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Parallel Programming in OpenMP

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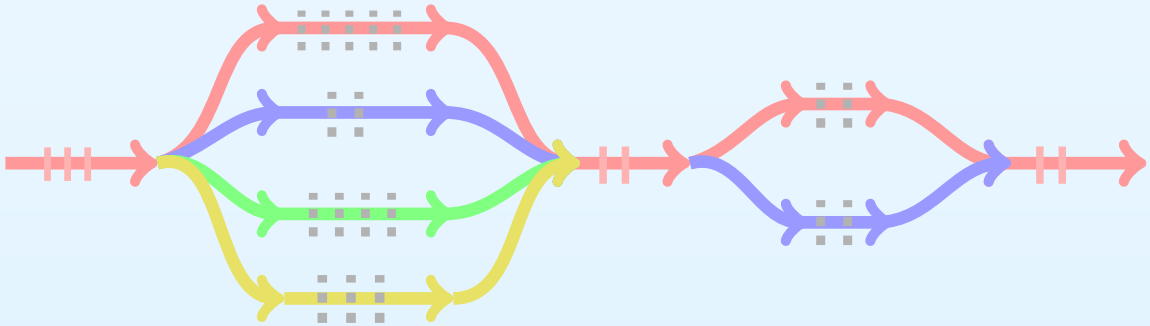

Overview

- Parallel programming
  - Prerequisite for parallel computing:
  - Constructs for **parallel execution**
  - **Data communications**
  - **Synchronization**
- OpenMP programming: directives/pragmas, environment variables, and run-time libraries
  - **Variables** peculiar to OpenMP programming;
  - **Loop** level parallelism;
  - **Nested** thread parallelism;
  - **Non-loop** level parallelism;
  - **Data race** and **false sharing**;
- Summary

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;

Shared-memory parallel programming

- System level and user's application level;
- **Pthreads** specification is from the IEEE POSIX standard;
  - Many control knobs at low level;
  - Difficult to use and relatively heavyweight threads;
- Intel **Cilk Plus**
  - C/C++ language extensions;
  - Supported by GCC and Intel C/C++ compilers;
  - Fork-join mechanism and efficient load-balancing via work-stealing;
- Intel **TBB** (Threading Building Blocks)
  - C++ libraries instead of language extension;
  - Supports task and loop-level parallelism;
- **OpenCL**
  - Offload work to devices, C/C++, Python, Java APIs;
  - Low-level model;

The "Three Knights" in OpenMP

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(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;

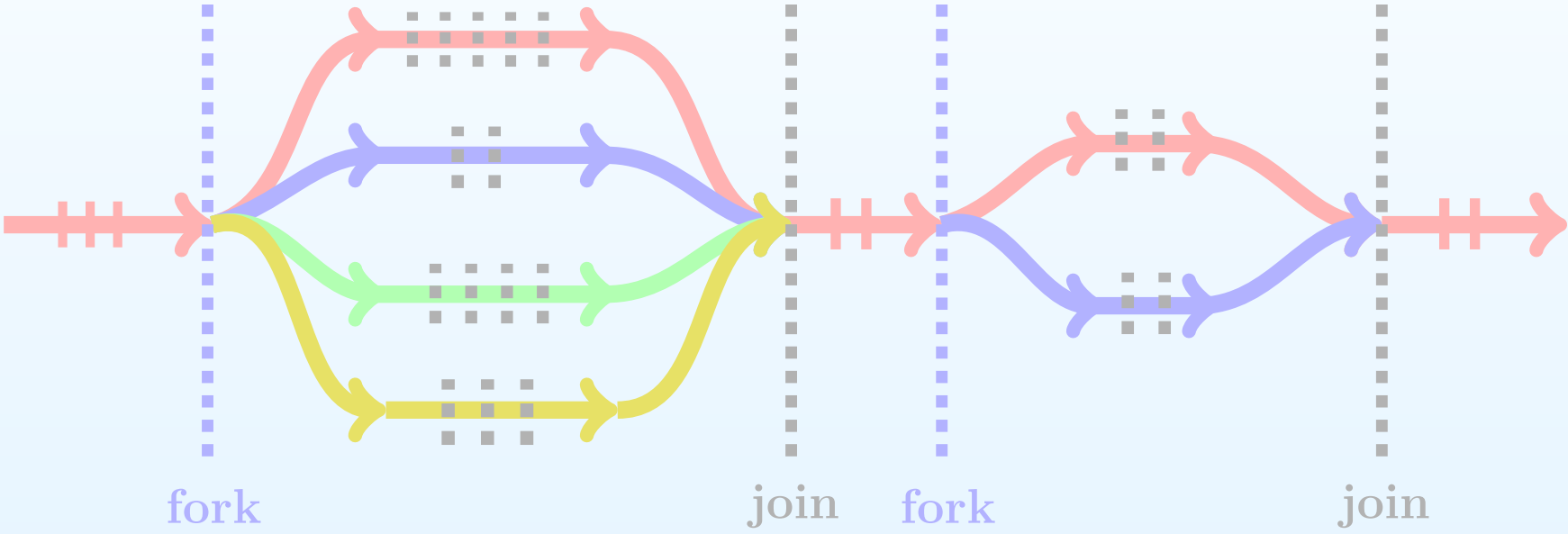
- How does OpenMP achieve parallel computing?
  - Specify parallel execution – parallel constructs allowing parallel execution;
  - Data communication – data constructs for communication among threads;
  - Synchronization – synchronization constructs;
- OpenMP directives/pragmas:

  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

- 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 it, 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 on **shared** variables 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 directives/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`

- Compilers support **conditional compilation** in disabling OpenMP. Intel compiler also provides the flag `-openmp-stubs` at the compiler level;
- 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]
```

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Loop level parallelism

First OpenMP "Hello World!" in Fortran and C

Fortran (hello_f.f90)

```
 1      program hello_world
 2      implicit none
 3
 4      integer ::  id, omp_get_thread_num
 5
 6  !$omp parallel
 7      id = omp_get_thread_num()
 8       write(*,'(1x,a,i3)') "Hello World! from", id
 9  !$omp end parallel
10
11      end program hello_world
```

```
$ export OMP_NUM_THREADS=16
   # on Mike-II in bash shell, or inline setting
$ ifort -o hello hello.f90 -openmp
```

First OpenMP "Hello World!" in Fortran and C

C (hello_c.c)

```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=16
  # on Mike-II in bash shell, or inline setting
$ icc -o hello hello.c -openmp
```

Loop-level parallelism

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

Fortran

```
1 !$omp parallel do [clauses]
2     do i = imin, imax, istep
3        loop body ...
4     end do
5 [!$omp end parallel do]
```

C/C++

```
1 #pragma omp parallel for [clauses]
2     for (i = imin; i <= imax; increment_expr)
3     {
4       loop body ...;
5     }
```

Loop-level parallelism

- Other form of parallel loops:

Fortran

```
1 !$omp parallel [clauses]
2 !$omp do [clauses]
3     do i = imin, imax, istep
4         loop body ...
5     end do
6 !$omp end do
7 !$omp end parallel
```

C/C++

```
1 #pragma omp parallel [clauses]
2 #pragma omp for [clauses]
3     for (i = imin; i <= imax; increment_expr)
4     {
5       loop body ...;
6     }
```

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)

```
1 for (i = imin; i < imax; increment_i)
2 {
3 #pragma omp parallel for
4     for (j = jmin; j <= jmax; increment_j)
5     { loop body ...; }
6 }
```

C/C++ (outer loop)

```
1 #pragma omp parallel for
2 for (i = imin; i <= imax; increment_i)
3 {
4     for (j = jmin; j <= jmax; increment_j)
5     { loop body ...; }
6 }
```

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 (but . . .);

How to control variables in loops?

- Once we have 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;
- 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** scope 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 variables in 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

```
1 ALLOCATE( da(1:nsize), db(1:nsize) )
2 !$omp parallel do default(none),        &
3 !$omp private(i,temp),                  &
4 !$omp shared(imin,imax,istep,scale,da,db)
5     do i = imin, imax, istep
6        temp = scale * da(i)
7        da(i) = temp + db(i)
8     end do
9 !$omp end parallel do
```

How to control variables in 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

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

What happens if we compile it?

How to control variables in 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 variables in 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++

```
1  double ashift = shift ;
2  #pragma omp parallel for default(none),          \
3                firstprivate(ashift), shared(a),   \
4                private(i)
5    {
6      for (i = imin; i <= imax; ++i)
7          {
8          ashift = ashift + (double) i ;
9          a[i] = a[i] + ashift ;
10         }
11   }
```

How to control variables in 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++

```
1 #pragma omp parallel for
2 for (i = imin; i <= imax; ++i)
3     {
4       for (j = jmin; j <= jmax; ++j)
5         a[i][j] = (double) (i + j) ;
6     }
```

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

How to control variables in 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++

```
1 #pragma omp parallel for private(i,j)
2 for (i = imin; i <= imax; ++i)
3     {
4       for (j = jmin; j <= jmax; ++j)
5         a[i][j] = (double) (i + j) ;
6     }
```

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

How to control loops?

- Parallelize multiple nested loops;
- The `collapse(n)` for nested parallel loops (`n` $\geqslant$ `1`);
- 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++

```
1 #pragma omp parallel for private(i,j), \
2         collapse(2)
3 for (i = imin; i <= imax; ++i)
4    {
5     for (j = jmin; j <= jmax; ++j)
6      a[i][j] = (double) (i + j) ;
7    }
```

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++

```
1 #pragma omp parallel for
2     {
3       for (i = imin; i <= imax; ++i)
4         r[i] = r[i] + r[i-1] ;
5     }
```

- **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;

Data dependence in loops

- How to identify data dependence and possibly remove it;
- A rule of thumb: **(1)** focus on those variables that are accessed **twice or more**. If the same memory location is only accessed (r/w) once, we don't have data dependence for that variable. **(2)** analyze all variables (mostly **array elements**) in a loop body. **(3)** pay attention to the **global** variables.

C/C++

```
1       for (i = imin; i <= imax; ++i)
2           { b[i] = b[i] + b[i-1] ; }
```

```
1       for (i = imin; i <= imax; ++i)
2           { b[i] = b[i] + a[i-1] ; }
```

```
1       for (i = 2; i <= imax; i+=2)
2           { a[i] = a[i] + a[i-1] ; }
```

Data dependence in loops

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- A rule of thumb: **(1)** focus on those variables that are accessed **twice or more**. If the same memory location is only accessed (r/w) once, we don't have data dependence for that variable. **(2)** analyze all variables (mostly **array elements**) in a loop body. **(3)** pay attention to the **global** variables.

C/C++

```
1       for (i = imin; i <= imax; ++i)
2           { b[i] = b[i] + b[i-1] ; }
```

```
1       for (i = imin; i <= imax; ++i)
2           { b[i] = b[i] + a[i-1] ; }
```

```
1       for (i = 1; i <= imax/2; ++i)
2           { b[i] = b[i] + b[i+imax/2] ; }
```

Data dependence in loops

- **Dataflow** analysis for potential data dependence;
- Access sequence in two or more statements is critical;
- **Three** types of dataflows:

  (1) flow dep. **(2)** anti-flow dep. **(3)** output dep.

```
1  for (i=0;i<10;++i)
2   { tmpi=sin(i);
3   b[i]=a[i]+tmpi; }
```

```
1  for (i=0;i<10;++i)
2   { tmpi=fact*c[i];
3   c[i]=b[i]+tmpi; }
```

Data dependence in loops

- **Dataflow** analysis for potential data dependence;
- Access sequence in two or more statements is critical;
- **Three** types of dataflows:

  (1) flow dep. **(2)** anti-flow dep. **(3)** output dep.

S_1 writes the var. S_2 reads the same var.	S_1 reads the var. S_2 writes the same var.
(1) Flow dependence	**(2) Anti-flow dep.**

Data dependence in loops

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S_1 writes the var. S_2 reads the same var.	S_1 reads the var. S_2 writes the same var.
(1) Flow dependence	**(2) Anti-flow dep.**

```
1          for (i = imin; i <= imax; ++i)
2              { tmp = a[i] + b[i];
3                c[3] = sin(tmp); }
```

Data dependence in loops

- **Dataflow** analysis for potential data dependence;
- Access sequence in two or more statements is critical;
- **Three** types of dataflows:

  (1) flow dep. **(2)** anti-flow dep. **(3)** output dep.

S_1 writes the var. S_2 reads the same var.	S_1 reads the var. S_2 writes the same var.
(1) Flow dependence	**(2) Anti-flow dep.**

```
1          for (i = imin; i <= imax; ++i)
2              { tmp = a[i] + b[i];
3                c[3] = sin(tmp); }
```

Multiple statements write to the same memory location

(3) Output dependence

Data dependence in loops

- Is it possible to remove **anti-flow** and **output** dependences?
- The answer is **yes** in most cases: change the **data structure**;
- Can we parallelize the following serial code?

```
1  // array a[] and b[] are ready to use.   v0 C/C++
2     for (i=0; i<nsize, i++)
3          a[i] = a[i+1] + b[i];
```

- This is a typical example of **anti-flow** dependence;

  (1) For the given `i`-th iteration, read `a[i+1]` (RHS, S_1);
  (2) In the next `i+1`-th iteration, write `a[i+1]` (LFS, S_2);

Data dependence in loops

- Is it possible to remove **anti-flow** and **output** dependences?
- The answer is **yes** in most cases: change the **data structure**;
- Data dependence follows a certain **pattern**;
- Define a new array with **shifted** indices;

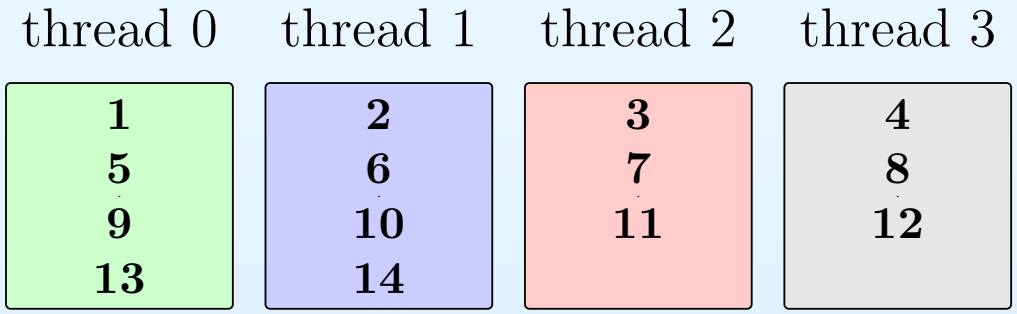
```
1  // make a new array by shifting index.  v1 C/C++
2  #pragma omp parallel for
3     for (i=0; i<nsize, i++) a_new[i] = a[i+1];
4
5  // array a[] and b[] are ready to use.
6  #pragma omp parallel for
7     for (i=0; i<nsize, i++)
8          a[i] = a_new[i] + b[i];
```

- Now the data dependences were removed;

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.



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;

False sharing

- Let's consider the following question: For a given **integer** matrix, how do we count the total number of **even** matrix elements?
- This is how the serial code looks like:

v0 C/C++

```
1 // count the number of even integers.
2     counter_even = 0;
3     for (i=0; i<nosize; i++)
4     for (j=0; j<nosize; j++)
5      { itmp = matrix[i][j]%2;
6        if (itmp == 0) ++counter_even;
7      }
8     printf("Number of even integers is %d\n", \
9          counter_even);
```

- How do we parallelize these two loops?

False sharing

- Generally, loop-level parallelism is considered **fine-grained** parallelism;
- Let's try something different: manually decompose the data;
- This is called **coarse-grained** parallelism:
  - We decompose the matrix in a **row-wise** and each thread takes care of one block (for the **outer** loop);
  - Then we define a counter array: each thread has its own counter;
  - Each thread counts the number of even matrix elements in its own block;
  - Finally, the **master** thread makes a summation;
- Reduce the overhead in the loop scheduling and maintain good **scalability** and **performance**;

False sharing

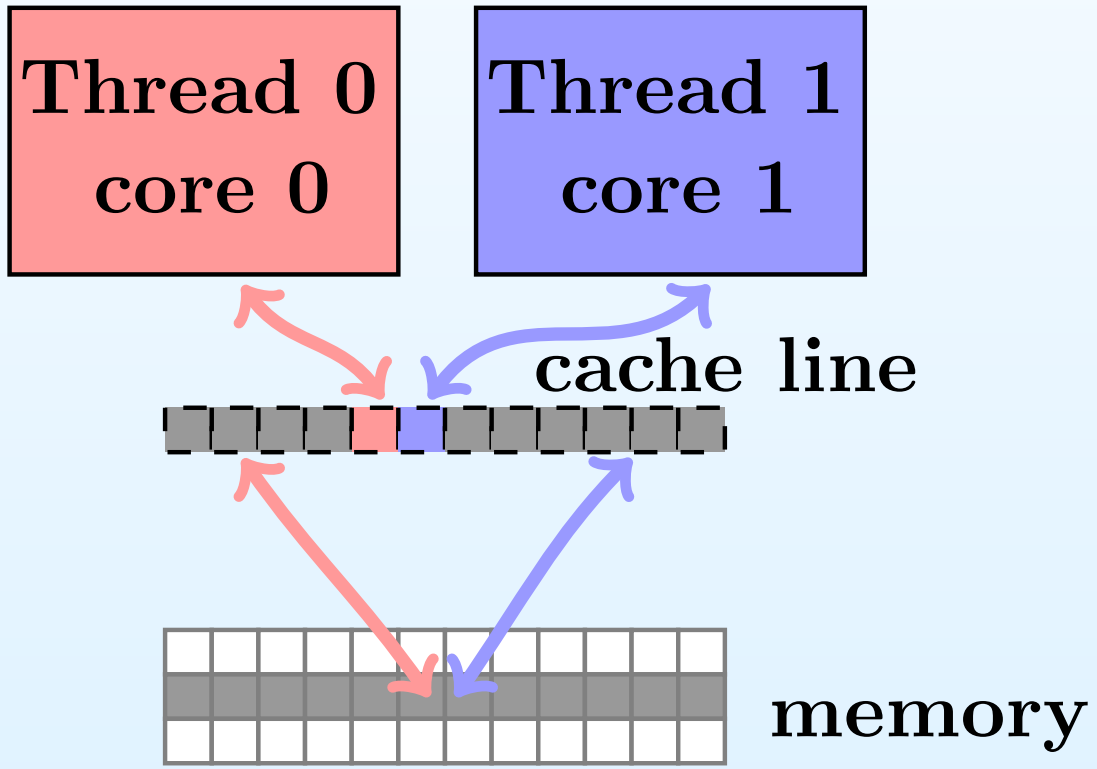
```
 1  // define the arrays.
 2  counter = (int*)malloc(nothread*sizeof(int));
 3  start_idx = (int*)malloc(nothread*sizeof(int));
 4 end_idx = (int*)malloc(nothread*sizeof(int));
 5  chunk_size = nosize / nothread + 1;
 6 for (id=0; id<nothread; id++)
 7  { start_idx[id] = id*chunk_size;
 8    end_idx[id] = MIN(start_idx[id]+chunk_size-1,\
 9    nosize-1);i }
10  for(id=0;id<nothread;id++) counter[id] = 0;
11  #pragma omp parallel private(id,i,j,itmp)
12    { id = omp_get_thread_num();
13    for (i=start_idx[id]; i<=end_idx[id]; i++)
14    for (j=0; j<nosize; j++)
15    { itmp = matrix[i][j]%2;
16    if (itmp == 0) ++counter[id]; } }
```

v1 C/C++

False sharing

- **False sharing** affects performance: the array `counter[]`;
- Thread only accesses its array element, but **adjacent**;
- What is **false sharing**? If **two** or **more** threads that access the **same** cache line, at least one of them is to **modify** (**write**) that cache line.

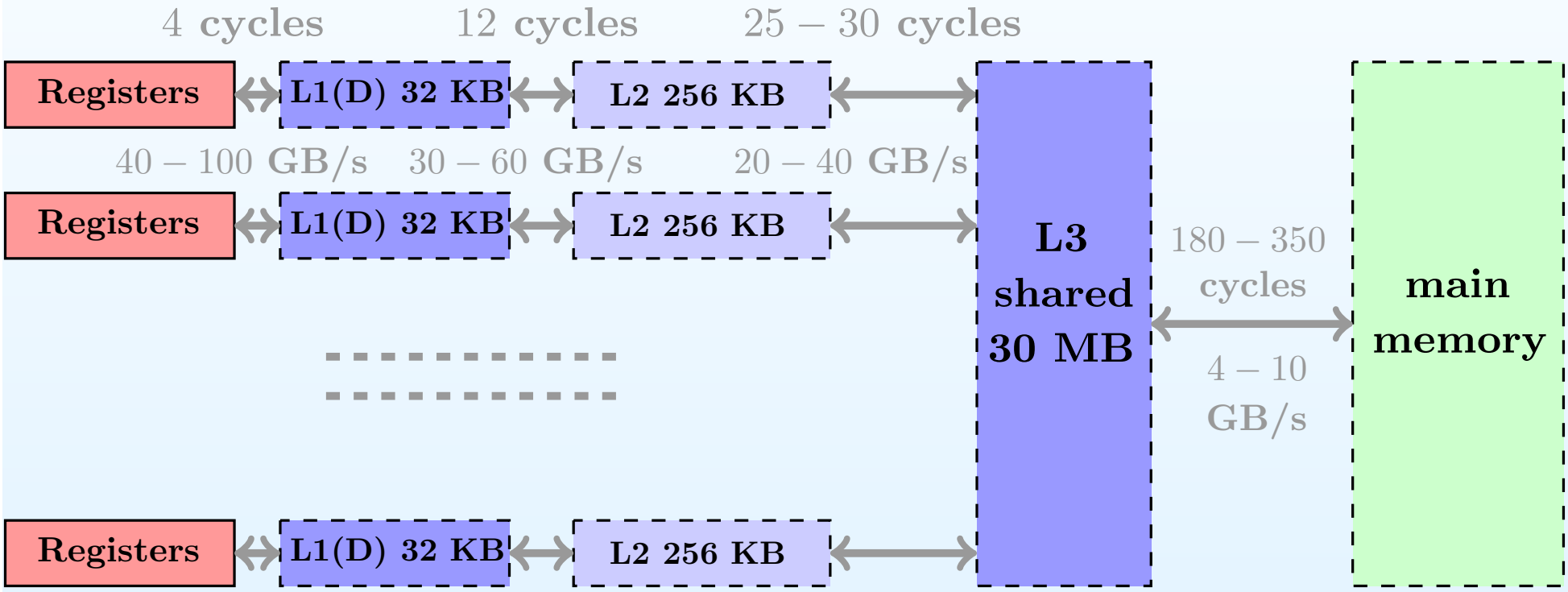
MESI protocol:
(1) Modified (M);
(2) Exclusive (E);
(3) Shared (S), and
(4) Invalid (I).



- Overhead to synchronize the cache and main memory;

False sharing

- Understand memory and cache **hierarchy**:
- Lower-level cache (smaller, faster), but higher-level cache (larger, slower);



Memory Hierarchy of Xeon Sandy-Bridge Processor

False sharing

- Can we **remove** the false sharing?
- The shared array `counter[]` is the root of the problems;

v2 C/C++

```
 1  #pragma omp parallel \
 2     private(id,i,j,itmp,counter_own)
 3  { counter_own = 0;
 4  id = omp_get_thread_num();
 5  for (i=start_idx[id]; i<=end_idx[id]; i++)
 6  for (j=0; j<nosize; j++)
 7  { itmp = matrix[i][j]%2;
 8  if (itmp == 0) ++counter_own; }
 9  counter[id] = counter_own; }
10  counter_even = 0;
11  for(id=0; id<nothread; id++) \
12     counter_even += counter[id];
```

False sharing

- Any improvement?
- Has the false sharing been removed **completely**?
- What happens if we simple do `parallel for`?

v3 C/C++

```
1 // count the number of even integers.
2    counter_even = 0;
3 #pragma omp parallel for private(i,j,itmp)
4    for (i=0; i<nosize; i++)
5    for (j=0; j<nosize; j++)
6    { itmp = matrix[i][j]%2;
7 #pragma omp critical
8    if (itmp == 0) ++counter_even;
9    }
```

- Using `critical` to **protect** the access to the **shared** variable;
- Any room to improve it?

False sharing

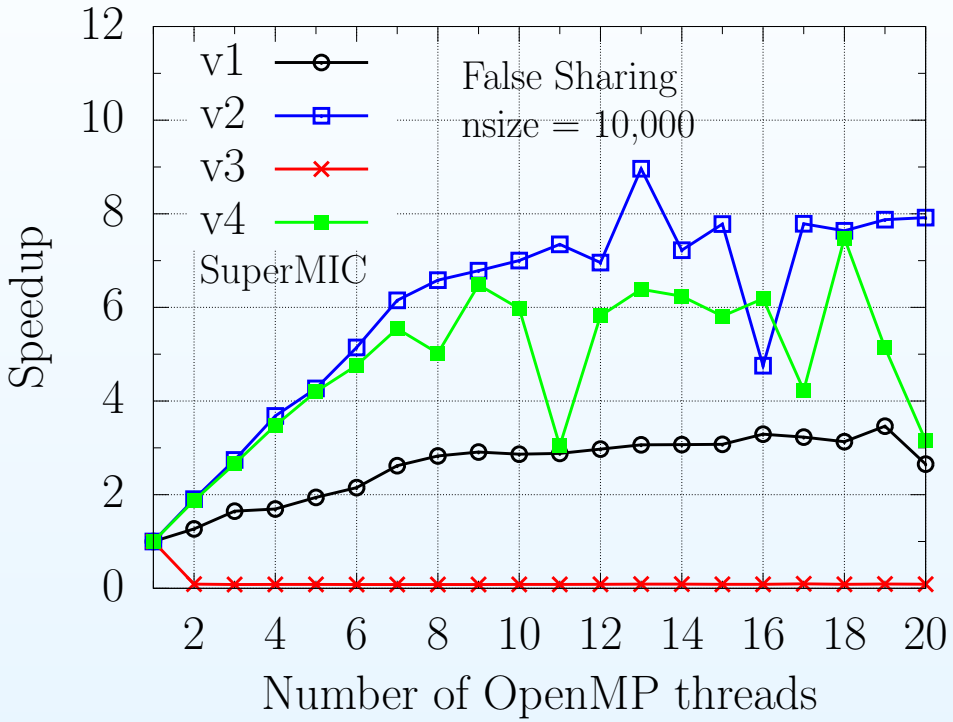
- Using **reduction** instead of **critical**:

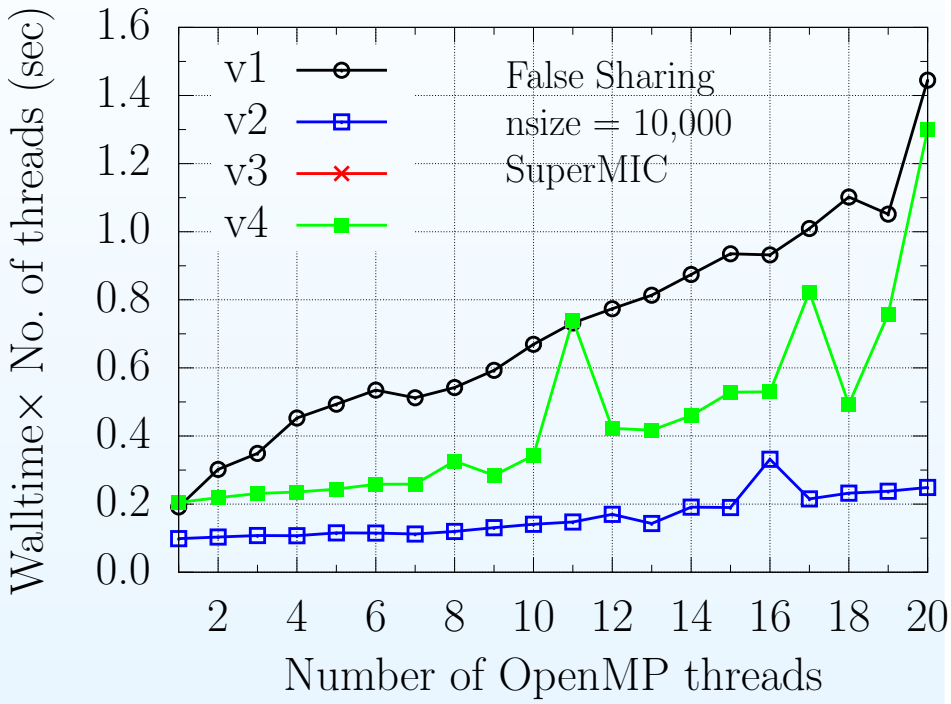
v4 C/C++

```
1  // start a timer.
2     time_start = omp_get_wtime();
3  // count the number of even integers.
4  counter_even = 0;
5  #pragma omp parallel for private(i,j,itmp) \
6     reduction(+:counter_even)
7     for (i=0; i<nosize; i++)
8     for (j=0; j<nosize; j++)
9     { itmp = matrix[i][j]%2;
10  if (itmp == 0) ++counter_even;
11     }
12     time_end = omp_get_wtime();
13  printf("Elapsed time (sec) is \
14     %.5f\n",time_end-time_start);
```

False sharing

- Compare the performance of the different versions;

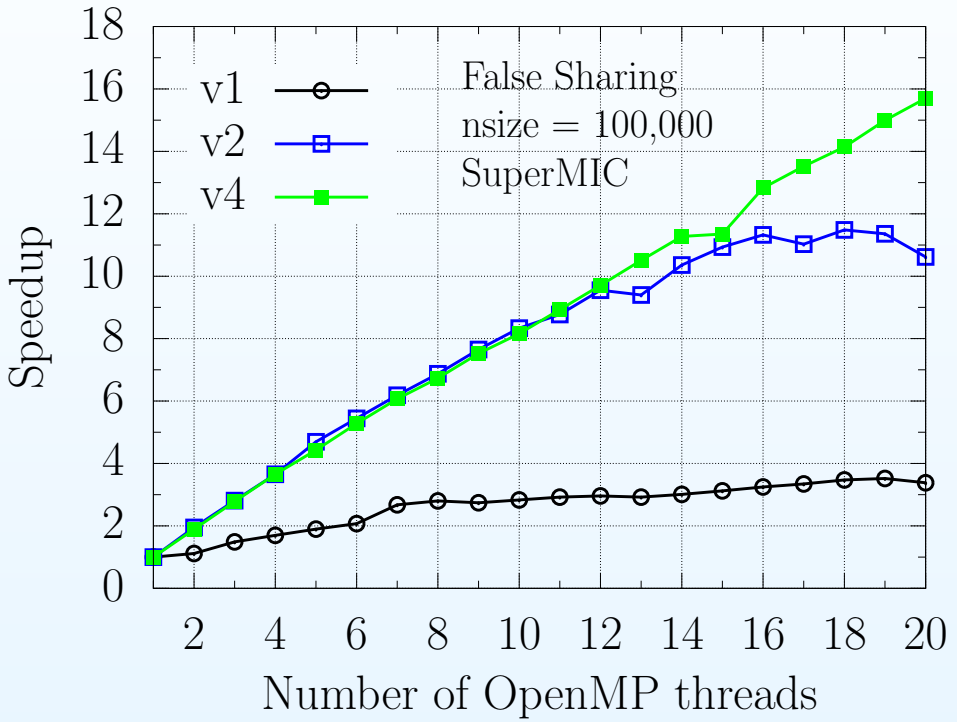


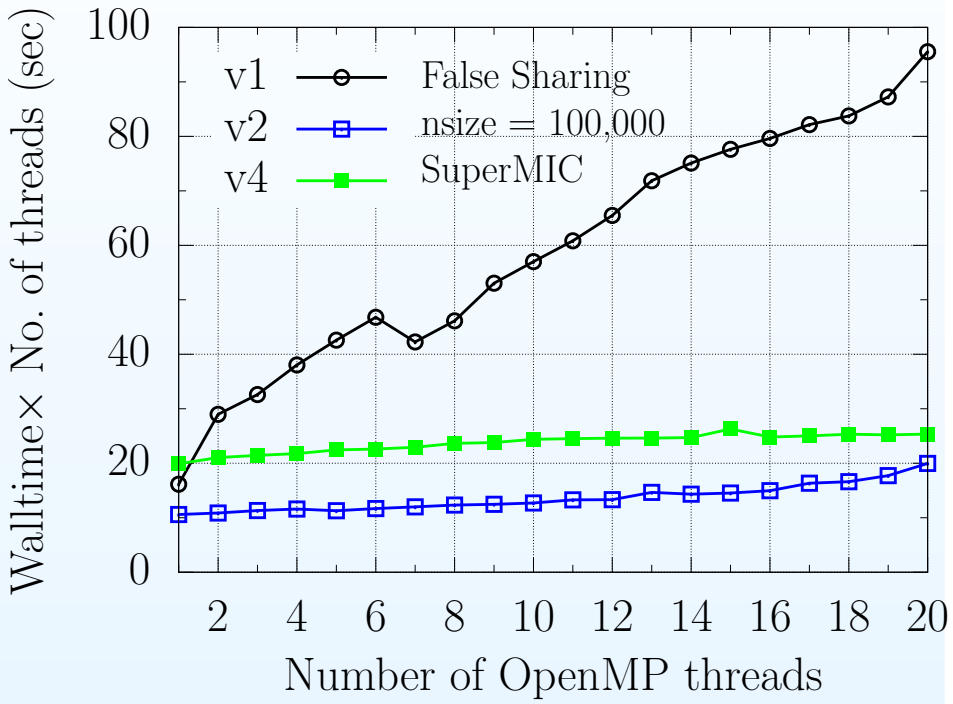


- Which version is the best?
- In the ideal case, the walltime $\times$ No. of threads is **flat**;
- The **coarse-grained** data decomposition(**v2**) is the best in terms of both speedup and walltime;

False sharing

- Compare the performance of the different versions;





- Which version is the best?
- Performance also depends on the **problem size**;
- The **coarse-grained** data decomposition(**v2**) is the best in terms of the speedup (**v4**) and walltime (**v2**);

False sharing

v1: manually decomposition with false sharing;
v2: manually decomposition with false sharing removed (almost);
v3: using `parallel for` with `critical`;
v4: using `parallel for` with `reduction`;

- Don't confuse **false sharing** with **data race**!
- **Data race** affects the **correctness** of your results;
- **False sharing** affects the code **performance**, but has nothing to do with the correctness of data;
- Both are caused by **shared** variables;

"*Sharing is the root of all contention!*" (H. Sutter 2009)

Nested thread parallelism

Nested thread parallelism

- The Intel MKL contains BLAS, LAPACK, Sparse BLAS and solvers, FFT routines, . . .
- All BLAS/LAPACK routines were written in Fortran, and Intel compiler provides the flag **-mkl** to link to it. It also supports a **CBLAS** wrapper for C/C++ code;
- In some cases we need to call the **MKL** routines in a **parallel** region. Note the problems of **oversubscribing** resources;
- `-mkl=parallel` Uses the threaded MKL routines. It is the same as `-mkl` (default);
- `-mkl=sequential` Uses the non-threaded MKL routine.
- `-mkl=cluster` Uses the **cluster** part and the **sequential** part of the MKL routines on **multiple** nodes. It is possible to link to the cluster part and parallel routines at the same time;

Nested thread parallelism

- Consider **matrix-matrix** products that need to be repeated multiple times;
- Link it to the MKL routine `dgemm` in Fortran or `cblas_dgemm` routine in C;

C/C++

```
1  // repeat "iteration" times:  C = A×B.
2  #pragma omp parallel for
3  for (k=0; k<iteration; k++)
5  {  cblas_dgemm(CblasRowMajor, CblasNoTrans, \
6     CblasNoTrans, nsize, nsize, nsize, \
7     alpha, matrix_a, nsize, matrix_b, nsize, \
8     beta, matrix_c, nsize);   }
```

- The MKL routine was embedded in the **parallel** region;
- **Explicit** OpenMP threading and **implicit** MKL threading;

Nested thread parallelism

- Compile it with `-openmp -mkl` flags;
- On a **compute node**, run the following commands and monitor the **load** average:

(1) Without setting anything but run `$ ./threaded_dgemm`
How many threads from **OpenMP parallel for** and how many threads from the implicit **MKL** routine?

(2) How do we **explicitly** control the no. of the **OpenMP** threads and the no. of the **MKL** threads?

```
$ OMP_NESTED=true MKL_DYNAMIC=false \
  OMP_NUM_THREADS=2 MKL_NUM_THREADS=4
  ./threaded_dgemm
```

In this case, we ask `2` OpenMP threads and each of them spawns `4` MKL threads;

Nested thread parallelism

- `OMP_NUM_THREADS` controls the number of **OpenMP** threads;
- `MKL_NUM_THREADS` controls the number of **MKL** threads;
- Setting `MKL_NUM_THREADS=1` at run-time is kind of equivalent to `-mkl=sequential` during compilation;
- What if we **don't** explicitly specify both of the thread counts?

```
$ OMP_NESTED=true MKL_DYNMAIC=false ./threaded_dgemm
```

- How many threads spawned in total?
- `OMP_NESTED` enable/disable **nested parallel regions**. If not defined, nested parallel regions are **disabled** by default;
- `MKL_DYNAMIC=true` allows the run-time system to detect and decide how many threads need to spawn. This is good to avoid `oversubscription`. If it is `false`, each **MKL** thread has a chance to spawn the max of thread counts, which is bad;

Nested thread parallelism

- The **default** value of `MKL_DYNAMIC` is `true`.
- By **default** the MKL routines will use only `1` thread if they are called in an OpenMP **parallel** region;
- "*I'm not a programmer, why should I be concerned about it?*"
- Some third-party applications or packages that were built on the top of the Intel MKL may **overwrite** the default behavior at run-time (call `omp_set_nested()` and `mkl_set_dynamic()`);

(1) Modify the `threaded_dgemm.c` code by adding
`omp_set_nested(1); mkl_set_dynamic(0);`
(2) Compile it and run it with `./thread_dgemm`
(3) Are there any problems and how can we fix it?
(4) Run it with `$ OMP_NUM_THREADS=4 ./threaded_dgemm`
How many threads in total?

- Use the env `OMP_NUM_THREADS` to control it;

Non-loop-level parallelism

Parallel regions

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

Fortran

```
1 !$omp parallel [clauses]
2     code block
3 !$omp end parallel
```

C/C++

```
1 #pragma omp parallel [clauses]
2     { 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

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

Fortran

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

Fortran

```
1 !$omp parallel do
2 do k = 1, 5
3     id = omp_get_thread_num()
4     write(*,*) "Hello World!  from ", id, k
5 end do
6 !$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;
- `common` 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

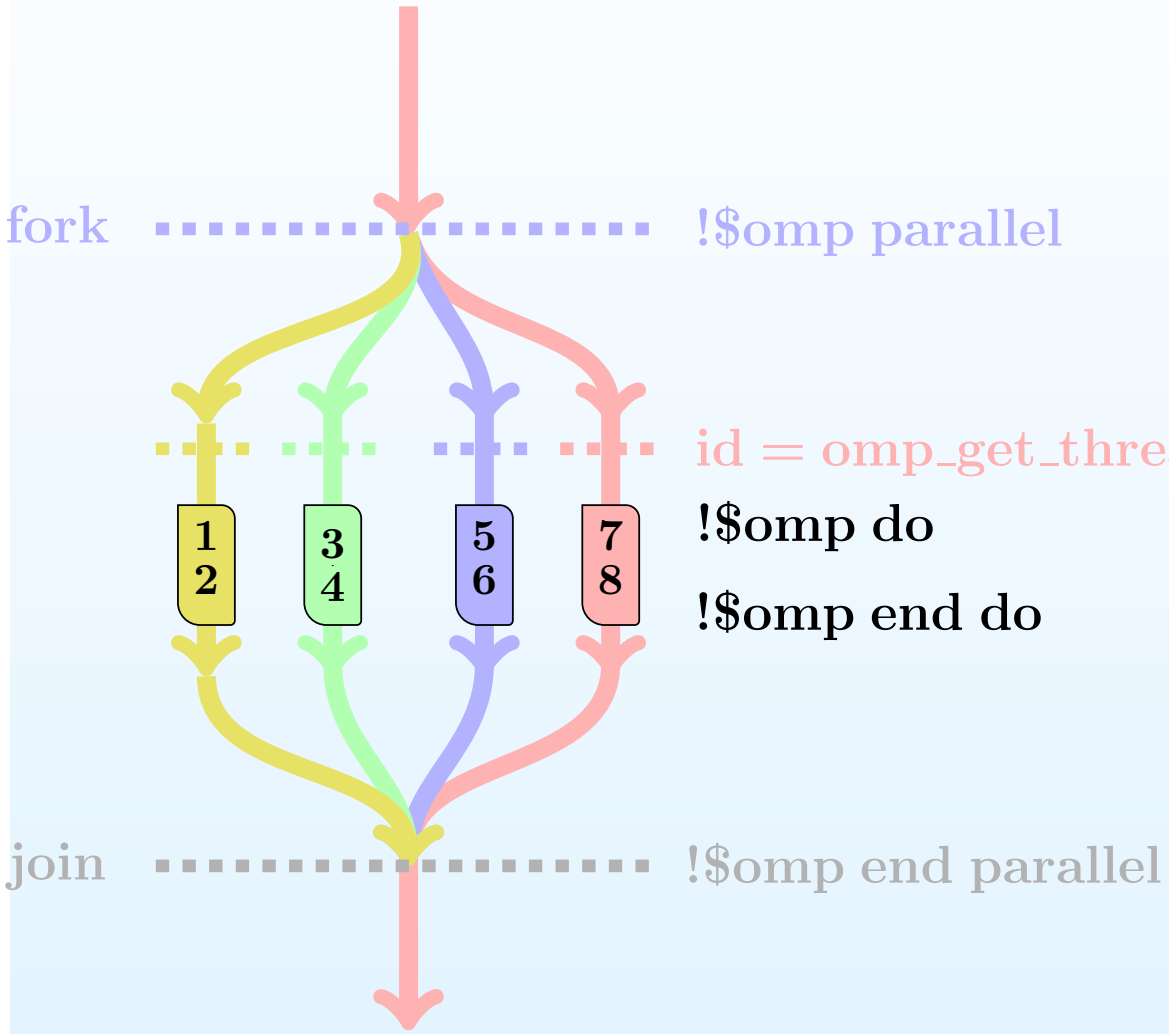
- `!$omp threadprivate (list_common_variables)` in Fortran;
- `#pragma omp threadprivate (list_variables)` in C/C++;
- We have **global** but **private** variables;
- The `threadprivate` variables are special private variables; thus thread `a` cannot access the `threaprivate` variables stored on thread `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 similar to the Intel `Xeon Phi` programming?

Work-sharing directives

Fortran

```
 1 program mapping
 2 implicit none
 3 integer ::  i,id,nothread,  &
 4           omp_get_thread_num, omp_get_num_threads
 5
 6 !$omp parallel private (k,id), shared(nothread)
 7    id = omp_get_thread_num()
 8    nothread = omp_get_num_threads()
 9 !$omp do
10   do k = 1, 40
11   write(*,'(1x,2(a,i4))') "id = ",id, " k = ",k
12   end do
13 !$omp end do [nowait]
14 !$omp end parallel
15 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

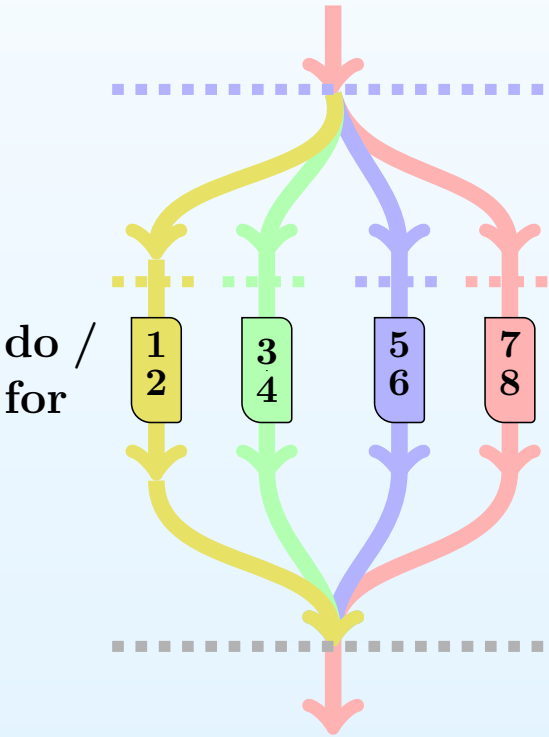
- Work-sharing constructs do **not** spawn multiple threads; they need to be **embedded** in a parallel region; if not, only one thread will run work-sharing constructs;
- There is an **implicit** barrier at the **end** of a work-sharing construct, but no implicit barrier upon the entry to it;
- **Three**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

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

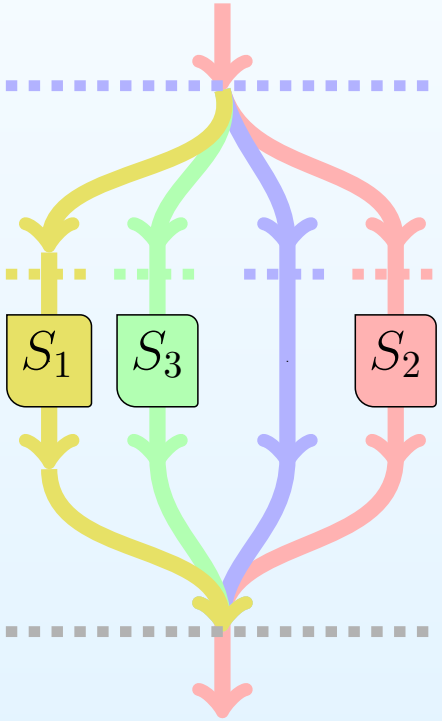
- A thread may work on zero, one, or more `omp sections`; but only one thread runs `omp single` at a given time;
- Be sure there are no data dependencies between `sections`;
- All threads must encounter the same workflow (though it may or may not execute the same code block at run-time);

Work-sharing directives

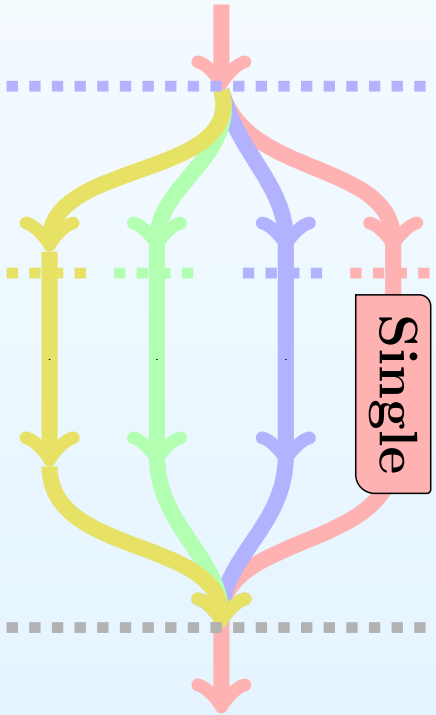
```
!$omp do
#pragma for
```




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




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



Work-sharing directives

C/C++

```
 1 #include <omp.h>
 2 #define nsize 500
 3 main() { int i, j, k ;
 4 double a[nsize], b[nsize], c[nsize] ;
 5 for (k = 0; k <= nsize, ++k) {
 6 a[k] = (double) k; b[k] = a[k]; c[k] = 0.5*a[k];}
 7
 8 #pragma omp parallel {
 9      #pragma omp sections {
10      #pragma omp section { code block_1; }
11      #pragma omp section { code block_2; }
12      #pragma omp section { code block_3; }
13                          }
14                        }
15          }
```

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 the `critical` section, but have to wait to enter the `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

```
1       tsum = 0.0d0 ; nsize = 10000
2  !$omp parallel private(temp), shared(tsum,nsize)
3       temp = 0.0d0
4  !$omp do
5       do i = 1, nsize
6           temp = temp + array(i)
7       end do
8  !$omp end do
9
10 !$omp critical
11          tsum = tsum + temp
12 !$omp end critical
13
14 !$omp end parallel
```

Synchronization

- Using `atomic` to protect a shared variable:

C/C++

```
 1 #include <omp.h>
 2 #include <stdio.h>
 3 #include <stdlib.h>
 4 #define nsize 1000
 5 int main () {
 6 int i; double x = 0.0, answer;
 7 #pragma omp parallel for private(i) shared(x) {
 8 for (i = 1; i <= nsize; ++i) {
 9      #pragma omp atomic
10      x += (double) i; }          }
11 answer = (double) 0.5*(nsize+1)*nsize;
12 printf("%f\n", x);
13 printf("correct answer is %f\n", answer);
14 }
```

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

Questions?

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