Tutorial: parallel coding OPENMP

Pascal Viot

October 5, 2020

Generalities

- Processors consist of a number of cores (or calculation units) which increases with time: initially, only one, then two, now often 4, or even 6 or 8 up to 24 for computing servers.

Generalities

- Processors consist of a number of cores (or calculation units) which increases with time: initially, only one, then two, now often 4, or even 6 or 8 up to 24 for computing servers.
- Compared to a parallelism where calculations are done on different machines, we can use the fact that on a single machine, the memory used by all computing units is the same and can be accessible theoretically simply by all.

Generalities

- Processors consist of a number of cores (or calculation units) which increases with time: initially, only one, then two, now often 4, or even 6 or 8 up to 24 for computing servers.
- Compared to a parallelism where calculations are done on different machines, we can use the fact that on a single machine, the memory used by all computing units is the same and can be accessible theoretically simply by all.
- We can calculate on the different units at the same time, provided that you do not want to walk on your feet (that is, not to write at the same time at the same memory locations).

Generalities

- Processors consist of a number of cores (or calculation units) which increases with time: initially, only one, then two, now often 4, or even 6 or 8 up to 24 for computing servers.
- Compared to a parallelism where calculations are done on different machines, we can use the fact that on a single machine, the memory used by all computing units is the same and can be accessible theoretically simply by all.
- We can calculate on the different units at the same time, provided that you do not want to walk on your feet (that is, not to write at the same time at the same memory locations).
- The OPENMP library contained in both Gnu and Intel compilers allows these operations to be performed.

Outline

- OPENMP: definition

Outline

- OPENMP: definition
- Definition of the computing world

Outline

- OPENMP: definition
- Definition of the computing world
- Compiling and running an OPENMP program, environment variables

Outline

- OPENMP: definition
- Definition of the computing world
- Compiling and running an OPENMP program, environment variables
- Parallel loop

Outline

- OPENMP: definition
- Definition of the computing world
- Compiling and running an OPENMP program, environment variables
- Parallel loop
- Internal functions

Outline

- OPENMP: definition
- Definition of the computing world
- Compiling and running an OPENMP program, environment variables
- Parallel loop
- Internal functions
- Reduction

Outline

- OPENMP: definition
- Definition of the computing world
- Compiling and running an OPENMP program, environment variables
- Parallel loop
- Internal functions
- Reduction
- Conclusion and references.

OPENMP: definition and several versions

- OPENMP:The current version is 5.0 and dated November 2018.

OPENMP: definition and several versions

- OPENMP:The current version is 5.0 and dated November 2018.
- Website: http://www.openmp.org/.

OPENMP: definition and several versions

- OPENMP:The current version is 5.0 and dated November 2018.
- Website: http://www.openmp.org/.
- The compilers contain the OPENMP library, i.e. the Gnu compiler and the Intel compiler

OPENMP: definition and several versions

- OPENMP:The current version is 5.0 and dated November 2018.
- Website: http://www.openmp.org/.
- The compilers contain the OPENMP library, i.e. the Gnu compiler and the Intel compiler
- OPENMP is a library for Fortran, C,C ++ and Python languages.

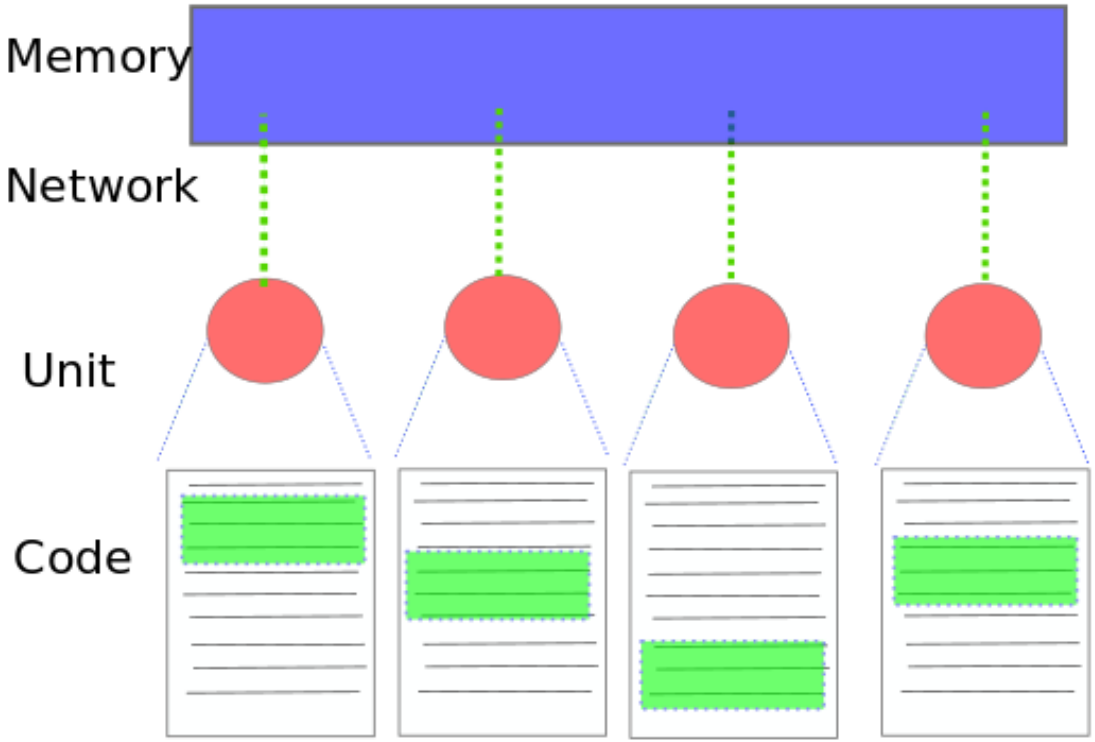
OPENMP: definition and several versions

- OPENMP:The current version is 5.0 and dated November 2018.
- Website: http://www.openmp.org/.
- The compilers contain the OPENMP library, i.e. the Gnu compiler and the Intel compiler
- OPENMP is a library for Fortran, C,C ++ and Python languages.
- Programming with OPENMP can be simple. It consists in inserting directives into an existing sequential program. In general, you do not destroy the original code! This means that the program can still operate sequentially or by using calculation units associated with a memory single center.

OPENMP: definition and several versions

- OPENMP:The current version is 5.0 and dated November 2018.
- Website: http://www.openmp.org/.
- The compilers contain the OPENMP library, i.e. the Gnu compiler and the Intel compiler
- OPENMP is a library for Fortran, C,C ++ and Python languages.
- Programming with OPENMP can be simple. It consists in inserting directives into an existing sequential program. In general, you do not destroy the original code! This means that the program can still operate sequentially or by using calculation units associated with a memory single center.
- Since computing sites are made up of one or more computers and networked, the ideal is to combine OPENMP and MPI, but it's more complicated for development.

Computing world: definition



Computing world: definition(2)

```
#include <iostream>
#include<omp.h>
using namespace std;
int main()
{
        #pragma omp parallel
        {
                cout<<"Hello, world!"<<endl;
        }
        cout<<"Ciao, mondo!"<<endl;
}
```

Compiling and running a program OPENMP, environment variables

- the #pragma omp parallel and the following braces indicate that the code of this block must be parallelized.

Compiling and running a program OPENMP, environment variables

- the #pragma omp parallel and the following braces indicate that the code of this block must be parallelized.
- Thus the Hello, World print will appear as many times as calculation (virtual) units have been solicited

Compiling and running a program OPENMP, environment variables

- the #pragma omp parallel and the following braces indicate that the code of this block must be parallelized.
- Thus the Hello, World print will appear as many times as calculation (virtual) units have been solicited
- To compile this program with gcc:
  gcc hello.c -fopenmp -o hello

Compiling and running a program OPENMP, environment variables

- the #pragma omp parallel and the following braces indicate that the code of this block must be parallelized.
- Thus the Hello, World print will appear as many times as calculation (virtual) units have been solicited
- To compile this program with gcc:
  gcc hello.c -fopenmp -o hello
- To compile this program with intel:
  icc hello.c -openmp -o hello

Compiling and running a program OPENMP, environment variables

- the #pragma omp parallel and the following braces indicate that the code of this block must be parallelized.
- Thus the Hello, World print will appear as many times as calculation (virtual) units have been solicited
- To compile this program with gcc:
  gcc hello.c -fopenmp -o hello
- To compile this program with intel:
  icc hello.c -openmp -o hello
- To build and run with codeblocks. To ensure the openmp functionality, open "Compiler and debugger settings", put "-fopenmp" in "other options", and "-lgomp -pthread" in "Other linker options".

Compiling and running a program OPENMP, environment variables

- the #pragma omp parallel and the following braces indicate that the code of this block must be parallelized.
- Thus the Hello, World print will appear as many times as calculation (virtual) units have been solicited
- To compile this program with gcc:
  gcc hello.c -fopenmp -o hello
- To compile this program with intel:
  icc hello.c -openmp -o hello
- To build and run with codeblocks. To ensure the openmp functionality, open "Compiler and debugger settings", put "-fopenmp" in "other options", and "-lgomp -pthread" in "Other linker options".
- If you run this program, it chooses the number of units available.

Compiling and running a program OPENMP, environment variables

- the #pragma omp parallel and the following braces indicate that the code of this block must be parallelized.
- Thus the Hello, World print will appear as many times as calculation (virtual) units have been solicited
- To compile this program with gcc:
  gcc hello.c -fopenmp -o hello
- To compile this program with intel:
  icc hello.c -openmp -o hello
- To build and run with codeblocks. To ensure the openmp functionality, open "Compiler and debugger settings", put "-fopenmp" in "other options", and "-lgomp -pthread" in "Other linker options".
- If you run this program, it chooses the number of units available.
- To fix the number of units, the environment variable in the terminal window must be set before launching the program

  export OMP_NUM _THREADS = 20

Compiling and running a program OPENMP, environment variables (2)

- The number of units is virtual, and does not necessarily correspond to the physical number of cores. However, for a simulation code, the number of units number should not be less ot equal to the number of cores. Indeed, in many cases, the running time can not decrease if you exceed this limit (to subtleties with multitheading).

Compiling and running a program OPENMP, environment variables (2)

- The number of units is virtual, and does not necessarily correspond to the physical number of cores. However, for a simulation code, the number of units number should not be less ot equal to the number of cores. Indeed, in many cases, the running time can not decrease if you exceed this limit (to subtleties with multitheading).
- The pragma instruction leads to execute N times the same group of instructions. It is therefore necessary to code properly for a calculation to be distributed and not executed N times.

Compiling and running a program OPENMP, environment variables (2)

- The number of units is virtual, and does not necessarily correspond to the physical number of cores. However, for a simulation code, the number of units number should not be less ot equal to the number of cores. Indeed, in many cases, the running time can not decrease if you exceed this limit (to subtleties with multitheading).
- The pragma instruction leads to execute N times the same group of instructions. It is therefore necessary to code properly for a calculation to be distributed and not executed N times.
- **Physical Limitations of an OMP Program** So that part of the code is executed by doing N units of computation, the system has to create threads, and finally destroy them. The time required is not always negligible.

Compiling and running a program OPENMP, environment variables (2)

- The number of units is virtual, and does not necessarily correspond to the physical number of cores. However, for a simulation code, the number of units number should not be less ot equal to the number of cores. Indeed, in many cases, the running time can not decrease if you exceed this limit (to subtleties with multitheading).
- The pragma instruction leads to execute N times the same group of instructions. It is therefore necessary to code properly for a calculation to be distributed and not executed N times.
- **Physical Limitations of an OMP Program** So that part of the code is executed by doing N units of computation, the system has to create threads, and finally destroy them. The time required is not always negligible.
- The time associated with this process is in the order of $0.1\mu s$. Again very much faster than clock time of the processor.

Parallel loop

- In order to have a parallel loop, one adds #pragma omp parallel for

Parallel loop

- In order to have a parallel loop, one adds #pragma omp parallel for
- The compiler will split the loop into different parts executed on virtual units. Once executed, the program destroys the threads.

Parallel loop

- In order to have a parallel loop, one adds #pragma omp parallel for
- The compiler will split the loop into different parts executed on virtual units. Once executed, the program destroys the threads.
- One can look at what happens with the unix instruction top in another terminal window that the percentage is greater than 100 %. This illustrates the fact that the program mobilizes multiple computing units at runtime.

Parallel loop

- In order to have a parallel loop, one adds #pragma omp parallel for
- The compiler will split the loop into different parts executed on virtual units. Once executed, the program destroys the threads.
- One can look at what happens with the unix instruction top in another terminal window that the percentage is greater than 100 %. This illustrates the fact that the program mobilizes multiple computing units at runtime.
- Additional instructions can be added to the previous statement that specify which variables are common to all threads and those that are internal. By default, the compiler is supposed to guess, but nothing prevents you from guiding it to make the right choices.

Parallel loop

- In order to have a parallel loop, one adds #pragma omp parallel for
- The compiler will split the loop into different parts executed on virtual units. Once executed, the program destroys the threads.
- One can look at what happens with the unix instruction top in another terminal window that the percentage is greater than 100 %. This illustrates the fact that the program mobilizes multiple computing units at runtime.
- Additional instructions can be added to the previous statement that specify which variables are common to all threads and those that are internal. By default, the compiler is supposed to guess, but nothing prevents you from guiding it to make the right choices.
- For a loop with a loop index called i, we can write
  # pragma omp parallel for default (shared), private (i)

Parallel loop

- In order to have a parallel loop, one adds #pragma omp parallel for
- The compiler will split the loop into different parts executed on virtual units. Once executed, the program destroys the threads.
- One can look at what happens with the unix instruction top in another terminal window that the percentage is greater than 100 %. This illustrates the fact that the program mobilizes multiple computing units at runtime.
- Additional instructions can be added to the previous statement that specify which variables are common to all threads and those that are internal. By default, the compiler is supposed to guess, but nothing prevents you from guiding it to make the right choices.
- For a loop with a loop index called i, we can write
  # pragma omp parallel for default (shared), private (i)
- By changing the OMP _NUM_THREADS statement, you can change the default number of threads used.

Parallel loop (2)

```
#include <iostream>
#include <cmath>
#include<vector>
#include<omp.h>
using namespace std;
double essai(double x)
{ return(5.0+10.0*x+x*x*exp(x)*log(x+0.1)+sqrt(fabs(x)))
    ;}

int main(){
        const int NITER=200000000;
        vector<double> a(NITER);
        #pragma omp parallel for default(shared)
        for (int j=0;j<NITER;j++){
                a[j] = essai(j*0.01);}
        exit(0);
}
```

Internal functions

- There are several internal functions that allow to have information about parallel processes and / or modifies inside of the program how the parallelization is carried out.

Internal functions

- There are several internal functions that allow to have information about parallel processes and / or modifies inside of the program how the parallelization is carried out.
- Among these functions, let's mention omp_get_num_threads () which gives the number of threads, omp_get_thread_num () which gives the thread label and omp_get_wtime which gives the time in decimal value

Internal functions (2)

```
...
int main(){
        const int NITER=200000000;
        vector<double> a(NITER);
        double deb,end;
        #pragma omp parallel
        if(omp_get_thread_num() == 0) {  deb=
            omp_get_wtime();}
        #pragma omp parallel for default(shared)
        for (int j=0;j<NITER;j++){
                a[j] = essai(j*0.01);}
        if(omp_get_thread_num() == 0) {end=omp_get_wtime
            ();
                cout<<"omp elasped time= "<< (end-deb)<<"
                    s"<<endl;}
        exit(0);
}
```

Reduction

- Data can be collected on each computing unit and operations performed elementary addition and multiplication.

Reduction

- Data can be collected on each computing unit and operations performed elementary addition and multiplication.
- the statement is added as argument of a pragma like reduction (operator: list)

Reduction

- Data can be collected on each computing unit and operations performed elementary addition and multiplication.
- the statement is added as argument of a pragma like reduction (operator: list)
- In addition to the usual operations, you can also search for the largest or smallest item in a list

First scientific program

```
#include <iostream>
#include <iomanip>
#include <cmath>
#include<ctime>
#include<vector>
#include<omp.h>
using namespace std;
double f(double a) { return (4.0 / (1.0 + a*a)); }
int main()
{
  const int ITER= 1000000000;
  double  pi,sum=0.0,h ;
  h=1.0 / (double) ITER;
  double startwtime = 0.0, endwtime;
#pragma omp parallel
  if (omp_get_thread_num() == 0)     {startwtime = omp_get_wtime();}
#pragma omp parallel for  reduction(+:sum)
  for (int i = 0; i <= ITER; i ++)
   { double x = h * (i - 0.5);
          sum += f(x);
        }
  pi = h * sum;
  if (omp_get_thread_num() == 0)
  { endwtime =  omp_get_wtime();
    cout<<"wall clock time = "<<endwtime-startwtime<<endl;
        cout<<"pi is approximately "<<setprecision(15)<<pi<<" , Error is "<< fabs(pi -
             M_PI)<<endl;
  }
  exit(0);
}
```

OPENMP clauses

- OpenMP is a shared memory library, so most code variables are visible, by default, by all threads.

OPENMP clauses

- OpenMP is a shared memory library, so most code variables are visible, by default, by all threads.
- Sometimes, private variables are needed to avoid conflicts in memory and it is necessary to pass values between the sequential part and in the parallel region. Data management is done through data attribute sharing clauses by adding them to the OpenMP instructions.

OPENMP clauses (2)

The different types of clauses are

- *shared*: data within a parallel region is shared, which means visible and accessible by all threads simultaneously. By default, all variables in the sharing region are shared except for the loop counter.

OPENMP clauses (2)

The different types of clauses are

- *shared*: data within a parallel region is shared, which means visible and accessible by all threads simultaneously. By default, all variables in the sharing region are shared except for the loop counter.
- *private*: the data within a parallel region is specific to each thread, which means that each thread will have a local copy and use it as a temporary variable.

OPENMP clauses (2)

The different types of clauses are

- *shared*: data within a parallel region is shared, which means visible and accessible by all threads simultaneously. By default, all variables in the sharing region are shared except for the loop counter.
- *private*: the data within a parallel region is specific to each thread, which means that each thread will have a local copy and use it as a temporary variable.
    1. a private variable is not initialized and the value is not retained for use outside the parallel region.

OPENMP clauses (2)

The different types of clauses are

- *shared*: data within a parallel region is shared, which means visible and accessible by all threads simultaneously. By default, all variables in the sharing region are shared except for the loop counter.
- *private*: the data within a parallel region is specific to each thread, which means that each thread will have a local copy and use it as a temporary variable.
  1. a private variable is not initialized and the value is not retained for use outside the parallel region.
  2. by default, loop iteration counters in OpenMP loop constructs are private.

OPENMP clauses (2)

The different types of clauses are

- *shared*: data within a parallel region is shared, which means visible and accessible by all threads simultaneously. By default, all variables in the sharing region are shared except for the loop counter.
- *private*: the data within a parallel region is specific to each thread, which means that each thread will have a local copy and use it as a temporary variable.
  1. a private variable is not initialized and the value is not retained for use outside the parallel region.
  2. by default, loop iteration counters in OpenMP loop constructs are private.
  3. *default* Allows the programmer to specify that the default value for data in a region
     The different options are either *shared*, *private*, *firstprivate* or *none*.

OPENMP clauses (2)

The different types of clauses are

- *shared*: data within a parallel region is shared, which means visible and accessible by all threads simultaneously. By default, all variables in the sharing region are shared except for the loop counter.
- *private*: the data within a parallel region is specific to each thread, which means that each thread will have a local copy and use it as a temporary variable.
  1. a private variable is not initialized and the value is not retained for use outside the parallel region.
  2. by default, loop iteration counters in OpenMP loop constructs are private.
  3. *default* Allows the programmer to specify that the default value for data in a region
     The different options are either *shared*, *private*, *firstprivate* or *none*.
  4. *none* The none option imposes to the programmer to declare each variable in the parallel region using the data attribute sharing clauses.

Synchronisation clauses

The fine surgery of OPENMP programming is done with synchronization guidelines

- *critical*: the code block will be executed by one thread at a time, and not executed simultaneously by several threads. It is often used to protect shared data to avoid conflict writings in memory.

Synchronisation clauses

The fine surgery of OPENMP programming is done with synchronization guidelines

- *critical*: the code block will be executed by one thread at a time, and not executed simultaneously by several threads. It is often used to protect shared data to avoid conflict writings in memory.
- *atomic*: update in memory (write or read-modify-write) in the next instruction will be executed atomically.

Synchronisation clauses

The fine surgery of OPENMP programming is done with synchronization guidelines

- *critical*: the code block will be executed by one thread at a time, and not executed simultaneously by several threads. It is often used to protect shared data to avoid conflict writings in memory.
- *atomic*: update in memory (write or read-modify-write) in the next instruction will be executed atomically.
- *ordered*: the structured block is executed in the order in which the iterations will be executed in a sequential loop

Synchronisation clauses

The fine surgery of OPENMP programming is done with synchronization guidelines

- *critical*: the code block will be executed by one thread at a time, and not executed simultaneously by several threads. It is often used to protect shared data to avoid conflict writings in memory.
- *atomic*: update in memory (write or read-modify-write) in the next instruction will be executed atomically.
- *ordered*: the structured block is executed in the order in which the iterations will be executed in a sequential loop
- *barrier* Each thread waits for all other threads until the team reaches this instruction. (Very useful!)

Synchronization clause: an instance

```
#include <iostream>
#include <cmath>
#include<ctime>
#include<vector>
#include<omp.h>
using namespace std;
double essai(double x)
{ return(5.0+10.0*x+x*x*exp(x)*log(x+0.1)+sqrt(fabs(x)));}

int main(){
        const int NITER=200000000;
        vector<double> a(NITER);
        double deb,end;
        int b=0;
        #pragma omp parallel
        if(omp_get_thread_num() == 0) {  deb=omp_get_wtime();}
        #pragma omp  parallel for default(shared)
        for (int j=0;j<NITER;j++){
                a[j] = essai(j/10.0);
                if((j%1000) ==0){
                #pragma omp atomic
                b++;
        }
}
if(omp_get_thread_num() == 0) {end=omp_get_wtime();
        cout<<"omp elasped time= "<< (end-deb)<<" s"<<endl;}
cout<<" valeur de b "<<b<<endl;;
exit(0);
}
```

Conclusion and References

- The OPENMP library has been developed for several languages (Fortran, C, C++)

Conclusion and References

- The OPENMP library has been developed for several languages (Fortran, C, C++)
- Developing an OPENMP program is easier than the one with the MPI library, but the number of cores (sharing the same memory) is generally less than ten, but significantly lower than by using many computers with the MPI library.