LAB : OpenMP Stampede

John Lockman III

Texas Advanced Computing Center
The University of Texas at Austin

July 9, 2013

Introduction

What you will learn

- How to compile Code (C and Fortran) with OpenMP
- How to parallelize code with OpenMP
  - Use the correct header declarations
  - Parallelize simple loops
- How to effectively hide OpenMP statements

What you will do

- Modify example code READ the CODE COMMENTS
- Compile and execute the example
- Compare the run-time of the serial codes and the OpenMP parallel codes with different scheduling methods

Accessing Lab Files

- Log on to Stampede using your train## account.
- Untar the file lab_OpenMP.tar file (in ~train00).
- The new directory (lab_openmp) contains sub-directories for exercises 1-3.
- cd into the appropriate subdirectory for an exercise.

You will be assigned this number.

```
ssh train##@stampede.tacc.utexas.edu
tar -xvf ~train00/lab_OpenMP.tar
cd lab_openmp
```

Running on compute nodes Interactively

YOU CAN DO THE LAB WITHOUT RUNNING ON COMPUTE NODES!!!

- You can compile* and execute your code on the login node (login1); or you can use one of the compute nodes (c###-###). Here is how to do that.

1hr, development queue, 16 cores.
If asked, put an account (-A …) here.

1.

```
login2$ srun -t 60 -p development -n 16  --pty /bin/bash -l
--> Verifying availability of home dir
(/home1/00770/milfeld)...OK
--> Verifying access to desired queue (devel)...OK
c559-802$
```

2. Once you have a command prompt, you are ready to go (you own the node- it isn't shared with any other user). E.g. compile and execute - note the login prompt is the node name.

(this is only an example)

```
c559-001% ifort hello.f90 -o hello
c559-001% ./hello
```

Compiling

- All OpenMP statements are activated by the OpenMP flag:
  - Intel compiler: icc/ifort -openmp -fpp source.<c,f90>
  - PGI compiler: pgcc/pgf90 -mp source.<c,f90>
- **On Stampede we will be using the Intel compiler**
- Compilation with the OpenMP flag (-openmp):

  Activates OpenMP comment directives (…) :

  Fortran: !$OMP ...

  C: #pragma omp ...

  Enables the macro named _OPENMP

  #ifdef _OPENMP evaluates to true

  (Fortraners: compile with –fpp)

  Enables ”hidden” statements (Fortran only!)

  !$ ...

Exercises – Lab 1

- Exercise 1: Kernel check
  - f_kernel.f90/c_kernel.c
  - Kernel of the calculation (see exercise 2)
  - Parallelize one Loop
- Exercise 2: Calculation of π
  - f_pi.f90/c_pi.c
  - Parallelize one Loop with a reduction
- Exercise 3: daxpy (a * x + b)
  - f_daxpy.f90/c_daxpy.c
  - Parallelize one Loop

Exercise I: π Integration Kernel Check

- cd exercise_1
- Codes: f_kernel.f90/c_kernel.c
- Number of intervals is varied (Trial loop)

Kernel

Trial Loop: itrial
Calculation of n and deltax
Loop over i
make sure area >0.0

1. Parallelize the code
2. Compile
3. Run with 1, 2, 4, 8,12, 16 threads

   e.g. export OMP_NUM_THREADS=4
   ./a.out
4. Compare the timings

1. Parallelize the Loop over i :
   Use **omp parallel do/for**
   Set appropriate variables to private

2. Compile with:
   ifort -openmp f_kernel.f90
   icc -openmp c_kernel.c

- ✓ Timings decrease with more threads.
- ✓ If you execute with more threads than cores the timings will NOT decrease. Why?

Exercise II: π Integration

- cd exercise_2
- Codes: f_pi.90/c_pi.c
- Number of intervals is varied (Trial loop)

π calculation

Trial Loop: itrial
Calculation of n and deltax
Loop over i

- Parallelize the code

1. Complete OpenMP statements
   - Initialization
   - omp get max threads
   - omp get thread num

1. Parallelize the Loop over **i** :
   Use **omp parallel do/for**
   with the default(none) clause

2. Compile with:
   make f_pi
   or
   make c_pi

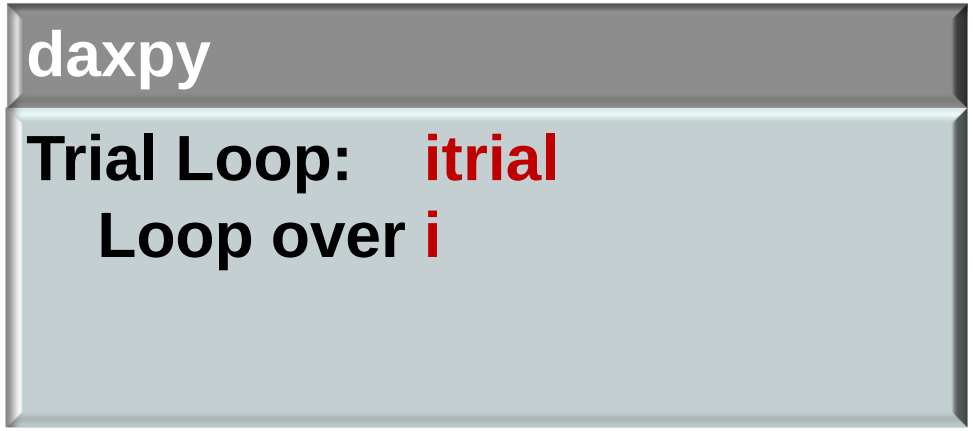
3. Run with 1, 2, 4, 8,12 threads
   e.g. export OMP_NUM_THREADS=4
   ./c_pi or ./f_pi

4. Compare timings

- ✓ Timings decrease with more threads
- ✓ What is the scale up at 12 threads?.

Exercise III: daxpy

- cd exercise_3
- Codes: f_daxpy.f90/c_daxpy.c
- Number of intervals is varied (Trial loop)



1. Parallelize the Loop over **i** :
   Use **omp parallel do/for**
   with the default(none) clause

2. Compile with:
   make f_daxpy
   or
   make c_daxpy

- Parallelize the code

1. complete OpenMP statements
   - Initialization
   - omp get max threads

3. Run with 1 and 12

4. Compare timings
   - Why is performance only doubled?

✓ Hint: Parallel performance can be limited by memory bandwidth– what is happening for every daxpy operation? (Is there cache reuse?)

Exercises – Lab 2

- Exercise 4: Update from neighboring cells (2 arrays)
  - f_neighbor.f90/c_neighbor.c
  - Create a Parallel Region
  - Use a Single construct to initialize
  - Use a Critical construct to update
  - Use dynamic or guided scheduling
- Exercise 5: Update from neighboring cells (same array)
  - f_red black.f90/c_red black.c
  - Parallelize 3 individual loops, use a reduction
  - Create a Parallel Region
  - Combine loops 1 and 2
  - Use a Single construct to initialize

Exercise IV: Neighbor Update; Part 1

- cd exercise_4
- Codes: f_neighbor.f90/c_neighbor.c

neighbor update

```
Parallel Region
Initialization: j_update
Parallelize loop i
Loop i
      Loop j
            increment j_update
            Loop k
                  b is calculated from a
```

- Try different schedules:
  static, dynamic, guided

Compile with: **make f_neighbor**
make c_neighbor

- Parallelize the Loop over **i**
- Use a **single** construct for initialization
- Would a **master** construct work, too?
- Use **critical** for increment of j_update
- Use omp parallel do/for with the default(none) clause

Exercise IV: Neighbor Update; Part 2

neighbor update

```
Parallel Region
Initialization: j_update
Parallelize loop i
Loop i
        Loop j
                single or master
                increment j_update
                end single or end master
                Loop k
                        b is calculated from a
```

Compile with: **make f_neighbor**
make c_neighbor

- Change the single to a master construct
- Run with 1 **and** 12 threads
- How does the number of j_update change?

Exercise V: Red-Black Update; Part 1

- cd exercise_5
- Codes: f_red_black.f90/c_red_black.c
- make a copy and create f_red_black_v1.f90/c_read_black_v1.c

red-black update

Iteration Loop: niter
  Loop: Update even elements
  Loop: Update odd elements
  Initialize error
  Loop-summation: error

Compile with: **make f_red_black_v1**
make c_red_black_v1

Part 1

- Parallelize each loop separately
- Use omp parallel do/for
  for the ‘‘Update’’-loops
- Use a reduction
  for the ‘‘Error’’-calculation
  with the default(none) clause

- Try static scheduling

Exercise V: Red-Black Update; Part 2

- cd exercise_5
- Start from version 1
- Codes: f_red_black.f90/c_red_black.c
- make a copy and create f_red_black_v2.f90/c_read_black_v2.c

Compile with: **make f_red_black_v2**
make c_red_black_v2

red-black update

Iteration Loop: niter
    Loop:
      Update even and odd el.
    Initialize error
    Loop-summation: error

Part 1

- Can the loops be combined?
- Why can the ‘‘update’’ loops be combined?
- Why can the ‘‘error’’ loop not be combined?
- Task:

Combine the “update” loops

- Try static scheduling

Solution V: Red-Black Update; Part 2

red-black update

```
!*** Update even elements
do i=2, n, 2
    a(i) = 0.5 * (a(i) + a(i-1))
enddo
!*** Update odd elements
do i=1, n-1, 2
    a(i) = 0.5 * (a(i) + a(i+1))
enddo
```

red-black update

```
!*** Update even and odd
!*** in one loop
do i=2, n, 2
    a(i) = 0.5 * (a(i) + a(i-1))
    a(i-1) = 0.5 * (a(i-1) + a(i))
enddo
```

Exercise V: Red-Black Update; Part 3

- cd exercise_5
- Start from version 2
- Codes: f_red_black.f90/c_red_black.c
- make a copy and create f_red_black_v3.f90/c_read_black_v3.c

Compile with: **make f_red_black_v3**
make c_red_black_v3

red-black update

Iteration Loop: niter
    parallel region
    Loop:
        Update even and odd el.
    single
    Initialize error
    end single
    Loop-summation: error
    end parallel region

Part 1

- Make one parallel region around both loops: ‘‘update’’ and ‘‘error’’.
- The initialization of error has to be done by one thread
- Use a single construct
- Would a master construct work?

Exercise VI: Orphaned work-sharing

- cd exercise_6
- Codes: f_print.f90/c_print.c
- make a copy and create f_red_black_v3.f90/c_read_black_v3.c

Orphaned work-sharing

```
parallel region
      print 1
parallel Loop
      print 2
call printer_sub
master
      print 5

subroutine print_sub
parallel Loop
      print 3
Loop
      print 4
```

Compile with: **make f_print**
make c_print

- Inspect the code
- Run with 1, 2, ... threads
- Explain the output
- How often are the 5 print statements executed?
- Why?