Introduction to OpenMP

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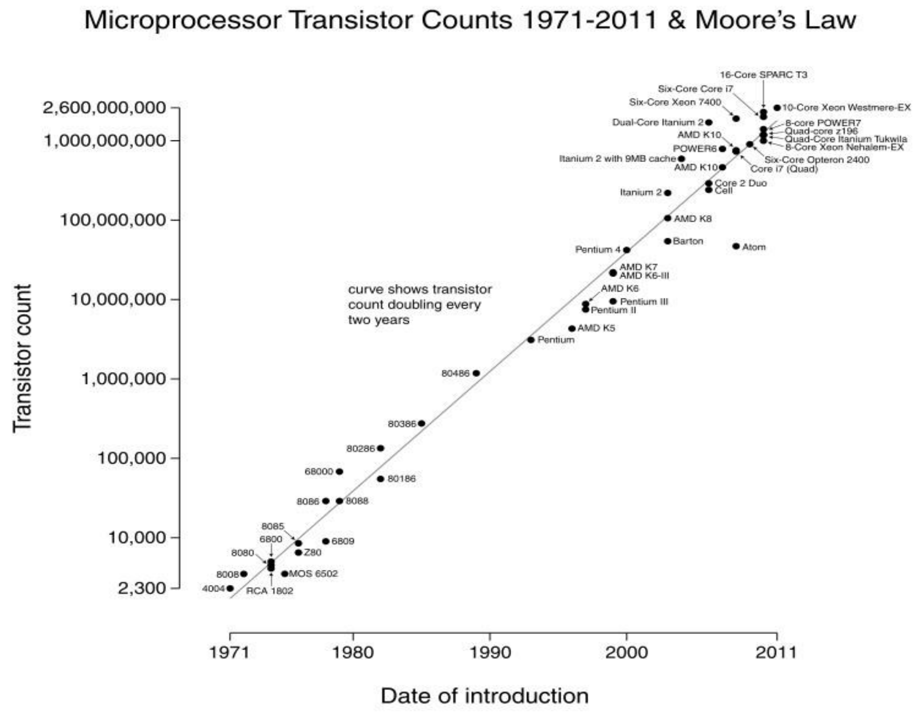
INTRODUCTION PARALLELIZATION

Why parallelization?

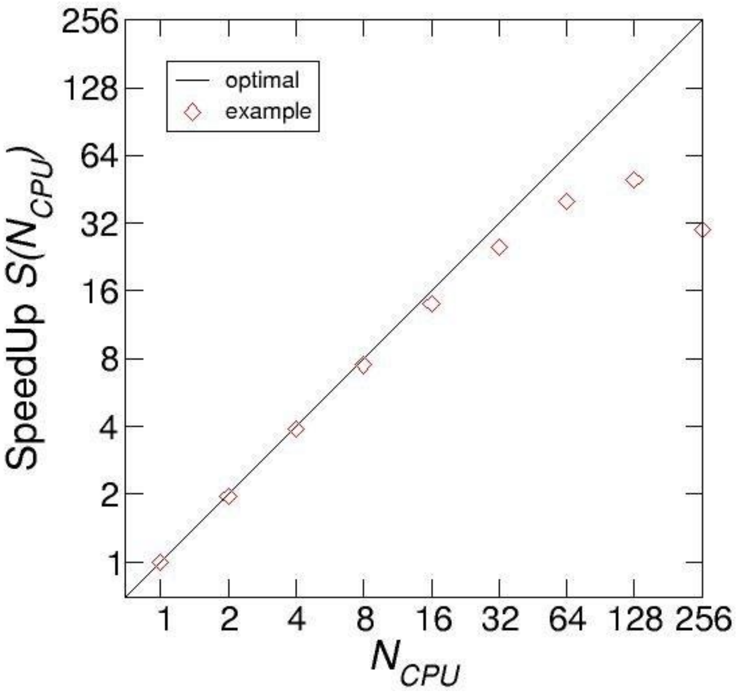
- Moore‘s law
  - The number of transistors on a chip will double every ~18 month
  - Frequency of todays CPUs
    → constant or decreasing
    (→ power consumption)
  - Increase only
    → more cores per CPU
- Problem too complex
  → time consuming
- Problem size
  → high memory needs



(source www.wikipedia.org)

Limit of parallelization - Scaling

- Speedup of the program when increasing number of processes / used cores
- Dependencies
  - Fraction of parallelization code P
  - Amount of communication / synchronization $C \sim O(N)$
  - Size / complexity of problem (e.g. number of unknown of an equation system)
  - Load balance (distribution of load on processors)
  - Hardware (latency/speed of network/memory access, cache coherence,…)

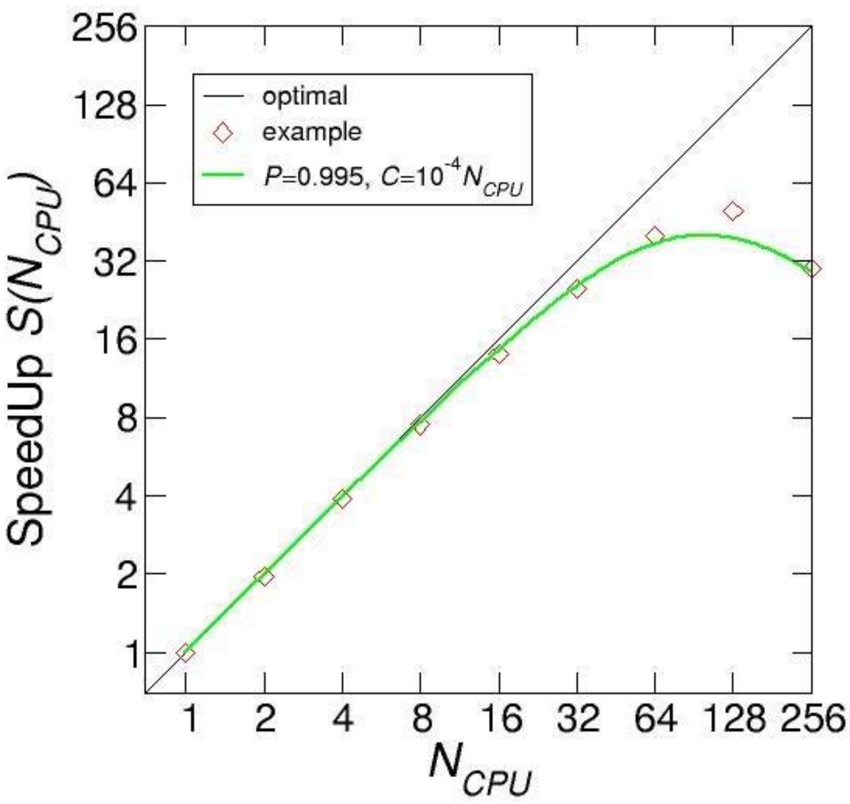


Limit of parallelization - Scaling

- *Strong scaling*
  - Problem size constant
  - Speedup $S(N)$ in time
  - Amdahl‘s law:

$$S(N) = \frac{1}{(1-P) + C + P/N}$$

- *Weak scaling*
  - Constant time frame
  - Speedup $S(N)$ by increasing problem size/
    number of solved problems
  - Gustavson‘s law:
    $S(N) = (1-P) + N \cdot P$



PARALLEL PROGRAMMING MODELS

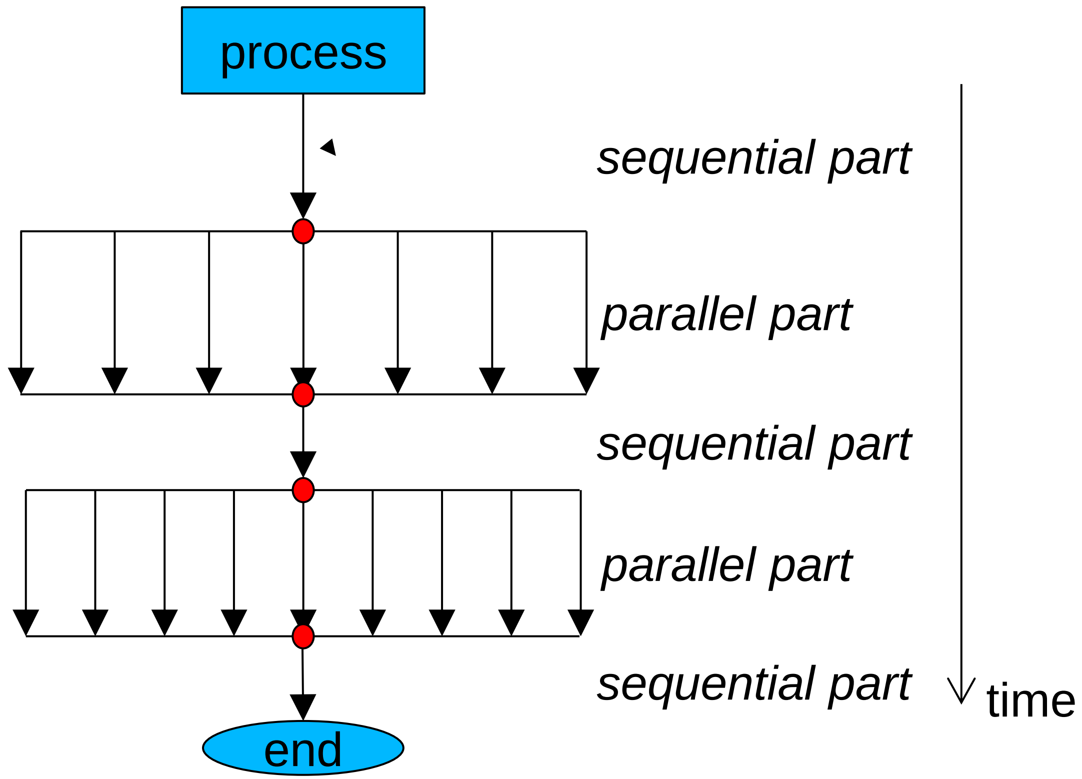
Parallel programming models

- Distributed memory
  - MPI (Message Passing Interface)
  - PVM (Parallel Virtual Machine)
- Distributed shared memory
  - PGAS (Partitioned Global Address Space)
- Shared memory
  - PThread (POSIX Threads)
  - OpenMP (Open Multi-Processing)
- Accelerator device
  - Nvidia's CUDA (Compute Unified Device Architecture)
  - OpenCL (Open Computing Language)

→ most common: MPI, PThread and OpenMP

Shared memory models - PThreads and OpenMP

- One process with multiple threads



- Use same memory segment
  → variables are accessible from every thread
  → can lead to race-conditions (need synchronization)

Shared memory models - PThreads and OpenMP

- OpenMP
  - C/C++:
    Pragma compiler statements
  - Fortran:
    Directives within comments
  - Minimal change of code
- PThreads
  - Library interface
  - Mutexes to avoid data collisions
  - Code has to be changed
- Note
  - Thread creation can be time consuming
  - Only usable on shared memory architectures!

OPENMP

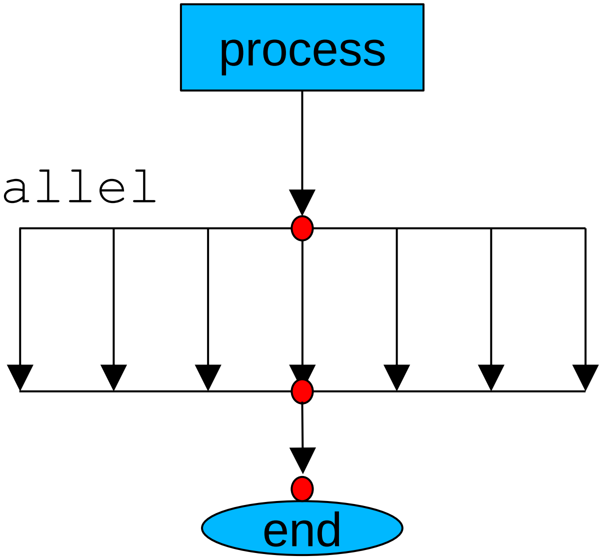
OpenMP code structure

<u>C/C++</u>

```
#pragma omp parallel
{
   code block
}
```

<u>Fortran</u>

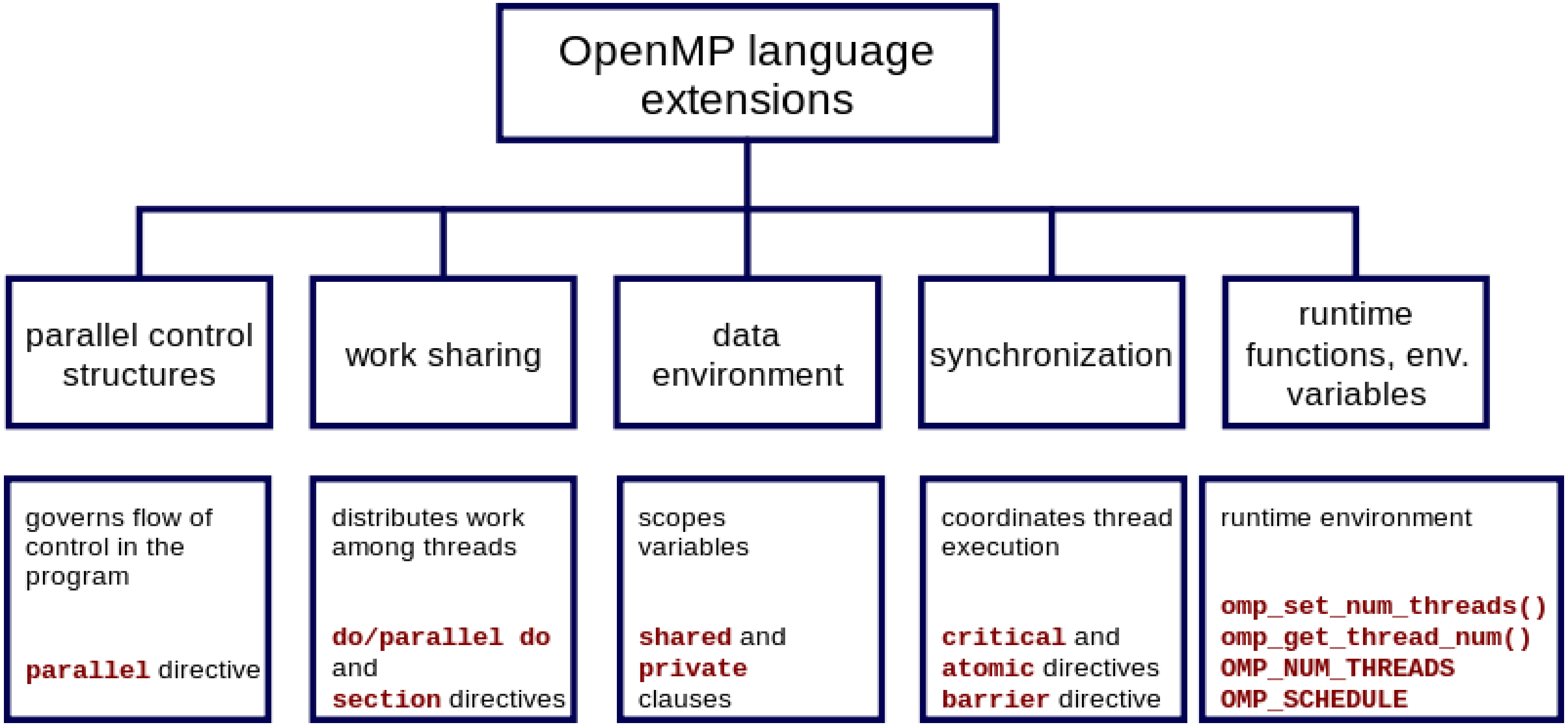
```
!$OMP PARALLEL

  code block
!$OMP END PARALLEL
```



Extension

```
#pragma omp [directive] [clause] [clause] …
!$OMP PARALLEL [directive] [clause] …
C$OMP PARALLEL [directive] [clause] …
```

OpenMP overview



from www.wikipedia.org

OpenMP runtime library

- additional routines by
  - C/C++: `#include <omp.h>`
  - Fortran: `use omp_lib` or `!$ INCLUDE ‘omp_lib.h’`
- feaures
  - setting and querying the number of threads (`omp_set_num_threads()` and `omp_get_num_threads()`)
  - querying the thread ID (`omp_get_thread_num()`)
  - querying if in a parallel region (`omp_in_parallel()`)
  - wall clock timers (`omp_get_wtime()`, `omp_get_wtick()`)
  - …
- environment variables enable control of runtime
  - setting the number of threads , e.g.
    `export OMP_NUM_THREADS=12`
  - setting the maximal number of threads, e.g.
    `export OMP_THREAD_LIMIT=24`

OpenMP “hello world”

C:

```
#include <omp.h>

int main(int argc,char *argv[])
{
#pragma omp parallel
  {
    printf(„Hello World! (%d)“, omp_get_thread_num());
  }
  return 0
}
```

Fortran:

```
 PROGRAM HELLOWORLD
!$ INCLUDE 'omp_lib.h'
!$OMP PARALLEL
     PRINT *, 'Hello World!’, OMP_GET_THREAD_NUM()
!$OMP END PARALLEL
     END
```

OpenMP “hello world”

```
flow01> make
gcc -fopenmp    -c helloWorld.c
gcc -fopenmp   helloWorld.o  -o helloWorld
flow01> ./helloWorld
Hello World! (1)
Hello World! (2)
Hello World! (3)
Hello World! (0)
flow01> ./helloWorld
Hello World! (0)
Hello World! (3)
Hello World! (1)
Hello World! (2)
```

→ Threads run in arbitrary order

OpenMP “hello world” 2

What happens here?

```
int main(int argc,char *argv[])
{
  int threadID, nThreads;

  #pragma omp parallel
  {
    threadID = omp_get_thread_num();
    printf("Hello World (%d)!\n", threadID);
    #pragma omp barrier
    if ( threadID == 0 ) {
      nThreads = omp_get_num_threads();
      printf("Using %d threads\n",nThreads);
    }
  }

  return 0;
}
```

OpenMP “hello world”

```
flow01> ./helloWorld
Hello World (0)!
Hello World (3)!
Hello World (1)!
Hello World (2)!
flow01> ./helloWorld
Hello World (1)!
Hello World (2)!
Hello World (3)!
Hello World (0)!
Using 4 threads
Using 4 threads
Using 4 threads
Using 4 threads
```

OpenMP "hello world" 2

Problem: Race conditions

```
int main(int argc,char *argv[])
{
  int threadID, nThreads;

  #pragma omp parallel
  {
    threadID = omp_get_thread_num();
    printf("Hello World (%d)!\n", threadID);
    #pragma omp barrier
    if ( threadID == 0 ) {
      nThreads = omp_get_num_threads();
      printf("Using %d threads\n",nThreads);
    }
  }

  return 0;
}
```

→ variable `threadID` is shared with all threads

OpenMP “hello world” 2

Correct way:

```
int main(int argc,char *argv[])
{
  int threadID, nThreads;

  #pragma omp parallel private(threadID)
  {
    threadID = omp_get_thread_num();
    printf("Hello World (%d)!\n", threadID);
    #pragma omp barrier
    if ( threadID == 0 ) {
      nThreads = omp_get_num_threads();
      printf("Using %d threads\n",nThreads);
    }
  }

  return 0;
}
```

→ variable `threadID` is now private for each thread

Clauses for parallel regions

- `private(`*`variable list`*`)`
  - definition of private variables in parallel region
  - variable are not initialized
  - variable have same name but different values in different threads
- `shared(`*`variable list`*`)`
  - define varaiable which are shared over threads
- `default(type)`
  - default for variables (`shared` or `private`)
- `reduction(`*`operator:list`*`)`
  - reduce values in a save way after joining threads
- `firstprivate(`*`variable list`*`)`
  - private variable will be initialized by the initial value
- `threadprivate(`*`variable list`*`)`
  - variables are replicated, each thread has its own copy

WORK SHARING DIRECTIVES

Work sharing directives

- usable in parallel regions
- directives specify how to work to threads
- no synchronization (barrier) at entry
- directives
  - `for` or `do` : (Fortran/C) split loops into parallel tasks
  - `sections` / `section` : definition of tasks for one thread
  - `single` : code block will executed only in one thread (synchronization at the end)
  - `master` : code block will executed only in master thread (no synchronization at the end)
  - `workshare` : Fortran directive for statements like `FORALL`, `WHERE` and array/scalar assignment
  - `task` : definition of a specific task

WORK SHARING DIRECTIVES FOR/DO

For/Do directive

```
int main(int argc,char *argv[])
{
  int i;
  const N=1000000;
  double x[N];

  #pragma omp parallel for
  for(i=0; i<N; i++)
  {
    x[i] = 1./(i+1.);
  }

  return 0;
}
```

- loop execute in parallel
- per default the range [0,N[is divided in $N_{threads}$ parts, e.g. $N_{threads}$=2: $i_{thread\ 0}$=0,…,N/2-1, $i_{thread\ 1}$=N/2,…,N-1

Clauses

- `lastprivate(`*`variable list`*`)`
  - variables get the last value of parallelized loop
- `collapse(n)`
  - collapse n loops to one loop (to get a better load balance)
- `ordered`
  - loop will run in the same order as in a serial code
- `schedule(type, [chunk size])`
  - specify how the loop will split up (optionally the chunk size)
    - `static` – fixed chunks, like in demo before
    - `dynamic` – waiting threads will get the next task
    - `guided` – decrease the chunk size to get a better load balance
    - `auto` – compiler decide best scheduling
- `nowait`
  - no implicit barrier at the end

Scheduling

Example on 3 threads

```
#pragma omp for
for(i=0; i<N; i++)
{
   ....
}
```

Distribution of `i` on thread IDs 0,1,2

i=	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
`static`	0	0	0	0	0	1	1	1	1	1	2	2	2	2	2	2
`dynamic`	0	1	2	0	2	1	0	2	1	2	0	1	2	0	1	2
`guided`	0	0	0	1	1	1	2	2	2	0	0	1	1	2	2	0
`auto`	*decided at runtime or from compiler*															

For/Do directive – 2nd example

```
int main(int argc,char *argv[])
{
  int i;
  const int N=1000000;
  double x[N];
  double nrm = 0.;

  #pragma omp parallel reduction(+:nrm)
  {
    /* init variables */
    #pragma omp for
    for(i=0; i<N; i++)
    {
      x[i] = 1./(i+1.);
    }

    /* calculate the norm */
    #pragma omp for
    for(i=0; i<N; i++)
    {
      nrm += x[i]*x[i];
    }
  }
  printf("Nrm = %g\n", sqrt(nrm));
...
```

Synchronization clauses

- `critical`
  - the code block will executed by only one thread per time
- `atomic`
  - memory updates within the block will be make atomically
- `ordered`
  - structured block (e.g. loops) will run in the same order as in a serial code
- `barrier`
  - each thread waits until all threads of a team reaches this point
- `nowait`
  - no implicit barrier at the end of a work share

For/Do directive – 2nd example alterantive

```
…
  double nrm = 0.;

  #pragma omp parallel shared(nrm)
  {
    double private_nrm = 0.;
    /* init variables */
    #pragma omp for
    for(i=0; i<N; i++)
    {
      x[i] = 1./(i+1.);
    }

    /* calculate the norm */
    #pragma omp for
    for(i=0; i<N; i++)
    {
      private_nrm += x[i]*x[i];
    }
    #pragma omp critical
    nrm += private_nrm;
  }
  printf("Nrm = %g\n", sqrt(nrm));
…
```

WORK SHARING DIRECTIVES SECTION

Sections directive

`sections` / `section` : definition of tasks for one thread

```
…
 #pragma omp parallel sections private(i)
  {
    {
      printf("Task %d has to do init x\n", omp_get_thread_num());
      for(i=0; i<N; i++)
        x[i] = 0.;
    }
    #pragma omp section
    {
      printf("Task %d has to do init y\n", omp_get_thread_num());
      for(i=0; i<N; i++)
        y[i] = 0.;
    }
    #pragma omp section
    {
      printf("Task %d has to do init z\n", omp_get_thread_num());
      for(i=0; i<N; i++)
        z[i] = 0.;
    }
  }
```

OpenMP “hello world”

Output:

```
flow01> ./section
Task 7 has to do init x
Task 3 has to do init y
Task 1 has to do init z
flow01> export OMP_NUM_THREADS=2
flow02> ./section
Task 1 has to do init y
Task 0 has to do init x
Task 0 has to do init z
```

→ each section will assigned to a thread

COMPILING

OpenMP Compililation

OpenMP compiler flags

- GNU compiler: `-fopenmp`
- Intel compiler: `-openmp`
- PGI compiler: `-mp`

PITFALLS

Implied flush

- consistent view on data in memory
  - data from cache will flushed implicitly only some points:
    - end of `do/for/sections/single/workshare`
    - at begin and end of `parallel/critical/ordered` blocks
    - `barrier`
  - on other points the shared variables may have temporarily different values
  - of need a consistent view use `flush(`*`varlist`*`)` directive
  - `nowait` directives

Race conditions, Dead locks and I/O

- race conditions
  - two or more threads access the same variable and at least one thread modify the variable and no synchronization is applied
  - lead to unpredictable results
  - use hellgrind of Intel Inspector for detecting race conditions
- deadlocks
  - two or more threads blocked and wait on each other
    → program run (wait) forever
- I/O
  - I/O within parallel regions from multiple threads can be unpredictable

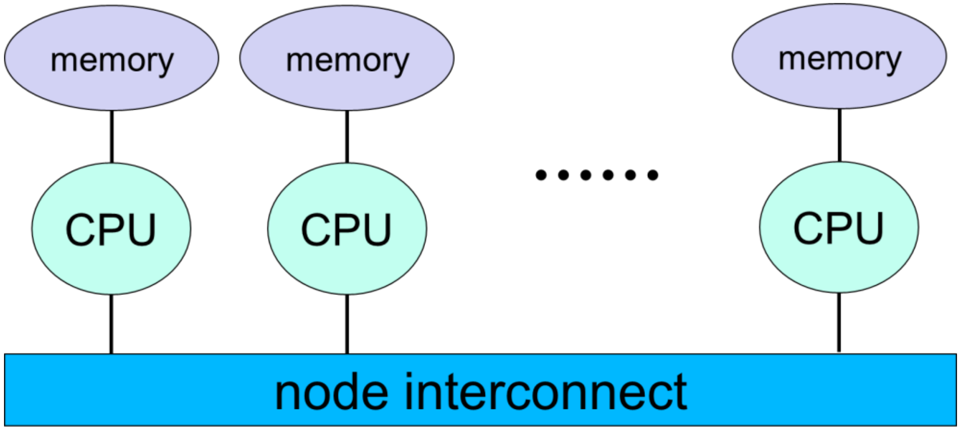
Overhead

Overhead

- synchronization/barriers
  → avoid unnecessary synchronization
- fork and join of parallel regions
  → try to build large parallel blocks
- so called *false-sharing*
  - two threads modify same memory block which is loaded in 2 different caches due to cache lines
  - e.g. by modification of an vector with dynamic scheduling

Optimization

- for multi-socket systems thinks about ccNUMA



→ variables attached to the socked where the first access happens (array allocated typically in 4Kb blocks, blocks can be assigned to memory at different sockets)

- pin threads to cores/cpus, e.g. by `numactl`

Summary

- usable by standardized compiler directives
- using threads within parallel regions
- simplify step by step parallelization
- can increase performance significatly
- disadvantages
  - limited to shared memory machines
  - race-conditions sometimes not easy to detect and to understand

Thanks a lot for your attention!

For further information please visit the HPC Wiki

http://wiki.hpcuser.uni-oldenburg.de

Exercises

- Login to FLOW/HERO
  `ssh -XY abcd1234@flow.hpc.uni-oldenburg.de`
  `ssh -XY abcd1234@hero.hpc.uni-oldenburg.de`

- Try to parallelize optimize sample code from yesterday
- Write submission script to test the program
- How does the code scale?