PHYS52015 Core Ib: Introduction to High Performance Computing (HPC)

Session III: OpenMP (3/3)

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Outline

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`atomic` operations

- `critical` directives protect *code blocks* from parallel access
- `atomic` directives protect *individual variables* from parallel access

atomic operations

- critical directives protect *code blocks* from parallel access
- atomic directives protect *individual variables* from parallel access

Recall the critical resolution of the inner product of a & b:

```
double result = 0.0;
#pragma omp parallel
{
  double myResult = 0.0;
  #pragma omp for
  for( int i=0; i<size; i++ ) {
    myResult += a[i] * b[i];
  }
  #pragma omp critical
  result += myResult;
}
```

atomic operations

Using an atomic update:

```
double result = 0.0;
#pragma omp parallel
{
  double myResult = 0.0;
  #pragma omp for
  for( int i=0; i<size; i++ ) {
    myResult += a[i] * b[i];
  }
  #pragma omp atomic
  result += myResult;
}
```

- The atomic clause tells the compiler that on the next line,
  - Thread acquires the lock
  - Thread updates the result
  - Thread releases the lock
- If updating different elements, i.e. x[k], then atomic will let x[k] and x[l] update simultaneously when $k \neq l$ (critical does not!).

Concept of building block

- Content
  - Introduce term atomic
  - Introduce atomic operator syntax
  - Study (potential) impact of atomic feature
- Expected Learning Outcomes
  - The student *knows* of atomics in OpenMP
  - The student can *identify* atomics in given codes
  - The student can *program* with atomics

Thread communication—repeated

We distinguish two different communication types:

- Communication through the join
- Communication inside the BSP part (not “academic” BSP)

Critical section: Part or code that is ran by at most one thread at a time.

Reduction: Join variant, where all the threads reduce a value into one single value.

$\Rightarrow$ Reduction maps a vector of $(x_0, x_1, x_2, x_3, \dots, x_{p-1})$ onto one value x, i.e. we have an all-to-one data flow

$\Rightarrow$ Inter-thread communication realised by data exchange through shared memory

$\Rightarrow$ Fork can be read as one-to-all information propagation (done implicitly by shared memory)

Collective operations

Collective operation: A collective operation is an operation that involves multiple cores/threads.

- Any synchronisation is a collective operation
- BSP/OpenMP implicitly synchronises threads, i.e. we have used synchronisation
- Synchronisation however does not compute any value

```
double result = 0.0;
#pragma omp parallel
{
  double myResult = 0.0;
  #pragma omp for
  for( int i=0; i<size; i++ ) {
    myResult += a[i] * b[i];
  }
  #pragma omp barrier
}
```

- The above fragment synchronises all threads
- This type is a special type of a *collective operation*
- Barriers are implicitly inserted by BSP programming model

Collective operations

Collective operation: A collective operation is an operation that involves multiple cores/threads.

- Challenge: Synchronisation does not compute any value

```
double result = 0.0;
#pragma omp parallel
{
  double myResult = 0.0;
  #pragma omp for
  for( int i=0; i<size; i++ ) {
    myResult += a[i] * b[i];
  }
  #pragma omp critical
  result += myResult;
}
```

- The above fragment mimics an all-to-one operation (all threads aggregate their data in the manager threads result variable)
- This type is called *reduction* which is a special type of a *collective operation*
- OpenMP provides a special clause for this

Reduction operator

- We have been looking at various ways to combine the results from parallel computation on a group of threads into a single value
- This is a classic parallel computing communication pattern – think about computing the norm of a vector!

$\Rightarrow$ This pattern is called a *reduction*

- Thread communication relies on shared memory
- Writing this communication manually is tedious – OpenMP provides a clause:

```
#pragma omp parallel for reduction([operator]:[variable])
```

Reduction operator

- We have been looking at various ways to combine the results from parallel computation on a group of threads into a single value
- This is a classic parallel computing communication pattern – think about computing the norm of a vector!
- ⇒ This pattern is called a *reduction*
- Thread communication relies on shared memory
- Writing this communication manually is tedious – OpenMP provides a clause:

```
#pragma omp parallel for reduction([operator]:[variable])
```

- Some restrictions for `reduction`:
  - `operator` must be binary associative; *e.g.*, $a \times (b \times c) \equiv (a \times b) \times c$
  - `operator` must have an identity value for initialisation – *e.g.*, 1 for $\times$
  - `variable` must be built-in type – *e.g.*, `int` or `double`
  - `variable` must not appear in (other) data clauses – `reduction` takes primacy

Reduction pragma

```
double result = 0;
#[1] #pragma omp parallel for reduction(*:result)
#[2] #pragma omp parallel for reduction(+:result)
#[3] #pragma omp parallel for private(result) reduction(+:result)
#[4] #pragma omp parallel for firstprivate(result) reduction(*:result)
for( int i=0; i<size; i++ ) {
  result += a[i] * b[i];
}
```

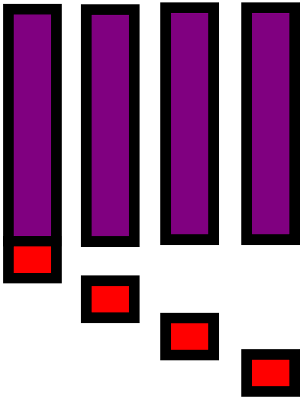
- Which `pragma` line is correct?

Reduction pragma

```
double result = 0;
#[1] #pragma omp parallel for reduction(*:result)
#[2] #pragma omp parallel for reduction(+:result)
#[3] #pragma omp parallel for private(result) reduction(+:result)
#[4] #pragma omp parallel for firstprivate(result) reduction(*:result)
for( int i=0; i<size; i++ ) {
  result += a[i] * b[i];
}
```

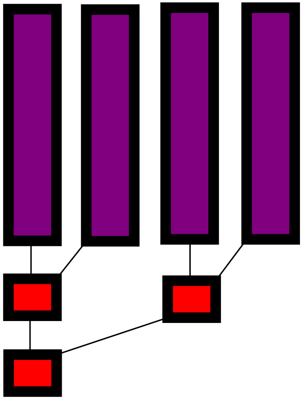
- Which `pragma` line is correct?
- Reduction keyword is parameterised with (commutative) operation (+,-,*,&,|,. . .)
- Reduction works solely for scalars.
- Keyword makes scalar private first but then merges the threads' scalars.
- Keyword initialises private copy with identity w.r.t. the operator.

Performance study



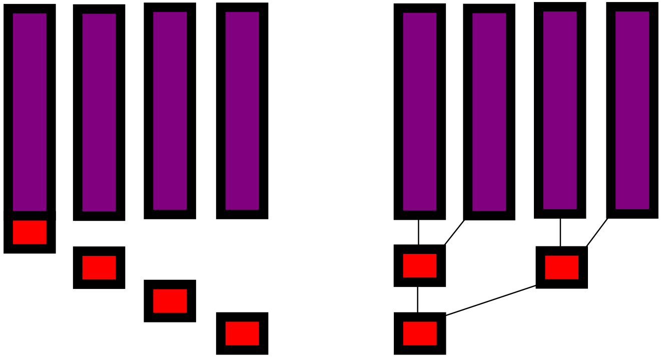
```
double result = 0.0;
#pragma omp parallel
{
  double myResult = 0.0;
  #pragma omp for
  for( int i=0; i<size; i++ ) {
    myResult += a[i] * b[i];
  }
  #pragma omp critical
  result += myResult;
}
```

Performance study



```
double result = 0;
#pragma omp parallel for reduction(+:result)
for( int i=0; i<size; i++ ) {
  result += a[i] * b[i];
}
```

Performance study



Concept of building block

- Content
  - Introduce term collective
  - Introduce reduction syntax
  - Study (potential) impact of reduction feature
- Expected Learning Outcomes
  - The student *knows* of reductions in OpenMP and their variants
  - The student can *identify* reductions in given codes
  - The student can *program* with reductions

My work is more varied than iterating over a loop...

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Sometimes we will have a large set of loosely-related subproblems with relatively shallow dependencies.

Or sometimes we will have multiple computations which are independent, but need to be combined in some way for another computation.

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Sometimes we will have a large set of loosely-related subproblems with relatively shallow dependencies.

Or sometimes we will have multiple computations which are independent, but need to be combined in some way for another computation.

The archetypal parallelization method for this type of problem is *tasking*.

If not all threads shall do the same

A manual task implementation:

```
#pragma omp parallel for schedule(static:1)
for (int i=0; i<2; i++) {
  if (i==0) {
    foo();
  }
  else {
    bar();
  }
}
```

Shortcomings:

- Syntactic overhead
- If `bar` depends at one point on data from `foo`, code deadlocks if ran serial
- Not a real task system, as two tasks are synchronised at end of loop

Tasks in OpenMP 3.0

- Introduce new task keyword:

```
#pragma omp task
```

- Parallel regions sets up queues:

```
#pragma omp parallel
```

- All tasks that are parallel to each other befill this queue
- Before OpenMP 3.0 there used to be a

```
#pragma omp section
```

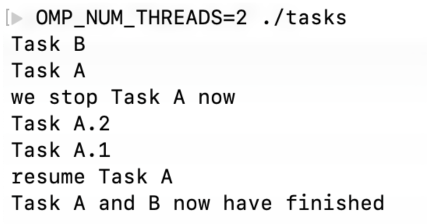
  command. The standard does not specify, whether sections can be stolen.
- Tasks may spawn additional tasks – classic example is recursive algorithms

Task example

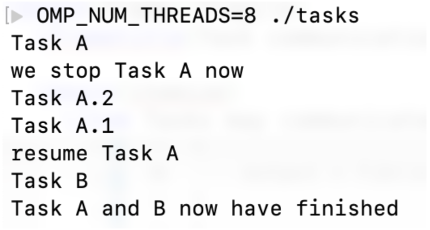
```
#pragma omp parallel
{
  #pragma omp single
  {
    #pragma omp task
    {
      printf( "Task A\n" );
      printf( "we stop Task A now\n" );
      #pragma omp task
      {
        printf( "Task A.1\n" );
      }
      #pragma omp task
      {
        printf( "Task A.2\n" );
      }
      #pragma omp taskwait
      printf( "resume Task A\n" );
    }
    #pragma omp task
    {
      printf( "Task B\n" );
    }
    #pragma omp taskwait
    #pragma omp task
    printf( "Task A and B now have finished\n" );
  }
}
```

- Which `printf` call prints first?

Experiment



```
[▶ OMP_NUM_THREADS=2 ./tasks
Task B
Task A
we stop Task A now
Task A.2
Task A.1
resume Task A
Task A and B now have finished
```



```
[▶ OMP_NUM_THREADS=8 ./tasks
Task A
we stop Task A now
Task A.2
Task A.1
resume Task A
Task B
Task A and B now have finished
```

- Either ‘Task A’ or ‘Task B’ lines print first
- Task A stop line always follows ‘Task A’
- ‘Task A.1’ and ‘Task A.2’ should precede ‘resume Task A’
- ‘Task A and B have finished’ is always last

Task communication

- Tasks may communicate through shared memory
- Critical sections remain available

```
#pragma omp parallel
{
  #pragma omp single
  {
    #pragma omp task
      foo();
    #pragma omp task
      bar();
  }
}
```

Observations:

- OpenMP pragmas are ignored if we compile without OpenMP

⇒ Code still deadlocks if `bar` depends on

⇒ Should work with `OMP_NUM_THREADS=1`

- There is still an implicit join where `omp parallel` terminates

⇒ Task paradigm is embedded into fork-join model

Task example

```
#pragma omp parallel
{
  #pragma omp single
  {
    #pragma omp task
    {
      printf( "Task A\n" );
      printf( "we stop Task A now\n" );
      #pragma omp task
      {
        printf( "Task A.1\n" );
      }
      #pragma omp task
      {
        printf( "Task A.2\n" );
      }
      #pragma omp taskwait
      printf( "resume Task A\n" );
    }
    #pragma omp task
    {
      printf( "Task B\n" );
    }
    #pragma omp taskwait
    #pragma omp task
    printf( "Task A and B now have finished\n" );
  }
}
```

- Can you draw the task dependency graph? It is the “inverse” of the spawn graph!

Tasking case study: Recursive Fibonacci

Recall the Fibonacci sequence: $f_0 = 0$, $f_1 = 1$, $f_n = f_{n-1} + f_{n-2}$

- Classic example of a (bad) recursive computation
- *This is pedagogical, not a recommendation for task parallelism . . .*
- Consider the serial implementation of `fib` below:

```c
#include <stdio.h>
#include <omp.h>
int fib(int n) {
    if (n < 2) return n;
    int x = fib(n - 1);
    int y = fib(n - 2);
    return x+y;
}
int main(int argc,char* argv[]){
    // ...
    fib(input);
    // ...
}
```

How would we use tasks for this . . .

```
int fib(int n) {
    if (n < 2) return n;
    int x, y;
    #pragma omp task shared(x)
    x = fib(n - 1);
    #pragma omp task shared(y)
    y = fib(n - 2);
    #pragma omp taskwait
    return x+y;
}
int main(int argc, char* argv[]){
    // ...
    #pragma omp parallel
    {
    #pragma omp single
    {
    fib(input);
    }
    }
    // ...
}
```

- One thread enters `fib` from `main`, spawns two initial work tasks
- Requires `taskwait` to recover intermediate `x` & `y` – not all child tasks
- From `main`, we we only need to call the `fib` function *once*.

Concept of building block

- Content
  - Introduce task parallelism
  - Discuss task features compared to “real” tasking systems
- Expected Learning Outcomes
  - The student *can analyse* OpenMP’s task concept and upcoming features
  - The student *can write* a task-based OpenMP code