OpenMP™

OpenMP Overview

openmp.org

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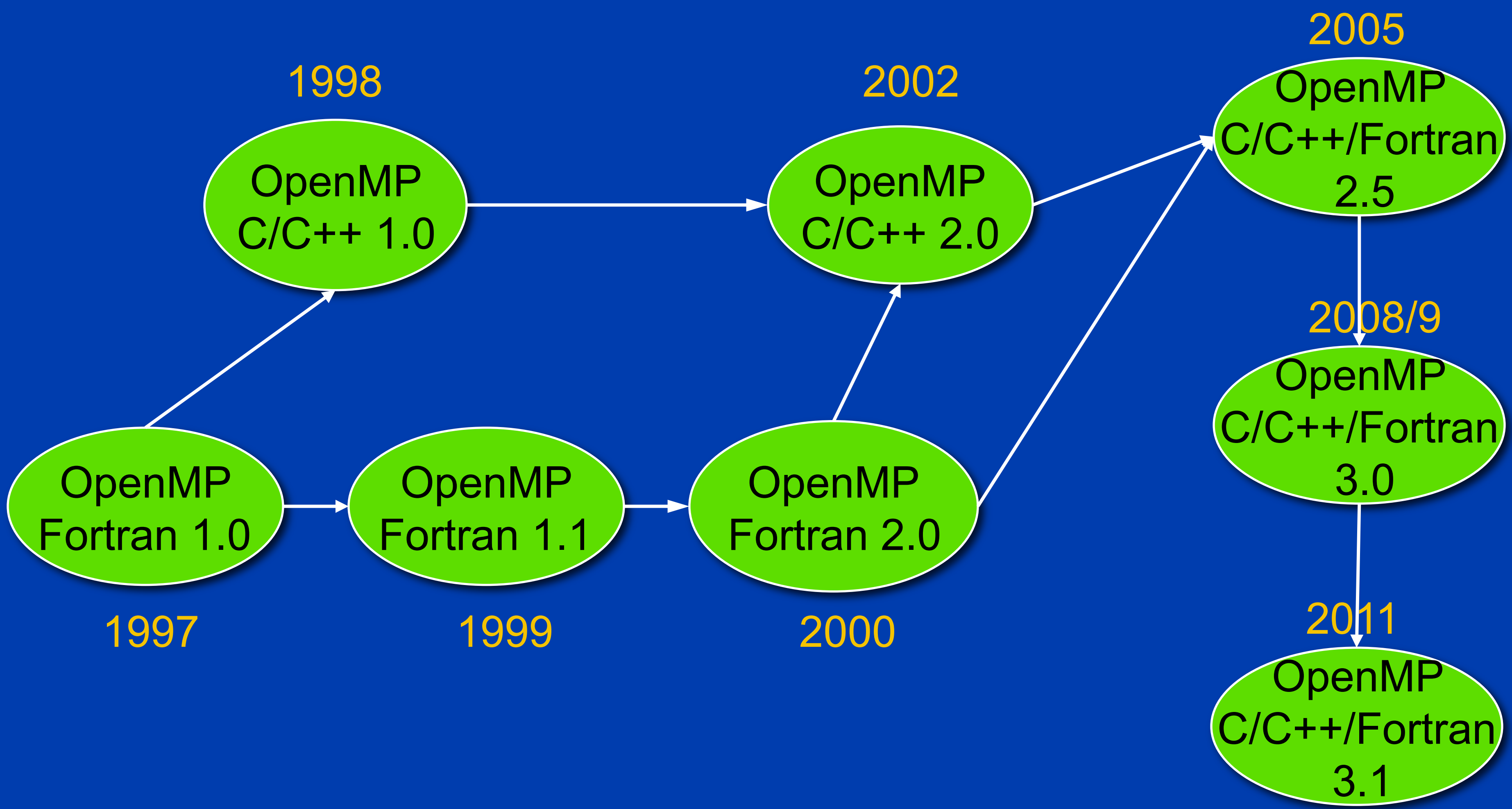
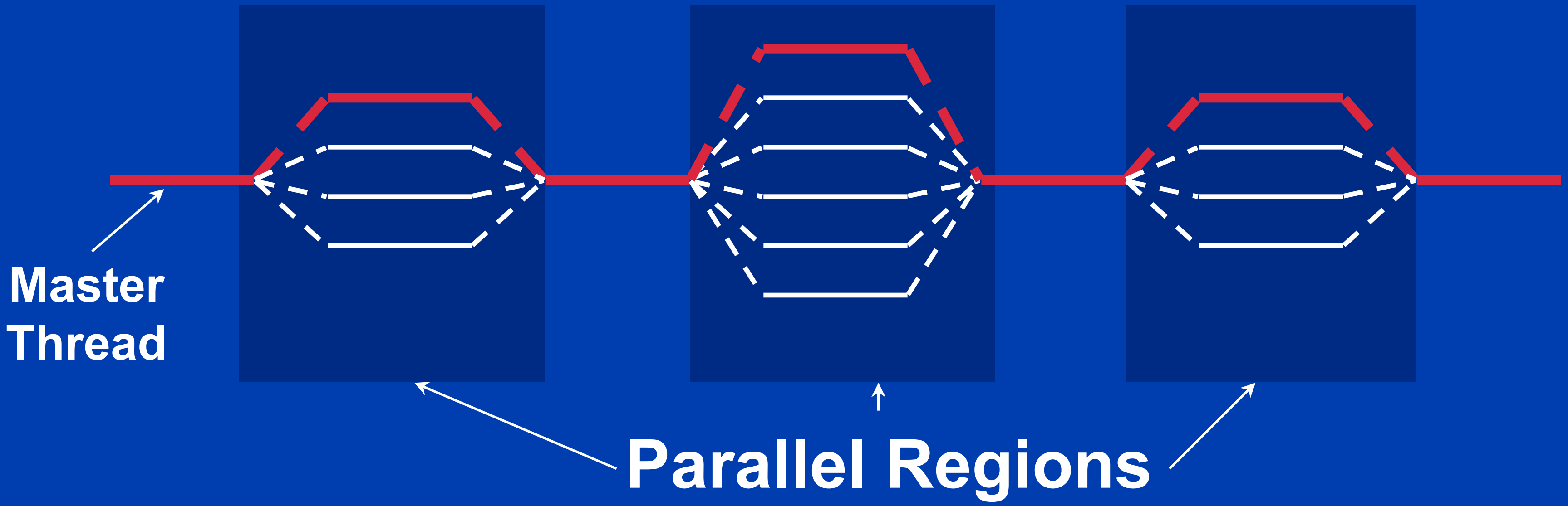
OpenMP Release History



OpenMP Programming Model:

Fork-Join Parallelism:

- ◆Master thread spawns a team of threads as needed.
- ◆Parallelism is added incrementally: i.e. the sequential program evolves into a parallel program.



(usually independent loops or "SPMD" sections)

How is OpenMP typically used?

- OpenMP is usually used to parallelize loops:
  - Find your most time consuming loops.
  - Split them up between threads.

Split-up this loop between multiple threads

```
      program example
      double precision Res(1000)


     do I=1,1000
        call huge_comp(Res(I))
      end do
      end
```

Sequential Program

```
      program example
      double precision Res(1000)
C$OMP PARALLEL DO
      do I=1,1000
         call huge_comp(Res(I))
      end do
      end
```

Parallel Program

How do threads interact?

- OpenMP is a shared memory model.
  - Threads communicate by sharing variables.
- Unintended sharing of data causes race conditions:
  - race condition: uncoordinated access to shared data; the program's outcome changes as the threads are scheduled differently.
- To control race conditions:
  - Use synchronization to protect data conflicts.
- Synchronization is expensive so:
  - Change how data is accessed to minimize the need for synchronization.

OpenMP:
Some syntax details to get us started

- Most of the constructs in OpenMP are compiler directives or pragmas.
  - For C and C++, the pragmas take the form:

    #pragma omp ***construct [clause [clause]…]***
  - For Fortran, the directives take one of the forms:

    C$OMP ***construct [clause [clause]…]***

    !$OMP ***construct [clause [clause]…]***

    $OMP** ***construct [clause [clause]…]
- Include file and the OpenMP lib module

```
#include <omp.h>
use omp_lib
```

OpenMP:
Structured blocks (C/C++)

- Most OpenMP* constructs apply to structured blocks.
  - Structured block: a block with one point of entry at the top and one point of exit at the bottom.
  - The only "branches" allowed are STOP statements in Fortran and exit() in C/C++.

```
#pragma omp parallel
{
          int id = omp_get_thread_num();
more:  res[id] = do_big_job(id);
          if(!conv(res[id]) goto more;
}
   printf(" All done \n");
```

A structured block

```
      if(go_now()) goto more;
#pragma omp parallel
{
          int id = omp_get_thread_num();
more:  res[id] = do_big_job(id);
          if(conv(res[id]) goto done;
          go to more;
}
done:      if(!really_done()) goto more;
```

<u>Not</u> A structured block

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OpenMP:
Structured blocks (Fortran)

- Most OpenMP constructs apply to structured blocks.
  - Structured block: a block of code with one point of entry at the top and one point of exit at the bottom.
  - The only "branches" allowed are STOP statements in Fortran and exit() in C/C++.

```
C$OMP PARALLEL
10    wrk(id) = garbage(id)
      res(id) = wrk(id)**2
      if(.not.conv(res(id)) goto 10
C$OMP END PARALLEL
     print *,id
```

A structured block

```
C$OMP  PARALLEL
10    wrk(id) = garbage(id)
30    res(id)=wrk(id)**2
      if(conv(res(id))goto 20
      go to 10
C$OMP END PARALLEL
     if(not_DONE) goto 30
20    print *, id
```

Not A structured block

OpenMP:

Structured Block Boundaries

- In C/C++: a block is a single statement or a group of statements between brackets {}

```
#pragma omp parallel
{
     id = omp_thread_num();
     res(id) = lots_of_work(id);
}
```

```
#pragma omp for
   for(I=0;I<N;I++){
         res[I] = big_calc(I);
         A[I] = B[I] + res[I];
   }
```

- In Fortran: a block is a single statement or a group of statements between directive/end-directive pairs.

```
C$OMP PARALLEL
10    wrk(id) = garbage(id)
      res(id) = wrk(id)**2
      if(.not.conv(res(id)) goto 10
C$OMP END PARALLEL
```

```
C$OMP PARALLEL DO
      do I=1,N
            res(I)=bigComp(I)
       end do
C$OMP END PARALLEL DO
```

OpenMP: Contents

- OpenMP's constructs fall into 5 categories:
  - Parallel Regions
  - Worksharing
  - Data Environment
  - Synchronization
  - Runtime functions/environment variables
- OpenMP is basically the same between Fortran and C/C++

The OpenMP* API

Parallel Regions

- **You create threads in OpenMP* with the "omp parallel" pragma.**
- **For example, To create a 4 thread Parallel region:**

```
double A[1000];
omp_set_num_threads(4);
#pragma omp parallel
{
        int ID = omp_get_thread_num();
        pooh(ID,A);
}
```

Runtime function to request a certain number of threads

Runtime function returning a thread ID

Each thread executes a copy of the the code within the structured block

- **Each thread calls pooh(ID,A) for `ID = 0 to 3`**

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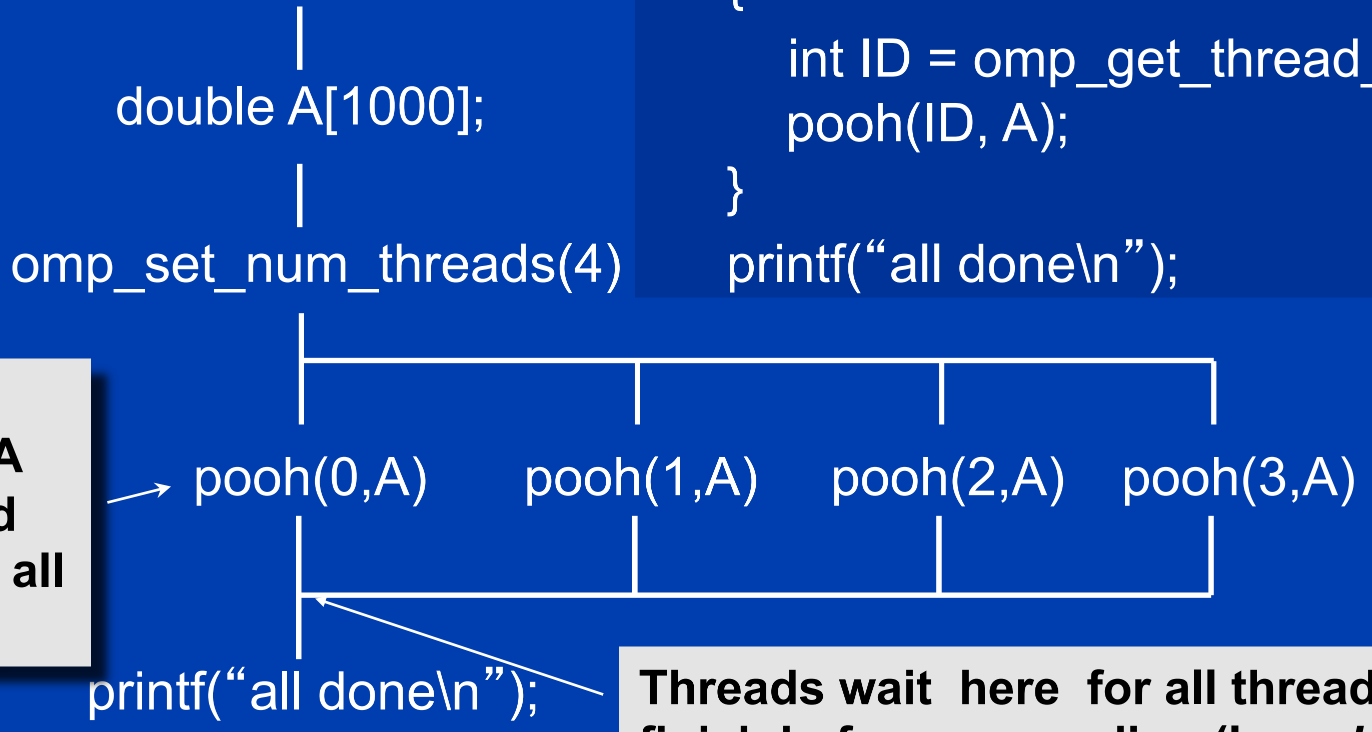
The OpenMP* API

Parallel Regions

- **Each thread executes the same code redundantly.**

```
double A[1000];
omp_set_num_threads(4);
#pragma omp parallel
{
    int ID = omp_get_thread_num();
    pooh(ID, A);
}
printf(“all done\n”);
```



A single copy of A is shared between all threads.

Threads wait here for all threads to finish before proceeding (I.e. a *barrier*)

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OpenMP: Contents

- OpenMP's constructs fall into 5 categories:
  - Parallel Regions
  - Work-sharing
  - Data Environment
  - Synchronization
  - Runtime functions/environment variables

OpenMP: Work-Sharing Constructs

- **The "for" Work-Sharing construct splits up loop iterations among the threads in a team**

```
#pragma omp parallel
#pragma omp for
        for (I=0;I<N;I++){
                NEAT_STUFF(I);
        }
```

By default, there is a barrier at the end of the "omp for". Use the "nowait" clause to turn off the barrier.

#pragma omp for nowait

"nowait" is useful between two consecutive, independent omp for loops.

Work Sharing Constructs
A motivating example

Sequential code

```
for(i=0;I<N;i++)   { a[i] = a[i] + b[i];}
```

OpenMP parallel region

```
#pragma omp parallel
{
        int id, i, Nthrds, istart, iend;
        id = omp_get_thread_num();
        Nthrds = omp_get_num_threads();
        istart = id * N / Nthrds;
        iend = (id+1) * N / Nthrds;
        for(i=istart;I<iend;i++)   { a[i] = a[i] + b[i];}
}
```

OpenMP parallel region and a work-sharing for-construct

```
#pragma omp parallel
#pragma omp for schedule(static)
        for(i=0;I<N;i++)   { a[i] = a[i] + b[i];}
```

OpenMP For/Do construct:
The schedule clause

- **The schedule clause effects how loop iterations are mapped onto threads**
  - ◆schedule(static [,chunk])
    - – Deal-out blocks of iterations of size “chunk” to each thread.
  - ◆schedule(dynamic[,chunk])
    - – Each thread grabs “chunk” iterations off a queue until all iterations have been handled.
  - ◆schedule(guided[,chunk])
    - – Threads dynamically grab blocks of iterations. The size of the block starts large and shrinks down to size “chunk” as the calculation proceeds.
  - ◆schedule(runtime)
    - – Schedule and chunk size taken from the OMP_SCHEDULE environment variable.

The Schedule Clause

Schedule Clause	When To Use
STATIC	Predictable and similar work per iteration
DYNAMIC	Unpredictable, highly variable work per iteration
GUIDED	Special case of dynamic to reduce scheduling overhead

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OpenMP: Work-Sharing Constructs

- The *Sections* work-sharing construct gives a different structured block to each thread.

```
#pragma omp parallel
#pragma omp sections
{
#pragma omp section
          X_calculation();
#pragma omp section
          y_calculation();
#pragma omp section
          z_calculation();
}
```

By default, there is a barrier at the end of the "omp sections". Use the "nowait" clause to turn off the barrier.

The OpenMP* API

Combined parallel/work-share

- OpenMP* shortcut: Put the “parallel” and the work-share on the same line

```
 double  res[MAX];  int i;
#pragma omp parallel
{
   #pragma omp for
   for (i=0;i< MAX; i++) {
       res[i] = huge();
   }
}
```

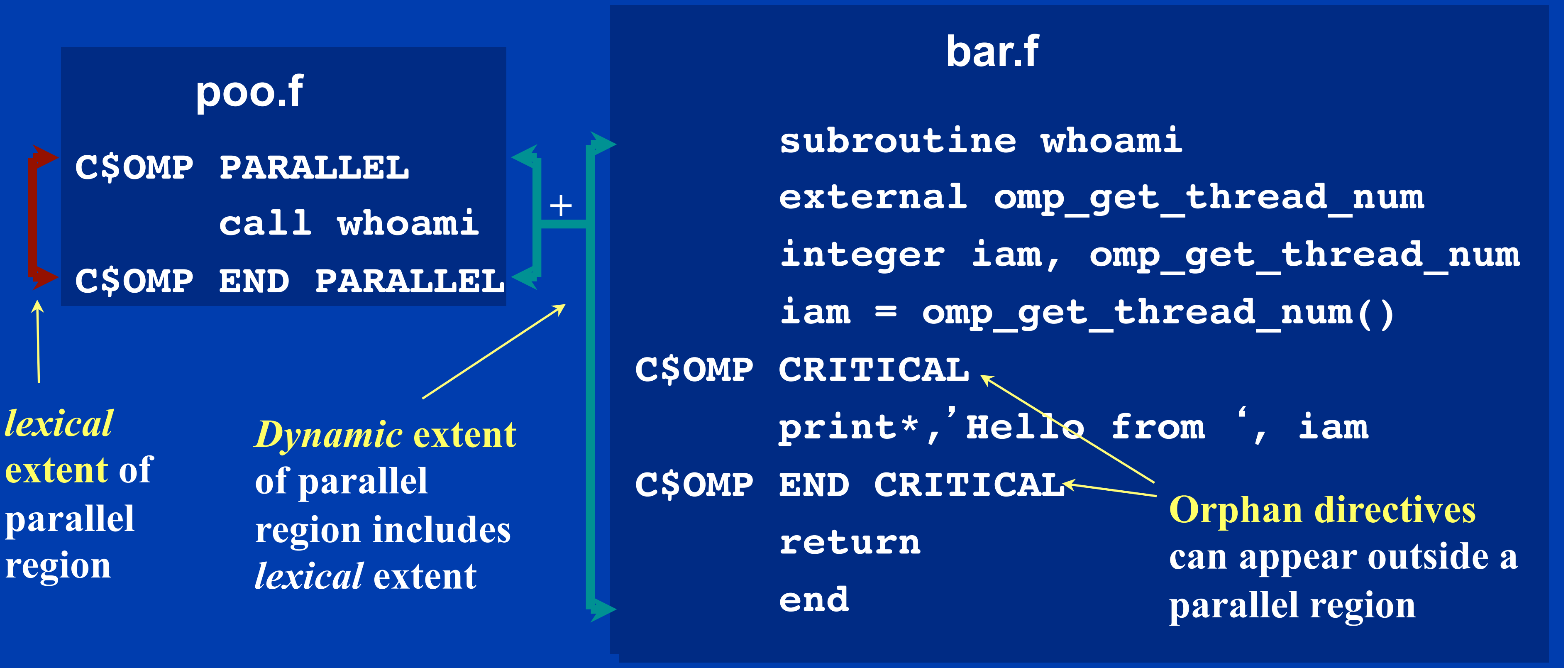
```
double  res[MAX];  int i;
#pragma omp parallel for
   for (i=0;i< MAX; i++) {
       res[i] = huge();
   }
```

These are equivalent

- There’s also a “parallel sections” construct.

OpenMP:
Scope of OpenMP constructs

OpenMP constructs can span multiple source files.



poo.f

```
C$OMP PARALLEL
      call whoami
C$OMP END PARALLEL
```

bar.f

```
      subroutine whoami
      external omp_get_thread_num
      integer iam, omp_get_thread_num
      iam = omp_get_thread_num()
C$OMP CRITICAL
      print*,’Hello from ‘, iam
C$OMP END CRITICAL
      return
      end
```

***lexical* extent of** parallel region

***Dynamic* extent** of parallel region includes *lexical* extent

Orphan directives can appear outside a parallel region

OpenMP: Contents

- OpenMP’s constructs fall into 5 categories:
  - ◆Parallel Regions
  - ◆Worksharing
  - ◆Data Environment
  - ◆Synchronization
  - ◆Runtime functions/environment variables

Data Environment:
Default storage attributes

- Shared Memory programming model:
  - Most variables are shared by default
- Global variables are SHARED among threads
  - Fortran: COMMON blocks, SAVE variables, MODULE variables
  - C: File scope variables, static
- But not everything is shared...
  - Stack variables in sub-programs called from parallel regions are PRIVATE
  - Automatic variables within a statement block are PRIVATE.

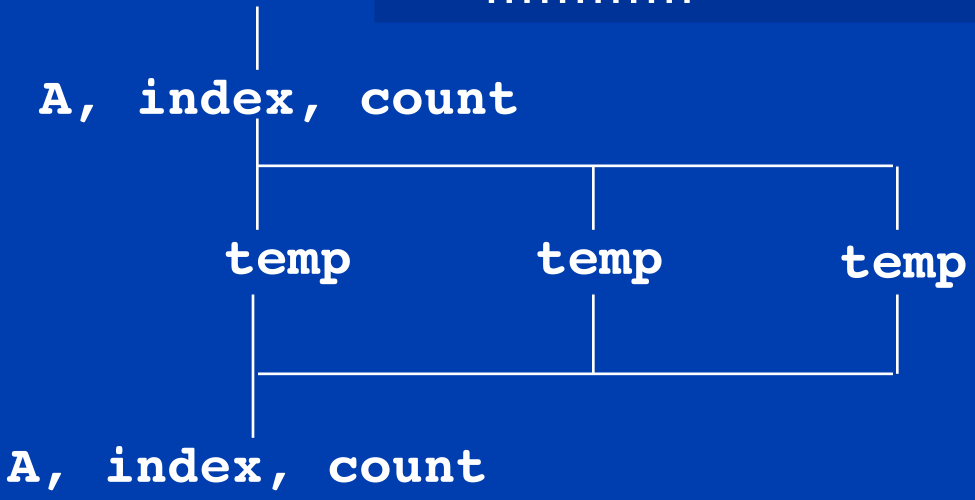
Data Sharing Examples

```
      program sort
      common /input/ A(10)
      integer index(10)
C$OMP PARALLEL
      call work(index)
C$OMP END PARALLEL
      print*, index(1)
```

```
subroutine work (index)
common /input/ A(10)
integer index(*)
real temp(10)
integer count
save count
      …………
```

A, index and count are shared by all threads.

temp is local to each thread



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Data Environment:
Changing storage attributes

- One can selectively change storage attributes constructs using the following clauses*
  - SHARED
  - PRIVATE
  - FIRSTPRIVATE
  - THREADPRIVATE

All the clauses on this page only apply to the *lexical extent* of the OpenMP construct.

- The value of a private inside a parallel loop can be transmitted to a global value outside the loop with:
  - LASTPRIVATE
- The default status can be modified with:
  - DEFAULT (PRIVATE | SHARED | NONE)

All data clauses apply to parallel regions and worksharing constructs except "shared" which only applies to parallel regions.

Private Clause

- private(var) creates a local copy of var for each thread.
  - The value is uninitialized
  - Private copy is *not* storage-associated with the original
  - The original is undefined at the end

```
      program wrong
      IS = 0
C$OMP PARALLEL DO PRIVATE(IS)
      DO J=1,1000
         IS = IS + J
      END DO
      print *, IS
```

IS was not initialized

Regardless of initialization, IS is undefined at this point

Firstprivate Clause

- Firstprivate is a special case of private.
  - Initializes each private copy with the corresponding value from the master thread.

```
      program almost_right
      IS = 0
C$OMP PARALLEL DO FIRSTPRIVATE(IS)
      DO J=1,1000
          IS = IS + J
1000  CONTINUE
      print *, IS
```

Each thread gets its own IS with an initial value of 0

Regardless of initialization, IS is undefined at this point

Lastprivate Clause

- Lastprivate passes the value of a private from the last iteration to a global variable.

```
      program closer
      IS = 0
C$OMP PARALLEL DO FIRSTPRIVATE(IS)
C$OMP+ LASTPRIVATE(IS)
      DO J=1,1000
          IS = IS + J
1000  CONTINUE
      print *, IS
```

Each thread gets its own IS with an initial value of 0

IS is defined as its value at the last iteration (I.e. for J=1000)

OpenMP:
A data environment test

- Consider this example of PRIVATE and FIRSTPRIVATE

```
        variables A,B, and C = 1
C$OMP PARALLEL PRIVATE(B)
C$OMP& FIRSTPRIVATE(C)
```

- Are A,B,C local to each thread or shared inside the parallel region?
- What are their initial values inside and after the parallel region?

Inside this parallel region ...

- "A" is shared by all threads; equals 1
- "B" and "C" are local to each thread.
  - B's initial value is undefined
  - C's initial value equals 1

Outside this parallel region ...

- The values of "B" and "C" are undefined.

Default Clause

- Note that the default storage attribute is DEFAULT (SHARED) (so no need to specify)
- To change default: DEFAULT(PRIVATE)
  - *each* variable in *static* extent of the parallel region is made private as if specified in a private clause
  - mostly saves typing
- DEFAULT(NONE)*:* *no* default for variables in static extent. Must list storage attribute for each variable in static extent

Only the Fortran API supports default(private).

C/C++ only has default(shared) or default(none).

Default Clause Example

```
        itotal = 1000
C$OMP PARALLEL PRIVATE(np, each)
      np = omp_get_num_threads()
      each = itotal/np
      .........
C$OMP END PARALLEL
```

```
      itotal = 1000
C$OMP PARALLEL DEFAULT(PRIVATE) SHARED(itotal)
      np = omp_get_num_threads()
      each = itotal/np
      .........
C$OMP END PARALLEL
```

Are these two codes equivalent?

$\downarrow$

$\boxed{\text{yes}}$

Threadprivate

- Makes global data private to a thread
  - Fortran: COMMON blocks
  - C: File scope and static variables
- Different from making them PRIVATE
  - with PRIVATE global variables are masked.
  - THREADPRIVATE preserves global scope within each thread
- Threadprivate variables can be initialized using COPYIN or by using DATA statements.

A threadprivate example

Consider two different routines called within a parallel region.

```
      subroutine poo
      parameter (N=1000)
      common/buf/A(N),B(N)
C$OMP THREADPRIVATE(/buf/)
      do i=1, N
        B(i)= const* A(i)
      end do
      return
      end
```

```
      subroutine bar
      parameter (N=1000)
      common/buf/A(N),B(N)
C$OMP THREADPRIVATE(/buf/)
      do i=1, N
        A(i) = sqrt(B(i))
      end do
      return
      end
```

Because of the threadprivate construct, each thread executing these routines has its own copy of the common block /buf/.

Copyin

You initialize threadprivate data using a copyin clause.

```
      parameter (N=1000)
      common/buf/A(N)
C$OMP THREADPRIVATE(/buf/)

C Initialize the A array
      call init_data(N,A)

C$OMP PARALLEL COPYIN(A)

 … Now each thread sees threadprivate array A initialied
 … to the global value set in the subroutine init_data()

C$OMP END PARALLEL

end
```

OpenMP: Reduction

- Another clause that effects the way variables are shared:

  reduction (op : list)

- The variables in “list” must be shared in the enclosing parallel region.
- Inside a parallel or a work-sharing construct:
  - A local copy of each list variable is made and initialized depending on the “op” (e.g. 0 for “+”).
  - Compiler finds standard reduction expressions containing “op” and uses them to update the local copy.
  - Local copies are reduced into a single value and combined with the original global value.

OpenMP:
Reduction example

```
#include <omp.h>
void main ()
{
        int i;
        double ZZ, func(), res=0.0;

#pragma omp parallel for reduction(+:res) private(ZZ)
        for (i=0; i< 1000; i++){
                ZZ = func(I);
                res = res + ZZ;
        }
}
```

OpenMP: Reduction example

- Remember the code we used to demo private, firstprivate and lastprivate.

```
      program closer
      IS = 0
      DO J=1,1000
           IS = IS + J
1000  CONTINUE
      print *, IS
```

- Here is the correct way to parallelize this code.

```
      program closer
      IS = 0
#pragma omp parallel for reduction(+:IS)
      DO J=1,1000
           IS = IS + J
1000  CONTINUE
      print *, IS
```

OpenMP:
Reduction operands/initial-values

- A range of associative operands can be used with reduction:
- Initial values are the ones that make sense mathematically.

Operand	Initial value
+	0
*	1
-	0
.AND.	All 1's

Operand	Initial value
.OR.	0
MAX	1
MIN	0
//	All 1's

OpenMP: Contents

- OpenMP’s constructs fall into 5 categories:
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  - ◆Worksharing
  - ◆Data Environment
  - ➡ ◆Synchronization
  - ◆Runtime functions/environment variables

OpenMP: Synchronization

- OpenMP has the following constructs to support synchronization:
  - critical section
  - atomic
  - barrier
  - flush
  - ordered
  - single
  - master

We will save flush for the advanced OpenMP tutorial.

We discuss this here, but it really isn't a synchronization construct. It's a work-sharing construct that may include synchronization.

We discus this here, but it really isn't a synchronization construct.

OpenMP: Synchronization

- Only one thread at a time can enter a critical section.

```
C$OMP PARALLEL DO PRIVATE(B)
C$OMP& SHARED(RES)
        DO 100 I=1,NITERS
                B =  DOIT(I)
C$OMP CRITICAL
                CALL CONSUME (B, RES)
C$OMP END CRITICAL
100   CONTINUE
```

Synchronization – critical section (in C/C++)

- Only one thread at a time can enter a **critical** section (with the same name).

```
float res;
#pragma omp parallel
{    float B;   int i;
     #pragma omp for
     for(i=0;i<niters;i++){
           B =  big_job(i);
#pragma omp critical <name>
           consum (B, RES);
     }
}
```

Threads wait their turn – only one at a time calls consume()

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OpenMP: Synchronization

- Atomic is a special case of a critical section that can be used for certain simple statements.
- It applies only to the update of a memory location (the update of X in the following example)

```
C$OMP PARALLEL PRIVATE(B)
          B =  DOIT(I)
tmp = big_ugly();

 C$OMP ATOMIC
          X = X + temp

C$OMP END PARALLEL
```

OpenMP: Synchronization

- **Barrier**: Each thread waits until all threads arrive.

```
#pragma omp parallel shared (A, B, C) private(id)
{
        id=omp_get_thread_num();
        A[id] = big_calc1(id);
#pragma omp barrier
#pragma omp for
        for(i=0;i<N;i++){C[i]=big_calc3(I,A);}
#pragma omp for nowait
        for(i=0;i<N;i++){ B[i]=big_calc2(C,  i); }
        A[id] = big_calc3(id);
}
```

implicit barrier at the end of a for work-sharing construct

no implicit barrier due to nowait

implicit barrier at the end of a parallel region

OpenMP: Synchronization

- The ordered construct enforces the sequential order for a block.

```
#pragma omp parallel private (tmp)
#pragma omp for ordered
        for (I=0;I<N;I++){
                tmp = NEAT_STUFF(I);
#pragma ordered
                res += consum(tmp);
        }
```

OpenMP: ~~Synchronization~~

- The **master** construct denotes a structured block that is only executed by the master thread. The other threads just skip it (no synchronization is implied).

```
#pragma omp parallel private (tmp)
{
          do_many_things();
#pragma omp master
          {     exchange_boundaries();   }
#pragma barrier
          do_many_other_things();
}
```

OpenMP: ~~Synchronization~~ work-share

- The single construct denotes a block of code that is executed by only one thread.
- A barrier is implied at the end of the single block.

```
#pragma omp parallel private (tmp)
{
        do_many_things();
#pragma omp single
        {    exchange_boundaries();   }
        do_many_other_things();
}
```

OpenMP:
Implicit synchronization

- Barriers are implied on the following OpenMP constructs:

```
end parallel
end do  (except when nowait is used)
end sections (except when nowait is used)
end single (except when nowait is used)
```

OpenMP: Contents

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  - ◆Data Environment
  - ◆Synchronization
  - ➡ ◆Runtime functions/environment variables

OpenMP: Library routines:

- Runtime environment routines:
  - Modify/Check the number of threads
    - omp_set_num_threads(),
    - omp_get_num_threads(),
    - omp_get_thread_num(),
    - omp_get_max_threads()
  - Are we in a parallel region?
    - omp_in_parallel()
  - How many processors in the system?
    - omp_num_procs()

OpenMP: Library Routines

- To fix the number of threads used in a program, (1) set the number threads, then (4) save the number you got.

```
#include <omp.h>
void main()
{   int num_threads;
    omp_set_num_threads( omp_num_procs() );
#pragma omp parallel
    {     int id=omp_get_thread_num();
#pragma omp single
             num_threads = omp_get_num_threads();
          do_lots_of_stuff(id);
    }
}
```

Request as many threads as you have processors.

Protect this op since Memory stores are not atomic

OpenMP: Environment Variables:

- **Control how "omp for schedule(RUNTIME)" loop iterations are scheduled.**
  - OMP_SCHEDULE "schedule[, chunk_size]"
- **Set the default number of threads to use.**
  - OMP_NUM_THREADS *int_literal*

Agenda

- Setting the stage
  - Parallel computing, hardware, software, etc.
- OpenMP: A quick overview
- OpenMP: A detailed introduction
- ➡ OpenMP use in the SPEC OMP Benchmarks

The SPEC OMPM2001 Benchmarks

Code	Applications	Language	lines
ammp	Chemistry/biology	C	13500
applu	Fluid dynamics/physics	Fortran	4000
apsi	Air pollution	Fortran	7500
art	Image Recognition\ neural networks	C	1300
fma3d	Crash simulation	Fortran	60000
gafort	Genetic algorithm	Fortran	1500
galgel	Fluid dynamics	Fortran	15300
equake	Earthquake modeling	C	1500
mgrid	Multigrid solver	Fortran	500
swim	Shallow water modeling	Fortran	400
wupwise	Quantum chromodynamics	Fortran	2200

Basic Characteristics

Code	Parallel Coverage (%)	Total Runtime (sec) Seq.	Total Runtime (sec) 4-cpu	# of parallel sections
ammp	99.11	16841	5898	7
applu	99.99	11712	3677	22
apsi	99.84	8969	3311	24
art	99.82	28008	7698	3
equake	99.15	6953	2806	11
fma3d	99.45	14852	6050	92/30*
gafort	99.94	19651	7613	6
galgel	95.57	4720	3992	31/32*
mgrid	99.98	22725	8050	12
swim	99.44	12920	7613	8
wupwise	99.83	19250	5788	10

* static sections / sections called at runtime

Wupwise

- Quantum chromodynamics model written in Fortran 90
- Parallelization was relatively straightforward
  - 10 OMP PARALLEL regions
  - PRIVATE and (2) REDUCTION clauses
  - 1 critical section
- Loop coalescing was used to increase the size of parallel sections

Major parallel loop in Wupwise

```
C$OMP PARALLEL
C$OMP+       PRIVATE (AUX1, AUX2, AUX3),
C$OMP+       PRIVATE (I, IM, IP, J, JM, JP, K, KM, KP, L, LM, LP),
C$OMP+       SHARED (N1, N2, N3, N4, RESULT, U, X)

C$OMP DO
   DO 100 JKL = 0, N2 * N3 * N4 - 1

     L = MOD (JKL / (N2 * N3), N4) + 1
     LP=MOD(L,N4)+1

     K = MOD (JKL / N2, N3) + 1
     KP=MOD(K,N3)+1

     J = MOD (JKL, N2) + 1
     JP=MOD(J,N2)+1

     DO 100 I=(MOD(J+K+L,2)+1),N1,2

        IP=MOD(I,N1)+1

       CALL GAMMUL(1,0,X(1,(IP+1)/2,J,K,L),AUX1)
       CALL SU3MUL(U(1,1,1,I,J,K,L),'N',AUX1,AUX3)

       CALL GAMMUL(2,0,X(1,(I+1)/2,JP,K,L),AUX1)
       CALL SU3MUL(U(1,1,2,I,J,K,L),'N',AUX1,AUX2)
       CALL ZAXPY(12,ONE,AUX2,1,AUX3,1)

       CALL GAMMUL(3,0,X(1,(I+1)/2,J,KP,L),AUX1)
       CALL SU3MUL(U(1,1,3,I,J,K,L),'N',AUX1,AUX2)
       CALL ZAXPY(12,ONE,AUX2,1,AUX3,1)

       CALL GAMMUL(4,0,X(1,(I+1)/2,J,K,LP),AUX1)
       CALL SU3MUL(U(1,1,4,I,J,K,L),'N',AUX1,AUX2)
       CALL ZAXPY(12,ONE,AUX2,1,AUX3,1)

       CALL ZCOPY(12,AUX3,1,RESULT(1,(I+1)/2,J,K,L),1)

 100  CONTINUE
C$OMP END DO
C$OMP END PARALLEL
```

Swim

- Shallow Water model written in F77/F90
- Swim is known to be highly parallel
- Code contains several doubly-nested loops
  The outer loops are parallelized

Example parallel loop

```
!$OMP PARALLEL DO
      DO 100 J=1,N
      DO 100 I=1,M
      CU(I+1,J) = .5D0*(P(I+1,J)+P(I,J))*U(I+1,J)
      CV(I,J+1) = .5D0*(P(I,J+1)+P(I,J))*V(I,J+1)
      Z(I+1,J+1) = (FSDX*(V(I+1,J+1)-V(I,J+1))-FSDY*(U(I+1,J+1)
                    -U(I+1,J)))/(P(I,J)+P(I+1,J)+P(I+1,J+1)+P(I,J+1))
      H(I,J) = P(I,J)+.25D0*(U(I+1,J)*U(I+1,J)+U(I,J)*U(I,J)
                    +V(I,J+1)*V(I,J+1)+V(I,J)*V(I,J))
  100 CONTINUE
```

Mgrid

- Multigrid electromagnetism in F77/F90
- Major parallel regions inrprj3, basic multigrid iteration
- Simple loop nest patterns, similar to Swim, several 3-nested loops
- Parallelized through the Polaris automatic parallelizing source-to-source translator

Applu

- Non-linear PDES time stepping SSOR in F77
- Major parallel regions in ssor.f, basic SSOR iteration
- Basic parallelization over the outer of 3D loop, temporaries held private

Up to 4-nested loops:

```
!$OMP PARALLEL DEFAULT(SHARED) PRIVATE(M,I,J,K,tmp2)
      tmp2 = dt
!$omp do
      do k = 2, nz - 1
         do j = jst, jend
            do i = ist, iend
               do m = 1, 5
                  rsd(m,i,j,k) = tmp2 * rsd(m,i,j,k)
               end do
            end do
         end do
      end do
!$omp end do
!$OMP END PARALLEL
```

Galgel

- CFD in F77/F90
- Major parallel regions in heat transfer calculation
- Loop coalescing applied to increase parallel regions, guided self scheduling in loop with irregular iteration times

Major parallel loop in subroutine syshtN.f of Galgel

```
!$OMP PARALLEL
!$OMP+  DEFAULT(NONE)
!$OMP+  PRIVATE (I, IL, J, JL, L, LM, M, LPOP, LPOP1),
!$OMP+  SHARED (DX, HtTim, K, N, NKX, NKY, NX, NY, Poj3, Poj4, XP, Y),
!$OMP+  SHARED (WXXX, WXXY, WXYX, WXYY, WYXX, WYXY, WYYX, WYYY),
!$OMP+  SHARED (WXTX, WYTX, WXTY, WYTY, A, Ind0)
           If (Ind0 .NE. 1) then
                                ! Calculate r.h.s.

C ++++++ - HtCon(i,j,l)*Z(j)*X(l) ++++++++++++++++++++++++++++++++++++

!$OMP DO SCHEDULE(GUIDED)
                Ext12: Do LM = 1, K
                 L = (LM - 1) / NKY + 1
                 M = LM - (L - 1) * NKY

                  Do IL=1,NX
                   Do JL=1,NY
                    Do i=1,NKX
                     Do j=1,NKY

                       LPOP( NKY*(i-1)+j, NY*(IL-1)+JL ) =
                             WXTX(IL,i,L) * WXTY(JL,j,M) + WYTX(IL,i,L) * WYTY(JL,j,M)
                     End Do
                    End Do
                   End Do
                  End Do

C .............. LPOP1(i) = LPOP(i,j)*X(j) ............................

                  LPOP1(1:K) = MATMUL( LPOP(1:K,1:N), Y(K+1:K+N) )

C ............. Poj3 = LPOP1 ......................................

                  Poj3( NKY*(L-1)+M, 1:K) = LPOP1(1:K)

C ............... Xp = <LPOP1,Z> ....................................

                Xp(NKY*(L-1)+M) =  DOT_PRODUCT (Y(1:K), LPOP1(1:K) )

C ............... Poj4(*,i) = LPOP(j,i)*Z(j) .........................

                  Poj4( NKY*(L-1)+M,1:N) =
                                    MATMUL( TRANSPOSE( LPOP(1:K,1:N) ), Y(1:K) )

                 End Do Ext12
!$OMP END DO

C ............ DX = DX - HtTim*Xp ...........................
!$OMP DO
                DO LM = 1, K
                 DX(LM) = DX(LM) - DOT_PRODUCT (HtTim(LM,1:K), Xp(1:K))
                END DO
!$OMP END DO NOWAIT

           Else

C ************ Jacobian ****************************************

C ...........A = A - HtTim * Poj3 ......................

!$OMP DO
                DO LM = 1, K
                A(1:K,LM) = A(1:K,LM) -
                                  MATMUL( HtTim(1:K,1:K), Poj3(1:K,LM) )
                END DO
!$OMP END DO NOWAIT

C ...........A = A - HtTim * Poj4 ......................

!$OMP DO
                DO LM = 1, N
                A(1:K,K+LM) = A(1:K,K+LM) -
                               MATMUL( HtTim(1:K,1:K), Poj4(1:K,LM) )
                END DO
!$OMP END DO NOWAIT

           End If
!$OMP END PARALLEL

       Return
      End
```

APSI

- 3D air pollution model
- Relatively flat profile
- Parts of work arrays used as shared and other parts used as private data

Sample parallel loop from run.f

```
!$OMP PARALLEL
!$OMP+PRIVATE(II,MLAG,HELP1,HELPA1)
!$OMP DO
      DO 20 II=1,NZTOP
        MLAG=NXNY1+II*NXNY
C
C               HORIZONTAL DISPERSION PART          2    2    2    2
C ----   CALCULATE WITH  DIFFUSION EIGENVALUES THE  K D C/DX ,K D C/DY
C                                                 X          Y
        CALL DCTDX(NX,NY,NX1,NFILT,C(MLAG),DCDX(MLAG),
                               HELP1,HELPA1,FX,FXC,SAVEX)
        IF(NY.GT.1) CALL DCTDY(NX,NY,NY1,NFILT,C(MLAG),DCDY(MLAG),
                                       HELP1,HELPA1,FY,FYC,SAVEY)
 20  CONTINUE
!$OMP END DO
!$OMP END PARALLEL
```

Gafort

- Genetic algorithm in C
- Most “interesting” loop: shuffle the population.
  - Original loop is not parallel; performs pair-wise swap of an array element with another, randomly selected element. There are 40,000 elements.
  - Parallelization idea:
    - Perform the swaps in parallel
    - Need to prevent simultaneous access to same array element: use one lock per array element → 40,000 locks.

Parallel loop In shuffle.f of Gafort

Exclusive access to array elements. Ordered locking prevents deadlock.

```
!$OMP PARALLEL PRIVATE(rand, iother, itemp, temp, my_cpu_id)
      my_cpu_id = 1
!$    my_cpu_id = omp_get_thread_num() + 1
!$OMP DO
      DO j=1,npopsiz-1
         CALL ran3(1,rand,my_cpu_id,0)
         iother=j+1+DINT(DBLE(npopsiz-j)*rand)
!$       IF (j < iother) THEN
!$          CALL omp_set_lock(lck(j))
!$          CALL omp_set_lock(lck(iother))
!$       ELSE
!$          CALL omp_set_lock(lck(iother))
!$          CALL omp_set_lock(lck(j))
!$       END IF
        itemp(1:nchrome)=iparent(1:nchrome,iother)
        iparent(1:nchrome,iother)=iparent(1:nchrome,j)
        iparent(1:nchrome,j)=itemp(1:nchrome)
        temp=fitness(iother)
        fitness(iother)=fitness(j)
        fitness(j)=temp
!$      IF (j < iother) THEN
!$          CALL omp_unset_lock(lck(iother))
!$          CALL omp_unset_lock(lck(j))
!$      ELSE
!$          CALL omp_unset_lock(lck(j))
!$          CALL omp_unset_lock(lck(iother))
!$      END IF
     END DO
!$OMP END DO
!$OMP END PARALLEL
```

Fma3D

- 3D finite element mechanical simulator
- Largest of the SPEC OMP codes: 60,000 lines
- Uses OMP DO, REDUCTION, NOWAIT, CRITICAL
- Key to good scaling was critical section
- Most parallelism from simple DOs
  - Of the 100 subroutines only four have parallel sections; most of them in fma1.f90
- Conversion to OpenMP took substantial work

Parallel loop in platq.f90 of Fma3D

```
!$OMP PARALLEL DO &
!$OMP   DEFAULT(PRIVATE), SHARED(PLATQ,MOTION,MATERIAL,STATE_VARIABLES), &
!$OMP   SHARED(CONTROL,TIMSIM,NODE,SECTION_2D,TABULATED_FUNCTION,STRESS),&
!$OMP   SHARED(NUMP4) REDUCTION(+:ERRORCOUNT),                      &
!$OMP   REDUCTION(MIN:TIME_STEP_MIN),                          &
!$OMP   REDUCTION(MAX:TIME_STEP_MAX)

     DO N = 1,NUMP4

      ... (66 lines deleted)

      MatID = PLATQ(N)%PAR%MatID

      CALL PLATQ_MASS ( NEL,SecID,MatID )

      ... (35 lines deleted)

      CALL PLATQ_STRESS_INTEGRATION ( NEL,SecID,MatID )

      ... (34 lines deleted)

!$OMP END PARALLEL DO
```

Contains large critical section

Subroutine platq_mass.f90 of Fma3D

```
 SUBROUTINE PLATQ_MASS ( NEL,SecID,MatID )

    ... (54 lines deleted)

!$OMP CRITICAL (PLATQ_MASS_VALUES)
      DO i = 1,4
        NODE(PLATQ(NEL)%PAR%IX(i))%Mass = NODE(PLATQ(NEL)%PAR%IX(i))%Mass + QMass
        MATERIAL(MatID)%Mass = MATERIAL(MatID)%Mass + QMass
        MATERIAL(MatID)%Xcm  = MATERIAL(MatID)%Xcm  + QMass * Px(I)
        MATERIAL(MatID)%Ycm  = MATERIAL(MatID)%Ycm  + QMass * Py(I)
        MATERIAL(MatID)%Zcm  = MATERIAL(MatID)%Zcm  + QMass * Pz(I)
!!
!! Compute inertia tensor B wrt the origin from nodal point masses.
!!
        MATERIAL(MatID)%Bxx = MATERIAL(MatID)%Bxx + (Py(I)*Py(I)+Pz(I)*Pz(I))*QMass
        MATERIAL(MatID)%Byy = MATERIAL(MatID)%Byy + (Px(I)*Px(I)+Pz(I)*Pz(I))*QMass
        MATERIAL(MatID)%Bzz = MATERIAL(MatID)%Bzz + (Px(I)*Px(I)+Py(I)*Py(I))*QMass
        MATERIAL(MatID)%Bxy = MATERIAL(MatID)%Bxy - Px(I)*Py(I)*QMass
        MATERIAL(MatID)%Bxz = MATERIAL(MatID)%Bxz - Px(I)*Pz(I)*QMass
        MATERIAL(MatID)%Byz = MATERIAL(MatID)%Byz - Py(I)*Pz(I)*QMass
      ENDDO
!!
!!
!! Compute nodal isotropic inertia
!!
      RMass = QMass * (PLATQ(NEL)%PAR%Area + SECTION_2D(SecID)%Thickness**2) / 12.0D+0
!!
!!
      NODE(PLATQ(NEL)%PAR%IX(5))%Mass = NODE(PLATQ(NEL)%PAR%IX(5))%Mass + RMass
      NODE(PLATQ(NEL)%PAR%IX(6))%Mass = NODE(PLATQ(NEL)%PAR%IX(6))%Mass + RMass
      NODE(PLATQ(NEL)%PAR%IX(7))%Mass = NODE(PLATQ(NEL)%PAR%IX(7))%Mass + RMass
      NODE(PLATQ(NEL)%PAR%IX(8))%Mass = NODE(PLATQ(NEL)%PAR%IX(8))%Mass + RMass
!$OMP END CRITICAL (PLATQ_MASS_VALUES)
!!
!!
      RETURN
      END
```

This is a large array reduction

Art

- Image processing
- Good scaling required combining two dimensions into single dimension
- Uses OMP DO, SCHEDULE(DYNAMIC)
- Dynamic schedule needed because of embedded conditional

Key loop in Art

```
#pragma omp for private (k,m,n, gPassFlag) schedule(dynamic)
  for (ij = 0; ij < ijmx; ij++)  {
    j = ((ij/inum) * gStride) + gStartY;
    i = ((ij%inum) * gStride) +gStartX;
    k=0;
    for (m=j;m<(gLheight+j);m++)
      for (n=i;n<(gLwidth+i);n++)
        f1_layer[o][k++].I[0] = cimage[m][n];

    gPassFlag =0;
    gPassFlag = match(o,i,j, &mat_con[ij], busp);

    if (gPassFlag==1) {
      if (set_high[o][0]==TRUE) {
        highx[o][0] = i;
        highy[o][0] = j;
        set_high[o][0] = FALSE;
      }
     if (set_high[o][1]==TRUE)  {
       highx[o][1] = i;
       highy[o][1] = j;
       set_high[o][1] = FALSE;
     }
    }
  }
```

Ammp

- Molecular Dynamics
- Very large loop in rectmm.c
- Good parallelism required great deal of work
- Uses OMP FOR, SCHEDULE(GUIDED), about 20,000 locks
- Guided scheduling needed because of loop with conditional execution.

Parallel loop in rectmm.c of Ammp

```
#pragma omp parallel for private (n27ng0, nng0, ing0, i27ng0, natoms, ii, a1, a1q, a1serial,
   inclose, ix, iy, iz, inode, nodelistt, r0, r, xt, yt, zt, xt2, yt2, zt2, xt3, yt3, zt3, xt4,
   yt4, zt4, c1, c2, c3, c4, c5, k, a1VP , a1dpx , a1dpy , a1dpz , a1px, a1py, a1pz, a1qxx ,
   a1qxy , a1qxz ,a1qyy , a1qyz , a1qzz, a1a, a1b, iii, i, a2, j, k1, k2 ,ka2, kb2, v0, v1, v2,
   v3, kk, atomwho, ia27ng0, iang0,  o ) schedule(guided)

    for( ii=0; ii<  jj; ii++)
    ...
                for( inode = 0; inode < iii; inode ++)
                   if( (*nodelistt)[inode].innode > 0) {
                     for(j=0; j< 27; j++)
                     if( j == 27  )
    ...
                                    if(  atomwho->serial > a1serial)
                                                   for( kk=0; kk< a1->dontuse; kk++)
                                                      if( atomwho == a1->excluded[kk])
    ...
                                    for( j=1; j< (*nodelistt)[inode].innode -1 ; j++)
    ...
                                                   if( atomwho->serial > a1serial)
                                                      for( kk=0; kk< a1->dontuse; kk++)
                                                                     if( atomwho == a1->excluded[kk]) goto SKIP2;
    ...
                for (i27ng0=0 ; i27ng0<n27ng0; i27ng0++)
    ...
    ...
                for( i=0; i< nng0; i++)
    ...
                   if( v3 > mxcut || inclose > NCLOSE )
    ...
    ...
```

(loop body contains 721 lines)

Performance Tuning Example 3: EQUAKE

- EQUAKE: Earthquake simulator in C
- EQUAKE is hand-parallelized with relatively few code modifications.
  - Parallelizing the four most time-consuming loops
  - inserted OpenMP pragmas for parallel loops and private data
  - array reduction transformation
  - A change in memory allocation made a big performance difference

EQUAKE Code Sample

```
 /* malloc w1[numthreads][ARCHnodes][3] */

#pragma omp parallel for
  for (j = 0; j < numthreads; j++)
    for (i = 0; i < nodes; i++) { w1[j][i][0] = 0.0; ...; }

#pragma omp parallel private(my_cpu_id,exp,...)
{
  my_cpu_id = omp_get_thread_num();

#pragma omp for
  for (i = 0; i < nodes; i++)
    while (...) {
      ...
      exp = loop-local computation;
      w1[my_cpu_id][...][1] += exp;
      ...
  }
}
#pragma omp parallel for
  for (j = 0; j < numthreads; j++) {
    for (i = 0; i < nodes; i++) { w[i][0] += w1[j][i]
[0]; ...;}
```

OpenMP Features Used

Code	regions	locks	guided	dynamic	critical	nowait
ammp	7	20k	2			
applu	22					14
apsi	24					
art	3			1		
equake	11					
fma3d	92/30				1	2
gafort	6	40k				
galgel	31/32*		7			3
mgrid	12					11
swim	8					
wupwise	10				1	

* static sections / sections called at runtime

“Feature” used to deal with NUMA machines: rely on *first-touch* page placement. If necessary, put initialization into a parallel loop to avoid placing all data on the master processor.