Multi Core Programming with OpenMP

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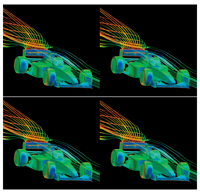


OpenMP: Open specification for Multi Processing

Shared address space model, based on *threads*

Thread:
- Light weight process, global addresses
- Private program counter, independent
- Private stack pointer, private data

=> All threads have access to global data, can run in parallel and have some private data on stack.

On a multi-core node the threads are scheduled over the CPU's to the different cores.
=> One node on IT-servers can run 8 parallel threads.

Insert compiler directives for parallelization of computations => high-level model

```
#pragma omp parallel for
 for (i=2;i<=N-1;i++)
    A[i]=F(B[i-1]+B[i]+B[i+1]);
```

Loop is automatically parallelized over all threads, different iterations on different theads. Arrays A and B are global data, loop variable i is private.

```
NLOC=N/NPROC
ALLOCATE (A(NLOC),B(NLOC))
. . .
```

(Standard send/recv avoiding deadlock)

```
IF (MOD(PID,2)==1) THEN
   CALL MPI_SEND(B(1),LEFT)
   CALL MPI_RECV(TEMP1,LEFT)
ELSEIF (MOD(PID,2)==0 AND PID<NPROC-1)
   CALL MPI_RECV(TEMP2,RIGHT)
   CALL MPI_SEND(B(NLOC),RIGHT)
END IF
IF (MOD(PID,2)==1 AND PID<NPROC-1) THEN
   CALL MPI_SEND(B(NLOC),RIGHT)
   CALL MPI_RECV(TEMP2,RIGHT)
ELSEIF (MOD(PID,2)==0 AND PID>0)
   CALL MPI_RECV(TEMP1,LEFT)
   CALL MPI_SEND(B(1),LEFT)
END IF
```

(Simpler with non-blocking communication MPI_Irecv followed by MPI_Send)

```
IF (PID>0) THEN
   A(1)=F(TEMP1+B(1)+B(2))
END IF
FOR (I=2; I<NLOC-1; I++)
   A(I)=F(B(I-1)+B(I)+B(I+1))
END DO
IF (PID<NPROC-1) THEN
   A(NLOC)=F(B(NLOC-1)+B(NLOC)+TEMP2)
END IF
```

OpenMP directives:

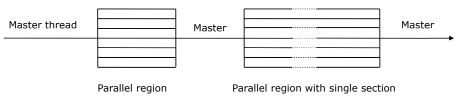
Parallel (main, fork threads)

Data sharing
- shared
- private
- firstprivate
- lastprivate
- threadprivate

Work sharing
- do/for
  - reduction
  - schedule
    - static, dynamic, guided
  - ordered
  - collapse
- sections
- tasks

Serial sections
- single
- master
- critical
- atomic
- ordered

Synchronization
- barrier
- flush
- nowait



OpenMP library functions:

- omp_set_num_threads
- omp_get_num_threads
- omp_get_max_threads
- omp_get_thread_num
- omp_set_nested
- and more (e.g. lock)

Allows for more flexible and user controlled (e.g. load balancing) programming than with the standard directives.

Environment variables: (export VARIABLE=value)
- OMP_NUM_THREADS
- OMP_SCHEDULE
- OMP_NESTED
- and more (stacksize, wait policy)

To run on 4 threads, before start of program do:
export OMP_NUM_THREADS=4

Directives: (Support only in Fortran/C/C++)

C/C++: #pragma omp *directive*
{ code block }

Fortran: !$omp *directive*
code block
!$omp end *directive*

Note: The directives are ignored by non-supporting compiler or if OpenMP-flag is turned off in compiling. => Portable code between single CPU, multi-core, and general parallel computers.

Also, possible to parallelize code incrementally (start with heaviest routine and continue until sufficient parallelism and performance are achived)

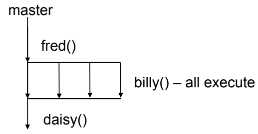
Parallel: (Fork-Join)

```
#pragma omp parallel [subdirectives]
{
"parallel code"
}
```

If no subdirectives, all data shared (global) and all code executed in parallel by all threads. At the end of parallel the threads are synchronized and joined.

Ex: program p1

```
...
call fred()
#pragma omp parallel
{ call billy() }
call daisy()
```



Example: helloworld.c

Data sharing:

- **shared**([list of variables]) - default
- **private**([list of variables])

Ex: program p2

```
...
a=10; b=0;
#pragma omp parallel private(a)
{
    a=a+10;
    b=b+a;
}
printf("a= %d, b= %d \n", a,b);
```

What is the result (assume 4 threads)?

Note: All private variables are allocated on the stack => uninitialized at entry and removed at exit, *original a* not equal to *private a*!

Note2: Shared variables must be protected from simultaneous writes by different threads! (Use a serial section directive.)

- **firstprivate**([list of variables])
  As private but the variables are initialized from the original variable (in master) before parallel.
- **lastprivate**([list of variables])
  At exit, the original variable gets the value from the thread executing the last iteration in a loop using the for-directive or the last section in the sections-directive.

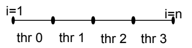
Work sharing (within parallel)

- Loop level parallelism – do/for
- Task parallelism – sections, tasks

do/for-directive:

```
!$omp do [subdirectives]
do i=1,n
    loop-body
end do
[ !$omp end do ]
```

```
#pragma omp for [subdirectives]
for (i=1; i<=n; i++)
    { loop-body }
```



Without subdirectives, loop counter is private, loop space is divided statically into nthr equal pieces, and run in parallel (different iterations in different threads). Threads are synchronized at end of the for-directive.

Note: We must have a perfectly parallel loop!

Example enumsort.c

Subdirectives:

- Private
- Firstprivate
- Lastprivate
- Reduction
- Schedule
- Ordered
- Collapse

Reduction(op:[list of variables])
Performs a global reduction using
op=+,-,*,max,min, or a logical operator

```
sum=0;
#pragma omp parallel for reduction(+:sum)
for (i=0;i<n;i++)
    sum=sum+a[i];
```

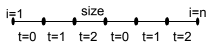
Same example without reduction:

```
sum=0;
#pragma omp parallel private(locsum)
{
    locsum=0;

    #pragma omp for
    for (i=0;i<n;i++)
        locsum=locsum+a[i];

    #pragma omp critical
    { sum=sum+locsum; }

}
```

Example enumsort.c

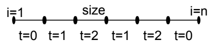
Schedule(type, [size])
Divides the iteration space into chunks=size and schedules the chunks to threads according to type. (size=n/nthr by default)

type=static:



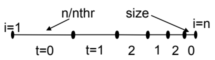
Assign the chunks cyclicly to threads

type=dynamic:



Dynamic scheduling, as soon as a thread is ready it gets a new chunk

type=guided:



As dynamic but the chunk size is decreasing exponentially. Minimizes synchronization time.

type=runtime:

Decide at runtime using the environment variable export *schedule=type* (where *type* is some above).

type=auto:

Let the run-time system and/or compiler decide automatically.

Note: Static scheduling is good for data locality (cache) while dynamic/guided good for load balance.

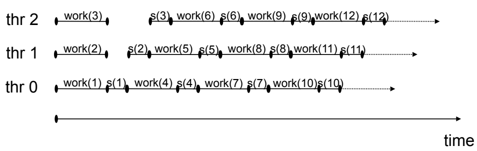
Ordered

Only one thread is allowed to the ordered block at a time and sequentially in loop order. Useful for I/O.

```
#pragma omp parallel
{
    #pragma omp for schedule(static,1) ordered
    for (i=0;i<n;i++)
    {
        call work(i)          ! parallel work

        #pragma omp ordered
        { call s(i) }         ! serial section
    }
}
```

Assume work(i)>>s(i) => Parallelism, pipelining effect

Static,1:



What happens if we use default scheduling (size=n/nthr)?

Collapse directive

Allow *collapsing* of perfectly nested loops, i.e., form a single loop and then parallelize that. Example: parallelize both i and j-loop in MxM

```
#pragma omp parallel
{
#pragma omp for collapse(2) private(i,j,k)
for (i=0;i<len;i++)
   for (j=0;j<len;j++)
    {
      c[i*len+j]=0.0;
      for (k=0;k<len;k++)
         c[i*len+j]+=a[i*len+k]*b[k*len+j];
    }
}
```

Task parallelism (static predefined tasks)

Sections

```
#pragma omp sections [subdirectives]
{
    #pragma omp section
        { task 1 }

    #pragma omp section
        { task 2 }

    etc.
}
```

Subdirectives:
- Private
- Firstprivate
- Lastprivate
- Reduction

The sections/tasks are scheduled (statically) to the threads and run in parallel. At end of sections the threads are synchronized. (No load balancing).

Nested parallelism (load balancing of sections)

```
omp_set_nested(1);
#pragma omp parallel sections omp_num_threads(2)
{
   #pragma omp section
   {
   #pragma omp parallel for omp_num_threads(P1)
   for (k=0;k<n;k++)
     call WORK1(A[K])
   }
   #pragma omp section
   {
   #pragma omp parallel for omp_num_threads(P2)
   for (k=0;k<n;k++)
     call WORK2(A[K])
   }
}
```

Assign appropriate number of threads to each section.

Task directive (dynamic tasks)

Can implement task-queues that are scheduled dynamically to all available threads in a parallel environment. Tasks can be generated at run-time.

Generate a task:
`#pragma omp task [if/untied/'`*`datasharing`*`']`
`{ task }`

Wait for all tasks to complete
`#pragma omp taskwait`

Task scheduling points at following locations:
1. Generation of task
2. Last instruction in task
3. Taskwait-directive
4. Implicit and explicit barriers

Serial sections

Avoid terminating threads, lose data in cache if threads rescheduled to different CPUs or cores (with fork-join model).

#pragma omp single [subdirectives]
The code-block within single is executed only by one thread, the others skip and wait at the end of block.
Subdirectives: - private
- firstprivate

#pragma omp master
The code-block is executed only by master thread, the other skip and continue (no barrier).

#pragma omp critical [name]
The code-block is executed by one thread at a time. As ordered but no predefined order.
If no name all critical sections have the same name. Only one critical section with the same name can be executed by one thread at a time.

#pragma omp atomic
Atomic update by one thread at a time. As critical but applies only for a one line expression. (Does not include a memory flush.)

Synchronization

Done implicitly at end of:
- parallel
- do/for
- sections
- single

Explicit barrier:
#pragma omp barrier

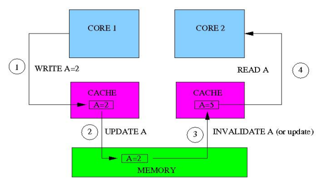
Can override with *nowait:*

```
!$omp do
do i=1,n
    code
end do
!$omp end do nowait
```

```
#pragma omp for nowait
for (i=0;i<n;i++)
    { code }
```

Note: If *nowait* be careful not to use data updated by other threads, *nowait* overrides memory flush!

In a **memory flush** all thread visible shared variables are refreshed (caches invalidated and memory updated). A memory flush is performed at all barriers (implicit and explicit) and before/after a critical directive.



Conceptual model

=> Be very careful with nowait !!! (Nowait removes 2 & 3)

OpenMP has a *relaxed-consistency* model, i.e., the threads can cache data not keeping exact consistency.

 Memory.c

Synchronization with locks

Can lock a code section and/or data only accessible to a specific thread. Routines include a flush.

```
omp_init_lock - omp_destroy_lock
omp_set_lock  - omp_unset_lock
omp_test_lock
```

Example:

```
omp_lock_t lockvar;
omp_init_lock(lockvar);
…
#pragma omp parallel {
…
   omp_set_lock(lockvar);
   sum=sum+a;
   omp_unset_lock(lockvar);
}
```


Performance obstacles in OpenMP:

- Fork/Join
  Time to create new threads, rescheduling
- Non-parallelized regions, serial sections
  Amdahl's law, Speedup < 1/s
- Synchronization
  Explicit/implicit barriers
- Load imbalance
  Trivial or naïve load balancing with OpenMP directives
- Cache misses => "communication"
  True/false sharing
- Non-optimal data placement on NUMA
  Costly remote memory accesses

Non-parallelized regions, serial sections:

* Split work at highest level => force code to be parallel.
* Overlap serial sections (ordered/single/master/critical) with other parallel activities, e.g., as using *ordered* above and as using *single* in iterative solver below. Have different names on different *critical* sections.

Synchronization:

* Minimize load imbalance.
* Analyze and remove implicit barriers between independent loops, using nowait.
* Use large parallel regions, avoid fork-join synch (also good for cache performance, threads not re-scheduled).
* Overlap activities to remove barriers (*Iterative solver*).
* Use locks to remove global barriers (*LU-factorization*).

Load imbalance:

* Use schedule-directive

```
#pragma omp parallel for schedule(type,[chunk])
for(i=0;i<n;i++)
    work(a[i]);
```

Where: type = static, dynamic, guided
static: regular work load, cache locality
dynamic, guided: irregular or unknown work load

* Use explicit load balancing

```
computeload(LB,UB,nthr);
#pragma omp parallel private(i,id)
 {
   id=omp_thread_num();
   for (i=LB(id);i<UB(id);i++)
       work(a[i]);
 }
```


Problems with the schedule directive:

Ex 1: 13 iterations, 6 threads
default schedule => 3,3,3,3,1,0
explicit partition => 3,2,2,2,2,2

Ex 2: How to perform a 2D-decomposition?
E.g., the Ocean modelling problem

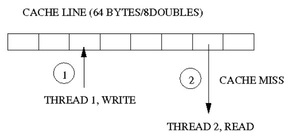
Ex 3: Consider 2 threads and 7 tasks with weights (run time): 5,2,3,4,5,2,10
Static => 14,17
dynamic,1 => 11,20
bin-pack => 16,15

=> Use explicit scheduling if bad performance

Cache misses: (“communication”)

* Cold/compulsory - first time access
* Conflict/capacity - “full” cache

* True sharing - invalid data
* False sharing - invalid cache line

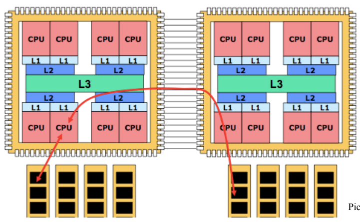


Minimize cache misses: (Application dependent)

* Re-use data as much as possible before replace, e.g., by cache blocking and loop fusion.
* Access data in sequence, e.g., by grouping data and by arranging loop order.
* Create dense data partitions, e.g., by using large chunk size following the data layout.

Note: schedule(static,1) generates a lot of false sharing, better with schedule(static,8) for scheduling whole cache lines.

Data placement, the NUMA problem:
(Consider multi-socket multicore nodes, e.g., AMD Magny Cores)



Picture by Erik Hagersten

Non-**U**niform **M**emory **A**ccess times, i.e., different access times to local memory close to your core and to remote memory close other cores.

=> Need control of data placement and localization of the data accesses (explicit user control)!

Memory placement often handled with *first touch,* i.e., memory is bound to the first touching thread with page granularity (typically 8KB).

=> Use parallel initalization with same access pattern as in the computations

(If serial init, all data allocated in touching thread's node. All other threads generate remote accesses and we get memory congestion.)

```
! Init
do i = 1, N
   do j = 1, M
      arrays(i,j) = ....
   end do
end do

!$OMP PARALLEL SHARED(arrays)
   .
!$OMP DO SCHEDULE(STATIC)
do i = 1, N
   do j = 1, M
      arrays(i,j) = ....
   end do
end do
   .
   .
```

Avoid serial init on NUMA

Note: Need static access pattern, e.g., using schedule(dynamic) destroys the data locality

Remedy: use user supplied load balancing

```
call loadbal(LB,UB,P)
!$OMP PARALLEL PRIVATE(ID,J)
   call OMP_THREAD_NUM(ID)
   DO J=LB(ID),UB(ID)
     A(J)=INIT(J)        !INIT, FIRST TOUCH
   END DO
   !$OMP BARRIER
   DO J=LB(ID),UB(ID)
     CALL WORK(A(J))     !WORK, STATIC ACCESS
   END DO
!$OMP END PARALLEL
```

Good for cache performance on a multicore node!

Case studies:

1. Iterative solver

```
while (norm>eps)
   y=Ax
   norm=||y-x||
   x=y
end while
```

E.g. - Jacobi for linear system of equations
- Conjugate Gradient for optimization
- Power method for eigenvalues

```
!$omp parallel
      do while(norm>eps)

           !$omp do private(j)
           do i=1,n
                do j=1,n
                     y(i)=y(i)+A(i,j)*x(j)
                end do
           end do
           !$omp end do

           !$omp single
           norm=0
           !$omp end single

           !$omp do reduction(+:norm)
           do i=1,n
                norm=norm+(y(i)-x(i))**2
           end do

           !$omp single
           swap(x,y)
           !$omp end single

      end do
!$omp end parallel
```

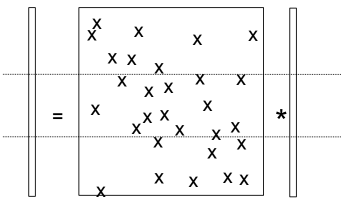
=> 4 barriers per iteration

Improve:
- Make x,y private
- Remove barriers between independent loops
- Unroll 2 iterations

=> 1 barrier per iteration


```
norm1=0; norm2=0;
!$omp parallel firstprivate(x,y)
do while (1)

     !$omp do private(j)
     do i=1,n
          do j=1,n
               y(i)=y(i)+A(i,j)*x(j)
          end do
     end do
     !$omp end do nowait

     !$omp single
     norm2=0
     !$omp end single nowait

     !$omp do reduction(+:norm1)
     do i=1,n
          norm1=norm1+(y(i)-x(i))**2
     end do

     swap(x,y)
     if (norm1<=eps) break

     !$omp do private(j)
     do i=1,n
          do j=1,n
               y(i)=y(i)+A(i,j)*x(j)
          end do
     end do
     !$omp end do nowait

     !$omp single
     norm1=0
     !$omp end single nowait

     !$omp do reduction(+:norm2)
     do i=1,n
          norm2=norm2+(y(i)-x(i))**2
     end do

     swap(x,y)
     if (norm2<=eps) break

end do
!$omp end parallel
```


2. Sparse matrix-vector multiplication (y=Ax)



thread 0

thread 1

thread 2

Use compressed sparse row format

val(nnz)	: nonzeros in matrix
col(nnz)	: column of nonzeros
row(nrows)	: starting pos of rows

Algorithm:

```
!$omp parallel do private(d,j)
do i=1,nrows
     d=0
     do j=row(i),row(i+1)-1
          d=d+val(j)*x(col(j))
     end do
     y(i)=d
end do
```

What are the parallel overheads?
(Assume MxV is part of an iterative solver, e.g., Conjugate-Gradient solver)

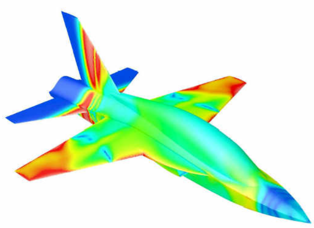
Schedule(static):
- Load imbalance, different number of non-zeros per row
- True sharing, need updates of x-vector
- Remote accesses if large bandwidth

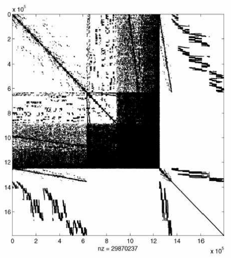
Schedule(dynamic):
- True sharing, need updates of x-vector
- False sharing, multiple updates of cache lines
- Remote accesses regardless of bandwidth

Note: Smaller bandwidth decreases true sharing remote accesses => Use bandwidth minimization, e.g., Reverse Cuthill-McKee

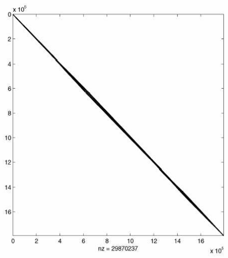
Real application, GEMS:

Maxwell's equations discretized with FEM-grid around a fighter jet => Ax=b with 1.8 million unknowns, solved with the CG method





Original matrix



Bandwidth minimized

Performance of GEMS solver:

	Original	RCM
Load	1.24	1.01
Time	336.7	234.6

S=1.44

Table 1: Sun E10K, UMA

	Original	RCM
Load	1.24	1.01
Time	131.3	74.8
L2 miss	427M	376M
Remote	125M	70M

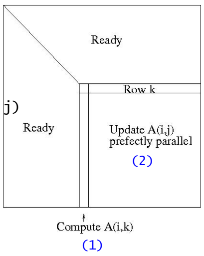
S=1.76

Table 2: Sun Fire 15K, NUMA

[Ref: H. Löf, J. Rantakokko, *Algorithmic Optimization of a Conjugate Gradient Solver on Shared memory systems*, International Journal of Parallel, Emergent and Distributed Systems, Vol 21, 2006.]

3. LU-factorization

```
    for k=1 to n
       for i=k+1 to n
(1)          A(i,k)=A(i,k)/A(k,k)
       end for
       for j=k+1 to n
          for i=k+1 to n
(2)             A(i,j)-=A(i,k)*A(k,j)
          end for
       end for
    end for
```



Parallelize update of A(i,j) over the j-loop*.

(* In C, change loop order and parallelize over i)

Parallel overheads:

- Frequent global synch of all threads (for each k)
- Non-static data partitions (the parallel loops shrink) lose data locality

Improvements:

- One large parallel region (including k-loop)
- Static partitioning cyclicly over columns
- First touch using parallel initialization
- Individual synchronization using locks


```
!-- Set up locks for each column
  do i=1,n
    call omp_init_lock(lck(i))
  end do

!$OMP PARALLEL PRIVATE(i,j,k,thrid)
  thrid=omp_get_thread_num();

!– Initate (parallel first touch)
!$OMP DO SCHEDULE(STATIC,chunk)
  do j=1,n
    do i=1,n
      A(i,j)=1.0/(i+j)
    end do
    call omp_set_lock(lck(j))
  end do
!$OMP END DO

!-- First column of L
  if (thrid==0) then
    do i=2,n
      A(i,1)=A(i,1)/A(1,1)
    end do
    call omp_unset_lock(lck(1))
  end if
```

```
!-- LU-factorization
  do k=1,n
    call omp_set_lock(lck(k))
    call omp_unset_lock(lck(k))
!$OMP DO SCHEDULE(STATIC,chunk)
    do j=1,n
      if (j>k) then
        do i=k+1,n
          A(i,j)=A(i,j)-A(i,k)*A(k,j)
        end do
        if (j==k+1) then
          do i=k+2,n
            A(i,k+1)=A(i,k+1)/A(k+1,k+1)
          end do
          call omp_unset_lock(lck(k+1))
        end if
      end if
    end do
!$OMP END DO NOWAIT
  end do

!$OMP END PARALLEL
```

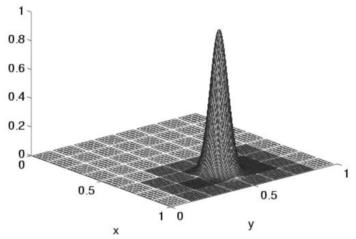

Performance: (Sun E10K)

Threads	LU-standard	LU-lock
1	31.4	29.7
2	5.83	3.32
4	3.44	1.69
8	2.37	0.97
16	2.62	0.63
24	3.20	0.44

=> 6 times performance improvement!
What about multi-core? Experiment at hands-on session.

4. Adaptive Mesh Refinement

(Research example of the data placement problem on NUMA)



Use higher resolution (block wise) in areas of interest

The problem:

- Pulse moves in the domain => The grid adaption is dynamic and follows the pulse.
- We do the parallelization over the blocks, i.e., each thread is responsible for a number of blocks.

↓

Work load per thread change as the blocks are refined or coarsened => Need to repartition data at runtime (even blocks that are not changed).

How? What do we need to consider?

- Optimize load balance, equal work load
- Minimize communication, i.e., neighbor blocks within the same partition as far as possible
- Minimize change of ownership for blocks

=> Use a *diffusion algorithm*, e.g., from Jostle or ParMetis.

Problem: Data locality is destroyed!

Remedy: `Migrate-on-next-touch*`

(* Sun specific solution, re-do first touch. On other systems, re-allocate blocks on new owners and do first touch.)

Performance results:

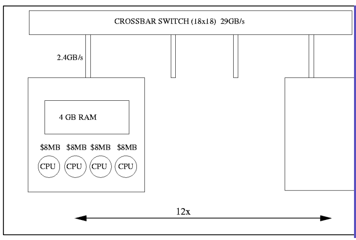
	No migration	Migration
CPU time	6.64h	3.99h
Remote acc	62.9%	8.1%

Performance: SunFire 15K

Data partitioning and explicit control of data => 66% performance improvement (2.6h)

[Ref: M. Norden, H. Löf, J. Rantakokko, S. Holmgren, *Dynamic data migration for structured AMR solvers*, International Journal of Parallel Programming, 2007]

SunFire 15K (2002), "Ngorongoro"



- 12x4 Ultra Sparc IIIcu, 900MHz + 1x4 US IV+ dual-core, 1.3GHz
- 12x4 GB (48GB RAM)
- Peak performance: 2x48x900MFlops = 86.4 Gflop/s
- List price: ~20M SEK