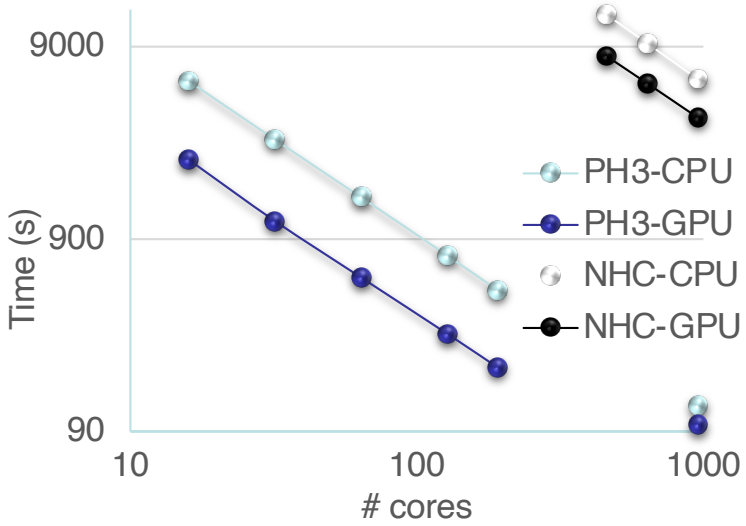
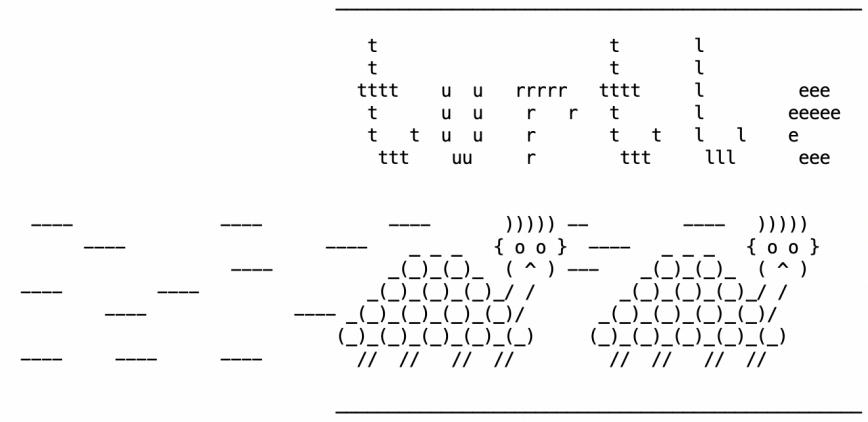
GPU programming with openMP





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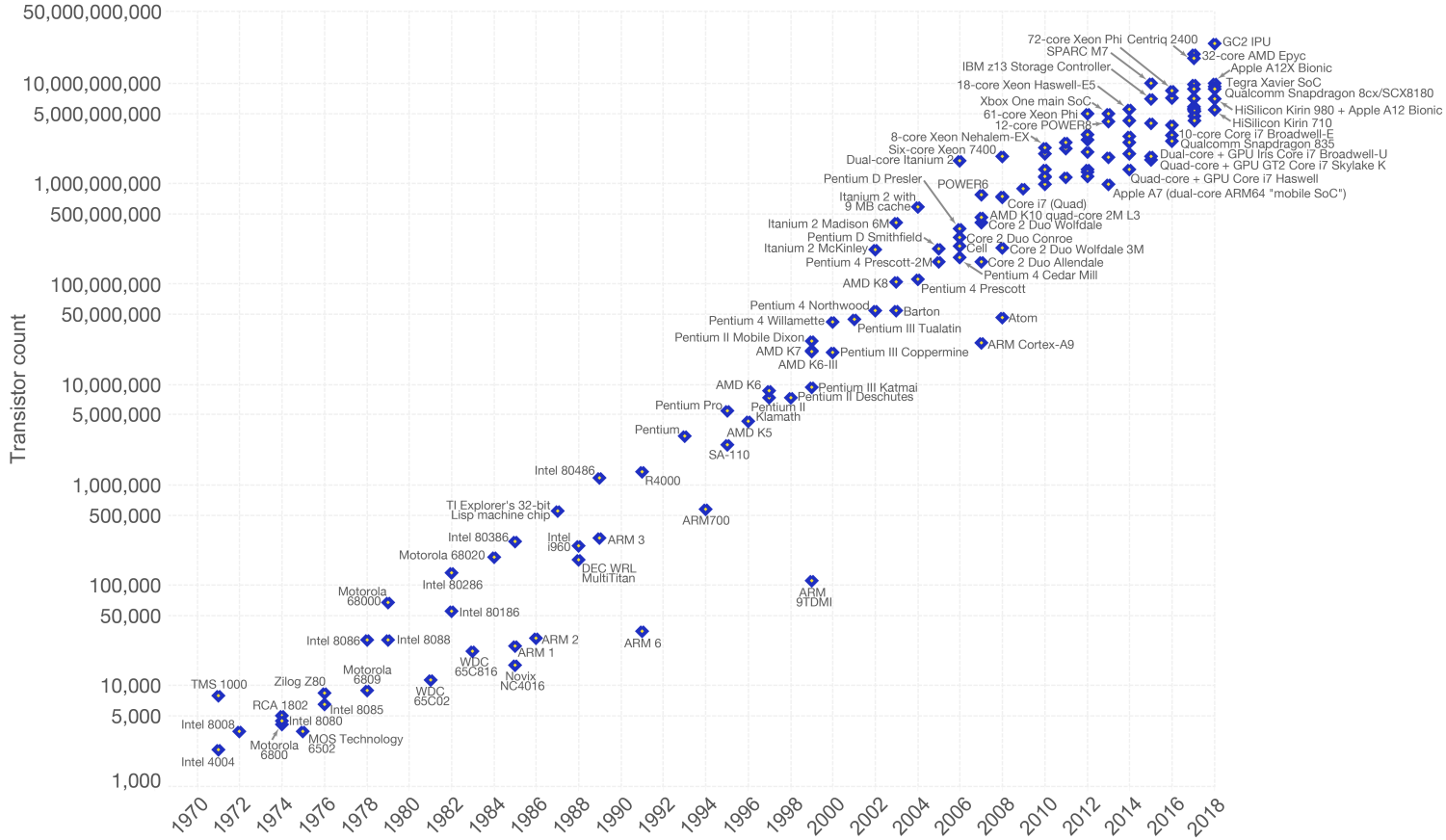
Overview

- Parallel programming with openMP and GPU offloading
  - Introduction
  - Basic steps
  - Examples
  - Hands-on session

Moore’s law

Moore’s Law – The number of transistors on integrated circuit chips (1971-2018)

Moore's law describes the empirical regularity that the number of transistors on integrated circuits doubles approximately every two years. This advancement is important as other aspects of technological progress – such as processing speed or the price of electronic products – are linked to Moore's law.



Data source: Wikipedia (https://en.wikipedia.org/wiki/Transistor_count)
The data visualization is available at OurWorldinData.org. There you find more visualizations and research on this topic.

Current supercomputers

- High node and core counts
- Equipped with accelerators

Summit at OLCF

Introduction to GPU with openMP

- CPU:
  - Fast clock
  - Multiple cores (8-64)
  - Complex cores

- GPU:
  - Slow clock
  - Thousands of cores
  - Lightweight cores

Why use openMP

- Methods to program heterogeneous systems:
  - Vendor specific library routines
    - cuBlas
  - Vendor specific frameworks
    - Cuda
  - Public domain frameworks
    - OpenCL
  - Compiler directive based API
    - OpenMP

Low programming effort, high performance, non portable

High programming effort, high performance, non portable

High programming effort, high performance, portable

Medium programming effort, high performance, portable

Advantages of openMP

- Compiler directives
- Runtime library routines
- Environment variables
- Heterogeneous programming since OpenMP 4.0
  - Integrates into existing openMP code
  - Supported by many compilers

openMP

- Compiler directive
  - Programmer inserted hint/command for the compiler
- Directive syntax
  - Fortran
    - Paired with matching *end* surrounding a code block

```
!$omp directive
    code
!$omp end directive
```

  - C
    - No *end* directive needed ({})

```
#pragma omp directive
{
code
}
```

openMP worksharing

- Parallel directive
  - Spawns a team of threads
  - Execution continues on all threads of team
  - All threads join at the end and the master thread continues

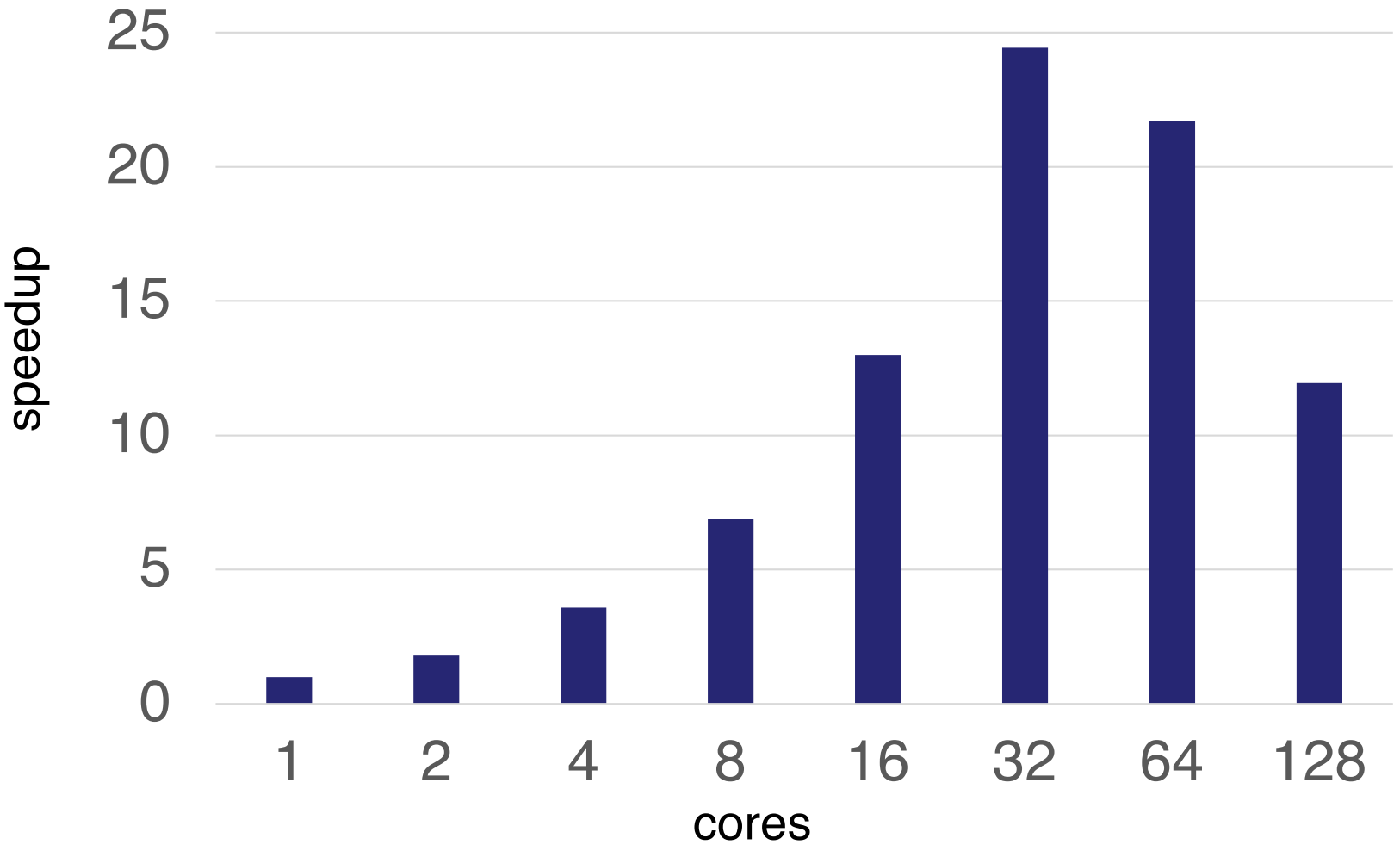
- FOR/DO (loop) directive
  - Divides the iterations of the next loop across the threads in the team

Matrix-matrix multiplication with openMP

```
      tstart=omp_get_wtime()
!$omp parallel do
      do i=1,ndim
        do j=1,ndim
          do k=1,ndim
            c(i,j)=c(i,j)+a(i,k)*b(k,j)
          enddo
        enddo
      enddo
      tend=omp_get_wtime()
```

Create a team of threads and workshare this loop across the threads

CPU version



GPU offloading

- gfortran v. 10
- AMD CPUs/GPUs and IBM Power 9 CPUs/GPUs
- Options:
  - -fopenmp [-foffload=amdgcn-amdhsa="-march=gfx906”]

```
      tstart=omp_get_wtime()
!$omp target
!$omp parallel do
      do i=1,ndim
        do j=1,ndim
          do k=1,ndim
            c(i,j)=c(i,j)+a(i,k)*b(k,j)
          enddo
        enddo
      enddo
      tend=omp_get_wtime()
```

Relocates execution to the Target (GPU) device

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GPU timing

Cores	Time (s)	Speedup
1	4698	1
2	2619	1.8
4	1313	3.6
8	681	6.9
16	362	13.0
GPU	27225	0.2

- No speedup! Only slow-down! Why?
- Parallel directive creates a single level of parallelism, and threads must be able to synchronize ⇒ GPU uses 1 thread block
- The *teams* directive to introduce a second level of parallelism

openMP teams

```
      tstart=omp_get_wtime()
!$omp target teams distribute
!$omp parallel do
      do i=1,ndim
        do j=1,ndim
          do k=1,ndim
            c(i,j)=c(i,j)+a(i,k)*b(k,j)
          enddo
        enddo
      enddo
      tend=omp_get_wtime()
```

Relocate execution to the target device, generate teams, distribute loop to teams and workshare

- Timing: 557 s; speedup: 8.4 x faster than serial version
- No synchronization between teams

Collapse clause

```
        tstart=omp_get_wtime()
!$omp target teams distribute
!$omp& parallel do collapse(2)
        do i=1,ndim
          do j=1,ndim
            do k=1,ndim
              c(i,j)=c(i,j)+a(i,k)*b(k,j)
            enddo
          enddo
        enddo
        tend=omp_get_wtime()
```

Collapse loops

ndim=4096

Machine	Time (s) No collapse	Time (s) Collapse
AMD - CPU	39.20	24.05
AMD - GPU	72.13	198.92
IBM - CPU	302.6	303.75
IBM - GPU	13.10	13.20

- Advantage not clear

Collapse clause (2)

```
      do while(error.gt.tol)
      error=0.0d0
      iter=iter+1
!$omp target teams distribute
!$omp& parallel do reduction(max:error)
!$omp& collapse(2) map(error)
      do i=2,ndim-1
        do j=2,ndim-1
          anew(j,i)=0.25*(a(j,i+1)+a(j,i-1)
     &     +a(j-1,i)+a(j+1,i))
          error=max(error,dabs(anew(j,i)-a(j,i)))
        enddo
      enddo
      …
      end do
```

Collapse loops

ndim=20000

Machine	Time (s) No collapse	Time (s) Collapse
AMD - CPU	558.22	519.98
AMD - GPU	7009.52	4228.25
IBM - CPU	2000.49	3174.13
IBM - GPU	250.57	251.58

- Collapse improves performance on AMD

Data movement – Power method

```
do while (error.gt.tol)
!$omp target teams …
  v2=a*v
!$omp target teams …
  dd=ddot(v2)
  val=dsqrt(dd)
!$omp target teams …
  v2=v2/val
!$omp target teams …
  error=ddot(v2-v)
  v=v2
end do
```

- Size of matrix: 10000

Machine	Time (s)
AMD - CPU	45.94
AMD - GPU	124.22
IBM - CPU	88.72

- Bad timings due to data movement

Data movement – Power method

```
!$omp target data map(v,v2,a)
do while (error.gt.tol)
!$omp target teams …
  v2=a*v
!$omp target teams …
  dd=ddot(v2)
  val=dsqrt(dd)
!$omp target teams …
  v2=v2/val
!$omp target teams …
  error=(v2-v)**2
  v=v2
end do
!$omp end target data
```

- Size of matrix: 10000

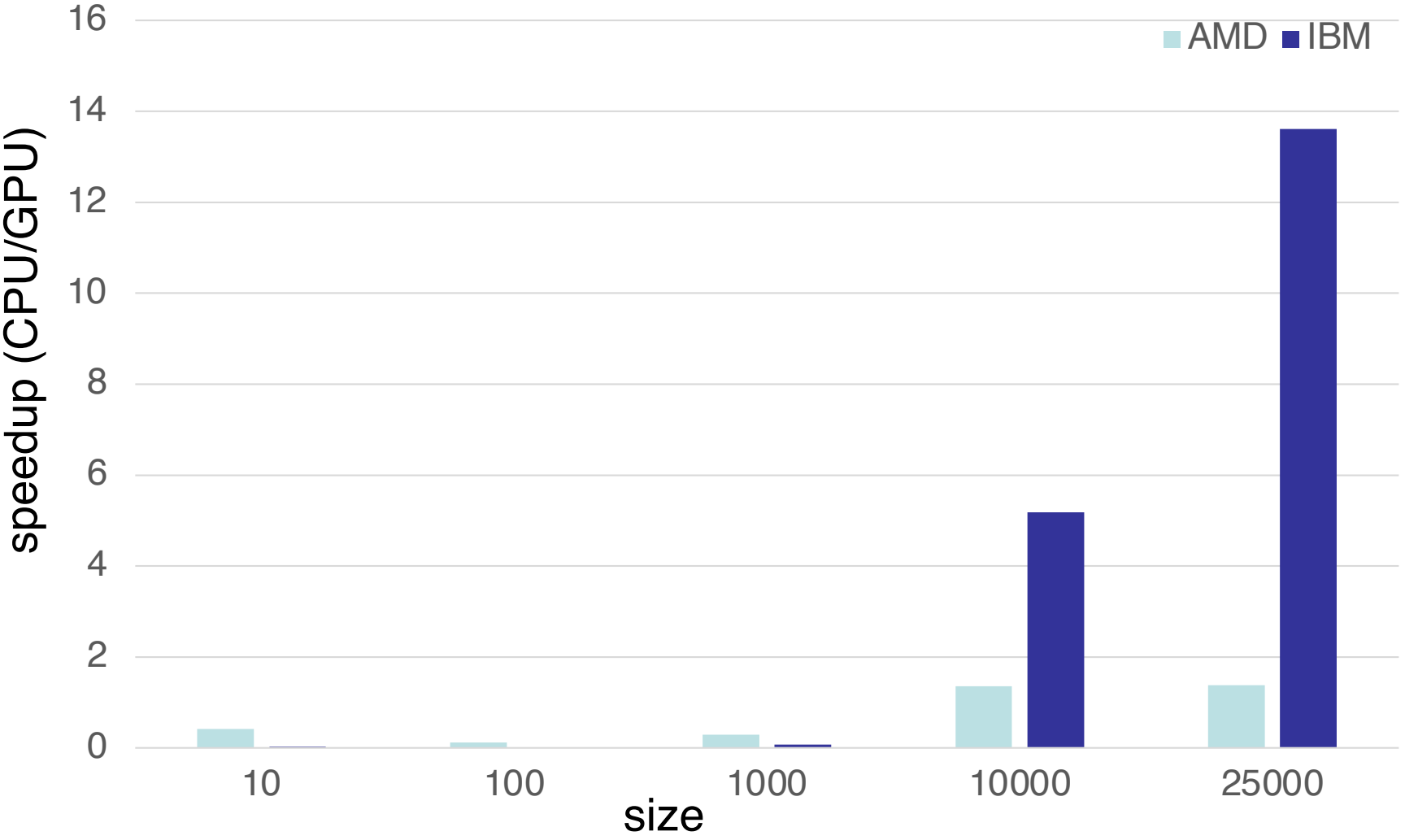
Machine	Time (s)
AMD - CPU	45.94
AMD - GPU	124.22
AMD - GPU2	33.69
IBM - CPU	88.72
IBM - GPU	--
IBM - GPU2	16.86

- Considerable improvement in performance

target data map

- target data map(<options>)
  - to – create space on the GPU and copy input data
  - from – create space on the GPU and copy output data
  - tofrom – create space on the GPU and copy input and output data
  - alloc – create space on the GPU, do not copy data

Power method, size dependence?



- GPU is not always faster! Only when the workload is high enough

openMP Host fallback

```
      tstart=omp_get_wtime()
!$omp target parallel do if(ndim>5000)
      do i=1,ndim
        do j=1,ndim
          do k=1,ndim
            c(i,j)=c(i,j)+a(i,k)*b(k,j)
          enddo
        enddo
      enddo
      tend=omp_get_wtime()
```

Only relocate execution to the device if the condition is met. Both a host and device version is built.

Device pointers

- use_device_ptr allows OpenMP device arrays to be passed to CUDA or accelerated libraries
- is_device_ptr clause allows CUDA arrays to be used within OpenMP target regions

```
!$omp target data map(x,y)
!$omp target teams distribute parallel do
        do i=1,ndim
          x(i)=1.0
          y(i)=2.0
        enddo
!$omp target data use_device_ptr(x,y)
        call cublasSaxpy(ndim,2.0,x,y,1)
```

Calling a function/subroutine

```
      program funct
      parameter (ndim=100)
      allocatable ival(:)
!$omp declare target(iff)
      allocate(ival(ndim))
!$omp target teams distribute parallel do map(from:ival)
      do i=1,ndim
         ival(i)=iff(i)
      enddo
!$omp end target teams distribute parallel do
      write(6,'(10I8)')(ival(i),i=1,ndim)
      end
      function iff(n)
!$omp declare target
      iff=n*n
      return
      end
```

Generate device code

Some openMP functions and environments

- OMP_DEFAULT_DEVICE
- omp_set_default_device/omp_get_default_device
- omp_get_num_devices
- omp_target_alloc/omp_target_free

Other options

- Launch kernel asynchronously (nowait)
- Depend clause
- OpenMP tasks
  - Define independent blocks of work
- Target enter/exit data construct
  - Map variables to the device data environment
    - Can span more than one function
- Target update: synchronize data with variable in device data environment

- Many more options:
  - See www.openmp.org

Hybrid MPI/openMP

- To fully exploit a machine, combine MPI with openMP

- Summit
  - 6 GPUs, 44 CPU cores
- AMD machine
  - 8 GPUs, 128 CPU cores
- Cartesius
  - 2 GPUs, 16 CPU cores

- Distribute work over GPUs and CPUs

- …

Important lessons

- Always use teams and distribute directive to expose all available parallelism
- Use the target data directive and map clauses to minimize data movement
- Aggressively collapse loops to increase available parallelism?
  - Test and tune!
- Use accelerated libraries
- Use host fallback to generate host and device code

Resources

- Jeff Larkin (NVIDIA) – OpenMP on GPUs, First Experiences and Best Practices
- James C. Beyer (NVIDIA) et al. – Advanced OpenMP Tutorial
- www.openmp.org
  - Openmp-examples
  - Openmp-4.5

- Many examples on the web

Acknowledgments

Hands-on session

- Write a program with some loop and possibility for data movement (multiple loops with same vectors)
  - For example (or one of the openACC examples):
    - ddot=ddot+v(i)*v(i)
    - a(i)=c*b(i)+d
    - …
- Parallelize it with openMP
- Introduce target directives
- Do some timings on the CPU (use different number of threads (OMP_NUM_THREADS environment))
- Compare with different GPU timings (openACC vs openMP)

Compiling on Cartesius

- module use /sw/arch/RedHatEnterpriseServer7/EB_testing/modulefiles
- module load compiler/GCCcore/10.2.0
- gfortran/gcc –fopenmp –o name.x name.f/c (or use make with makefile)

- Interactive usage:
  - ssh gcn1
  - ./name.x
  - (check in another terminal with nvidia-smi the GPU usage)

- Batch usage
  - Make a batch script name
  - sbatch name
  - (Check with squeue on which node it runs
    - ssh to the node, and check with nvidia-smi GPU usage)

Batch script

```
#!/bin/bash
#SBATCH --job-name=name
#SBATCH --output=name.o%J
#SBATCH --time=0:30:00
#SBATCH --nodes=1
#SBATCH --reservation=prace_gpu_day_4
#SBATCH --ntasks-per-node=1

./program.x
```

- Use ‘sbatch *script*’ to submit job
- Example: /scratch/shared/ccur0054/example.tar