University of Minho
Informatics Department

Parallel Computing Paradigms (UCE CPD)

OpenMP

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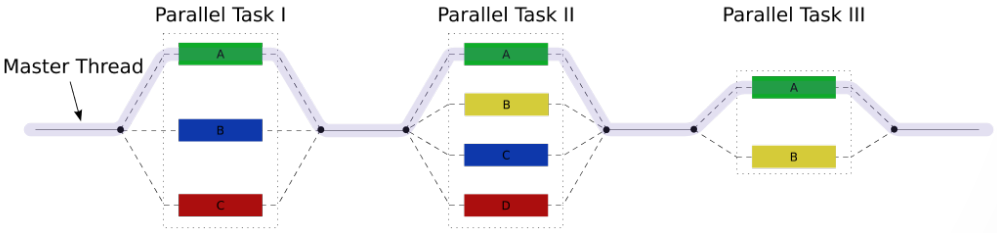
Introduction to OpenMP

- OpenMP is an API to support Shared Memory (SM) parallelization on multi-core machines.
  - Based on: Compiler directives, Library routines and Environmental variables;
  - Supports C/C++ and Fortran programming languages.
- Uses multithreading based on the **fork-join** model of parallel execution.



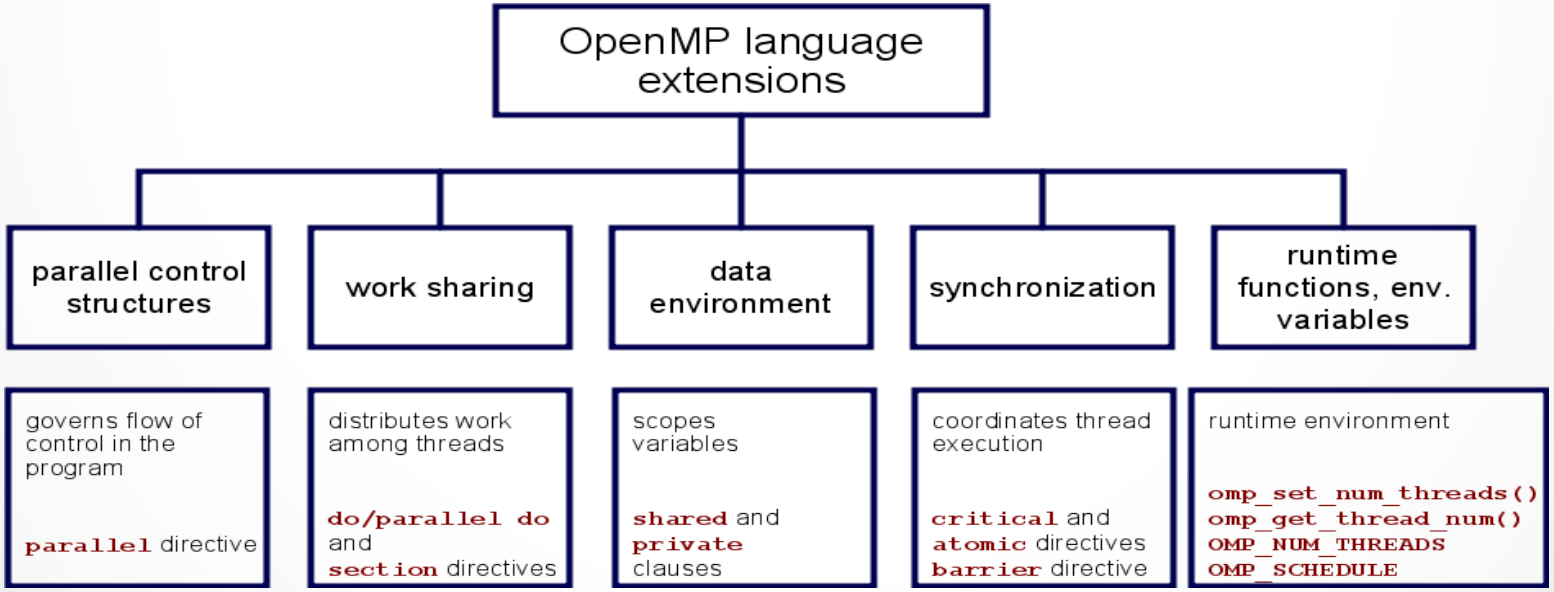
- It is through directives, added by the programmer to the code, that the compiler adds parallelism

OpenMP considerations:

- OpenMP itself **does not** solve problems as :
  - Starvation, deadlock or poor load balancing (among others).
  - But, offers routines to solve problems like:
    - Load balancing or memory consistency.
  - However, starvation and deadlock are the programmer's responsibility.
- The creation/managing of threads are delegated to the compiler & OpenMP runtime:
  - + Easier to parallelize application;
  - - Less control over the threads' behaviour.
- By default, the number of parallel activities is defined in run-time according to available resources
  - e.g. 2 cores -> 2 threads
  - HT capability counts as a core
- OpenMP does **not** support **distributed memory systems** & more complex parallelization must resort to library calls.

OpenMP: Programming Model

- The openMP program begins as a single thread (**master thread**).
- **Parallel regions** create a team of parallel activities;
- **Work-sharing** constructs/generates work for the team to process;
- **Data sharing** clauses specify how variables are shared within a parallel region;



OpenMP Programming

- OpenMP directives format for C/C++ applications:
  - ***#pragma omp*** *directive-name [clause[[,] clause]...] new-line*
- **Parallel Constructs**
  - ***#pragma omp parallel*** **-> Creates a team of threads.**
- **Work-sharing Constructs**
  - ***#pragma omp for*****-> Assignment of iterations to threads.**
  - **#pragma omp sections -> Assignment of blocks of code (section) to threads.**
  - **#pragma omp single -> Restrict a code of block to be executed by only one thread.**
- **Tasking Constructs**
  - **#pragma omp task -> Creation of a pool of tasks to be executed by the thread.**
- **Master & Synchronization Constructs**
  - **#pragma omp master -> A block of code to be executed only the master thread of the team.**
  - **#pragma omp critical -> Restricts the execution of a given block of code to a single thread at a time.**
  - **#pragma omp barrier -> Makes all threads in a team to wait for the remaining.**
  - **#pragma omp taskwait -> wait for the completion of the current task child's.**
  - **#pragma omp atomic -> Ensures that a specific storage location is accessed atomically.**
  - **#pragma omp flush -> Makes a thread's temporary view of memory consistent with memory.**
  - **#pragma omp ordered -> Specifies a block of code in a loop region that will be executed in the order of the loop iterations.**

Data Sharing

- What happens to variables in parallel regions?
  - Variables declared inside are local to each thread;
  - Variables declared outside are shared
- Data sharing clauses:
  - **private(varlist)** => each variable in varlist becomes private to each thread, initial values no specified.
  - **firstprivate(varlist) =>** Same as private, but variables are initalized with the same value outside the region.
  - **lastprivate(varlist) =>** same as private, but the final value is the last loop iteration's value.
  - **reduction (op:var)** => same as lastprivate, but the final value is the result of reduction using the operator "op".
- Directives for data sharing:
  - #pragma omp threadlocal => each thread gets a local copy of the value.
  - **copyin clause** copies the values from thread master to the others threads.

Parallel Region

- When a thread encounters a parallel construct, a team of threads is created (**FORK**);
- The thread which encounters the parallel region becomes the **master** of the new team;
- All threads in the team (including the master) execute the region;
- At end of parallel region, all threads synchronize, and join master thread (**JOIN**).

Parallel region syntax

```
#pragma omp parallel [clauses]
{
        code_block
}
```

Where clause can be:

if (*scalar-expression*)

num_threads (*integer-expression*)

private (*list*)

firstprivate (*list*)

shared (*list*)

reduction (*operator*: *list*)

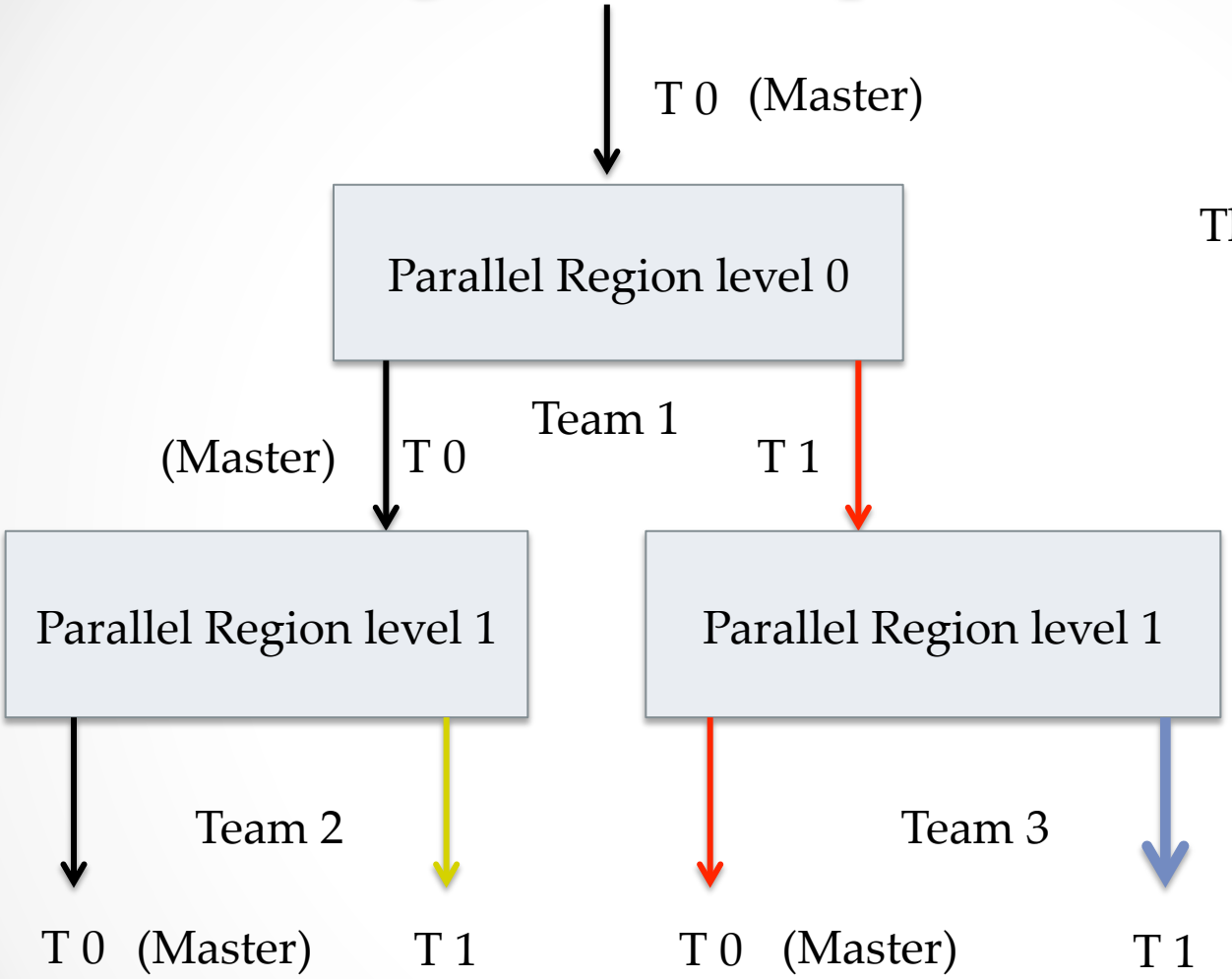
Nested Parallel Region

- If a thread in a team executing a parallel region encounters another parallel directive, it creates a new team, and becomes the master of this team;

- If **nested parallelism** is disabled, then no additional team of threads will be created.

- To enable/disabled -> **omp_set_nested(x);**

Nested region example



Thread marked with red is slave on team 1 but master on team 2.

Loop Construct

- The for loop iterations are distributed across threads **in the team;**
  - The distribution is based on:
    - Chunk_size, by default = 1;
    - Parallel for schedule, by default = static.
- Loop schedule:
  - **Static –** Iterations divided into chunks of size ***chunk_size*** assigned to the threads in a team in a **round-robin** fashion;
  - **Dynamic –** the chunks are assigned to threads in the team as the threads request them;
  - **Guided** - similar to dynamic but the chunk size decreases during execution.
  - **Auto –** the chose scheduling is delegated to the compiler.

Parallel region syntax

```
#pragma omp for[clauses]
{
        code_block
}
```

Where clause can be:

```
private(list)
firstprivate(list)
lastprivate(list)
reduction(operator: list)
schedule(kind[, chunk_size])
collapse(n)
ordered
nowait
```

Loop Constructors

- schedule(**static**) vs schedule(**dynamic**)
  - **Static** has lower overhead;
  - **Dynamic** has a better load balance approach;
  - Increasing the chuck size in the dynamic for:
    - Diminishing of the scheduling overhead;
    - Increasing the possibility of load balancing problems.

- Lets f() be a given function and we want to parallelize the loop using 2 threads:

```
#pragma omp parallel for schedule ( ?)
 for(I = 0; I < 100; I++)
    f();
```

What is the most appropriated type of scheduling?

Parallel for with ordered clause

- ```
  #pragma omp for schedule(static) ordered
  for (i = 0; i < N; ++i)
  {
    // Do something here.
    #pragma omp ordered
    {
     printf("test() iteration %d\n", i);
    }
  }
  ```
  ```

Parallel execution of code sections

- Supports heterogeneous tasks:

```
#pragma omp parallel
{
   #pragma omp sections
    {
      #pragma omp section
      {
                taskA();
      }
      #pragma omp section
      {
                taskB();
      }
      #pragma omp section
      {
                taskC();
      }
   }
}
```

- The section blocks are divided among threads in the team;
- Each section is executed only once by threads in the team.
- There is an implicit barrier at the end of the section construct unless a nowait clause is specified
- Allow the following clauses:
  - private (list);
  - firstprivate(list);
  - lastprivate(list);
  - reduction(operator:list)

Task constructor:

```
int fib(int n)
{
  int i, j;
  if (n<2) return n;
  else
    {
       #pragma omp task shared(i) firstprivate(n)
       i=fib(n-1);

       #pragma omp task shared(j) firstprivate(n)
       j=fib(n-2);

       #pragma omp taskwait
       return i+j;
    }
}

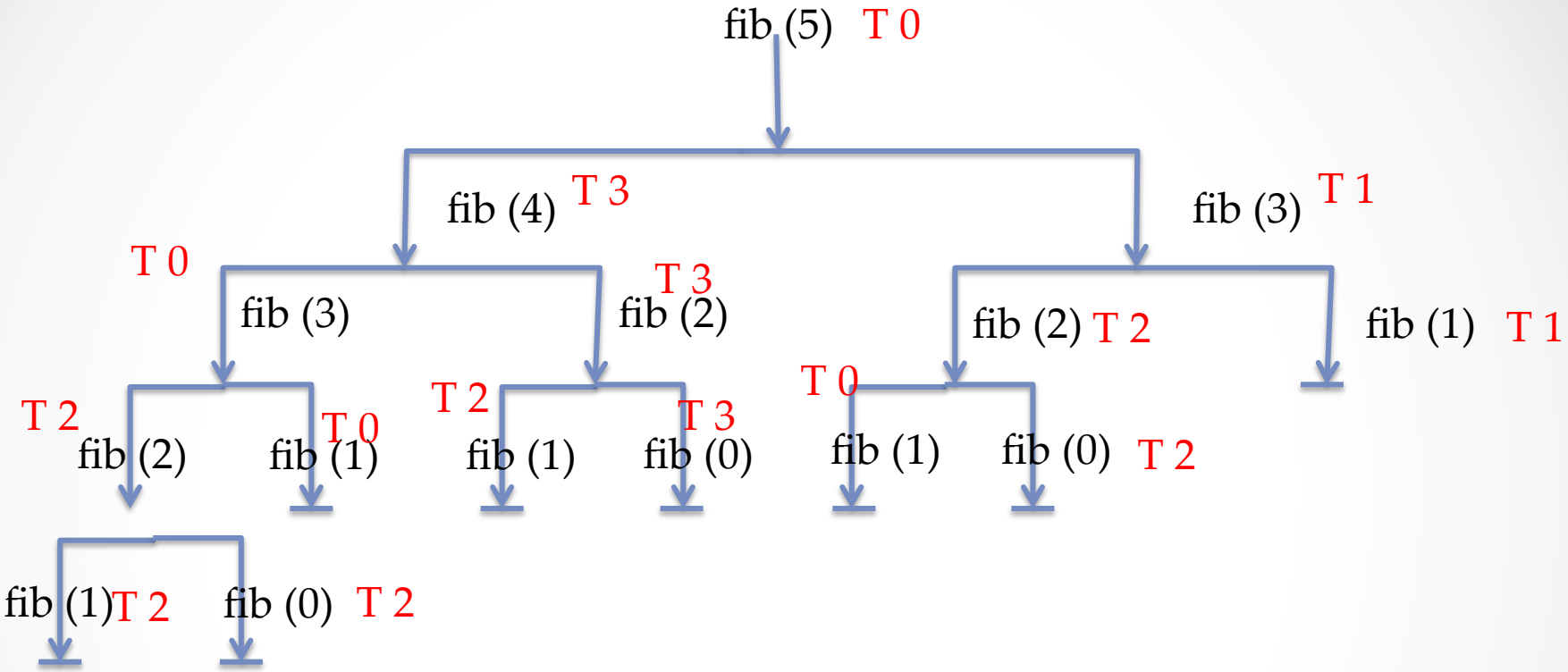
int main()
{
  int n = 10;

  omp_set_num_threads(4);

  #pragma omp parallel shared(n)
  {
    #pragma omp single
    printf ("fib(%d) = %d\n", n, fib(n));
  }
}
```

- When a thread encounters a task construct, a task is generated;
- Thread can immediately execute the task, or can be executed latter one by any thread on the team;
- OpenMP creates a pool of tasks to be executed by the active threads in the team;
- The **taskwait** directive ensures that the 2 tasks generated are completed before the return statements.
- Although, only one thread executes the **single** directive and hence the call to fib(n), **all four threads** will participate in executing the tasks generated.

Execution Tree Exemplified



Synchronization Constructs:

- Critical regions (executed in mutual exclusion):
  - #pragma omp critical [name]

    updateParticles();
  - Restricts execution of the associated structured blocks to a single thread at a time;
  - Works inter-teams.
  - An optional name may be used to identify the critical construct, all critical without name are considered to have the same unspecified name.

- Atomic Operations (fine-grain synchronization):
  - #pragma omp atomic

    A[i] += x;
  - The memory in will be updated atomically. It does not make the entire statement atomic; only the memory update is atomic.
  - A compiler might use special hardware instructions for **better** performance than when using ***critical***.

Avoid/reduce synchronisation

- Reduction of multiple values (in parallel):

```
sum = 0;
    # pragma omp parallel for reduction(+:sum)
      for(int i = 0;  i<100; i++) {
        sum += array[i];
      }
```

- Thread reuse across parallel regions

```
    # pragma omp parallel {
    #pragma omp for
      for(int i = 0;  i<100; i++)
        …
    #pragma omp for
      for(int j= 0; j<100; j++)
        …
    }
```

Environment variables

- **OMP_SCHEDULE**
  - sets the *run-sched-var* ICV for the runtime schedule type and chunk size. It can be set to any of the valid OpenMP schedule types (i.e., **static**, **dynamic**, **guided**, and **auto**).
- **OMP_NUM_THREADS**
  - sets the *nthreads-var* ICV for the number of threads to use for **parallel** regions.
- **OMP_DYNAMIC**
  - sets the *dyn-var* ICV for the dynamic adjustment of threads to use for **parallel** regions.
- **OMP_NESTED**
  - sets the *nest-var* ICV to enable or to disable nested parallelism.
- **OMP_STACKSIZE**
  - sets the *stacksize-var* ICV that specifies the size of the stack for threads created by the OpenMP implementation.
- **OMP_WAIT_POLICY**
  - sets the *wait-policy-var* ICV that controls the desired behavior of waiting threads.
- **OMP_MAX_ACTIVE_LEVELS**
  - sets the *max-active-levels-var* ICV that controls the maximum number of nested active parallel regions.
- **OMP_THREAD_LIMIT**
  - sets the *thread-limit-var* ICV that controls the maximum number of threads participating in the OpenMP program.

OpenMP Rotines

- omp_set_num_threads / omp_get_num_threads
- omp_get_max_threads
- omp_get_thread_num.
- omp_get_num_procs.
- omp_in_parallel.
- omp_set_dynamic / omp_get_dynamic.
- omp_set_nested / omp_get_nested.
- omp_set_schedule / omp_get_schedule
- omp_get_thread_limit.
- omp_set_max_active_levels / omp_get_max_active_levels
- omp_get_level.
- omp_get_ancestor_thread_num.
- omp_get_team_size.
- omp_get_active_level

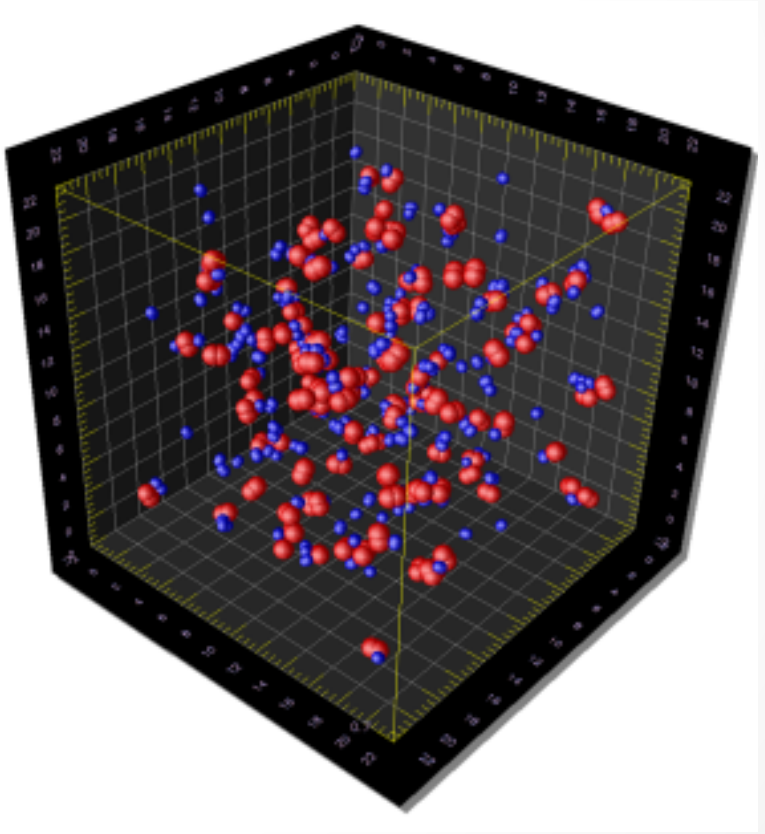
- Locks
  - void omp_init_lock(omp_lock_t *lock);
  - void omp_destroy_lock(omp_lock_t *lock);
  - void omp_set_lock(omp_lock_t *lock);
  - void omp_unset_lock(omp_lock_t *lock);
  - int omp_test_lock(omp_lock_t *lock);
- Timers
  - double omp_get_wtime(void);
  - double omp_get_wtick(void);

OpenMP versions and compiler support

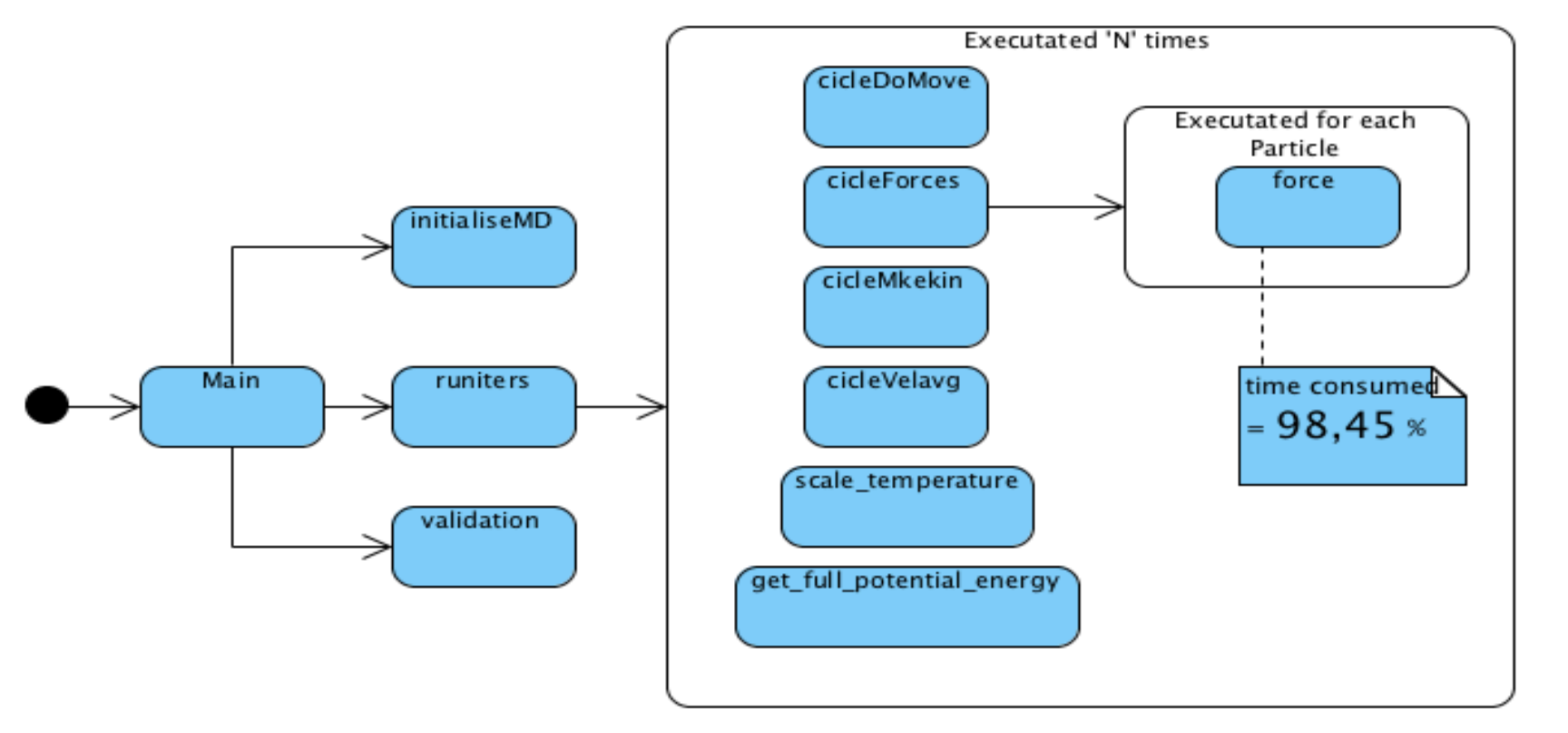
OpenMP version	Principal new features	Compiler support	
2.5 (May 2005)		gcc 4.2	
3.0 (May 2008)	- Task / taskwait	gcc4.4	Icc 11.1
3.1 (July 2011)	- Final/mergeable - Taskyield - Min/max reductions in C++ - OMP_PROC_BIND	gcc4.7	Icc 12.1
4.0 (July 2013)	- Cancel - Declare reduction - SIMD - Taskgroup - Device construct	gcc4.8.2 / gcc4.9	Icc 13.1 (?)

Molecular Dynamic

- Simulation of particle's interactions;
- Use of mathematical models such as Lennard-Jones Potential;
- Interaction calculation based on:
  - Position;
  - Velocity;
  - Force.



MD: Call Graph



MD code

Molecular Dynamic Simulation

```
for (md->move = 0; md->move < md->movemx; md->move++)
{
     cicleDoMove                    (md,particulas);
     cicleForces                    (md,particulas);
     cicleMkekin                    (md,particulas);
     cicleVelavg                    (md,particulas);
     scale_temperature              (md,particulas);
     get_full_potential_energy      (md);
}
```

Force Calculation of all Particles

```
void cicleForces()
{
     ...
     for(int i = 0; i < MAX_PARTICLES; i++)
         calForce(i);
}
```

Force Calculation of one particle with the remaining

```
void force(int particleI)
{
    for(int i = particleI + 1; i < MAX_PARTICLES; i++)
    {
        int distance = calDist(i,particleI);

        if(distance <= RADIUS)
        {
            forceAcumulada += forceBetween(particleI,i);
            aplicar3LeiNewton(i);
            updateVariaveisControlo();
        }
    }
    updateForce(particleI,forceAcumulada);
}
```

Parallelizing the Application

```
void cicleForces()
{
      #pragma omp parallel for
      for(int i = 0; i < MAX_PARTICLES; i++)
          calForce(i);
}
```

- Load balancing problems (due 3º Newton's Law).
- Solution ?

Parallelizing the Application

```
void cicleForces()
{
      #pragma omp parallel for schedule (dynamic)
      for(int i = 0; i < MAX_PARTICLES; i++)
          calForce(i);
}
```

- ~~Load balancing problems (due 3º Newton's Law).~~
- There is the overhead problem ☹
- Solution ?

Parallelizing the Application

```
void cicleForces()
{
     int a,b;
     int halfPart= MAX_PARTICLES/2;


     #pragma omp parallel for private (a,b)
     {
     int thrID = omp_get_thread_num();
     int numThr = omp_get_num_threads();


     for(a = thrID; a < halfPart; a += numThr)
         calForce(a);

     for(b = MAX_PARTICLES - thrID - 1; b >= halfPart; b -= numThr)
         calForce(b);
     }

}
```

- ~~Load balancing problems (due 3º Newton's Law).~~
- ~~There is the overhead problem ☹~~
- No task distribution synchronization overhead!
- But there are cases of load balancing -> **halfPart % numThr != 0**

Checking data Dependencies (Critical clause)

```
void force(int particleI)
{
    for(int i = particleI + 1; i < MAX_PARTICLES; i++)
    {

        int distance = calDist(i,particleI);

        if(distance <= RADIUS)
        {
            forceAcumulada += forceBetween(particleI,i);
            #pragma omp critical
            {
            aplicar3LeiNewton(i);
            updateVariaveisControlo();
            }
        }
    }
    #pragma omp critical
    {
    updateForce(particleI,forceAcumulada);
    }
}
```

- Mutual exclusion is ensured.
  - Very high synchronization overhead;
  - Unnecessary synchronization.
- Solution ?
  - Fine grain synchronization.

Checking data Dependences (Lock per Particle)

```
omp_lock_t locks[MAX_PARTICLES];

void force(int particleI)
{
    for(int i = particleI + 1; i < MAX_PARTICLES; i++)
    {

        int distance = calDist(i,particleI);

        if(distance <= RADIUS)
        {
            forceAcumulada += forceBetween(particleI,i);

            omp_set_lock(&locks[i]);
            aplicar3LeiNewton(i);
            updateVariaveisControlo();
            omp_unset_lock(&locks[i]);
        }
    }

    omp_set_lock(&locks[particleI]);
    updateForce(particleI,forceAcumulada);
    omp_unset_lock(&locks[particleI]);
}
```

- ~~Mutual exclusion is ensured.~~
  - ~~Very high synchronization overhead;~~
  - ~~Unnecessary synchronization.~~
- Solution ?
  - Fine grain synchronization.
- Lot less synchronization.
  - But there is still overhead ☹
- Solution?.
  - Data redundancy.

Removing some synchronization overhead

```
#pragma omp parallel private (i)
{
for (i = 0; i < MAX_ITERATIONS; i++)
{

     #pragma omp master
     cicleDoMove                    (md,particulas);

     #pragma omp barrier
     cicleForces                    (md,particulas);
     #pragma omp barrier

     #pragma omp master
     {
      cicleMkekin                    (md,particulas);
      cicleVelavg                    (md,particulas);
      scale_temperature              (md,particulas);
      get_full_potential_energy      (md);
     }
  }
}
```

```
void cicleForces()
{
     int a,b;
     int halfPart= MAX_PARTICLES/2;

     #pragma omp for private (a,b)
     {
      //   ...
     }

}
```