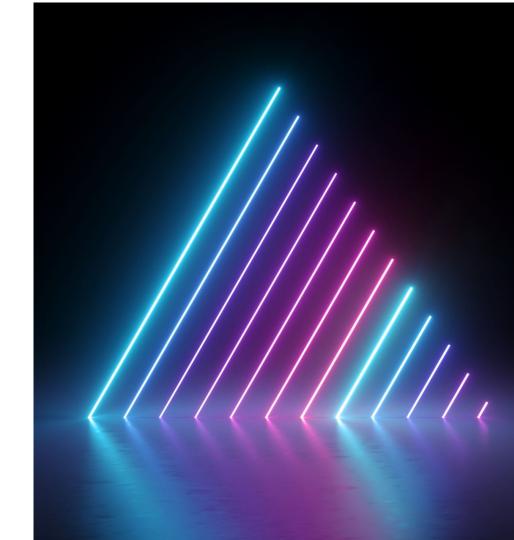
Schedule

- **Beyond Threads**
- Tasking
- SIMD
- Affinity
- C++
- **OpenMP Offloading**
 - GPUs in HPC
 - Introduction to the offloading paradigms
 - OpenMP target directive
 - **OpenMP Mapping**
 - OpenMP Variants, Metadata, interoperabilites

OpenMP beyond basics

CSC Summer Institute
October 9-11, 2023

Kent Milfeld (TACC)
Emanuele Vitali (CSC)



Slides available at:



General



Parallelize for orders of magnitude better performance. CPU/GPU=> teams/grids =>threads+SIMD/SMT

Teach basics with concepts, not just syntax

- This is the debut for this course the schedule may vary
- Content is about Concepts: Describes Features, Syntax, and use with examples (+labs).
- Some content comes from other tutorials/classes/documents (sources are referenced)



Outline of Intro



- History of OpenMP
- Summary of the Basics
- Hints, tricks and and Tips for OpenMP development
- Getting setup for Lumi/Frontera





OpenMP

tinyurl.com/tacc-csc-2023-omp



OpenMP beyond threads



OpenMP is NOT just about threads

OpenMP deals with multiple levels of Parallelism

target

Across Devices



parallel do/for, task

Across Cores



simd

Across SIMD Lanes





OpenMP beyond threads



OpenMP is NOT just about threads

OpenMP deals with Memory

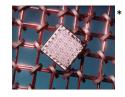
Affinity

HW thrds, cores, sockets



Allocations

API memory routines



Code Transformation

loop transform directives

 $for(i,j,k) \rightarrow for(l,m,n)$

^{*} https://commons.wikimedia.org/wiki/File:Electronic Memory.jpg



OpenMP -- board and membership



The OpenMP Architecture Review Board (ARB) published first OpenMP Specification in 1997. It is a non-profit organization with the following members:





OpenMP -- Information



Specifications, Examples and Reference Guide (Cheat Sheet) and stackoverflow link are available at:

https://openmp.org -- click on Specifications

https://stackoverflow.com/questions/tagged/openmp

- Recommended forum for technical questions is <u>Stack Overflow</u>, using the tag OpenMP
- Alternatively post messages on:
 - Twitter: <u>@OpenMP_ARB</u>
 - LinkedIn: <u>OpenMP Users</u>
 - Facebook: OpenMP Group
 - Email: info@openmp.org

https://www.openmp.org/resources/openmp-compilers-tools/



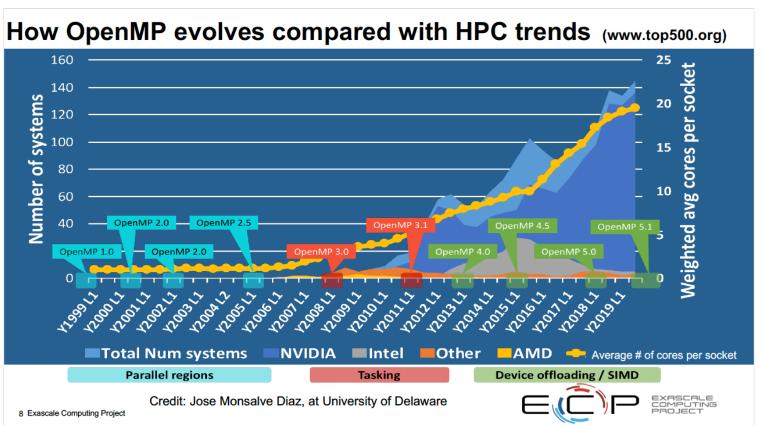
OpenMP Releases



OpenMP Version	Year (Release)	_OPENMP (YYYYMM)	Examples (YY-MM)
5.2	2021	202111	2022-11
5.1	2020	202011	2021-08
5.0	2018	201811	2020-05
4.5	2015	201511	2016-11
4.0	2013	201307	2015-03
3.1	2011	201107	
3.0	2008	200805	



OpenMP -- Evolution



https://www.openmp.org/resources/openmp-compilers-toois/





OpenMP -- early development in some areas

```
2.5->3.0 May 2008
        Environment Variables and setter:
        Tasking, thread limit, active levels, stack size, wait policy,
        set_num_threads, get ancestor thread num.get levels
3.0->3.1 Jul 2011
        Tasking (final, mergeable, taskyield)
        Affinity (PROC'BIND)
3.1->4.0 Jul 2013
        target directives (data, update, declare, teams, distribute..., )
        SIMD directive
        User Defined Reduction
        Affinity (OMP_PLACES)
        Tasking (defined scheduling points, taskgroup, depend clause)
        OMP DIŠPLAY ENV
```





Summary of Basics

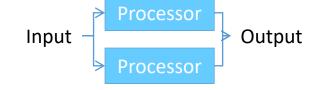


Why Parallel?



Power =
$$CV^2F$$





Freq
$$= 1.0f$$

Power =
$$1.0cv^2f$$

Do same work with 2 processors at 0.5 freq.

Voltage ~ Frequency 2x more wires ->

~2x Capacitance

Cap = 2.2c

Volts = 0.6v

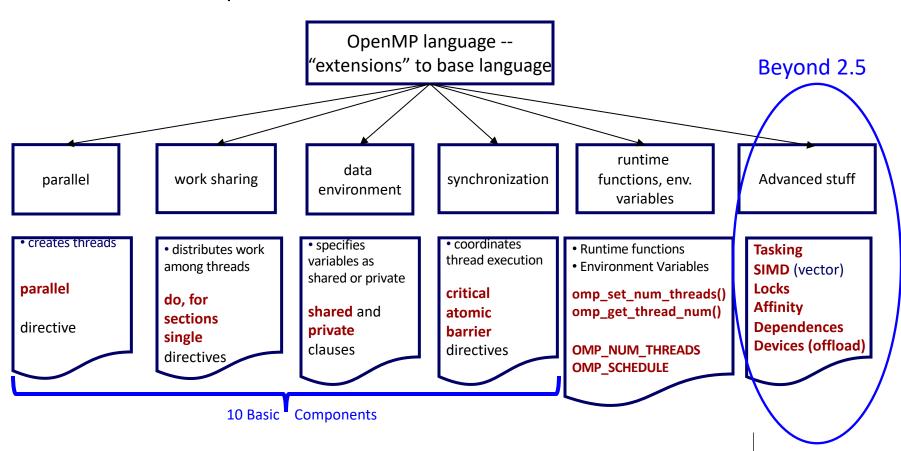
Freq = 0.5f

Power = $0.4cv^2f$

https://www.youtube.com/watch?v=cMWGeJyrc9w&index=2&list=PLLX-Q6B8xqZ8n8bwjGdzBJ25X2utwnflows.pdf.



OpenMP 2.5 Basics Constructs





OpenMP Syntax



Compiler directive syntax:

```
#pragma omp construct [clause [[,]clause]...] C

!$omp construct [clause [[,]clause]...] F90
```

Example

```
Fortran
print*,"serial"

!$omp parallel num_threads(4)
...
!$omp end parallel

print*,"serial"
```

```
c/C++
printf("serial\n");

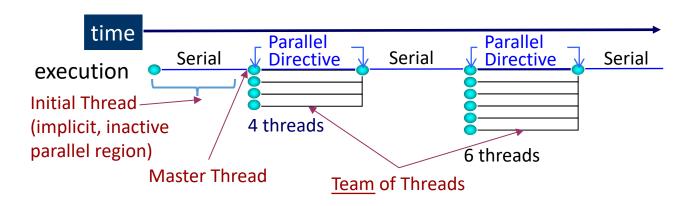
#pragma omp parallel num_threads(4)
{
    ... // can be statements or just function call w.o. {}
}
printf("serial\n");
```



Early (2.5 legacy) Execution Model



- Programs begin as a single, initial thread.
- A thread encountering a parallel construct it becomes a *master thread*.
- After executing the statements in the parallel region, team threads synchronize and terminate (join) but initial thread continues



Note:

<u>threads</u> – concept of task comes in 3.0.



OpenMP Directive Scope



* Fortran Fixed Format: !\$OMP, C\$OMP or *\$OMP

OpenMP directives are comments/pragmas in source:

F90 : !\$omp free-format*

C/C++: #pragma omp sentinel

Parallel regions are marked by enclosing parallel directives

F90 : !\$omp parallel ... !\$omp end parallel

C/C++: #pragma omp on block { ...}, or single statement

Work-sharing loops are marked by parallel do/for

```
Fortran
!$omp parallel
...
!$omp end parallel
!$omp parallel
call foo(...)
!$omp end parallel
```

```
C/C++
#pragma omp parallel
   {...
}
#pragma omp parallel
   foo(...);
```

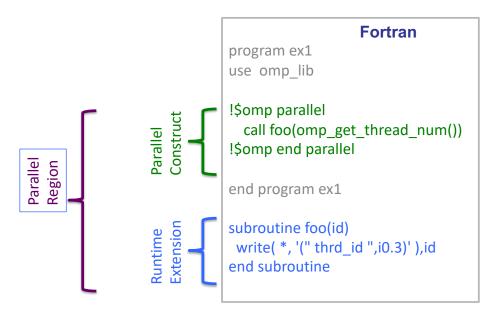
Any directive that uses omx or ompx in the sentinel is implementation defined



OpenMP Directive Scope



- construct the lexical extent of executable directive
- region all code encountered in a construct (construct + routines)



```
C/C++
#include "omp.h"
void foo(int);
int main(){
 #pragma omp parallel
   foo(omp get thread num());
void foo(int id){
 printf("thrd id %0.3d\n",id);
```



Parallel Region & work ID



F90

For example, to create a 4-thread parallel region.

Each thread executes the code within the structured block

Thread numbers range from 0 to Nthreads-1

Each thread calls foo(ID,A) with a different ID {= 0 to 3}



Parallel Region & work ID



C/C++

For example, to create a 4-thread Parallel region.

Each thread executes the code within the structured block

Thread numbers range from 0 to Nthreads-1

Each thread calls foo(ID,A) with a different ID {= 0 to 3}



Parallel Region & Worksharing



Use OpenMP directives to specify Parallel Region & Worksharing constructs

!\$ and #pragma not shown here.

Work-sharing Directives assign threads to units of work.

There is an **implied barrier** at the end of a worksharing construct!

The master directive has no barrier, and is therefore not worksharing.



Parallel Region and Worksharing



Line 1 Team of threads formed (parallel region).

Line 3-7 Loop iterations are split among threads. implied barrier at }

Each loop iteration must be independent of other iterations.



Parallel Region and Worksharing



- Line 1 Team of threads formed (parallel region).
- Line 3-4 Loop iterations are split among threads by DO construct.
- Line 5 !\$OMP END DO is optional after the enddo.
- Line 5 Implied barrier at enddo.

Each loop iteration must be independent of other iterations.



Parallel Region & Combined Constructs



```
Fortran
!$omp parallel
  !$omp do
    do ...
    end do
  !$omp end do
!$omp end parallel
!$omp parallel do
  end do
```

```
C/C++
# pragma omp parallel
  #pragma omp for
  for (...) {...}
# pragma omp parallel for
  for(){...}
```

^{*} Since Fortran DO has a block structure "!\$omp end do" Is not required

Parallel Region & Combined Constructs

!\$OMP PARALLEL

{code}

do i = 1,N*4



Replicated: Work blocks are executed by all threads.

!\$OMP DO

end do

Work-Sharing: Work is divided among threads.

4 Threads

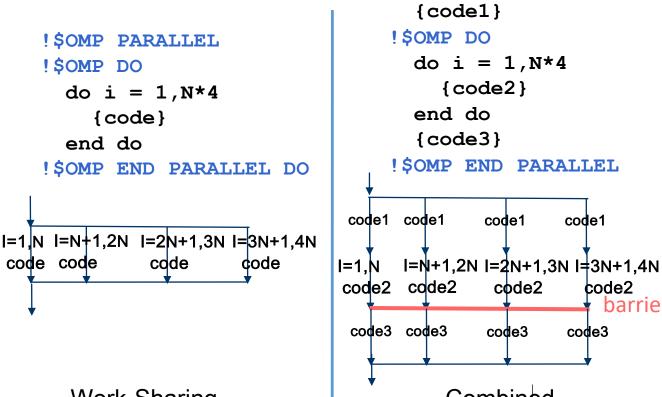
!\$OMP PARALLEL {code}

!\$OMP END PARALLEL

code code code

Work-Sharing Replicated

code code



!SOMP PARALLEL

code

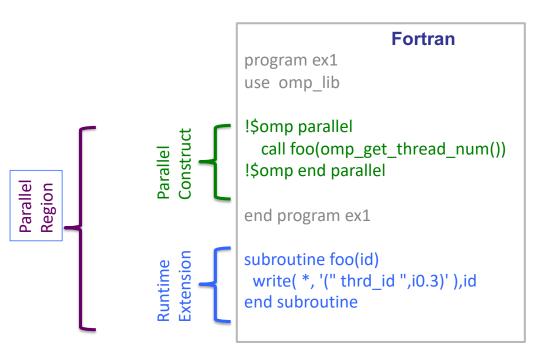
barrier



OpenMP Directive Scope



- construct the lexical extent of executable directive
- region all code encountered in a construct (construct + routines)



```
C/C++
#include "omp.h"
void foo(int);
int main(){
 #pragma omp parallel
   foo(omp get thread num());
void foo(int id){
 printf("thrd id %0.3d\n",id);
```



Schedule Clause for Worksharing

schedule(static)

Each CPU receives one set of contiguous iterations

schedule(static, C)

Iterations are divided round-robin fashion in chunks of size C

schedule(dynamic, C)

Iterations handed out in chunks of size C as CPUs become available

schedule(guided, C)

Each of the iterations are handed out in pieces of exponentially decreasing size, with C minimum number of iterations to dispatch each time

schedule (runtime)

Schedule and chunk size taken from the OMP SCHEDULE environment variable

schedule(auto)

Decision is delegated to compiler and/or runtime

schedule(monotonic: ...)

Each thread executes the chunks that it is assigned in increasing logical iteration order (nonmonotonic – any order).

schedule(simd: ...) simd size is considered in chunk size—see SIMD.

Kind Modifier



!\$omp do schedule(...)

do i=1,128 A(i)=B(i)+C(i)

enddo

#pragma omp schedule(.
 for(i=0;i<128;++i)
 A[i]=B[i]+C[i]:</pre>

A[i]=B[i]+C[i];



OpenMP Data Environments



Clauses control the data(-sharing) attributes of vars within a parallel region:

shared, private, reduction, firstprivate, lastprivate

Default variable scope (in parallel region):

- 1. Variables declared in main/program (C/F90) are shared by default
- 2. Global variables are shared by default
- 3. Automatic variables within routines called within a parallel region are private (reside on a stack private to each thread)
- 4. Loop index of worksharing loops are private.
- 5. Default scoping rule can be changed with **default** clause

Private and Shared Data



```
!$omp parallel do &
!$omp& shared(a,b,c,n) private(i)
  do i = 1,n
      a(i) = b(i) + c(i)
  enddo

C/C++
```

```
#pragma omp parallel for \
    shared(a,b,c,n) private(i)
    for (i=0; i<n; i++) {
        a[i] = b[i] + c[i];
    }
    F90</pre>
```



Reductions



- Operation that combines multiple elements to form a single result
- A variable that accumulates the result is called a reduction variable
- In parallel loops reduction operators and variables must be declared

```
float asum=0.0, aprod=1.0;
#pragma omp parallel for \
    reduction(+:asum) \
    reduction(*:aprod)

for (i=0; i<n; i++) {
    asum = asum + a[i];
    aprod = aprod * a[i];
}
    c/c++</pre>
```

```
real asum=0.0, aprod=1.0
!$omp parallel do
!$omp& reduction(+:asum) &
!$omp& reduction(*:aprod)
   do i = 1,n
                    + a(i)
            = asum
      aprod = aprod * a(i)
   enddo
                           F90
```

Each thread has a private **asum** and **aprod**, initialized to the operator's identity **After the loop execution, the master thread collects the private values of each thread and finishes the (global) reduction**



Synchronization



- Synchronization is used to impose order constraints and to protect access to shared data
- High-Level Synchronization
 - critical
 - atomic Now has acquire and release semantics!
 - barrier
 - ordered
- Low-Level Synchronization
 - locks



Parallel Region & Combined Constructs



When only one thread at a time can execute a section of code (to avoid race conditions), create a **critical** region. In essence the code executes (and can even run worse than) serially.

Use an **atomic** directive for ("simple") atomic operations that possibly have hardware atomic support. The expression must have canonical (recognizable) form.

```
!$omp parallel shared(sum,x,y)
...
!$omp critical
   update(x);
   update(y);
   sum=sum+1;
!$omp end critical

!$omp end parallel
```

4 threads

-time



nowait clause (non) synchronization



When a work-sharing region is executed, a barrier is implied - all threads must reach the barrier before any can proceed.

A nowait clause at the end of a worksharing region can remove an implied barrier.

```
#pragma omp parallel
  #pragma omp for nowait
         for (i=0; i<n; i++)
           {work(i);}
  #pragma omp for schedule(guided,k)
         for (i=0; i<m; i++)
           {x[i]=y[i]+z[i];}
                                C/C++
```

```
!$OMP PARALLEL
   !$OMP DO
      do i=1,n
         work(i)
      enddo
   !$OMP END DO NOWAIT
   !$OMP DO schedule(quided,k)
      do i=1,m
         x(i) = y(i) + z(i)
      enddo
   !$OMP END DO
!$OMP END PARALLEL
                                F90
```



Minimize number of fork/join

Optimize

1 thread per 'core'

Optimize scheduling

Remove implicit barriers

Do not serialize everything

See 'min. fork/join'

Utilize all cores

Utilize vector lanes

Interplay MPI/OpenMP

OpenMP	Summary	of tho	hacies
Opernivir	Summary	OI IIIE	Dasics

Concept	<u>'</u>	What to leave			1	
	Openivir	Summary	OI	me	Dasics	

What do the threads do?

Why/how to shelter data

Condensing a result from pieces

One thread, and only one thread

Vectorization with OpenMP

All threads, but one thread at a time

How to compile

'omp do/for'

MPI + OpenMP

Irregular problems

concept

Levei

Basic

Easy

Work-sharing: easy

Replicated: medium

Will take effort!

medium

medium

harder

harder

medium

medium

hard

hard

Work-sharing/replicated work

Avoiding race conditions

Thread/memory pinning

tinyurl.com/tacc-csc-2023-omp

- Private variables

- Critical/atomic

- Single/master

- reduction

Advanced

- Hybrid

- SIMD

- Tasking

Setup

Parallel region

OMP NUM THREADS Forking/joining threads



Hints, Tricks and Tips for OpenMP development





OpenMP Version (Compliance)

Timers

Warm up

OMP_SCHEDULE

Programming style

omp_get... _num_thread(), _thread_num(), etc.



The Compliance Table



Specification and Technical Report	Compliance Version	_OPENMP (YYYYMM)
TR: Nov 2022	for 6.0	
Spec: Nov 2021	5.2	202111
Spec: Nov 2020	5.1	202011
Spec: Nov 2018	5.0	201811
Spec: Nov 2015	4.5	201511
Spec: Jul 2013	4.0	201307
Spec: Jul 2011	3.1	201107

Releases now occur at SuperComputing (in Nov).

Some compilers specify _OPENMP with a TR report --if they have early-adapter implementations

There are many earlier TRs.

If you don't memorize the table, see openmp.org/specifications where the Spec and TR links are specified with versions and dates.

See Cray man page intro_openmp (it has details about feature implementation)!



timers -- gettimeofday



Usually accurate to ns.
Call syntax may vary.
Fortran can easily call the C version

```
double gtod_secbase = 0.0E0;
double gtod_timer_() {
   struct timeval tv;
   double sec;
   gettimeofday(&tv, NULL);
// Always remove the LARGE sec value for improved accuracy
   if(gtod secbase == 0.0E0)
      gtod_secbase = (double)tv.tv sec;
   sec = (double)tv.tv sec - gtod secbase;
   return sec + 1.0E-06*(double)tv.tv usec;
```



timers -- time stamp counter (tsc)



Highly specific to HW (x86 below, with 2 32-bit registers)
Every Clock Period (CP) counter is updated.
Accuracy is about 20 CP!
But, to get seconds, use the "clock rate", most often just report CPs.

```
static __inline unsigned long long tsc(void){
  unsigned long a, d;
  unsigned long long d2;
   _asm__ __volatile__ ("rdtsc" : "=a" (a), "=d" (d));
                         read time stamp counter
  return (unsigned long long) a | (d2 << 32);</pre>
};
unsigned long long tsc timer(void){ return tsc(); }
unsigned long long tsc timer (void) { return tsc(); }
```



timers -- class timer



Collects time with a label – good for measuring multiple events. Easy to use and incorporate. Uses gettimeofday

```
#include "timer.hpp"
Timer timer;
timer.start("for loop: 1");
  for(...)...;
timer.stop()
timer.start("function: 2");
 fun();
timer.stop()
timer.print();
```

```
use mod timer
type(cls_timer) :: timer
call timer%start("do loop: 1")
   do i=1,N ...
call timer%stop
call timer%start("function: 2")
call foo2()
call timer%stop
call timer%print
```





OpenMP Version (Compliance)

Timers

Warm up

OMP_SCHEDULE

Programming style

omp_get... _num_thread(), _thread_num(), etc.



warm up



- It may take considerable time to get threads from the OS for the first parallel region
- When benchmarking, always request the threads first in a do-nothing parallel region, for doing timings.

```
#include <omp.h>
#pragma omp parallel
if(omp get num threads()<
   omp_get_thread_num()) exit(1);
timer.start("parallel loop: 1");
  #pragma omp parallel for
    for(...)...;
timer.stop()
timer.print();
```

```
use omp lib
!$omp parallel
 if( omp get num threads()< &
     omp get thread num() ) stop
 call timer%start("do loop: 1")
     !$omp parallel do
     do i=1,N ...
 call timer%stop
 call timer%print
```



OMP_SCHEDULE env. var.



• When evaluating performance, you can quickly change the schedule kind by setting the schedule clause to runtime and setting the OMP_SCHEDULE environment variable to the kind.





OpenMP Version (Compliance)

Timers

Warm up

OMP_SCHEDULE

Programming style

omp_get... _num_thread(), _thread_num(), etc.



Program styles



- Consistent style can help organize across program files/projects
- Remember, it will be read again by a person and the compiler
 Use a style that allows a reader to easily evaluate what you have done (and yourself 6 months later)
- Personal experience (KFM) for Fortran coders, for any non-trivial procedure use implicit none. (Also, in subroutines use omp_lib, only: omp_get... lets readers know what is used.)
- Sometimes, going outside the style box helps in reading and debugging code.

Which "style" is easier to read, understand the logic, and modify?

```
subroutine func2(A)
                                          subroutine func2(A)
   implicit none
                                             implicit none
   double precision
                      :: A(100,100)
                                             double precision
                                                                :: A(100,100)
   integer :: i1,i2,j1,j2
                                                                :: i1, i2, j1, j2
                                             integer
   do i1 = 1, 100, 4
                                             do i1 = 1, 100, 4
                  = j1, min(j1+15,100)
  end do: end do: end do: end do
                                             end do: end do; end do; end do
end subroutine
                                          end subroutine
```



OpenMP API routines



There are many API routines that can help you

* Threads and Teams: Count, number(ID), max -- getters and setters

* Target: Device count, number, Is Initial Device

* Parallel: In parallel region

* Memory allocation routines (host and device)

* Affinity Information – display and setters

Most are self descriptive:



Most are self descriptive:

omp_set_num_threads omp_get_num_threads omp_get_max_threads omp_get_thread_num omp in parallel

omp set schedule omp get schedule omp get thread limit omp get team size omp get proc bind

omp get num places omp get place num procs

omp set affinity format omp get affinity format omp display affinity omp capture affinity

omp get num teams omp get team num omp set num teams omp get max teams omp set teams thread limit omp get teams thread limit omp get num procs omp set default device omp get default device omp get num devices

omp get device num

omp is initial device

omp get initial device

omp target alloc omp target free omp_target_is_present omp_target_is_accessible omp_target_memcpy omp_target_memcpy_rect omp_target_memcpy_async omp_target_memcpy_rect_async omp target associate ptr omp_target_disassociate_ptr

omp init lock omp_init_lock_with_hint omp_init_nest_lock_with_hint omp destroy lock omp set lock omp unset lock omp test lock

omp_get_mapped_ptr

omp_get_wtime

omp get wtick omp init allocator omp destroy allocator omp set default allocator omp get default allocator omp_alloc omp_free omp_calloc omp realloc

.....NOT all included!



Program Information Displays



DISPLAY Environment Variable (EV) info
 export OMP_DISPLAY_ENV=TRUE | FALSE

Shows ICVs associated with the EVs after runtime evaluates EVs (or their defaults).

Use VERBOSE to show values of runtime variables that may be modified by vendor-specific.

*ICV = internal control variables associated with a data environment

API routine:



Program Information



_OPENMP: YYYYMM

Year & Month of Spec.

201511 – 4.5

201811 - 5.0

202011 - 5.1

202111 - 5.2

Some vendors are Technical Report compliant 202008 – TR9 202107 – TR10

202211 - TR11

```
OPENMP DISPLAY ENVIRONMENT BEGIN
OPENMP='202011'
[host] OMP_NUM_THREADS: value is not defined
[host] OMP_MAX_ACTIVE_LEVELS='1'
[host] OMP_SCHEDULE='static'
[host] OMP_STACKSIZE='4M'
[host] OMP_DISPLAY_AFFINITY='FALSE'
[host] OMP_AFFINITY_FORMAT='(null)'
[host] OMP_PLACES: value is not defined
[host] OMP_PROC_BIND: value is not defined
[host] OMP_TARGET_OFFLOAD=DEFAULT
[host] OMP_DEFAULT_DEVICE='0'
```

[host] OMP_ALLOCATOR='omp_default_mem_alloc'

[host] OMP_MAX_TASK_PRIORITY='0'

OPENMP DISPLAY ENVIRONMENT END

Not all ENV VARs shown. Order has been changed.

Program Information Displays



Display Affinity Info

ENV. VAR:

API routine:

export OMP_DISPLAY_AFFINITY=TRUE I FALSE omp_display_affinity(NULL) //CIC++ call omp_display_affinity("") / !! F90

Can put format string here.

Wall Clock Timer



- Every developer should have an easy why to evaluate performance for code optimization and changes
- Total time:

```
wrapper: /usr/bin/time -p./a.out
```

wrapped: date +%s

./a.out

date +%s #in secs.

\$ /usr/bin/time -p a.out real 5.00 user 4.50

\$ nstimer echo Hello World

- 002101725

0.01

```
$ date; ./a.out; date
1693573722
1693573727
```

Bash function nanosecond timer:

```
nstimer(){ t0=`date +%s.%N`; $*; t1=`date +%s.%N`; bc <<<"$t1 - $t0" ; }
```



thread number



- API routine: omp_get_thread_num()
- In normal programming used for task-parallel work assignment in a parallel region.
- Identifying threads is useful for (debugging):
 - ✓ Making sure multiple threads are executing tasks
 - ✓ Critical in resolving affinity problems
 - ✓ Resolving race conditions by slowing down one thread in a race.



New Terminology



primary thread

An OpenMP thread that has thread number 0. A primary thread may be an initial thread or the thread that encounters a parallel construct, creates a team, generates a set of implicit tasks, and then executes one of those tasks as thread number 0.

Example of Class Timer for C/C++/F90 codes

```
    See timer.hpp and timer.f90

#include "timer.hpp";
                               #include "timer.f90"
int main(){
                               program main
  Timer timer;
                                 use mod_timer
                                 type(cls_timer) :: timer
  timer.start("CPU:foo1");
                                 call timer%start("CPU:foo1")
                                 call foo1()
  foo1();
  timer.stop();
                                 call timer%stop
  timer.start("CPU:foo2");
                                 call timer%start("CPU:foo2")
  foo2();
                                 call foo2()
  timer.stop();
                                 call timer%stop
  timer.print();
                                 call timer%print
```



Output from Class Timer for C/C++/F90 codes

1.0e-06



• OUTPUT:

```
Action :: time/s Time resolution = 1e-06
-----
CPU:foo1 :: 1.9e-05
```

CPU:foo2 ::

Useful Unix Utils

TAC

- |& tee file for displaying stdout/err and saving to file
- Contributions welcome:



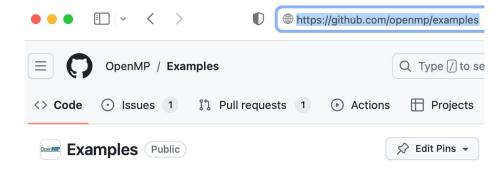
Remember how to get to these references



OpenMP References

https://www.openmp.org Look under Specifications
OpenMP API 5.2 Specification
OpenMP API 5.2.1 Examples
OpenMP API 5.2 Reference Guide

https://github.com/openmp/examples get example codes here







For Exercises, git clone

https://github.com/csc-training/advancedOpenMP.git

```
$ cd OpenMP_cpu
$ cd adv_intro
```

```
$ ls
1_env_apis
2_timers
3_private_if_clauses
```

```
README_dev_access.md
README.md
job_lumi_C
```