i = 1; i < m-1; i++) {
    Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                         A[j-1][i] + A[j+1][i]);
    error = max(error, abs(Anew[j][i] - A[j][i]);
  }
}
```

A, Anew resident on accelerator

Copy

A, Anew resident on host

```
    ...
}
```

These copies happen every iteration of the outer while loop!*

*Note: there are two #pragma acc kernels, so there are 4 copies per while loop iteration!

Golden rule: check the compiler report!

```
pgcc  -acc -ta=nvidia -Minfo=accel
laplace2d.c
main:
  57, Generating copyin(A[:4095][:4095])
      Generating
copyout(Anew[1:4094][1:4094])
  .........
  69, Generating copyout(A[1:4094][1:4094])
      Generating copyin(Anew[1:4094][1:4094])
  .........
```

- The compiler tries to minimize the CPU-GPU data movements
- In the previous case
  - in the first loop :
    - A is copied in, from CPU to GPU
    - Anew is copied out, from GPU to CPU
  - in the second loop:
    - Anew is copied in
    - A is copied out

DATA MANAGEMENT

Explicit data control: the naive way

- It is possible to explicitely control the data movements at the opening of the **acc parallel** regions using **data clauses**

```
#pragma acc parallel loop reduction(max:error) copyin(A) copyout(Anew)
   for( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {
      Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                           A[j-1][i] + A[j+1][i]);
      error = max(error, abs(Anew[j][i] - A[j][i]);
    }
  }
#pragma acc parallel loop copyin(Anew) copyout(A)
  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }
```

- **But we cannot lower down the amount of copies because the scope of the GPU variables is limited to the accelerated regions. What now?**

Data Construct

C

```
#pragma acc data [clause …]
   { structured block }
```

Fortran

```
!$acc data [clause …]
   structured block
!$acc end data
```

- Manages explicitely data movements
- Crucial to handle GPU data persistence
- Allows for decoupling the scope of GPU variables from that of the accelerated regions
- May be nested
- Data clauses define different possible behaviours
  - the usage is similar to that of data clauses in parallel regions

Data Clauses

`copy ( list )` **Allocates memory on GPU and copies data from host to GPU when entering region and copies data to the host when exiting region.**

`copyin ( list )` **Allocates memory on GPU and copies data from host to GPU when entering region.**

`copyout ( list )` **Allocates memory on GPU and copies data to the host when exiting region.**

`create ( list )` **Allocates memory on GPU but does not copy.**

`present ( list )` **Data is already present on GPU from another containing data region.**

and `present_or_copy[in|out]`, `present_or_create`, `deviceptr`.

Array Shaping

- The compiler sometimes cannot determine the sizes of arrays
  - you must specify them by using data clauses and array “shape”
  - you may need just a section of an array
  - sub-array syntax is allowed, in Fortran it is language-native
- C

  #pragma acc data copyin(a[1:size]), copyout(b[s/4:3*s/4+1])

- Fortran

  !$pragma acc data copyin(a(1:size)), copyout(b(s/4:s))

- Data clauses can be used on data, kernels or parallel

Update Executable Directive

Fortran

```
!$acc update [clause …]
```

C

```
#pragma acc update [clause …]
```

Clauses:

```
host( list ) or self(list)
              device( list )
```

- Used to synchronize data among existing data when they change in the corresponding copy (e.g. update device copy after host copy changes)
- Note: subarray may be updated but updated memory must be contiguous
- Moves data from GPU to host, or host to GPU
- Data movement can be conditional and asynchronous

Exercise 4: Jacobi Data Directives

- Task: use **acc data** to minimize transfers in the Jacobi example
- Start from given laplace2d.c In the `002-laplace2d-data` directory
  - Add directives where needed
- Q: What speedup can you get with data + kernels directives?
  - Versus 1 CPU core? Versus 8 CPU cores?

Exercise 4: Performance

2 eight-core Intel(R) Xeon(R) CPU E5-2687W @ 3.10GHz

GPU: Nvidia Tesla K20s

Execution	Time (s) - PGI
CPU 1 OpenMP thread	21.9
CPU 8 OpenMP threads	3.7
OpenACC GPU-parallel	**30**
OpenACC GPU-collapse	**30**
OpenACC GPU-data	**0.9**

14x compared to 1 core!
4x compared to 8 cores!

Declare data

- It is possible to further extend the scope of data on the device
  - it significantly enhances code readability and maintainability

- The **declare** directive specifies that a variable or array has to be allocated in the device memory for the duration of the implicit data region of a function
  - used in the declaration section of a function
  - may specify whether the data have to be transferred and how
  - for global scope variables, the implicit region is the whole program

C

```
float a[100];
#pragma acc declare create(A)
```

Fortran

```
real A(100)
!$acc declare create(A)
```

Declare data - 2

- Standard data clauses may be specified
  - copy, copyin, copyout, create, present, ... (restrictions apply for global variables)
  - specific data clauses may be employed, too
- **device_resident**
  - the memory has to be allocated on the accelerator memory and not on the host memory
- **link**
  - only a global link for the named variable should be statically created in the accelerated memory
  - to be used for large global host static data referenced within an accelerated routine
- The compiler implementations may still lag behind

Exercise 5

- Employ the **declare** directive to manage the data persistence and transfer
- Ensure that the data are correctly synchronized before and after the accelerated regions
  - beware: the default behavior for arrays is **present_or_copy** and only one number is interpreted as the size
  - hence, you need to **update** data on device or host

check the support of your compiler for declare!

Data and functions

- What happens when calling a function from a data region?
  - e.g., consider that the updating of A, including the loops, is performed by a function
  - the data region opened by the calling function applies
  - default behaviours when considering each parallel region
  - in C you just have to take care of the reduction variable using a temporary variable

```
void update_A(int n, int m, double *error)
{
double error_loc = 0.0;
#pragma acc parallel loop \
        reduction(max: error_loc)
for( int j = 1; j < n-1; j++)
{
 for( int i = 1; i < m-1; i++ )
 {
  Anew[j][i] = 0.25 * ( A[j][i+1] +
     A[j][i-1]+ A[j-1][i] + A[j+1][i]);
  error_loc = fmax(error_loc,
           abs(Anew[j][i] - A[j][i]));
  }
}
*error = error_loc ;
}
```

Default behaviours and Privatization

- For arrays present_or_copy: no GPU allocation nor CPU-GPU copies are performed if the variable exists in a surrounding data region
  - i.e., the default behavior is shared, but private clause may be enforced to loop
- For scalars the rules are not trivial
  - for acc parallel regions, the default is firstprivate (private but initialized with the global value)
  - for kernels, default is copy (in and out), and private cannot be specified
  - if needed, it is usually best to specify private at the loop construct level

```
void copy_A(int n, int m) {
#pragma acc parallel loop
for( int j = 1; j < n-1; j++) {
   #pragma acc loop private(Asca)
   for( int i = 1; i < m-1; i++ )  {
      Asca = Anew[j][i];
      A[j][i] = Asca;
    }
 } }
```

check the compiler report!
PGI compiler performs a live-in/live-out analysis to help you

Exercise 6

- Add directives for the case with called functions
  - Look at the compiler messages: what about intermediate copies of A and Anew? Why?
- Add also the value of A(2,2) printed together to iter,error
- Update subarray rules:
  - **In fortran v(start_x:end_x,start_y:end_y)**
    - **if start or end are not specified, the array bounds are used**
    - **and only one number is interpreted as the end**
  - **In C v[start_x:size_x][start_y:size_y]**
    - **if start or size are not specified, the array bounds are used, if known**
    - **and only one number is interpreted as the size**

multidimensional section updates not supported by CAPS 3.4.1, update the whole matrix

Calling functions

- What happens if an accelerated region calls a function?
  - e.g., performing the updating for each grid point

```
#pragma acc parallel loop
for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
            update_grid_point(m,n,i,j);
            error = fmax( error, fabs(Anew[j][i] - A[j][i]));
        }
}
```

- According to OpenACC1.0, the only solution is to inline the function
  - it can be done manually
  - or by relying on smart usage of the preprocessor
  - or the compiler may inline the function, using adequate options

Inlining tricks

- Inlining of functions depends on the compiler skills
- But you can help the compiler
- Two important points when using PGI

  –Minline=name:<function name>

  – automatic arrays defined inside the function must be avoided: pass them even if you do not need their values in the calling program
  – in Fortran, reshaping arrays (different shapes of array from caller to dummy arguments) must be explicitely requested specifying

    –Minline=reshape

Linking accelerated functions

- From OpenACC 2.0, the **acc routine** allows for effective separate compilation and correct linking
  - it tells the compiler that there will be a device copy of the routine

```
#pragma acc routine
extern void update_grid_point(n,m,i,j);

#pragma acc parallel loop
for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ )        {
           update_grid_point(m,n,i,j);
           error = fmax( error, fabs(Anew[j][i] - A[j][i]));
       }
}
#pragma acc routine
extern void update_grid_point(n,m,i,j) {
...
}
```

Linking accelerated functions / 2

- Crucial to keep the existing code modularity
- Check if available with your compiler!
- It is possible to rename the device function using the bind clause
  - it tells the compiler that there will be a device version of the routine with a different name
  - and when defining the function nohost avoid the host compilation

```
#pragma acc routine bind(update_grid_point_dev)
extern void update_grid_point(n,m,i,j);

#pragma acc parallel loop
......

#pragma acc routine nohost
extern void update_grid_point_dev(n,m,i,j) {
...
}
```

Further speedups

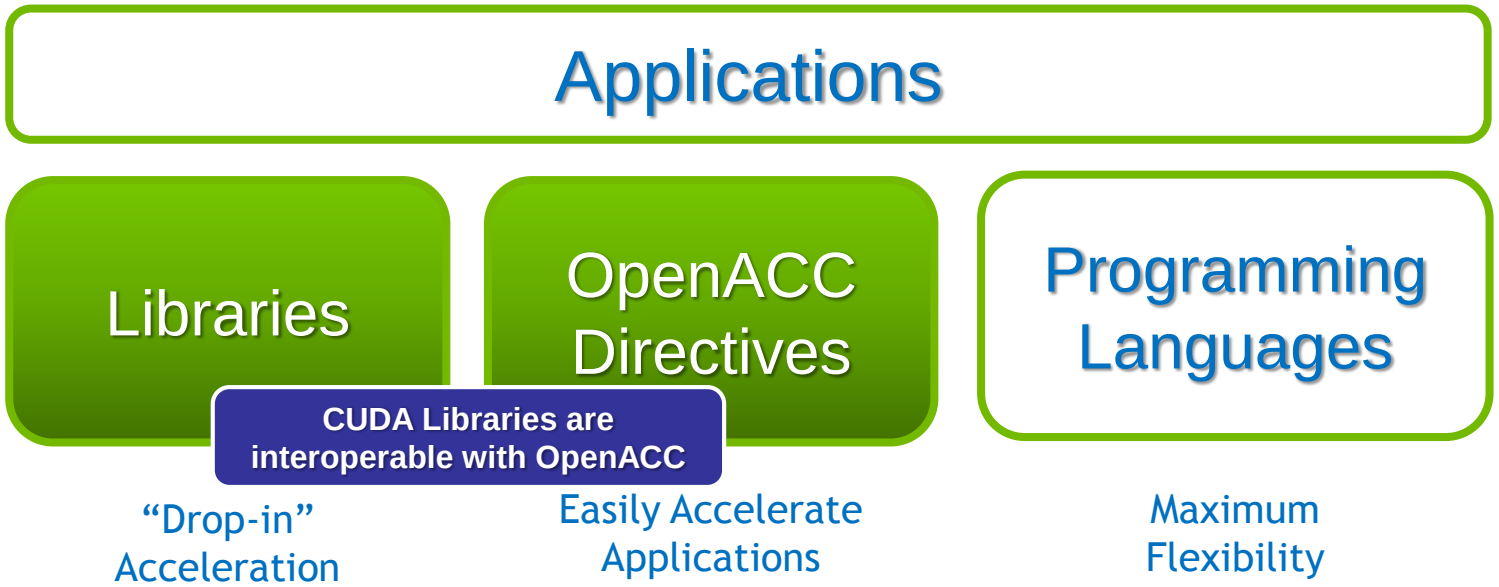
- OpenACC gives us more detailed control over parallelization
  - Via gang, worker, and vector clauses
- By understanding more about OpenACC execution model and GPU hardware organization, we can get higher speedups on this code
- By understanding bottlenecks in the code via profiling, we can reorganize the code for higher performance
- Will tackle these in later exercises

Tips and Tricks

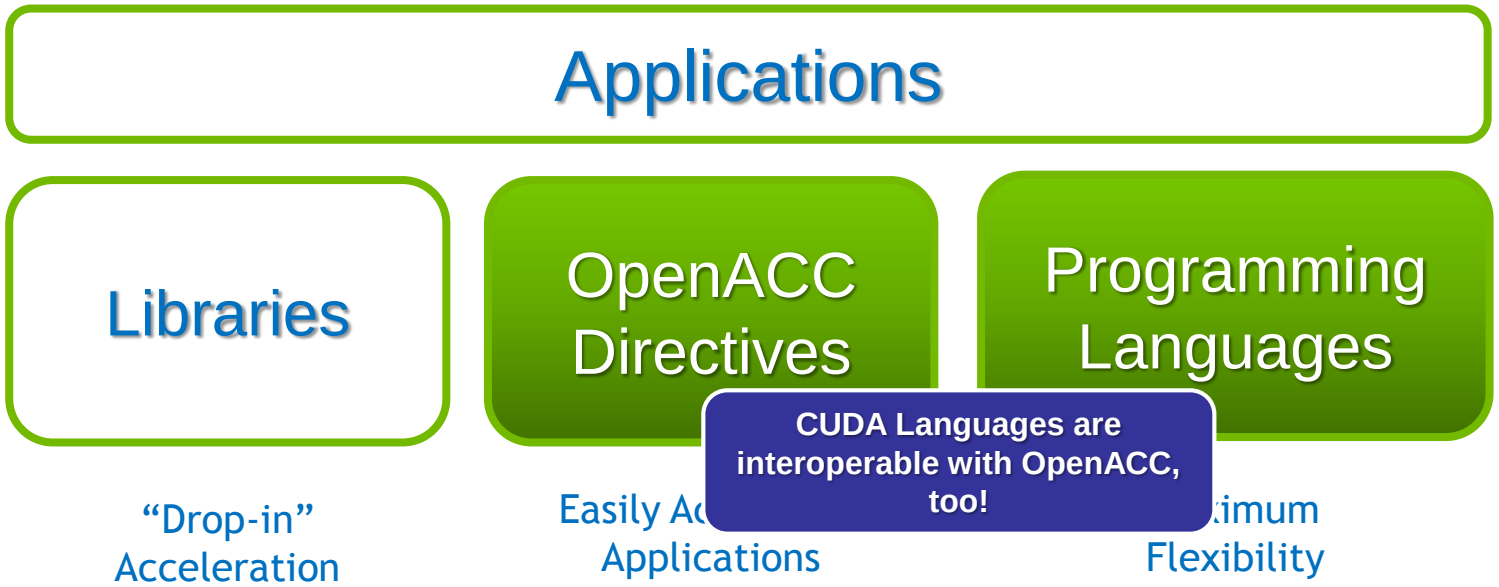
- (PGI) Use time option to learn where time is being spent
  - -ta=nvidia,time
- Eliminate pointer arithmetic
- Inline function calls in directives regions
  - (PGI): -inline or –inline,levels(<N>)
- Use contiguous memory for multi-dimensional arrays
- Use data regions to avoid excessive memory transfers
- Conditional compilation with _OPENACC macro

OpenACC and CUDA interoperability

3 Ways to Accelerate Applications



3 Ways to Accelerate Applications



Sharing data with libraries

- CUDA libraries and OpenACC both operate on device arrays
- OpenACC provides mechanisms for interop with library calls
  - deviceptr data clause
  - host_data construct
- Note: same mechanisms useful for interop with custom CUDA C/C++/Fortran code

deviceptr Data Clause

`deviceptr( list )` Declares that the pointers in *list* refer to device pointers that need not be allocated or moved between the host and device for this pointer.

Example:

C

```
#pragma acc data deviceptr(d_input)
```

Fortran

```
$!acc data deviceptr(d_input)
```

host_data Construct

Makes the address of device data available on the host.

`host_data( list )` Tells the compiler to use the device address for any variable in *list.* Variables in the list must be present in device memory due to data regions that contain this construct

Example

C

```
#pragma acc host_data use_device(d_input)
```

Fortran

```
$!acc host_data use_device(d_input)
```

Example: 1D convolution using CUFFT

- Perform convolution in frequency space
  1. Use CUFFT to transform input signal and filter kernel into the frequency domain
  2. Perform point-wise complex multiply and scale on transformed signal
  3. Use CUFFT to transform result back into the time domain

- We will perform step 2 using OpenACC

Source Excerpt

```
// Transform signal and kernel
 error = cufftExecC2C(plan, (cufftComplex *)d_signal,
                      (cufftComplex *)d_signal, CUFFT_FORWARD);
 error = cufftExecC2C(plan, (cufftComplex *)d_filter_kernel,
                      (cufftComplex *)d_filter_kernel, CUFFT_FORWARD);

 // Multiply the coefficients together and normalize the result
 printf("Performing point-wise complex multiply and scale.\n");
 complexPointwiseMulAndScale(new_size,
                             (float *restrict)d_signal,
                             (float *restrict)d_filter_kernel);

 // Transform signal back
 error = cufftExecC2C(plan, (cufftComplex *)d_signal,
                      (cufftComplex *)d_signal, CUFFT_INVERSE);
```

This function must execute on device data

OpenACC convolution code

```
void complexPointwiseMulAndScale(int n, float *restrict signal,
                                 float *restrict filter_kernel)
{
// Multiply the coefficients together and normalize the result
#pragma acc data deviceptr(signal, filter_kernel)
    {
#pragma acc parallel loop
        for (int i = 0; i < n; i++) {
            float ax = signal[2*i];
            float ay = signal[2*i+1];
            float bx = filter_kernel[2*i];
            float by = filter_kernel[2*i+1];
            float s = 1.0f / n;
            float cx = s * (ax * bx - ay * by);
            float cy = s * (ax * by + ay * bx);
            signal[2*i] = cx;
            signal[2*i+1] = cy;
        }
    }
}
```

If the OpenACC compiler does not support structs in OpenACC loops, then we cast the Complex* pointers to float* pointers and use interleaved indexing

Linking CUFFT

- `#include “cufft.h”`
- Compiler command line options:

```
CUDA_PATH = /usr/local/pgi/linux86-64/2012/cuda/4.0
CCFLAGS = -I$(CUDA_PATH)/include -L$(CUDA_PATH)/lib64
          -lcudart -lcufft
```

Must use PGI-provided CUDA toolkit paths

Must link libcudart and libcufft

Results

```
[harrism@kollman0 cufft-acc]$ ./cufft_acc
Transforming signal cufftExecC2C
Performing point-wise complex multiply and scale.
Transforming signal back cufftExecC2C
Performing Convolution on the host and checking correctness

Signal size: 500000, filter size: 33
Total Device Convolution Time: 11.461152 ms (0.242624 for point-wise
convolution)
Test PASSED
```

CUFFT + cudaMemcpy

OpenACC

Summary

- Use deviceptr data clause to pass pre-allocated device data to OpenACC regions and loops
- Use host_data to get device address for pointers inside acc data regions

- The same techniques shown here can be used to share device data between OpenACC loops and
  - Your custom CUDA C/C++/Fortran/etc. device code
  - Any CUDA Library that uses CUDA device pointers

Exercise 7

- Try to mix OpenACC and CUDA paradigms for the Laplace example
- The basic idea is to focus on some sections of code and optimize them employing CUDA APIs
- As an example, try to implement the second loop calling a cudaMemcpy, a DeviceToDevice copy
  - use the **host_data** directive to make the data visible to the host
  - you need to define an extern C function which calls the cudaMemcpy
  - passing the arrays and the extents
- Compilation, modify the Makefile consistently
  - compile the CUDA function using nvcc and the openacc code using PGI
  - then, link the objects together

Exercise 7 - Makefile

```
CUDA_PATH  = /cineca/prod/compilers/pgi/13.10/none/linux86-64/2013/cuda/5.0/
PGCC       = pgcc -g -acc -ta=nvidia,time,cuda5.0,cc35 -Minfo=accel -O3 -DPGI
GCC        = gcc -O3 -DCAPS #-Wall -Wextra
CAPSMC     = capsmc --codelet-required # --debug -g -G
CUDA_FLAGS   = -I$(CUDA_PATH)/include -L$(CUDA_PATH)/lib64 -lcudart

pgi: laplace2d_acc_pgi.o cudaFun.o
	$(PGCC) laplace2d_acc_pgi.o cudaFun.o $(CUDA_FLAGS) -o laplace2d_acc_pgi_withcuda
laplace2d_acc_pgi.o: laplace2d.c
	$(PGCC) -c -o laplace2d_acc_pgi.o $<
caps: laplace2d_acc_caps.o cudaFun.o
	$(CAPSMC) $(GCC) laplace2d_acc_caps.o cudaFun.o $(CUDA_FLAGS) -o laplace2d_acc_caps_withcuda
laplace2d_acc_caps.o: laplace2d.c
	$(CAPSMC) $(GCC) -c -o laplace2d_acc_caps.o $<
cudaFun.o: cudaFun.cu
	nvcc -c cudaFun.cu -o cudaFun.o
```

Exercise 7: Performance

2 eight-core Intel(R) Xeon(R) CPU E5-2687W @ 3.10GHz

GPU: Nvidia Tesla K20s

Execution	Time (s) - PGI
CPU 1 OpenMP thread	21.9
CPU 8 OpenMP threads	3.7
OpenACC GPU-parallel	**30**
OpenACC GPU-collapse	**30**
OpenACC GPU-data	**0.9**
OpenACC GPU-withcuda	**0.8**

no significant improvement for this simple case

Exercise 8

- Up to now, we used statically allocated memory
  - Using OpenACC for dynamically allocated data is possible
  - data extents need to be explicitely specified
- It may be more difficult for the compiler to assess the independence of iterations
  - this is obviously crucial adopting the kernels directive
  - but, it may be important even using parallel directive, for the internal loops
  - best practice: use explicit loop directive or collapse clause to strongly control the parallelization of each loop
- Try to accelerate the code in the directory 009-laplace2D-dynamic
    - **using parallel directive**
    - **using kernel directive**

OpenACC and C++

- C++ is supported according to the OpenACC standard
  - **but compilers may significantly lag behind!**
- In **data** constructs
  - if a variable or array of struct or class is specified, all the data members of the struct or class are allocated and copied, as appropriate
  - if a struct or class member is a pointer type, the data addressed by that pointer are not implicitely copied
- At present, using PGI or CAPS, the code needs to be adapted recovering a C-like style
  - PGI has its own C++ compiler while CAPS relies on an underlying compiler
  - use **_OPENACC** macro to differentiate the code
  - it clearly limits the code maintainability

Exercise 9

- Implement OpenACC acceleration to the Laplace C++ code
  - the code employs vector containers and multi-index-like overloading
  - you need to extract the pointer to the data, overloading the () could be an idea

```
class field {
  int n;   int m;   vector<double> vec;
public:
  field(int nn, int mm) : n(nn), m(mm) { vec.assign(nn*mm,0.); }
  double& operator() (int i, int j) { return vec[m*i+j]; }
  double* operator() () { return &(vec[0]); }
};
```

  - to access vector indexes, a macro could be employed

```
#define IDX(i,j) ((i)*(NM)+(j))
```

Exercise 9 - Solution

```
double *A_p, *Anew_p;
..........
field A(n,m); field Anew(n,m);
..........
A_p = A();  Anew_p = Anew();
#pragma acc data copy(A_p[0:NN*NM]), create(Anew_p[0:NN*NM])
{
while ( error > tol && iter < iter_max )  {
error = 0.0;
#pragma acc parallel loop collapse(2) reduction(max: error)
for( j = 1; j < n-1; j++) {
   for( i = 1; i < m-1; i++) {
#ifdef _OPENACC
      Anew_p[IDX(j,i)] = 0.25*( A_p[IDX(j,i+1)]+A_p[IDX(j,i-1)]+A_p[IDX(j-1,i)]+A_p[IDX(j+1,i)]);
      error = fmax( error, fabs(Anew_p[IDX(j,i)] - A_p[IDX(j,i)]));
#else
      Anew(j,i) = 0.25 * ( A(j,i+1) + A(j,i-1)  + A(j-1,i) + A(j+1,i));
      error = fmax( error, fabs(Anew(j,i) - A(j,i)));
#endif
} }
.......
```

OpenACC and MPI

- OpenACC may be used to accelerate the codes featuring MPI parallelization
  - **each MPI process may be accelerated, just like what happens when adding OpenMP simple constructs to MPI codes**
- When dealing with MPI communications, obvious data synchronizations must be performed
  - update host before sending data
  - update device after receiving data
- In the simplest approach, each MPI process controls a different GPU
  - again, use runtime library routines
  - possibly, some MPI processes use GPUs while other processes use the host as the computing unit

Exercise 10

- Add OpenACC directives to the MPI laplace code in the directory 010-laplace2D-mpi/
  - the baseline features a 2D MPI Cartesian decomposition
  - before evolving the field data, halo data are copied into buffers and MPI exchanges are performend
- The association of MPI processes to GPUs is already prepared considering a machine with a defined number of GPUs

```
#define NGPU_PER_NODE 4
mygpu = rank%NGPU_PER_NODE;
```

  - employ MPI colours to make it more general
- Remember to specify the array extents to be created or updated
  - when dealing with MPI, dynamic memory is a common choice

Exercise 10: Performance

2 eight-core Intel(R) Xeon(R) CPU E5-2687W @ 3.10GHz

GPU: Nvidia Tesla K20s

Execution	Time (s) - PGI
CPU 8 OpenMP threads	3.7
OpenACC GPU-parallel	**30**
OpenACC GPU-collapse	**30**
OpenACC GPU-data	**0.9**
OpenACC GPU-withcuda	**0.8**
OpenACC GPU 2 MPI procs	**0.5**

significant scalability

Optimizing OpenACC parallelization

Cache Directive

- The cache directive may appear at the top of (inside of) a loop
  - it specifies array elements or subarrays that should be fetched into the higheset level of the cache for the body of the loop
  - obviously the actual performance gain strongly depends on the analyzed loop

```
#pragma acc parallel loop collapse(2) reduction(max:error)
for( j = 1; j < n-1; j++) {
   for( i = 1; i < m-1; i++ ) {
#pragma acc cache(A[i-1:2][j-1:2])
       Anew[j][i] = 0.25 * ( A[j][i+1] + A[j][i-1]
                           + A[j-1][i] + A[j+1][i]);
       error = fmax( error, fabs(Anew[j][i] - A[j][i]));
       }
   }
```

Parallel Construct

Fortran

```
!$acc parallel [clause …]
    structured block
!$acc end parallel
```

C

```
#pragma acc parallel [clause …]
    { structured block }
```

Clauses

```
if( condition )
async( expression )
num_gangs( expression )
num_workers( expression )
vector_length( expression )
```

```
private( list )
firstprivate( list )
reduction( operator:list )
```

Also any data clause

Parallel Clauses

`num_gangs ( expression )`	Controls how many parallel gangs are created (CUDA **`gridDim`**).
`num_workers ( expression )`	Controls how many workers are created in each gang (CUDA **`blockDim`**).
`vector_length ( list )`	Controls vector length of each worker (SIMD execution).
`private( list )`	A copy of each variable in list is allocated to each gang.
`firstprivate ( list )`	**`private`** variables initialized from host.
`reduction( operator:list )`	**`private`** variables combined across gangs.

Loop Construct

Fortran

```
!$acc loop [clause …]
    loop
!$acc end loop
```

C

```
#pragma acc loop [clause …]
    { loop }
```

Combined directives

```
!$acc parallel loop [clause …]
!$acc kernels loop [clause …]
```

Detailed control of the parallel execution of the following loop.

Loop Clauses

`collapse( n )`	Applies directive to the following `n` nested loops.
`seq`	Executes the loop sequentially on the GPU. Often, something went wrong...
`private( list )`	A copy of each variable in list is created for each iteration of the loop. It is default behavior
`reduction( operator:list )`	**`private`** variables combined across iterations.

Loop Clauses Inside parallel Region

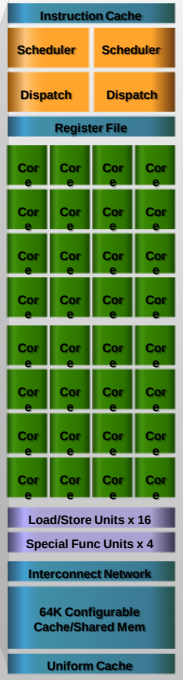
`gang`	Shares iterations across the gangs of the parallel region.
`worker`	Shares iterations across the workers of the gang.
`vector`	Execute the iterations in SIMD mode

Loop Clauses Inside kernels Region

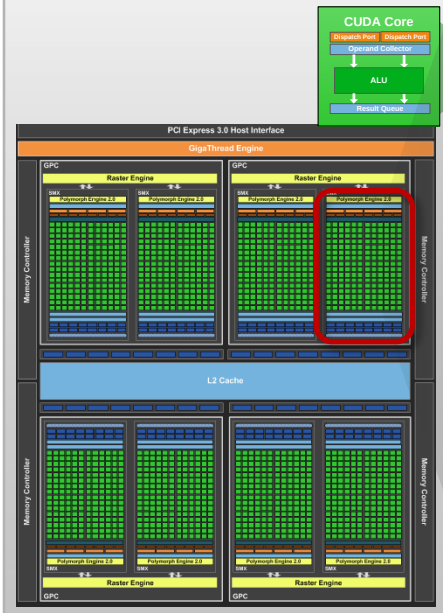
`gang [( num_gangs )]`	Shares iterations across at most `num_gangs` gangs.
`worker [( num_workers )]`	Shares iterations across at most `num_workers` of a single gang.
`vector [( vector_length )]`	Executes the iterations in SIMD mode with maximum `vector_length`.
`independent`	Specifies that the loop iterations are independent.

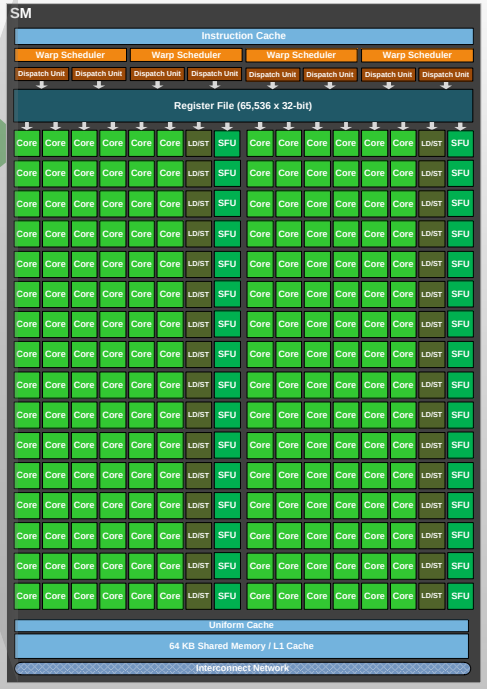
Fermi and Kepler architecuters sketches

Fermi



Kepler

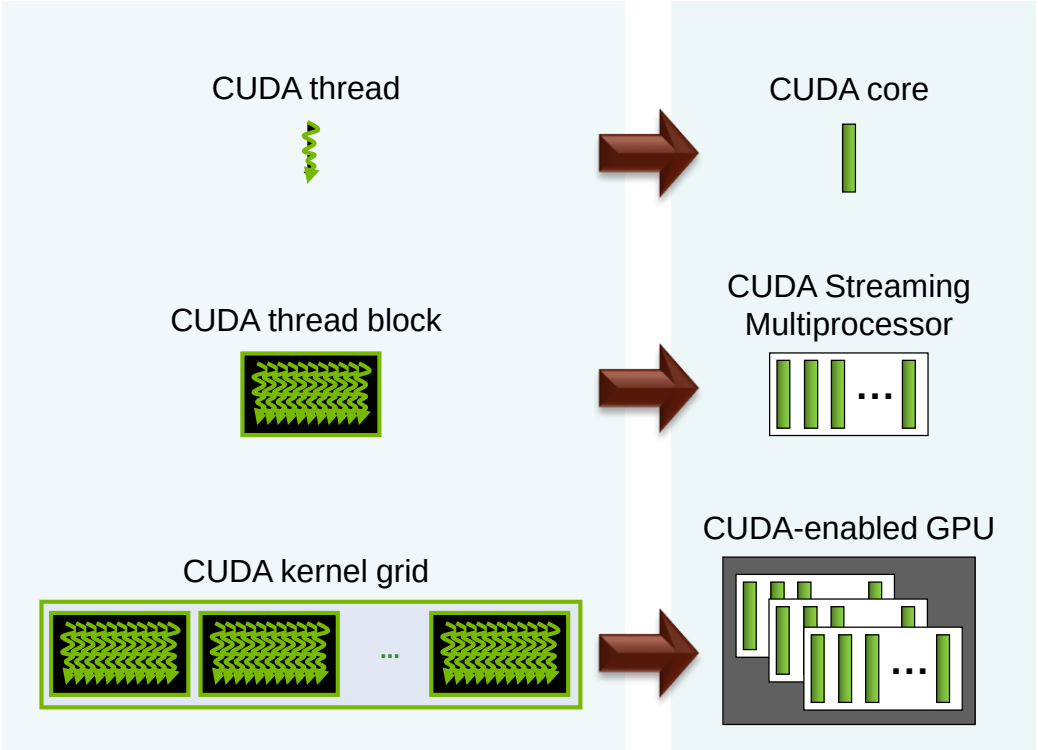




OpenACC and targets

- OpenACC on NVIDIA GPUs compiles to target the CUDA platform
  - CUDA is a parallel computing platform and programming model invented by NVIDIA.
- OpenACC may potentially target different architectures
  - NVIDIA GPU, AMD GPU, Intel MIC, many-cores and CPUs, too
  - CAPS compiler allows for producing OpenCL code instead of CUDA code
  - PGI is testing OpenACC on AMD Radeon cards
- The mapping between OpenACC parallel levels and target is performed by the compiler

CUDA and Kernel Execution



- Each thread is executed by a core

- Each block is executed by one SM and does not migrate
- Several concurrent blocks can reside on one SM depending on the blocks' memory requirements and the SM's memory resources

- Each kernel is executed on one device
- Multiple kernels can execute on a device at one time

OpenACC execution Model

- The OpenACC execution model has three levels:
  - gang, worker and vector
- This is supposed to map to an architecture that is a collection of Processing Elements (PEs)
  - Each PE is multithreaded and each thread can execute vector instructions
- For GPUs one possible mappings could be
  - **gang==block, worker==warp, vector==threads in a warp**
  - **omit “worker” and just have gang==block, vector==threads of a block**
- Depends on what the compiler thinks is the best mapping for the problem

Mapping OpenACC to CUDA threads and blocks

```
#pragma acc kernels
   for( int i = 0; i < n; ++i ) y[i] += a*x[i];
```

Let the compiler decide: probably 16 blocks, 256 threads each

```
#pragma acc kernels loop gang(100) vector(128)
   for( int i = 0; i < n; ++i ) y[i] += a*x[i];
```

100 thread blocks, each with 128 threads, each thread executes one iteration of the loop, using kernels

```
#pragma acc parallel num_gangs(100) vector_length(128)
{
   #pragma acc loop gang vector
   for( int i = 0; i < n; ++i ) y[i] += a*x[i]; }
```

100 thread blocks, each with 128 threads, each thread executes one iteration of the loop, using parallel

Mapping OpenACC to CUDA threads and blocks

```
#pragma acc parallel num_gangs(100)
{
   for( int i = 0; i < n; ++i ) y[i] += a*x[i]; }
```

100 thread blocks, each with apparently 1 thread, each thread redundantly executes the loop

```
#pragma acc parallel num_gangs(100)
{
   #pragma acc loop gang
   for( int i = 0; i < n; ++i ) y[i] += a*x[i]; }
```

compiler can notice that only 'gangs' are being created, so it might decide to create threads instead, say 2 thread blocks of 50 threads.

Mapping OpenACC to CUDA threads and blocks

```
#pragma acc kernels loop gang(100) vector(128)
   for( int i = 0; i < n; ++i ) y[i] += a*x[i];
```

100 thread blocks, each with 128 threads, each thread executes one iteration of the loop, using kernels

```
#pragma acc kernels loop gang(50) vector(128)
   for( int i = 0; i < n; ++i ) y[i] += a*x[i];
```

50 thread blocks, each with 128 threads. Each thread does two elements worth of work

Doing multiple iterations per thread can improve performance by amortizing the cost of setup

Tuning loops

- Selecting the optimal strategy to match the 3 OpenACC layers to the code loops is usually a compiler job
  - **not easy to manually optimize a code selecting *magic* numbers**
  - **In case you need to optimize more, probably the use of CUDA and/or CUDA libraries is the best choice for specific sections of code**
  - **but using OpenACC allows for a much greater portability**
  - **device_type clause may be employed to have multiple tuning**

```
void matvecmul( float* x, float* a,
                float* v, int m, int n ){
#pragma acc parallel loop \
  device_type(nvidia) num_gangs(200) \
  device_type(radeon) num_ganges(400)
 for( int i = 0; i < m; ++i )
{
    ……..
}
```

Advanced parallelization

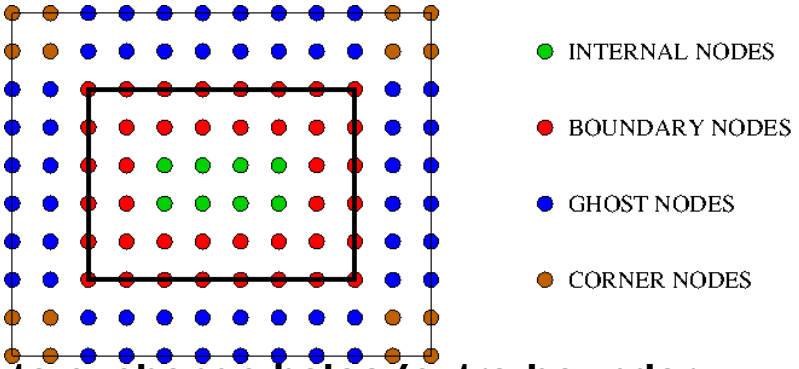
- On the other hand, a control of the OpenACC loop layers may be crucial when the loop structure to parallelize is not trivial
  - i and xx are privates as for the gang level
  - but xx is reduction as for the worker level

```
void matvecmul( float* x, float* a,
                float* v, int m, int n ){
#pragma acc parallel loop gang
for( int i = 0; i < m; ++i ){
   float xx = 0.0;
#pragma acc loop worker reduction(+:xx)
  for( int j = 0; j < n; ++j )
    xx += a[i*n+j]*v[j];

  x[i] = xx;
}
}
```

CPU: MPI and Asynchronism

- **For CPU parallel MPI programs, employing the asynchronism may significantly improve performances**
  - **the main idea is to overlap communications to computations**
  - **the overlapping between computing and communications may be achieved using non-blocking MPI calls**
- **A basic pattern suitable for one iteration of the Laplace program is based on splitting the domain into bulk, boundary and halo points**
  - **boundary updating**
  - **MPI Send/Recv non-blocking calls to exchange halos (extra-boundary points)**
  - **bulk updating**
  - **MPI Wait calls**



CPU+device, MPI and Asynchronism

- **For GPU-enabled codes, the asynchronism has additional features**
  - **the programming model has two main actors: host – coprocessor**
  - **usually, the basic objective is still the overlapping of tasks**
- **CPU and GPU computations may be overlapped**
  - **but, the computing power of the GPU is often larger and decomposing the work-load is not trivial**
  - **however, special tasks may be better executed by the CPU**
- **As for overlapping communications, CPU-device copies have to be taken into account**
  - **different patterns are required**
  - **achieving overlapping becomes more important (CPU-GPU copies are expensive)**

OpenACC async and wait

- OpenACC allows for asynchronous compute regions and data updates with the **async** clause
- It is also possible to have a number of **async** queues by adding a value expression to the async clause
  - activities with the same async value will be executed as they are enqueued by the host thread

```
#pragma acc parallel async
{ ..... }
#pragma acc update device(...) async
{ ..... }
#pragma acc wait
```

```
#pragma acc parallel async(1)
{ ..... }
#pragma acc parallel async(2)
{ ..... }
#pragma acc wait(1)
{ ..... }
#pragma acc wait(2)
```

A CPU-GPU asynchronous pattern for Laplace

- A basic pattern to hide communications between GPU and GPU considering GPU->host and host -> GPU intermediate copies
  - update boundary – synchronous
  - update bulk – asynchronous
  - MPI halo exchange - blocking or not blocking with MPI waits
  - OpenACC wait for update bulk

- Use CUDA-streams or OpenACC **async** to implement it

What we left out

- A few directives, e.g.:
  - `atomic`
  - `enter data/exit data`
- More on targeting platforms
  - e.g., compiler extensions
- Some clauses, e.g., `tile`
- (Much) more on the run-time library

Perspectives

- The main reference: www.openacc-standard.org
- PGI and CAPS full implementations of OpenACC 2.0
- Future improvements of the standard
  - at present, no standard way to support arrays inside C++ classes, C structs or Fortran derived data types
- Multi-platform implementations and tests:
  - AMD GPUs, Intel MICs,...
- Open-Source OpenACC implementations
  - OpenACC extension will be supported in mainstream GCC compilers

OpenMP 4 and accelerators by examples

OpenMP 4.0: new features

- Support for compute devices
- SIMD constructs
- Task enhancements
- Thread affinity
- Other improvements

OpenMP 4.0 and accelerators

- Effort to support a wide variety of compute devices
  - GPUs, Xeon Phis, ...
- Adds mechanisms to describe regions of code where data and/or computation should be moved to another computing device
  - Some ideas follow the OpenACC approach
- Accelerator
  - different functionality (optimized for something special) and instruction set
  - each accelerator attached to one host device
  - it may or may not share memory with the device (shared memory?)
- Execution model:
  - host-centric

Target Construct

```
extern void init(float*, float*, int);
extern void output(float*, int);
void vec_mult(int N)
{
int i;
float p[N], v1[N], v2[N];
init(v1, v2, N);
#pragma omp target
#pragma omp parallel for private(i)
for (i=0; i<N; i++)
p[i] = v1[i] * v2[i];
output(p, N);
}
```

map Clause

```
extern void init(float*, float*, int);
extern void output(float*, int);
void vec_mult(int N)
{
int i;
float p[N], v1[N], v2[N];
init(v1, v2, N);
#pragma omp target map(v1, v2, p)
#pragma omp parallel for
for (i=0; i<N; i++)
p[i] = v1[i] * v2[i];
output(p, N);
}
```

map Clause with to/from

```
extern void init(float*, float*, int);
extern void output(float*, int);
void vec_mult(int N)
{
int i;
float p[N], v1[N], v2[N];
init(v1, v2, N);
#pragma omp target map(to: v1, v2) map(from: p)
#pragma omp parallel for
for (i=0; i<N; i++)
p[i] = v1[i] * v2[i];
output(p, N);
}
```

map Clause with array sections

```
extern void init(float*, float*, int);
extern void output(float*, int);
void vec_mult(float *p, float *v1, float *v2, int N)
{
int i;
init(v1, v2, N);
#pragma omp target map(to: v1[0:N], v2[:N]) map(from: p[0:N])
#pragma omp parallel for
for (i=0; i<N; i++)
p[i] = v1[i] * v2[i];
output(p, N);
}
```

target data Construct

```
extern void init(float*, float*, int);
extern void output(float*, int);
void vec_mult(float *p, float *v1, float *v2, int N)
{
int i;
init(v1, v2, N);
#pragma omp target data map(to: v1[0:N], v2[:N]) map(from: p[0:N])
{
#pragma omp target
#pragma omp parallel for
for (i=0; i<N; i++)
p[i] = v1[i] * v2[i];
}
output(p, N);
}
```

target update Construct

```
void vec_mult(float *p, float *v1, float *v2, int N)
{
int i; init(v1, v2, N);
#pragma omp target data map(to: v1[:N], v2[:N]) map(from: p[0:N])
{
#pragma omp target
#pragma omp parallel for
for (i=0; i<N; i++) p[i] = v1[i] * v2[i];
init_again(v1, v2, N);
#pragma omp target update to(v1[:N], v2[:N])
#pragma omp target
#pragma omp parallel for
for (i=0; i<N; i++) p[i] = p[i] + (v1[i] * v2[i]);
}
output(p, N);
}
```

declare target for functions

```
#pragma omp declare target
extern void fib(int N);
#pragma omp end declare target
#define THRESHOLD 1000000
void fib_wrapper(int n)
{
#pragma omp target if(n > THRESHOLD)
{
fib(n);
}
}
```

declare target for variables

```
#define N 1000
#pragma omp declare target
float p[N], v1[N], v2[N];
#pragma omp end declare target
extern void init(float *, float *, int);
extern void output(float *, int);
void vec_mult()
{
int i; init(v1, v2, N);
#pragma omp target update to(v1, v2)
#pragma omp target
#pragma omp parallel for
for (i=0; i<N; i++)
p[i] = v1[i] * v2[i];
#pragma omp target update from(p)
output(p, N);
}
```

using teams, distribute

```
#include <stdio.h>
#include <omp.h>
int main() {
int ntprocs;
#pragma omp target map(from:ntprocs)
ntprocs = omp get num procs();
int ncases=2240, nteams=4, chunk=ntprocs*2;
#pragma omp target
#pragma omp teams num teams(nteams) thread limit(ntprocs/nteams)
#pragma omp distribute
for (int starti=0; starti<ncases; starti+=chunk)
#pragma omp parallel for
for (int i=starti; i<starti+chunk; i++)
printf("case i=%d/%d by team=%d/%d thread=%d/%d\n",
i+1, ncases,
omp_get_team_num()+1, omp_get_num_teams(),
omp_get_thread_num()+1, omp_get_num_threads());
}
```

OpenAcc / OpenMP differences

- **Parallelism**
  - OpenACC offload and parallel startup tied together (parallel and kernels
  - OpenMP: offload and parallel startup disconnected (target, parallel & teams)
- **Loops**
  - OpenAcc: one construct loop, multiple parallelism types, nested parallelism implicit
  - OpenMP: three constructs (distribute, for, simd), nested parallelism explicit
- **Variables copies**:
  - OpenAcc: copy without present allowed
  - OpenMP: map always implies present test

OpenMP & OpenAcc loops

```
#pragma omp target device(0) map(tofrom:B)
#pragma omp parallel for
for (i=0; i<N; i++)
   B[i] += sin(B[i]);
```

OpenMP 4.0 for Intel Xeon Phi

```
#pragma omp target device(0) map(tofrom:B)
#pragma omp teams num_teams(num_blocks) thread_limit(bsize)
#pragma omp distribute
for (i=0; i<N; i += bsize)
#pragma omp parallel for
for (b = i; b < bsize; b++)
    B[b] += sin(B[b]);
```

OpenMP 4.0 for Nvidia GPU

```
#pragma acc parallel copy(B[0:N]) num_gangs(numblocks)\
        vector_length(bsize)
#pragma acc loop gang vector
for (i=0; i<N; ++i)
    B[i] += sin(B[i]);
```

OpenACC for NVIDIA GPU

Using OpenMP scheduling

```
#define N 1024*1024
float dotprod(float B[], float C[], int N)
{
    float sum = 0;
    int i;
    #pragma omp target map(to: B[0:N], C[0:N])
    #pragma omp teams num_teams(8) thread_limit(16)
    #pragma omp distribute parallel for reduction(+:sum) \
                dist_schedule(static, 1024) schedule(static, 64)
    for (i=0; i<N; i++)
        sum += B[i] * C[i];
    return sum;
}
```

OpenMP 4.0 implementation

- Intel compiler 2015 implements OpenMP 4.0 target directives but presently supports only Intel Xeon Phi devices

- GNU compiler is going to provide support to different type of accelerators
  - keep updated!

References

- OpenACC standard
  - **http://www.openacc.org/sites/default/files/OpenACC.2.0a_1.pdf**
- OpenACC technical report on structured types
  - **http://www.openacc.org/sites/default/files/TR-14-1.pdf**
- PGI
  - https://www.pgroup.com/resources/accel.htm
- OpenMP
  - http://www.openmp.org/mp-documents/OpenMP4.0.0.pdf

Credits

Mark Harris - NVIDIA
John Urbanic - Pittsburgh Supercomputing Center
Sarah Tariq - NVIDIA
Jeff Larkin – NVIDIA
Christian Terboven