

HPC Lab

Session 2: OpenMP

Carsten Uphoff, Chaulio Ferreira, Michael Bader
TUM – SCCS

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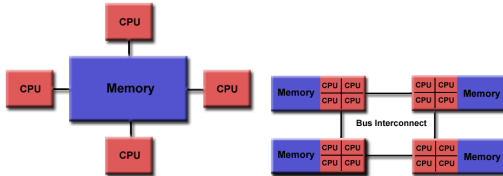
What is OpenMP?

“OpenMP is a specification for a set of compiler directives, library routines, and environment variables that can be used to specify high-level parallelism in Fortran and C/C++ programs”

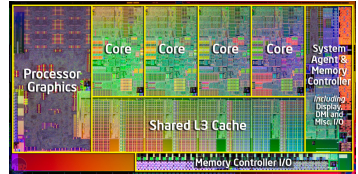
<http://openmp.org/openmp-faq.html#WhatIs>

Shared-Memory-Parallelism

- Transparent programming view: Cores access “same” memory
- In hardware: Be aware of layout, e.g. NUMA



<https://computing.llnl.gov/tutorials/openMP/>



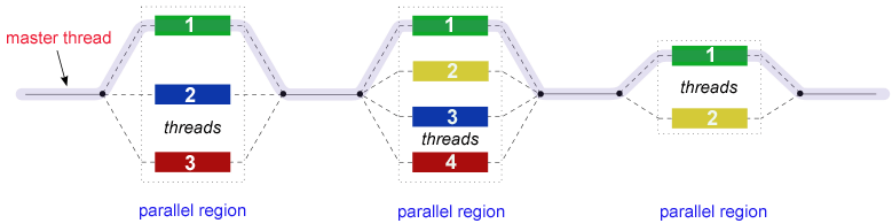
Sandy Bridge CPU,

<http://www.bit-tech.net/hardware/cpus/2011/01/03/intel-sandy-bridge-review/1>



Knights Corner and Knights Landing,
<http://www.zdnet.com/sc13-intel-reveals-knights-landing-high-performance-cpu-7000023393/>

Fork-Join Model



<https://computing.llnl.gov/tutorials/openMP/#ProgrammingModel>

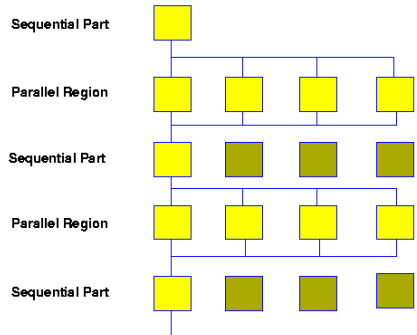
A Simple Loop

```

1 #include <omp.h>
2 // some initialization
3
4 #pragma omp parallel for
5 for (i = 0; i < n; i++) {
6     for (j = 0; j < n; j++) {
7         // do some work
8     }
9 }

```

OpenMP Execution Model



OpenMP - Parallel programming on shared memory systems

<https://www.lrz.de/services/software/parallel/openmp/>

OMP: An Overview

- Compiler-directives:
`#pragma omp ...[clause[[],] clause]...`
 - Parallel region
`#pragma omp parallel`
 - Work-sharing
`#pragma omp for ...`, and many more
 - Synchronization
`#pragma omp barrier`, and many more
- Data Scope Clauses
`shared`, `private`, `firstprivate`, `reduction`, ...
- Library routines
`omp_get_num_threads()`, `omp_get_thread_num()`, ...

Compilation and Execution

- compile with additional Compiler-Flag `-qopenmp`:
`icpc -qopenmp -o my_algorithm alg.c`
- export `OMP_NUM_THREADS=number_of_threads`
`./my_algorithm`

Parallel Region

```
1 | #pragma omp parallel [clause[[,] clause]...]  
2 | structured block
```

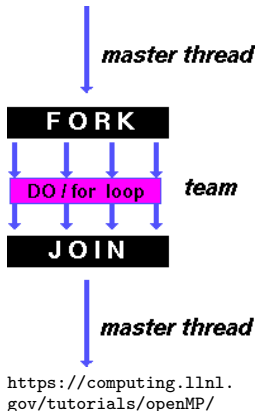
- code within parallel region is executed by all threads

```
1 | #include <omp.h>  
2 | // more initialization ...  
3 |  
4 | #pragma omp parallel  
5 | {  
6 |     int size = omp_get_num_threads();  
7 |     int rank = omp_get_thread_num();  
8 |     printf("Hello World! (Thread %d of %d)", rank, size);  
9 | }
```


Work Sharing: `for`

```
#pragma omp for [clause[[,] clause]...]
for-loop
```

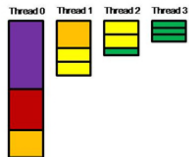
- within a *parallel* region and directly in front of a *for*-loop
- iterations are scheduled across different threads
- implicit synchronization at the end of *for*-loop (can be disabled with *nowait* clause)
- shortcut possible: `#pragma omp parallel for`



Work Sharing: for

```
#pragma omp for [clause[[],] clause]...
for-loop
```

- *schedule* clause determines how to map iterations to threads
 - *schedule(static[, chunk size])* default chunk size is #iterations divided by #threads
 - *schedule(dynamic[, chunk size])* default chunk size is 1
 - *schedule(guided[, chunk size])* similar to dynamic but initial chunk size as in static
 - *schedule(runtime)* Scheduling is given by environment variable OMP_SCHEDULE



(a) Unbalanced assignment of tasks to threads



(b) Balanced assignment of tasks to threads

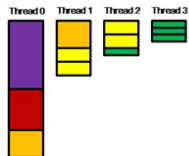
Intel, Load Balance and Parallel Performance,
<https://software.intel.com/en-us/articles/load-balance-and-parallel-performance>

Work Sharing: task

```
#pragma omp task [clause[[,] clause]...]
structured block
where clause can be...
```

- `final(expression)`: if *expression* is *true*, task is executed sequentially; no recursive task generation
- `untied`: the execution of a task is not tied to one single thread
- `shared | firstprivate | private [...]`

```
#pragma omp taskwait: waits for children completion
```



(a) Unbalanced assignment of tasks to threads



(b) Balanced assignment of tasks to threads

Intel, Load Balance and Parallel Performance,
<https://software.intel.com/en-us/articles/load-balance-and-parallel-performance>

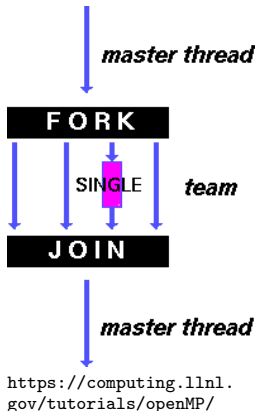
“Work Sharing”: single

```
#pragma omp single [clause[[],] clause]...
structured block
where clause can be...
```

- use only one (arbitrary) thread
- implicit synchronization (can be disabled with `nowait` clause)

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

- use only master thread for structured block
- NO synchronization at the end



Synchronization

- `#pragma omp barrier`: block execution until all threads have reached the barrier
- `#pragma omp critical`:
structured block
 - only one thread at a time can execute the structured block encapsulated by critical
 - *Warning*: Use carefully; can definitely kill performance.

Reduction

reduction(operator: list)

- executes a reduction of variables in list using operator
- available operators: +, *, -, &&, ||
since OpenMP 3.1: min, max

```
1 | #pragma omp parallel for private(r), reduction(+: sum)
2 | for(i = 0; i < n; i++) {
3 |     r = compute_r(i);
4 |     sum = sum + r;
5 | }
```

Scopes

- `private(list)`: *declares* variables in list as private for each thread (*no copy*)
- `shared(list)`: variables in list are used by all threads (race conditions are possible), write accesses have to be handled by the programmer
- `firstprivate(list)`: private variables *and* init them with the latest valid value before parallel region
- `lastprivate(list)`: variable in the serial part receives the value from the thread executing the last parallel iteration
- ...
- default data scope is shared, but exceptions exist \Rightarrow be precise
 - local variables are always *private*
 - loop-variables of *for*-loops are private

Fill the Gaps

```
1 | k = compute_k();  
2 |  
3 | #pragma omp parallel for private(?), shared(?), firstprivate(?), lastprivate(?),  
   |     reduction(?)  
4 | for (i = 0; i < n; i++) {  
5 |     k = compute_my_k(i, k);  
6 |     r = compute_r(i, k, h);  
7 |     sum = sum + r;  
8 | }
```


Nested parallelism

Enable with `OMP_NESTED` or `omp_set_nested(1)`.

```
1 | omp_set_nested(1);
2 |
3 | #pragma omp parallel num_threads(4)
4 | {
5 |     printf("outer thread id %d\n", omp_get_thread_num());
6 |     #pragma omp parallel num_threads(2)
7 |     {
8 |         printf("inner thread id %d\n", omp_get_thread_num());
9 |     }
10| }
```

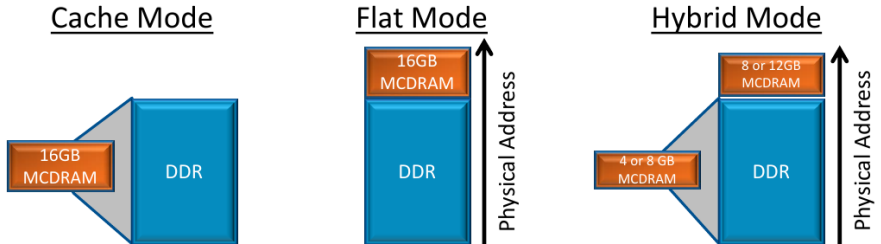
- Not nested: 4 threads
- Nested: 8 threads

KNL memory modes

Two kinds of memory.

- DDR: up to 384 GB, off-chip, slow
- MCDRAM: 16 GB, on-chip, fast

Memory mode selected at boot time:



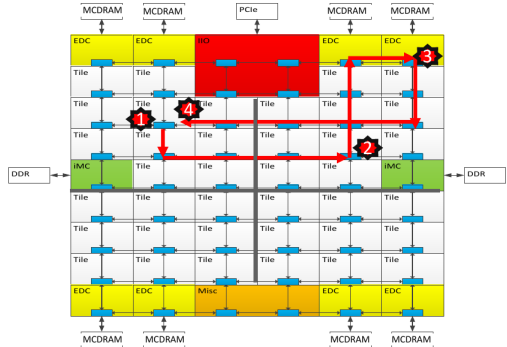
<https://www.alcf.anl.gov/files/HC27.25.710-Knights-Landing-Sodani-Intel.pdf>

KNL cluster modes

<https://www.alcf.anl.gov/files/HC27.25.710-Knights-Landing-Sodani-Intel.pdf>

Three agents:

1. Core – Initiates a memory request
2. Tag directory – Memory request is forwarded to tag directory which knows the dedicated memory channel
3. Memory channel – Memory channel sends request to memory

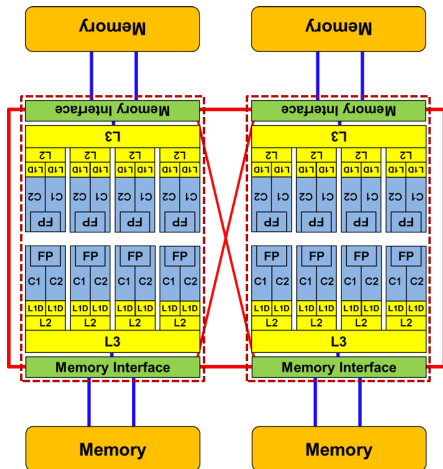


1) L2 miss, 2) Directory access, 3) Memory access, 4) Data return

Cluster mode (All2All, Quadrant, SNC-2/4) determines affinity of tag directory and memory channel. SNC exposes quadrants as NUMA domains.

NUMA

- Non-uniform memory access (NUMA): Not all cores access all memory in the same manner
- Pinning: Use close-to-core memory as far as possible
 - Linux first touch policy: *not the malloc counts but the first (write) access*
 - numactl is a useful tool



Georg Hager's Blog,
<http://blogs.fau.de/hager/>