Outline:

- Parallel computing
- Amdahl’s law
- Speed up, strong and weak scaling
- OpenMP

Reading:

- class notes: bibliography for general books on parallel programming
- class notes: OpenMP section of Bibliography
Amdahl’s Law

Typically only part of a computation can be parallelized.

Suppose 50% of the computation is inherently sequential, and the other 50% can be parallelized.

**Question:** How much faster could the computation potentially run on many processors?
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**Question:** How much faster could the computation potentially run on many processors?

**Answer:** At most a factor of 2, no matter how many processors.

The sequential part is taking half the time and that time is still required even if the parallel part is reduced to zero time.
Suppose 10% of the computation is inherently sequential, and the other 90% can be parallelized.

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**Question:** How much faster could the computation potentially run on many processors?

**Answer:** At most a factor of 10, no matter how many processors.

The sequential part is taking 1/10 of the time and that time is still required even if the parallel part is reduced to zero time.
Amdahl’s Law

Suppose $1/S$ of the computation is inherently sequential, and the other $(1 - 1/S)$ can be parallelized.

Then can gain at most a factor of $S$, no matter how many processors.
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Note that

$$T_P \to (1/S)T_S \quad \text{as} \quad P \to \infty$$
Amdahl’s Law

Suppose $1/S$ of the computation is inherently sequential $\implies$

$$T_P = (1/S)T_S + (1 - 1/S)T_S/P$$

**Example:** If 5% of the computation is inherently sequential ($S = 20$), then the reduction in time is:

<table>
<thead>
<tr>
<th>$P$</th>
<th>$T_P$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$T_S$</td>
</tr>
<tr>
<td>2</td>
<td>0.525$T_S$</td>
</tr>
<tr>
<td>4</td>
<td>0.288$T_S$</td>
</tr>
<tr>
<td>32</td>
<td>0.080$T_S$</td>
</tr>
<tr>
<td>128</td>
<td>0.057$T_S$</td>
</tr>
<tr>
<td>1024</td>
<td>0.051$T_S$</td>
</tr>
</tbody>
</table>
The ratio $T_S/T_P$ of time on a sequential machine to time running in parallel is the speedup.

This is generally less than $P$ for $P$ processors.
   Perhaps much less.

Amdahl’s Law plus overhead costs of starting processes/threads, communication, etc.
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Amdahl’s Law plus overhead costs of starting processes/threads, communication, etc.

**Caveat**: May (rarely) see speedup greater than $P$...

For example, if data doesn’t all fit in one cache but does fit in the combined caches of multiple processors.
Some algorithms \textit{scale} better than others as the number of processors increases.

Typically interested on how well algorithms work for large problems requiring lots of time, e.g.
- Particle methods for \( n \) particles,
- algorithms for solving systems of \( n \) equations,
- algorithms for solving PDEs on \( n \times n \times n \) grid in 3D,
Some algorithms **scale** better than others as the number of processors increases.

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For large $n$, there **may** be lots of inherent parallelism.

**But this depends on many factors:**
- dependencies between calculations,
- communication as well as flops,
- nature of problem and algorithm chosen.
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**Strong scaling:** How does the algorithm perform as the number of processors $P$ increases for a **fixed problem size** $n$?

Any algorithm will eventually break down (consider $P > n$)
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**Strong scaling:** How does the algorithm perform as the number of processors $P$ increases for a fixed problem size $n$?

Any algorithm will eventually break down (consider $P > n$)

**Weak scaling:** How does the algorithm perform when the problem size increases with the number of processors?

E.g. If we double the number of processors can we solve a problem “twice as large” in the same time?
What does “twice as large” mean?

Depends on how algorithm complexity scales with $n$.

**Example:** Solving $n \times n$ linear system with Gaussian elimination requires $O(n^3)$ flops.

Doubling $n$ requires 8 times as many operations.
Weak scaling

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(Or may be better to count memory accesses!)
Solving steady state heat equation on $n \times n \times n$ grid.

$n^3$ grid points $\implies$ linear system with this many unknowns.

If we used Gaussian elimination (very bad idea!) we would require $\sim (n^3)^3 = n^9$ flops.

Doubling $n$ would require $2^9 = 512$ times more flops.
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Developing better algorithms is as important as better hardware!!
Speedup for problems like steady state heat equation

Fig. 2  Comparison of the contributions of mathematical algorithms and computer hardware.

“Open Specifications for MultiProcessing”

Standard for shared memory parallel programming. For shared memory computers, such as multi-core.

Can be used with Fortran (77/90/95/2003), C and C++.

Complete specifications at http://www.openmp.org
OpenMP References

- http://www.openmp.org
- http://www.openmp.org/wp/resources/

Other references in

- class notes bibliography: OpenMP
- class notes bibliography: Other courses
Explicit programmer control of parallelization using fork-join model of parallel execution

- all OpenMP programs begin as single process, the master thread, which executes until a parallel region construct encountered
- FORK: master thread creates team of parallel threads
- JOIN: When threads complete statements in parallel region construct they synchronize and terminate, leaving only the master thread.
OpenMP — Basic Idea

- **Rule of thumb**: One thread per processor (or core),
- User inserts *compiler directives* telling compiler how statements are to be executed
  - which parts are parallel
  - how to assign code in *parallel regions* to threads
  - what data is *private* (local) to threads
- Compiler generates explicit threaded code
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  - which parts are parallel
  - how to assign code in *parallel regions* to threads
  - what data is *private* (local) to threads
- Compiler generates explicit threaded code
- *Dependencies* in parallel parts require *synchronization* between threads
- User’s job to *remove dependencies* in parallel parts or use *synchronization*. (Tools exist to look for *race conditions.*)
OpenMP compiler directives

Uses **compiler directives** that start with ![ ] (pragmas in C.)

These look like comments to standard Fortran but are recognized when compiled with the flag `-fopenmp`.

**OpenMP statements:**

Ordinary Fortran statements conditionally compiled:

```fortran
!$ print *, "Compiled with -fopenmp"
```

**OpenMP compiler directives, e.g.**

```fortran
!$omp parallel do
```

**Calls to OpenMP library routines:**

```fortran
use omp_lib       ! need this module
!$ call omp_set_num_threads(2)
```
OpenMP directives

$omp directive [clause ...]
if (scalar_expression)
private (list)
shared (list)
default (shared | none)
firstprivate (list)
reduction (operator: list)
copyin (list)
num_threads (integer-expression)
A few OpenMP directives

```plaintext
!$omp parallel [clause]
   ! block of code
!$omp end parallel

!$omp parallel do [clause]
   ! do loop
!$omp end parallel do

!$omp barrier
   ! wait until all threads arrive
```

Several others we’ll see later...
API also provides for (but implementation may not support):

- Nested parallelism (parallel constructs inside other parallel constructs)
- Dynamically altering number of threads in different parallel regions

The standard says nothing about parallel I/O.

OpenMP provides "relaxed-consistency" view of memory.

Threads can cache their data and are not required to maintain exact consistency with real memory all the time.

\$omp flush

can be used as a memory fence at a point where all threads must have consistent view of memory.
program test
    use omp_lib
    integer :: thread_num

    ! Specify number of threads to use:
    !$ call omp_set_num_threads(2)

    print *, "Testing openmp ..."

    !$omp parallel
    !$omp critical
    !$ thread_num = omp_get_thread_num()
    !$ print *, "This thread = ", thread_num
    !$omp end critical
    !$omp end parallel
end program test
Compiled with OpenMP:

```
$ gfortran -fopenmp test.f90
$ ./a.out

Testing openmp ...
This thread = 0
This thread = 1
```
(or threads might print in the other order!)

Compiled without OpenMP:

```
$ gfortran test.f90
$ ./a.out
Testing openmp ...
```
OpenMP test code

! Specify number of threads to use:
!$ call omp_set_num_threads(2)

Can specify more threads than processors, but they won’t execute in parallel.

The number of threads is determined by (in order):

- Evaluation of \texttt{if} clause of a directive
  (if evaluates to zero or false $\Rightarrow$ serial execution)
- Setting the \texttt{num_threads} clause
- the \texttt{omp_set_num_threads()} library function
- the \texttt{OMP_NUM_THREADS} environment variable
- Implementation default
OpenMP test code

!$omp parallel
!$omp critical
!$ thread_num = omp_get_thread_num()
!$ print *, "This thread = ", thread_num
!$omp end critical
!$omp end parallel

The !$omp parallel block spawns two threads and each one works independently, doing all instructions in block.

Threads are destroyed at !$omp end parallel.

However, the statements are also in a !$omp critical block, which indicates that this section of the code can be executed by only one thread at a time, so in fact they are not done in parallel.

So why do this? The function omp_get_thread_num() returns a unique number for each thread and we want to print both of these.
OpenMP test code

Incorrect code without critical section:

```c
$omp parallel
thread_num = omp_get_thread_num()
print *, "This thread = ", thread_num
$omp end parallel
```

Why not do these in parallel?

1. If the prints are done simultaneously they may come out **garbled** (characters of one interspersed in the other).

2. `thread_num` is a **shared variable**. If this were not in a critical section, the following would be possible:

   Thread 0 executes function, sets `thread_num=0`
   Thread 1 executes function, sets `thread_num=1`
   Thread 0 executes print statement: "This thread = 1"
   Thread 1 executes print statement: "This thread = 1"

There is a **data race** or **race condition**.
OpenMP test code

Could change to add a **private** clause:

```c
!$omp parallel private(thread_num)

!$ thread_num = omp_get_thread_num()

!$omp critical
!$ print *, "This thread = ", thread_num
!$omp end critical
!$omp end parallel
```

Then each thread has it’s own version of the **thread_num** variable.
OpenMP parallel do loops

```c
 !$omp parallel do
 do i=1,n
   ! do stuff for each i
   enddo
 !$omp end parallel do  ! OPTIONAL
```

indicates that the do loop can be done in parallel.

**Requires:**
what’s done for each value of \( i \) is independent of others
Different values of \( i \) can be done in any order.

The iteration variable \( i \) is **private** to the thread: each thread has its own version.

By default, all other variables are **shared** between threads unless specified otherwise.