Introduction to OpenACC

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Acknowledgement: Most of examples and pictures are from PSC (https://www.psc.edu/images/xsedetraining/OpenACC_Nov2017/OpenACC_Introduction_To_OpenACC.PDF)

Logistics of this webinar

- Login to Midway using your CNetID username/password
  - Using terminal:
    - `ssh -Y cnetid@midway.rcc.uchicago.edu`
  - Using ThinLinc:
    - https://midway.rcc.uchicago.edu)
- Once you are logged in, download the workshop material by running:
  - `git clone https://github.com/rcc-uchicago/openacc-intro.git`

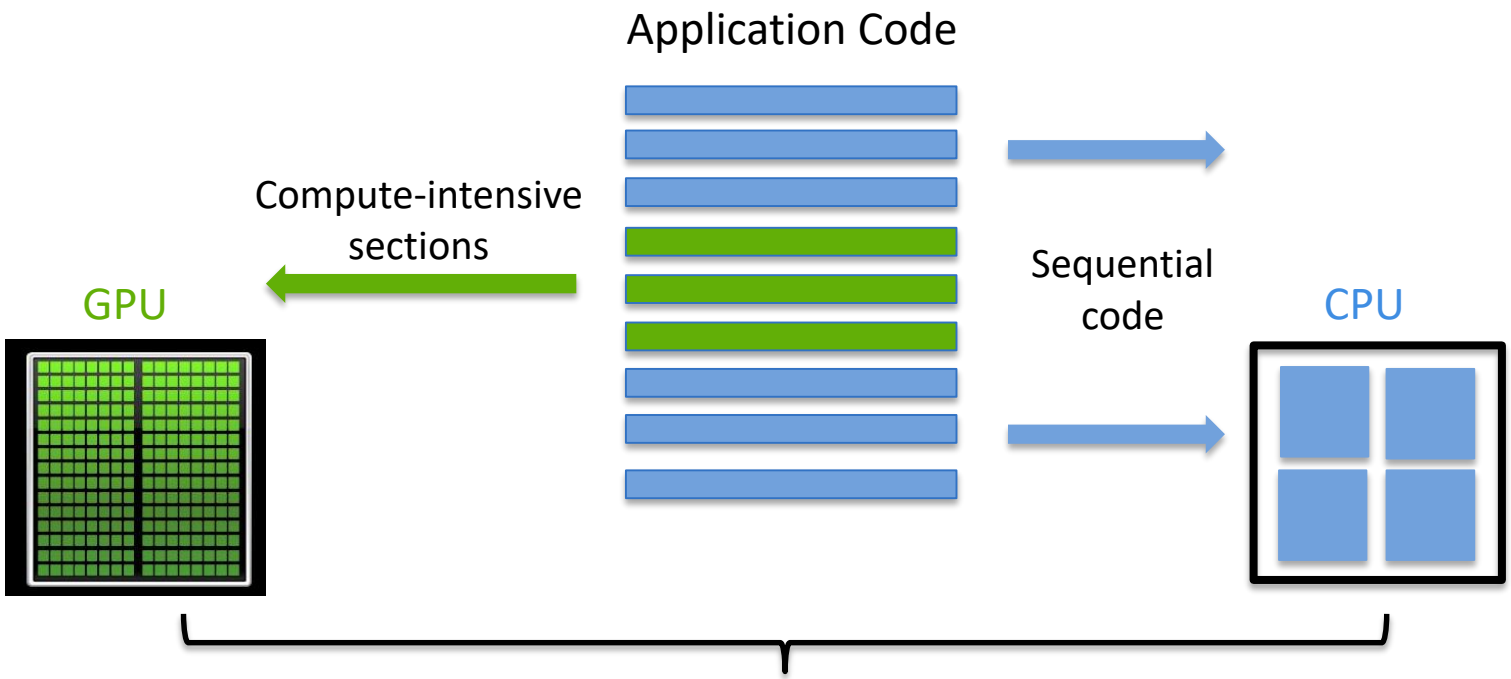
Logistics of this webinar

- Please run the `module load pgi/2017` command to access the PGI compilers
- We will use the gpu partition on Midway2
  - Please run `rcchelp sinfo -p gpu` to see the specification of nodes
- Please use editors such as vim, nano, etc. to edit the files
  - Please refrain from transferring the files to Windows, editing, and transferring them back to Parallel
  - Copying codes/commands from slides may result in unexpected error messages

GPU: Graphical Processing Unit

- Designed for graphics
- Optimized for parallel tasks with hundreds of cores
- Good at doing simple and repeated calculations
- High memory bandwidth and flops/watt
- We will use NVIDIA GPUs in this workshop

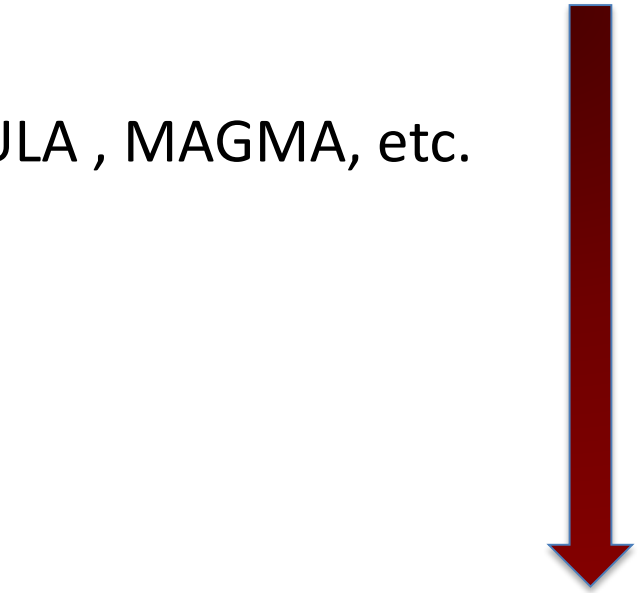
Heterogeneous computing



Picture is adapted from https://computing.llnl.gov/tutorials/2014.09.15-16.NVIDIA-OpenACC.pdf

GPU computing

- Libraries
  - NVIDIA Math Libraries, CULA , MAGMA, etc.
- Compiler directives
  - OpenACC
- Programming languages
  - NVIDIA CUDA toolkit for C/C++, PGI CUDA Fortran, NVIDIA OpenCL, PyCUDA



Increased flexibility and complexity

OpenACC

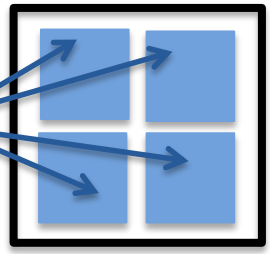
- Programming standard developed by NVIDIA, Cray, CAPS, and PGI
- Includes GPU directives to annotate C/C++ and Fortran code
- Can be used on different GPUs (NVIDIA and AMD)

Key advantages

- High-level
  - No involvement of OpenCL, CUDA, etc.
- Single source
  - Compile the same program for accelerators or serial execution
- Efficient
  - Comparable to the low-level implementations of the same algorithm
- Performance portable
  - Supports GPU accelerators and co-processors from multiple vendors
- Incremental

OpenACC is similar to OpenMP

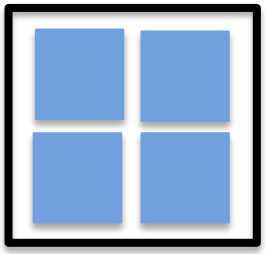
CPU



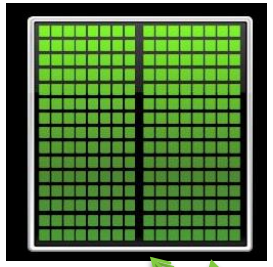
```
main(){
  double pi = 0.0;long i;

#pragma omp parallel for reduction(+:pi)
  for(i=0;i < N;i++)
  {
    double t = (double)((i+0.05)/N);
    pi += 4.0/(1.0+t*t);
  }
  printf("pi = %f\n",pi/N);
}
```

CPU



GPU



```
main(){
  double pi = 0.0;long i;

#pragma acc kernels
  for(i=0;i < N;i++)
  {
    double t = (double)((i+0.05)/N);
    pi += 4.0/(1.0+t*t);
  }
  printf("pi = %f\n",pi/N);
}
```

Basics

- In C/C++ all OpenACC directives start with `#pragma acc`
  - These lines will be skipped by non-OpenACC compilers
    - You may get a warning message but it should be OK

```
#pragma acc <directive> [clause]
{
  …
}
```

- In Fortran all OpenACC directives start with `!$acc`

```
!$acc <directive> [clause]
 …
!$acc end directive
```

`kernels` directive

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

```
#pragma acc kernels
{
  for(i=1;i<n;i++){
    a[i] = 0.0;
    b[i] = 1.0;
  }
  for(i=0;i < n;i++)
    a[i] = b[i] + 5;
}
```

Kernel 1

Kernel 2

Kernel: A parallel routine to run on the GPU

`parallel loop` directive

C

```
#pragma acc parallel loop
{
  …
}
```

Fortran

```
!$acc parallel loop
  …
!$acc end parallel loop
```

Similar to OpenMP we can use `parallel for` in C and `parallel do` in Fortran. To keep it consistent, `parallel loop` can be used in both.

`kernels` vs. `parallel loop`

- `kernels`
  - Gives more flexibility to compiler to parallelize loops
  - Covers larger sections of code

- `parallel loop`
  - Requires programmer to analyze the dependencies
  - Is a simple transition from OpenMP

SAXPY

```
#include "ticktock.h”
int main(){
  int n=1e7; float a = 5./3.;int i;
  float *x = malloc(sizeof(float)*n);
  float *y = malloc(sizeof(float)*n);

  //initialize vectors
  for (i=0; i<n; i++){
    x[i] = 2.0f;
    y[i] = (i+1.)*(i-1.);
  }
  tick_tock tt;
  tick(&tt);
  saxpy(n,a,x,y);
  tock(&tt);
  free(x);
  free(y);
  return 0;
}
```

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

The `restrict` keyword: C99 standard

- Important for optimization of serial as well as OpenACC and OpenMP code.

- Promise to the compiler for a pointer

```
float *restrict y
```

  - Meaning: “for the lifetime of y, only it or a value directly derived from it (such as y + 1) will be used to access the object to which it points”

- Limits the effects of pointer aliasing

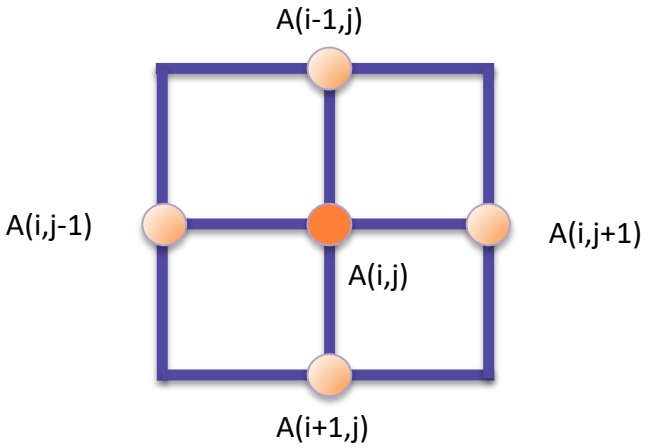
Compile and run

```
$pgcc -acc -Minfo=accel saxpy.c ticktock.c -o saxpy
$pgf90 -acc -Minfo=accel saxpy.f90 ticktock.f90  -o saxpy

saxpy.c:
saxpy:
  5, Generating implicit copy(y[:n])
     Generating implicit copyin(x[:n])
  6, Loop is parallelizable
     Accelerator kernel generated
     Generating Tesla code
    6, #pragma acc loop gang, vector(128)/* blockIdx.x threadIdx.x */
$./saxpy
```

Fundamental example

- Laplace equation for two dimensional heat conduction problem:



$$A(i,j) = \frac{A(i-1,j)+A(i+1,j)+A(i,j-1)+A(i,j+1)}{4}$$

- Jacobi iteration:

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

From PSC (https://www.psc.edu/images/xsedetraining/OpenACC_Nov2017/OpenACC_Introduction_To_OpenACC.PDF), Copyright John Urbanic.

Serial code

```
while ( dt > MAX_TEMP_ERROR && iteration <= max_iterations ) {
  for(i = 1; i <= ROWS; i++)
    for(j = 1; j <= COLUMNS; j++)
      Temperature[i][j] = 0.25 * (Temperature_last[i+1][j] +
              Temperature_last[i-1][j]+ Temperature_last[i][j+1] +
              Temperature_last[i][j-1]);

  dt = 0.0;

  for(i = 1; i <= ROWS; i++)
    for(j = 1; j <= COLUMNS; j++){
      dt = fmax( fabs(Temperature[i][j]-Temperature_last[i][j]), dt);
      Temperature_last[i][j] = Temperature[i][j];
    }

  if((iteration % 100) == 0) {
    track_progress(iteration);
  }
  iteration++;
}
```

Compute

Update

Print

Helper functions

```
void initialize(){
  int i,j;
  for(i = 0; i <= ROWS+1; i++)
    for(j = 0; j <= COLUMNS+1; j++)
      Temperature_last[i][j] = 0.0;

  // these boundary conditions never change throughout run
  // set left side to 0 and right to a linear increase
  for(i = 0; i <= ROWS+1; i++){
    Temperature_last[i][0] = 0.0;
    Temperature_last[i][COLUMNS+1] = (100.0/ROWS)*I;
  }

  // set top to 0 and bottom to linear increase
  for(j = 0; j <= COLUMNS+1; j++){
    Temperature_last[0][j] = 0.0;
    Temperature_last[ROWS+1][j] = (100.0/COLUMNS)*j;
  }
}
```

```
void track_progress(int iteration){
  int i;
  printf("-- Iteration: %d --\n", iteration);
  for(i = ROWS-5; i <= ROWS; i++)
    printf("[%d,%d]: %5.2f ", i, i,
           Temperature[i][i]);
  printf("\n");
}
```

OpenACC version

```
while ( dt > MAX_TEMP_ERROR && iteration <= max_iterations ) {
  #pragma acc kernels
  for(i = 1; i <= ROWS; i++)
    for(j = 1; j <= COLUMNS; j++)
      Temperature[i][j] = 0.25 * (Temperature_last[i+1][j] +
              Temperature_last[i-1][j]+ Temperature_last[i][j+1] +
              Temperature_last[i][j-1]);
  dt = 0.0;
  #pragma acc kernels
  for(i = 1; i <= ROWS; i++)
    for(j = 1; j <= COLUMNS; j++){
      dt = fmax( fabs(Temperature[i][j]-Temperature_last[i][j]), dt);
      Temperature_last[i][j] = Temperature[i][j];
    }

  if((iteration % 100) == 0) {
    track_progress(iteration);
  }
  iteration++;
}
```

Compile and run

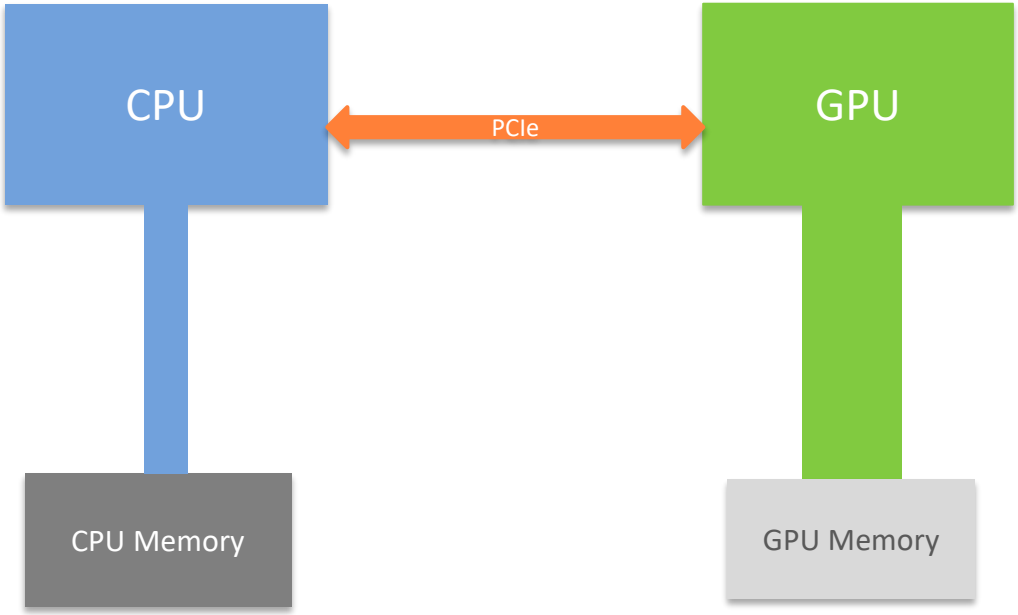
```
$pgcc -acc -Minfo=accel jacobi_acc.c -o jacobi_acc
$pgf90 -acc -Minfo=accel jacobi_acc.f90 -o jacobi_acc
main:
     36, Generating implicit copyin(Temperature_last[:][:])
         Generating implicit copyout(Temperature[1:1000][1:1000])
     37, Loop is parallelizable
     38, Loop is parallelizable
         Accelerator kernel generated
         Generating Tesla code
         37, #pragma acc loop gang, vector(4) /* blockIdx.y threadIdx.y */
         38, #pragma acc loop gang, vector(32) /* blockIdx.x threadIdx.x */
     44, Generating implicit copyin(Temperature[1:1000][1:1000])
         Generating implicit copy(Temperature_last[1:1000][1:1000])
     45, Loop is parallelizable
     46, Loop is parallelizable
         Accelerator kernel generated
         Generating Tesla code
         45, #pragma acc loop gang, vector(4) /* blockIdx.y threadIdx.y */
         46, #pragma acc loop gang, vector(32) /* blockIdx.x threadIdx.x */
         47, Generating implicit reduction(max:dt)
$./laplace_acc
```

Slower than serial and much slower than OpenMP version!!

Running with profiling on

```
main  NVIDIA  devicenum=0
    time(us): 2,600,570
    36: compute region reached 600 times
        38: kernel launched 600 times
            grid: [32x250]  block: [32x4]
             device time(us): total=66,868 max=114 min=111 avg=111
            elapsed time(us): total=82,196 max=499 min=134 avg=136
    36: data region reached 1200 times
        36: data copyin transfers: 600
             device time(us): total=478,660 max=841 min=793 avg=797
        42: data copyout transfers: 600
             device time(us): total=479,890 max=854 min=795 avg=799
    44: compute region reached 600 times
        44: data copyin transfers: 600
             device time(us): total=5,470 max=19 min=8 avg=9
        46: kernel launched 600 times
            grid: [32x250]  block: [32x4]
             device time(us): total=93,708 max=163 min=140 avg=156
            elapsed time(us): total=122,285 max=367 min=185 avg=203
        46: reduction kernel launched 600 times
            grid: [1]  block: [256]
             device time(us): total=13,817 max=32 min=23 avg=23
            elapsed time(us): total=24,132 max=85 min=38 avg=40
        46: data copyout transfers: 600
             device time(us): total=9,508 max=46 min=13 avg=15
    44: data region reached 1200 times
        44: data copyin transfers: 1200
             device time(us): total=966,408 max=843 min=796 avg=805
        51: data copyout transfers: 600
             device time(us): total=486,241 max=852 min=802 avg=810
```

Data movement



Data management

C

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

Fortran

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

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.
    - Principal use: For many important data structures in your code, this is a logical default to input, modify and return the data.
- `copyin( list )`
  - Allocates memory on GPU and copies data from host to GPU when entering region.
    - Principal use: Think of this like an array that you would use as just an input to a subroutine.
- `copyout( list )`
  - Allocates memory on GPU and copies data to the host when exiting region.
    - Principal use: A result that isn't overwriting the input data structure.
- `create( list )`
  - Allocates memory on GPU but does not copy.
    - Principal use: Temporary arrays.

Array shaping

- Compilers sometimes cannot determine the size of arrays, so we must specify explicitly using data clauses with an array “shape”.
  - The compiler will let you know if you need to do this. Sometimes, you do it for your own efficiency reasons.
- C

```
#pragma acc data copyin(a[0:size]), copyout(b[s/4:3*s/4])
```

- Fortran

```
!$acc data copyin(a(1:size)), copyout(b(s/4:3*s/4))
```

- Fortran uses start:end and C uses start:length

`update` directive

```
#pragma acc update host(a)
```

`host`: copies data from the device (GPU) to the host (CPU)

`device`: copies from the host to the device

- Explicitly transfers data between the host and the device

- Useful when you want to update data in the middle of a data region Clauses:

OpenACC solution with data clause

```
#pragma acc data copy(Temperature_last) create(Temperature)
while ( dt > MAX_TEMP_ERROR && iteration <= max_iterations ) {
  #pragma acc kernels
  for(i = 1; i <= ROWS; i++)
    for(j = 1; j <= COLUMNS; j++)
      Temperature[i][j] = 0.25 * (Temperature_last[i+1][j] +
              Temperature_last[i-1][j]+ Temperature_last[i][j+1] +
              Temperature_last[i][j-1]);
  dt = 0.0;
  #pragma acc kernels
  for(i = 1; i <= ROWS; i++)
    for(j = 1; j <= COLUMNS; j++){
      dt = fmax( fabs(Temperature[i][j]-Temperature_last[i][j]), dt);
      Temperature_last[i][j] = Temperature[i][j];
    }
  if((iteration % 100) == 0) {
    #pragma acc update host(Temperature)
    track_progress(iteration);
  }
  iteration++;
}
```

Conclusion

- OpenACC is an easy and quick way to make use of GPUs to run your code faster

- Data dependency and data movement are two important challenges to get a good speedup from GPU-based code

References

- References and useful links:
  - http://www.openacc.org
  - https://www.psc.edu/images/xsedetraining/OpenACC_Nov2017/OpenACC_Introduction_To_OpenACC.PDF
  - http://courses.cms.caltech.edu/cs101gpu/
  - http://on-demand.gputechconf.com/gtc/2017/presentation/S7133-jiri-kraus-multi-gpu-programming.PDF