Introduction to OpenMP

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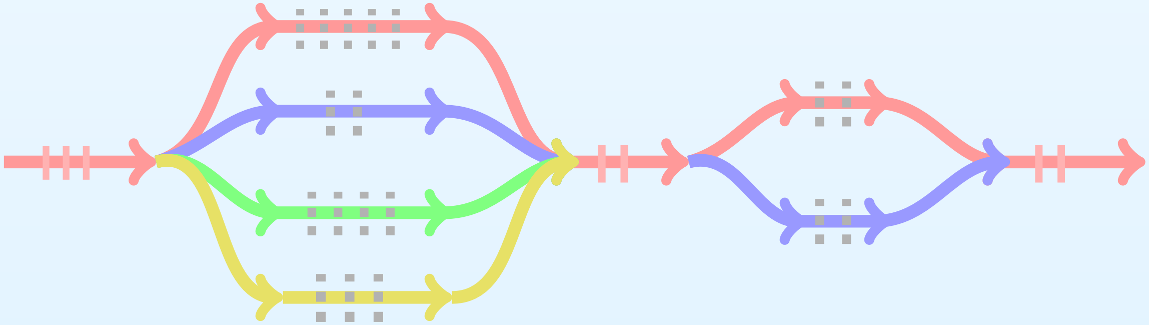

Overview

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- Parallel Programming on **Shared**-Memory and **Distributed**-Memory Machines

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- Parallel Programming on **Shared**-Memory and **Distributed**-Memory Machines
- Introduction to OpenMP
  - Prerequisite for Parallel Computing;
  - Constructs for **Parallel Execution**;
  - **Data Communications**;
  - **Synchronization**;

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- Parallel Programming on **Shared**-Memory and **Distributed**-Memory Machines
- Introduction to OpenMP
  - Prerequisite for Parallel Computing;
  - Constructs for **Parallel Execution**;
  - **Data Communications**;
  - **Synchronization**;
- OpenMP Programming: Directives/Pragams, Environment Variables, and Run-time Libraries
  - Variables Peculiar to OpenMP Programming;
  - Loop Level Parallelism;
  - Non-Loop Level Parallelism;

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- Parallel Programming on **Shared**-Memory and **Distributed**-Memory Machines
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- OpenMP Programming: Directives/Pragams, Environment Variables, and Run-time Libraries
  - Variables Peculiar to OpenMP Programming;
  - Loop Level Parallelism;
  - Non-Loop Level Parallelism;
- Summary and Further Reading

Overview of parallel computing

- Why parallel or concurrency computing?
- Goes beyond the single-core capability (memory and flops per unit time), and therefore increase performance;
- Reduces wall-clock time, and saves energy;
- Finish those impossible tasks in my lifetime;
- Handles larger and larger-scale problems;
- **There is no free lunch, however!**
- Different techniques other than serial coding are needed;
- Effective parallel algorithms in terms of performance;
- Increasing flops per unit time is one of our endless goals in the HPC community;
- Think in parallel;
- Start parallel programming as soon as possible;

Parallel programming

- Parallel programming environment;
  - Essential language extensions to the existing language (Fortran 95);
  - New constructs for directives/pragmas to existing serial programs (**OpenMP** and HPF);
  - Run-time libraries that support data communication and synchronization (**MPI** and Pthreads);
- **OpenMP** stands for **Open M**ulti-**P**rocessing (API);
- **OpenMP** is one of the directives/pragmas approaches that support parallelism on **shared** memory systems;
- **OpenMP** is supported by Fortran, and C/C++;
- **OpenMP** allows us to start from a serial code and provides an incremental approach to express parallelism;

The “Three Knights” in OpenMP

(1) Directives/pragmas need to express parallelism;
(2) Run-time libraries can dynamically control or change code execution at run-time;
(3) Environment variables specify the run-time options;

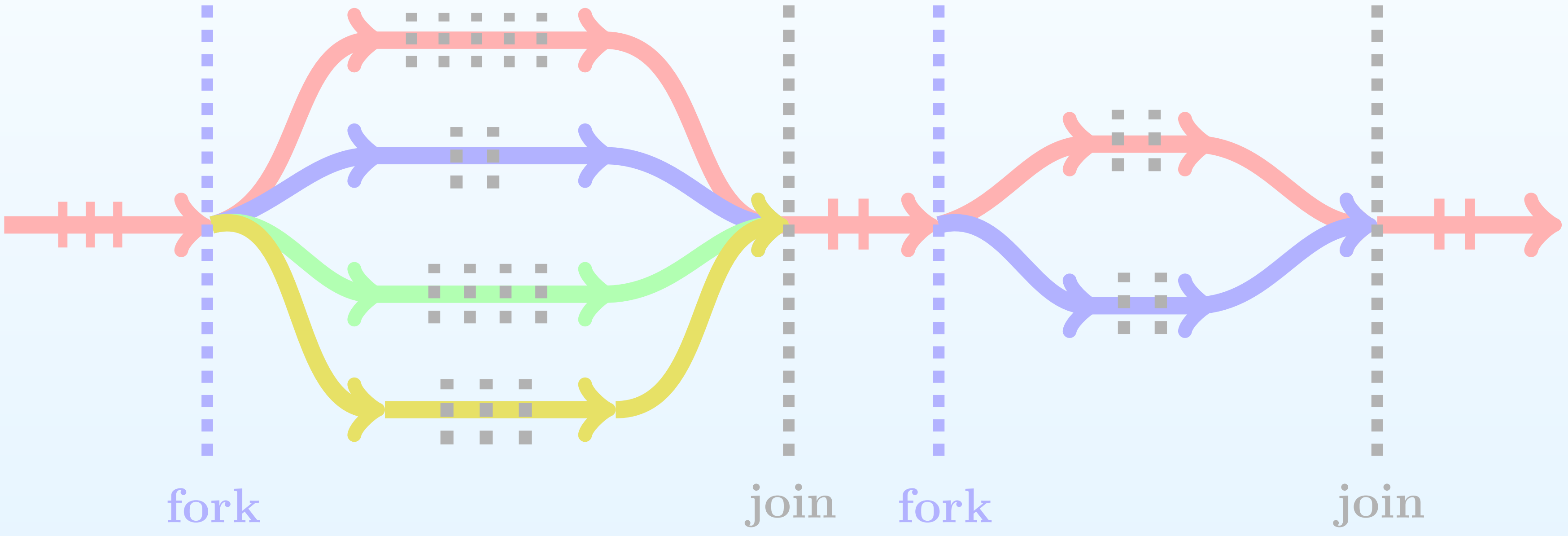
- How does OpenMP achieve parallel computing?
  - ○ Specify parallel execution – parallel constructs allowing parallel execution;
  - ○ Data communication – data constructs for communication among threads;
  - ○ Synchronization – synchronization constructs;
- OpenMP directives/pragmas:

  Fortran: `!$omp`, `c$omp`, or `*$omp [clauses]`

  C/C++: `#pragma [clauses]`

Parallel execution

- Constructs for parallel execution: OpenMP starts with a single thread, but it supports the directives/pragmas to spawn multiple threads in a fork-join model;



- OpenMP `do` and `parallel` directives;
- OpenMP also allows you to change the number of threads at run-time;

Data communication

- When multiple threads were spawned, each thread was assigned to a unique thread ID from 0 to $N-1$. Here N is the total number of threads;
- The key point is that there are three types of variables: `private`, `shared`, and `reduction` variables;
- At run-time, there is always a common region in global memory that allows all threads to access, and this memory region is used to store all `shared` variables;
- Each thread was also assigned a private memory region to store all `private` variables; Thread `a` cannot access the private variables stored in the private memory space for thread `b`;
- Data Communications are achieved through `read` and `write` operations among the threads;

Synchronization

- In OpenMP, synchronization is used to **(1)** control the access to **shared** variables and **(2)** coordinate the workflow;
- Event and mutual exclusion synchronization;
- **Event synchronization** includes **barrier** directives, which are either explicit or implicit; a thread has to wait until all threads reach the same point;
- **Mutual exclusion** is supported through **critical**, **atomic**, **single**, and **master** directives. All these are used to control how many threads, which thread, or when a thread can execute a specified code block or modify shared variables;
- Be careful with synchronization!

Compile OpenMP code

- Compiler options that enable OpenMP directive/pragmas:

Compiler	Fortran	C	C++
Intel	ifort -**openmp**	icc -**openmp**	icpc -**openmp**
PGI	pgf90 -**mp**	pgcc -**mp**	pgCC -**mp**
GCC	gfortran -**fopenmp**	gcc -**fopenmp**	g++ -**fopenmp**

- If the above flags are left out, OpenMP code is compiled as serial code (except Intel compilers but -openmp-stubs needed);
- Load modules on the HPC or LONI machines:

```
$ module load [package name]
$ soft add [+package name] (resoft)
```

intel, pgi, or gcc.

- Set up an environment variable:

```
$ export OMP_NUM_THREADS=[number of threads]
```

Loop level parallelism

First OpenMP “Hello World!” in Fortran and C

Fortran (hello.f90)

```
   program hello_world
   implicit none

   integer ::  id, omp_get_thread_num

!$omp parallel
   id = omp_get_thread_num()
   write(*,'(1x,a,i3)') "Hello World! from", id
!$omp end parallel

   end program hello_world
```

```
$ export OMP_NUM_THREADS=20
```

# for instance, on SuperMIC in bash shell

```
$ ifort -o hello hello.f90 -openmp
```

First OpenMP “Hello World!” in Fortran and C

C (hello.c)

```
#include <stdio.h>
#include <stdlib.h>
#include <omp.h>

int main( ) {
int id;

#pragma omp parallel {
id = omp_get_thread_num();
printf("Hello World! from %3d\n", id);
                      }
}
```

```
$ export OMP_NUM_THREADS=20
```

# for instance, on SuperMIC in bash shell

```
$ icc -o hello hello.c -openmp
```

Loop-level parallelism

- Loop-level parallelism is one of the fine-grained approaches supported by OpenMP;
- `parallel do` directives in Fortran and `parallel for` pragmas in C/C++;

Fortran

```
!$omp parallel do [clauses]
    do i = imin, imax, istep
       loop body ...
    end do
[!$omp end parallel do]
```

C/C++

```
#pragma omp parallel for [clauses]
    for (i = imin; i < imax; increment_expr)
    {
      loop body ...;
    }
```

Loop-level parallelism

Fortran

```fortran
!$omp parallel [clauses]
!$omp do [clauses]
    do i = imin, imax, istep
       loop body ...
    end do
!$omp end do
!$omp end parallel
```

C/C++

```c
#pragma omp parallel [clauses]
  {
#pragma omp for [clauses]
    for (i = imin; i < imax; increment_expr)
    {
      loop body ...;
    }
  }
```

Loop-level parallelism

- How about nested multiple loops? Where do we add `parallel for`, right above outer loop or inner loop?

C/C++ (inner loop)

```
for (i = imin; i < imax; increment_i)
{
#pragma omp parallel for
   for (j = jmin; j < jmax; increment_j)
   { loop body ...; }
}
```

C/C++ (outer loop)

```
#pragma omp parallel for
for (i = imin; i < imax; increment_i)
{
   for (j = jmin; j < jmax; increment_j)
   { loop body ...; }
}
```

More words on parallel loops

- OpenMP only supports Fortran `do` loops and C/C++ for loops that the number of loop iterations is known for at run-time;
- However, it doesn't support other loops, including `do-while` and `repeat-until` loops in Fortran and `while` loops and `do-while` loops in C/C++. In these cases, the trip count of loop is unknown before entering the loop;
- Loop body has to follow `parallel do` or `parallel for` immediately, and nothing in between them!
- There is an implicit `barrier` at the end of `parallel do` or `for` loops;
- All loops must have a single entry point and single exit point. We are **not** allowed to jump into a loop or branch out of a loop;

How to control loops?

- Once we entered the parallel region, for some variables multiple threads need to use the same named variables, but they store different values at different memory locations; these variables are called **private** variables;
- This leads to the fact that all private variables are **undefined** or **uninitialized** before entry and after exit from parallel regions;
- The **shared** variables are also necessary to allow data communication between threads;
- **Default** scopes for variables: By default all the variables are considered to be **shared** in parallel regions, unless they are explicitly declared as **private**, **reduction**, or **other** types;
- Remember Fortran and C/C++ may have different settings regarding default rules;

How to control loops?

- Let's see how we can do it, for instance, in parallel loops;
- OpenMP provides a means to change the default rules;
- Clauses `default(none)`, `default(private)`, and `default(shared)` in Fortran;
- But only `default(none)` and `default(shared)` in C/C++;

Fortran

```
ALLOCATE( da(1:nsize), db(1:nsize) )
!$omp parallel do default(none),        &
!$omp private(i,temp),                  &
!$omp shared(imin,imax,istep,scale,da,db)
    do i = imin, imax, istep
        temp = scale * da(i)
        da(i) = temp + db(i)
    end do
!$omp end parallel do
```

How to control loops?

- OpenMP `reduction` operations;
- The reduction variable is very special that it has both characters of private and shared variables;
- Compiler needs to know what type of operation is associated with the `reduction` variable; `operation` = `+`, `*`, `max`, `min`, etc;
- `reduction(operation : variables_list)`

Fortran

```
ALLOCATE( da(1:nsize) )
      prod = 1.0d0
!$omp parallel do default(none), private(i),  &
!$omp reduction(* : prod)
   do i = imin, imax, istep
      prod = prod * da(i)
   end do
!$omp end parallel do
```

What happens if we compile it?

How to control loops?

- Two special "private" variables: `firstprivate` and `lastprivate`; they are used to initialize and finalize some `private` variables;
- `firstprivate`: upon entering a `parallel do/for`, the private variable for each **slave** thread has a copy of the **master** thread's value;
- `lastprivate`: upon exiting a `parallel do/for`, no matter which thread executed the **last** iteration (sequential), the private variable was copied back to the **master** thread;
- Why do we need them? **(1)** all private variables are **undefined** outside of a parallel region, **(2)** they provide a simply way to exchange data to some extent through these special **private** variables;

How to control loops?

- In a parallel region, a given variable can only be one of `private`, `shared`, or `reduction`, but it can be both of `firstprivate` and `lastprivate`;

C/C++

```
double ashift = shift ;
#pragma omp parallel for default(none),       \
            firstprivate(ashift), shared(a),  \
            private(i)
  {
    for (i = imin; i <= imax; ++i)
       {
       ashift = ashift + (double) i ;
       a[i] = a[i] + ashift ;
       }
  }
```

How to control loops?

- Exception of the default rules: Fortran and C/C++ behave differently;
- The index in a parallel loop is always **private**. The index in a sequential loop is also **private** in Fortran, but is **shared** in C by default!
- Is the following code correct?
- Has the loop `j` been parallelized?

C/C++

```
#pragma omp parallel for
for (i = imin; i <= imax; ++i)
   {
    for (j = jmin; j <= jmax; ++j)
     a[i][j] = (double) (i + j) ;
   }
```

- Do we have the same issues in the Fortran version?

How to control loops?

- Exception of the default rules. Fortran and C/C++ behave differently;
- The index in a parallel loop is always **private**. The index in a sequential loop is also **private** in Fortran, but is **shared** in C by default!
- Is the following code correct?
- Has the loop `j` been parallelized?

C/C++

```
#pragma omp parallel for private(i,j)
for (i = imin; i <= imax; ++i)
   {
    for (j = jmin; j <= jmax; ++j)
     a[i][j] = (double) (i + j) ;
   }
```

- Do we have the same issues in the Fortran version?

How to control loops?

- Parallelize multiple nested loops;
- The `collapse(n)` ($n \geqslant 1$) for nested parallel loops;
- Each thread takes a chunk of the `i` loop and a chunk of the `j` loop at the same time;
- No statements in between;

C/C++

```
#pragma omp parallel for private(i,j), \
        collapse(2)
for (i = imin; i <= imax; ++i)
   {
    for (j = jmin; j <= jmax; ++j)
     a[i][j] = (double) (i + j) ;
   }
```

Restrictions on parallel loops

- Not all loops are parallelizable. What can we do?
- Think parallely and change your algorithms;
- We have to maintain the correctness of the results;
- One of the common mistakes is `data race`;

C/C++

```
#pragma omp parallel for
   {
    for (i = imin; i <= imax; ++i)
     r[i] = r[i] + r[i-1] ;
   }
```

- **Data race** means that in a parallel region, the same memory location is referred by **two** or **more** statements, and at least one of them is a **write** operation;
- Data race requires more attention and might lead to incorrect results!

Restrictions on parallel loops

- A closer look at at the data race: let's run it on `2` threads and assume that `r[0]=a`; `r[1]=b`; `r[2]=c`; and `imin=1`; `imax=2`;
- Note `r[1]` is referred twice, and thus we have two scenarios:

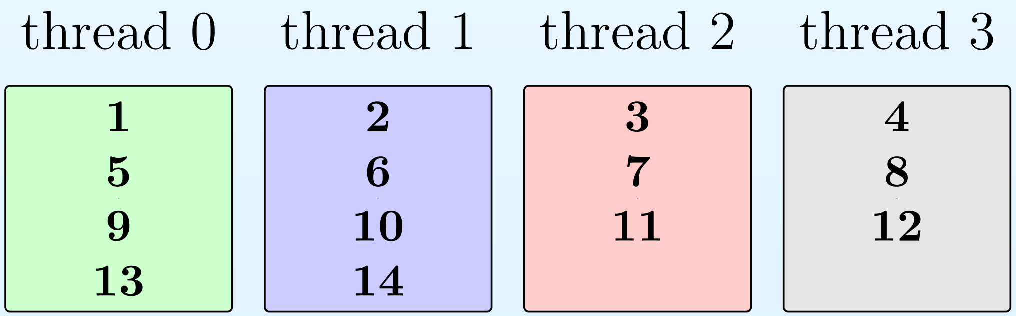
if `thread 0` finished first		if `thread 1` finished first	
`thread 0`	`thread 1`	`thread 1`	`thread 0`
`i = 1`	`i = 2`	`i = 2`	`i = 1`
`r[0]=a`		`r[1]=b`	`r[0]=a`
`r[1]=a+b`	`r[2]=a+b+c`	`r[2]=b+c`	`r[1]=b+a`
→ time		→ time	

- OpenMP standard does not guarantee which thread finishes first or later;

How to control loops again?

- OpenMP supports three loop schedulings as clauses: `static`, `dynamic`, and `guided` in the code, plus `run-time` scheduling;
- `schedule( type[, chunk_size] )`

For `static`, if `chunk_size` is given, loop iterations are divided into multiple blocks and each block contains `chun_size` iterations. The iterations will be assigned to threads in a round-robin fashion. If `chunk_size` is not present, the loop iterations will be (nearly) evenly divided and assigned to each thread.



thread 0	thread 1	thread 2	thread 3
1 5 9 13	2 6 10 14	3 7 11	4 8 12

14 iterations
on 4 threads
in round-robin fashion

How to control loops again?

- For `dynamic`, if `chunk_size` is given, the partition is almost the same as those of `static`. The difference is that with `static`, the mapping between loop iterations and threads are done during **compilation**, while for `dynamic`, it will be done at **run-time** (therefore, more potentially overhead); if `chunk_size` is not present, then it was set to `1`.
- The `guided` scheduling means the `chunk_size` assigned to threads decreases exponentially;
- Run-time scheduling: set the environment variable `OMP_SCHEDULE`;
- `$ export OMP_SCHEDULE=10`, for instance;
- Each scheduling has its own pros and cons, so be careful with `chunk_size` and potential overhead;

Non-loop-level parallelism

Parallel regions

- In addition to `parallel do` or `for`, most importantly OpenMP supports the parallelism beyond loop levels;

Fortran

```
!$omp parallel [clauses]
    code block
!$omp end parallel
```

C/C++

```
#pragma omp parallel [clauses]
    { code block ; }
```

- Each thread in the parallel team executes the same block of code, but with different data;
- In `parallel` directives, **clauses** include:

`private(list)`, `shared(list)`, `reduction(operation : list)`, `default(none | private | shared)`, `if(logical operation)`, `copyin(list)`;

Any differences?

Fortran

```
!$omp parallel
   id = omp_get_thread_num()
   write(*,*) "Hello World!  from ", id
!$omp end parallel
```

Fortran

```
!$omp parallel
do k = 1, 5
   id = omp_get_thread_num()
   write(*,*) "Hello World!  from ", id, k
end do
!$omp end parallel
```

Fortran

```
!$omp parallel do
do k = 1, 5
   id = omp_get_thread_num()
   write(*,*) "Hello World!  from ", id, k
end do
!$omp end parallel do
```

Global variables in OpenMP

- In addition to **automatic** or **static** variables in Fortran and C/C++, we also need **global** variables;
- `Command blocks` or `modules` in Fortran, while `globals` in C/C++, and we might have issues with private variables;
- **Global**/**local** variables between different code units for a given thread;
- **Private**/**shared** variables between multiple threads in a given code unit;
- The default data scoping rule is only apply to its **lexical** region, and all rest are **shared**; How can we make **private** variables “propagate” to **other** code units?
- OpenMP introduced the `threadprivate` directive to solve data scoping issues;

Global variables in OpenMP

- `!$omp threadprivate (list_common_variables)` in Fortran;
- `#pragma omp threadprivate (list_variables)` in C/C++;
- We have **global** but **private** variables;
- The `threadprivate` variables are special private variables; thus thread `a` cannot access the `threaprivate` variables stored on thread `b`;
- The `threadprivate` variables persist from one parallel region to another, because they are globals;
- Furthermore, OpenMP supports the `copyin (list)` clause to initialize global variables on slave threads to be the values on the master thread;
- `#pragma omp parallel copyin (a,b,c) { code block; }`
- Sounds familiar with the Intel `Xeon Phi` programming?

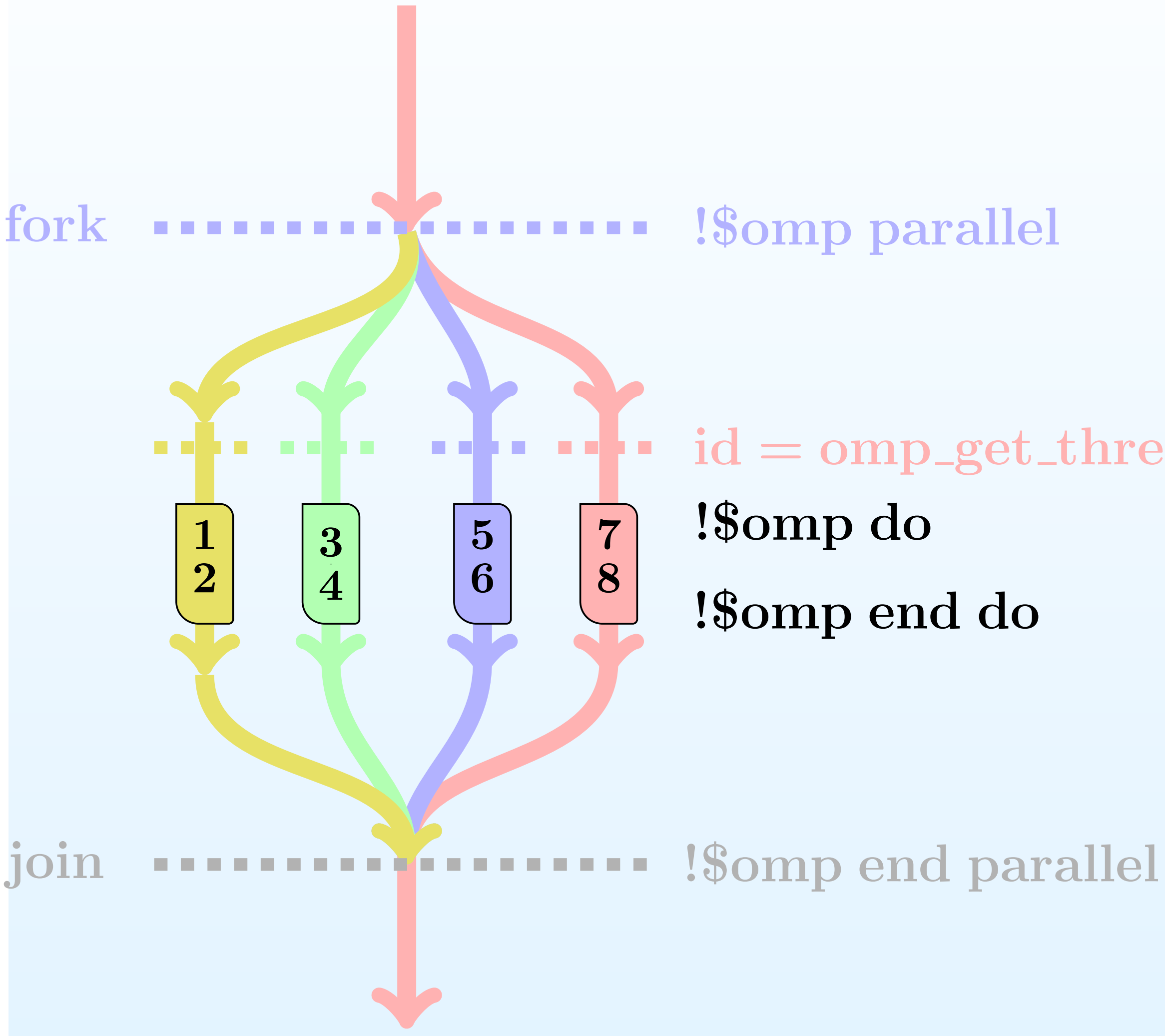
Work-sharing directives

Fortran

```
program mapping
implicit none
integer ::  i,id,nothread,  &
        omp_get_thread_num, omp_get_num_threads

!$omp parallel private (k,id), shared(nothread)
    id = omp_get_thread_num()
    nothread = omp_get_num_threads()
!$omp do
  do k = 1, 40
  write(*,’(1x,2(a,i4))’) "id = ",id, " k = ",k
  end do
!$omp end do [nowait]
!$omp end parallel
end program mapping
```

Work-sharing directives



The point is that `!$omp do` directive does not spawn threads. Instead, only `!$omp parallel` spawns multiple threads!

`!$omp do` needs to be embedded in an existing parallel region.

Work-sharing directives

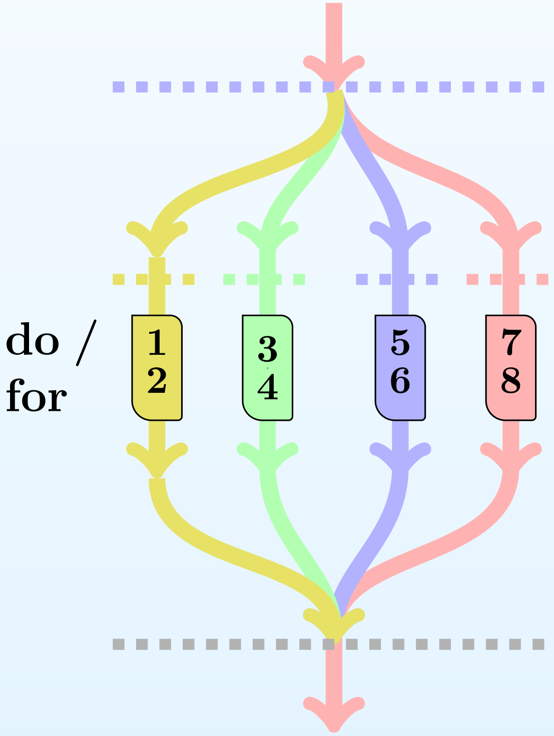
- Work-sharing constructs do **not** spawn multiple threads; they need to be **embedded** in a parallel region; if not, only one thread will run work-sharing constructs;
- There is an **implicit** barrier at the **end** of a work-sharing construct, but no implicit barrier upon the entry to it;
- **Three** work-sharing constructs:

```
!$omp do                 #pragma for
!$omp section            #pragma section
!$omp single             #pragma single
```

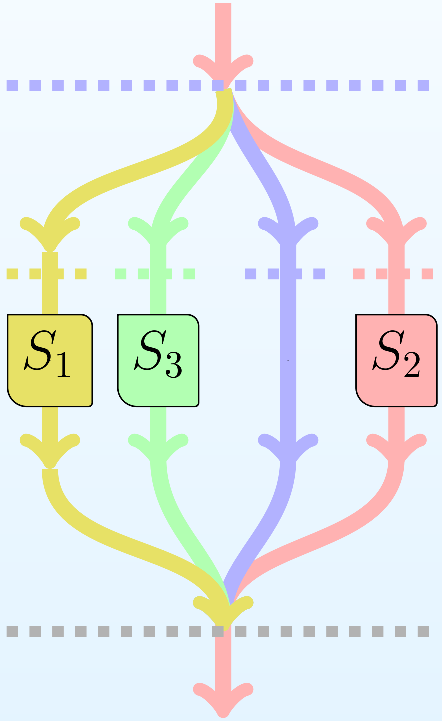
- A given thread may work on zero, one or more `omp sections`; but only one thread runs `omp single` at a given time;
- Be sure there are no data dependencies between `sections`;
- All threads must encounter the same workflow (though it may or may not execute the same code block at run-time);

Work-sharing directives

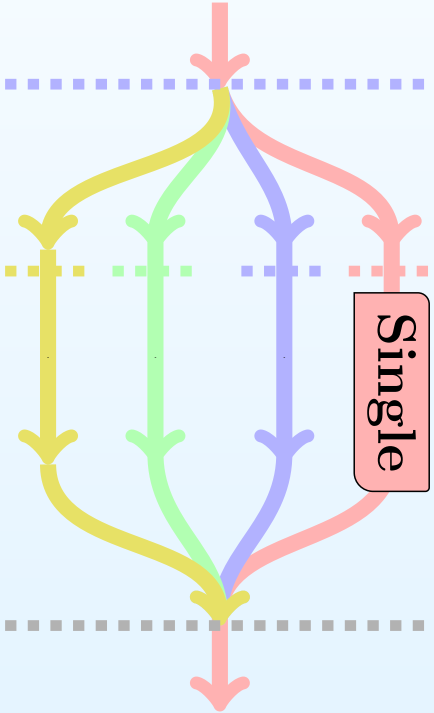
```
!$omp do
#pragma for
```



```
!$omp section
#pragma section
```



```
!$omp single
#pragma single
```



Work-sharing directives

C

```
#include <omp.h>
#define nsize 500
main() { int i, j, k ;
double a[nsize], b[nsize], c[nsize] ;
for (k = 0; k <= nsize, ++k) {
a[k] = (double) k; b[k] = a[k]; c[k] = 0.5*a[k];}

#pragma omp parallel {
    #pragma omp sections {
    #pragma omp section { code block_1; }
    #pragma omp section { code block_2; }
    #pragma omp section { code block_3; }
                          }
                     }
        }
```

Synchronization

Synchronization

- OpenMP provides the constructs for **mutual exclusion**: `critical`, `atomic`, `master`, `barrier`, and `run-time` routines;
  `!$omp critical [name] code block`
  `!$omp end critical [name]` in Fortran;
  `#pragma omp critical [name] {code block;}` in C/C++;
- [name] is an optional; But in Fortran, name here should be unique (cannot be the same as those of `do` loops or `if/endif` blocks, etc);
- At a given time, `critical` only allows **one** thread to run it, and all other threads also need to go through `critical` section, but have to wait to enter `critical` section;
- Don't jump into or branch out of a critical section;
- It is useful in a parallel region;
- It might have a tremendous impact on code performance;

Synchronization

- The other way to think of `reduction` variable (say addition):

Fortran

```
    tsum = 0.0d0 ; nsize = 10000
!$omp parallel private(temp), shared(tsum,nsize)
    temp = 0.0d0
!$omp do
    do i = 1, nsize
       temp = temp + array(i)
    end do
!$omp end do

!$omp critical
      tsum = tsum + temp
!$omp end critical

!$omp end parallel
```

Synchronization

- Using atomic to protect a shared variable:

C

```
#include <omp.h>
#include <stdio.h>
#include <stdlib.h>
#define nsize 1000
int main () {
int i; double x = 0.0, answer;
#pragma omp parallel for private(i) shared(x) {
for (i = 0; i < nsize; ++i) {
    #pragma omp atomic
    x += (double) i; }        }
answer = (double) 0.5*(nsize-1)*nsize;
printf("%f\n", x);
printf("correct answer is %f\n", answer);
}
```

OpenMP run-time libraries

- `integer omp_get_num_threads()`
  `int omp_get_num_threads(void)`
  # No. of threads in the current collaborating parallel region;
- `integer omp_get_thread_num()`
  `int omp_get_thread_num(void)`
  # Return the thread IDs in a parallel team;
- `integer omp_get_num_procs()`
  `int omp_get_num_procs(void)`
  # Get the number of “processors” available to the code;
- `call omp_set_num_threads(num_threads)`
  `omp_set_num_threads(num_threads)`
  # Set number of threads to be `num_threads` for the following parallel regions;
- `omp_get_wtime()` # Measure elapsed wall-clock time (in seconds) relative to an arbitrary reference time;

Summary and Further Reading

- OpenMP loop-level, non-loop level parallelism, synchronization, and run-time libraries;
- How to protect **shared** variables; pay attention to them and synchronization; data races;
- Global and local variables in OpenMP programming (**global private** variables);
- Develop a defensive programming style;

Parallel Programming in OpenMP, R. Chandra et al. (Morgan Kaufmann Publishers, 2001).

Questions?

sys-help@loni.org