Parallel Programming with OpenMP

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Parallel Programming with OpenMP

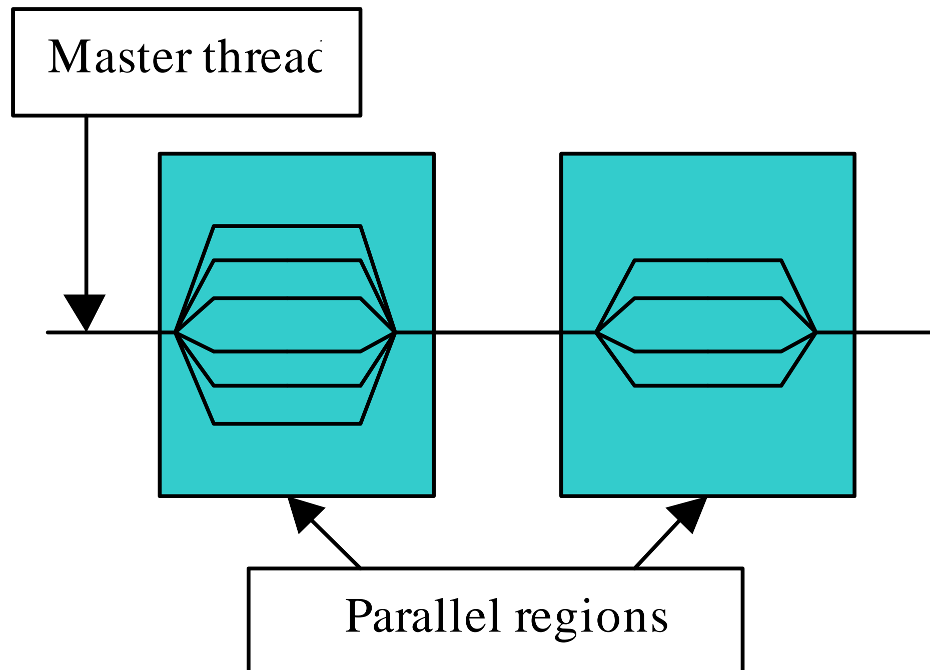
- Introduction
- The Basics of OpenMP
- Synchronization Constructs
- Some Advanced Features of OpenMP
- Debugging OpenMP Code
- Performance Tuning and OpenMP
- Other Sources of Information
- Problem Set

Introduction to OpenMP

- **OpenMP is an API for writing multi-threaded applications in a shared memory environment**
- **It consists of a set of compiler directives and library routines**
- **Relatively easy to create multi-threaded applications in Fortran, C, and C++**
- **Standardizes the last 15 or so years of SMP development and practice**
- **Currently supported by**
  - Hardware vendors
    - Cray, HP, IBM, Intel, SGI, Sun
  - Software tools vendors
    - Intel, PGI, Absoft
  - Applications vendors
    - ANSYS, Fluent, Oxford Molecular, NAG, Livermore Software, ...
- **Support is common and growing**

The OpenMP Programming Model

- A *master* thread spawns *teams* of threads as needed
- Parallelism is added incrementally; the serial program evolves into a parallel program



The OpenMP Programming Model

- **Programmer inserts OpenMP directives (Fortran comments, C `#pragmas`) at key locations in the source code**
- **Compiler interprets these directives and generates library calls to parallelize code regions**

Serial:

```
void main()
{
  double x[1000];
  for (int i=0; i<1000; i++)
   {
     big_calc(x[i]);
   }
}
```

Parallel:

```
void main()
{
  double x[1000];
#pragma omp parallel for
  for (int i=0; i<1000; i++)
   {
     big_calc(x[i]);
   }
}
```

Split up loop iterations among a team of threads

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The OpenMP Programming Model

- **Number of threads can be controlled from within the program, or by using the environment variable** `OMP_NUM_THREADS`
- **The programmer is responsible for managing synchronization and data dependencies!**
- **Compiling on OSC cluster systems:**

```
ifort -openmp prog.f
ifort -openmp prog.f90
icc -openmp prog.c
```

How Do Threads Interact?

- **Shared memory model**
  - Threads communicate by sharing variables.
- **Unintended sharing of data can lead to "race conditions"**
  - When the program's outcome changes as the threads are scheduled differently.
- **To control race conditions, use synchronization to avoid data conflicts**
- **Synchronization is expensive!**
  - Think about changing how data is organized, to minimize the need for synchronization.

Pros and Cons of OpenMP

Pros

- Very simple programming model
- Portable
- Can “mark up” a serial program to make it parallel

Cons

- Requires built-in support from compilers
- Requires shared memory
- Memory placement directives not part of the specification

The Basics of OpenMP

- General syntax rules
- The parallel region
- Execution modes
- OpenMP directive clauses
- Work-sharing constructs
- Combined parallel work-sharing constructs
- Environment variables
- Runtime environment routines
- Interlude: data dependencies

General Syntax Rules

- **Most OpenMP constructs are compiler directives or C `pragmas`**
  - For C and C++, `pragma`s take the form:

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

  - For Fortran, directives take one of the following forms:

```
c$omp construct [clause [clause]...]
!$omp construct [clause [clause]...]
*$omp construct [clause [clause]...]
```

- **Since these are essentially comments, compilers that don’t support OpenMP can still compile OpenMP programs (serially, of course!)**

General Syntax Rules (cont'd.)

- **Most OpenMP directives apply to structured blocks**
  - A block of code with one entry point at the top, and one exit point at the bottom. The only branches allowed are `STOP` statements in Fortran and `exit()` in C/C++.

```
c$omp parallel

10     wrk(id) = junk(id)
       res(id) = wrk(id)**2
       if (conv(res)) goto 10

c$omp end parallel

       print *, id
```

A structured block

```
c$omp parallel

10     wrk(id) = junk(id)
30     res(id) = wrk(id)**2
       if (conv(res)) goto 20
       goto 10

c$omp end parallel

       if (not_done) goto 30
20     print *, id
```

Not a structured block!

The Parallel Region

- **The fundamental construct that initiates parallel execution**
- **Fortran syntax:**

```
c$omp parallel
c$omp& shared(var1, var2, …)
c$omp& private(var1, var2, …)
c$omp& firstprivate(var1, var2, …)
c$omp& reduction(operator|intrinsic:var1, var2, …)
c$omp& if(expression)
c$omp& default(private|shared|none)

   a structured block of code

c$omp end parallel
```

The Parallel Region (cont'd.)

- **C/C++ syntax:**

```
#pragma omp parallel                            \
        private (var1, var2, …)                 \
        shared (var1, var2, …)                  \
        firstprivate(var1, var2, …)             \
        copyin(var1, var2, …)                   \
        reduction(operator:var1, var2, …)       \
        if(expression)                          \
        default(shared|none)                    \
{

   …a structured block of code…

}
```

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The Parallel Region (cont'd.)

- **The number of threads created upon entering the parallel region is controlled by the value of the environment variable** `OMP_NUM_THREADS`
  - Can also be controlled by a function call from within the program.
- **Each thread executes the block of code enclosed in the parallel region**
- **In general, there is no synchronization between threads in the parallel region!**
  - Different threads reach particular statements at unpredictable times.
- **When all threads reach the end of the parallel region, all but the master thread go out of existence and the master continues alone**

The Parallel Region (cont'd.)

- **Each thread has a thread number, which is an integer from `0` (the master thread) to the number of threads minus one**
  - Can be determined by a call to **`omp_get_thread_num().`**
- **Threads can execute different paths of statements in the parallel region**
  - Typically achieved by branching on the thread number:

```
#pragma omp parallel
{
   myid = omp_get_thread_num();
   if (myid == 0)
     do_something();
   else
      do_something_else(myid);
}
```

Parallel Regions: Execution Modes

- Dynamic mode (the default)
  - The number of threads used in a parallel region can vary, under control of the operating system, from one parallel region to the next.
  - Setting the number of threads just sets the *maximum* number of threads; you might get fewer!
- Static mode
  - The number of threads is fixed by the programmer; you must always get this many (or else fail to run).
- **Parallel regions may be nested, but a compiler may choose to "serialize" the inner parallel region, i.e., run it on a single thread**
- **Execution mode is controlled by**
  - The environment variable **`OMP_DYNAMIC`.**
  - The OMP function **`omp_set_dynamic()`.**

OpenMP Directive Clauses

- `shared(var1,var2,…)`
  - Variables to be shared among all threads (threads access same memory locations).
- `private(var1,var2,…)`
  - Each thread has its own copy of the variables for the duration of the parallel code.
- `firstprivate(var1,var2,…)`
  - Private variables that are initialized when parallel code is entered.
- `lastprivate(var1,var2,…)`
  - Private variables that save their values at the last (serial) iteration.
- `if(expression)`
  - Only parallelize if `expression` is true.
- `default(shared|private|none)`
  - Specifies default scoping for variables in parallel code.
- `schedule(type [,chunk])`
  - Controls how loop iterations are distributed among threads.
- `reduction(operator|intrinsic:var1,var2…)`
  - Ensures that a reduction operation (e.g., a global sum) is performed safely.

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The `private`, `default`, and `if` Clauses

private & default

```
c$omp  parallel shared(a)
c$omp& private(myid,x)
      myid=omp_get_thread_num()
      x = work(myid)
      if (x < 1.0) then
        a(myid) = x
      end if
c$omp end parallel
```

Equivalent is:

```
c$omp parallel do default(private)
c$omp& shared(a)
      …
```

- **Each thread has its own private copy of `x` and `myid`**
- **Unless `x` is made private, its value is indeterminate during parallel operation**
- **Values for private variables are undefined at beginning and end of the parallel region!**
- **`default` clause automatically makes `x` and `myid` private**

if(expression)

- **Don't want to parallelize a loop if the overhead outweighs the speedup**

```
c$omp parallel do if(n.ge.2000)
      do i = 1, n
        a(i) = b(i)*c + d(i)
      enddo
```

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firstprivate

- **Variables are private (local to each thread), but are initialized to the value in the preceding serial code**

```
program first
  integer :: myid,c
  integer,external :: omp_get_thread_num
  c=98
!$omp parallel private(myid)
!$omp& firstprivate(c)
  myid=omp_get_thread_num()
  write(6,*) 'T:',myid,' c=',c
!$omp end parallel
end program first
-----------------------------------
T:1 c=98
T:3 c=98
T:2 c=98
T:0 c=98
```

- **Each thread has a private copy of `c`, initialized with the value 98**

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OpenMP Work-Sharing Constructs

- Parallel `for/DO`
- Parallel `sections`
- `single` directive
- Placed inside parallel regions
- Distribute the execution of associated statements among existing threads
  - No *new* threads are created.
- No implied synchronization between threads at the start of the work-sharing construct!

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OpenMP Work-Sharing Constructs - `for`/`DO`

- **Distribute iterations of the immediately following loop among threads in a team**

```
#pragma omp parallel shared(a,b) private(j)
{
   #pragma omp for
     for (j=0; j<N; j++)
        a[j] = a[j] + b[j];
}
```

- **By default there is a barrier at the end of the loop**
  - Threads wait until all are finished, then proceed.
  - Use the **`nowait`** clause to allow threads to continue without waiting.

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Detailed Syntax - `for`

```
#pragma omp for [clause [clause]…]
    for loop
```

where each `clause` is one of

- `private(`*`list`*`).`
- `firstprivate(`*`list`*`).`
- `lastprivate(`*`list`*`).`
- `reduction(`*`operator: list`*`).`
- `ordered.`
- `schedule(`*`kind [, chunk_size]`*`).`
- `nowait.`

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Detailed Syntax - DO

```
c$omp do [clause [clause]…]
    do loop
[c$omp end do [nowait]]
```

where each `clause` is one of

- `private(`*`list`*`).`
- `firstprivate(`*`list`*`).`
- `lastprivate(`*`list`*`).`
- `reduction(`*`operator: list`*`).`
- `ordered.`
- `schedule(`*`kind [, chunk_size]`*`).`

- **For Fortran 90, use `!$OMP` and F90-style line continuation**

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lastprivate

- **Like `private` within the parallel construct - each thread has its own copy**
- **The value corresponding to the last iteration of the loop (in serial mode) is saved following the parallel construct**

```
c$omp  do shared(x)
c$omp& lastprivate(i)
      do i = 1, N
        x(i)=a
      enddo

      n = i
```

- **When the loop is finished, `i` is saved as the value corresponding to the last iteration in serial mode (i.e., `n=N+1`)**
- **If `i` is declared `private` instead, the value of `n` is undefined!**

`reduction(operator|intrinsic:var1[,var2])`

- **Allows safe global calculation or comparison**
- **A private copy of each listed variable is created and initialized depending on `operator` or `intrinsic` (e.g., `0` or `+`)**
- **Partial sums and local `mins` are determined by the threads in parallel**
- **Partial sums are added together from one thread at a time to get global sum**
- **Local `mins` are compared from one thread at a time to get `gmin`**

```
c$omp do shared(x) private(i)
c$omp&  reduction(+:sum)
      do i = 1, N
         sum = sum + x(i)
      enddo
```

```
c$omp do shared(x) private(i)
c$omp&  reduction(min:gmin)
      do i = 1,N
         gmin =
min(gmin,x(i))
      end do
```

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`reduction(operator|intrinsic:var1[,var2])`

- **Listed variables must be `shared` in the enclosing parallel context**
- **In Fortran**
  - `operator` can be `+`, `*`, `-`, `.and.`, `.or.`, `.eqv.`, `.neqv.`
  - `intrinsic` can be `max`, `min`, `iand`, `ior`, `ieor`.
- **In C**
  - `operator` can be `+`, `*`, `-`, `&`, `^`, `|`, `&&`, `||`.
  - pointers and reference variables are not allowed in reductions!

OpenMP Work-Sharing Constructs - sections

```
c$omp parallel
c$omp sections

c$omp section
      call computeXpart()
c$omp section
      call computeYpart()
c$omp section
      call computeZpart()

c$omp end sections
c$omp end parallel
      call sum()
```

- **Each parallel `section` is run on a separate thread**
- **Allows functional decomposition**
- **Implicit barrier at the end of the sections construct**
  - Use the `nowait` clause to suppress this.

OpenMP Work-Sharing Constructs - `sections`

- **Fortran syntax:**

```
c$omp sections [clause[,clause]...]
c$omp section
      code block
[c$omp section
      another code block
[c$omp section
      …]]
c$omp end sections [nowait]
```

- **Valid clauses:**
  - `private(`*`list`*`).`
  - `firstprivate(`*`list`*`).`
  - `lastprivate(`*`list`*`).`
  - `reduction(`*`operator|intrinsic:list`*`).`

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OpenMP Work-Sharing Constructs - `sections`

- **C syntax:**

```
#pragma omp sections [clause [clause...]]
{
   #pragma omp section
      structured block
  [#pragma omp section
      structured block
   …]
}
```

- **Valid clauses:**
  - `private(list).`
  - `firstprivate(list).`
  - `lastprivate(list).`
  - `reduction(operator:list).`
  - `nowait.`

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OpenMP Work-Sharing Constructs - `single`

- Ensures that a code block is executed by only one thread in a parallel region
- The thread that reaches the `single` directive first is the one that executes the `single` block
- Equivalent to a `sections` directive with a single section - but a more descriptive syntax
- All threads in the parallel region must encounter the single directive
- Unless `nowait` is specified, all non-involved threads wait at the end of the `single` block

```
c$omp parallel private(i)
shared(a)
c$omp do
      do i = 1, n
        …work on a(i) …
      enddo

c$omp single
   … process result of do …
c$omp end single

c$omp do
      do i = 1, n
      … more work …
    enddo
c$omp end parallel
```

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OpenMP Work-Sharing Constructs - `single`

- **Fortran syntax:**

```
c$omp single [clause [clause…]]
      structured block
c$omp end single [nowait]
```

where `clause` is one of

- `private(list)`.
- `firstprivate(list)`.

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OpenMP Work-Sharing Constructs - `single`

- **C syntax:**

```
#pragma omp single [clause [clause…]]
      structured block
```

where `clause` is one of

- `private(list)`.
- `firstprivate(list)`.
- `nowait`.

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Combined Parallel Work-Sharing Constructs

- **Short cuts for specifying a parallel region that contains only one work-sharing construct (a parallel `for`/`DO` or parallel `sections`)**
- **Semantically equivalent to declaring a parallel section followed immediately by the relevant work-sharing construct**
- **All clauses valid for a parallel section and for the relevant work-sharing construct are allowed, except `nowait`**
  - The end of a parallel section contains an implicit barrier anyway.

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Parallel DO/for Directive

```
c$omp parallel do [clause [clause…]]
      do loop
[c$omp end parallel do]
```

```
#pragma omp parallel for [clause [clause…]]
        for loop
```

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Parallel sections Directive

```
c$omp parallel sections [clause [clause…]]
[c$omp section]
        structured block
[c$omp section
        structured block]
…
c$omp end parallel sections
```

```
#pragma omp parallel sections [clause [clause…]]
{
    [#pragma omp section]
        structured block
    [#pragma omp section
        structured block
     …]
}
```

OpenMP Environment Variables

- **`OMP_NUM_THREADS`**
  - Sets the number of threads requested for parallel regions.
- **`OMP_SCHEDULE`**
  - Set to a string value that controls parallel loop scheduling at runtime.
  - Only loops that have schedule type `RUNTIME` are affected.
- **`OMP_DYNAMIC`**
  - Enables or disables dynamic adjustment of the number of threads actually used in a parallel region (due to system load).
  - Default value is implementation-dependent.
- **`OMP_NESTED`**
  - Enables or disables nested parallelism.
  - Default value is `FALSE` (nesting disabled).

OpenMP Environment Variables

- **Examples:**

```
[ipf-login1]$ export OMP_NUM_THREADS=16

[ipf-login1]% setenv OMP_SCHEDULE “guided,4”

[ipf-login1]$ export OMP_DYNAMIC=false

[ipf-login1]% setenv OMP_NESTED TRUE
```

Note: values are case-insensitive!

OpenMP Runtime Environment Routines

- **`(void) omp_set_num_threads(int *num_threads*)`**
  - Sets the number of threads to be requested for subsequent parallel regions.
- **`int omp_get_num_threads()`**
  - Returns the number of threads currently in the team.
- **`int omp_get_max_threads()`**
  - Returns the maximum value that may be returned by `omp_get_num_threads()`.
  - Generally used to allocate data structures that have a maximum size per thread when `OMP_DYNAMIC` is set to `TRUE`.
- **`int omp_get_thread_num()`**
  - Returns the thread number, an integer from `0` to the number of threads minus `1`.
- **`int omp_get_num_procs()`**
  - Returns the number of physical processors available to the program.

OpenMP Runtime Environment Routines

- **`(int/logical) omp_in_parallel()`**
  - Returns "true" (logical `.TRUE.` in Fortran; a non-zero integer in C) if called from a parallel region, "false" (logical `.FALSE.` in Fortran, 0 in C) otherwise.
- **`(void) omp_set_dynamic(`*`expr`*`)`**
  - Enables (*`expr`* is "true") or disables (*`expr`* is "false") dynamic thread allocation.
- **`(int/logical) omp_get_dynamic()`**
  - Returns "true" or "false" if dynamic thread allocation is enabled/disabled, respectively.
- **`void omp_set_nested(int/logical `*`expr`*`)`**
  - Enables (*`expr`* is "true") or disables (*`expr`* is "false") nested parallelism.
- **`(int/logical) omp_get_nested()`**
  - Returns "true" or "false" if nested parallelism is enabled/disabled, respectively.

OpenMP Runtime Environment Routines

- **In Fortran, routines that return a value (integer or logical) are functions, while those that set a value (i.e., take an argument) are subroutines**
- **In Fortran, functions must be declared as the appropriate datatype**
- **In C, be sure to** `#include <omp.h>`
- **Changes to the environment made by function calls have precedence over the corresponding environment variables**
  - For example, a call to **`omp_set_num_threads()`** overrides any value that **`OMP_NUM_THREADS`** may have.

Interlude: Data Dependencies

- In order for a loop to parallelize, the work done in one loop iteration cannot depend on the work done in any other iteration
- In other words, the order of execution of loop iterations must be irrelevant
- Loops with this property are called data independent
- Some data dependencies may be broken by changing the code

Data Dependencies (cont'd.)

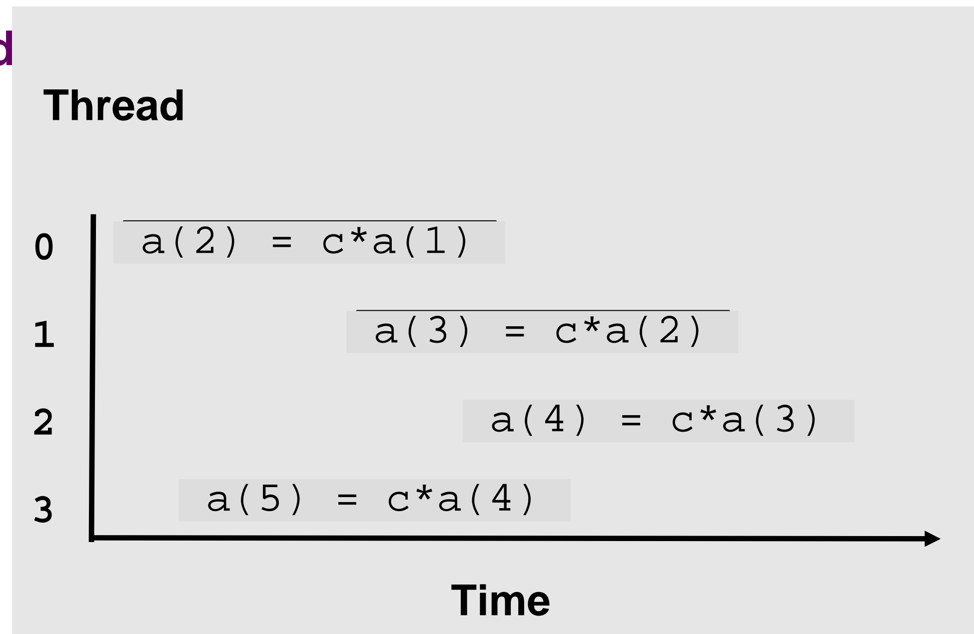
- **Only variables that are written in one iteration and read in another iteration will create data dependencies**
- **A variable cannot create a dependency unless it is shared**
- **Often data dependencies are difficult to identify. Compiler tools can help by identifying the dependencies automatically**

Is there a dependency here?

```
do i = 2,N,2
 a(i) = c*a(i-1)
enddo
```

Recurrence:

```
do i = 2,5
     a(i) = c*a(i-1)
enddo
```



Data Dependencies (cont'd.)

- **Unless declared as `private`, a temporary variable may be shared and will cause a data dependency**

Function Calls

```
do i = 1,n
  call myroutine(a,b,c,i)
enddo

subroutine myroutine(a,b,c,i)
…
a(i) = 0.3 * (a(i-1)+b(i)+c)
…
return
```

Temporary Variable Dependency

```
do i = 1,n
    x = cos(a(i))
    b(i) = sqrt(x * c)
enddo
```

- **In general, loops containing function calls can be parallelized**
- **The programmer must make certain that the function or subroutine contains no dependencies or other side effects**
- **In Fortran, make sure there are no `static` variables in the called routine**
- **Intrinsic functions are safe**

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Data Dependencies (cont'd.)

- **Similar to the temporary variable dependency, a reduction dependency is eliminated simply by using the `reduction` clause to the `parallel do` directive**

Reductions

```
do i = 1,n
 xsum = xsum + a(i)
 xmul = xmul * a(i)
 xmax = max(xmax,a(i))
 xmin = min(xmin,a(i))
enddo
```

Indirect Indexing

```
do i = 1,n
  a(i) = c * a(idx(i))
enddo

do i = 1,n
  a(ndx(i)) = b(i)+c (i)
enddo
```

- **If `idx(i)` not equal to `i` on every iteration, then there is a dependency**
- **If `ndx(i)` ever repeats itself, there is a dependency**

Data Dependencies (cont'd.)

- **Loops with conditional exits should not be parallelized. Requires ordered execution**

Conditional Loop Exit

```
do i = 1,n
    a(i) = b(i) + c(i)
    if (a(i).gt.amax) then
      a(i) = amax
      goto 100
    endif
enddo

100 continue
```

Nested Loop Order

```
do k = 1, n
 do j = 1, n
  do i = 1, n
   a(i,j)=a(i,j)+b(i,k)*c(k,j)
  enddo
 enddo
enddo
```

- **If the `k`-loop is parallelized, then there is a dependency related to `a(i,j)`**
- **This can be fixed by making the `k`-loop the innermost loop**

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Minimizing the Cost of a Recurrence

- Move the dependency into a separate loop
- Parallelize the loop without the dependency
- Make sure benefits outweigh the cost of loop overhead

```
do i = 1, NHUGE
   a(i) = ...lots of math...
 &        + a(i-1)
   enddo
```

```
c
c   Parallel Loop
c
c$omp  parallel do shared(junk)
c$omp& private(i)
      do i = 1, NHUGE
       junk(i) = ...lots of math...
      enddo

c
c   Serial Loop
c
       do i = 1, NHUGE
         a(i) = junk(i) + a(i-1)
       enddo
```

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Loop Nest Parallelization Possibilities

All examples shown run on 8 threads with `schedule(static)`

- **Parallelize the outer loop:**

```
!$omp parallel do private(i,j) shared(a)
      do i=1,16
        do j=1,16
          a(i,j) = i+j
        enddo
      enddo
```

- **Each thread gets two values of `i` (T0 gets `i`=1,2; T1 gets `i`=3,4, etc.) and *all* values of `j`**

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Loop Nest Parallelization Possibilities

- **Parallelize the inner loop:**

```
      do i=1,16
!$omp parallel do private(j) shared(a,i)
        do j=1,16
          a(i,j) = i+j
        enddo
      enddo
```

- **Each thread gets two values of `j` (T0 gets `j`=1,2; T1 gets `j`=3,4, etc.) and *all* values of `i`**

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OpenMP Synchronization Constructs

- `critical`
- `atomic`
- `barrier`
- `master`
- `ordered`
- `flush`

OpenMP Synchronization - `critical` Section

Ensures that a code block is executed by only one thread at a time in a parallel region

- **Syntax:**

```
#pragma omp critical [(name)]
        structured block
```

```
!$omp critical [(name)]
      structured block
!$omp end critical [(name)]
```

- **When one thread is in the critical region, the others wait until the thread inside exits the critical section**
- ***name* identifies the critical region**
- **Multiple critical sections are independent of one another unless they use the same name**
- **All unnamed critical regions are considered to have the same identity**

OpenMP Synchronization - `critical` Section Example

```
integer :: cnt1, cnt2

c$omp parallel private(i)
c$omp& shared(cnt1,cnt2)

c$omp do
   do i = 1, n
      …do work…
      if(condition1)then
c$omp critical (name1)
         cnt1 = cnt1+1
c$omp end critical (name1)
      else
c$omp critical (name1)
         cnt1 = cnt1-1
c$omp end critical (name1)
      endif
      if(condition2)then
c$omp critical (name2)
         cnt2 =cnt2+1
c$omp end critical (name2)
      endif
   enddo
c$omp end parallel
```

OpenMP - `critical` Section Problem

Is this correct?

```
…
c$omp parallel do
      do i = 1,n
        if (a(i).gt.xmax) then
c$omp critical
        xmax = a(i)
c$omp end critical
        endif
      enddo
…
```

What about this?

```
…
c$omp parallel do
      do i = 1,n
c$omp critical
        if (a(i).gt.xmax) then
          xmax = a(i)
        endif
c$omp end critical
      enddo
…
```

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OpenMP Synchronization - `atomic` Update

Prevents a thread that is in the process of (1) accessing, (2) changing, and (3) restoring values in a shared memory location from being interrupted at any stage by another thread

- Syntax:

```
#pragma omp atomic
        statement
```

```
!$omp atomic
      statement
```

- Alternative to using the `reduction` clause (it applies to same kinds of expressions)
- Directive in effect only for the code statement immediately following it

OpenMP Synchronization - `atomic` Update

```
integer, dimension(8) :: a,index
data index/1,1,2,3,1,4,1,5/

c$omp parallel private(i),shared(a,index)
c$omp do
  do i = 1, 8
c$omp  atomic
    a(index(I)) = a(index(I)) + index(I)
  enddo
c$omp end parallel
```

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OpenMP Synchronization - `barrier`

Causes threads to stop until all threads have reached the barrier

- Syntax:

```
!$omp barrier
```

```
#pragma omp barrier
```

- A red light until all threads arrive, then it turns green
- Example:

```
c$omp parallel
c$omp do
      do i = 1, N
        <assignment>
c$omp barrier
        <dependent work>
      enddo
c$omp end parallel
```

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OpenMP Synchronization - `master` Region

Code in a `master` region is executed only by the master thread

- **Syntax:**

```
#pragma omp master
        structured block
```

```
!$omp master
        structured block
!$omp end master
```

- **Other threads skip over entire master region (no implicit barrier!)**

OpenMP Synchronization - `master` Region

```
!$omp parallel shared(c,scale) &
!$omp private(j,myid)
      myid=omp_get_thread_num()
!$omp master
   print *,'T:',myid,' enter scale'
   read *,scale
!$omp end master
!$omp barrier
!$omp do
   do j = 1, N
      c(j) = scale * c(j)
   enddo
!$omp end do
!$omp end parallel
```

OpenMP Synchronization - `ordered` Region

Within an `ordered` region, loop iterations are forced to be executed in sequential order

- **Syntax:**

```
c$omp ordered
      structured block
c$omp end ordered
```

```
#pragma omp ordered
      structured block
```

- **An `ordered` region can appear only in a parallel loop**
- **The parallel loop directive must contain the `ordered` clause (new)**
- **Threads enter the ordered region one at a time**

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OpenMP Synchronization - `ordered` Region

```
  integer, external :: omp_get_thread_num
  call omp_set_num_threads(4)
c$omp parallel private(myid)
  myid=omp_get_thread_num()
c$omp do private(i) ordered
  do i = 1, 8
c$omp ordered
     print *,'T:',myid,' i=',i
c$omp end ordered
  enddo
c$omp end parallel
--------------------
T:0 i=1
T:0 i=2
T:1 i=3
T:1 i=4
T:2 i=5
T:2 i=6
T:3 i=7
T:3 i=8
```

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OpenMP Synchronization - `flush` Directive

Causes the present value of the named shared variable to be immediately written back ("flushed") to memory

- Syntax:

```
c$omp flush(var1[,var2]…)
```

```
#pragma omp flush(var1[,var2]…)
```

- Enables signaling between threads by using a shared variable as a semaphore
- When other threads see that the shared variable has been changed, they know that an event has occurred and proceed accordingly

Sample Program: `flush` Directive

```
program flush
  integer, parameter :: M=1600000
  integer, dimension(M) :: c
  integer :: stop,sum,tid
  integer, dimension(0:1) :: done
  integer, external :: omp_get_thread_num

  call omp_set_num_threads(2)
  c=1
  c(345)=9
!$omp parallel default(private) shared(done,c,stop)
  tid=omp_get_thread_num()
  done(tid)=0
  if(tid==0) then
     neigh=1
  else
     neigh=0
  end if
!$omp barrier
```

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Sample Program: `flush` Directive (cont'd.)

```
 if (tid==0) then
     do j=1,M
        if(c(j)==9) stop=j
     end do
  end if
  done(tid)=1

!$omp flush(done)
  do while(done(neigh).eq.0)
!$omp flush(done)

  end do

  if (tid==1) then
     sum=0
     do j=1,stop-1
        sum=sum+c(j)
     end do
  end if
!$omp end parallel

end program flush
```

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Debugging OpenMP Code

- **Shared memory parallel programming opens up a range of new programming errors arising from unanticipated conflicts between shared resources**
- **Race Conditions**
  - When the outcome of a program depends on the detailed timing of the threads in the team.
- **Deadlock**
  - When threads hang while waiting for a locked resource that will never become available.

Examples: Race Conditions

```
c$omp parallel sections
      A = B + C
c$omp section
      B = A + C
c$omp section
      C = B + A
c$omp end parallel sections
```

- **The result varies unpredictably, depending on the order in which threads execute the sections**
- **Wrong answers are produced without warning!**

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Examples: Race Conditions

```
c$omp parallel shared(x) private(tmp)
        id = omp_get_thread_num()
c$omp do reduction(+:x)
    do j=1,100
        tmp = work(j)
            x = x + tmp
    enddo
c$omp end do nowait
    y(id) = work(x,id)
c$omp end parallel
```

The result varies unpredictably because the value of `x` isn't correct until the barrier at the end of the `do` loop is reached

- Wrong answers are produced without warning!
- Be careful when using `nowait`!

Examples: Race Conditions

```
   real :: tmp,x
c$omp parallel do reduction(+:x)
   do j=1,100
      tmp = work(j)
      x = x + tmp
   enddo
c$omp end do
   y(id) = work(x,id)
```

- **The result varies unpredictably because access to the shared variable `tmp` is not protected**
- **Wrong answers are produced without warning!**
- **Probably want to make `tmp` private**

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Examples: Deadlock

```
        call OMP_INIT_LOCK(lcka)
        call OMP_INIT_LOCK(lckb)
c$omp parallel sections
        call OMP_SET_LOCK(lcka)
        call OMP_SET_LOCK(lckb)
        call useAandB(res)
        call OMP_UNSET_LOCK(lckb)
        call OMP_UNSET_LOCK(lcka)
c$omp section
        call OMP_SET_LOCK(lckb)
        call OMP_SET_LOCK(lcka)
        call useBandA(res)
        call OMP_UNSET_LOCK(lcka)
        call OMP_UNSET_LOCK(lckb)
c$omp end parallel sections
```

- **If A is locked by one thread and B by another, you have deadlock**
- **If both are locked by the same thread, you have a race condition!**
- **Avoid nesting different locks**

Examples: Deadlock

```
          call OMP_INIT_LOCK(lcka)
c$omp parallel sections
          call OMP_SET_LOCK(lcka)
          ival = work()
          if (ival.eq.tol) then
            call OMP_UNSET_LOCK(lcka)
          else
            call error(ival)
          endif
c$omp section
          call OMP_SET_LOCK(lcka)
          call useBandA(res)
          call OMP_UNSET_LOCK(lcka)
c$omp end parallel sections
```

- **If A is locked in the first section and the `if` statement branches around the unset lock, then threads in the other section will deadlock waiting for the lock to be released**
- **Make sure you release your locks!**

Other Danger Zones

- **Are the libraries you are using thread-safe?**
  - Standard libraries should always be okay.
- **I/O inside a parallel region can interleave unpredictably**
- **`private` variables can mask globals**
- **Understand when shared memory is coherent**
  - When in doubt, use `FLUSH`.
- **`NOWAIT` removes implicit barriers**

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Performance Tuning and OpenMP

- Basic strategies
- Automatic parallelization
- Example 1
- Example 2
- The memory hierarchy
- Cache locality
- Data locality

Basic Strategies

- **If possible, use auto-parallelizing compiler as a first step**
- **Use profiling to identify time-consuming code sections (loops)**
- **Add OpenMP directives to parallelize the most important loops**
- **If a parallelized loop does not perform well, check for/consider**
  - Parallel startup costs.
  - Small loops.
  - Load imbalances.
  - Many references to shared variables.
  - Low cache affinity.
  - Unnecessary synchronization.
  - Costly remote memory references (in NUMA machines).

Automatic Parallelization

- Most widely used languages often have compilers that will automatically parallelize your code
- The compiler stage that performs this is called the Automatic Parallelizer (AP)
- The AP will insert OpenMP directives into your code if a loop can be parallelized. If not, it will tell you why
- "Safe" parallel optimization implies there are no dependencies
- Only loops can be parallelized automatically
- Should be considered, at best, as a first step toward getting your code parallelized
- The next step should be inserting your own directives, and tuning the various parallel sections for optimum performance

Strategy for Using Auto-Parallelization

- **Run AP on source files, and examine the listing**
  - Convenient to break code up into separate source files (use `fsplit(1)` and `make(1)`).
- **For loops that don't automatically parallelize, try to eliminate inhibiting dependencies by modifying the source code**
- **Use the listing to implement parallelization by hand using OpenMP directives**
- **Stop when you are satisfied with performance**

Performance Tuning: Example 1

- **Original code:**

```
c1 = x(1)>0
c2 = x(1:10)>0

DO i=1,n
   DO j=i,n
      if (c1) then r(1:100) = …
    …
      if (c2) then … = r(1:100)
      sum(j) = sum(j) + …
   ENDDO
ENDDO
```

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Example 1 (cont'd.)

- **First, parallelize the loop**
  - Prefer to parallelize the outer loop - higher iteration count.
  - Note `c2` is never true unless `c1` is also true - can make `r` private!
  - Also parallelize the reduction.
- **But, the loop is "triangular"! By default, iterations may be unbalanced between processors**
  - Use the `schedule` clause to enforce more efficient load balancing.

Example 1 - Parallel Version

```
c1 = x(1)>0
c2 = x(1:10)>0
ALLOCATE(xsum(1:nprocs,n))

c$omp  parallel do private(i,j,r,myid)
c$omp& schedule(static,1)
DO i=1,n
   myid = omp_get_thread_num()
   DO j=i,n
      if (c1) then r(1:100) = …
    …
      if (c2) then … = r(1:100)
      xsum(myid,j) = sum(myid,j) + …
   ENDDO
ENDDO

c$omp parallel do
DO i=1,n
   sum(i) = sum(i) + xsum(1:nprocs,i)
ENDDO
```

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Performance Tuning: Example 2

- **Increasing parallel loop granularity using the `nowait` clause:**

```
!$omp parallel private(ld1,ld2,ldi,j,ld,k)
    do k = 2,ku-2
!$omp do
       do j = jlo, jhi
        ld2 = a(j,k)
        ld1 = b(j,k)+ld2*x(j,k-2)
        ld  = c(j,k)+ld1*x(j,k-1)+ld2*y(j,k-1)
        ldi = 1./ld
        f(j,k,1) = ldi*(f(j,k,1)-f(j,k-2,1)*ld2
        f(j,k,1) = ldi*(f(j,k,2)-f(j,k-2,2)*ld1
        x(j,k) = ldi*(d(j,k)-y(j,k-1)*ld1
        y(j,k) = e(j,k)*ld
        enddo
!$omp end do nowait
    end do
!$omp end parallel
```

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The Memory Hierarchy

- **Most parallel systems are built from CPUs with a memory hierarchy**
  - Registers.
  - Primary (L1) cache.
  - Secondary (L2) cache.
  - Additional levels of cache.
  - Local memory.
  - Remote memory - accessed through the interconnect network.
- **As you move down this list, the time to retrieve data increases by about an order of magnitude for each step!**
- **Therefore:**
  - Make efficient use of local memory (caches).
  - Minimize remote memory references.

Performance Tuning - Cache Locality

- **The basic rule for efficient use of local memory (caches):**

  Use a memory stride of one

- **This means array elements are accessed in the same order they are stored in memory**
- **Fortran: “Column-major” order**
  - Want the leftmost index in a multi-dimensional array varying most rapidly in a loop.
- **C: “Row-major” order**
  - Want rightmost index in a multi-dimensional array varying most rapidly in a loop.
- **Interchange nested loops if necessary (and possible!) to achieve the preferred order**

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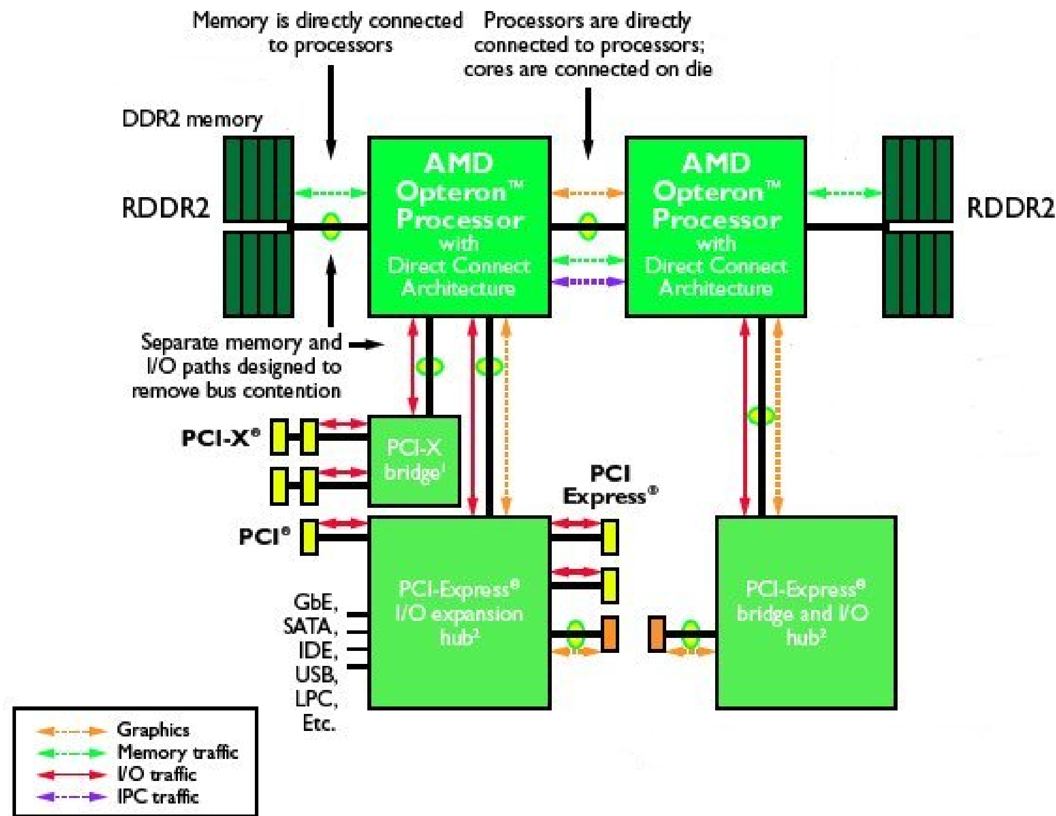
Performance Tuning - Data Locality

- **On NUMA ("non-uniform memory access") platforms, it may be important to know**
  - Where threads are running.
  - What data is in their local memories.
  - The cost of remote memory references.
- **OpenMP itself provides no mechanisms for controlling**
  - The binding of threads to particular processors.
  - The placement of data in particular memories.
- **OpenMP was designed with true SMP (i.e., UMA) in mind**
  - For NUMA, the possibilities are many and highly machine-dependent.
  - NUMA machines are becoming increasingly common.
- **Often there are system-specific mechanisms for addressing these problems**
  - Additional directives for data placement.
  - Ways to control where individual threads are running.

NUMA Architectures: AMD Opteron Dual Socket



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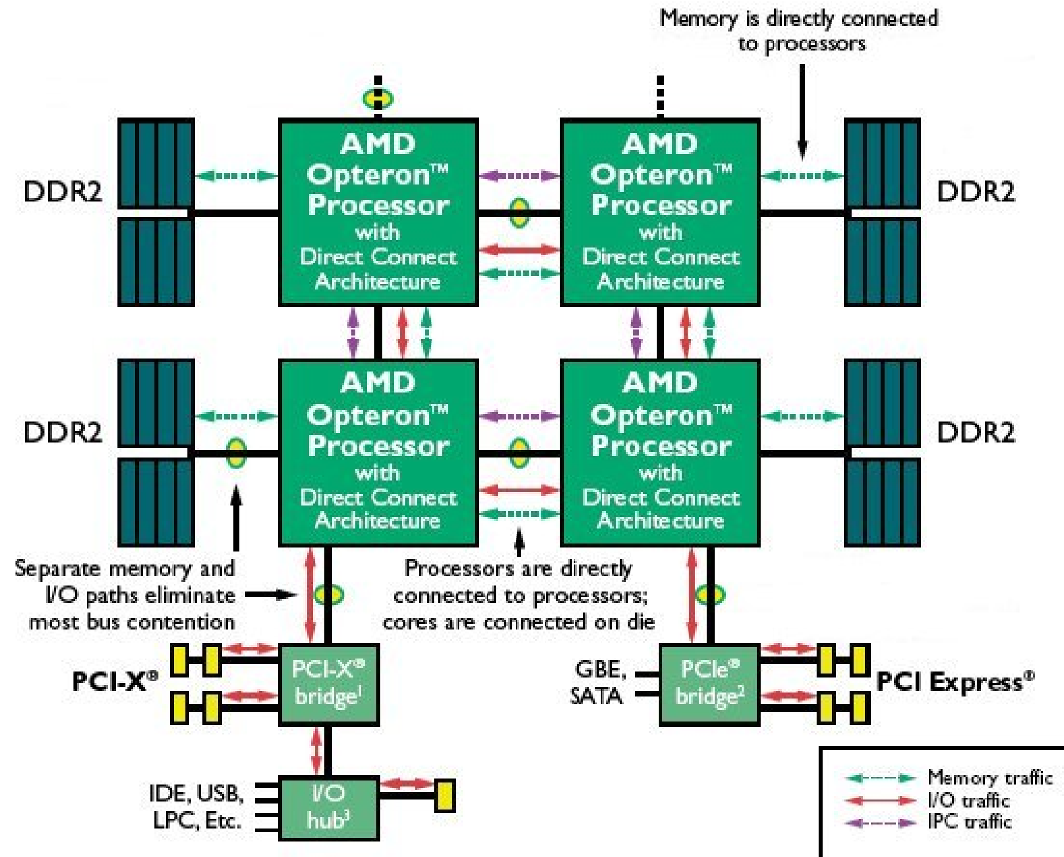
NUMA Architectures: AMD Opteron Quad Socket



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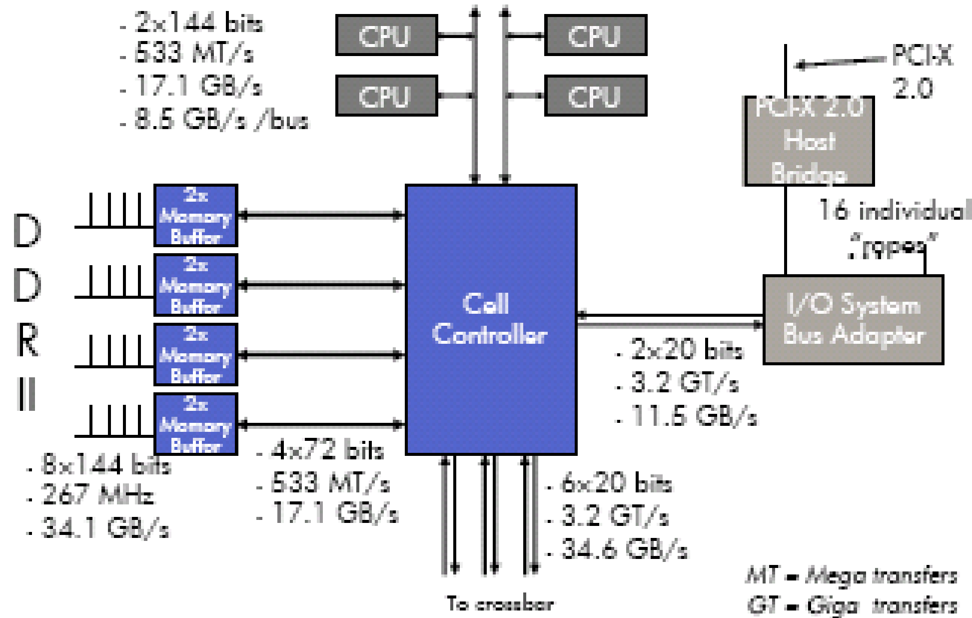
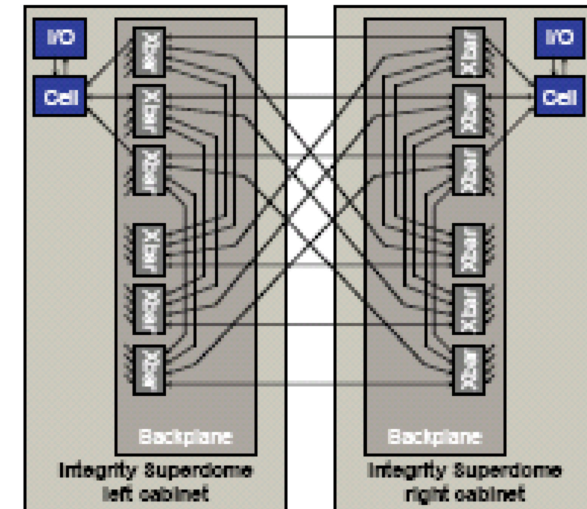
NUMA Architectures: HP Superdome sx2000





From *Meet the HP Integrity Superdome Server with the HP Super-Scalable Processor Chipset sx2000*, HP, 2006.

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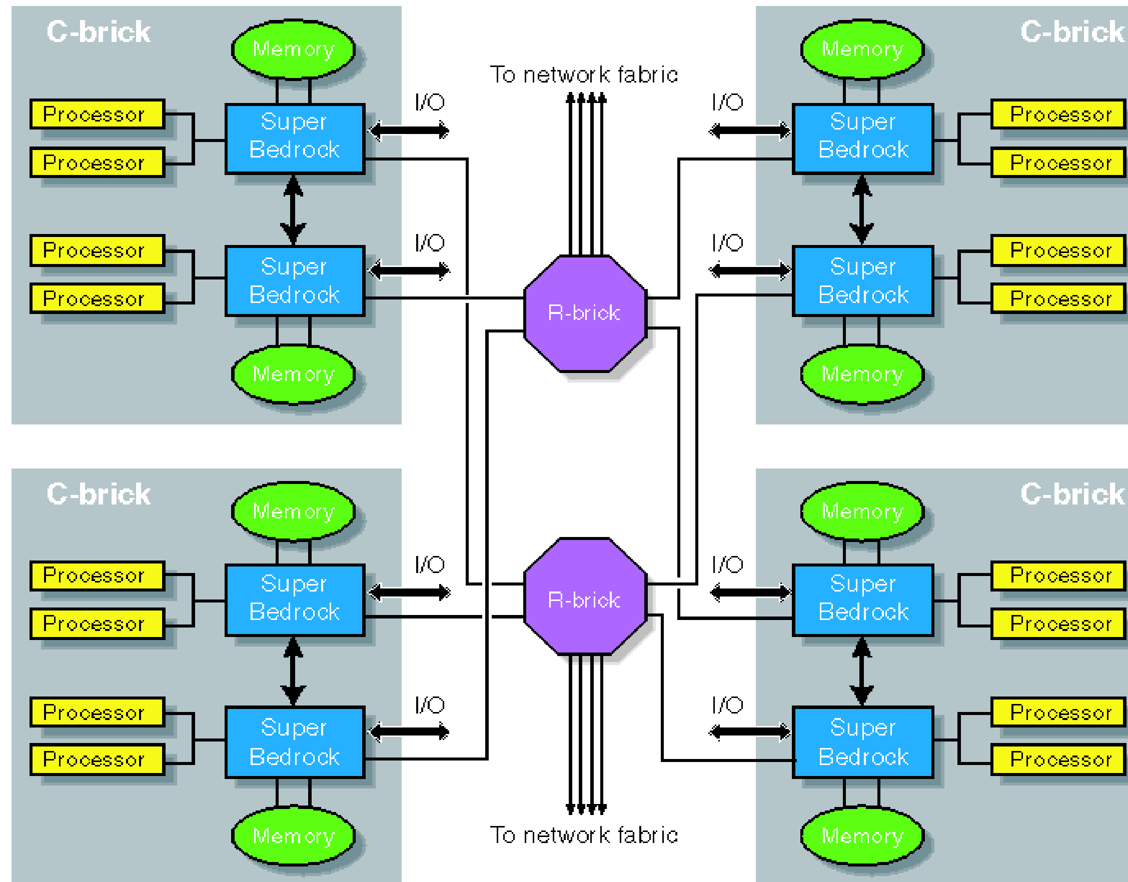
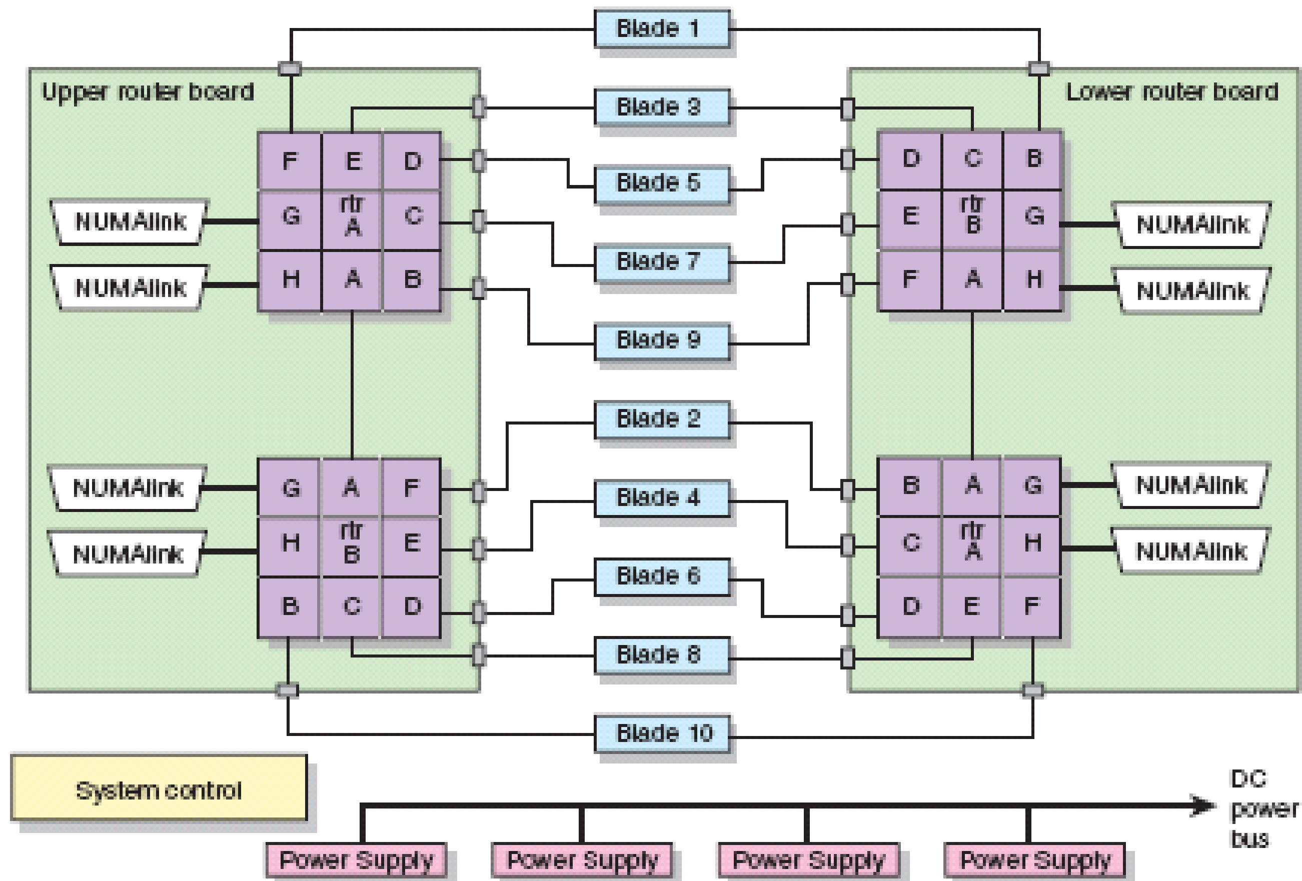
NUMA Architectures: SGI Altix 3000 Series



From Figure 3.4 of *SGI Altix 3000 User's Guide*, SGI, 2003.

NUMA Architectures: SGI Altix 4000 Series



From Figure 3.4 of *SGI Altix 4000 User's Guide*, SGI, 2006.

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Other Sources of Information

- **Online manuals**
- **Related workshop courses**

Online Manuals

- Like most UNIX-like systems, Linux includes a set of reference manuals as part of the operating system. These can be accessed by typing `man cmdname`, where `cmdname` is the name of the command or library routine for which you need information

- You can also do a keyword search of all of the currently accessible manual pages by running `man -k keyword`

Related Workshop Courses

OSC offers several other courses that may be of interest:

- C Programming
- Features of the C++ Programming Language
- An Introduction to Fortran 90
- Parallel Programming with MPI
- Using the ScaLAPACK Parallel Numerical Library
- Parallel I/O Techniques
- Performance Tuning for Microprocessor Architectures

More information on these courses and more can be found at

http://www.osc.edu/hpc/training/

OpenMP Problem Set

1. Write a program where each thread prints the message 'Hello World!', along with its thread ID number and the total number of threads used. Run with 8 threads and run your program several times. Does the order of the output change? Repeat using 4,16, 33, and 50 threads.
2. Modify your solution to Problem 1 so that only even-numbered threads print out the information message.
3. Write a program that declares an array `A` to have 16000 integer elements and initialize `A` so that each element has its index as its value. Then create a real array `B` that will contain the running average of array `A`. That is,

   ```
   B(I)=(A(I-1) + A(I) +A(I+1)/3.0
   ```

   except at the end points. Your code should do the initialization of `A` and the running average in parallel using 8 threads. Experiment with all four scheduling types for the running average loop by timing the loop with different schedules.

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OpenMP Problem Set (cont'd.)

4. Write a program so that the parallel threads print out 'Backwards' and their thread ID number in *reverse order* of thread number. That is, each time your program is run, the last thread prints out first, then the second to last, and so on. There are at least five different ways to solve this problem. Find as many as you can.
5. Compile the code `mystery.f` and run on 16 threads. What is wrong with this program? (You may have to run it several times.) Fix the code so that it works correctly. As with problem 4 there are several ways to fix the code; try to find them all.
6. Write a program to read in the x,y,z coordinates from a file `points.dat` (which you will be given) and calculate the geometric center, which is the average x value, the average y value, and the average z value. Do the calculation in parallel. Write two versions of your program: the first using loop-level parallelism, the next using functional decomposition. (The points data file is ASCII with one x,y,z triplet per line.)

OpenMP Problem Set (cont'd.)

7. **Using the functional decomposition version of program 6, calculate the average coordinate value given by the equation**

   $$(\Sigma x_i + \Sigma y_i + \Sigma z_i)/3N$$

   where N is the number of data points. Implement using a global sum and critical regions.

8. **Write a program to multiply two large matrices together**
   a) Compile for single-processor execution. Time the program.
   b) Compile for multiple processor execution (OpenMP directives) and time for 4,8,16, and 32 threads.

9. **Compile the program `alias.f` and run on four threads. Can you see the inefficiency in the program? Write a new version that is more efficient.**