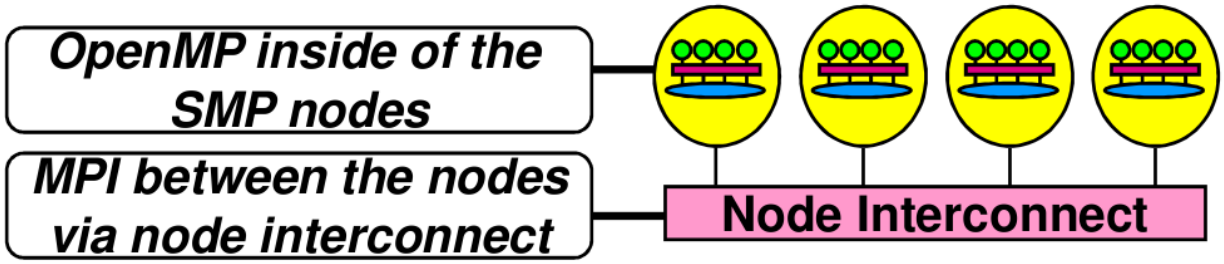
Parallel programming

Modern parallel programing has two pillars: **open-MP** and **MPI**.

- **openMP**:
  - is used only for parallelization across multiple cores on the same node.
  - is part of the compiler, and is typically invoked by ”-openmp” (or ”-fopenmp”) option when compiling. The code needs to contain ”#pragma” statements.
- **MPI** :
  - is primarily used for parallelization across multiple nodes (although it works also on a single node).
  - is implemented as add-on library of commands. A proper set of MPI calls to the library will allow parallel code execution.
  - **Hybrid**: This is the combination of **MPI** and **openMP** parallelization whereby **openMP** is used inside a single node, and **MPI** across different nodes.



A fundamental difference between **MPI** and **openMP** is that in the latter all threads can access the same memory (so called shared memory available to all threads), while in **MPI** every thread can access only its own memory. To communicate between threads, **MPI** command needs to be issued, which is typically very expensive.

On the harware level, every **MPI** commands results in the network traffic between nodes, which is expensive (latency problem). In **openMP** all threads are running on the same motherboard, and hence access the same RAM.

M P I = Message Passing Interface.

It is a standardized collection of routines (functions) which is implemented for each programing language (fortran, C, C++, Python).

It was first standardized in 1994 (MPI-1.0) and second in 1997 (MPI-2.0) and (MPI-3.0) after 2012. Currently MPI-2.0 is most widely used.

Standard is available at `https://www.mpi-forum.org/docs/`

Many implementations of the standard are available (see `http://en.wikipedia.org/wiki/Message_Passing_Interface`)

The two most widely used implementations are MPICH

`http://www.mpich.org`

and open-MPI

`http://www.open-mpi.org`

(Note that open-MPI has nothing to do with openMP)

I will demonstrate examples using open-MPI (`http://www.open-mpi.org`) and for Python implementation mpi4py

(https://mpi4py.readthedocs.io/en/stable/.

If you want to follow, you might want to install both.

There is a lot of literature available (”google MPI”).

- http://mpitutorial.com
- http://www.llnl.gov/computing/tutorials/mpi/#What
- https://www.youtube.com/watch?v=kHV6wmG35po

Brief history:

- 1980s - early 1990s: Distributed memory, parallel computing develops, as do a number of incompatible software tools for writing such programs - usually with tradeoffs between portability, performance, functionality and price. Recognition of the need for a standard arose. MPI Evolution
- April, 1992: Workshop on Standards for Message Passing in a Distributed Memory Environment, sponsored by the Center for Research on Parallel Computing, Williamsburg, Virginia. The basic features essential to a standard message passing interface were discussed, and a working group established to continue the standardization process. Preliminary draft proposal developed subsequently.
- November 1992: - Working group meets in Minneapolis. MPI draft proposal (MPI1) from ORNL presented. Group adopts procedures and organization to form the MPI Forum. MPIF eventually comprised of about 175 individuals from 40 organizations including parallel computer vendors, software writers, academia and application scientists.
- November 1993: Supercomputing 93 conference - draft MPI standard presented.
- Final version of draft released in May, 1994 - available on the at:

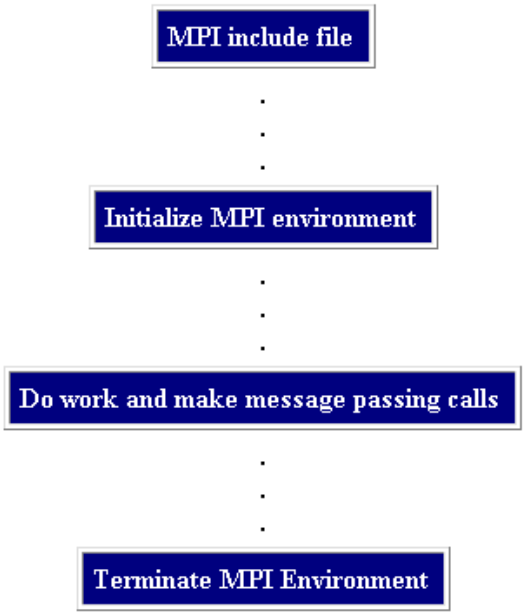
http://www-unix.mcs.anl.gov/mpi.

- MPI-2 picked up where the first MPI specification left off, and addressed topics which go beyond the first MPI specification. The original MPI then became known as MPI-1. MPI-2 is briefly covered later. Was finalized in 1996.
- Today, MPI-2 is widely used.

MPI is available for **Fortran**, **C** and **C++** and Python... We will present examples for **C++** and **Python**. Commands have the same name in all languages, but calls to routines differ slightly.

- MPI is large! It includes 152 functions.
- MPI is small! Many programs need only 6 basic functions.

Typical structure of a parallel code is organized as follows:



minimal C++ code (see http://www.physics.rutgers.edu/~haule/509/MPI_Guide_C++.pdf for details)

```
#include <mpi.h>
#include <iostream>
using namespace std;

int main(int argc, char *argv[])
{
  MPI_Init(&argc, &argv);
  int mpi_size, my_rank;
  MPI_Comm_size(MPI_COMM_WORLD, &mpi_size);
  MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
  cout<<"Hello world from core "<<my_rank<<" out of all "<<mpi_size<<endl;
  MPI_Finalize();
  return 0;
}
```

minimal Python code using my4py:

```
#!/usr/bin/env python
from mpi4py import MPI

comm = MPI.COMM_WORLD
mpi_size = comm.Get_size()
rank = comm.Get_rank()
name = MPI.Get_processor_name()

print "I am processor %d of %d with name %s." % (rank, mpi_size, name)
```

To compile C++ code, we need to execute

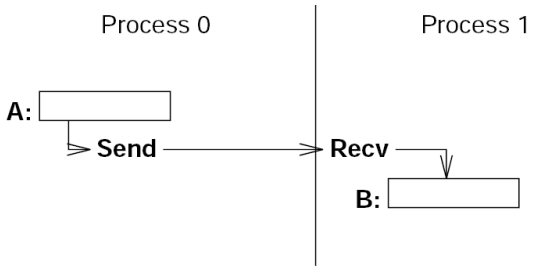
```
mpic++ -o example1 example1.cc
```

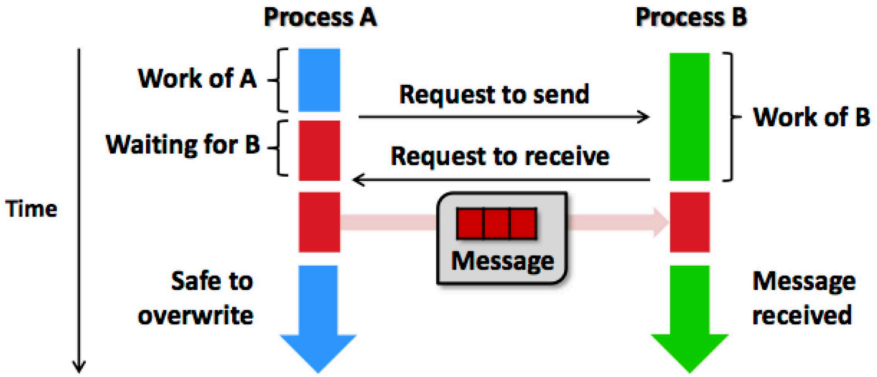
To execute the example, we should issue

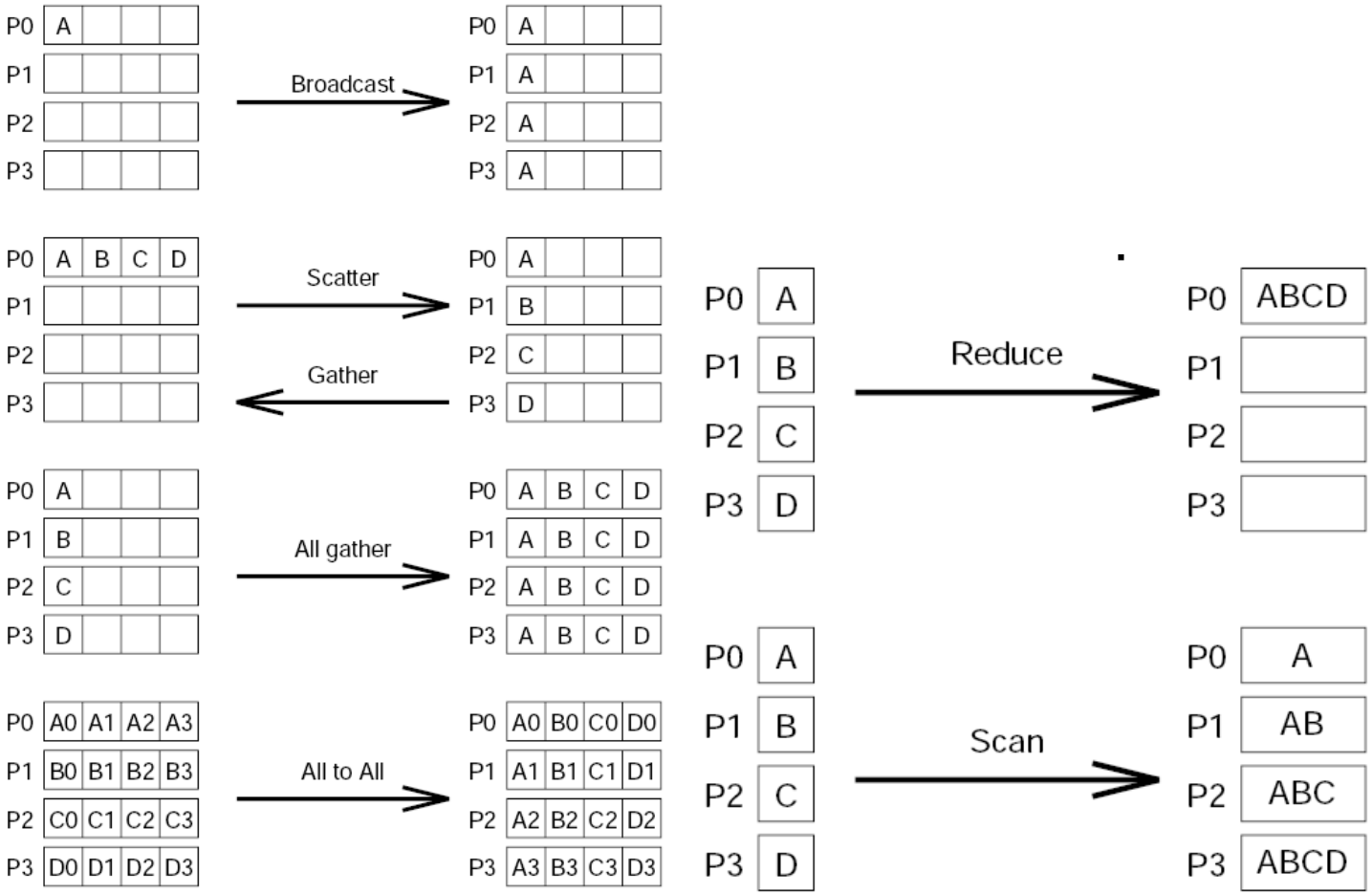
```
mpirun -n 4 example1
```

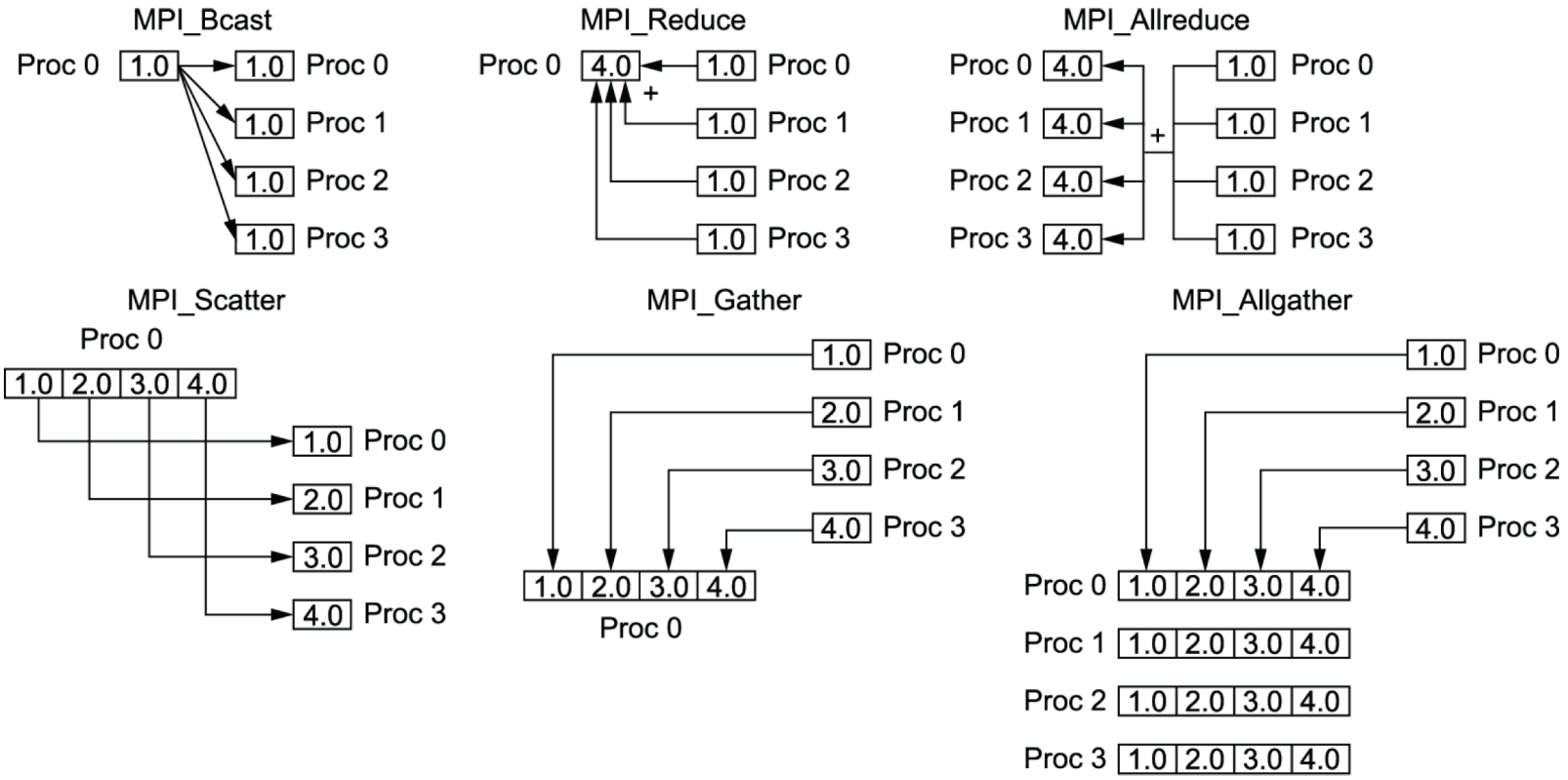
This will run the code on 4 cores on the local node. If one wants to run on multiple nodes, these nodes need to be properly configured into the common network. User needs to provide ”machine file” (list of machine names) and and the following option to mpirun

```
mpirun -hostfile <hostfile> -n 4 example1
```


Process 0
Process 1
A:
Send
Recv
B:


Process A
Process B
Work of A
Waiting for B
Request to send
Request to receive
Work of B
Time
Message
Safe to overwrite
Message received


P0 A
P1
P2
P3
Broadcast
P0 A
P1 A
P2 A
P3 A
P0 A B C D
P1
P2
P3
Scatter
Gather
P0 A
P1 B
P2 C
P3 D
P0 A
P1 B
P2 C
P3 D
All gather
P0 A B C D
P1 A B C D
P2 A B C D
P3 A B C D
P0 A0 A1 A2 A3
P1 B0 B1 B2 B3
P2 C0 C1 C2 C3
P3 D0 D1 D2 D3
All to All
P0 A0 B0 C0 D0
P1 A1 B1 C1 D1
P2 A2 B2 C2 D2
P3 A3 B3 C3 D3
P0 A
P1 B
P2 C
P3 D
Reduce
P0 ABCD
P1
P2
P3
P0 A
P1 B
P2 C
P3 D
Scan
P0 A
P1 AB
P2 ABC
P3 ABCD


MPI_Bcast
Proc 0
1.0
1.0 Proc 0
1.0 Proc 1
1.0 Proc 2
1.0 Proc 3
MPI_Reduce
Proc 0
4.0
+
1.0 Proc 0
1.0 Proc 1
1.0 Proc 2
1.0 Proc 3
MPI_Allreduce
Proc 0 4.0
Proc 1 4.0
Proc 2 4.0
Proc 3 4.0
+
1.0 Proc 0
1.0 Proc 1
1.0 Proc 2
1.0 Proc 3
MPI_Scatter
Proc 0
1.0 2.0 3.0 4.0
1.0 Proc 0
2.0 Proc 1
3.0 Proc 2
4.0 Proc 3
MPI_Gather
1.0 Proc 0
2.0 Proc 1
3.0 Proc 2
4.0 Proc 3
1.0 2.0 3.0 4.0
Proc 0
MPI_Allgather
1.0 Proc 0
2.0 Proc 1
3.0 Proc 2
4.0 Proc 3
Proc 0 1.0 2.0 3.0 4.0
Proc 1 1.0 2.0 3.0 4.0
Proc 2 1.0 2.0 3.0 4.0
Proc 3 1.0 2.0 3.0 4.0

Example of Monte Carlo integration on multiple cores using MPI

```
#include <cmath>
#include <iostream>
#include <mpi.h>
using namespace std;

static const double exact = 1.393203929685676859184246260325 5;

double g(double* x)
{
  return 1./(1.0 - cos(x[0])*cos(x[1])*cos(x[2]))/(M_PI*M_PI*M_PI);
}


int main(int argc, char *argv[])
{
  /* Brute force Monte Carlo to compute an integral of the 3D function:
       1/(1-Cos[x]*Cos[y]*Cos[z])
       in the interval (x,y,z) in [0,Pi],[0,Pi],[0,Pi]
  */
  MPI_Init(&argc, &argv);
  int mpi_size, my_rank;                        // How cores and which processor is this
  MPI_Comm_size(MPI_COMM_WORLD, &mpi_size);
  MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);

  int iseed = time(0)+10*my_rank;               // Each processor should start from different random sequence.
  srand48(iseed);                               // Set iseed

  int N = 10000000;
  double ave=0.0;  // average
  double av2=0.0;  // average^2
  for (int i=0; i<N; i++){
    double kv[3] = {drand48()*M_PI, drand48()*M_PI, drand48()*M_PI};
    double f = g(kv);
    ave += f;
```

```
    av2 += f*f;
  }
  ave=ave/N;  // now we have average
  av2=av2/N;  //     and average^2
  double Vol = M_PI*M_PI*M_PI;  // Volume of the region
  double Int = Vol*ave;         // Integrals is Vol*<f>
  double Int2 = Vol*Vol*av2;    // For error we also need Vol^2 * <f^2>
  double err = sqrt((Int2-Int*Int)/N); // This is standard deviation/N :  sigma^2 =  ( (<f>*Vol)^2 - <f^2>*Vol^2 )
  cout<<"Integral="<<Int<<" Error="<<err<<" approximation-exact="<<Int-exact<<endl;

  double res[2]={Int,Int2};
  double res_sum[2];
  MPI_Reduce(res, res_sum, 2, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);

  if (my_rank==0){
    cout<<"*** Average over all processors ***"<<endl;
    double Int = res_sum[0]/mpi_size;          // Average just sums up
    double Int2 = res_sum[1]/mpi_size;         // Also average^2 just sums up
    double err = sqrt((Int2-Int*Int)/(N*mpi_size)); // New error, which is now divided by (N*mpi_size),
    cout<<"Total Int="<<Int<<" Total err="<<err<<" approximation-exact="<<Int-exact<<endl;
  }

  MPI_Finalize();
  return 0;
}
```

The same algorithm in Python using Pypar:

```
#!/usr/bin/env python
from scipy import *
import pypar    # The Python-MPI interface
import random

def g(x):
  return 1./(1.0 - cos(x[0])*cos(x[1])*cos(x[2]))/pi**3

if __name__ == '__main__':

    mpi_size = pypar.size()
    my_rank =  pypar.rank()
    my_name =  pypar.get_processor_name()

    random.jumpahead(my_rank)   # different random number start on each processor

    N = 100000
    ave=0.0
    av2=0.0
    for i in range(N):
        f = g(array([random.random(),random.random(),random.random()])*pi)
        ave += f
        av2 += f*f

    ave=ave/N   # now we have average
    av2=av2/N   #     and average^2
    Vol = pi**3 # Volume of the region
    Int = Vol*ave          # Integrals is Vol*<f>
    Int2 = Vol*Vol*av2     # For error we also need Vol^2 * <f^2>
    Error = sqrt((Int2-Int*Int)/N) # This is standard deviation  sigma^2 =  ( (<f>*Vol)^2 - <f^2>*Vol^2 )/N
    print "Integral=", Int, "Error=", Error

    res=array([Int,Int2])
    sum_res=zeros(2)
```

```
pypar.reduce(res, pypar.SUM, 0, buffer=sum_res)  #  This is the crucial MPI call

if my_rank==0:
    Int = sum_res[0]/mpi_size
    Int2 = sum_res[1]/mpi_size
    Error = sqrt((Int2-Int*Int)/(N*mpi_size))
    print "Final Integral=", Int, "Error=", Error

pypar.finalize()
```

We again compile C++ code with the command

```
mpic++ -o example2 example2.cc
```

and execute by

```
mpirun -n 4 example2
```

The Python code does not need compilation. Make the Python script executable (chmod a+x example2.py). Then execute by

```
mpirun -n 4 example2.py
```

Some useful tips:

- Alwyas parallelize the most outside loop. Do not parallelize inside loops! This will minimize the communication.
- Avoid using many MPI calls. Try to combine MPI calls. Do not use multiple 'send-receive' calls if you can use Broadcast or Gather,....
- Every MPI call takes some minimum amount of time (it is expensive) and typically all processors need to wait at the point of MPI call. MPI call slows down all processors.
- Always develop and test serial code first. Parallel job is very hard to debug!
- Some algorithms are easy to parallelize. Some inpossible. Test if more processors gives you better performance. Sometimes gives you even worse!
- In parallel programming, the "minimum amount of work" strategy does not apply. The amount of communication has to be minimized because communication is usually slow.

For example.

- Master reads some data. Other processors wait for the master
- MPI::Broadcast is used to transfer the data to slaves
- Each processors performs part of the work
- The common part of the work could be performed on master only. Let's call MPI::Gather or MPI::Reduce and perform common part of the computation on Master. When finished, master distributes the result by MPI::Broadcast
- Each processor continues with its own task
- Finally the results are merged together with MPI::Gather or MPI::Reduce

Much more efficient sheme is

- Every processor reads the data and immediately starts with work.
- Each processors performs part of the work
- Each processor performs the common part of the work. It does not take more time. All processors repeat the same calculation, but the MPI call can be skipped.
- Each processor continues with its own task
- Finally the results are merged together with MPI::Gather or MPI::Reduce