Using OpenMP 4.5 Target Offload for Programming Heterogeneous Systems

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NASA Advanced Supercomputing Division

Outline

- Introduction
  - Concepts of Programming Heterogeneous Architectures
- OpenMP Heterogeneity Support Basics
  - Off-loading Work and Data to the GPU
  - Expressing Parallelism and Data Locality
- Using OpenMP 4.5 on Pleiades GPU Nodes
- Learning by Example
  - Laplace Kernel
- More OpenMP 4.5 Constructs and Clauses
- References

Question? Use the Webex chat facility to ask the Host

Heterogeneous Systems

- A general purpose processor connected to an accelerator device
- An example is an Intel Xeon processor connected to a Nvidia GPU

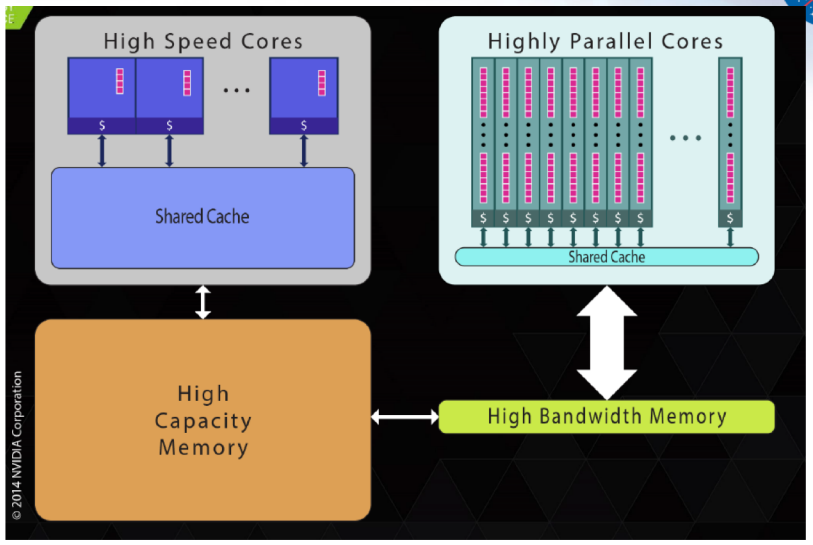


Image courtesy of Nvidia

- CPU
  - Fast clock (2.4-2.9 GHz on Pleiades)
  - Multiple cores (16-40 on Pleiades)
  - Complex cores
    - Large caches, complex branch prediction, OOO execution, multi-threading
  - Parallelism
    - Deep pipelines, multiple cores, vector units, SIMD execution

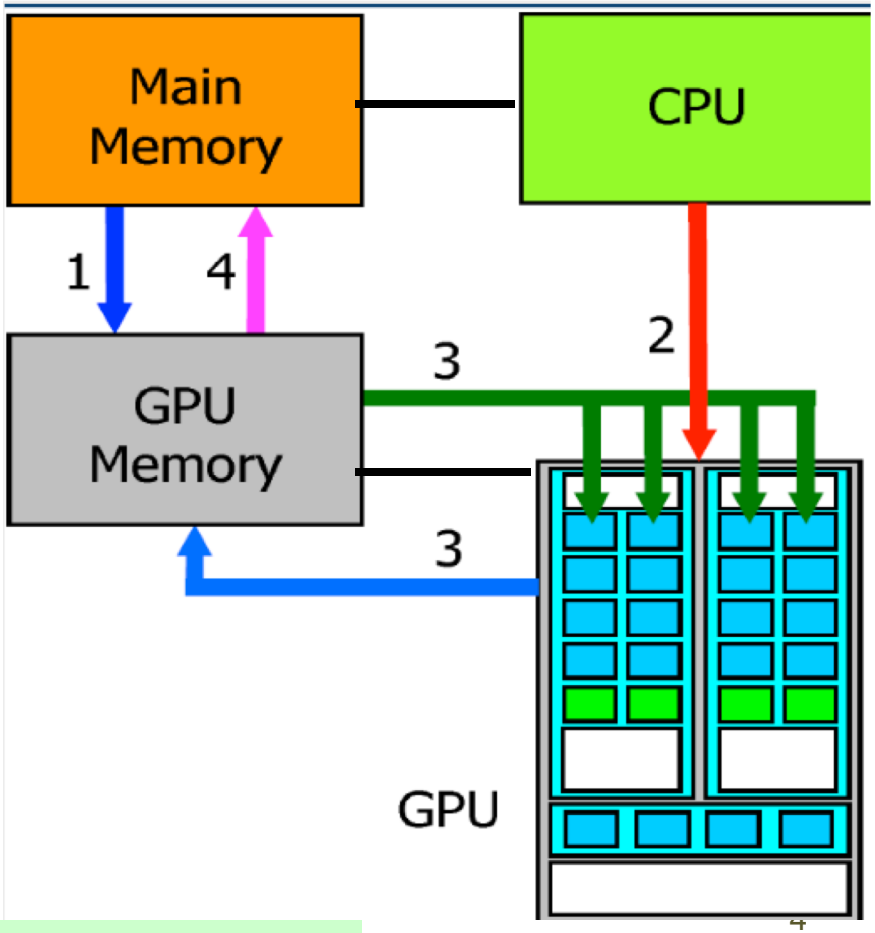
- Device
  - Slow clock (0.8-1.0 GHz)
  - Thousands of cores
    - 2880 SP cores on Pleiades
  - Lightweight cores:
    - Small caches, little branch prediction, in-order execution, multi-threading
  - Parallelism: Theoretically enormous!
    - In practice limited; SIMT execution

Question? Use the Webex chat facility to ask the Host

Programming Heterogeneous Systems

- Necessary steps to be taken
  - Identification and offloading of compute kernels from host to device
  - Expressing parallelism within the kernel
  - Manage data transfer between CPU and Device
- Execution flow
  1. Data copy from main to device memory
  2. CPU initiates kernel for execution on the device
  3. Device executes the kernel using device memory
  4. Data copy from device to main memory

Example:
Device is a GPU



Question? Use the Webex chat facility to ask the Host

Why Use OpenMP?

- Methods to program heterogeneous systems:
  - **Vendor specific** library routines
    - Examples: cuBlas, cufftw, …
  - **Vendor specific** frameworks
    - Example: Cuda
  - Public domain frameworks
    - Example: OpenCL
  - Compiler directive based API
    - OpenMP

- OpenMP:
  - Compiler directives
  - Runtime library routines
  - Environment variables
- Well established since 1997
- Heterogeneous programming since OpenMP 4.0
  - Seamlessly integrates into existing OpenMP code
  - Supported by many compilers: gcc, Intel icc, IBM xl, Cray cc

Low programming effort, high performance, **non-portable**

High programming effort, high performance, suitable for any kernel, **non-portable**

Medium programming effort with acceptable performance, portable

High programming effort, high performance, suitable for any kernel, portable

Question? Use the Webex chat facility to ask the Host

OpenMP Directive Syntax

- Compiler Directive
  - Programmer inserted hint/command for the compiler
- Directive Syntax
  - Fortran
    - Mostly paired with a matching **end** directive surrounding a structured code block

```
!$omp directive [clause [,] [clause] …]
    code
!$omp end directive
```

  - C
    - No **end** directive needed as the structured block is bracketed

```
#pragma omp directive [clause [,] [clause] …]
{
    code
}
```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OpenMP Heterogeneity Basic Support

`#pragma omp target` or
`!$omp target/end target`

- A device data environment is created for the marked region
- The marked code region is mapped to the device and executed.

`#pragma omp target teams` or
`!$omp teams/end teams`

- A **league** of thread teams is created
- The master thread of each team executes the code region

`#pragma omp target teams distribute`

- Worksharing construct: Share work across the teams

`#pragma omp parallel for` or `!$omp parallel do`

- Worksharing across threads within a team

We have seen those before….

`#pragma omp simd`

- Worksharing across vector length

`#pragma omp target map(map-type: list)`

- Map a variable to/from the device data environment

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Stencil Kernel in OpenMP 4.5

```
{
#pragma omp target teams   distribute  num_teams(4)
   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 = fmax( error, fabs(Anew[j][i] - A[j][i]));
          }        }
```

- League of teams is started via **target *teams***
- All teams execute the target region

- Work is distributed across the teams via ***distribute***

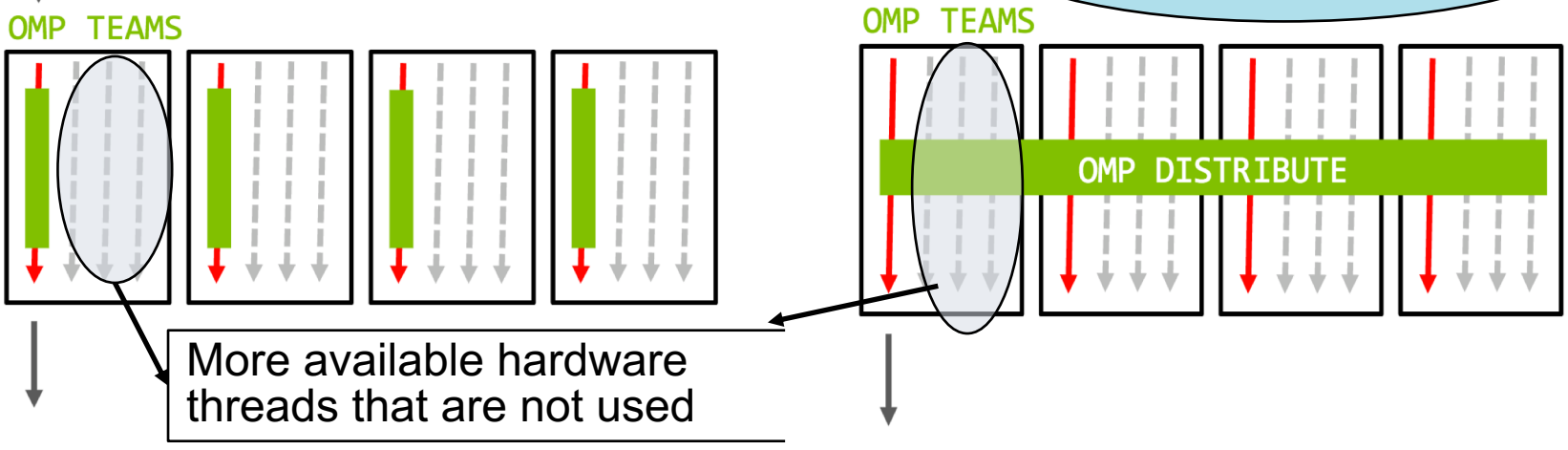
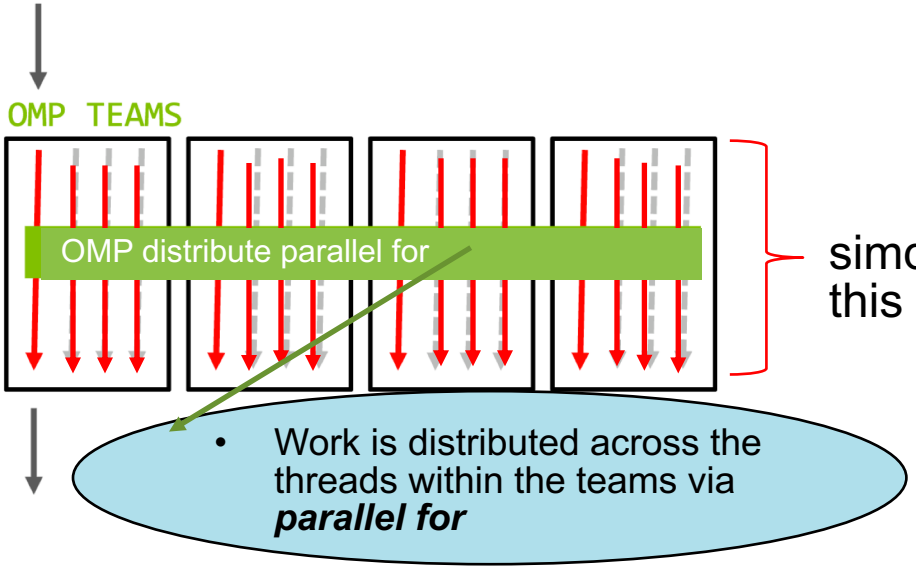


Image courtesy of Nvidia

Stencil Kernel in OpenMP 4.5

```
{
#pragma omp target teams distribute num_teams(4) parallel for thread_limit(4)
   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 = fmax( error, fabs(Anew[j][i] - A[j][i]));
          }         }
```



For more details check out the presentation by Jeff Larkin, Nvidia:
http://on-demand.gputechconf.com/gtc/2016/presentation/s6510-jeff-larkin-targeting-gpus-openmp.pdf

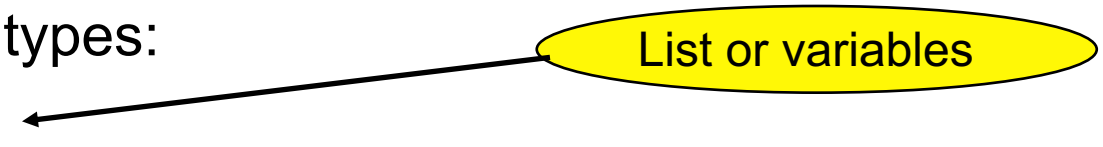
Image courtesy of Nvidia

Structured Data Management

- The device data region:
  - A region of the program within which data is accessible to the device
  - It can be explicitly defined to reduce data copies
  - The `target data` construct is used to mark such regions

```
#pragma omp target data map(map-type: list)
```

- Example map types:



`to (list)`

  - Allocates memory on the device and copies data in when entering the region, the values are not copied back

`from (list)`

  - Allocates memory on the device and copies the data to the host when exiting the region

`alloc (list)`

  - Allocates memory on the device
  - If the data is already present on the device a reference counter is incremented

Question? Use the Webex chat facility to ask the Host

Compiling and Running on Pleiades

- Pleiades GPU nodes:
  - 64 Sandy Bridge nodes with one Tesla K40 GPU
- Compilation:
  - Intel icc/ifort does not generate code for Nvidia GPU execution ☹
  - PGI pgcc/pgf90 does not support the OpenMP target construct ☹
  - **Experimental gcc 8.1 with GPU support is available on Pleiades ☺**

```
module purge
module load cuda
module load /home1/gjost/public/modules/gcc8.1-module
gcc --version
gcc or gfortran  -fopenmp -foffload="-lm"   test.c or test.f90
```

- Submit to GPU node

```
qsub -l select=1:ncpus=16:model=san_gpu -q k40
```

- Run the executable

```
./a.out
```


Question? Use the Webex chat facility to ask the Host

Example: 2D Laplace Solver

```
#pragma omp target data map(to:Anew) map(A)
while ( error > tol && iter < iter_max ) {
        error = 0.0;

#pragma omp target teams distribute parallel for reduction(max:error)
map(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 = fmax( error, fabs(Anew[j][i] - A[j][i]));}}
#pragma omp target teams distribute parallel for
         for( int j = 1; j < n-1; j++) {
            for( int i = 1; i < m-1; i++ ) {
                A[j][i] = Anew[j][i]; }}

if(iter % 100 == 0) printf("%5d, %0.6f\n", iter, error);
iter++;} // end of while loop
```

or alloc

total: 167.7766 seconds on Pleiades

Example: 2D Laplace Solver Separated


```
#pragma omp target data map(to:Anew) map(A)
while ( error > tol && iter < iter_max ) {
        error = 0.0;

#pragma omp target teams distribute reduction(max:error) map(error)
        for( int j = 1; j < n-1; j++){
#pragma omp parallel for reduction(max:error)
            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 = fmax( error, fabs(Anew[j][i] - A[j][i]));}}
#pragma omp target teams distribute
         for( int j = 1; j < n-1; j++){
#pragma omp parallel for
            for( int i = 1; i < m-1; i++ ){
                A[j][i] = Anew[j][i]; }}

 if(iter % 100 == 0) printf("%5d, %0.6f\n", iter, error);
 iter++;}
```

total: 155.659801 seconds on Pleiades

- Other possibilities, eg use collapse clause
- Depends on problem sizes and system

Question? Use the Webex chat facility to ask the Host

Example: 2D Laplace Solver in Fortran


```
!$omp target data map(to:Anew) map(A)
  do while ( error .gt. tol .and. iter .lt. iter_max )
    error=0.0_fp_kind
!$omp target teams distribute parallel do reduction(max:error) map(error)
    do j=1,m-2
      do i=1,n-2
        Anew(i,j) = 0.25_fp_kind * ( A(i+1,j  ) + A(i-1,j  ) + &
                                     A(i  ,j-1) + A(i  ,j+1) )
        error = max( error, abs(Anew(i,j)-A(i,j)) )
      end do
    end do
!$omp end target teams distribute parallel do
    if(mod(iter,100).eq.0 ) write(*,'(i5,f10.6)') iter, error
    iter = iter + 1
!$omp target teams distribute parallel do
    do j=1,m-2
      do i=1,n-2
        A(i,j) = Anew(i,j)
      end do
    end do
!$omp end target teams distribute parallel do
  end do
!$omp end target data
```


Question? Use the Webex chat facility to ask the Host

Performance Challenges

- Function calls in inner loops:
  - Challenging for the compiler's dependence analysis
    - Possibly use `!$omp declare target` to compile routine for the device (p. 20)
    - manually in-line
- IF-Branches:
  - Can get expensive if threads take different execution paths
    - Move your branches up to a level in your code where all threads go down the same code branch
    - Avoid branches in inner loops
- Structures with complex and/or dynamic components:
  - Might prevent stride 1 memory access
  - Example: NPB FT uses complex data; performance increase via manual linearization
  - Unstructured data management for structures with dynamic components (next slide)
- Loop strides/memory layout
  - Inner loop should be long and move along the fastest dimension

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Unstructured Data Management: Enter/Exit Data Constructs

- Real life applications, just like real life, are not always a nicely structured sequence of code regions
  - Example: C++ Structures or Fortran user defined types with dynamic arrays
- Unstructured data directives

```
!$omp target enter data map(map_type:list)
```

  - Allocate memory on the device for the remainder of the program or until explicitly deleted
  - Possible map types are `to, alloc`

```
!$omp target exit data map(map_type:list)
```

  - Deallocate the memory on the device
  - Possible map types are `from, release`, or `delete`
- Multiple `enter/exit data` constructs, branched across different function calls are allowed

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Unstructured Data Management


```
module matrix_mod
  implicit none
  type matrix
    integer :: num_rows
    integer :: nnz
    integer, pointer :: row_offsets(:)
    integer, pointer :: cols(:)
    real(8), pointer :: coefs(:)
  end type matrix
  public :: allocate_3d
  ….

  subroutine  allocate_3d (a, n)
    implicit none
    type(matrix) :: a
    allocate(a%row_offsets(num_rows+1))
    allocate(a%cols(nnz))
    allocate(a%coefs(nnz))
    arrow_offsets => a%row_offsets
    acols => a%cols
    acoefs => a%coefs
!$omp target enter data map(to:a)
!$omp target enter data map(to:acols(1:nnz)…
end subroutine allocate_3d
end module matrix_mod
```

```
subroutine free_3d(a)
    implicit none
    type(matrix) :: a
     …
    arow_offsets => a%row_offsets
    acols => a%cols
    acoefs => a%coefs

    !$omp exit data map(delete:acols(1:nnz),…)
    !$omp exit data map (delete: a)
    deallocate(arow_offsets)
    deallocate(acols)
    deallocate(acoefs)
  end subroutine free_matrix
```

Call `allocate_3d` and `free_3d` as often as you need to, also across subroutine calls

Routines and global variables

!$omp declare target

- Specifies that variables, functions and subroutines are mapped to a device for the duration of the program

in LBM.cpp

```
#pragma omp target teams distribute parallel do
for (int index1 = 0; index1 < a_numPts; ++index1)
     {
       Real feq[NUMV];
       getFEQ(feq,index1);
```

in LBM.H

```
#pragma omp declare target
inline void getFEQ(Real* const __restrict a_feq,
                   const int a_index1)
#pragma omp end declare target
```

Synchronize host and device buffers

!$omp target update clause

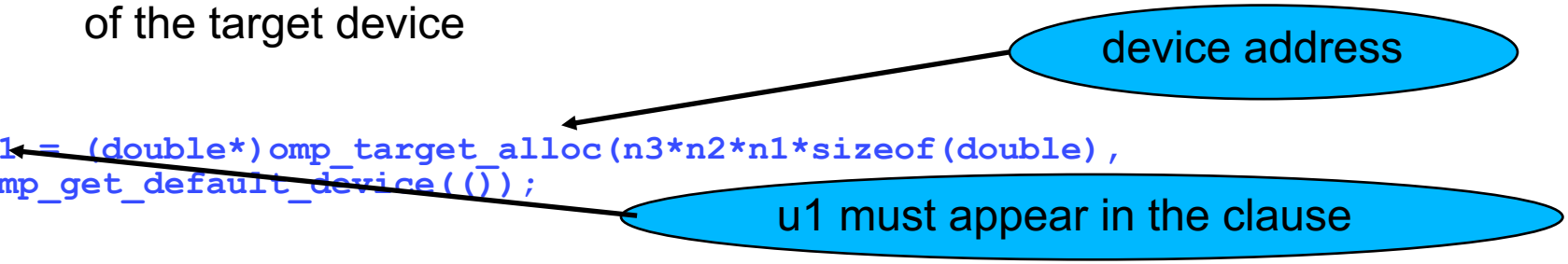
- Makes the variables on the device consistent with the original variables
- Possible motion clauses are to or from

```
#pragma omp declare target
void work_on_device_work(int* srcA, int* result);
#pragma omp end declare target

#pragma omp target data map(to:a[0:size)map(from:c[0:size])
{
   #pragma omp target
   {
      work_on_device_work(a, c);
   }
   /* Copy modified target data to the host */
   #pragma omp target update from(c[0:size])

   work_on_host(c);
   #pragma omp target
   {
      work_on_device_work(a, c);
   }
```


Question? Use the Webex chat facility to ask the Host

Device Pointers

- Pointer variable on the host containing device address
- Device memory routines
  - Support of allocation and management of pointers in the data environment of the target device




```
u1 = (double*)omp_target_alloc(n3*n2*n1*sizeof(double),
omp_get_default_device());
…

#pragma omp target map(tofrom: ou[0:n3*n2*n1]) is_device_ptr(u1)

#pragma omp teams distribute
 for (i3 = 1; i3 < n3-1; i3++) {

#pragma omp parallel for collapse(2)
    for (i2 = 1; i2 < n2-1; i2++) {
            for (i1 = 0; i1 < n1; i1++) {
                 I3D(u1, n1, n2, i3, i2, i1) =
                                    I3D(ou, n1, n2, i3, i2-1, i1)
                                  + I3D(ou, n1, n2, i3, i2+1, i1)
                                  + I3D(ou, n1, n2, i3-1, i2, i1)
                                  + I3D(ou, n1, n2, i3+1, i2, i1); }}}

Note :
#define I3D(array,n1,n2,i3,i2,i1) (array[(i3)*n2*n1 + (i2)*n1 + (i1)])
```


Question? Use the Webex chat facility to ask the Host

References

Using GPUs codes on Pleiades HECC KB

https://www.nas.nasa.gov/hecc/support/kb/using-gpu-nodes_298.html

Jeff Larkin Presentation

(see slide) https://www.nas.nasa.gov/publications/ams/2015/04-21-15.html

- OpenMP Home Page and Books

http://www.openmp.org/

http://www.openmp.org/tech/using-openmp-next-step/

https://mitpress.mit.edu/books/using-openmp

Fortran Target Routines

```
module mod_fib
contains
  subroutine fib(N)
     integer :: N
     !$omp declare target
     ! ….
   end subroutine
   end module
program my_fib
  !$omp target if (N > 1000)
      call fib(N)
  !$omp end target
 end program
```

in a module

```
program my_fib
Integer :: N=8
!$omp declare target(fib)
  !$omp target
      call fib(N)
  !$omp end target
 end program
 subroutine fib(N)
 integer :: N
 !$omp declare target
    print*, “hello from fib”
    !...
  end subroutine
```

external

Host/Device Asynchronous Execution

```
#pragma omp target map(a,b,c,d) nowait
{
    {
    #pragma parallel for
    for (i=0; i<N; i++) (
        a[i] = b[i] * c + d;
    }
 }
 F(b); //Execute in parallel with target task

 #pragma omp taskwait //wait for target task to finish
```

Example: 2D Laplace Solver Collapse

```
#pragma omp target data map(to:Anew) map(A)
while ( error > tol && iter < iter_max ) {
        error = 0.0;

#pragma omp target teams distribute parallel for reduction(max:error)
map(error) collapse (2)
      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 = fmax( error, fabs(Anew[j][i] - A[j][i]));}}
#pragma omp target teams distribute parallel for collapse(2)
       for( int j = 1; j < n-1; j++){
            for( int i = 1; i < m-1; i++ ) {
                A[j][i] = Anew[j][i]; }}

if(iter % 100 == 0) printf("%5d, %0.6f\n", iter, error);
iter++;}
```

total: 167.67 seconds on Pleiades

Get to know your GPU

```
PBS r313i1n2 51> module load cuda
PBS r313i1n2 52> nvidia-smi
Mon Mar 18 14:58:08 2019
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 384.81                 Driver Version: 384.81                    |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|===============================+======================+======================|
|   0  Tesla K40m          Off  | 00000000:02:00.0 Off |                    0 |
| N/A   25C    P0    67W / 235W |      0MiB / 11439MiB |     95%      Default |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                       GPU Memory |
|  GPU       PID   Type   Process name                             Usage      |
|=============================================================================|
|  No running processes found                                                 |
+-----------------------------------------------------------------------------+
```

nvprof textual Profiles

Sparse Matvec Better

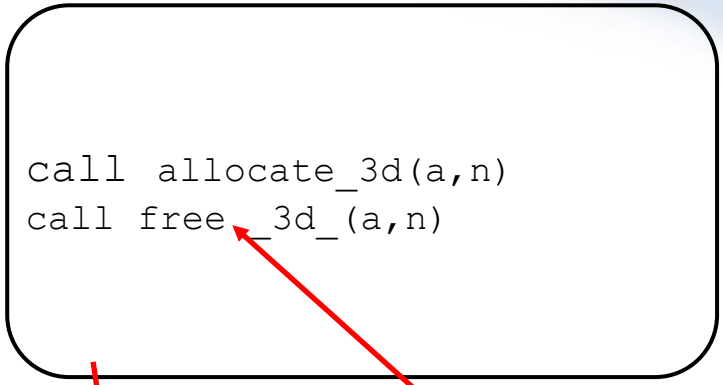
```
 Total Iterations:          100 Time (s):    16.21501
==95387== Profiling result:
Time(%)      Time     Calls       Avg       Min       Max  Name
 97.02%  15.8332s       101  156.76ms  156.50ms  156.90ms  matvec_114_gpu
  1.91%  311.27ms       302  1.0307ms  696.17us  1.0377ms  waxpby_60_gpu
  0.89%  145.68ms       200  728.41us  620.77us  843.05us  dot_46_gpu
  0.18%  29.020ms       200  145.10us  144.10us  146.27us  dot_46_gpu_red
  0.00%  422.63us       200  2.1130us  2.0800us  2.7840us  [CUDA memcpy DtoH]
  0.00%  186.50us       200     932ns     896ns  1.6320us  [CUDA memcpy HtoD]
```

nvprof ./cg.exe

Sparse Matvec Best

```
 Total Iterations:          100 Time (s):    5.814235
Profiling application: ./cg.x
==64924== Profiling result:
Time(%)      Time     Calls       Avg       Min       Max  Name
 87.90%  5.36086s       101  53.078ms  53.044ms  53.107ms  matvec_118_gpu
  5.07%  309.17ms       302  1.0237ms  680.83us  1.0302ms  waxpby_64_gpu
  4.17%  254.03ms       370  686.57us     896ns  1.7418ms  [CUDA memcpy HtoD]
  2.37%  144.67ms       200  723.35us  622.12us  831.88us  dot_50_gpu
  0.47%  28.874ms       200  144.37us  143.39us  145.63us  dot_50_gpu_red
  0.01%  641.54us         2  320.77us  320.55us  320.99us  initialize_vector_26_gpu
  0.01%  414.98us       200  2.0740us  2.0480us  2.8480us  [CUDA memcpy DtoH]
```

Unstructured Data Management




```
module matrix_mod
  implicit none
  type matrix
    integer :: num_rows
    integer :: nnz
    integer, pointer :: row_offsets(:)
    integer, pointer :: cols(:)
    real(8), pointer :: coefs(:)
  end type matrix
  public :: allocate_3d
  ….
  subroutine  allocate_3d (a, n)
    implicit none
    type(matrix) :: a
    allocate(a%row_offsets(num_rows+1))
    allocate(a%cols(nnz))
    allocate(a%coefs(nnz))
    arrow_offsets => a%row_offsets
    acols => a%cols
    acoefs => a%coefs
!$omp target enter data map(to: a)
!$omp target enter data map(to : a%row_offsets,a%cols,a%coefs)…
end subroutine allocate_3d
end module matrix_mod
```

```
!$omp target exit data map(delete: a)
```

Call as often as you need to, also across subroutine calls

Question? Use the Webex chat facility to ask the Host