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Parallel Programming with OpenMP and MPI

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Lecture 5: More basics of OpenMP

High Performance Computing

Outline of course

- Basics of parallel computer architecture
- Basics of parallel computing
- Introduction to shared-memory programming with OpenMP
- OpenMP performance issues
- Introduction to the Message Passing Interface (MPI)
- Advanced MPI
- MPI performance issues
- Hybrid MPI+OpenMP programming

OpenMP reductions

Operations on data across threads

- Recurring problem: Operations across thread-local instances of a variable

```
int i,N;
double a[N], b[N];
...
s=0.;
#pragma omp parallel firstprivate(s)
{
#pragma omp for
  for(i=0; i<N; ++i)
      s = s + a[i] * b[i];
  // How to sum up the different s?
}
```

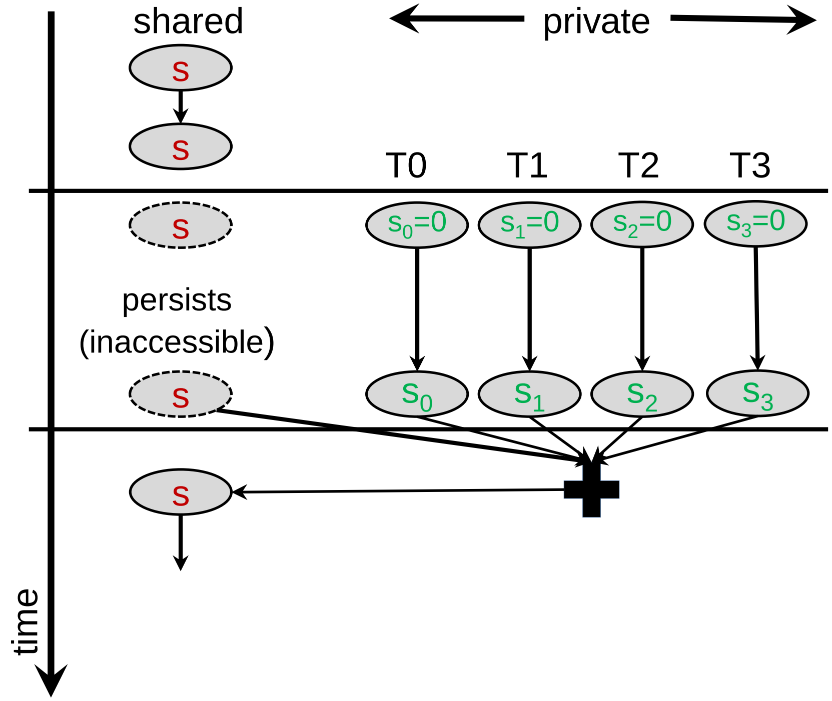
- Solution: `reduction` clause

Reduction clause on parallel region or workshared loop

```
int i,N;
double a[N], b[N];
...
s=0.;
#pragma omp parallel
{
// s is still shared here
#pragma omp for reduction(+:s)
  for(i=0; i<N; ++i)
      s = s + a[i] * b[i];
// s is shared again here
}
```

At synchronization point:

- reduction operation is performed
- result is transferred to master copy
- restrictions similar to **`firstprivate`**



Reduction variable must be shared in enclosing context!

Reduction operations: general considerations

Fortran has an analogous set

Oper-ation	Initial value
`+`	0
`-`	0
`*`	1
`&`	`~0`
`|`	0
`^`	0
`&&`	1
`||`	0
`max`	`MINVAL(type)`
`min`	`MAXVAL(type)`

Multiple reductions:

```
float x, y, z;
#pragma omp for reduction(+:x, y, z)
```

```
#pragma omp for reduction(+:x, y) \
                reduction(*:z)
```

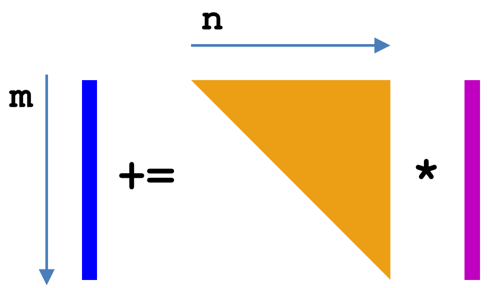
Consistency required!

`x = expr - x` is not allowed

Don’t lie.

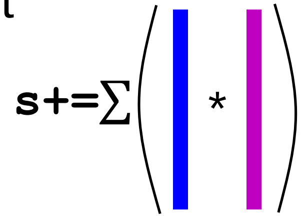
Reduction operations: Example

```
double s, a[size*size], x[size], y[size];
...
s=0.;
#pragma omp parallel
{
#pragma omp for schedule(???)
    for(int m=0; m<size; m++){
      for(int n=m; n<size; n++){
        y[m] += a[m*size+n] * x[n];
      }
    }
...
#pragma omp for reduction(+:s)
    for(int m=0; m<size;m++) {
      s += x[m] * y[m];
    }
...
}
```



dense triangular MVM

scalar product



Reductions on arrays

- Elementwise reductions on arrays (or slices thereof)

```
#pragma omp parallel for reduction(+:y[0:rows])
for(int c=0; c<cols; ++c)
  for(int r=0; r<rows; ++r)
     y[r] += a[r+c*rows] * x[c];
```

C/C++: Array slice syntax is mandatory

Fortran: No slice necessary on full array reduction

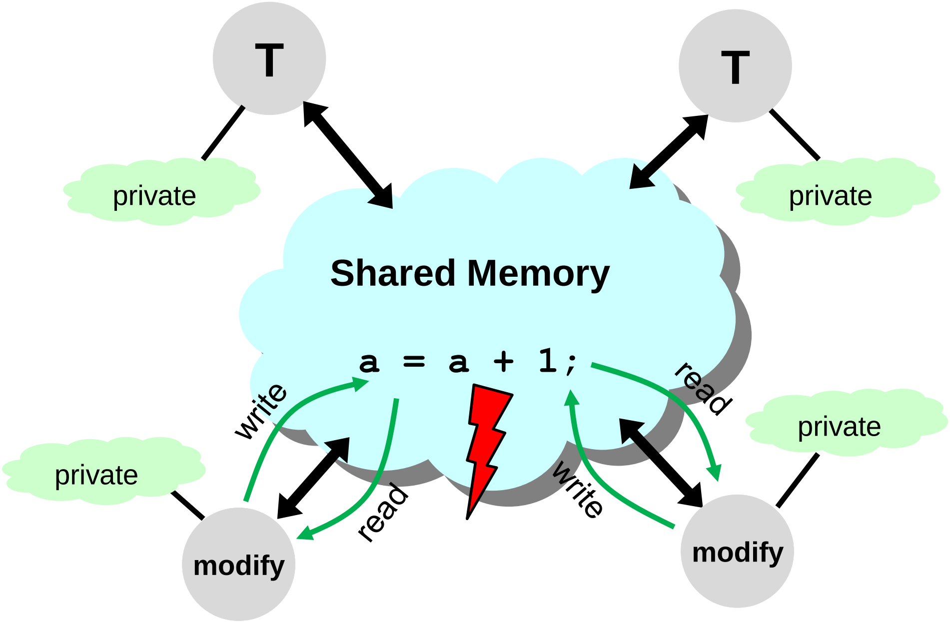
```
!$omp parallel do reduction(+:y)
do c = 1 , C
  do r = 1 , R
     y(r) = y(r) + A(r,c) * x(c)
  enddo
enddo
!$omp end parallel do
```

OpenMP synchronization

Ensuring consistency

Why synchronization?

Example: variable update (read – modify – write)



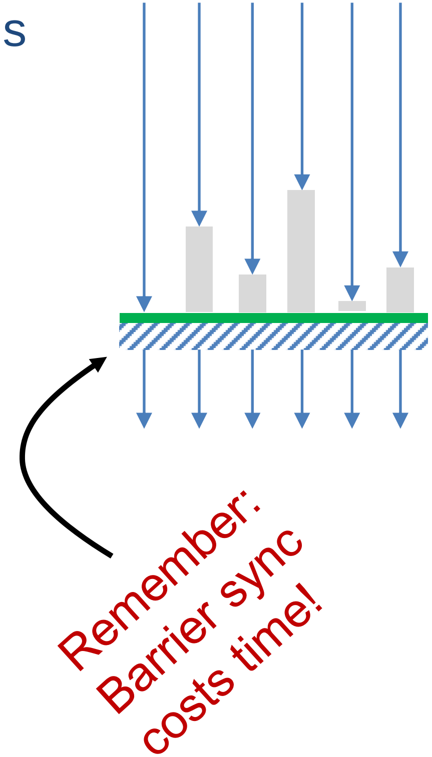
Multiple threads access shared variable, and at least one writes to it
→ “race condition”

Synchronization = means to manage conflicting/uncontrolled accesses

Barrier synchronization

- **`#pragma omp barrier`**
  - Each thread blocks upon reaching the barrier until all threads have reached the barrier
  - All accessible shared variables are flushed to the memory hierarchy (similar to **`volatile`** attribute in C/C++)
  - barrier may not appear within work-sharing construct (e.g., **`omp for`** block) → potential of deadlock

- Implicit barrier:
  - at the beginning and end of parallel regions
  - at the end of worksharing constructs unless a **`nowait`** clause is present



Relaxing synchronization requirements

- The **nowait** clause
  - removes the implicit barrier at end of worksharing construct
  - potential performance **improvement** (especially if load imbalance occurs within construct)
  - Programmer is responsible for preventing race conditions!

```
#pragma omp parallel
{
    #pragma omp for nowait
      for(int i=0; i<N; ++i) {
        a[i] = some_stuff(i);
      }
      // ... More parallel work (don't reference a[])
    #pragma omp barrier
      ... = a(i);    // after deferred barrier
}
```

No barrier here

Case study: reducing barrier cost for dense MVM

- General advice: Parallelize as far out as possible!

```
void dmvm(int n, int m, double *lhs,
          double *rhs, double *mat){
...
#pragma omp parallel for
  for(int c=0; c<n; ++c)
    int offset = m * c;
    for(int r=0; r<m; ++r)
      lhs[r] += mat[r + offset] * rhs[c];

}
```

Only one barrier…

… but race condition on `lhs[]`

Reducing barrier cost: dense MVM

- Inner loop parallel → correct result

```
void dmvm(int n, int m, double *lhs,
          double *rhs, double *mat){
...
#pragma omp parallel
{
  for(int c=0; c<n; ++c)
    int offset = m * c;
    #pragma omp for
    for(int r=0; r<m; ++r)
      lhs[r] += mat[r + offset] * rhs[c];
}
}
```

Only one parallel region

… but **n** implicit barriers

Result is correct: threads work on separate parts of **lhs[]**

Reducing barrier cost: dense MVM

- Inner loop parallel → correct result, and use **`nowait`** to avoid barriers

```
void dmvm(int n, int m, double *lhs,
          double *rhs, double *mat){
...
#pragma omp parallel
{
  for(int c=0; c<n; ++c)
    int offset = m * c;
    #pragma omp for schedule(static) nowait
    for(int r=0; r<m; ++r)
      lhs[r] += mat[r + offset] * rhs[c];
}
}
```

Only one parallel region

No implicit barriers on workshared loop

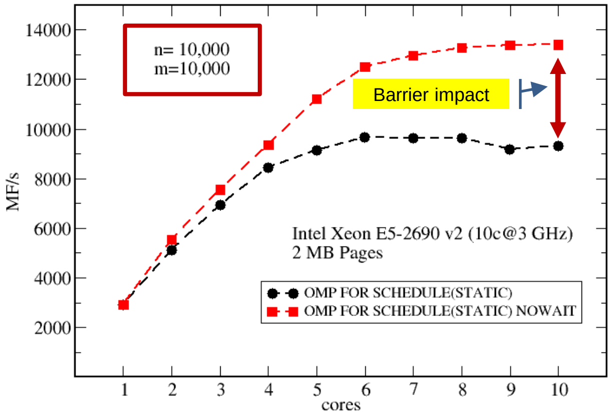
Ensure same iteration-to-thread mapping

One implicit barrier

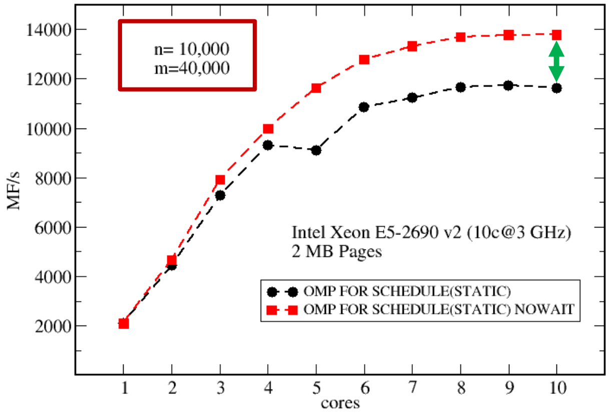
Result is correct: threads work on separate parts of **`lhs[]`**

Reducing barrier cost: dense MVM

- Barrier overhead may substantially decrease performance
- Performance impact decreases as inner loop length (work per barrier) increases (see m=40,000 vs. m=10,000)



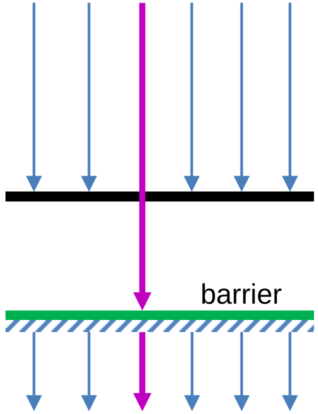
- Use **`nowait`** with due care (correctness)!



- Is the performance as expected? What does the barrier cost?
  - → homework

The `single` directive

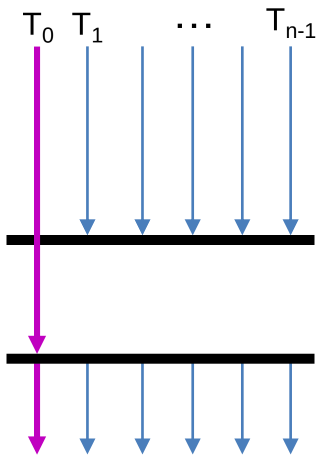
- `#pragma omp single [clause[[,]clause]…]`
  `    structured-block`
- Structured block is executed by exactly one thread, which one is unspecified
  - Actually a worksharing directive
- Remaining threads skip the structured block and continue execution.
- Implied barrier at the exit of the single section!



- Do not use within another worksharing construct (deadlock!)
- `nowait` clause suppresses barrier

The `master` directive

- `#pragma omp master [clause[[,]clause]…]`
  `structured-block`
- Only thread zero executes the structured block
- Other threads continue without synchronization
- Not all threads have to reach the construct

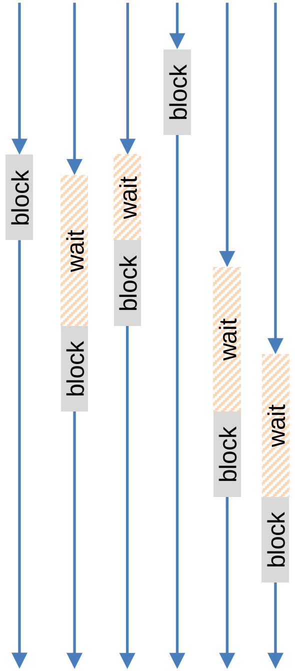


- Essentially equivalent to:

```
#ifdef _OPENMP
if(omp_get_thread_num()==0)
#endif
   structured-block;
```

Critical region

- `#pragma omp critical`
  `structured-block`
- Only one thread at a time can execute the block
- … but every thread that encounters it will eventually execute it
- Order of execution is undefined!
- All unnamed critical regions are mutually exclusive across the whole program
  - Beware of deadlocks!



Named critical regions

- What if I want several independent critical regions?
  - Named critical regions to the rescue!
- Regions with different names are mutually independent
- Name can be chosen freely
  - No association with data to be “protected”
- Unnamed critical regions share the same (invisible) name

```
double func(double v) {
  double x;
#pragma omp critical(prand)
    x = v + random_func();
  return x;
}
...
#pragma omp parallel for private(x)
for(int i=0; i<N; ii+) {
  x = sin(2.*M_PI*i/N);
  #pragma omp critical(psum)
    sum += func(x);
}
```

Atomic updates

- `#pragma omp atomic [clause[[,] clause] ... ]`
  `expression-stmt`
- Ensures that a storage location is accessed atomically, i.e., the full access cannot be interrupted
- Applies only to the statement immediately following it
- **`expression-stmt`** can be:

```
x++;
x--;
++x;
--x;
x binop= expr;
x = x binop expr;
x = expr binop x;
```

- Variants of **`atomic`** for pure read, pure write, and capture are also available

Why `atomic`?

Can't I just use a critical region?

1. **`atomic`** *may* be more efficient due to hardware support (no guarantee!)
2. **`atomic`** allows for protecting updates to individual data elements

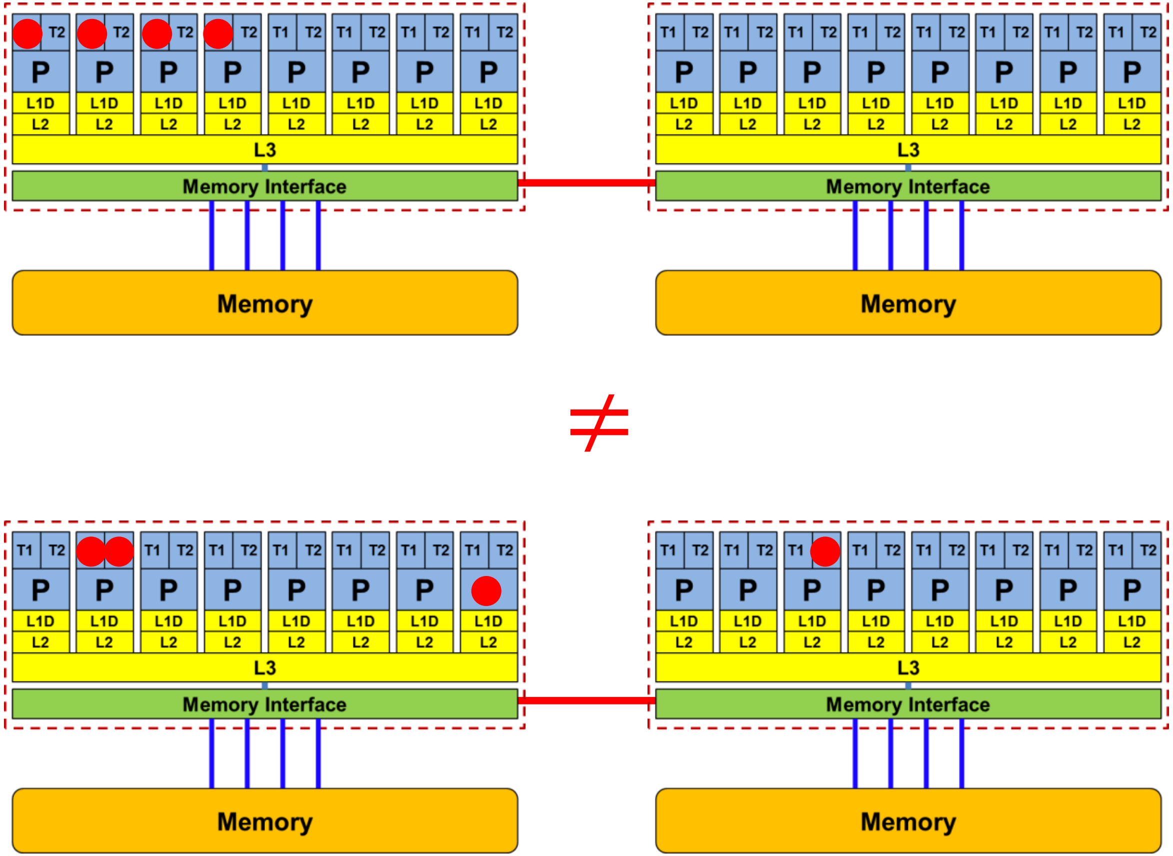
```
#pragma omp parallel for
for (i=0; i<n; i++) {
  double t = func(table[i]);
  if(t < 0.) {
    #pragma omp atomic
      x[table[i]]++;
  }
  y[i] += other(i);
}
```

Updates of different **`x[]`** entries do not block each other

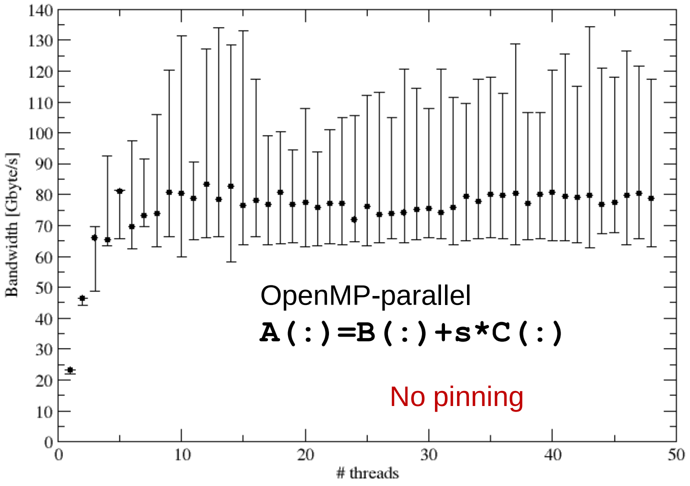
OpenMP affinity

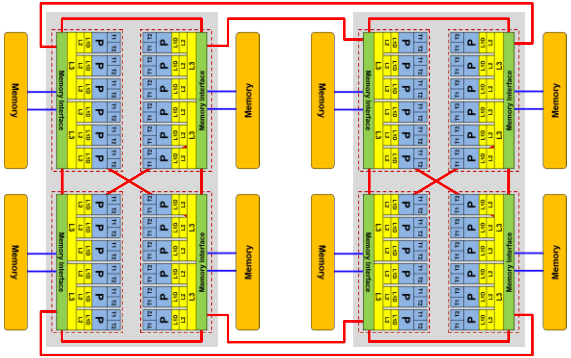
OpenMP affinity: it matters!

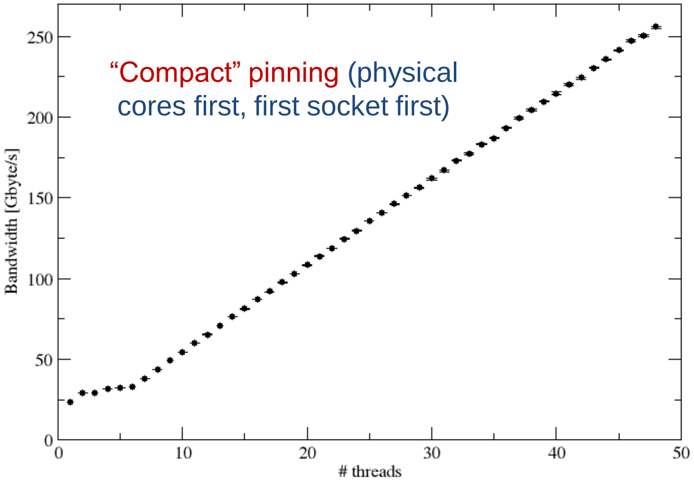
- Remember all the hardware bottlenecks!
- It *does* matter where the threads are running
- Yes, it’s up to you
- No, the system will not magically guess what’s best



STREAM benchmark on 2x24-core AMD “Naples”: Anarchy vs. thread pinning







There are several reasons for caring about affinity:

- Eliminating performance variation
- Making use of architectural features
- Avoiding resource contention

OMP_PLACES and Thread Affinity

- Processor: smallest entity able to run a thread or task (SMT/hyper-thread)
- Place: one or more processors → thread pinning is done place by place
- Free migration of the threads on a place between the processors of that place.

abstract name

OMP_PLACES	Place ==
`threads`	Hardware thread (hyper-thread)
`cores`	All HW threads of a single core
`sockets`	All HW threads of a socket
`abstract_name(num_places)`	Restrict # of places available

Or use explicit numbering, e.g. 8 places, each consisting of 4 processors:

- `OMP_PLACES="{0,1,2,3},{4,5,6,7},{8,9,10,11}, … {28,29,30,31}"`
- `OMP_PLACES="{0:4},{4:4},{8:4}, … {28:4}"` — <lower-bound>:<number of entries>[:<stride>]
- `OMP_PLACES="{0:4}:8:4"`

Caveat: Actual behavior is implementation defined!

OMP_PROC_BIND variable / proc_bind() clause

Determines how places are used for pinning:

OMP_PROC_BIND	Meaning
FALSE	Affinity disabled
TRUE	Affinity enabled, implementation defined strategy
CLOSE	Threads bind to consecutive places
SPREAD	Threads are evenly scattered among places
MASTER	Threads bind to the same place as the master thread that was running before the parallel region was entered

If there are more threads than places, consecutive threads are put into individual places (“balanced”)

Example:

```
$ OMP_NUM_THREADS=4 OMP_PROC_BIND=close OMP_PLACES=cores ./a.out
```

Some simple OMP_PLACES examples

Intel Xeon w/ SMT, 2x10 cores, 1 thread per physical core, fill 1 socket

```
OMP_NUM_THREADS=10
OMP_PLACES=cores
OMP_PROC_BIND=close
```

Always prefer abstract places instead of hardware thread IDs!

Intel Xeon Phi with 72 cores, 4-way SMT
32 cores to be used, 2 threads per physical core

```
OMP_NUM_THREADS=64
OMP_PLACES=cores(32)
OMP_PROC_BIND=close    # spread will also do
```

Intel Xeon, 2 sockets, 4 threads per socket (no binding within socket!)

```
OMP_NUM_THREADS=8
OMP_PLACES=sockets
OMP_PROC_BIND=close    # spread will also do
```

Intel Xeon, 2 sockets, 4 threads per socket, binding to cores

```
OMP_NUM_THREADS=8
OMP_PLACES=cores
OMP_PROC_BIND=spread
```

Wrap-up: beginner’s OpenMP toolbox

- Parallel region
- Workshared loop construct
- Data scoping (shared, private, firstprivate)
- Basic reductions with standard operators
- Simple synchronization constructs
  - barrier, nowait
  - (named) critical, atomic
  - single (actually worksharing), master
- OpenMP affinity as defined in the standard

- But wait, there’s more…