An introduction to OpenMP

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Before We Start

- The OpenMP web site is a good source of information:

`openmp.org`

  - tutorials and examples from beginner to advanced
  - the standard (which is easy to understand for a standard)
  - quick reference guides

Multicore

The Free Lunch

- For a long time high-performance computing had a "free-lunch"
  - The density of transistors in chips increased, decreasing the size of integrated circuits
    - same number of transistors with less power
    - more transistors to add functionality
  - The clock speeds steadily rose, increasing the number of operations per second (from MHz to GHz)
- But the free lunch has been over for a few years now
  - We are reaching the limitations of transistor density
  - Increasing clock frequency requires too much power

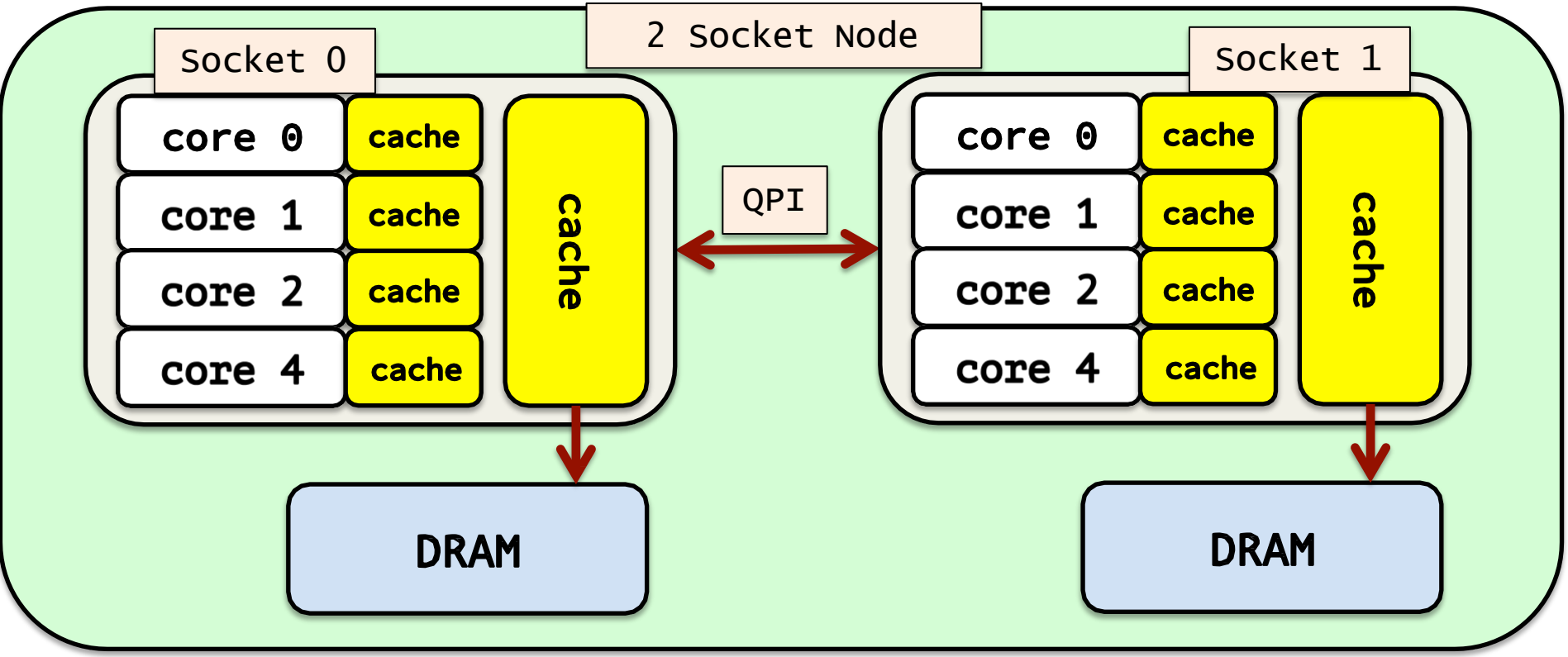
we used to focus on floating point operations **per second**
now we also think about floating point operations **per Watt**

The Solution: Multicore

- The number of transistors is still increasing
  - Sandy Bridge 28 nm, Haswell 22 nm, Broadwell 14 nm
  - Projected hard limit of 5–7 nm
- This has lead to three trends
  - more cores
    - the Haswell/Broadwell processors on Daint has 12/18 cores
    - KNL processors on Tave have 64 cores (x4 HT)
  - reducing clock speed
  - simplify/specialize cores
    - An extreme example of this is GPUs, which have in the order of 100/1000s of cores specialized for tasks common in graphics

Multicore HPC Nodes

- A CPU-based node can have multiple sockets, each with multiple cores.
  - cores on a socket share cache and uniform DRAM access



Piz Daint: using lstopo

- the `lstopo` command can be used to visualize node topology
- Multicore nodes have 2 sockets with 18 cores each

The **Flat** MPI Model

- MPI is the dominant parallelization model in HPC
  - The problem being solved is broken into chunks, one chunk per MPI process
  - Processes communicate via message passing
- The flat MPI model was well-suited to few cores per socket/node
  - Each MPI process sees one core with its cache and memory.
  - It is a logical abstraction for the underlying hardware
- You will learn about MPI later in this course

The **Hybrid** MPI-OpenMP Model

- The flat MPI model assigns one process per core
  - for 8/16/32/64 ranks per multi-core node
  - can have scaling problems with many nodes/MPI ranks: the amount of data passed around in messages increases as number of ranks increases
  - to take advantage of shared cache and DRAM on a socket, why not use threads on the socket/node, and pass messages between sockets/nodes?
- The hybrid MPI-OpenMP model has light-weight threads that share on-node memory.

This course is about OpenMP, however you could use other threading technologies like **pthreads, Intel Threading Building Blocks, HPX** or **C++11 threads.**

NUMA

- On a multi-socket node each socket has its own DRAM memory
- However the operating system presents all memory as one unified memory space
  - threads can read and write to memory that is local to other sockets.
  - non-local accesses (to local memory on another socket) are slower than local accesses
- This memory architecture is called Non-Uniform Memory Access (NUMA)
  - "NUMA effects" arise when threads frequently access memory on a different NUMA domain.

Avoiding NUMA Effects

- Avoid them: hybrid MPI-OpenMP with at least one rank per NUMA node
  - threads in an MPI rank all run on the same NUMA node
  - explicit message passing via MPI between NUMA nodes
- Use first-touch memory allocation
  - by default the Linux kernel assigns memory pages to the NUMA node that first "touches" the memory
  - it is not the allocation of memory, but the first write to the memory that is important
    - the thread that will be accessing a part of memory should initialize it
    - memory allocation methods that initialize memory values are to be avoided, e.g. `calloc` and `std::allocator<>`

NUMA First Touch Example

```
const int N = 1000000000;

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

// initialize memory as it will be used
#pragma omp parallel for
for (i = 0; i < n; ++i) {
    x[i] = ...;
    y[i] = ...;
    z[i] = ...;
}

#pragma omp parallel for
for (i = 0; i < n; ++i)
    z[i] = x[i] + y[i];
```

Affinity

- CPU affinity is the pinning of a process or thread to a core
  - If the operating system interrupts the thread, it doesn't migrate it to another core
  - For most HPC scenarios where only one application is running on a node, these interruptions are short
  - Some multi-core architectures (e.g. IBM BG/Q) require multiple threads/core to achieve peak performance
  - On x86 the best results are obtained with 1 or 2 threads per core
- Memory affinity is allocation of memory as closely as possible to the cores that will be accessing it
  - achieved by first touch or MPI between NUMA nodes

Controlling Thread Affinity on Daint

- On systems using native SLURM, the `srun` command is used to launch jobs: provides flags for setting thread affinity
  - see the man page for all options

```
> man srun
```

- The best configuration can be system and application dependent
- Letting the runtime schedule threads is useful when using libraries that create additional threads

8 cores

```
> srun -n1 -c8 -hint=nomultithread ./a.out
> srun -n2 -c4 -hint=nomultithread ./a.out
```

2 MPI ranks with 4 cores each

OpenMP

What is OpenMP?

Open Multi Processing

- The OpenMP standard is an API with compiler directives, a run time library, and environment variables for writing parallel shared memory applications in C, C++ and Fortran.
  - supported by compiler vendors in HPC, including GNU, Intel, Cray and PGI compilers. Also Clang and MSVC.
- OpenMP compilers allow programmers to tell the compiler where and how to parallelize key loops and tasks with directives
  - The user does not have the complication of explicitly managing threads, as would be the case with a low level threading library like pthreads.

Goals of OpenMP

- Standardization
- Lean
  - concise and simple set of directives
  - possible to get good speedup with a handful of directives
  - but each new release gets more complicated (now at 4.5)
- Ease of use
  - you can incrementally add it to code without major changes
  - in practice refactoring is required to get performance
- Portability
  - Supported by range of compilers and platforms

Should I use OpenMP?

- OpenMP + MPI often doesn't perform as well as flat MPI on multicore
  - at least not without significant developer effort
- But for many-core architectures like Xeon Phi flat MPI won't scale as well
  - lightweight threading is required
- OpenMP is the defacto standard for Fortran, and path of least resistance existing codes
- Other options exist for C and C++
  - look into them if developing new code
  - e.g. Intel TBB, Stella HPX, Cilk++

OpenMP Compiler Directives

- In C and C++ parallel regions are scopes that are marked with #pragma omp parallel

```
#pragma omp parallel
{
  // executed in parallel
}
```

parallel region is enclosed in scope {curly braces}

- In Fortran parallel regions are indicated with specially-formatted comments

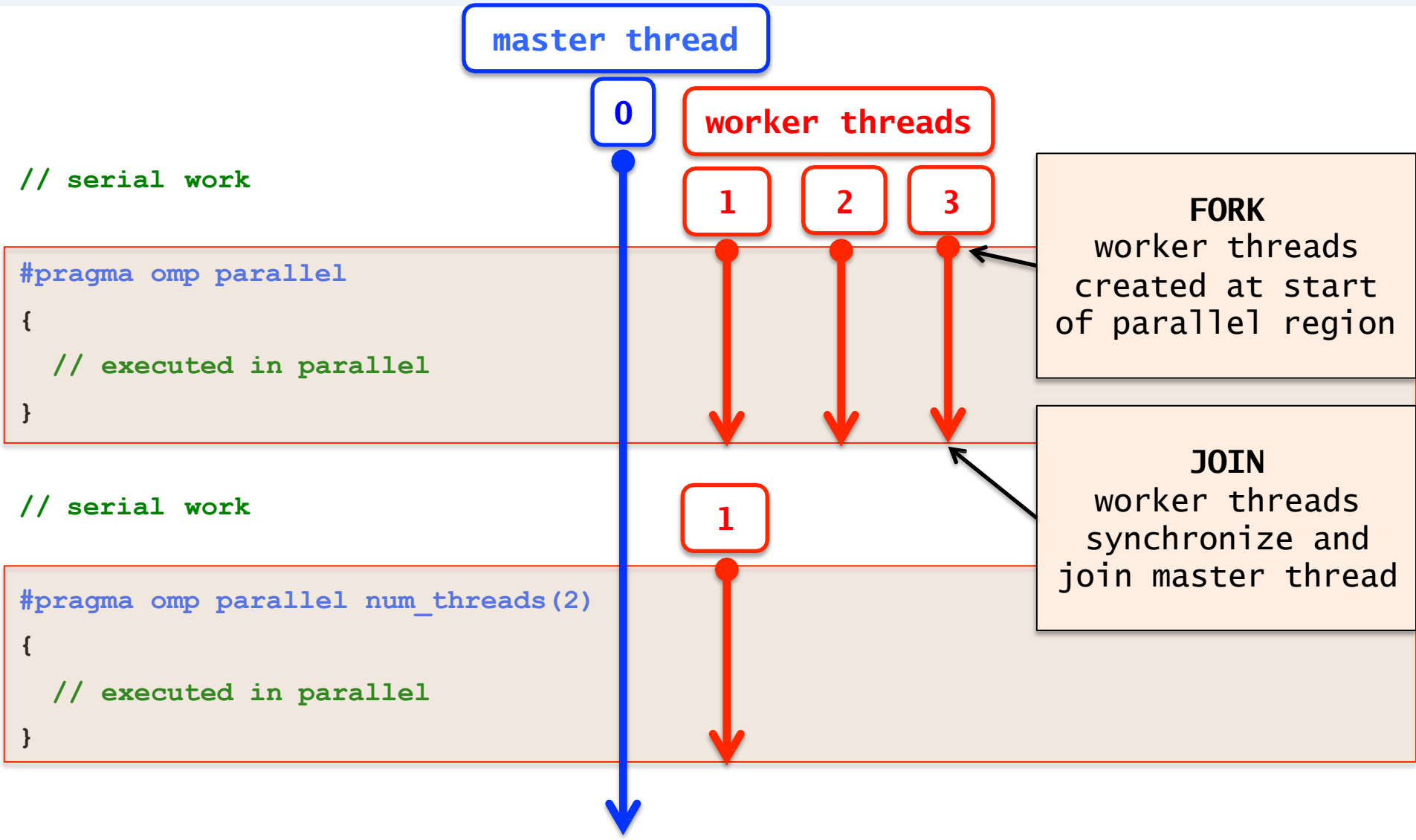
```
!$omp parallel
! executed in parallel
!$omp end parallel
```

must have comment at start and end of parallel region

Fork and Join Model

- OpenMP uses a fork and join model for threading
- The application starts with a master thread
  - FORK: a team of parallel worker threads is started at the beginning of each parallel block
  - the block is executed in parallel by each thread
  - JOIN: the worker threads are synchronized at the end of the parallel block and join with the master thread.
- Threads are numbered 0:N-1, where N is the total number of threads
- The master thread is always numbered 0.

Fork and Join Illustrated



Compiling OpenMP

- Most compilers require a flag to enable OpenMP compilation
  - without a flag the #pragma or !$omp directives are ignored by the compiler and a serial application is created
- compilers that don't understand OpenMP will simply ignore the directives (no portability problems).

```
Cray    : on by default for -O1 and greater, disable with -h noomp
Intel   : off by default, enable with -openmp
GNU     : off by default, enable with -fopenmp
PGI     : off by default, enable with -mp
```

Running OpenMP applications

- The default number of threads is set with an environment variable `OMP_NUM_THREADS`
- There has to be at least one core per thread
  - multiple threads on a single core have to share resources on the core
  - Typically we assign as many cores as there are threads, and let the runtime schedule them

```
> ftn -fopenmp app.ftn -o app.exe
> export OMP_NUM_THREADS=8
> srun -n1 -c8 --hint=nomultithread ./app.exe
```

compile openmp code

set 8 threads

run on 8 cores (on Cray)

Exercises: before starting

- The source code for exercises and slides are in the repository
  - to get a copy in your local path

```
> ssh -X username@ela.cscs.ch
> ssh -X daint
> cd $SCRATCH
> git clone https://github.com/eth-cscs/SummerSchool2017
```

let us know if you have a problem getting the code

  - for these examples we will use the gnu compiler, for which a script to set up the environment is provided

```
> CC hello_world.cpp -fopenmp
> ftn hello_world.f90 -fopenmp
```

we use the GNU compiler because the Cray compiler aggressively replaces simple loops with BLAS calls in the absence of OpenMP directives, which make it difficult to compare OpenMP versions of a code.

Exercise 1: Compiling and running

- Open the test code `hello_world.cpp/f90`
  - what do you expect the output to be?
- Compile:

choose C++ or Fortran version

```
> module swap PrgEnv-cray PrgEnv-gnu
> CC hello_world.cpp -fopenmp
> ftn hello_world.f90 -fopenmp
```

- Then run

```
> OMP_NUM_THREADS=1 srun -c1 -n1 -hint=nomultithread ./hello_world.exe
...
...
> OMP_NUM_THREADS=8 srun -c8 -n1 -hint=nomultithread ./hello_world.exe
```

shorthand for setting number of threads

- Is the output what you expected? Why?

Exercise 1: Affinity

- go to the `openmp/exercises/affinity` path
- Compile:

```
> cd SummerSchool2016/openmp/exercises/affinity
> make
```

- Experiment with affinity
  - try different numbers of threads and srun flags

```
> srun ./test.mpi
> OMP_NUM_THREADS=1 srun -hint=nomultithread ./test.mpi
> OMP_NUM_THREADS=1 srun ./test.mpi
> OMP_NUM_THREADS=8 srun -c8 ./test.mpi
> OMP_NUM_THREADS=8 srun -c8 -n1 ./test.mpi
> OMP_NUM_THREADS=8 srun -c8 -n1 -hint=nomultithread ./test.mpi
```

Runtime Library

- OpenMP has runtime library routines for controlling your application, including
  - `int omp_get_thread_num()`
    - get id of current thread
  - `int omp_get_num_threads()`
    - number of threads in current parallel region
  - `int omp_get_max_threads()`
    - default number of threads in parallel regions: corresponds to OMP_NUM_THREADS environment variable
  - `double omp_get_wtime()`
    - accurate timing function: returns double
- There are many others, however these are the most commonly used

Runtime Library

- The runtime library requires that the omp header/ module is included

```c
#include <omp.h>
...
int threads = omp_get_max_threads();
int outside = omp_get_num_threads();
int inside;
#pragma omp parallel
{
  inside = omp_get_num_threads();
}
printf("%d in, %d out, %d max \n",
       inside, outside, threads);
```

```
use omp_lib
...
integer :: threads, inside, outside
threads = omp_get_max_threads()
outside = omp_get_num_threads()
!$omp parallel
inside = omp_get_num_threads()
!$omp end parallel
print *, inside, ' in ', outside, ' out ',
         threads, ' max'
```

```
> OMP_NUM_THREADS=8 ./a.out
8 in, 1 out, 8 max
```

Synchronization

- Sometimes you need to synchronize threads inside a parallel region, for example
  - tasks that have to be done by only one thread
  - when multiple threads have to update memory, and we need to ensure that the value in memory is consistent
  - threads have to wait for others to finish before continuing
- OpenMP provides directives that can be used to indicate such regions
- WARNING: synchronization and serial code regions can quickly limit the potential speed up from parallelism.

Synchronization Example

- The intention of the code below is to print a hello world message, similarly to the hello world example earlier:

```
#pragma omp parallel
{
  int tid = omp_get_thread_num();
  printf("hello world from thread %d", tid);
}
```

```
> OMP_NUM_THREADS=8 ./a.out
???
```

  - each thread gets a private copy of `tid`, but the output could get messed up because all threads write to stdout at the same time.

`master` Directive

- The master directive indicates sections that are to be executed only by the master thread
  - the master thread is always thread 0

```
#pragma omp parallel
{
  int tid = omp_get_thread_num();
  #pragma omp master
  printf("hello world from thread %d", tid);
}
```

```
> OMP_NUM_THREADS=2 ./a.out
hello world from thread 0
```

  - only the master thread prints its `tid` value.

`single` Directive

- Block will only be executed by the first thread to arrive at the block
  - varies from one run to the next

```
#pragma omp parallel
{
  int tid = omp_get_thread_num();
  #pragma omp single
  printf("hello world from thread %d", tid);
}
```

```
> OMP_NUM_THREADS=8 ./a.out
hello world from thread 3
> OMP_NUM_THREADS=8 ./a.out
hello world from thread 6
```

  - only one thread will print message.

`critical` Directive

- All threads will execute block, one at a time
  - in order that the threads arrive at the block: varies each time application is run

```
#pragma omp parallel
{
  int tid = omp_get_thread_num();
  #pragma omp critical
  printf("hello world from thread %d", tid);
}
```

```
> OMP_NUM_THREADS=3 ./a.out

hello world from thread 1
hello world from thread 0
hello world from thread 2
```

  - each thread prints one message, in order of thread arrival at the critical block

`barrier` Directive

- All threads wait at barrier until all of the threads are at barrier, before continuing

```
#pragma omp parallel
{
  int tid = omp_get_thread_num();
  #pragma omp barrier
  printf("hello world from thread %d", tid);
}
```

```
> OMP_NUM_THREADS=3 ./a.out
hello world from thread 0 hello world from thread 2


hello world from thread 1
```

  - in this case, this doesn't solve anything: all threads try to write to stdout at the same time when they simultaneously leave the barrier

Exercise 2

- Go back to the `hello_world.cpp/f90` example, and add appropriate synchronization directives
  - do you see expected behavior now?
- Look at `sum_threads.cpp/f90`
  - what was the intended output?
  - run the example and compare the actual output.
  - can you add a synchronization directive to get the expected result?

```
> source setup.sh
> CC sum_threads.cpp -fopenmp
... or
> ftn sum_threads.f90 -fopenmp
> OMP_NUM_THREADS=8 srun -c8 -n1 -hint=nomultithread ./a.out
```

Shared Memory Model

- OpenMP uses a shared memory model
- All threads can read and write to the same memory locations simultaneously
- By default variables are shared, so one copy is used by all threads
- The result of computations where multiple threads attempt to read/write to a variable are undefined
  - see the sum_threads example in the previous exercises for a simple example
  - this is a very common parallel programming bug called a race condition

Variable Scoping

- OpenMP provides clauses that describe how variables should be shared between threads
  - shared: all variables access the same copy of a variable.
    - this is the default behavior
    - WARNING: take care when writing to shared variables
  - private: each thread gets its own copy of the variable
    - private copy is uninitialized
    - use firstprivate to initialize variable with value from master

Variable Scoping

```
int tid;
const int num_threads = omp_get_num_threads();
#pragma omp parallel shared(num_threads) private(tid)
{
  tid = omp_get_thread_num();
  #pragma omp critical
  printf("hello world from thread %d of %d", tid, num_threads);
}
```

Private Variables in C99/C++

- Variables that are declared inside a parallel region are private by default
  - this isn't possible in Fortran because variables must be declared at the top of each subroutine/program/function

using private clause

```
int tid;
#pragma omp parallel private(tid)
{
  tid = omp_get_thread_num();
  // ... use tid for local computation
}
```

best practice: declare variable in scope

```
#pragma omp parallel
{
  int tid = omp_get_thread_num();
  // ... use tid for local computation
}
```

Exercises 3

- Now we finally have all the tools needed to fix hello_world.cpp/f90

Work Sharing: for/do loops

- A common target for parallelization is loops without loop carried dependencies
  - for example, adding two vectors:

```
double *x, *y, *z;
int n;
for(int i=0; i<n; ++i) {
  z[i] = x[i] + y[i];
}
```

C++

```
real(kind=8) :: x(:), y(:), z(:)
integer      :: i, n
do i=1,n
  z(i) = x(i) + y(i)
end do
```

Fortran

- we could attempt to parallelize this using the techniques that we have learnt so far...

for/do loops the hard way

```
double *x, *y, *z;
int n;
...
for(int i=0; i<n; ++i) {
  z[i] = x[i] + y[i];
}
```

serial

What a mess!
And error-prone too: does this approach still work if n<num_threads?

```
double *x, *y, *z;
int n;
...
#pragma omp parallel
{
  int tid = omp_get_thread_num();
  int num_threads = omp_get_num_threads();
  int work = n/num_threads;
  int s = tid*work;
  int e = (tid==num_threads-1) ? n : s+work;
  for(int i=s; i<e; ++i)
    z[i] = x[i] + y[i];
}
```

calculate loop bounds for this thread's chunk

parallel

parallel for

- OpenMP provides a directive for `for/do` loops

loop index variable `i` is private by default

```
double *x, *y, *z;
int n, i;
#pragma omp parallel
{
  #pragma omp for
  for(i=0; i<n; ++i) {
    z[i] = x[i] + y[i];
  }
}
```

C++

```
real(kind=8) :: x(:), y(:), z(:)
integer      :: i, n
!$omp parallel
!$omp do
do i=1,n
  z(i) = x(i) + y(i)
end do
!$omp end do
!$omp end parallel
```

Fortran

- Compiler handles loop bounds for you
- there is a compact single-line directive:

```
#pragma omp parallel for
for(i=0; i<n; ++i) {
    z[i] = x[i] + y[i];
}
```

C++

```
!$omp parallel do
do i=1,n
  z(i) = x(i) + y(i)
end do
!$omp end parallel do
```

Fortran

Example: Vector Normalize

1. Open `dot.cpp/f90`
   - this code finds the dot product of two vectors
   - add OpenMP directives to parallelize the code
2. Open `normalize.cpp/f90`
   - write a parallel version of the function/subroutine normalize_vector()
     - find the norm of the vector v
     - scale the vector by the norm

Reductions

- Reduction operations reduce a set of values to a single value according to an operation `op`

```
a = initial value
for i = 1,n
  a = a op expr
```

e.g. C++ sum reduction

```
double sum = 0.0, v[n];
for(int i=0; i<n; ++i)
  sum = sum + v[i];
```

- OpenMP provides a clause of the form `reduction(op:list)` for performing reductions
  - a is a scalar variable in list
  - expr is a scalar expresion that does not reference `a`
  - only certain expressions allowed e.g. (+, –, *, /, binary ops)

```
double sum = 0.0, v[n];
#pragma omp parallel for
#pragma omp reduction(+:sum)
for(int i=0; i<n; ++i)
  sum = sum + v[i];
```

Exercise

- Revisit the `dot.cpp/f90` exercise, and rewrite it to use a reduction.
  - use `test.sh` to see how it scales from 1 to 12 threads
  - try arrays of length 10'000, 100'000 and 1'000'000
    - how does this affect scaling?
- We can apply everything that we have learnt to the example `pi.cpp/f90`, which computes pi using the trapezoidal rule
  - use `test.sh` to test its scaling from 1 to 8 threads
  - is its scaling better or worse? why?

Nested Loops

- If you apply directives nested loops, the outer loop will be parallelized.
- the collapse directive will merge the loops and parallelize both

```
double sum = 0.0, v[n];
#pragma omp parallel for
for(int j=0; j<n; ++j) {
  for(int i=0; i<m; ++i)
    A[j][i] = f(B[j][i]);
}
```

n parallel work items

```
double sum = 0.0, v[n];
#pragma omp parallel for collapse(2)
for(int j=0; j<n; ++j) {
  for(int i=0; i<m; ++i)
    A[j][i] = f(B[j][i]);
}
```

n*m parallel work items

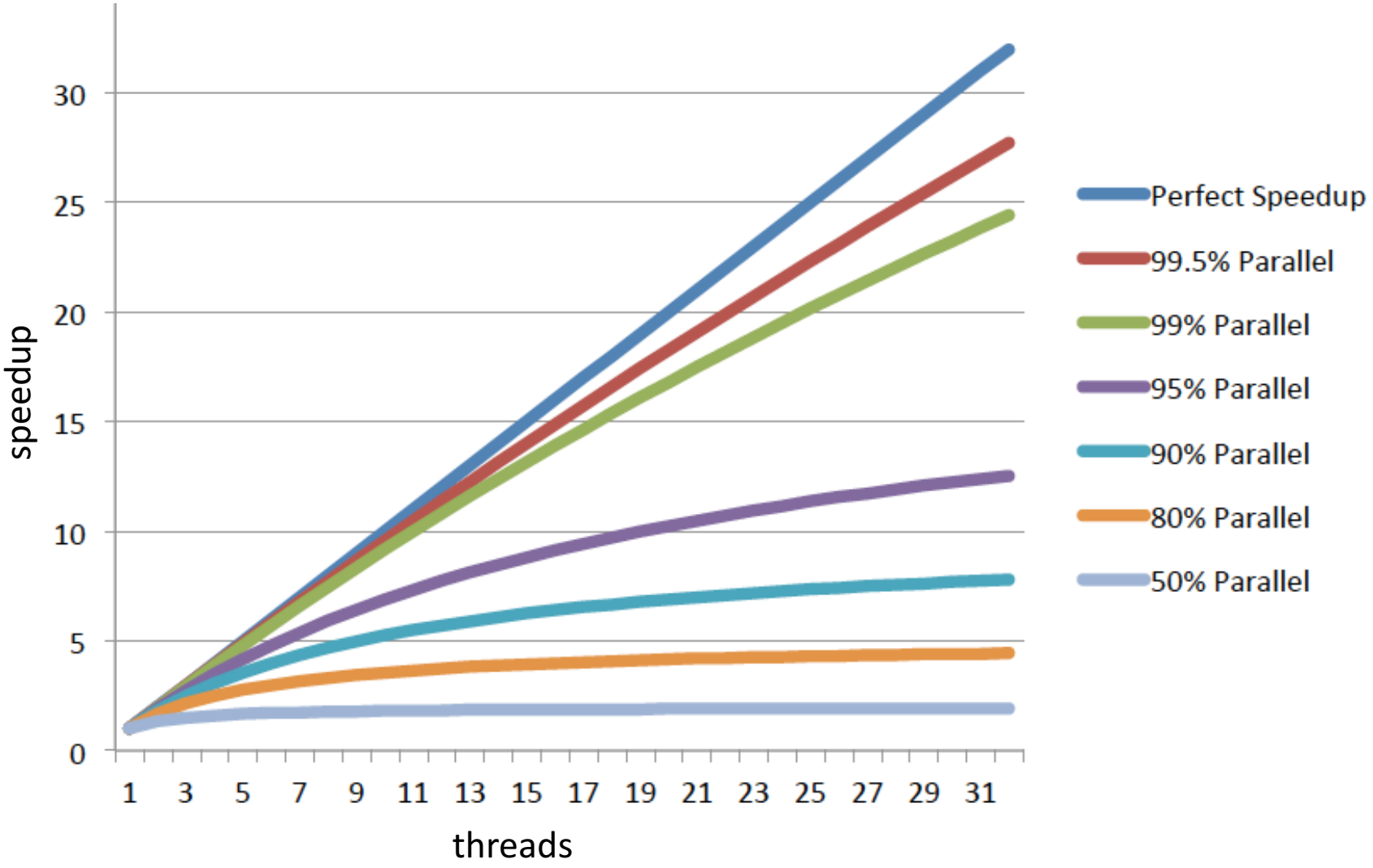
- use if n is small relative to OMP_NUM_THREADS and/or the amount of work in f is significant

Limitations to Parallel Speedup

Limitations To Parallel Speedup

- The amount of speedup that you will get from OpenMP is dependent on many factors including
  - having enough work to keep all threads busy
  - the ratio of sequential to parallel work
- Amdahl's Law is used to define the maximum possible speedup when only parts of a code can be parallelized
  - $T(n) = T(1) * (B+(1-B)/n)$
    - i.e. as $n \rightarrow \infty$, the best speedup possible is $B*T(1)$
  - where T(n) is time to solution for n threads, and B is the fraction of the algorithm that is strictly serial

Amdahl Illustrated



Amdahl's Law

- Our application would ideally scale to many threads
- But just 1% serial code in an algorithm means that it won't scale more than 100 times: no matter how many threads/nodes we use.
- While adding OpenMP directives to an existing sequential code is easy, the modifications required to get really good scaling might require significant restructuring
  - there is no free lunch!

OpenMP and Accelerators

- Current version OpenMP 4.5
- OpenMP 4.0 adds directives for using accelerators
  - Including GPUs and Intel Phi (MIC & KNL)
  - GCC 5.0 and the Intel compilers support of Xeon Phi offload
  - Currently there is no OpenMP 4.0 GPU offload in GCC
- Similar concept to the OpenACC directives that you will see for GPUs next week

Should You use OpenMP?

- Disclaimer: this might be controversial
- you should consider OpenMP if
  - you are using Fortran
  - you have to port an application that relies on OpenMP libraries
- However, if using C++ there are alternatives
  - namely Intel TBB & Stellar HPX
  - these are vanilla C++: not language extensions
  - Can be used to express more different types of parallelism more easily
    - e.g. task based parallelism