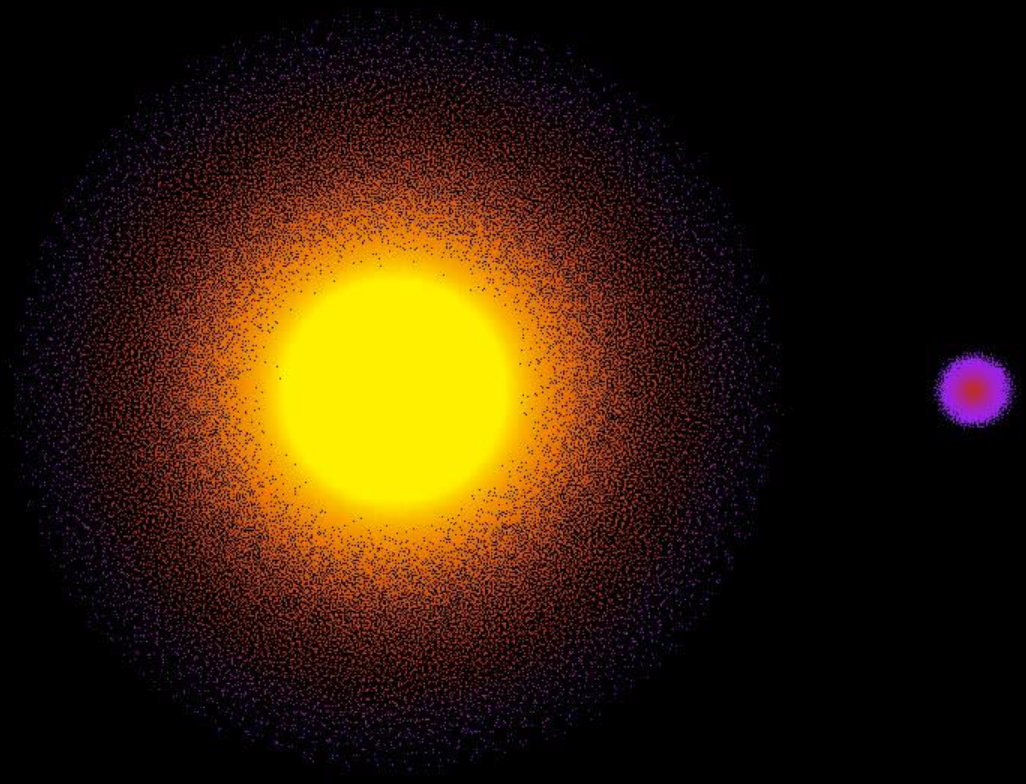
Introduction to Parallel Computing



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Dr. Aurélien Cavelan

sciCORE
Center for scientific computing

University of Basel

OpenMP

Outline

Introduction

OpenMP

- ❑ Scheduling
- ❑ Variables scope
- ❑ Reduction
- ❑ Atomic
- ❑ Collapse
- ❑ Orphaned directives

Python

- ❑ Multiprocessing
- ❑ Numba

OpenMP and GPU offloading

MPI (just a smidge)

Launching in clusters (SLURM)

09:00 – 10:30: Lecture
10:30 – 10:45: Coffee break
10:45 – 12:00: Lecture

12:00 – 13:30: Lunch

13:30 – 15:00: Lecture
15:00 – 15:15: Coffee break
15:15 – 17:00: Lecture

First thing to do:

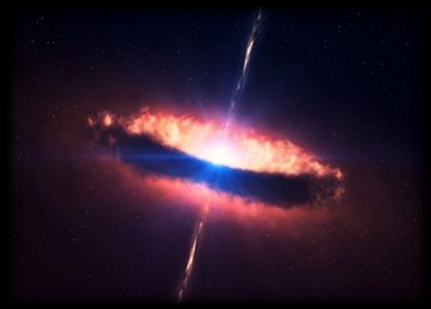
Download the slides of the course:

From the browser: https://bit.ly/scicore_openmp

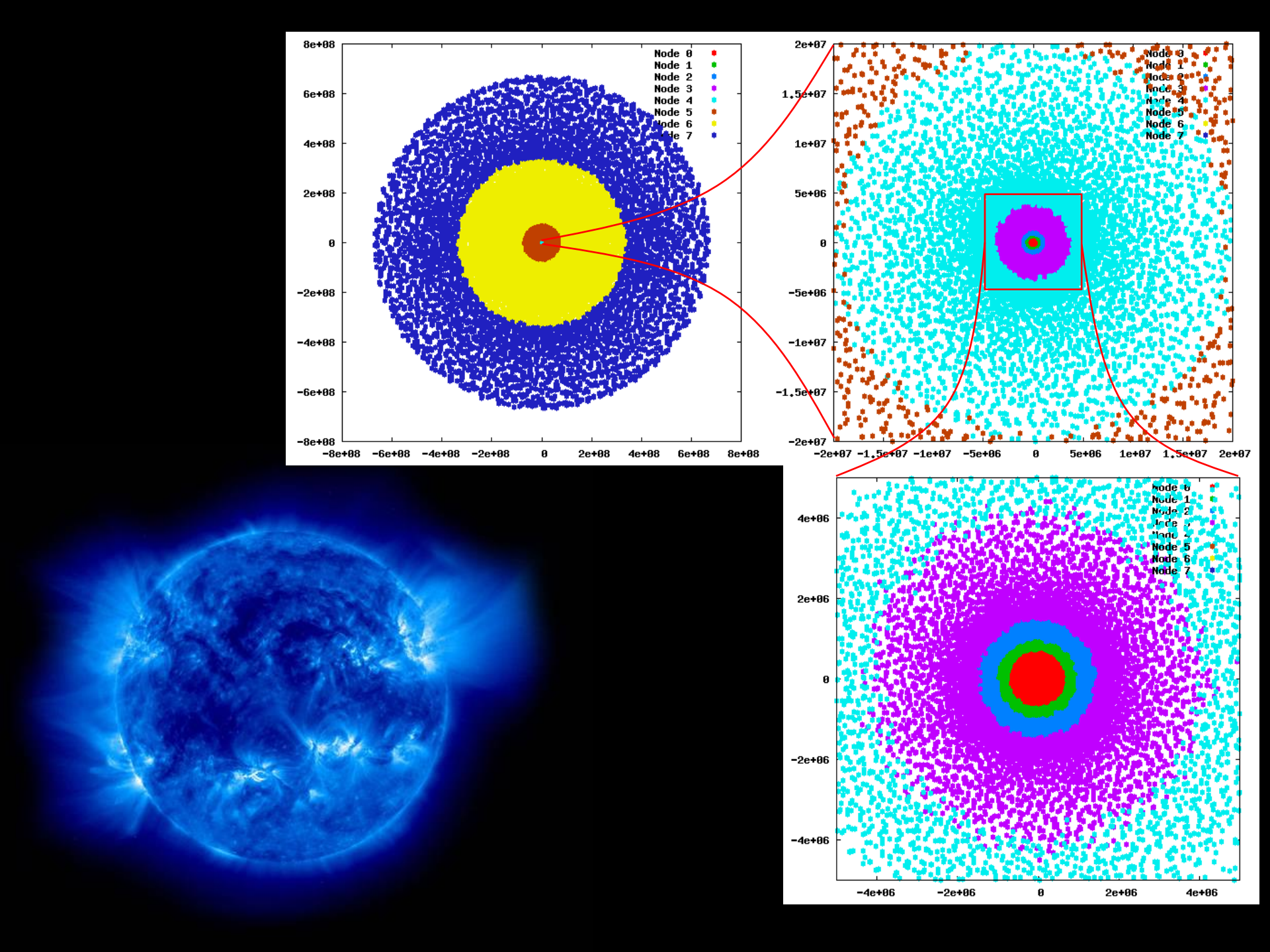
From the terminal: wget https://bit.ly/scicore_openmp

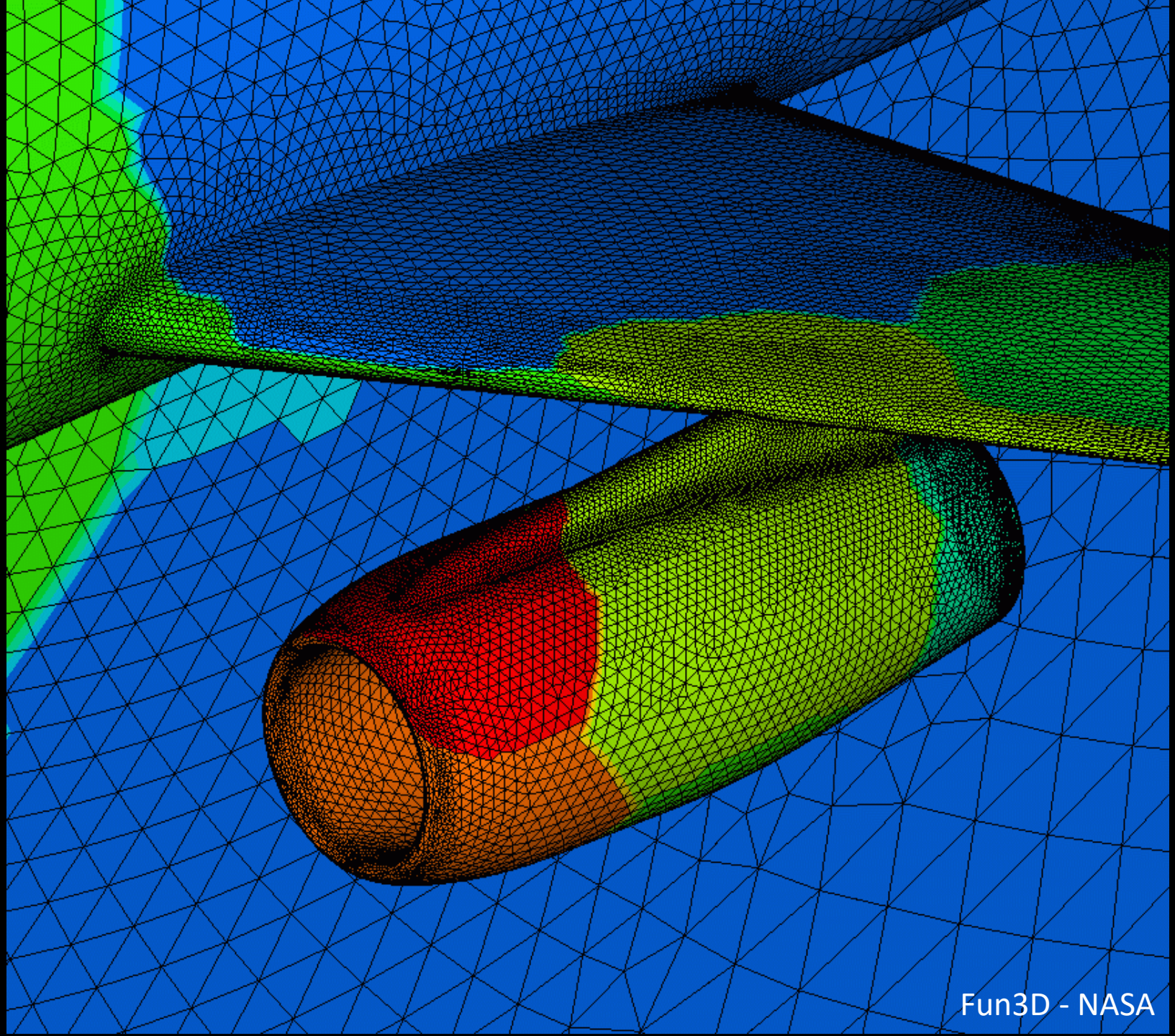
You can find there the slides of the course (exercises are redacted)

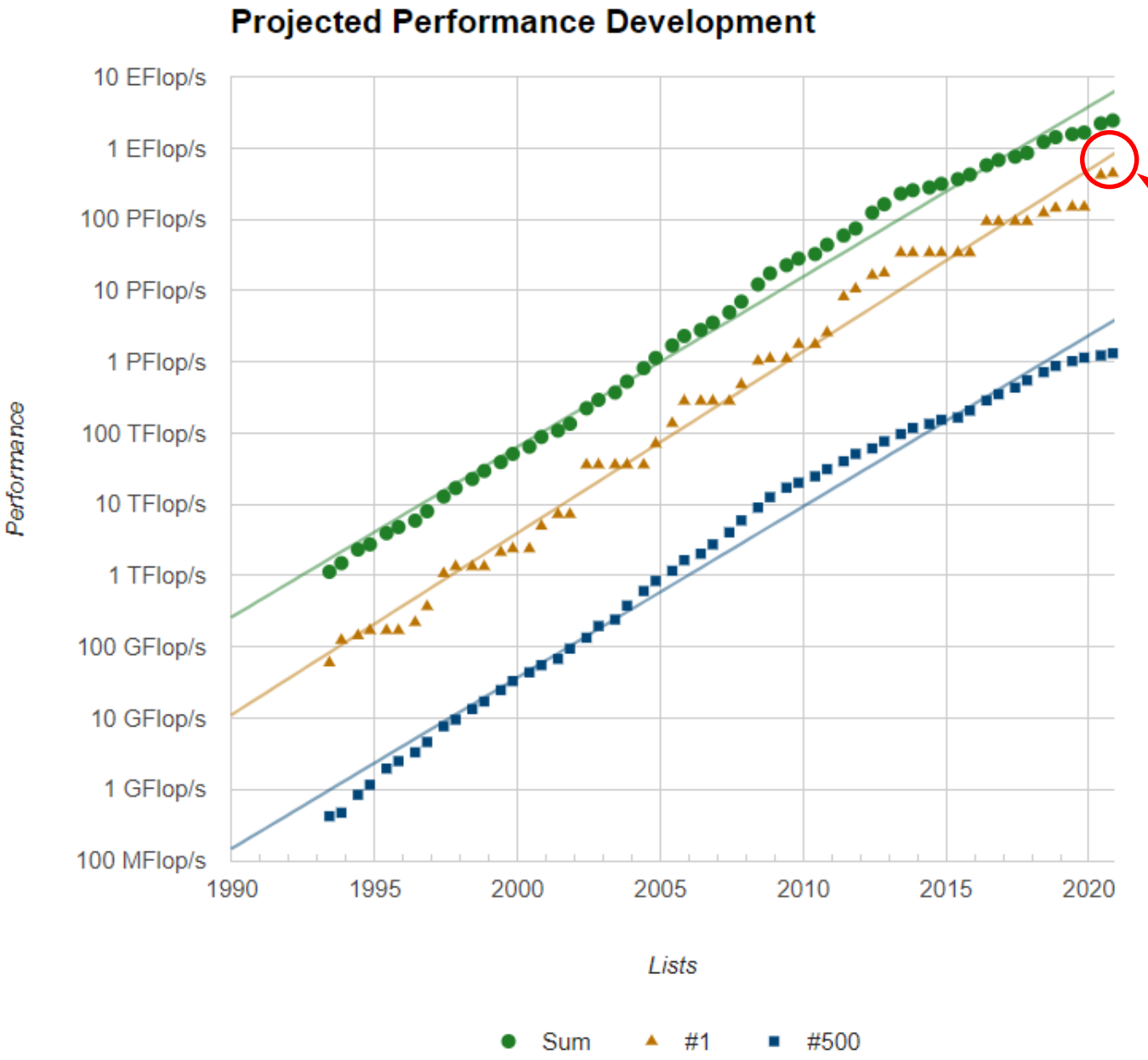
Multiple executions of the same code, applied to different sections of the input data.



Split the problem in subdomains that are partially solved independently.


Node 0
Node 1
Node 2
Node 3
Node 4
Node 5
Node 6
Node 7
8e+08
6e+08
4e+08
2e+08
0
-2e+08
-4e+08
-6e+08
-8e+08
2e+07
1.5e+07
1e+07
5e+06
-5e+06
-1e+07
-1.5e+07
-2e+07
4e+06
2e+06
-2e+06
-4e+06

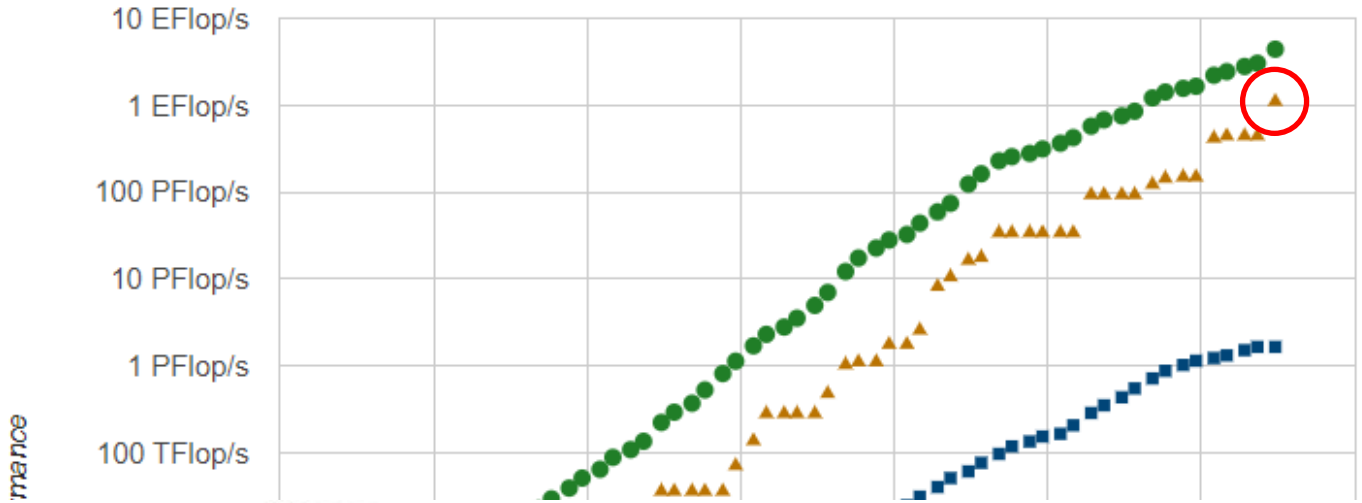

Fun3D - NASA

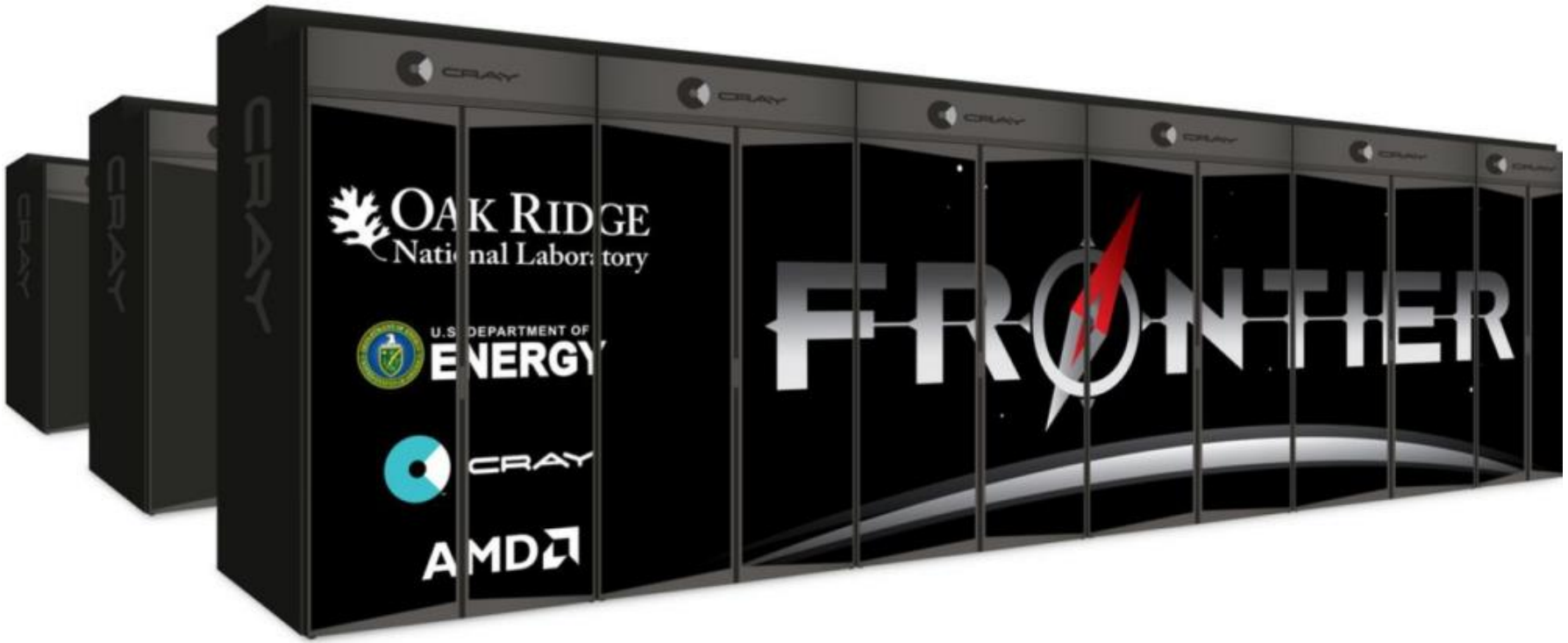


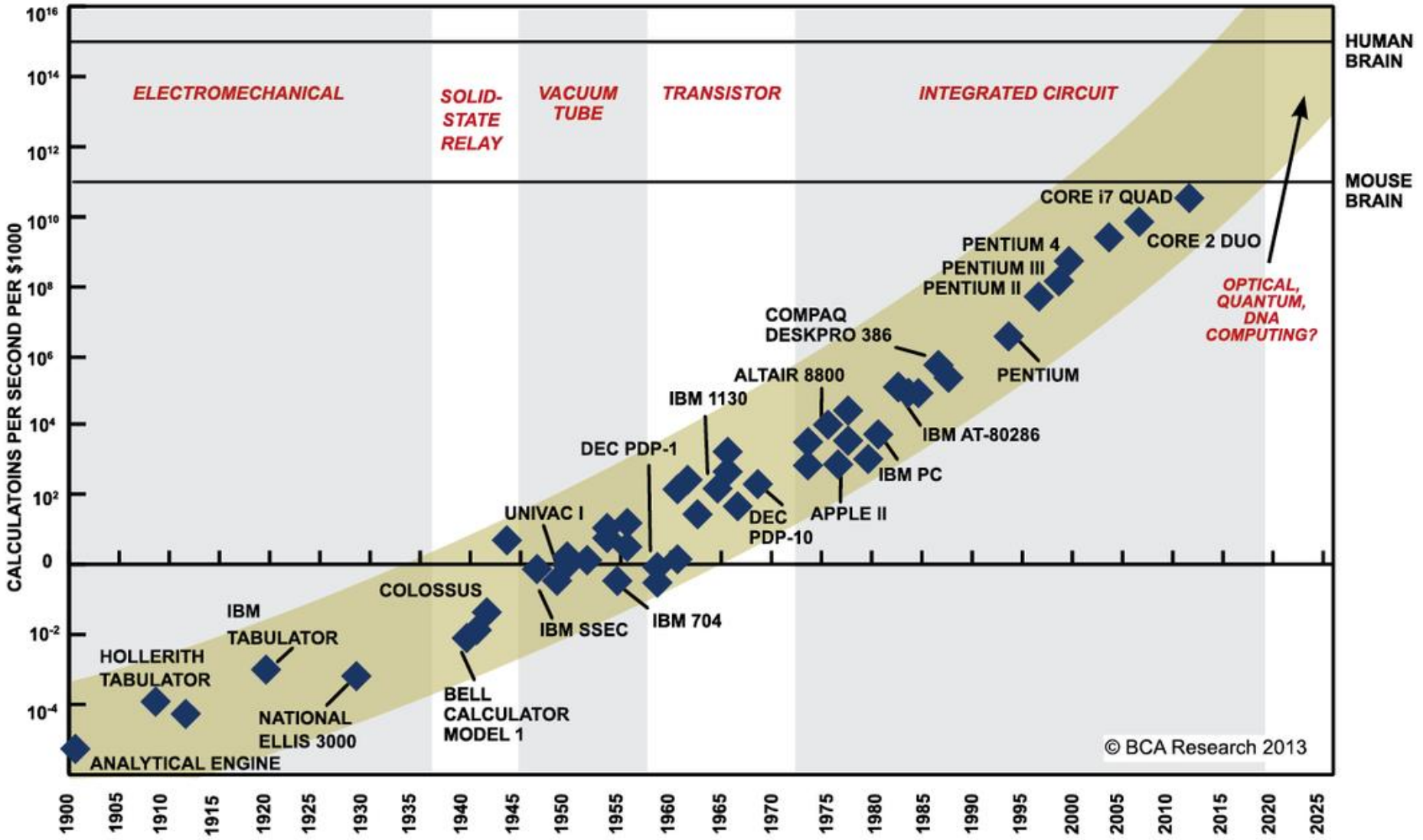
Exascale will be reached close to 2022

- Aerospace, Airframes, Jet Turbines
- Astrophysics
- Biological and medical systems
- Climate and weather
- Combustion
- Materials science
- Fusion energy
- National security
- Nuclear engineering

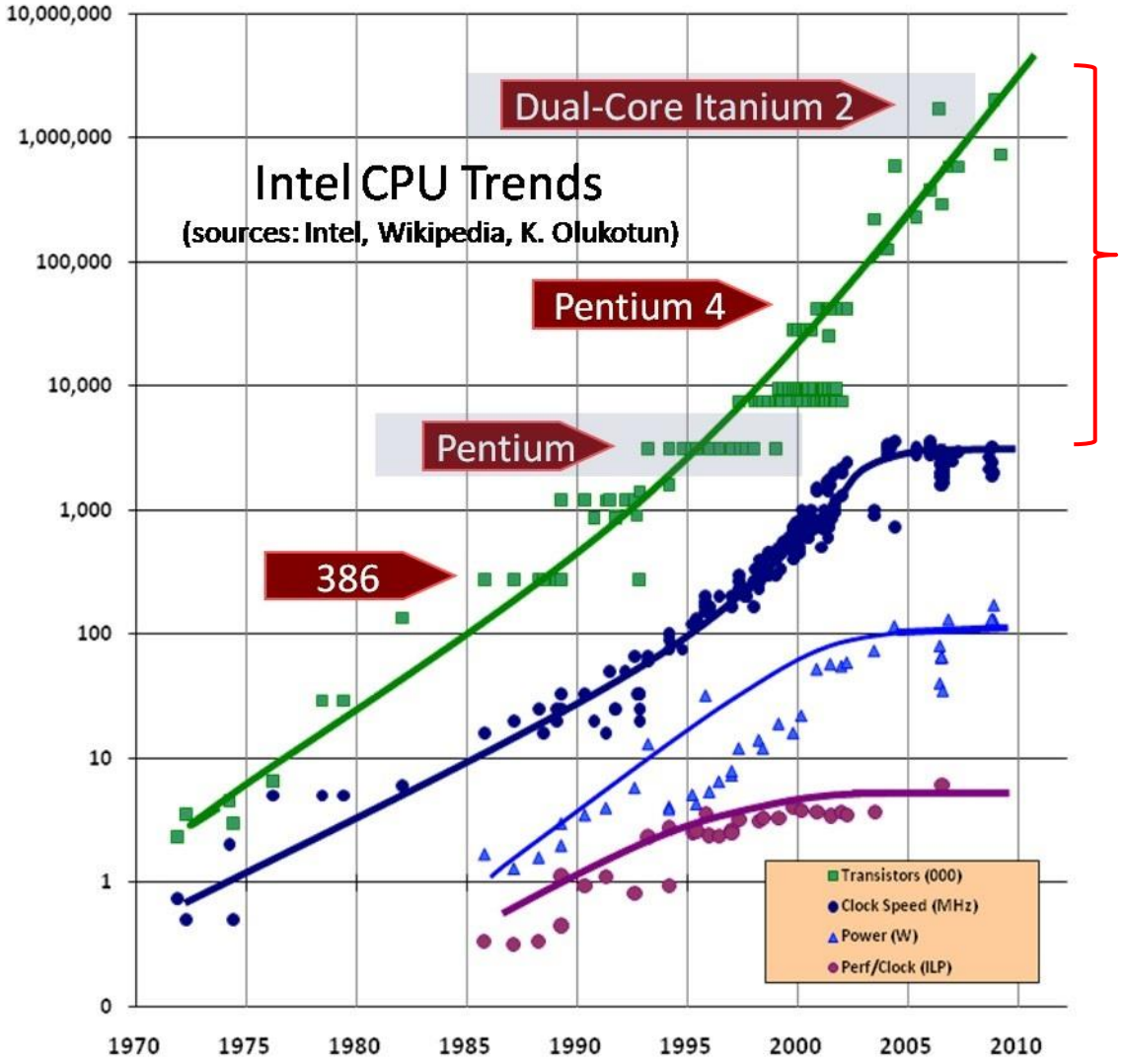
Performance Development



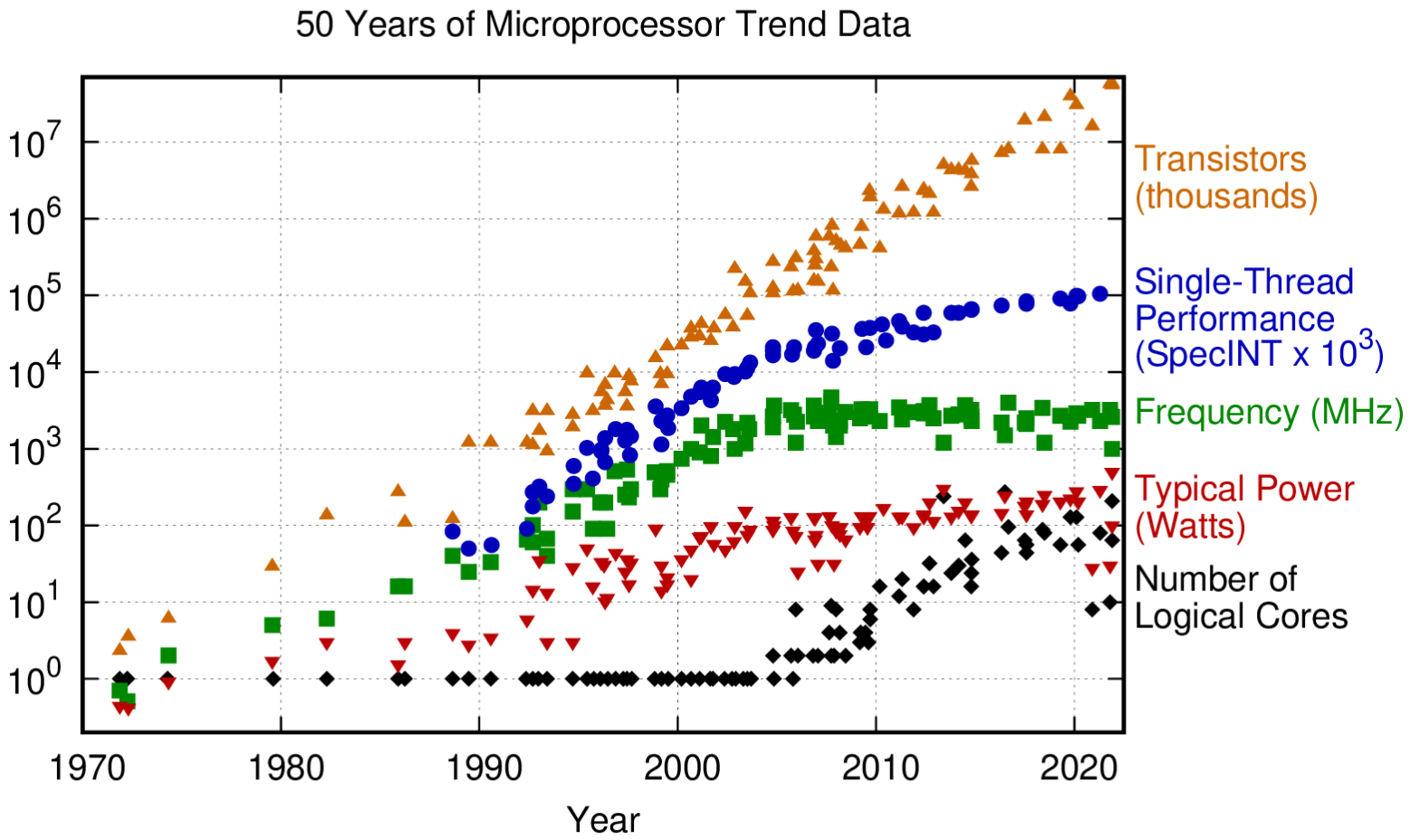




SOURCE: RAY KURZWEIL, "THE SINGULARITY IS NEAR: WHEN HUMANS TRANSCEND BIOLOGY", P.67, *THE VIKING PRESS*, 2006. DATAPOINTS BETWEEN 2000 AND 2012 REPRESENT BCA ESTIMATES.



More transistors do not mean faster anymore!

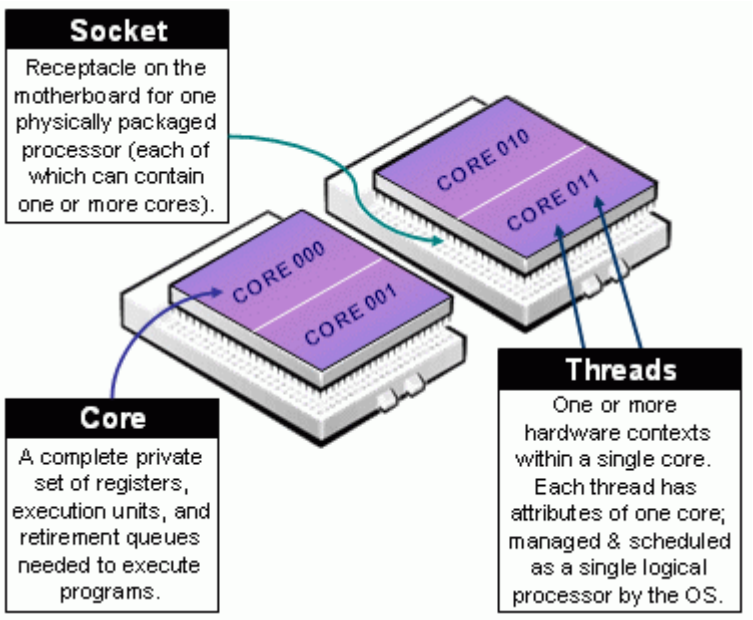


Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten
New plot and data collected for 2010-2021 by K. Rupp

Increase in performace is done nowadays via **parallelization**

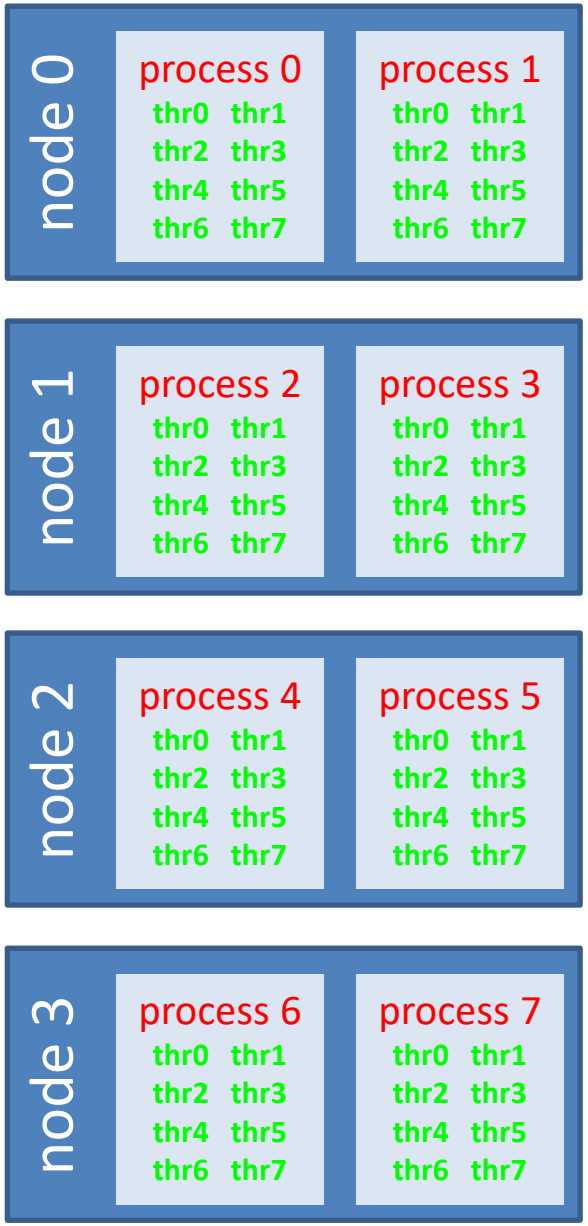
Usually a hybrid MPI+X approach is taken

(X=OpenMP, OpenMP offloading, OpenACC, CUDA)



Hyperthreading is usually deactivated in HPC facilities by default.
Ask the sysadmin!

logical cores = # physical cores * # threads/core



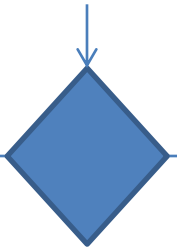
In general, the problem can be reduced to a logical repetitive structure:

```
do i = 1, n

<calculations>

end do
```

Are these <calculations> completely **independent** from each other?



Yes

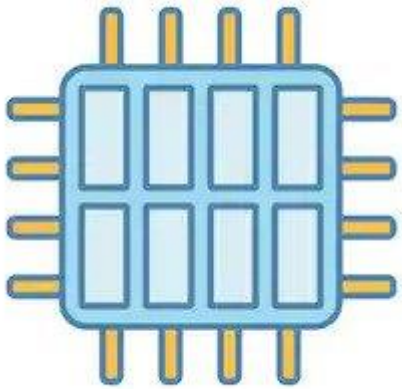
No

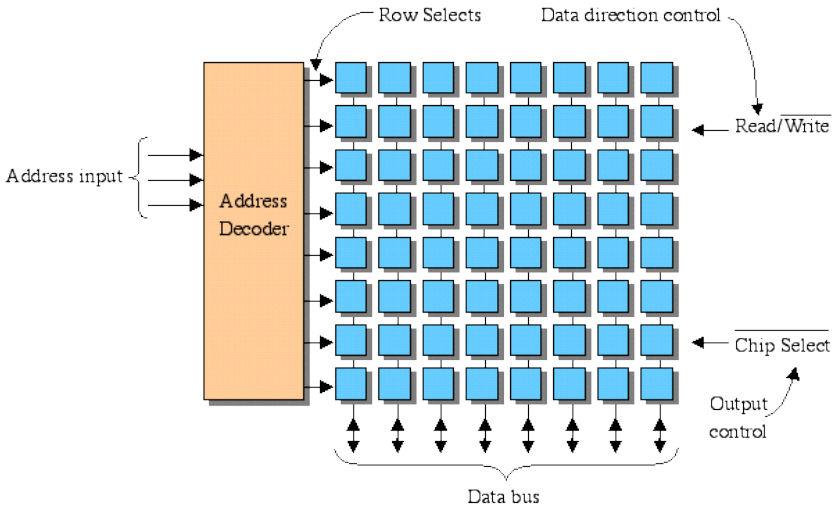
- What's the degree of dependency?
- Can I rewrite/factorize to eliminate the dependency?
- Do variables share contents? Is it necessary?

OpenMP

Open **M**ulti-**P**rocessing

Works in shared memory systems
Can use as many cores as there are in the compute node
Uses threads to split the work
Threads have both private and shared variables
Uses preprocessor directives in commented lines





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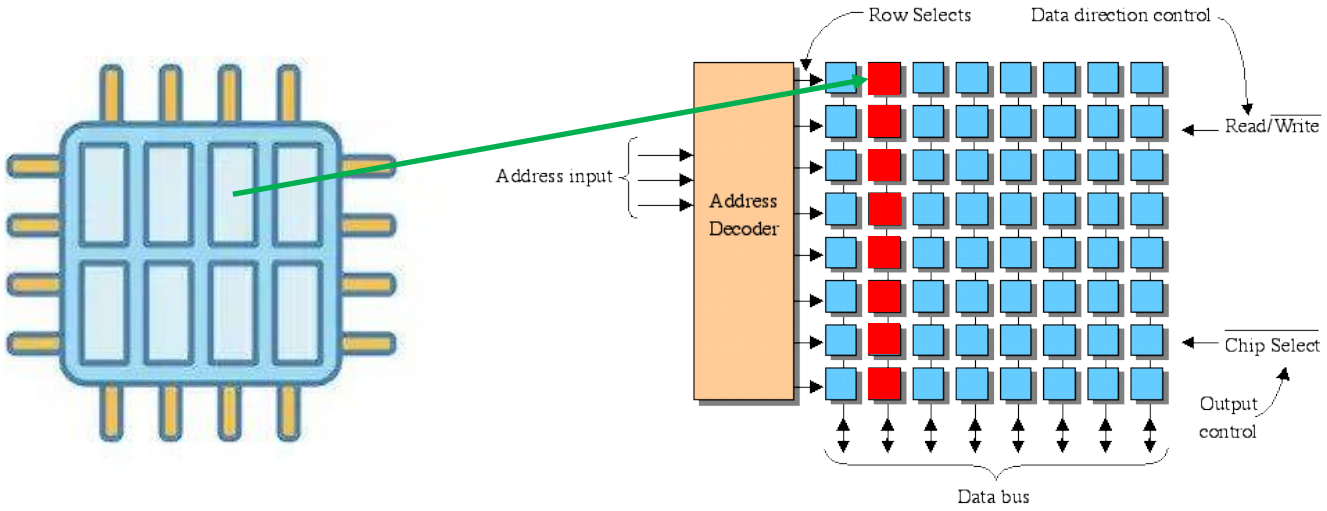

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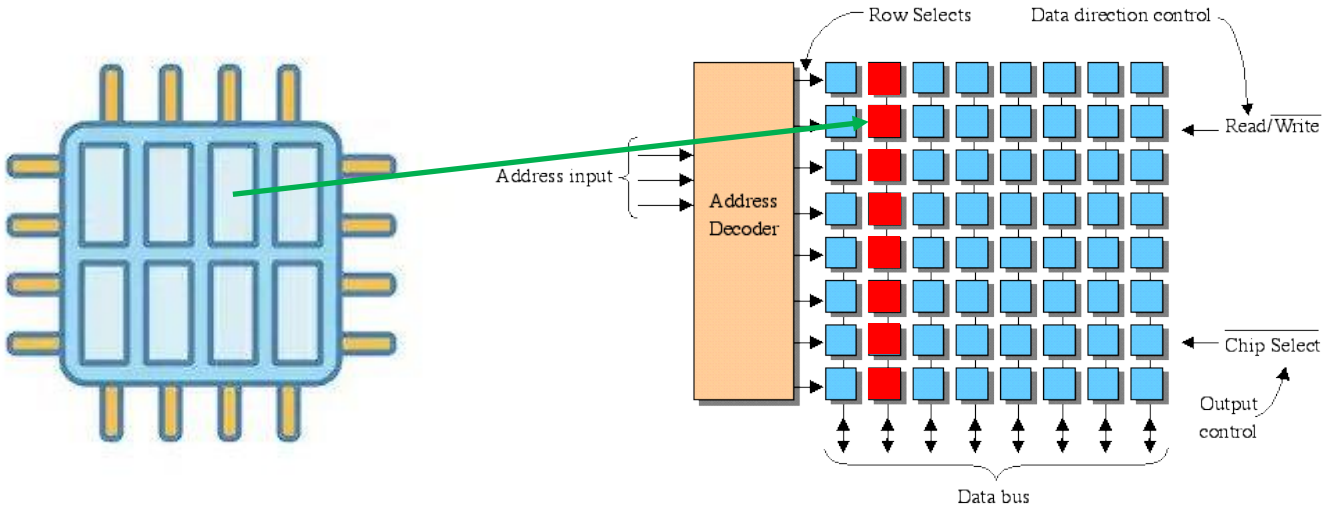

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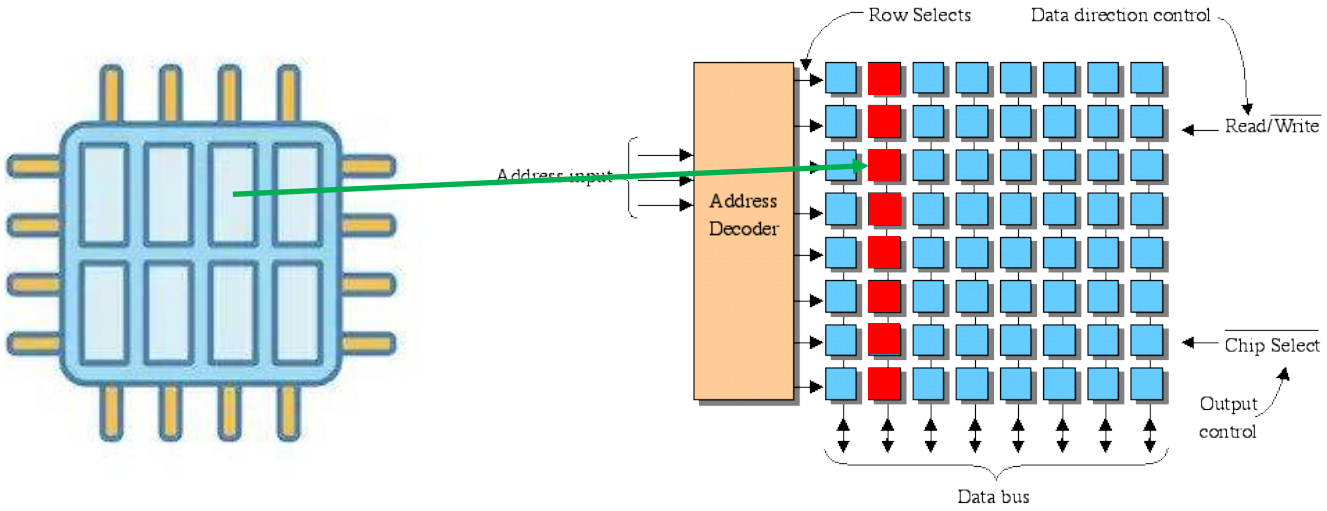

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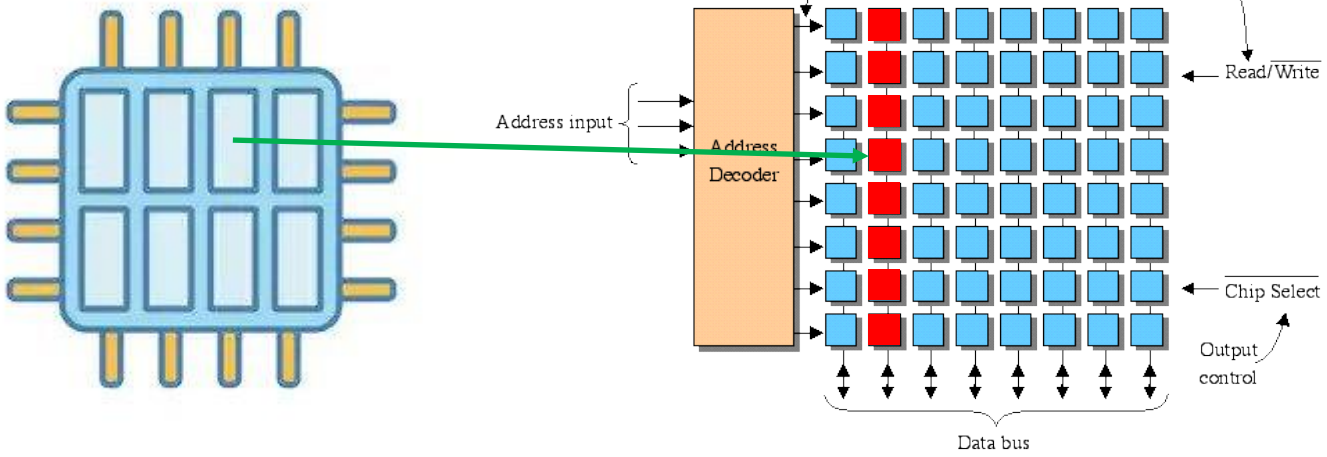

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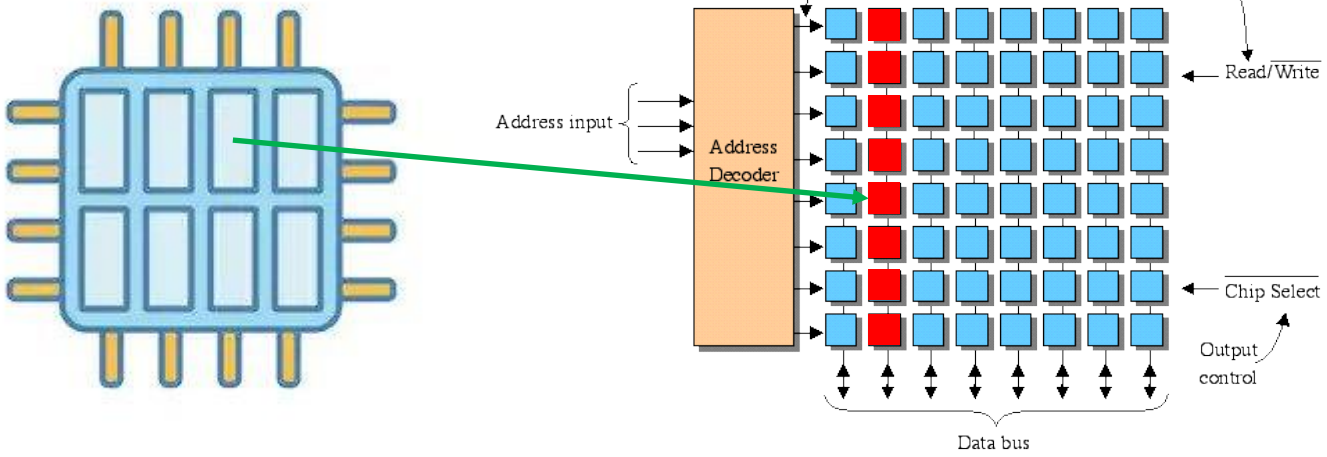

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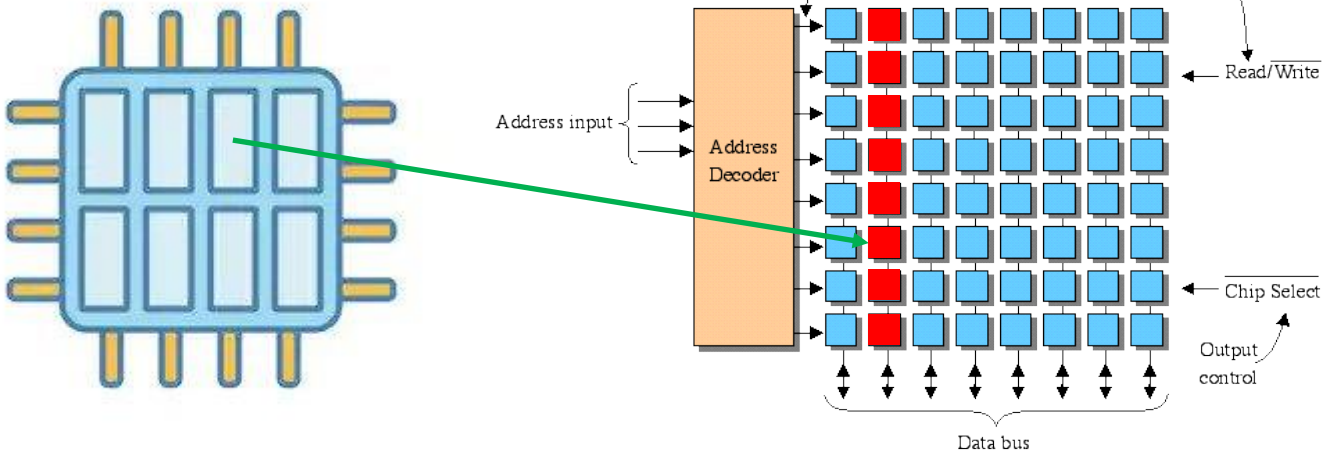

OpenMP™

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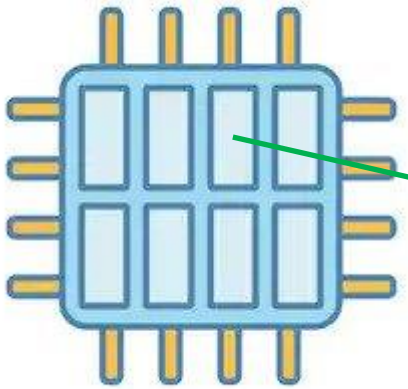

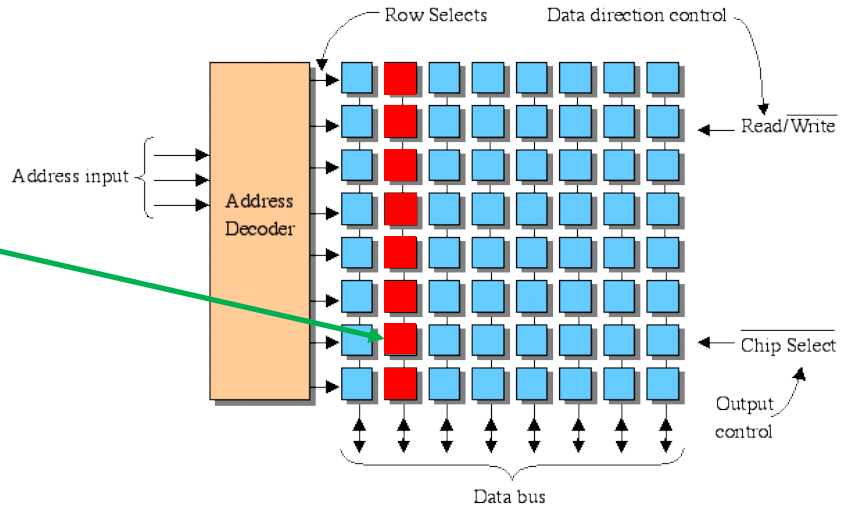

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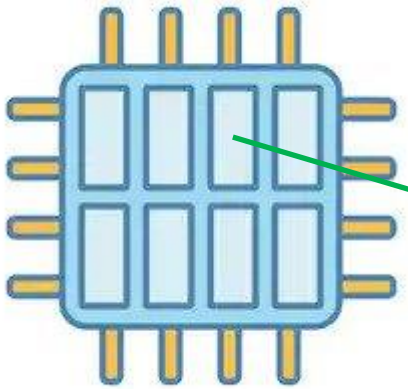

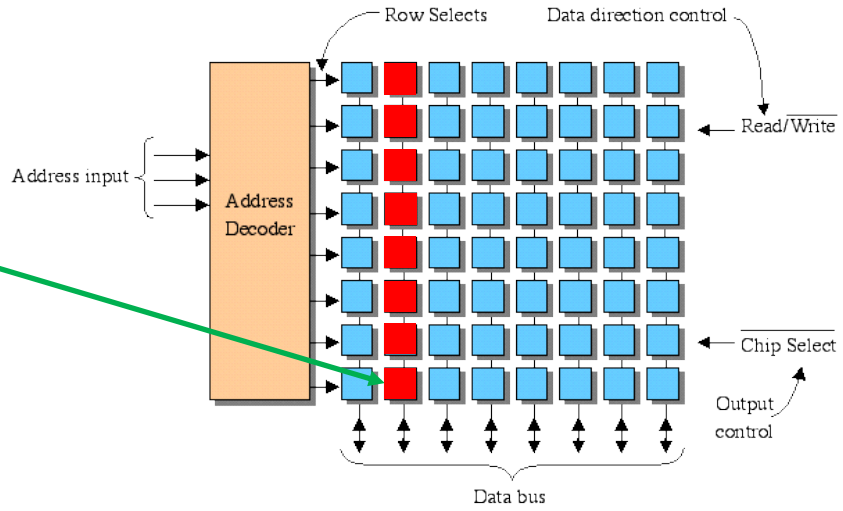

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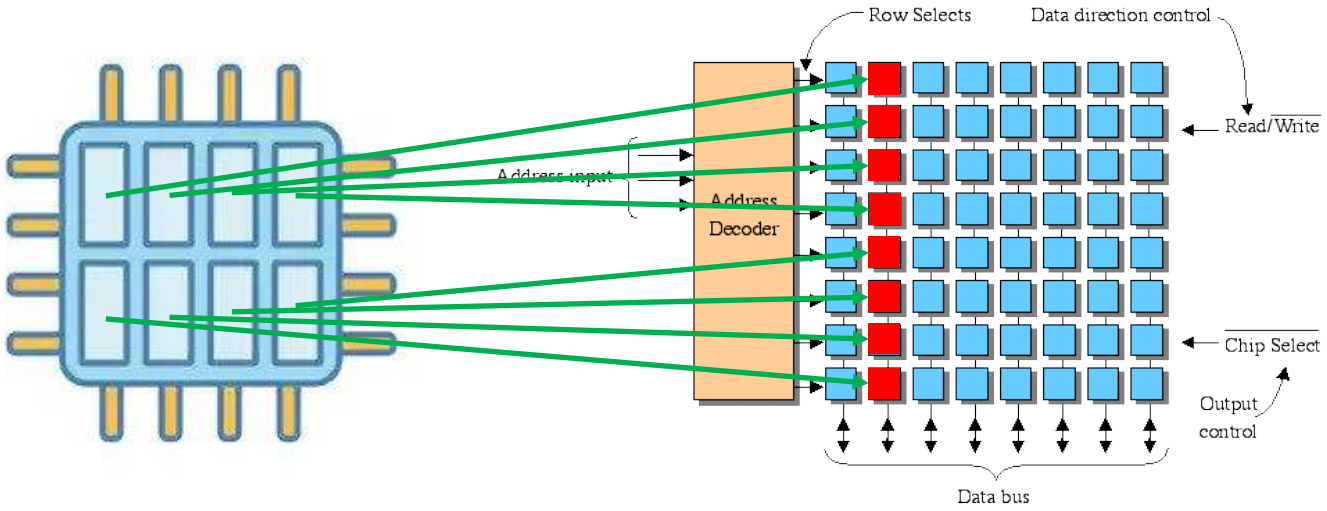


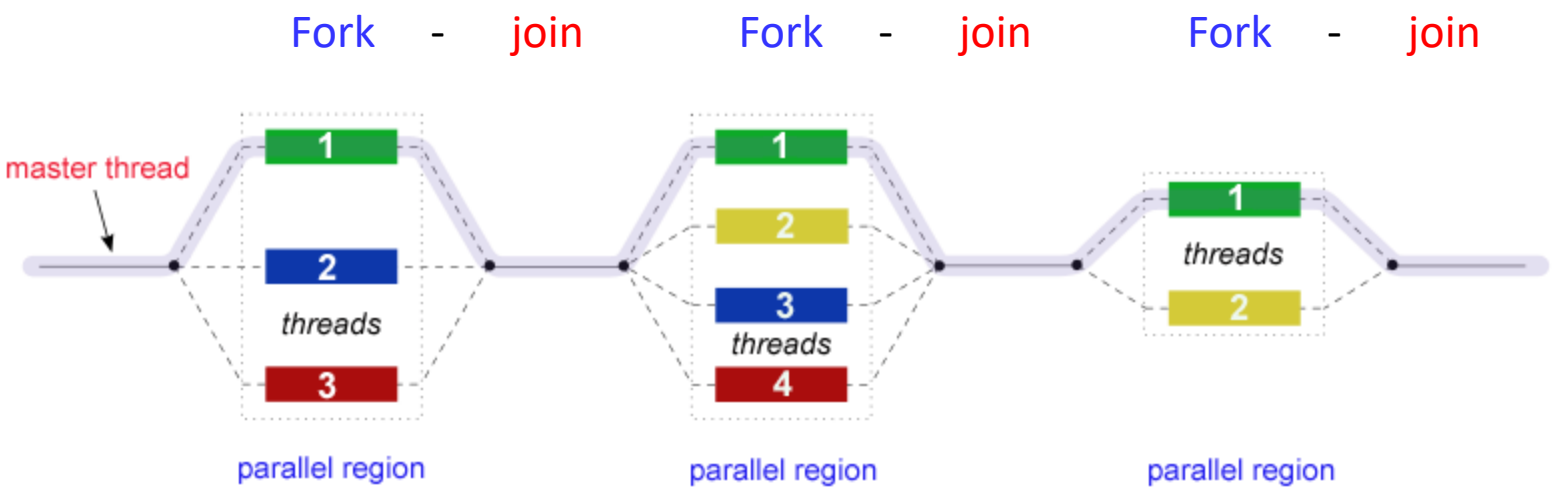
Some resources

- Main references:
  https://www.openmp.org/wp-content/uploads/OpenMPRefCard-5-2-web.pdf
  https://www.openmp.org/compunity/

- Examples & tutorials:
  https://www.openmp.org/wp-content/uploads/openmp-examples-5.1.pdf
  https://hpc-tutorials.llnl.gov/openmp/
  https://www.youtube.com/playlist?list=PLLX-Q6B8xqZ8n8bwjGdzBJ25X2utwnoEG
  https://numba.pydata.org/numba-doc/latest/user/5minguide.html
  https://mpi4py.readthedocs.io/en/stable/tutorial.html

- Books:
  The OpenMP Common Core: Making OpenMP Simple Again (Mattson, et al. 2019)

- In-person Courses:
  Unibas Master and PhD course, https://hpc.dmi.unibas.ch/HPC/Teaching.html
  In particular: Foundations of Distributed Systems (45402-01/HS): F. Ciorba, H. Schuldt, C. Tschundin
  High-Performance Computing (17164-01/FS): F. Ciorba


Fork - join
Fork - join
Fork - join
master thread
1
2
threads
3
parallel region
1
2
3
threads
4
parallel region
1
threads
2
parallel region

FORTRAN

```
use omp_lib


!$omp parallel
...
!$omp do
do ...
enddo
!$omp end do
...
!$omp end parallel
```

C/C++

```
#include <omp.h>


#pragma omp parallel
{
  ...
  #pragma omp for
  for(...){
  ...
  }
}
```

- Serial and parallel program share the same source code.
- Serial compiler simply overlooks parallel directives (they are comments).
- Modifying parallel directives cannot break the serial code.
- Modifying the serial code outside of parallel regions cannot break the parallelization.
- Easy to maintain.
- Compact code.

```
!$omp parallel private(id)
id=omp_get_thread_num()
print *,'I am thread: ',id
!$omp end parallel
```

Runtime library rutine.

- omp_get_num_threads()
- omp_set_num_threads()
- omp_get_wtime()
- …

```
I am thread 0
I am thread 1
I am thread 2
I am thread 3
```

```
I am thread 0
I am thread 3
I am thread 2
I am thread 1
```

```
I am thread 2
I am thread 1
I am thread 0
I am thread 3
```

```
I am thread 0
I am thread 1
I am thread 2
I am thread 3
```

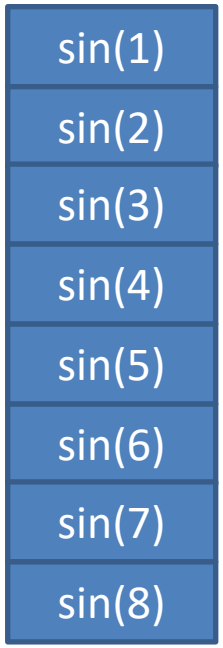
We cannot ensure that the threads will execute and finish in order!

```
do i = 1, n

   f(i) = sin(dble(i))

end do
```

f(i) =

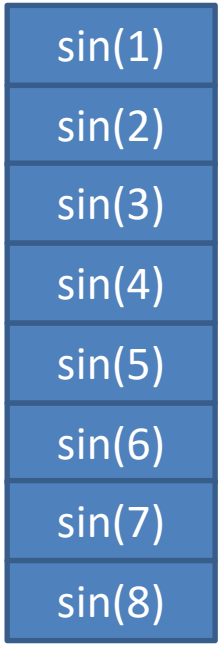



```
!$omp parallel
!$omp do
do i = 1, n

   f(i) = sin(dble(i))

end do
!$omp end do
!$omp end parallel
```

f(i) =



```
do i = 1, n

   f(i) = sin(dble(i))

end do
```

```
!$omp parallel
!$omp do
do i = 1, n

   f(i) = sin(dble(i))

end do
!$omp end do
!$omp end parallel
```

f(i) =

sin(1)
sin(2)
sin(3)
sin(4)
sin(5)
sin(6)
sin(7)
sin(8)

Check env. variable, f.e.:
$OMP_NUM_THREADS=4

f(i) =

sin(1)
sin(2)
sin(3)
sin(4)
sin(5)
sin(6)
sin(7)
sin(8)

```
do i = 1, n

   f(i) = sin(dble(i))

end do
```

```
!$omp parallel
!$omp do
do i = 1, n

   f(i) = sin(dble(i))

end do
!$omp end do
!$omp end parallel
```

f(i) =

sin(1)
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f(i) =

sin(1)
sin(2)
sin(3)
sin(4)
sin(5)
sin(6)
sin(7)
sin(8)

Creates 4 threads and distributes the work evenly

```
do i = 1, n

   f(i) = sin(dble(i))

end do
```

```
!$omp parallel
!$omp do
do i = 1, n

   f(i) = sin(dble(i))

end do
!$omp end do
!$omp end parallel
```

f(i) =

sin(1)
sin(2)
sin(3)
sin(4)
sin(5)
sin(6)
sin(7)
sin(8)

Check env. variable, f.e.:
$OMP_NUM_THREADS=4

f(i) =

sin(1)	thread 0
sin(2)	thread 0
sin(3)	thread 1
sin(4)	thread 1
sin(5)	thread 2
sin(6)	thread 2
sin(7)	thread 3
sin(8)	thread 3

x4 Speed-up!

Creates 4 threads and distributes the work evenly

OpenMP

```
!$omp parallel
!$omp do
do i = 1, n

   f(i) = sin(dble(i))

end do
!$omp end do
!$omp end parallel
```

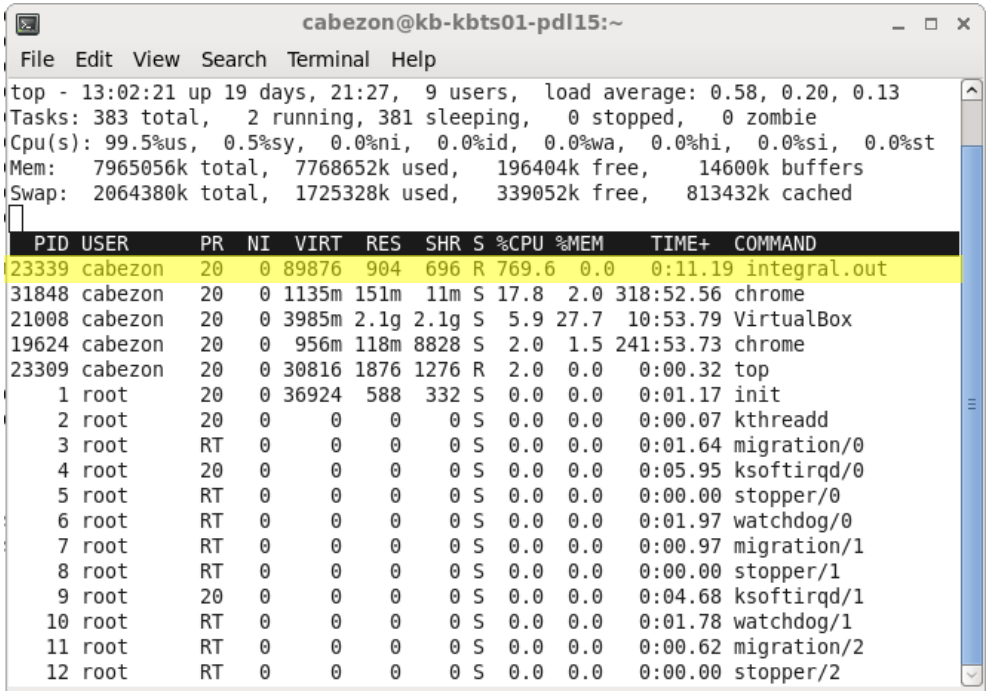
Establish parallel section

Parallel loop evenly divided among the threads

The number of threads is given by the environment variable: $OMP_NUM_THREADS
If not defined, OpenMP assumes OMP_NUM_THREADS = # cores in the computer.
Can be changed with: export OMP_NUM_THREADS = <integer>
(consider adding it to .bashrc)

These are comments!
They are understood by the compiler only when compiled with –openmp option (or similar). Otherwise they are ignored.

An OpenMP calculation will appear as using more than 100% of CPU



OpenMP

```
!$omp parallel
!$omp do schedule(static)
do i = 1, n

   f(i) = sin(dble(i))

end do
!$omp end do
!$omp end parallel
```

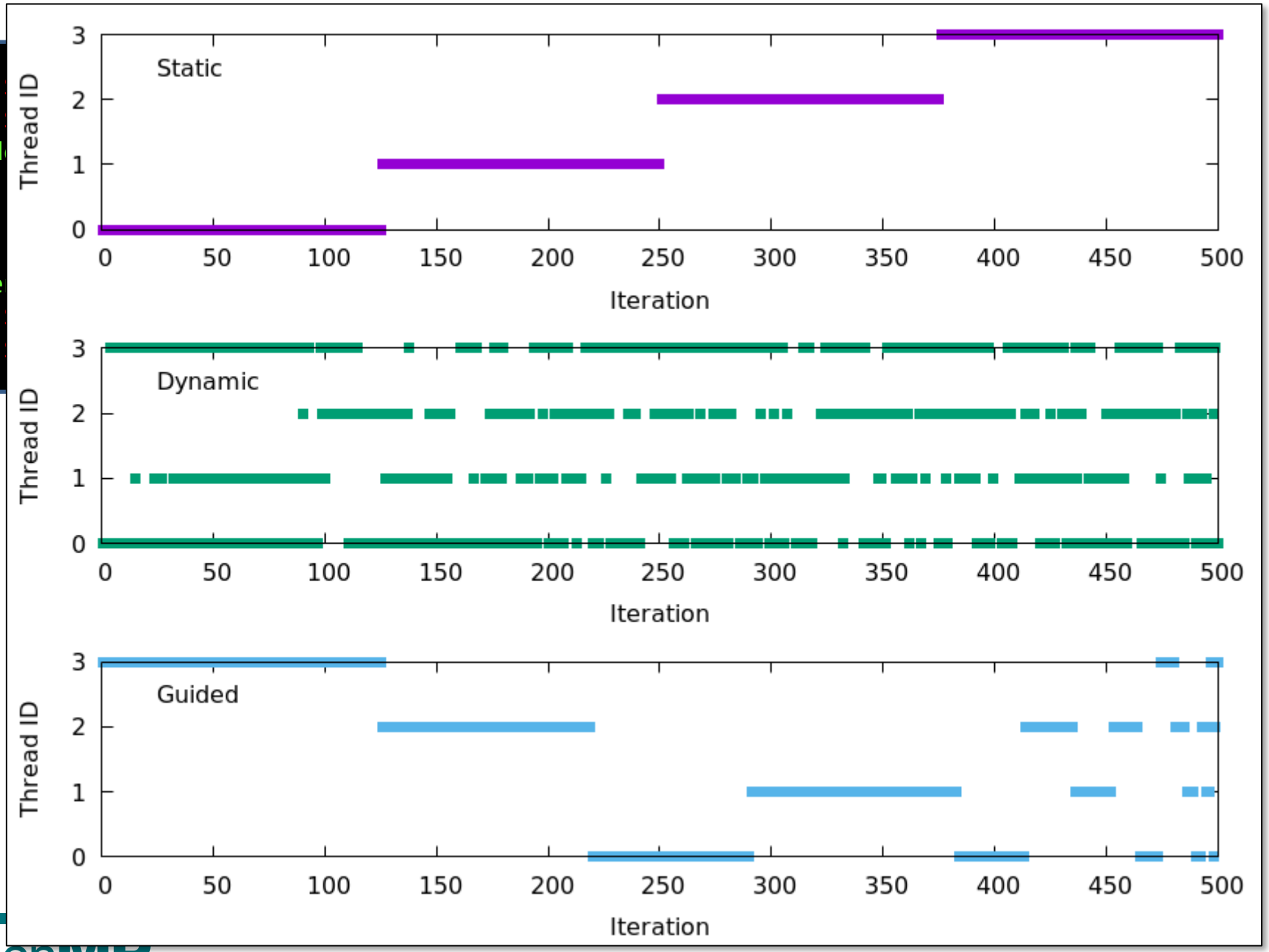
Parallel loop evenly divided among the threads

$$\text{chunk} = \frac{\text{loop count}}{\text{\# threads}}$$

static schedule

Other options are available: `!$omp do schedule(<kind> [,chunk_size])`

Kind	Description
static	Divides the loop in equal-sized chunks (or as equal as possible).
dynamic	When a thread finishes, it retrieves the next chunk from the internal queue. Be aware of the extra overhead! (defaul chunk size = 1).
guided	Similar to dynamic, but starts off large and decreases to better handle imbalace. (defaul chunk size = same as static).
auto	Decision regarding scheduling is delegated to the compiler.
runtime	Uses OMP_SCHDEULE env. Variable to select the schdeluding type.


Static
Thread ID
Iteration
Dynamic
Thread ID
Iteration
Guided
Thread ID
Iteration
0
1
2
3
0
50
100
150
200
250
300
350
400
450
500

```
factorial(1) = 1



do i = 2, 6

   factorial(i) = i * factorial(i-1)

end do
```

factorial(i) =

1
2
6
24
120
720
5040

```
factorial(1) = 1

!$omp parallel
!$omp do schedule(static)
do i = 2, 6

   factorial(i) = i * factorial(i-1)

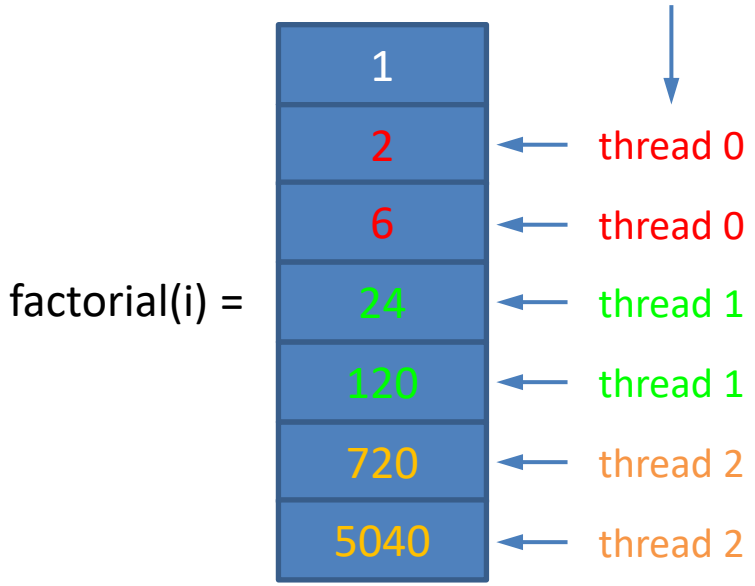
end do
!$omp end do
!$omp end parallel
```

There is something wrong here!

We cannot ensure this!

factorial(i) =

1
2
6
24
120
720
5040



```
factorial(1) = 1

!$omp parallel
!$omp do schedule(static)
do i = 2, 6

   factorial(i) = i * factorial(i-1)

end do
!$omp end do
!$omp end parallel
```

factorial(i) =

1
2
6
24
120
720
5040

Threads access data in a disordered way

factorial(i) =

1
2

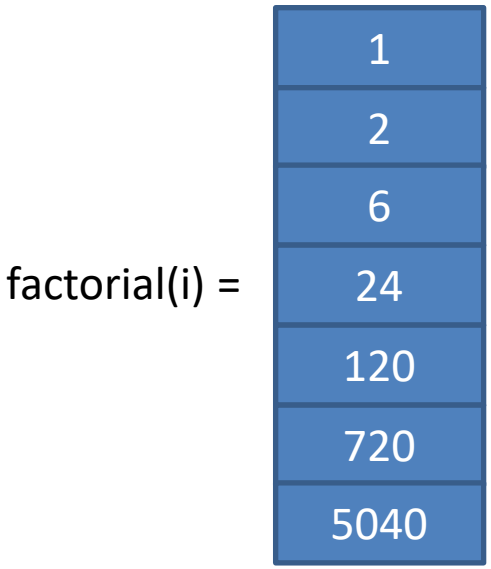
thread 0

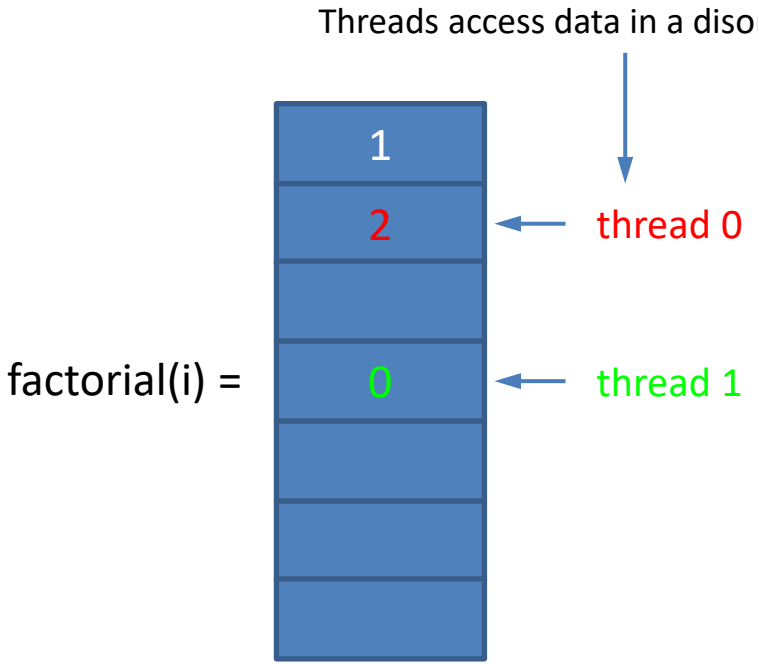
```
factorial(1) = 1

!$omp parallel
!$omp do schedule(static)
do i = 2, 6

   factorial(i) = i * factorial(i-1)

end do
!$omp end do
!$omp end parallel
```



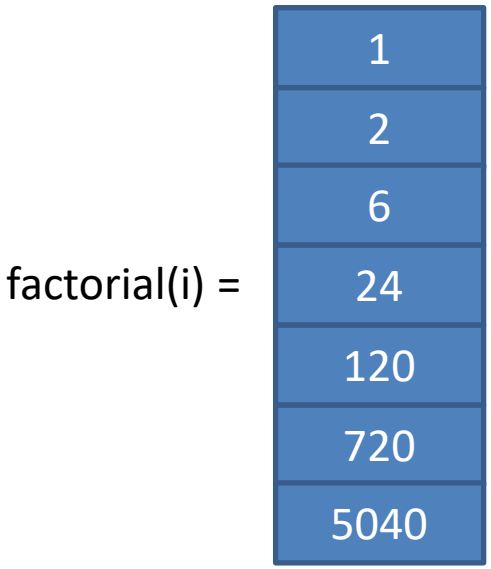


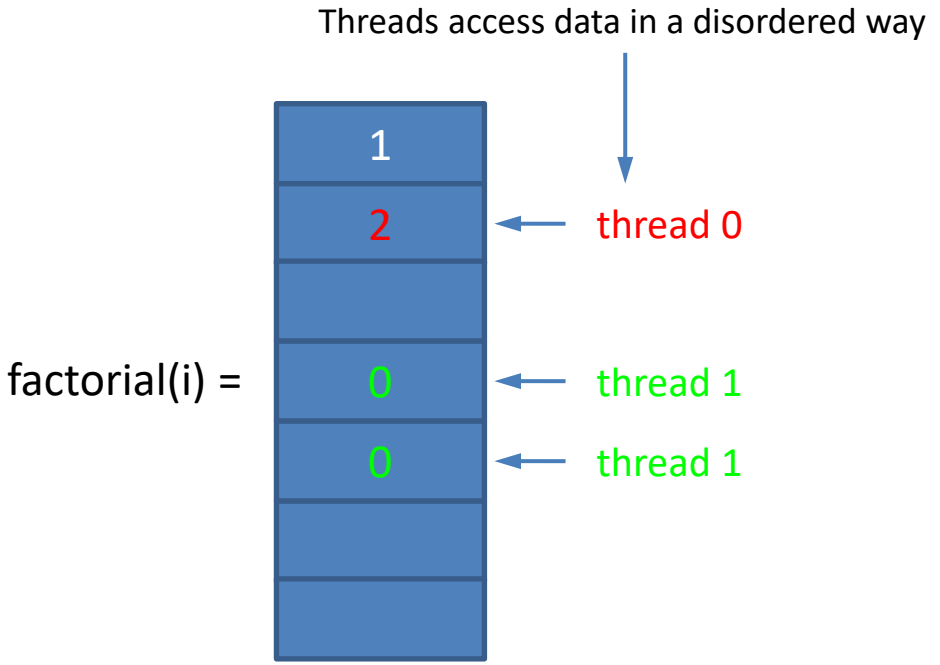
```
factorial(1) = 1

!$omp parallel
!$omp do schedule(static)
do i = 2, 6

   factorial(i) = i * factorial(i-1)

end do
!$omp end do
!$omp end parallel
```



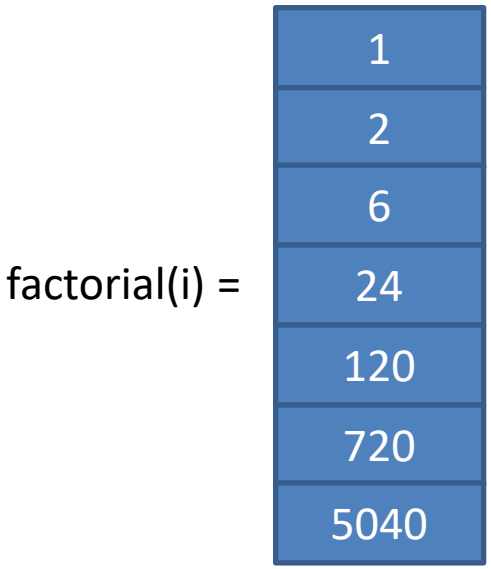


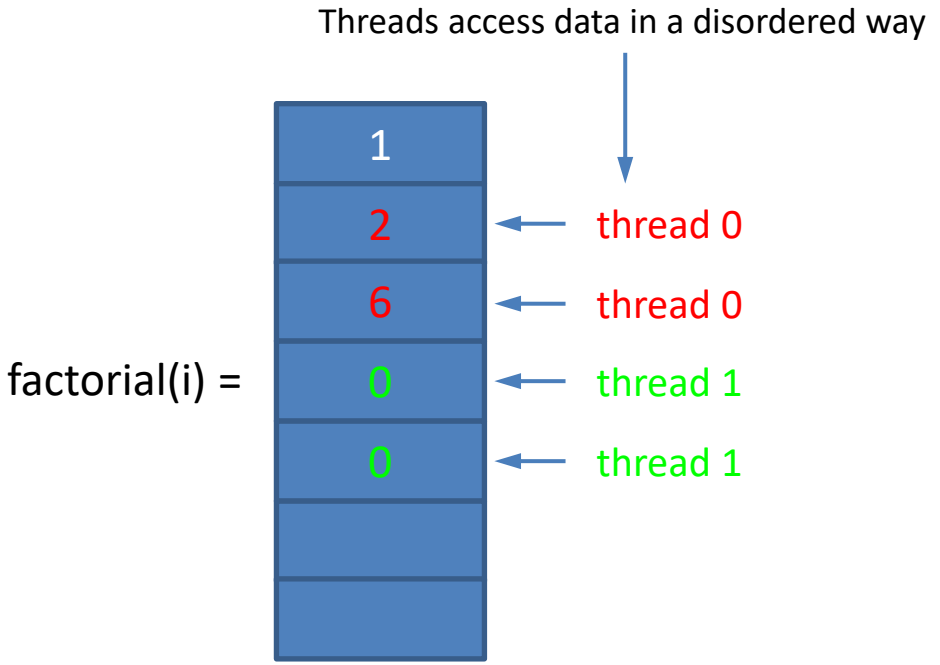
```
factorial(1) = 1

!$omp parallel
!$omp do schedule(static)
do i = 2, 6

   factorial(i) = i * factorial(i-1)

end do
!$omp end do
!$omp end parallel
```





```
factorial(1) = 1

!$omp parallel
!$omp do schedule(static)
do i = 2, 6

   factorial(i) = i * factorial(i-1)

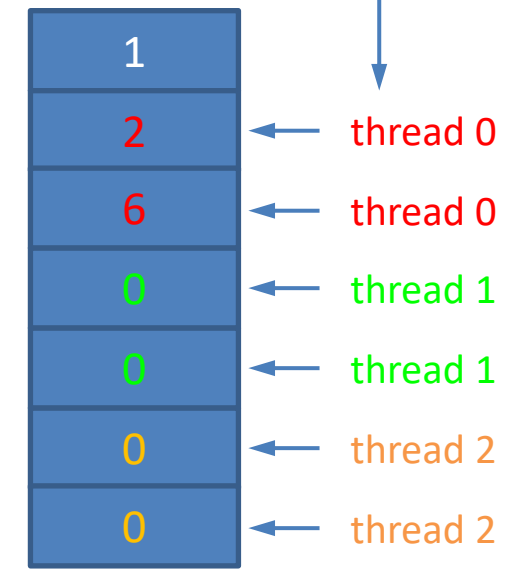
end do
!$omp end do
!$omp end parallel
```

factorial(i) =

1
2
6
24
120
720
5040

Threads access data in a disordered way

factorial(i) =



OpenMP

```
factorial(1) = 1

!$omp parallel
!$omp do schedule(static)
do i = 2, 6

   factorial(i) = i * factorial(i-1)

end do
!$omp end do
!$omp end parallel
```

This is called **Race Condition**

It can even be worse if factorial was not properly initialized!

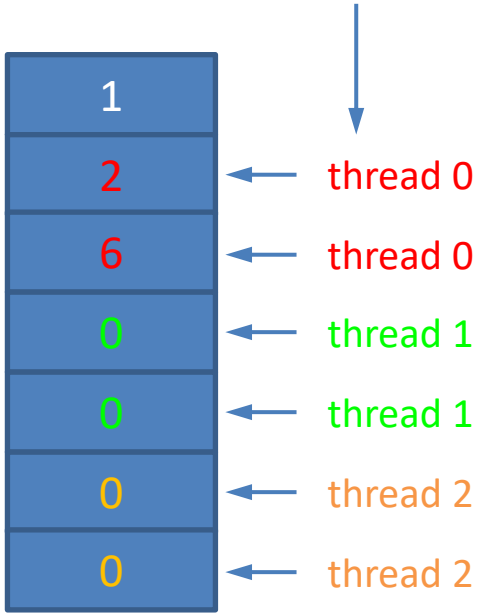
Difficult to detect because for a given case, system or run, the threads may win the race in an order that happens to make the program run correctly.

factorial(i) =

1
2
6
24
120
720
5040

Threads access data in a disordered way

factorial(i) =



OpenMP

```
!$omp parallel
!$omp do schedule(static)
do i = 1, 6

   x = i
   y(i) = x * 2

end do
!$omp end do
!$omp end parallel
```

Another example of **Race Condition**

y(i) =

2
4
6
8
10
12

y(i) =

x	y(i)
1	

← thread 0

```
!$omp parallel
!$omp do schedule(static)
do i = 1, 6

   x = i
   y(i) = x * 2

end do
!$omp end do
!$omp end parallel
```

Another example of **Race Condition**

y(i) =

2
4
6
8
10
12

y(i) =

x	y(i)	
1	2	← thread 0

```
!$omp parallel
!$omp do schedule(static)
do i = 1, 6

   x = i
   y(i) = x * 2

end do
!$omp end do
!$omp end parallel
```

Another example of **Race Condition**

y(i) =

2
4
6
8
10
12

y(i) =

x	y(i)	
1	2	← thread 0
2		← thread 0

```
!$omp parallel
!$omp do schedule(static)
do i = 1, 6

   x = i
   y(i) = x * 2

end do
!$omp end do
!$omp end parallel
```

Another example of **Race Condition**

y(i) =

2
4
6
8
10
12

y(i) =

x	y(i)	
1	2	← thread 0
2		← thread 0
5		← thread 2

```
!$omp parallel
!$omp do schedule(static)
do i = 1, 6

   x = i
   y(i) = x * 2

end do
!$omp end do
!$omp end parallel
```

Another example of **Race Condition**

y(i) =

2
4
6
8
10
12

y(i) =

x	y(i)	
1	2	← thread 0
2	10	← thread 0
5		← thread 2

```
!$omp parallel
!$omp do schedule(static)
do i = 1, 6

   x = i
   y(i) = x * 2

end do
!$omp end do
!$omp end parallel
```

Another example of **Race Condition**

y(i) =

2
4
6
8
10
12

y(i) =

x	y(i)	
1	2	← thread 0
2	10	← thread 0
3		← thread 1
5		← thread 2

```
!$omp parallel
!$omp do schedule(static)
do i = 1, 6

   x = i
   y(i) = x * 2

end do
!$omp end do
!$omp end parallel
```

Another example of **Race Condition**

y(i) =

2
4
6
8
10
12

y(i) =

x	y(i)	
1	2	← thread 0
2	10	← thread 0
3		← thread 1
5	6	← thread 2

```
!$omp parallel
!$omp do schedule(static)
do i = 1, 6

   x = i
   y(i) = x * 2

end do
!$omp end do
!$omp end parallel
```

Another example of **Race Condition**

y(i) =

2
4
6
8
10
12

y(i) =

x	y(i)	
1	2	← thread 0
2	10	← thread 0
3	6	← thread 1
5	6	← thread 2

```
!$omp parallel
!$omp do schedule(static)
do i = 1, 6

   x = i
   y(i) = x * 2

end do
!$omp end do
!$omp end parallel
```

Another example of **Race Condition**

y(i) =

2
4
6
8
10
12

y(i) =

x	y(i)	
1	2	← thread 0
2	10	← thread 0
3	6	← thread 1
4		← thread 1
5	6	← thread 2

```
!$omp parallel
!$omp do schedule(static)
do i = 1, 6

   x = i
   y(i) = x * 2

end do
!$omp end do
!$omp end parallel
```

Another example of **Race Condition**

y(i) =

2
4
6
8
10
12

y(i) =

x	y(i)	
1	2	← thread 0
2	10	← thread 0
3	6	← thread 1
4		← thread 1
5	6	← thread 2
6		← thread 2

```
!$omp parallel
!$omp do schedule(static)
do i = 1, 6

   x = i
   y(i) = x * 2

end do
!$omp end do
!$omp end parallel
```

Another example of **Race Condition**

To solve this we have the **private** clause.

y(i) =

2
4
6
8
10
12

y(i) =

x	y(i)	
1	2	thread 0
2	10	thread 0
3	6	thread 1
4	12	thread 1
5	6	thread 2
6	12	thread 2

```
!$omp parallel private (x)
!$omp do schedule(static)
do i = 1, 6

   x = i
   y(i) = x * 2

end do
!$omp end do
!$omp end parallel
```

Another example of **Race Condition**

To solve this we have the **private** clause.

With this, each thread has its private copy of x and the problem is solved.

This comes at the cost of an overhead in memory.

y(i) =

2
4
6
8
10
12

y(i) =

x_0	x_1	x_2	y(i)	
1			2	← thread 0
2			4	← thread 0
	3		6	← thread 1
	4		8	← thread 1
		5	10	← thread 2
		6	12	← thread 2

OpenMP

By default everything is shared inside the OMP section, but loop indexes, which are private.
Nevertheless, I recommend to explicitely declare private everything that it has to be private.

Can you declare all private variables of the following code?

NOTE: jumpx and w1d are outputs of the corresponding subroutine calls.

```
!$omp parallel private (???)
!$omp do schedule(static)
do i = ini, end
   ii = 1+dim*(i-1)
   do k = 1, nvi(i)
      j = neighbors(i,k)
      call apply_PBC(i,k,0,jumpx)
      d1 = a(ii) – a(jj) – jumpx
      d05 = sqrt(d1)
      v1 = d05/h(i)
      call Wkernel(v1,w1d)
      dter = pk(i)*w1d
      sumwh(i) = sumwh(i) + xmass(j) * dter
      if (equ) then
         dlw1d = log10(w1d)/indice(i)
      end if
   end do
   do it = 1, nut
      do ie = 1, ne
         f(ie, it) = kfactor * alpha( ie, it, i)
         ftot(ie, it, i) = f(ie, it) / dens(i)
      end do
    end do
end do
!$omp end do
!$omp end parallel
```

Automatized help: Intel Inspector

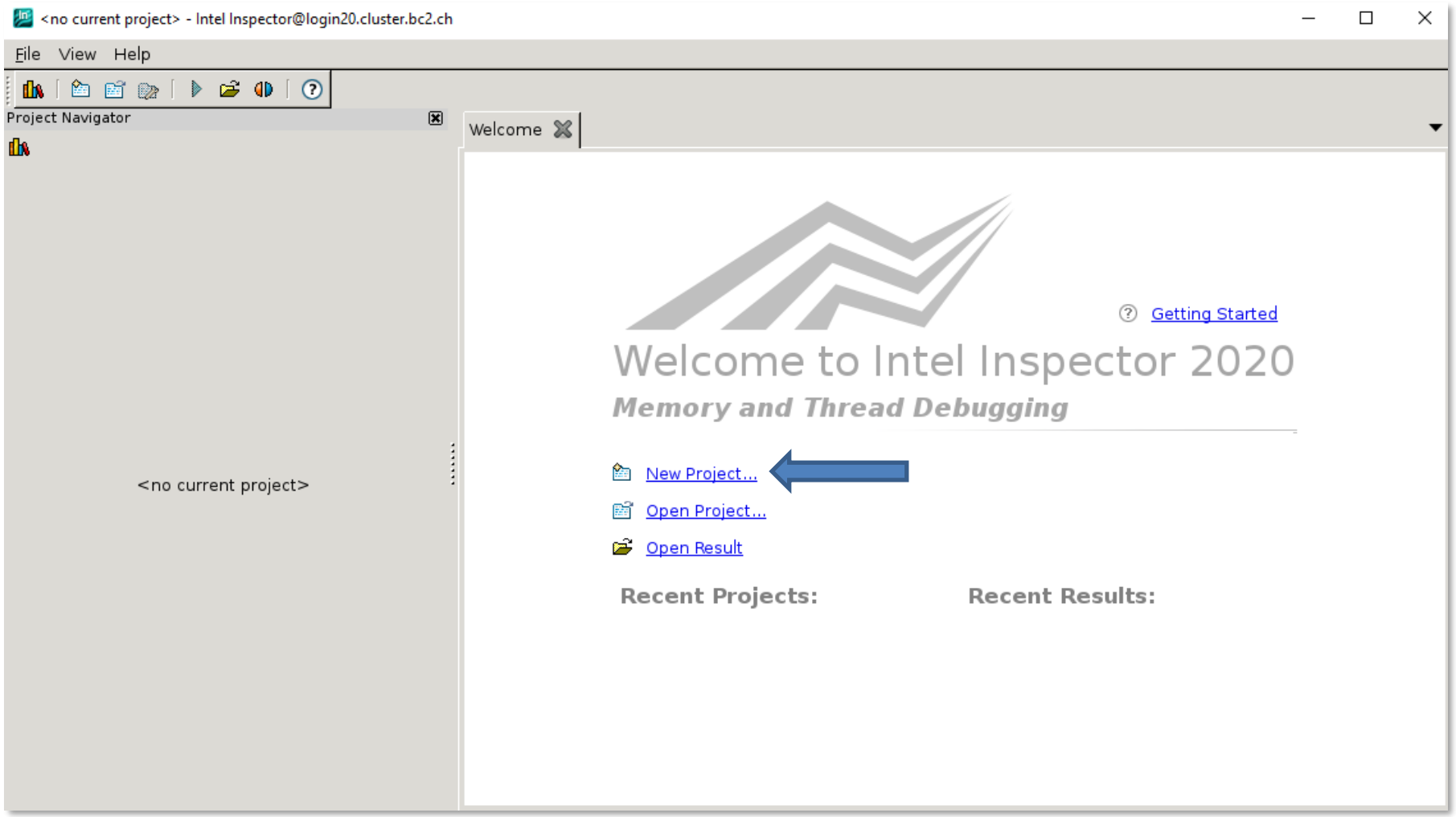
Commercial tool, but free licenses for academia and open source projects.
https://www.intel.com/content/www/us/en/developer/articles/tool/oneapi-standalone-components.html#inspector

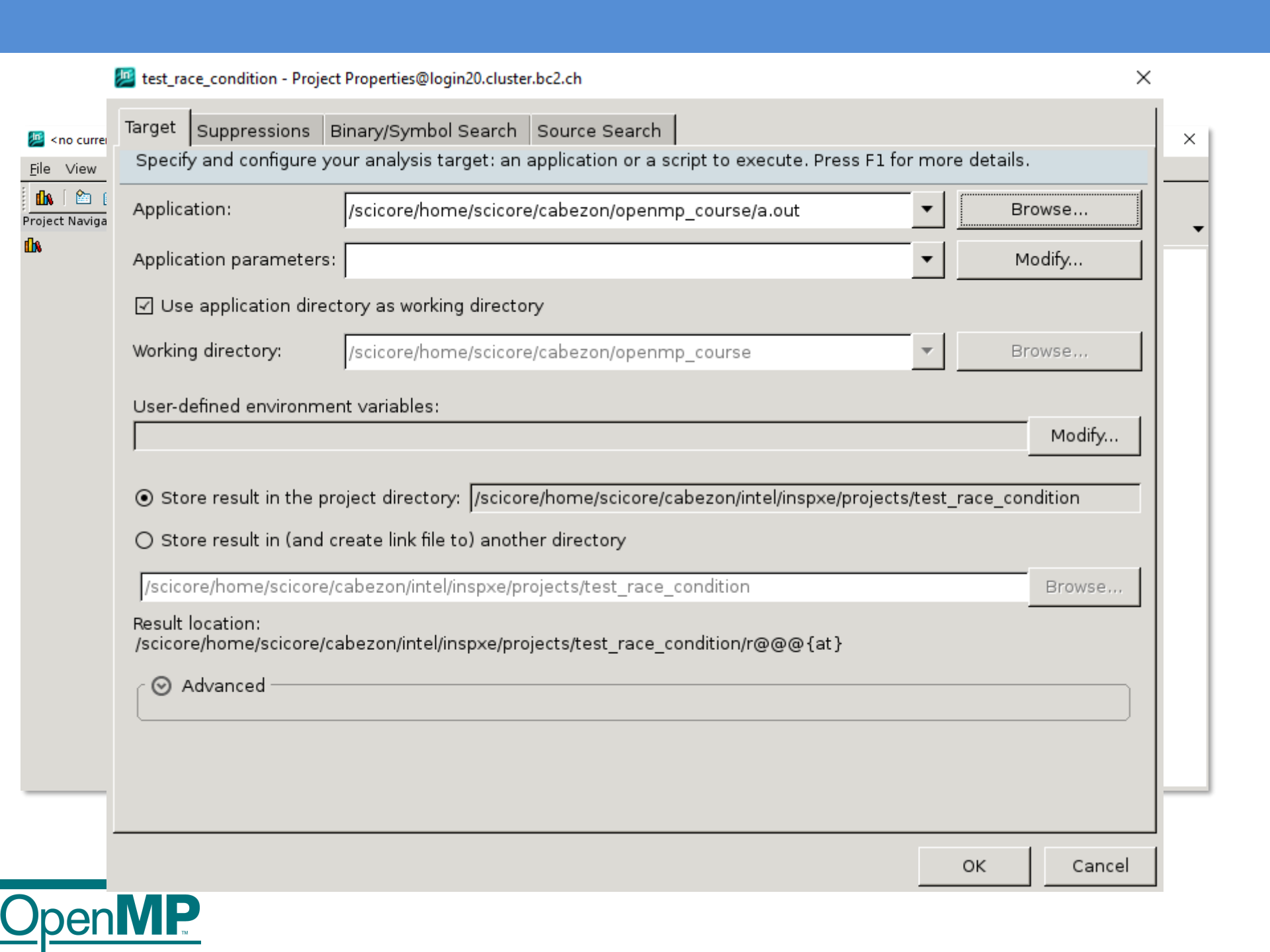
Available for Linux and Windows. Supports C, C++, and Fortran. GUI + command line.
10 min intro: https://www.intel.com/content/www/us/en/developer/videos/introduction-to-intel-inspector.html

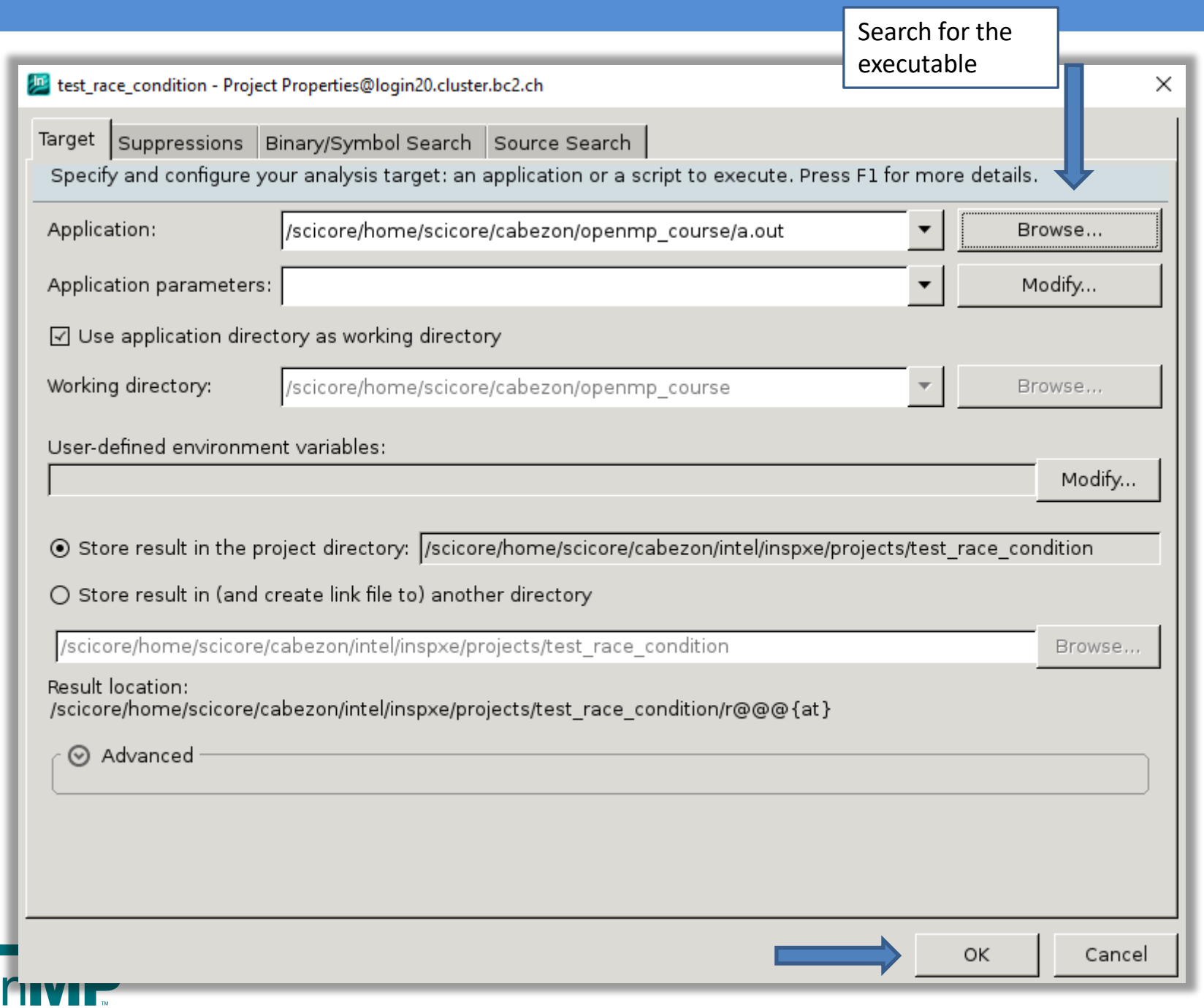
Detects Race conditions and Deadlocks.

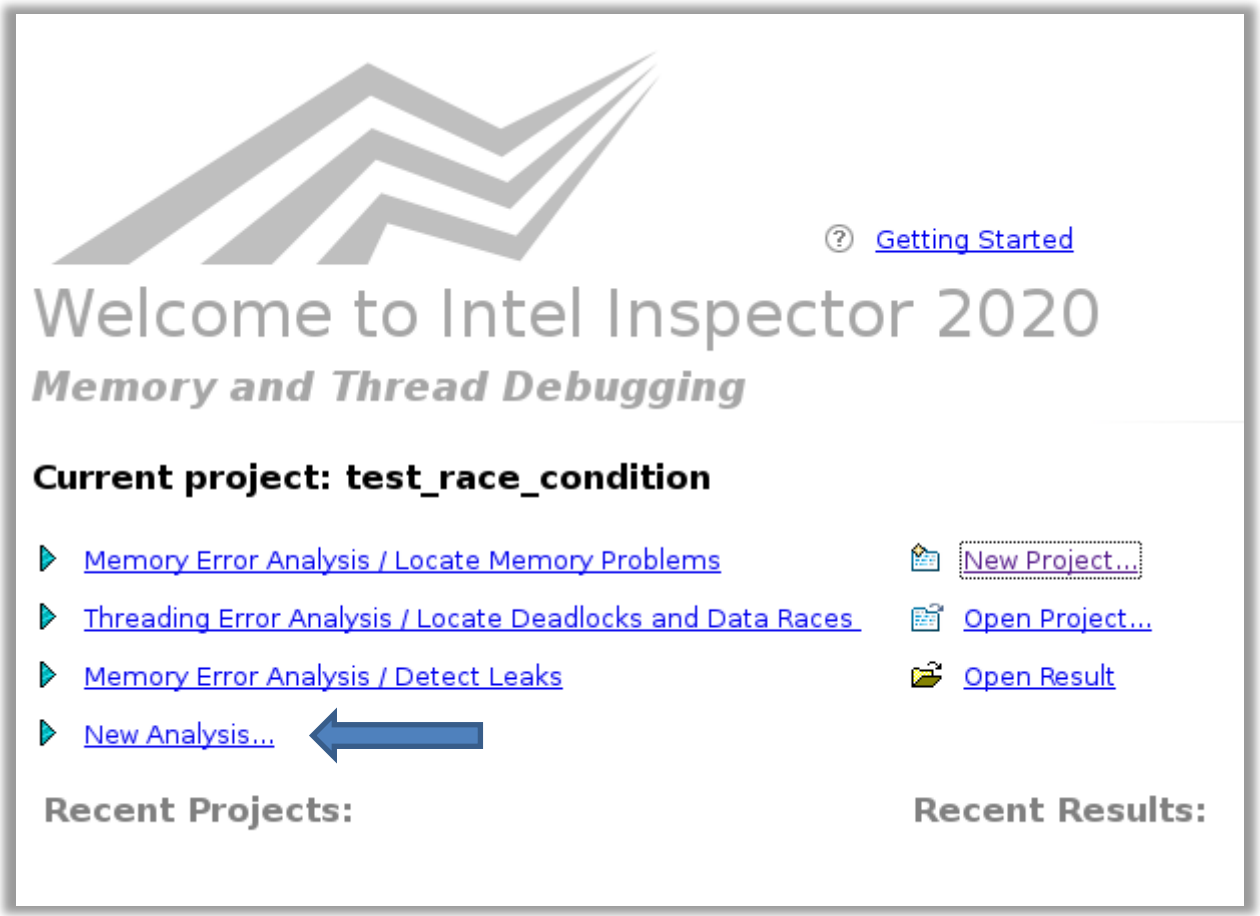

```
> ifort -g -openmp myprogram.f90 -o myprogram

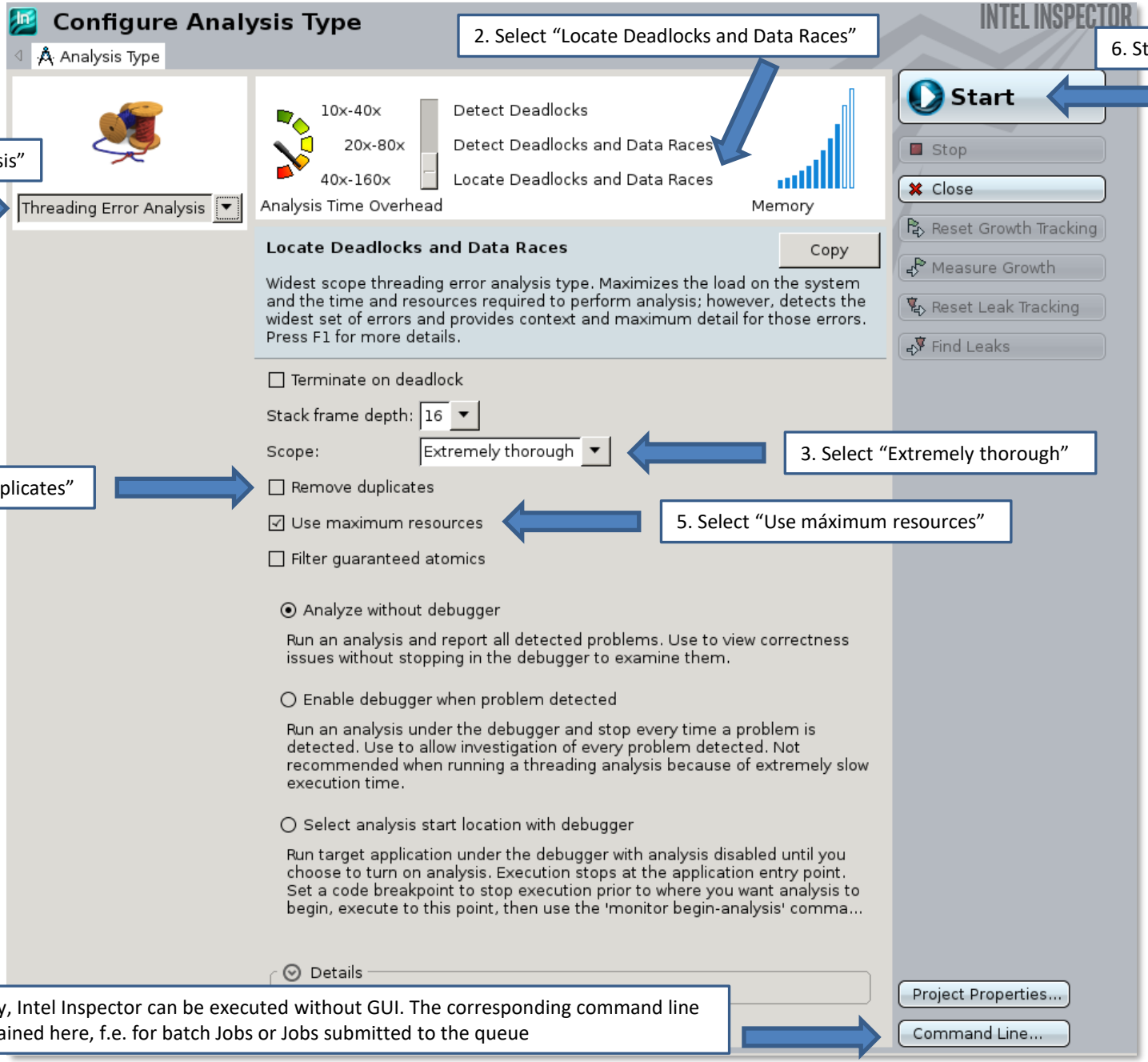
> export NUM_THREADS_OMP=2
> inspxe-gui
```


<no current project> - Intel Inspector@login20.cluster.bc2.ch
File View Help
Project Navigator
<no current project>
Welcome
Getting Started
Welcome to Intel Inspector 2020
Memory and Thread Debugging
New Project...
Open Project...
Open Result
Recent Projects:
Recent Results:

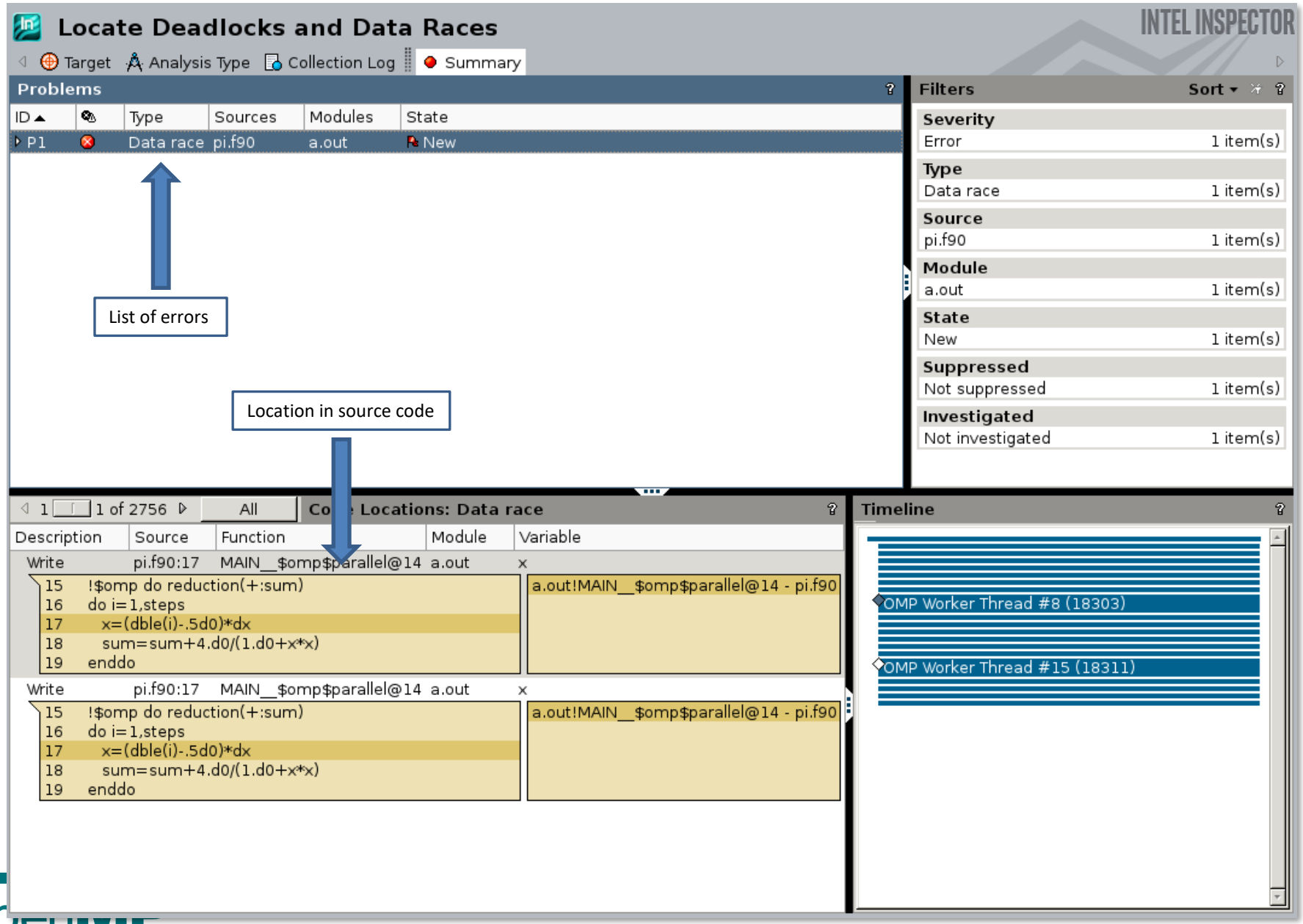

test_race_condition - Project Properties@login20.cluster.bc2.ch
Target
Suppressions
Binary/Symbol Search
Source Search
Specify and configure your analysis target: an application or a script to execute. Press F1 for more details.
Application:
/scicore/home/scicore/cabezon/openmp_course/a.out
Browse...
Application parameters:
Modify...
Use application directory as working directory
Working directory:
/scicore/home/scicore/cabezon/openmp_course
Browse...
User-defined environment variables:
Modify...
Store result in the project directory:
/scicore/home/scicore/cabezon/intel/inspxe/projects/test_race_condition
Store result in (and create link file to) another directory
/scicore/home/scicore/cabezon/intel/inspxe/projects/test_race_condition
Browse...
Result location:
/scicore/home/scicore/cabezon/intel/inspxe/projects/test_race_condition/r@@@{at}
Advanced
OK
Cancel
File
View
Project Naviga


Search for the executable
test_race_condition - Project Properties@login20.cluster.bc2.ch
Target
Suppressions
Binary/Symbol Search
Source Search
Specify and configure your analysis target: an application or a script to execute. Press F1 for more details.
Application:
/scicore/home/scicore/cabezon/openmp_course/a.out
Browse...
Application parameters:
Modify...
Use application directory as working directory
Working directory:
/scicore/home/scicore/cabezon/openmp_course
Browse...
User-defined environment variables:
Modify...
Store result in the project directory:
/scicore/home/scicore/cabezon/intel/inspxe/projects/test_race_condition
Store result in (and create link file to) another directory
/scicore/home/scicore/cabezon/intel/inspxe/projects/test_race_condition
Browse...
Result location:
/scicore/home/scicore/cabezon/intel/inspxe/projects/test_race_condition/r@@@{at}
Advanced
OK
Cancel


Getting Started
Welcome to Intel Inspector 2020
Memory and Thread Debugging
Current project: test_race_condition
Memory Error Analysis / Locate Memory Problems
Threading Error Analysis / Locate Deadlocks and Data Races
Memory Error Analysis / Detect Leaks
New Analysis...
New Project...
Open Project...
Open Result
Recent Projects:
Recent Results:



If necessary, Intel Inspector can be executed without GUI. The corresponding command line can be obtained here, f.e. for batch Jobs or Jobs submitted to the queue


Locate Deadlocks and Data Races
INTEL INSPECTOR
Target
Analysis Type
Collection Log
Summary
Problems
ID
Type
Sources
Modules
State
P1
Data race
pi.f90
a.out
New
List of errors
Location in source code
Filters
Sort
Severity
Error
1 item(s)
Type
Data race
1 item(s)
Source
pi.f90
1 item(s)
Module
a.out
1 item(s)
State
New
1 item(s)
Suppressed
Not suppressed
1 item(s)
Investigated
Not investigated
1 item(s)
1 of 2756
All
Locations: Data race
Description
Source
Function
Module
Variable
Write
pi.f90:17
MAIN__ompparallel@14
a.out
15 !$omp do reduction(+:sum)
16 do i=1,steps
17 x=(dble(i)-.5d0)*dx
18 sum=sum+4.d0/(1.d0+x*x)
19 enddo
a.out!MAIN__ompparallel@14 - pi.f90
Write
pi.f90:17
MAIN__ompparallel@14
a.out
15 !$omp do reduction(+:sum)
16 do i=1,steps
17 x=(dble(i)-.5d0)*dx
18 sum=sum+4.d0/(1.d0+x*x)
19 enddo
a.out!MAIN__ompparallel@14 - pi.f90
Timeline
OMP Worker Thread #8 (18303)
OMP Worker Thread #15 (18311)

A note regarding private variables: They are not initialized!

```
result = 20

!$omp parallel private(result)
result = result + 10
print *, ‘Thread ‘,omp_get_thread_num(), result
!$omp end parallel

print *, result
```

To control the initialization of private variables we have **firstprivate**

```
Thread 3 10
Thread 0 10
Thread 1 71
Thread 2 10

20
```

If you are lucky, result may access a section of the memory that is empty. Otherwise, any value can be used to initialize result.

A note regarding private variables: They are not initialized!

```
result = 20

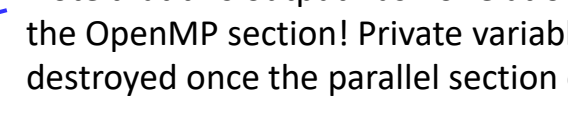
!$omp parallel firstprivate(result)
result = result + 10
print *, ‘Thread ‘,omp_get_thread_num(), result
!$omp end parallel

print *, result
```

To control the initialization of private variables we have **firstprivate**

```
Thread 3 30
Thread 0 30
Thread 1 30
Thread 2 30

20
```



Note that this output has no relation with the OpenMP section! Private variables are destroyed once the parallel section ends.

Consider now this code. Is it correct?

```
sum = 0

!$omp parallel
!$omp do
do i = 1, 6

   sum = sum + i

end do
!$omp end do
!$omp end parallel
```

The variable sum should be private to give the correct answer, but it should be also shared to be accessed by all threads!

Consider now this code. Is it correct?

```
sum = 0

!$omp parallel
!$omp do reduction(+: sum)
do i = 1, 6

   sum = sum + i

end do
!$omp end do
!$omp end parallel
```

The variable sum should be private to give the correct answer, but it should be also shared to be accessed by all threads!

We can solve this with reduction

This allows each thread to have a private copy of sum where they store their partial calculation and then, when the threads exit, it groups all partial values from all threads using the defined operation (+ in this case) in one global variable.

Reduction variables have to meet the following requirements:

- They can only be listed in one reduction
- Cannot be declared constant
- Cannot be declared private in the parallel contruct

Consider now this code. Is it correct?

```
sum = 0

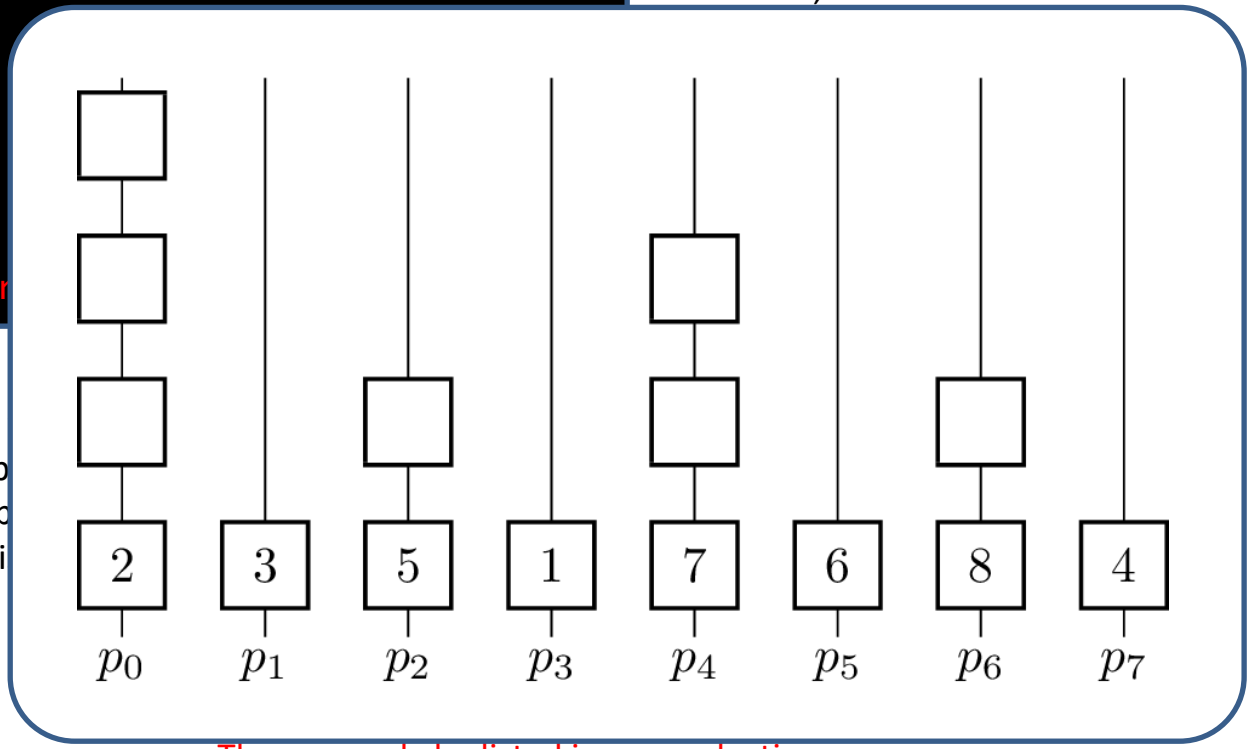
!$omp parallel
!$omp do reduction(+: sum)
do i = 1, 6

   sum = sum

end do
!$omp end do
!$omp end par
```

The variable sum should be private to give the correct answer, but it should be also shared to be accessed by

This allows each
they store their p
exit, it groups all p
operation (+ in thi



Source: wikipedia

- They can only be listed in one reduction
- Cannot be declared constant
- Cannot be declared private in the parallel contruct

Getting the course exercises

Clone the repository of the exercises:
git clone https://git.scicore.unibas.ch/scicore/openmp_course.git

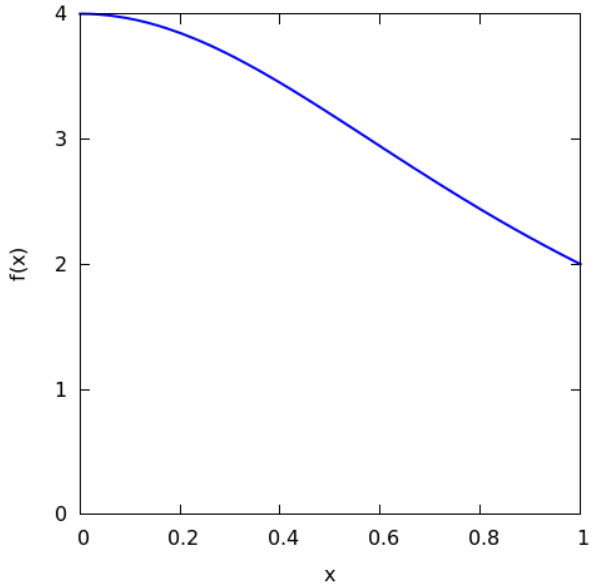
Or download them directly and extract:
https://git.scicore.unibas.ch/scicore/openmp_course/-/archive/master/openmp_course-master.tar.gz

Enter in openmp_course/:
cd openmp_course

Exercise: Numerical integration

We know that:

$$\int_0^1 \frac{4}{(1+x^2)} dx = \pi$$



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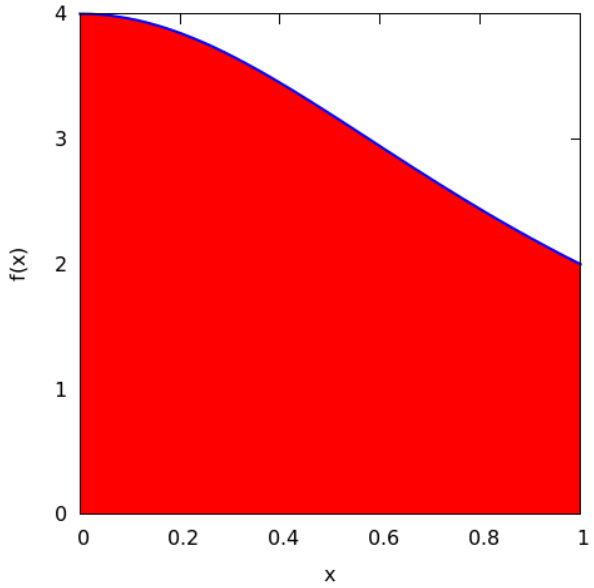

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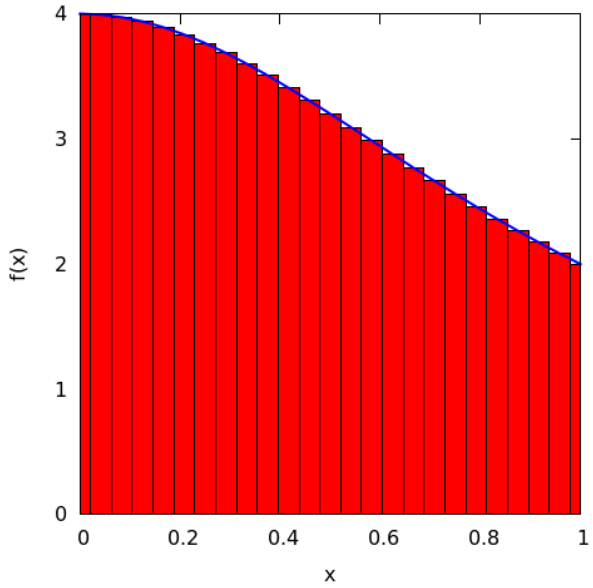

Using the composite formula we can approximate the integral as:

$$\int_a^b f(x)dx \approx \left(\sum_{i=0}^{n} f(x_i)\right)\frac{b-a}{n}$$

Exercise: Numerical integration

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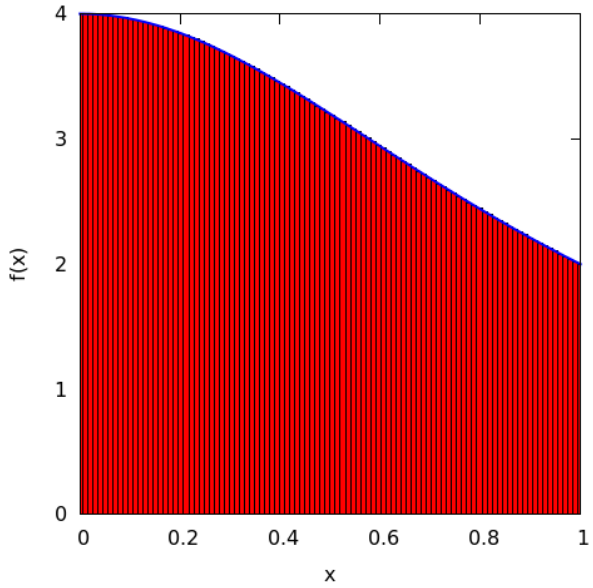


Using the composite formula we can approximate the integral as:

$$\int_a^b f(x)dx \approx \left(\sum_{i=0}^{n} f(x_i)\right)\frac{b-a}{n}$$

Exercise: Numerical integration

Parallelize the following program with openMP

```
steps = 1000000000
dx = 1./dble(steps)
sum = 0.
do i = 1, steps
   x = (dble(i)-0.5)*dx
   sum = sum + 4./(1. + x*x)
end do
sum = sum * dx
```

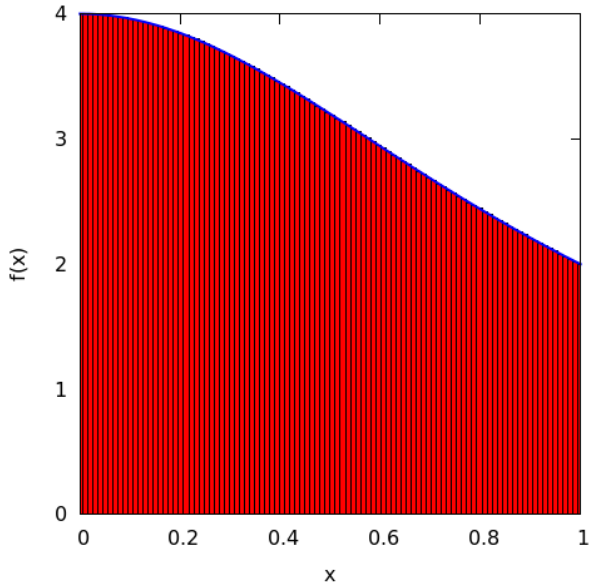
Compile with: **gfortran –fopenmp pi.f90**

Fix the number of threads: **export OMP_NUM_THREADS=4**

Execute with: **time ./a.out**

We know that:

$$\int_0^1 \frac{4}{(1+x^2)} dx = \pi$$



Using the composite formula we can approximate the integral as:

$$\int_a^b f(x)dx \approx \left(\sum_{i=0}^{n} f(x_i)\right)\frac{b-a}{n}$$

What happens if we have nested loops?

```
do i = 1, ni
   do j = 1, nj
      do k = 1, nk
         <calculations>
      end do
   end do
end do
```

What happens if we have nested loops?

Not much… we simply parallelize the outer loop.

```
!$omp parallel private(i,j,k)
!$omp do
do i = 1, ni
   do j = 1, nj
      do k = 1, nk
         <calculations>
      end do
   end do
end do
!$omp end do
!$omp end parallel
```

But this depends on the number of iterations for each loop.

What happens if we have nested loops?

Not much… we simply parallelize the outer loop.

```
!$omp parallel private(i,j,k)
!$omp do
do i = 1, 4
   do j = 1, 20
      do k = 1, 10000
         <calculations>
      end do
   end do
end do
!$omp end do
!$omp end parallel
```

But this depends on the number of iterations for each loop.

Having such small count of iterations in the outer loop is not efficient. We might even have less iterations than threads!

What happens if we have nested loops?

Not much… we simply parallelize the outer loop.

```
!$omp parallel private(i,j,k)
!$omp do
do k = 1, 10000
   do j = 1, 20
      do i = 1, 4
         <calculations>
      end do
   end do
end do
!$omp end do
!$omp end parallel
```

But this depends on the number of iterations for each loop.

Having such small count of iterations in the outer loop is not efficient. We might even have less iterations than threads!

Re-arranging the nested loops will solve it!

But this is not always possible, or maybe all loops have relatively small counts!

What happens if we have nested loops?

Not much… we simply parallelize the outer loop.

```
!$omp parallel private(i,j,k)
!$omp do
do i = 1, 10
   do j = 1, 10
      do k = 1, 10
         <calculations>
      end do
   end do
end do
!$omp end do
!$omp end parallel
```

But this depends on the number of iterations for each loop.

Having such small count of iterations in the outer loop is not efficient. We might even have less iterations than threads!

Re-arranging the nested loops will solve it!

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What happens if we have nested loops?

Not much… we simply parallelize the outer loop.

```
!$omp parallel private(i,j,k)
!$omp do collapse(3)
do i = 1, 10
   do j = 1, 10
      do k = 1, 10
         <calculations>
      end do
   end do
end do
!$omp end do
!$omp end parallel
```

To solve this we have the clause **collapse(n)**

It specifies how many nested loops will be collapsed in a single loop.

But this depends on the number of iterations for each loop.

Having such small count of iterations in the outer loop is not efficient. We might even have less iterations than threads!

Re-arranging the nested loops will solve it!

But this is not always possible, or maybe all loops have relatively small counts!

```
!$omp parallel private(ii,i,j,k)
!$omp do
do ii = 1, 1000
   i = mod(ii/100, 10)+1
   j = mod(ii/10, 10)+1
   k = mod(ii, 10)+1
   <calculations>
end do
!$omp end do
!$omp end parallel
```

What about subroutines? We can use orphaned directives

```
!$omp parallel private(i,j,k)

call calculate_manythings()

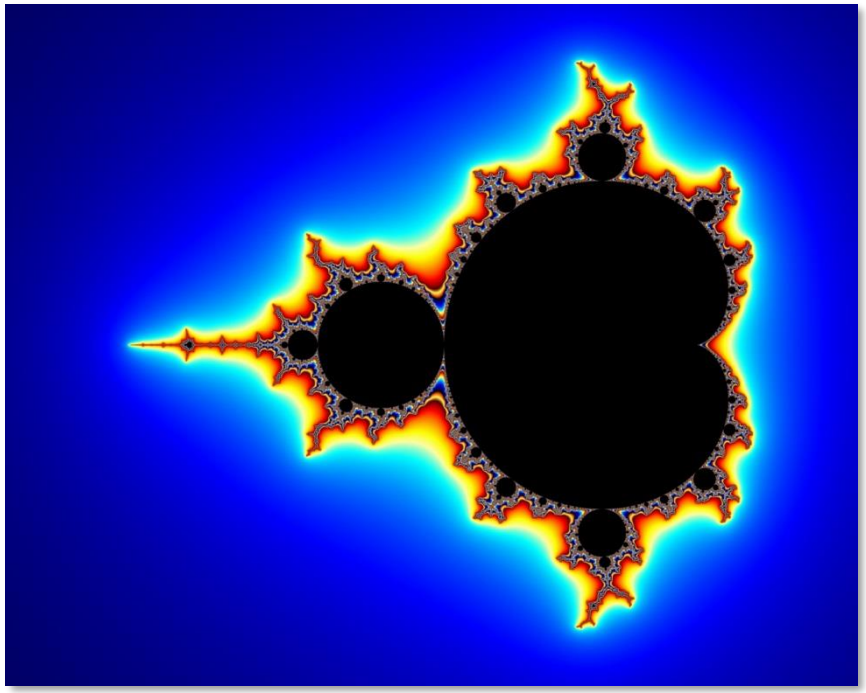
!$omp end parallel
```

```
subroutine calculate_manythings()

!$omp do schedule(static)
      do i=1,n
           <calculations>
      enddo
!$omp end do

return
end subroutine
```

Mandelbrot set area calculation



Mathematically it can be calculated exactly as:

$$A = \pi\left(1 - \sum_{n=1}^{\infty} n\, b_n^2\right)$$

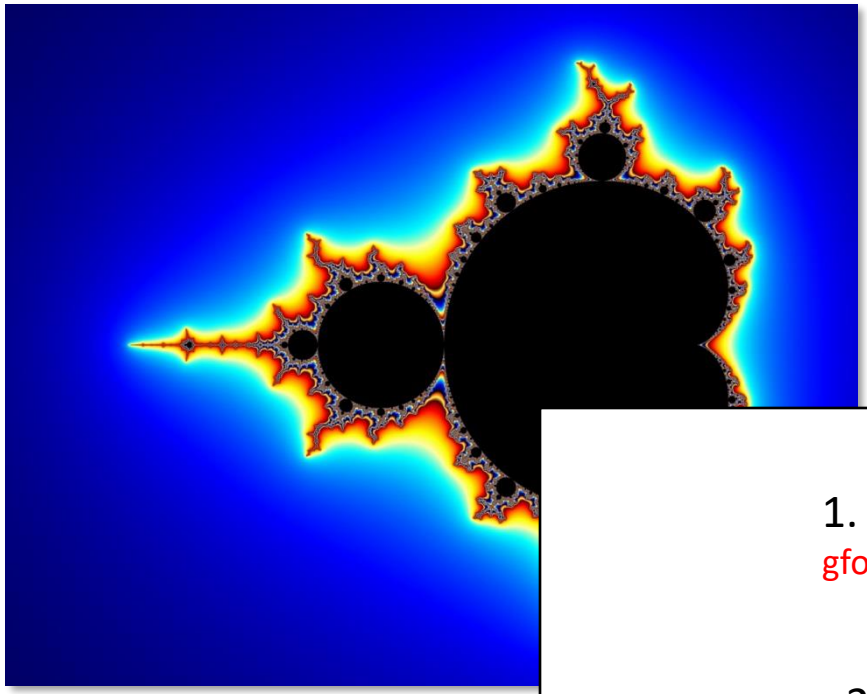
But this series converges VERY slowly. It needs 10^{118} terms to get the first two digits, and 10^{1181} to get the third!

The area obtained by pixel counting is:

$1.50659177 \pm 0.00000008$

(Munafo et al. OEIS A098403, 2000)

Mandelbrot set area calculation



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(Munafo et al. OEIS A098403, 2000)

1. Compile and execute the serial code

```
gfortran mandelbrot.f90 –o mandelbrot_serial
time ./mandelbrot_serial
```

2. Parallelize the code with OpenMP

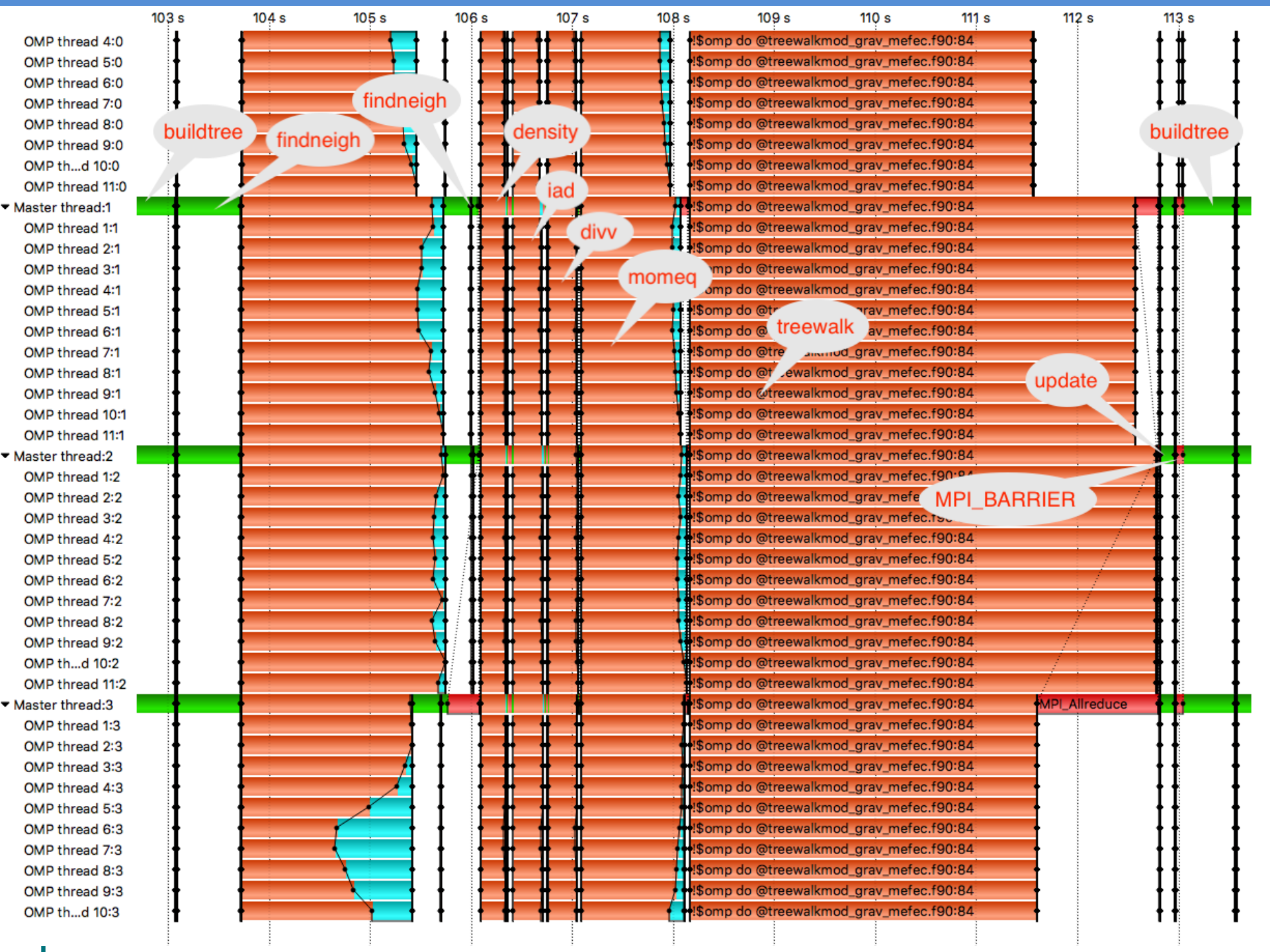
3. Compile and execute the parallel code

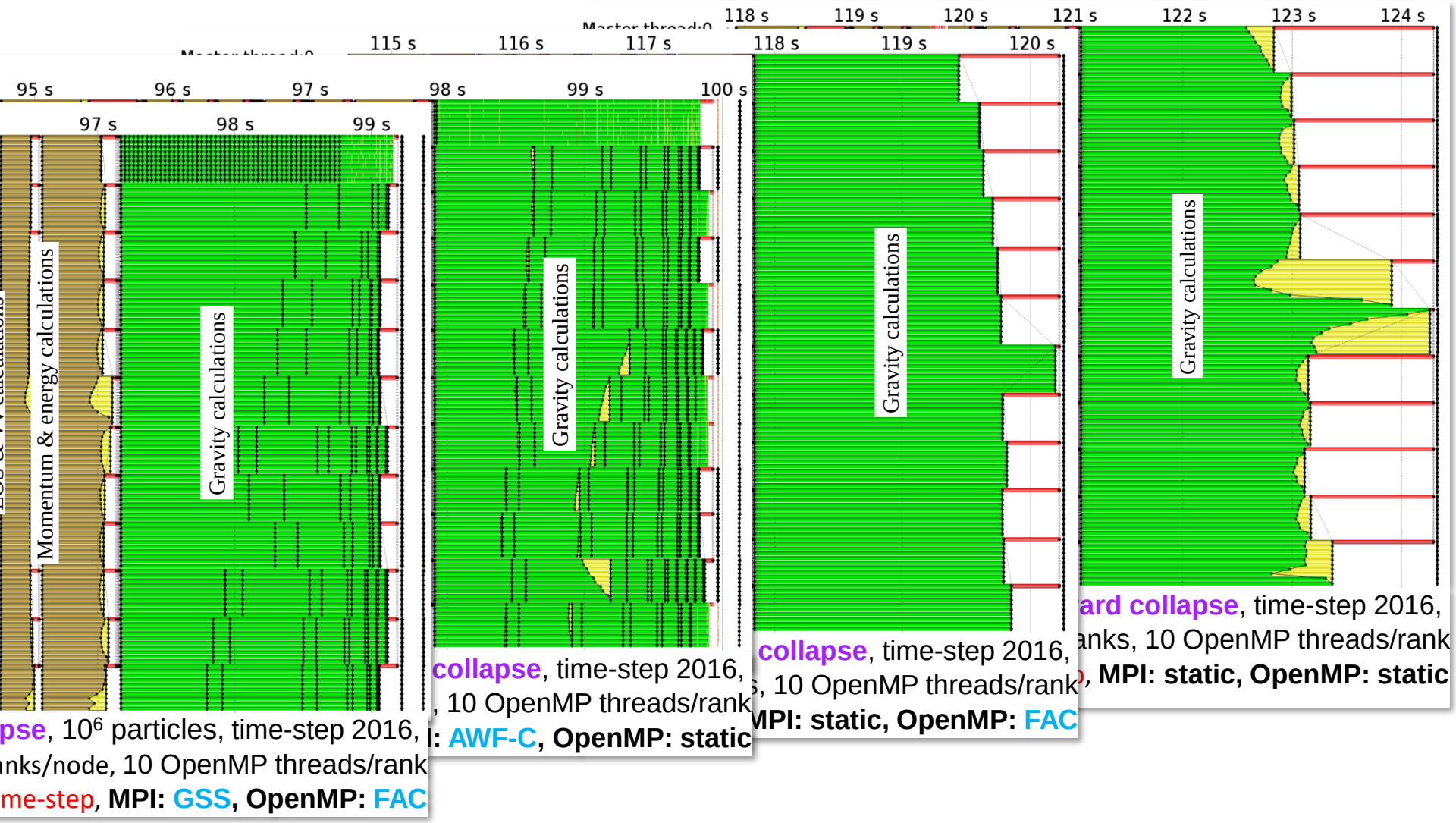
```
gfortran –fopenmp mandelbrot.f90 –o mandelbrot_parallel
time ./mandelbrot_parallel
```

4. Change the number of threads (2-4) and check if it scales

```
export OMP_NUM_THREADS = <# of threads>
```

OpenMP


103 s
104 s
105 s
106 s
107 s
108 s
109 s
110 s
111 s
112 s
113 s
OMP thread 4:0
OMP thread 5:0
OMP thread 6:0
OMP thread 7:0
OMP thread 8:0
OMP thread 9:0
OMP th...d 10:0
OMP thread 11:0
Master thread:1
OMP thread 1:1
OMP thread 2:1
OMP thread 3:1
OMP thread 4:1
OMP thread 5:1
OMP thread 6:1
OMP thread 7:1
OMP thread 8:1
OMP thread 9:1
OMP thread 10:1
OMP thread 11:1
Master thread:2
OMP thread 1:2
OMP thread 2:2
OMP thread 3:2
OMP thread 4:2
OMP thread 5:2
OMP thread 6:2
OMP thread 7:2
OMP thread 8:2
OMP thread 9:2
OMP th...d 10:2
OMP thread 11:2
Master thread:3
OMP thread 1:3
OMP thread 2:3
OMP thread 3:3
OMP thread 4:3
OMP thread 5:3
OMP thread 6:3
OMP thread 7:3
OMP thread 8:3
OMP thread 9:3
OMP th...d 10:3
!$omp do @treewalkmod_grav_mefec.f90:84
buildtree
findneigh
findneigh
density
iad
divv
momeq
treewalk
update
buildtree
MPI_BARRIER
MPI_Allreduce



pse, 10^6 particles, time-step 2016,
nks/node, 10 OpenMP threads/rank
me-step, **MPI: GSS, OpenMP: FAC**

collapse, time-step 2016,
, 10 OpenMP threads/rank
I: AWF-C, OpenMP: static

collapse, time-step 2016,
s, 10 OpenMP threads/rank
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ard collapse, time-step 2016,
anks, 10 OpenMP threads/rank
, MPI: static, OpenMP: static

OpenMP

Two-level dynamic load balancing for high performance scientific applications
Mohammed, A. et al (Siam PP20)

Can we do any of this in Python? **Kind of…**

```
from multiprocessing import Process


def func1():
  j=0
  print ('func1: starting')
  for i in range(1000000000):
      j=j+1
  print ('func1: finishing',j)

def func2():
  j=0
  print ('func2: starting')
  for i in range(1000000000):
      j=j+1
  print ('func2: finishing',j)

def func3():
  j=0
  print ('func3: starting')
  for i in range(1000000000):
      j=j+1
  print ('func3: finishing',j)


if __name__ == '__main__':
  p1 = Process(target=func1)
  p1.start()
  p2 = Process(target=func2)
  p2.start()
  p3 = Process(target=func3)
  p3.start()
  p1.join()
  p2.join()
  p3.join()
```

```
top - 11:28:00 up 2 days,  2:02,  1 user,  load average: 0,57, 0,56, 0,48
Tasks: 306 total,   4 running, 301 sleeping,   0 stopped,   1 zombie
%Cpu(s): 38,3 us,  0,4 sy,  0,0 ni, 61,1 id,  0,1 wa,  0,0 hi,  0,1 si,  0,0 st
KiB Mem :  8079052 total,   294168 free,  5072908 used,  2711976 buff/cache
KiB Swap: 19529724 total, 19506740 free,    22984 used.  1438376 avail Mem

  PID USER      PR  NI    VIRT    RES    SHR S  %CPU %MEM     TIME+ COMMAND
26027 ruben     20   0   50896   8488   3072 R 100,0  0,1   0:09.43 python
26028 ruben     20   0   50896   8488   3072 R 100,0  0,1   0:09.43 python
26026 ruben     20   0   50896   8488   3072 R  99,0  0,1   0:09.43 python
24587 ruben     20   0 4736720 2,196g 2,119g S   4,0 28,5   7:45.81 VirtualBox
 1128 root      20   0  756332 231528 197116 S   1,0  2,9  11:15.62 Xorg
 7796 ruben     20   0 1325324 184588  52036 S   1,0  2,3  21:43.70 skypeforli+
26032 ruben     20   0  437152  21932  18568 S   1,0  0,3   0:00.25 gnome-scre+
    1 root      20   0  185332   4984   3008 S   0,0  0,1   0:01.58 systemd
```

```
ruben@jarvis:~/test/parallelpython$ time python test.py
func1: starting
func2: starting
func3: starting
func3: finishing 1000000000
func2: finishing 1000000000
func1: finishing 1000000000
[1]+  Done                    emacs test.py

real    0m36.208s
user    1m50.284s
sys     0m0.544s
```

Can we do any of this in Python? **Kind of…**

```
from multiprocessing import Process


def func1():
  j=0
  print ('func1: starting')
  for i in range(1000000000):
      j=j+1
  print ('func1: finishing',j)

def func2():
  j=0
  print ('func2: starting')
  for i in range(1000000000):
      j=j+1
  print ('func2: finishing',j)

def func3():
  j=0
  print ('func3: starting')
  for i in range(1000000000):
      j=j+1
  print ('func3: finishing',j)

def runInParallel(*fns):
  proc = []
  for fn in fns:
    p = Process(target=fn)
    p.start()
    proc.append(p)
  for p in proc:
    p.join()


if __name__ == '__main__':
    runInParallel (func1, func2, func3)
```

```
top - 11:28:00 up 2 days,  2:02,  1 user,  load average: 0,57, 0,56, 0,48
Tasks: 306 total,   4 running, 301 sleeping,   0 stopped,   1 zombie
%Cpu(s): 38,3 us,  0,4 sy,  0,0 ni, 61,1 id,  0,1 wa,  0,0 hi,  0,1 si,  0,0 st
KiB Mem :  8079052 total,   294168 free,  5072908 used,  2711976 buff/cache
KiB Swap: 19529724 total, 19506740 free,    22984 used.  1438376 avail Mem

  PID USER      PR  NI    VIRT    RES    SHR S  %CPU %MEM     TIME+ COMMAND
26027 ruben     20   0   50896   8488   3072 R 100,0  0,1   0:09.43 python
26028 ruben     20   0   50896   8488   3072 R 100,0  0,1   0:09.43 python
26026 ruben     20   0   50896   8488   3072 R  99,0  0,1   0:09.43 python
24587 ruben     20   0 4736720 2,196g 2,119g S   4,0 28,5   7:45.81 VirtualBox
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```
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func1: starting
func2: starting
func3: starting
func3: finishing 1000000000
func2: finishing 1000000000
func1: finishing 1000000000
[1]+  Done                    emacs test.py

real    0m36.208s
user    1m50.284s
sys     0m0.544s
```

http://stackabuse.com/parallel-processing-in-python/

We want to sum up the integer half-value of the first 3e8 integers.

```python
from multiprocessing import Process,Manager

def func1(id,results):
    j=0
    print('func1: starting')
    for i in range(100000000):
        j=j+i/2
    print('func1: finishing')
    results[id]=j

def func2(id,results):
    j=0
    print('func2: starting')
    for i in range(100000001,200000000):
        j=j+i/2
    print('func2: finishing')
    results[id]=j

def func3(id,results):
    j=0
    print('func3: starting')
    for i in range(200000001,300000000):
        j=j+i/2
    print('func3: finishing')
    results[id]=j

def runInParallel(*fns):
    proc=[]
    for i,fn in enumerate(fns):
        p = Process(target=fn,args=(i,results))
        p.start()
        proc.append(p)
    for p in proc:
        p.join()
    print(results)
    print(sum(results.values()))


if __name__ == '__main__':
    results=Manager().dict()
    runInParallel (func1,func2,func3)
```

```
[cabezon@login10 openmp]$ time python python_multiproc_2.py
func1: starting
func2: starting
func3: starting
func3: finishing
func2: finishing
func1: finishing
{0: 2499999950000000, 1: 7499999900000000, 2: 12499999850000000}
22499999700000000

real    0m12.819s
user    0m27.136s
sys     0m8.865s
[cabezon@login10 openmp]$
```

Note that threads finish in an unstructured way!

We store the results in a dictionary and sum them up.
(mimicking a ‘reduce’ in OpenMP)

More elegant way to do this is using ‘numba’. https://numba.pydata.org/

Adding a decorator numba compiles the code on-the-fly creating an optimized machine code

```
from numba import jit

@jit()
def func1():
    j=0
    print('func1: starting')
    for i in range(300000000):
        j=j+i/2
    print('func1: finishing',j)

if __name__ == '__main__':
    func1()
```

```
[cabezon@login10 openmp]$ time python python_multiproc_2.py
func1: starting
func2: starting
func3: starting
func3: finishing
func2: finishing
func1: finishing
{0: 2499999950000000, 1: 7499999900000000, 2: 12499999850000000}
22499999700000000

real    0m12.819s
user    0m27.136s
sys     0m8.865s
[cabezon@login10 openmp]$
```

```
[cabezon@login10 openmp]$ source numbatest/bin/activate
(numbatest) [cabezon@login10 openmp]$ time python python_numba.py
func1: starting
func1: finishing 2.249999988355443e+16

real    0m1.142s
user    0m1.205s
sys     0m1.294s
(numbatest) [cabezon@login10 openmp]$
```

More elegant way to do this is using ‘numba’. https://numba.pydata.org/

Adding a decorator numba compiles the code on-the-fly creating an optimized machine code

```
[cabezon@login10 openmp]$ time python python_multiproc_2.py
func1: starting
func2: starting
func3: starting
func3: finishing
func2: finishing
func1: finishing
{0: 2499999950000000, 1: 7499999900000000, 2: 12499999850000000}
22499999700000000

real    0m12.819s
user    0m27.136s
sys     0m8.865s
```

```
from numba import jit

@jit()
def func1():
    j=0
    print('func1: starting'
    for i in range(30000000
        j=j+i/2
    print('func1: finishing

if __name__ == '__main__':
    func1()
```

We need to install numba. For that we will install a virtual environment of Python:

virtualenv testnumba

source testnumba/bin/activate

2. Install numba

pip install numba

3. Execute the serial version with the numba decorator

(don’t forget to import jit at the beginning of the Python script)

time python python_serial.py

More elegant way to do this is using ‘numba’. https://numba.pydata.org/

We are using just 1 core with numba, but we can also use all cores in the machine, just like with OpenMP, with prange:

```
cabezon@shi101:~/openmp_course $time python python_serial.py
func: starting (from 1 to 30000000000)
func1: finishing 2.2500000000007956e+20

real    0m31.206s
user    0m32.340s
sys     0m2.832s
cabezon@shi101:~/openmp_course $
```

```
cabezon@shi101:~/openmp_course $time python python_serial.py
func: starting (from 1 to 30000000000)
func1: finishing 2.2500000000005246e+20

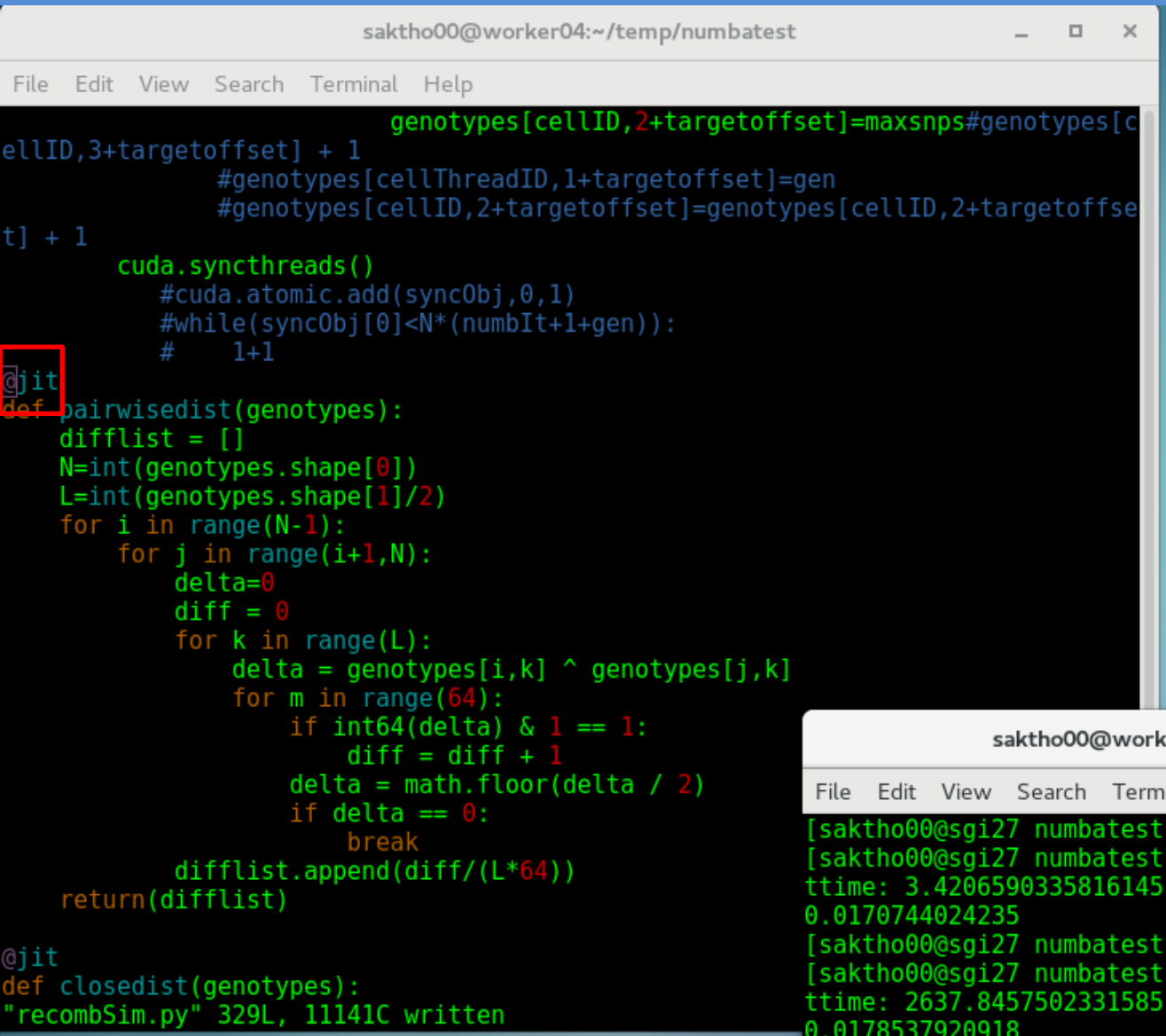
real    0m1.781s
user    0m41.160s
sys     0m3.124s
cabezon@shi101:~/openmp_course $
```

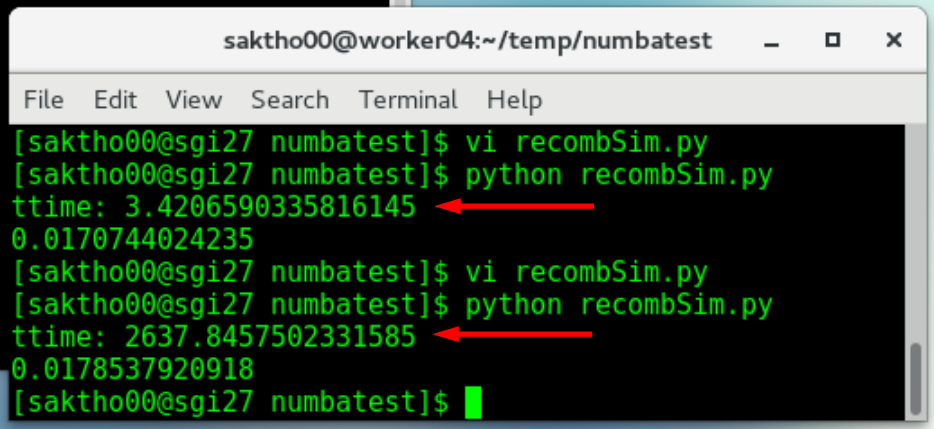
```
from numba import jit,prange

@jit(parallel=True)
def func1():
    j=0
    print('func: starting (from 1 to 300000000)')
    for i in prange(1,30000000001):
        j=j+i/2
    print('func1: finishing',j)

if __name__ == '__main__':
    func1()
```

NOTE: we are doing x100 more iterations in this example than in the previous one so that we can actually see differences in the times between 1 and many cores.

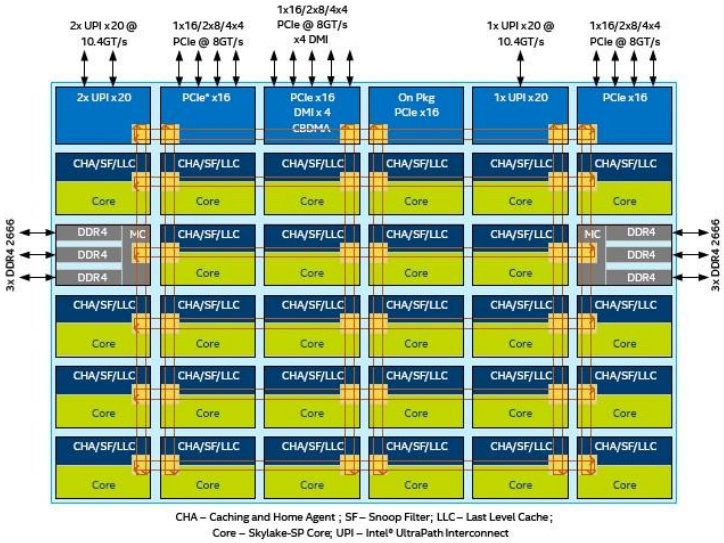




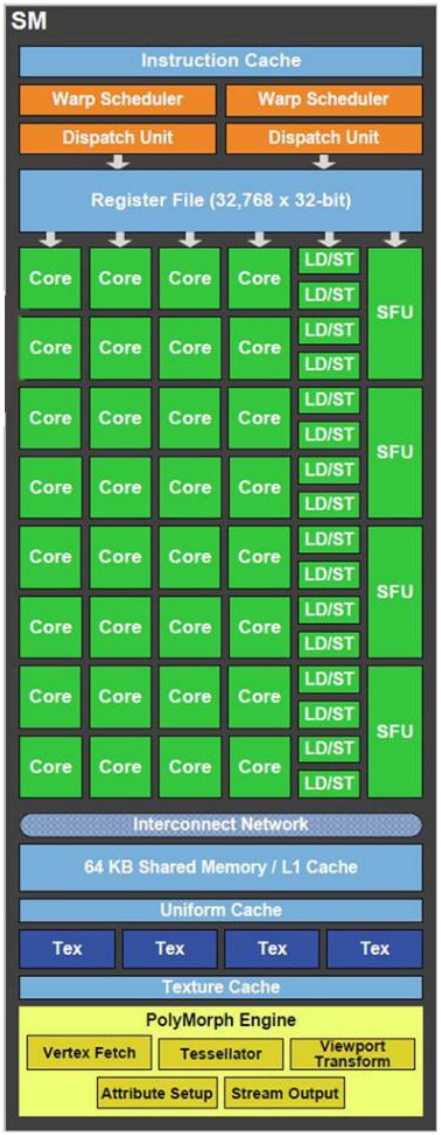
Thomas Sakoparnig

What about GPU?

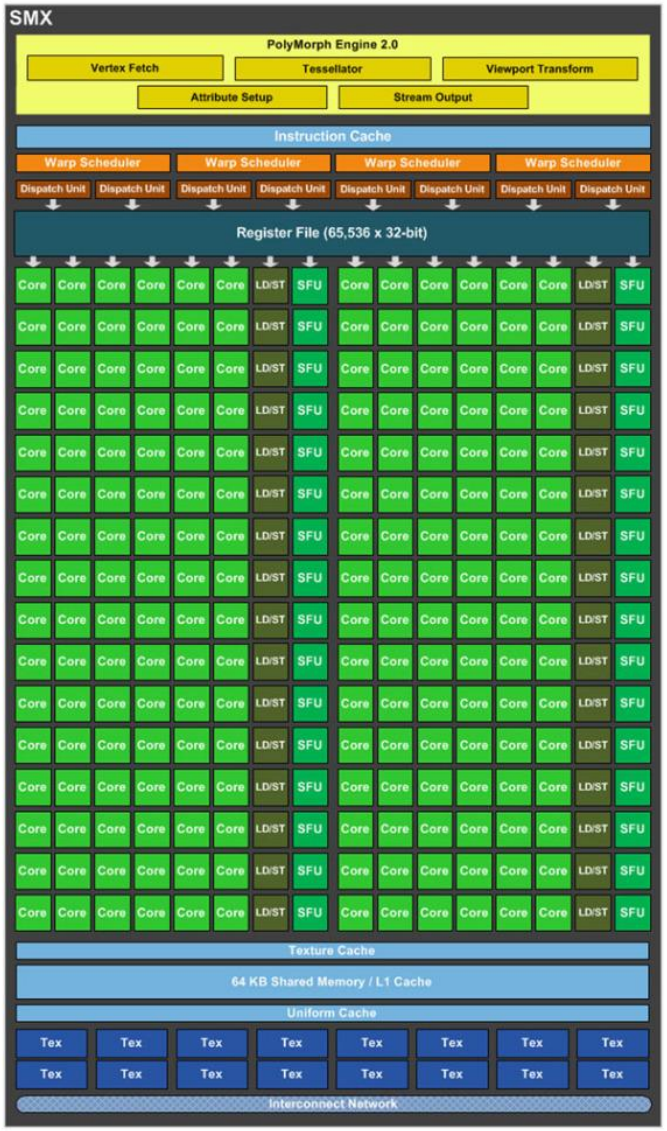
Intel Skylake (2017)



Tesla SM unit (2007)



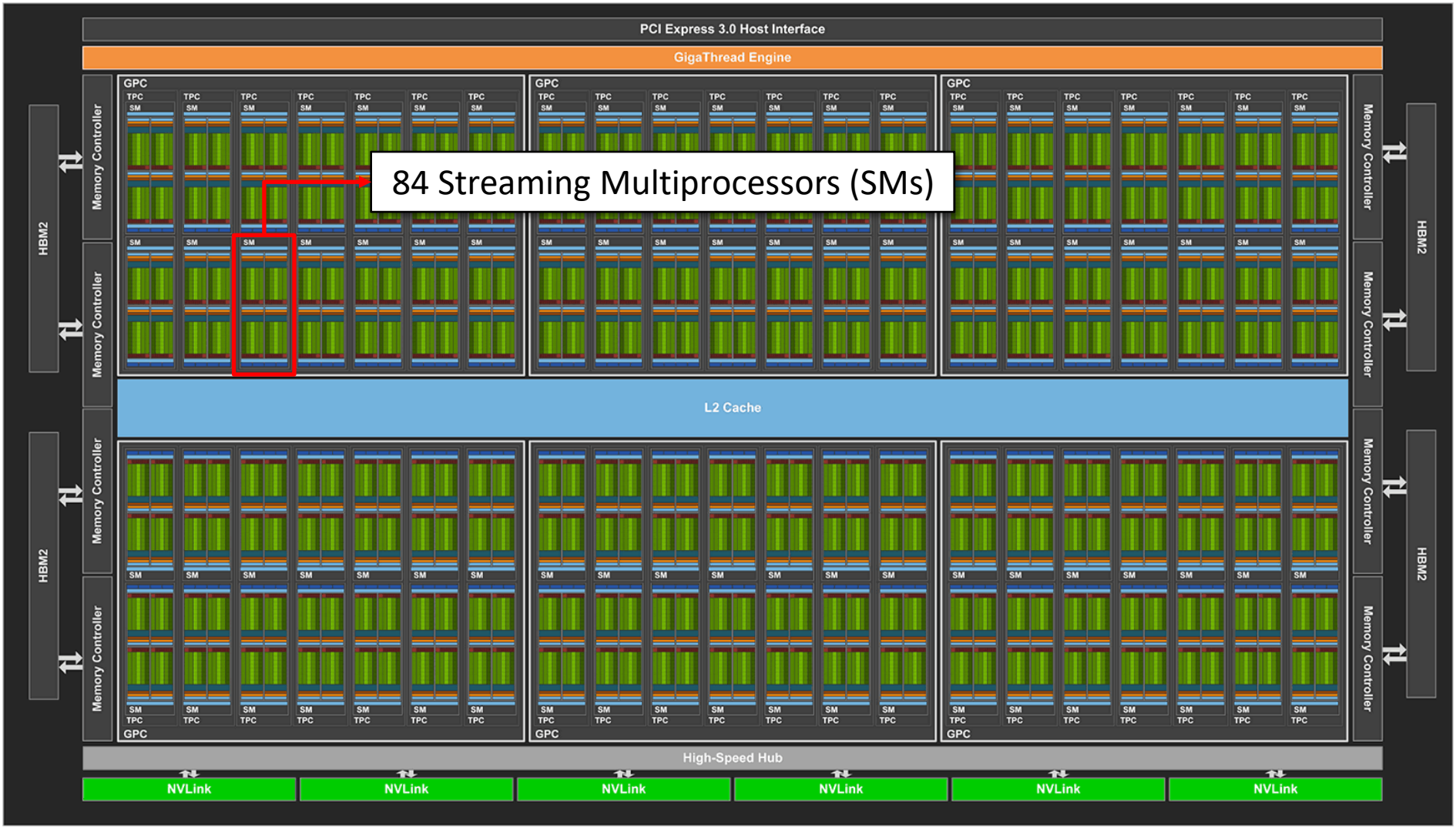
Fermi SMX unit (2011)



Volta (2017)


PCI Express 3.0 Host Interface
GigaThread Engine
GPC
TPC
SM
Memory Controller
HBM2
L2 Cache
High-Speed Hub
NVLink

Volta (2017)


PCI Express 3.0 Host Interface
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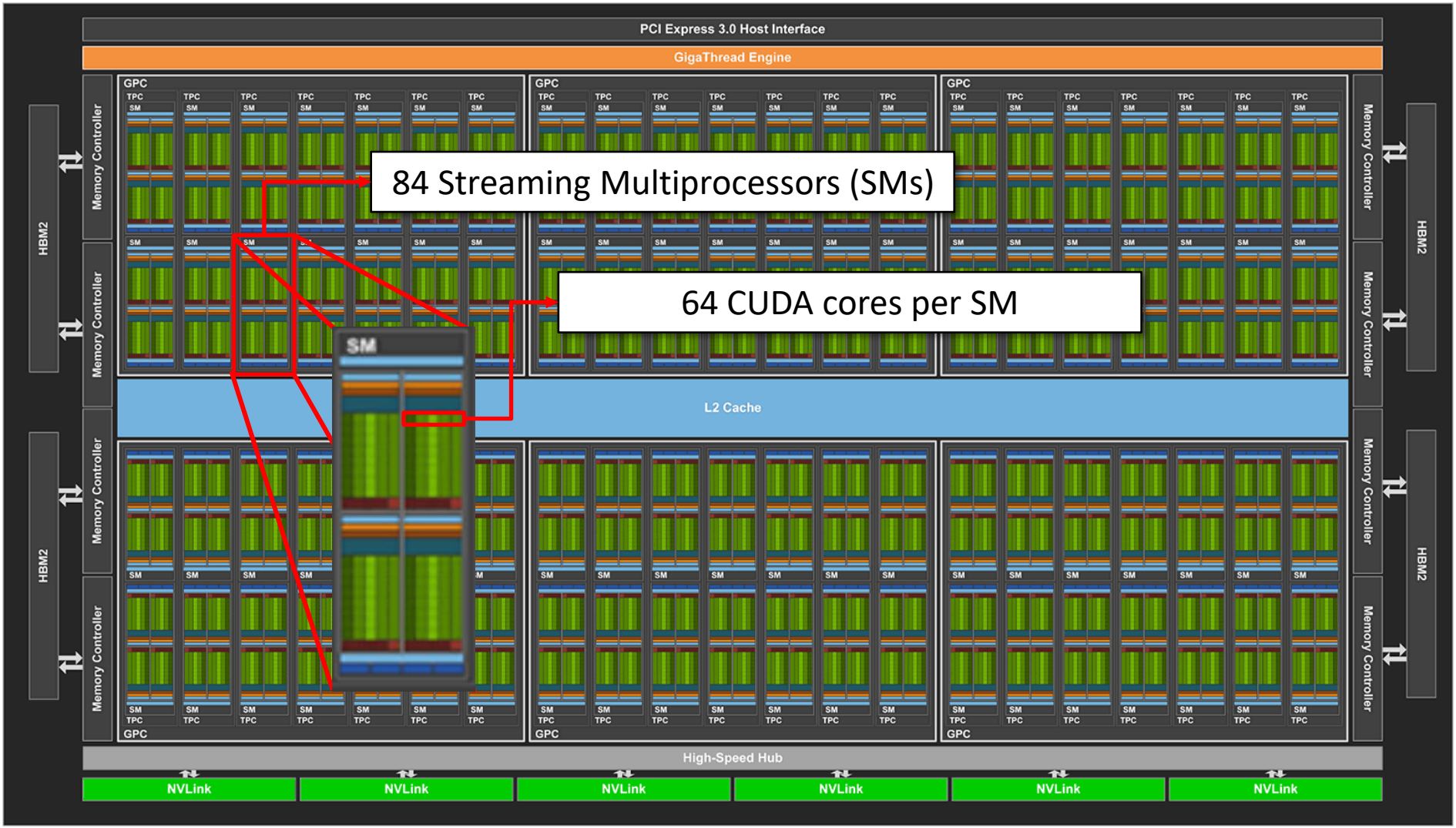
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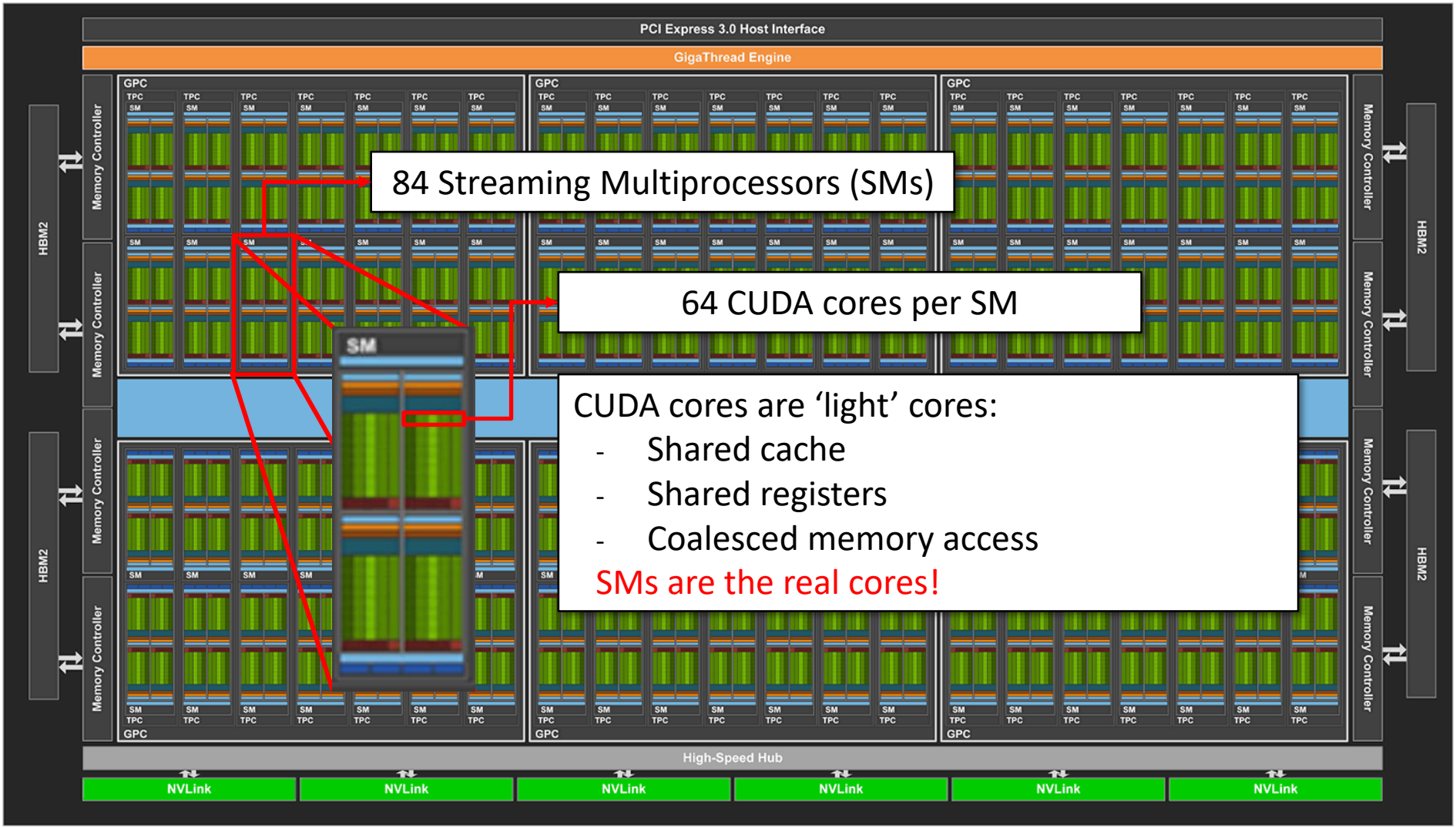
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- Shared registers
- Coalesced memory access
SMs are the real cores!
High-Speed Hub
NVLink

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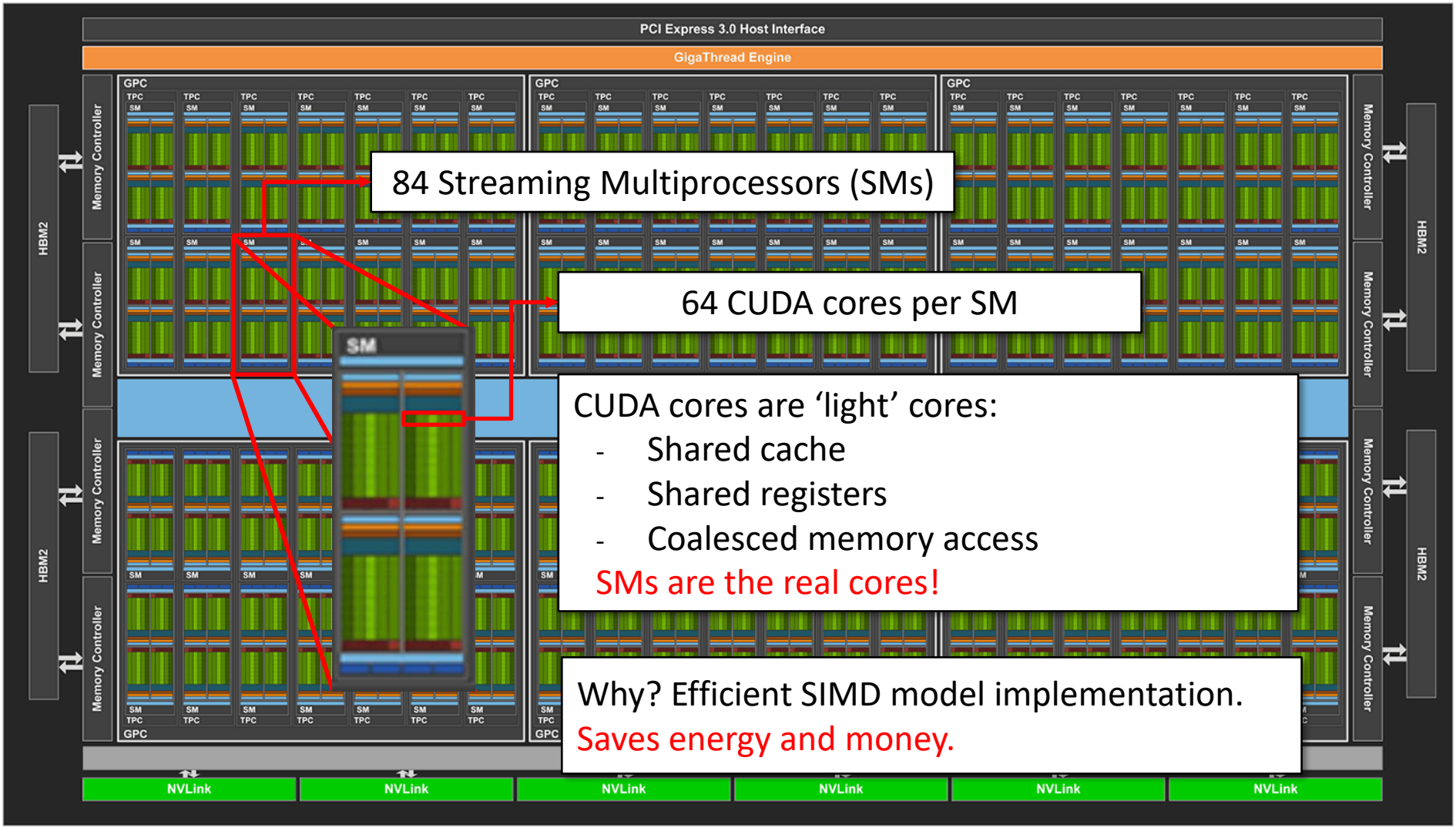
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CUDA cores are ‘light’ cores:
- Shared cache
- Shared registers
- Coalesced memory access
SMs are the real cores!
Why? Efficient SIMD model implementation.
Saves energy and money.
NVLink

Since version 4.0, openMP can do GPU offloading.

```
int A[1] = {-1};
#pragma omp target
{
   A[0] = omp_is_initial_device();
}
if (!A[0]) {
    printf("Able to use offloading!\n");
}
```

omp_is_initial_device() returns 0 when called from the accelerator

You can control the transfer of data

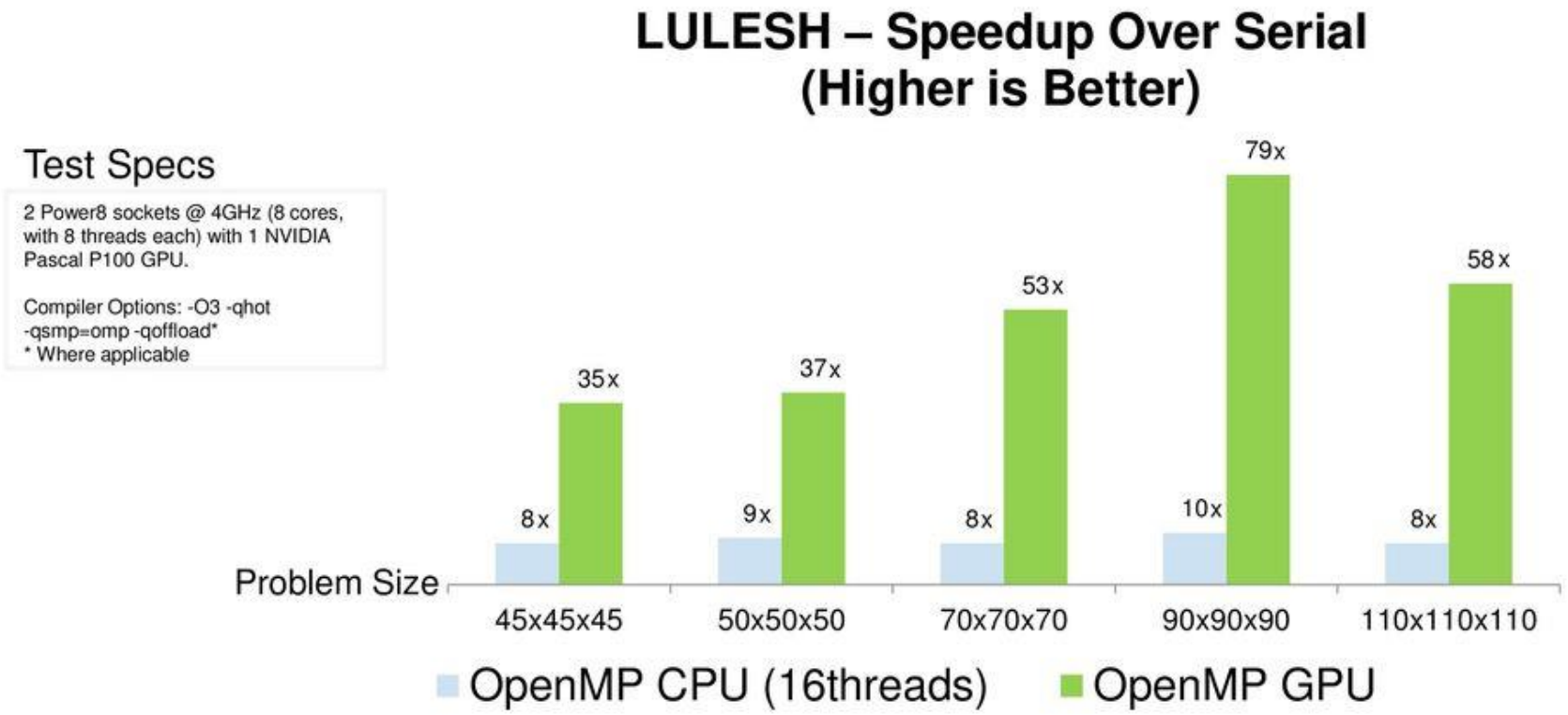
```
#pragma omp target data map(to: b[:n])
{
    // 'b' copied onto device

    // This region is offloaded to device
    #pragma omp target map(tofrom: a[:n])
    {
        // 'a' copied onto device
        #pragma omp teams distribute
        for(int ii = 0; ii < n; ++ii)
        {
            a[ii] = a[ii] + alpha * b[ii];
        }
    }
    // 'a' copied back

    // ... potentially more target regions
}
// 'b' is discarded by device
```

Since version 4.0, openMP can do GPU offloading.

Performance Results – End to End

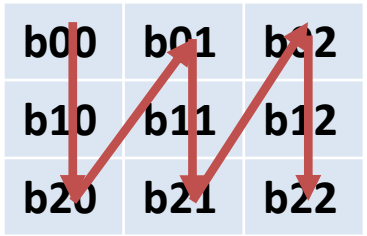


Full example: matrix multiplication

Sub-optimal memory access will kill the performance…

The less efficient way (column-major):

```
for(int i=0; i<n; ++i)
   for(int j=0; j<n; ++j)
      for(int k=0; k<n; ++k)
          c[i*n+j] += a[i*n+k] * b[k*n+j];
```



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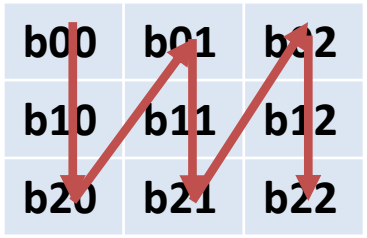
      for(int k=0; k<n; ++k)
         c[i*n+j] += a[i*n+k] * b[k*n+j];
```



- Processors **load data into their cache** for fast reuse
- They always load a bunch of data at the same time
- They do **branch-prediction** and **pre-fetching**!

However here we are not helping him…

Processor cache

Cache Misses: 0

a00	a01	a02	a10	a11	a12	a20	a21	a22
b00	b01	b02	b10	b11	b12	b20	b21	b22
c00	c01	c02	c10	c11	c12	c20	c21	c22

i	j	k
0	0	0

Full example: matrix multiplication

Sub-optimal memory access will kill the performance…

The less efficient way (column-major):

```
for(int i=0; i<n; ++i)
   for(int j=0; j<n; ++j)
      for(int k=0; k<n; ++k)
         c[i*n+j] += a[i*n+k] * b[k*n+j];
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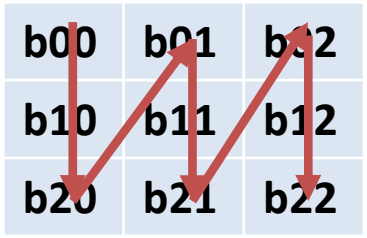

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Processor cache

Cache Misses: 1

a00	a01	a02	a10	a11	a12	a20	a21	a22
b00	b01	b02	b10	b11	b12	b20	b21	b22
c00	c01	c02	c10	c11	c12	c20	c21	c22

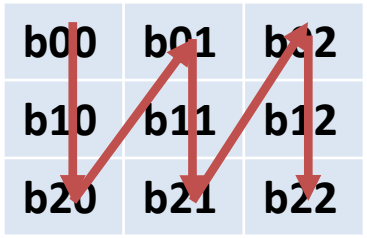
i	j	k
0	0	1

Full example: matrix multiplication

Sub-optimal memory access will kill the performance…

The less efficient way (column-major):

```
for(int i=0; i<n; ++i)
   for(int j=0; j<n; ++j)
      for(int k=0; k<n; ++k)
          c[i*n+j] += a[i*n+k] * b[k*n+j];
```



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However here we are not helping him…

Processor cache

Cache Misses: 2

a00	a01	a02	a10	a11	a12	a20	a21	a22
b00	b01	b02	b10	b11	b12	b20	b21	b22
c00	c01	c02	c10	c11	c12	c20	c21	c22

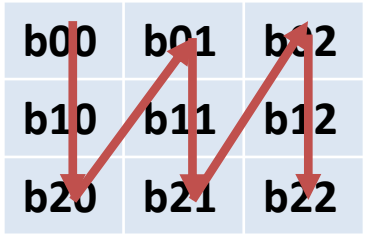
i	j	k
0	0	2

Full example: matrix multiplication

Sub-optimal memory access will kill the performance…

The less efficient way (column-major):

```
for(int i=0; i<n; ++i)
   for(int j=0; j<n; ++j)
      for(int k=0; k<n; ++k)
          c[i*n+j] += a[i*n+k] * b[k*n+j];
```



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However here we are not helping him…

Processor cache

Cache Misses: 3

a00	a01	a02	a10	a11	a12	a20	a21	a22
b00	b01	b02	b10	b11	b12	b20	b21	b22
c00	c01	c02	c10	c11	c12	c20	c21	c22

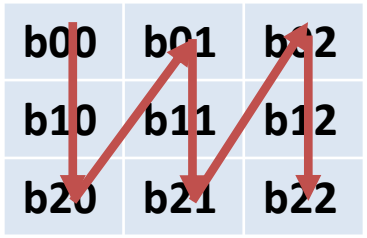
i	j	k
0	1	0

Full example: matrix multiplication

Sub-optimal memory access will kill the performance…

The less efficient way (column-major):

```
for(int i=0; i<n; ++i)
   for(int j=0; j<n; ++j)
      for(int k=0; k<n; ++k)
         c[i*n+j] += a[i*n+k] * b[k*n+j];
```



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However here we are not helping him…

Processor cache

Cache Misses: 4

a00	a01	a02	a10	a11	a12	a20	a21	a22
b00	b01	b02	b10	b11	b12	b20	b21	b22
c00	c01	c02	c10	c11	c12	c20	c21	c22

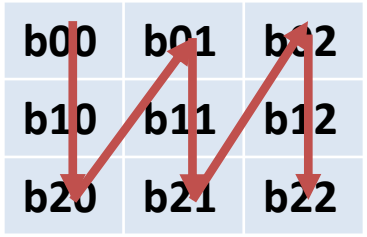
i	j	k
0	1	1

Full example: matrix multiplication

Sub-optimal memory access will kill the performance…

The less efficient way (column-major):

```
for(int i=0; i<n; ++i)
   for(int j=0; j<n; ++j)
      for(int k=0; k<n; ++k)
         c[i*n+j] += a[i*n+k] * b[k*n+j];
```



- Processors **load data into their cache** for fast reuse
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However here we are not helping him…

Processor cache

Cache Misses: 5

a00	a01	a02	a10	a11	a12	a20	a21	a22
b00	b01	b02	b10	b11	b12	b20	b21	b22
c00	c01	c02	c10	c11	c12	c20	c21	c22

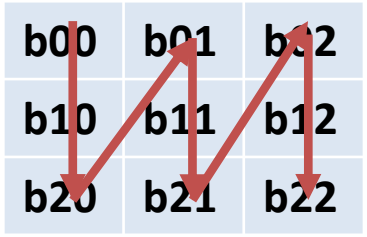
i	j	k
0	1	2

Full example: matrix multiplication

Sub-optimal memory access will kill the performance…

The less efficient way (column-major):

```
for(int i=0; i<n; ++i)
   for(int j=0; j<n; ++j)
      for(int k=0; k<n; ++k)
          c[i*n+j] += a[i*n+k] * b[k*n+j];
```



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Processor cache

Cache Misses: 6

a00	a01	a02	a10	a11	a12	a20	a21	a22
b00	b01	b02	b10	b11	b12	b20	b21	b22
c00	c01	c02	c10	c11	c12	c20	c21	c22

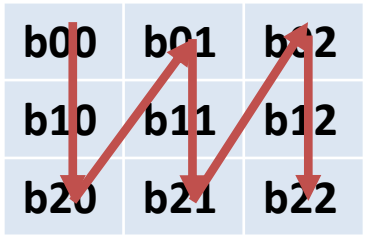
i	j	k
0	2	0

Full example: matrix multiplication

Sub-optimal memory access will kill the performance…

The less efficient way (column-major):

```
for(int i=0; i<n; ++i)
   for(int j=0; j<n; ++j)
      for(int k=0; k<n; ++k)
          c[i*n+j] += a[i*n+k] * b[k*n+j];
```



- Processors **load data into their cache** for fast reuse
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However here we are not helping him…

Processor cache

Cache Misses: 7

a00	a01	a02	a10	a11	a12	a20	a21	a22
b00	b01	b02	b10	b11	b12	b20	b21	b22
c00	c01	c02	c10	c11	c12	c20	c21	c22

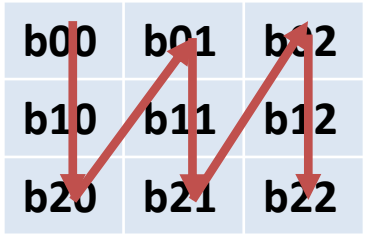
i	j	k
0	2	1

Full example: matrix multiplication

Sub-optimal memory access will kill the performance…

The less efficient way (column-major):

```
for(int i=0; i<n; ++i)
   for(int j=0; j<n; ++j)
      for(int k=0; k<n; ++k)
         c[i*n+j] += a[i*n+k] * b[k*n+j];
```



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Processor cache

Cache Misses: 8

a00	a01	a02	a10	a11	a12	a20	a21	a22
b00	b01	b02	b10	b11	b12	b20	b21	b22
c00	c01	c02	c10	c11	c12	c20	c21	c22

i	j	k
0	2	2

Full example: matrix multiplication

Sub-optimal memory access will kill the performance…

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```
for(int i=0; i<n; ++i)
   for(int j=0; j<n; ++j)
      for(int k=0; k<n; ++k)
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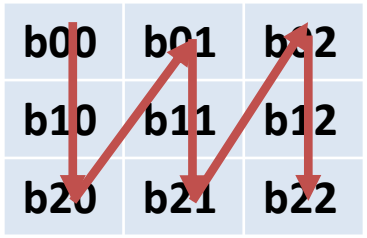
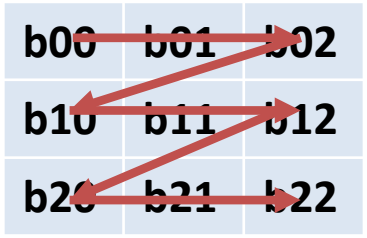
```



The better way (row-major):

```
for(int i=0; i<n; ++i)
   for(int k=0; k<n; ++k)
       for(int j=0; j<n; ++j)
          c[i*n+j] += a[i*n+k] * b[k*n+j];
```



Let's go…

a00	a01	a02	a10	a11	a12	a20	a21	a22
b00	b01	b02	b10	b11	b12	b20	b21	b22
c00	c01	c02	c10	c11	c12	c20	c21	c22

i	k	j
0	0	0

Full example: matrix multiplication

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```
for(int i=0; i<n; ++i)
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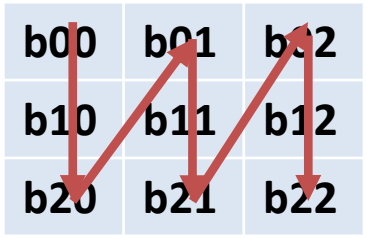

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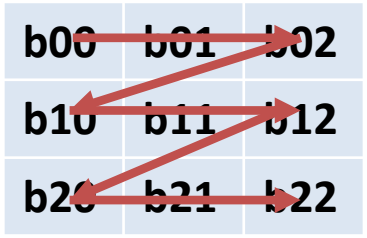

Cache Misses: 0

a00	a01	a02	a10	a11	a12	a20	a21	a22
b00	b01	b02	b10	b11	b12	b20	b21	b22
c00	c01	c02	c10	c11	c12	c20	c21	c22

i	k	j
0	0	1

Full example: matrix multiplication

Sub-optimal memory access will kill the performance…

The less efficient way (column-major):

```
for(int i=0; i<n; ++i)
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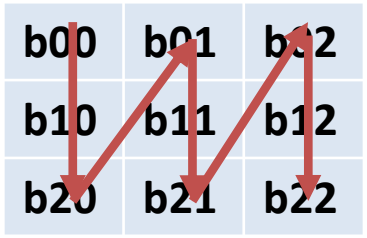

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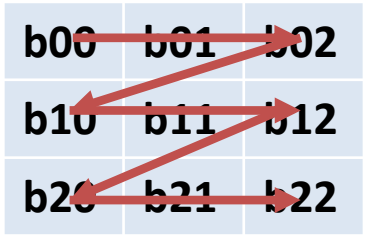


Cache Misses: 0

a00	a01	a02	a10	a11	a12	a20	a21	a22
b00	b01	b02	b10	b11	b12	b20	b21	b22
c00	c01	c02	c10	c11	c12	c20	c21	c22

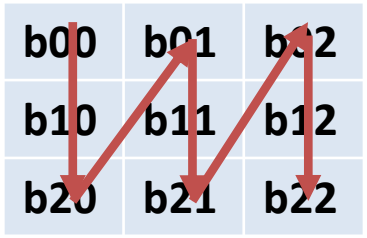
i	k	j
0	0	2

Full example: matrix multiplication

Sub-optimal memory access will kill the performance…

The less efficient way (column-major):

```
for(int i=0; i<n; ++i)
   for(int j=0; j<n; ++j)
      for(int k=0; k<n; ++k)
          c[i*n+j] += a[i*n+k] * b[k*n+j];
```



The better way (row-major):

```
for(int i=0; i<n; ++i)
   for(int k=0; k<n; ++k)
       for(int j=0; j<n; ++j)
          c[i*n+j] += a[i*n+k] * b[k*n+j];
```

Cache Misses: 1

a00	a01	a02	a10	a11	a12	a20	a21	a22
b00	b01	b02	b10	b11	b12	b20	b21	b22
c00	c01	c02	c10	c11	c12	c20	c21	c22

i	k	j
0	1	0

Full example: matrix multiplication

Sub-optimal memory access will kill the performance…

The less efficient way (column-major):

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for(int i=0; i<n; ++i)
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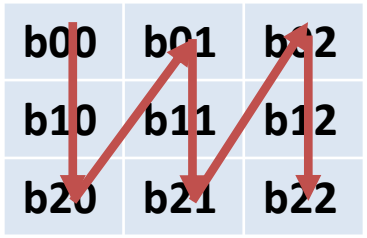

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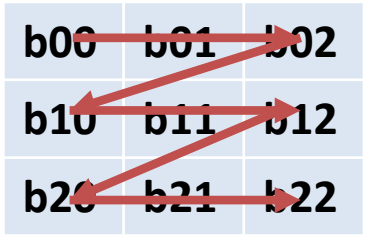

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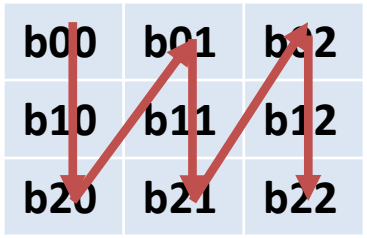

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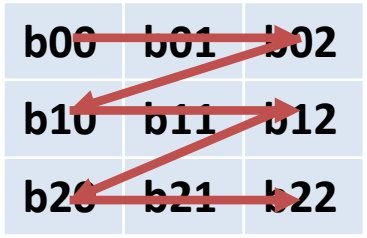

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c00	c01	c02	c10	c11	c12	c20	c21	c22

i	k	j
0	1	2

Full example: matrix multiplication

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```
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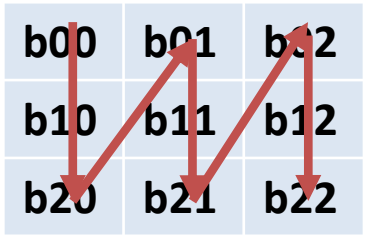

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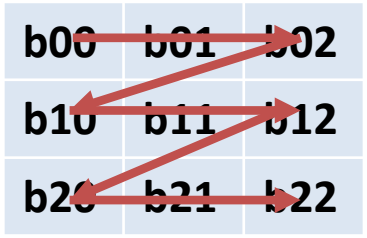

Cache Misses: 2

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b00	b01	b02	b10	b11	b12	b20	b21	b22
c00	c01	c02	c10	c11	c12	c20	c21	c22

i	k	j
0	2	0

Full example: matrix multiplication

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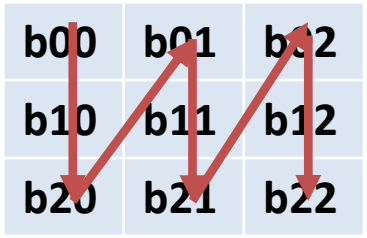

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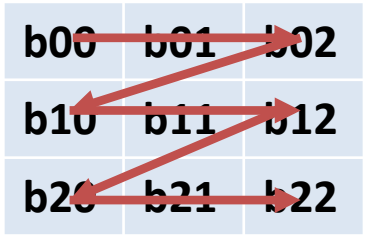

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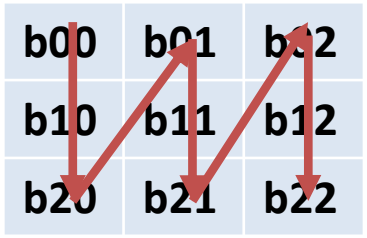
```



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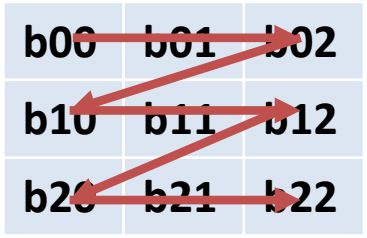

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i	k	j
0	2	2

Full example: matrix multiplication with OpenMP / Numba

```
#pragma omp parallel for
for(int i=0; i<size; ++i)
   for(int k=0; k<size; ++k)
      for(int j=0; j<size; ++j)
         c[i*size+j] += a[i*size+k] * b[k*size+j];
```

C++

```
!$omp parallel private(i,j,k)
!$omp do schedule(static)
do i=0,size-1
   do k=0,size-1
      do j=0,size-1
         c(i*size+j) = c(i*size+j) + a(i*size+k) * b(k*size+j)
      enddo
   enddo
enddo
!$omp end do
!$omp end parallel
```

FORTRAN

```
@jit(Parallel=True)
def mat_mul(a,b,c,size):
    for i in prange(size):
        for k in range(size):
            for j in range(size):
                c[i*size+j] += a[i*size+k] + b[k*size+j]
```

Python

Full example: matrix multiplication with GPU offloading (OpenMP 4.5+)

```
!$omp target map(tofrom:c) map(to:a,b)
!$omp teams distribute parallel do private(i,j,k) collapse(2)
do i=0,size-1
   do k=0,size-1
      do j=0,size-1
         c(i*size+j) = c(i*size+j) + a(i*size+k) * b(k*size+j)
      enddo
   enddo
enddo
!$omp end target
```

FORTRAN

```
#pragma omp target map(to: a[0:n2], b[0:n2]), map(tofrom: c[0:n2])
#pragma omp teams distribute parallel for collapse(2)
for(int i=0; i<size; ++i)
    for(int j=0; j<size; ++j)
        for (int k = 0; k < size; k++)
          c[i*size+j] += a[i*size+k] * b[k*size+j];
```

C++

Full example: matrix multiplication with CUDA

```
__global__ void cuda_mul(float* a, float* b, float* c, int size) {
    int row = blockIdx.y*blockDim.y+threadIdx.y;
    int col = blockIdx.x*blockDim.x+threadIdx.x;
    for (int i = 0; i < size; i++)
        c[row*size+col] += a[row*size+i] * b[i*size+col];
}
```

CUDA Kernel

```
cudaMemcpy(dm1, a, sizeof(float)*size*size, cudaMemcpyHostToDevice);
cudaMemcpy(dm2, b, sizeof(float)*size*size, cudaMemcpyHostToDevice);
cudaMemcpy(dm3, c, sizeof(float)*size*size, cudaMemcpyHostToDevice);

dim3 blockSize = dim3(16, 16);
dim3 gridSize = dim3(size / blockSize.x, size/ blockSize.y);

cuda_mul<<<gridSize, blockSize>>>(dm1, dm2, dm3, size);

cudaMemcpy(c, dm3, sizeof(float)*size*size, cudaMemcpyDeviceToHost);
```

Kernel Call

Full example: matrix multiplication with CUDA

```
__global__ void cuda_mul(float* a, float* b, float* c, int size) {
    int row = blockIdx.y*blockDim.y+threadIdx.y;
    int col = blockIdx.x*blockDim.x+threadIdx.x;
    for (int i = 0; i < size; i++)
        c[row*size+col] += a[row*size+i] * b[i*size+col];
}
```

CUDA Kernel

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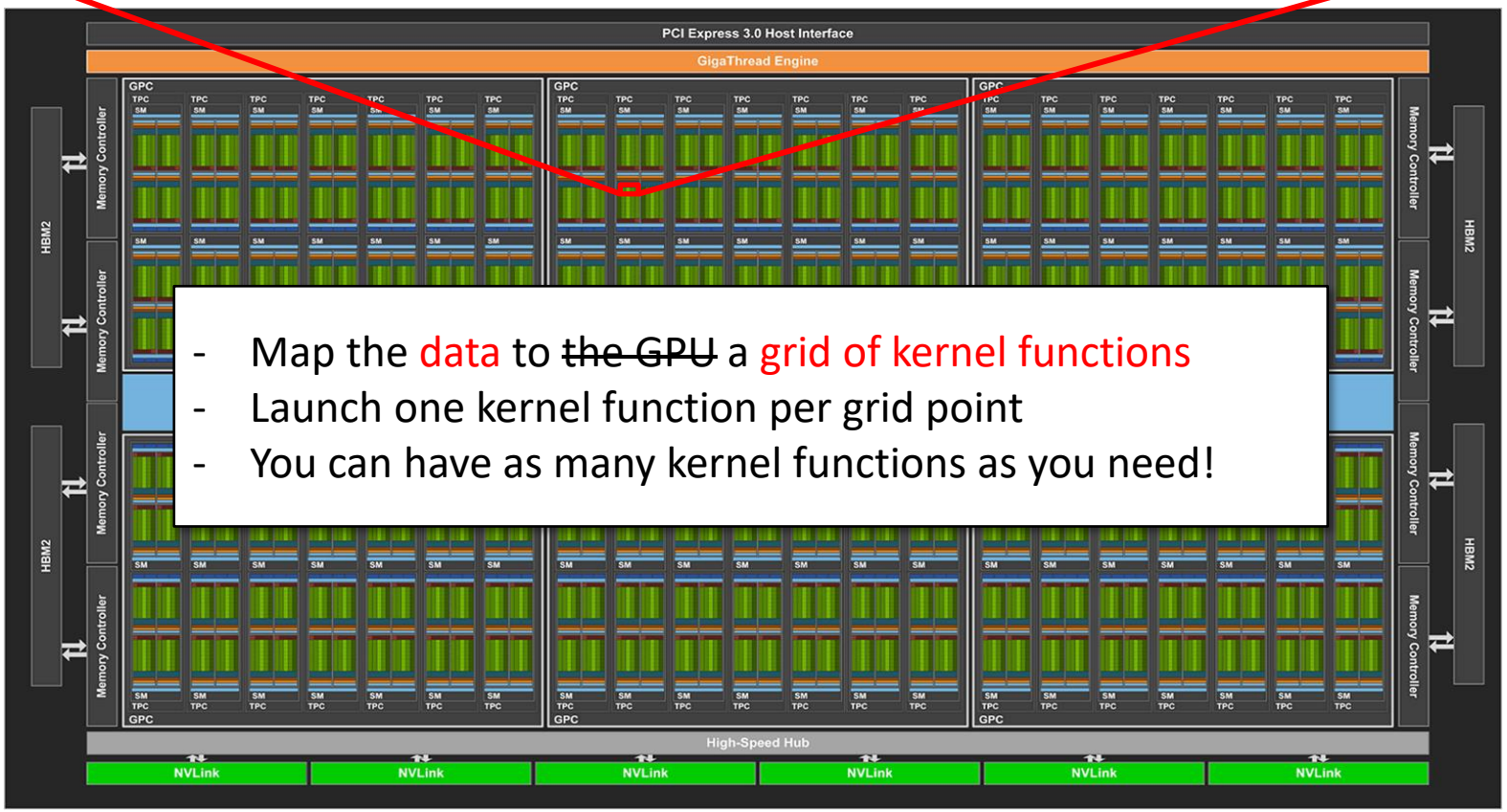
}
```

CUDA Kernel



- Map the data to ~~the GPU~~ a grid of kernel functions
- Launch one kernel function per grid point
- You can have as many kernel functions as you need!

Full example: matrix multiplication with CUDA and Numba

```
@cuda.jit
def mat_mul(a,b,c,size):
    row=cuda.blockIdx.y*cuda.blockDim.y+cuda.threadIdx.y
    col=cuda.blockIdx.x*cuda.blockDim.x+cuda.threadIdx.x
    for i in range(size):
        c[row*size+col] += a[row*size+i] * b[i*size+col]
```

CUDA Kernel

```
threadsperblock = (16,16)
blockspergrid_x = int(np.ceil(size_array / threadsperblock[0]))
blockspergrid_y = int(np.ceil(size_array / threadsperblock[1]))
blockspergrid = (blockspergrid_x, blockspergrid_y)

mat_mul[blockspergrid, threadsperblock](a,b,c,size_array)
```

Kernel Call

Full example: matrix multiplication with CUDA and Numba

```
@cuda.jit
def mat_mul(a,b,c,size):
    row=cuda.blockIdx.y*cuda.blockDim.y+cuda.threadIdx.y
    col=cuda.blockIdx.x*cuda.blockDim.x+cuda.threadIdx.x
    for i in range(size):
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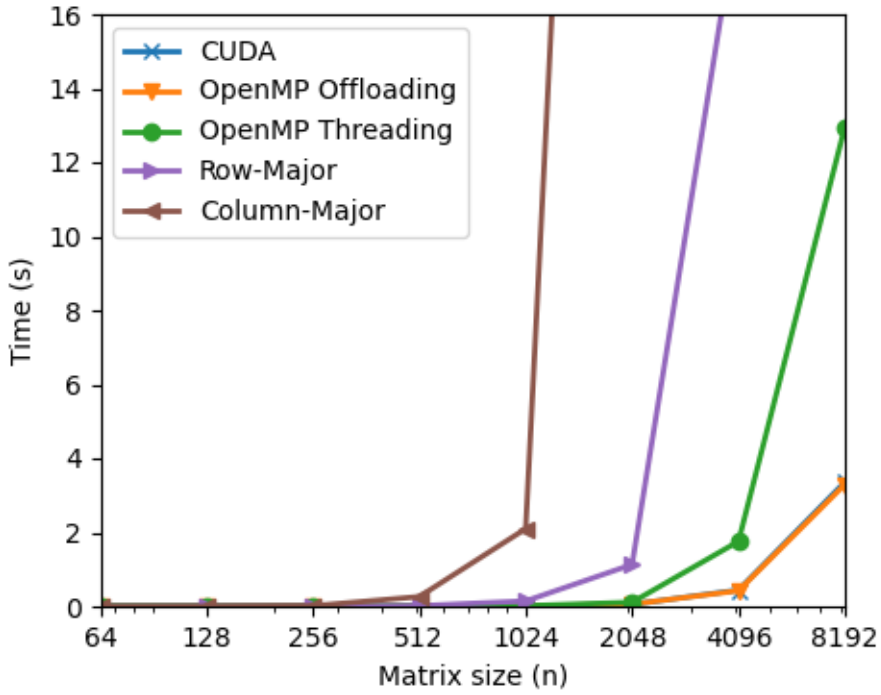
```

Kernel Call

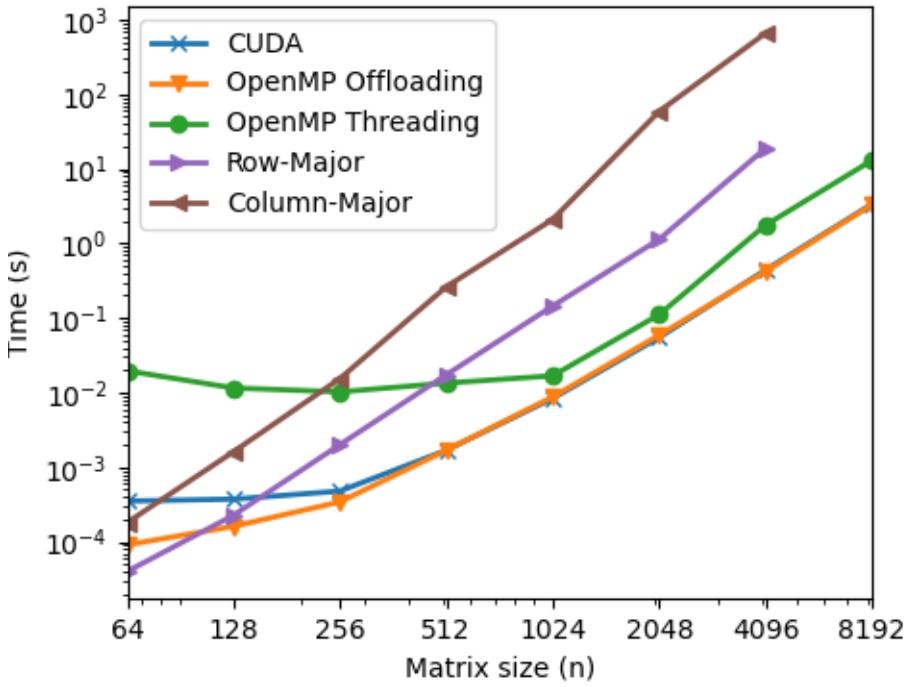
Matrix Multiplication Demo

Full example: matrix multiplication performance

Linear / log scale



Log / log scale



N = 4096
Column-Major: 658s
OpenMP 4.5/CUDA GPU: 0.43s

=> 1500x performance speedup!

There are two main ways of parallelizing a code

OpenMP™

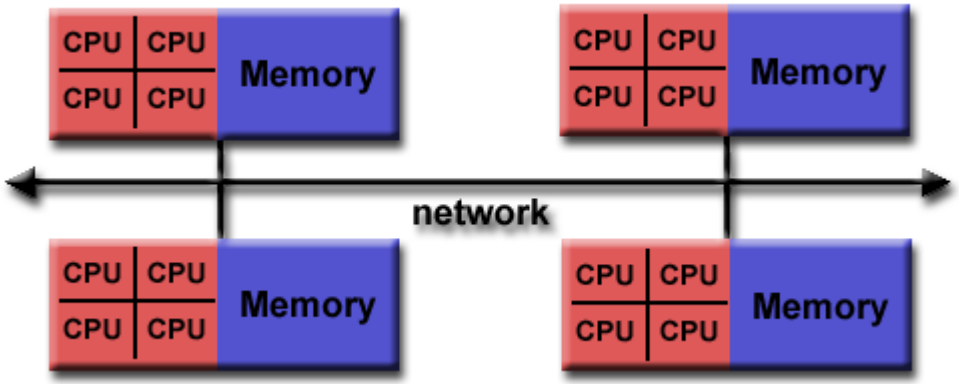
Open **M**ulti-**P**rocessing

MPI

Message **P**assing **I**nterface

Both are APIs for C/C++ and Fortran

Works in shared memory systems	Works in shared and distributed memory systems
Can use as many cores as there are in the compute node	Can use as many cores as there are in the cluster
Uses threads to split the work	Uses procesess to split the work
Threads have both private and shared variables	Processes have only private variables
Uses preprocessor directives in commented lines	Loads a library and uses specific commands



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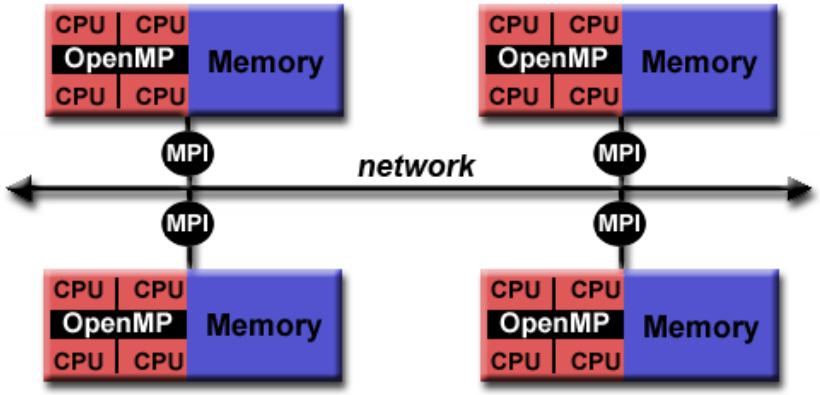

What about MPI?

Loads a library and uses specific commands

```
include ‘mpif.h’

<variable declarations>

call MPI_INIT(ierr)
call MPI_COMM_RANK(MPI_COMM_WORLD,id,ierr)
call MPI_COMM_SIZE(MPI_COMM_WORLD,nproc,ierr)

<calculations>

call MPI_FINALIZE(ierr)
```

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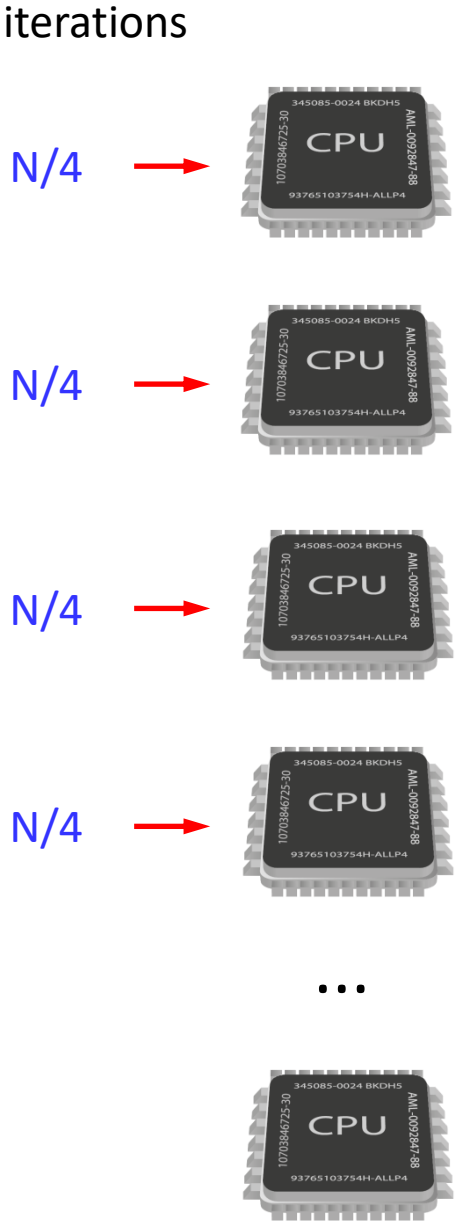
<variable declarations>

call MPI_INIT(ierr)
call MPI_COMM_RANK(MPI_COMM_WORLD,id,ierr)
call MPI_COMM_SIZE(MPI_COMM_WORLD,nproc,ierr)

do i=1,N
   <calculations>
enddo

call MPI_FINALIZE(ierr)
```



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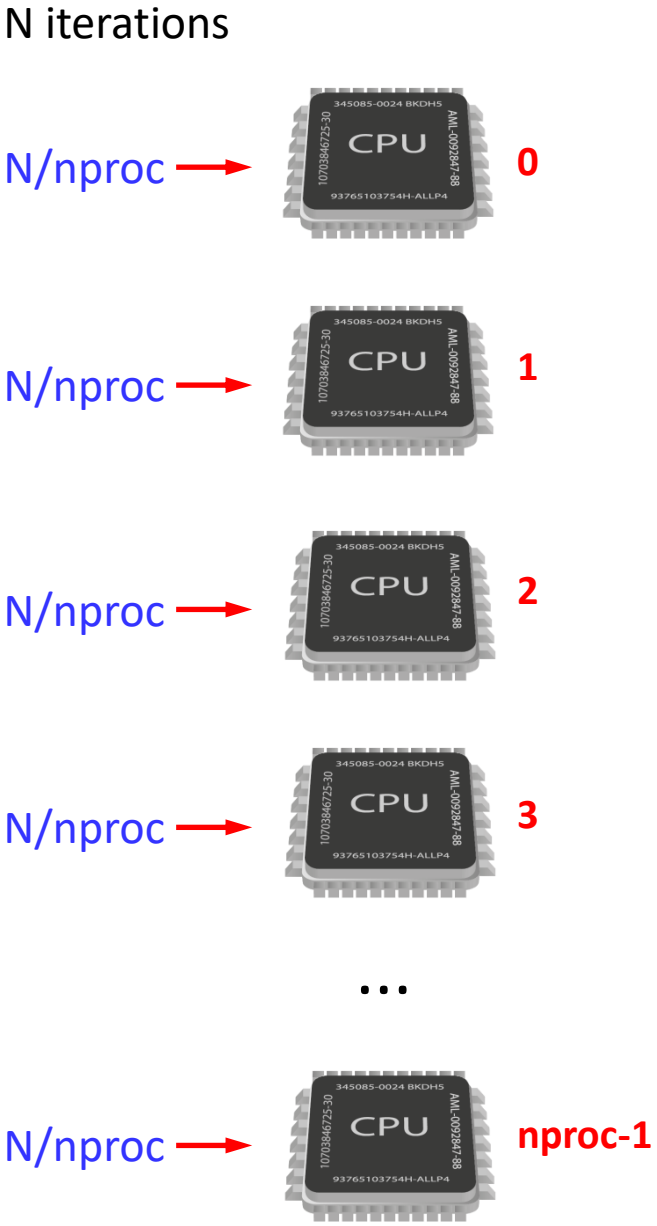

Open MPI

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Loads a library and uses specific commands

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include ‘mpif.h’

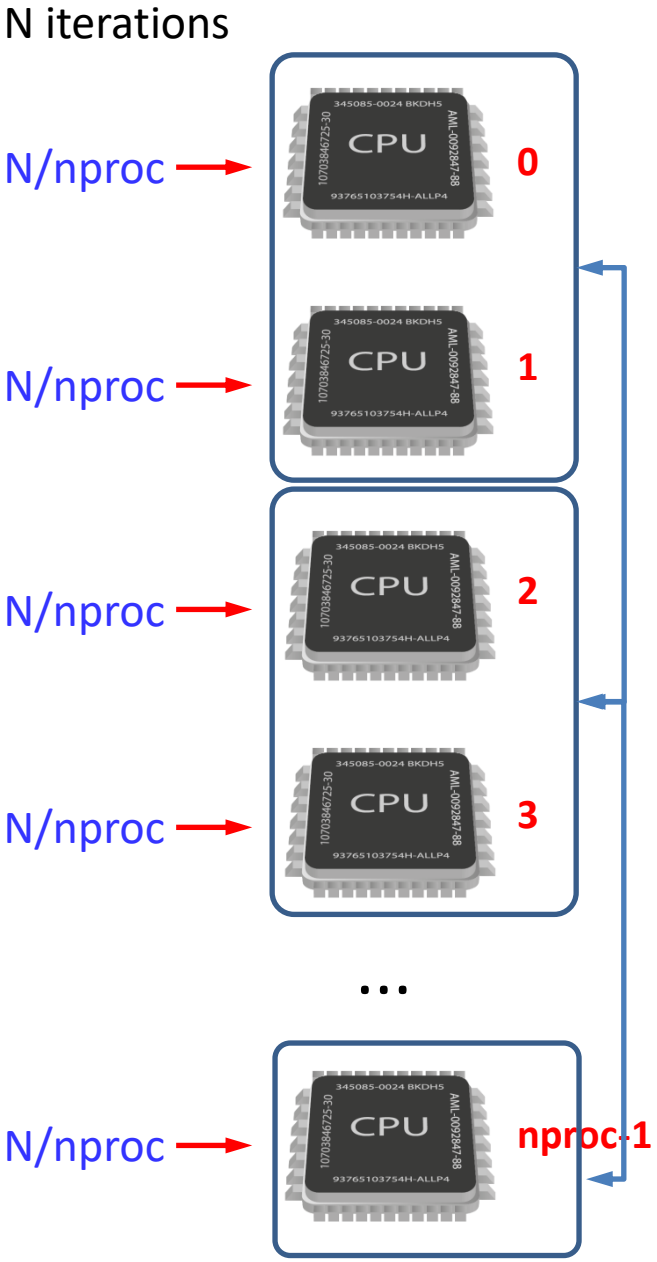
<variable declarations>

call MPI_INIT(ierr)
call MPI_COMM_RANK(MPI_COMM_WORLD,id,ierr)
call MPI_COMM_SIZE(MPI_COMM_WORLD,nproc,ierr)

ini=id*(N/nproc)+1
fin=(id+1)*(N/nproc)

do i=ini,fin
   <calculations>
enddo

call MPI_FINALIZE(ierr)
```



OPEN MPI


345085-0024 BKDH5
CPU
10703846725-30
AML-0092847-88
93765103754H-ALLP4

0


345085-0024 BKDH5
CPU
10703846725-30
AML-0092847-88
93765103754H-ALLP4

1


345085-0024 BKDH5
CPU
10703846725-30
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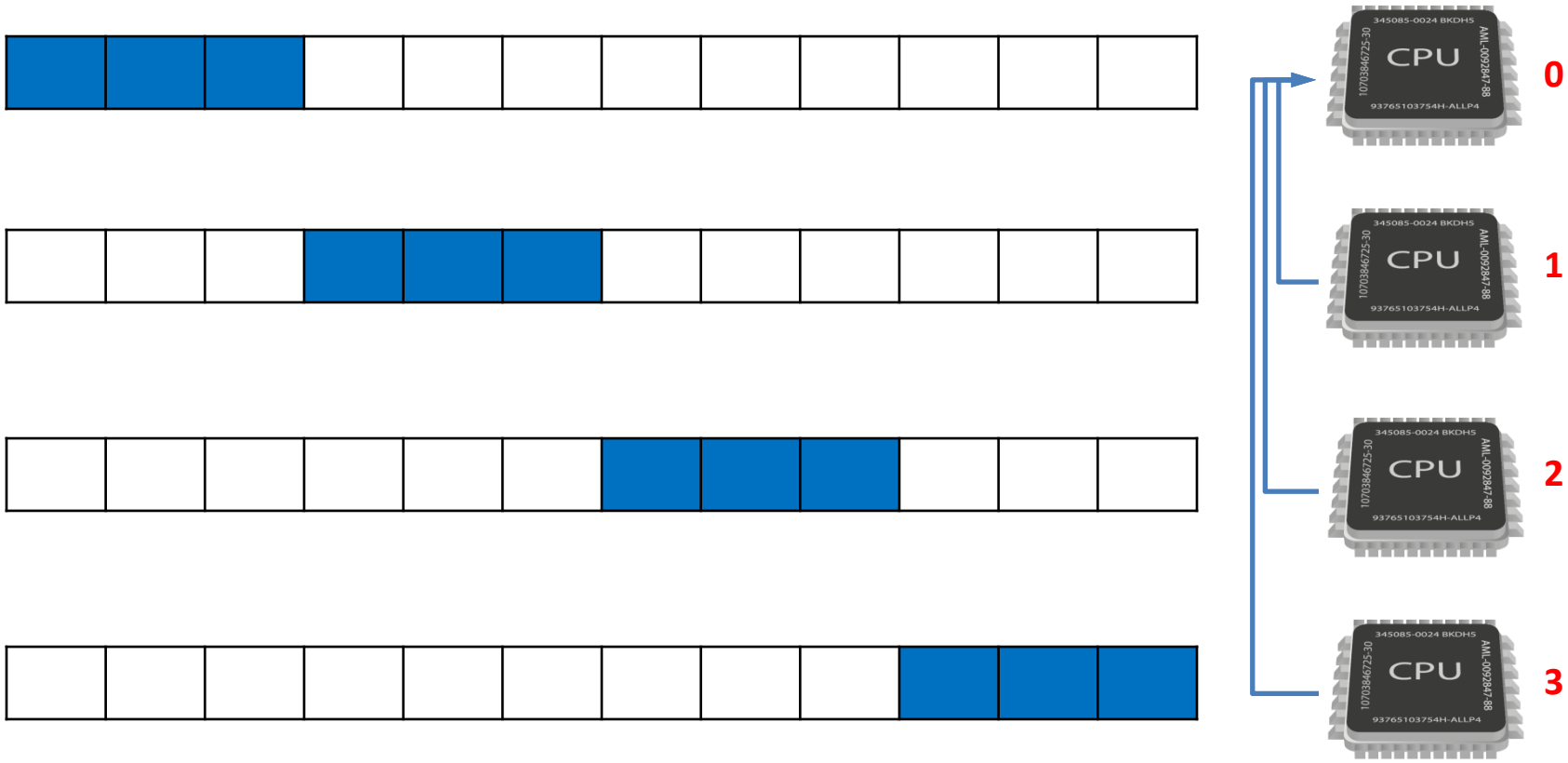
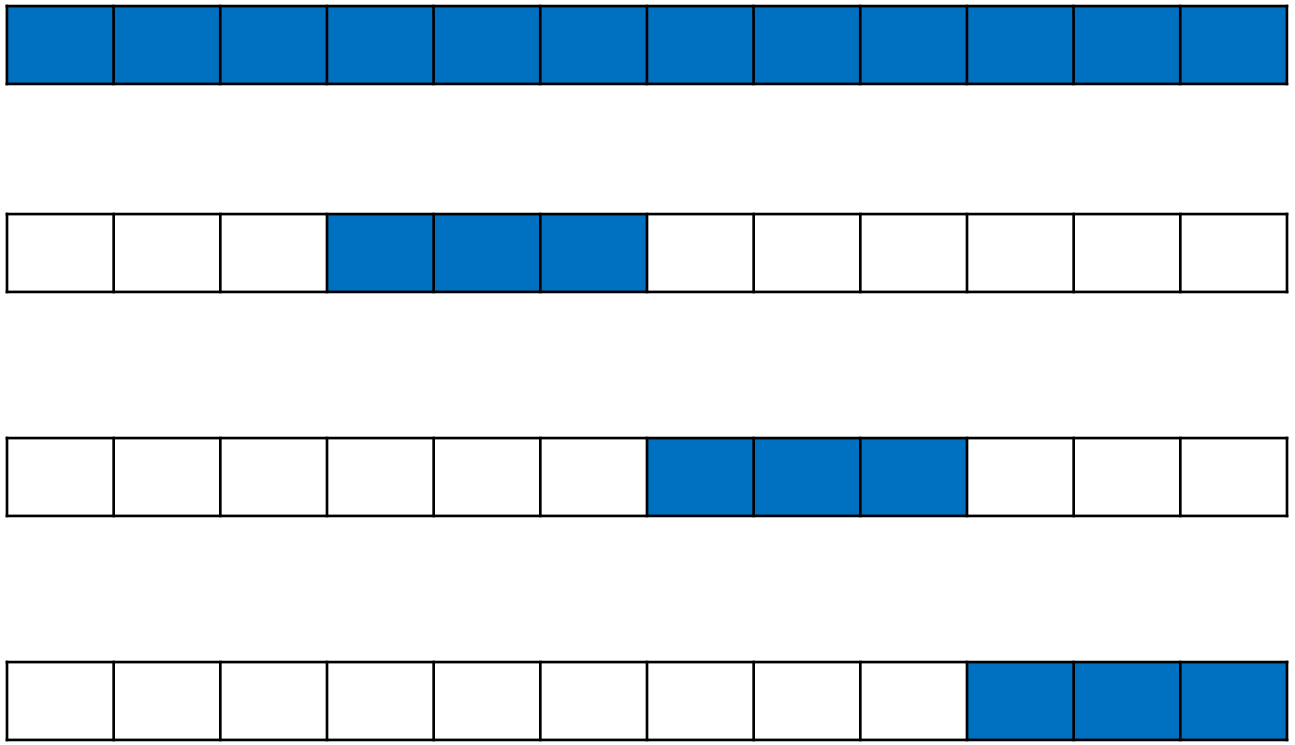
3


OPEN MPI



Open MPI

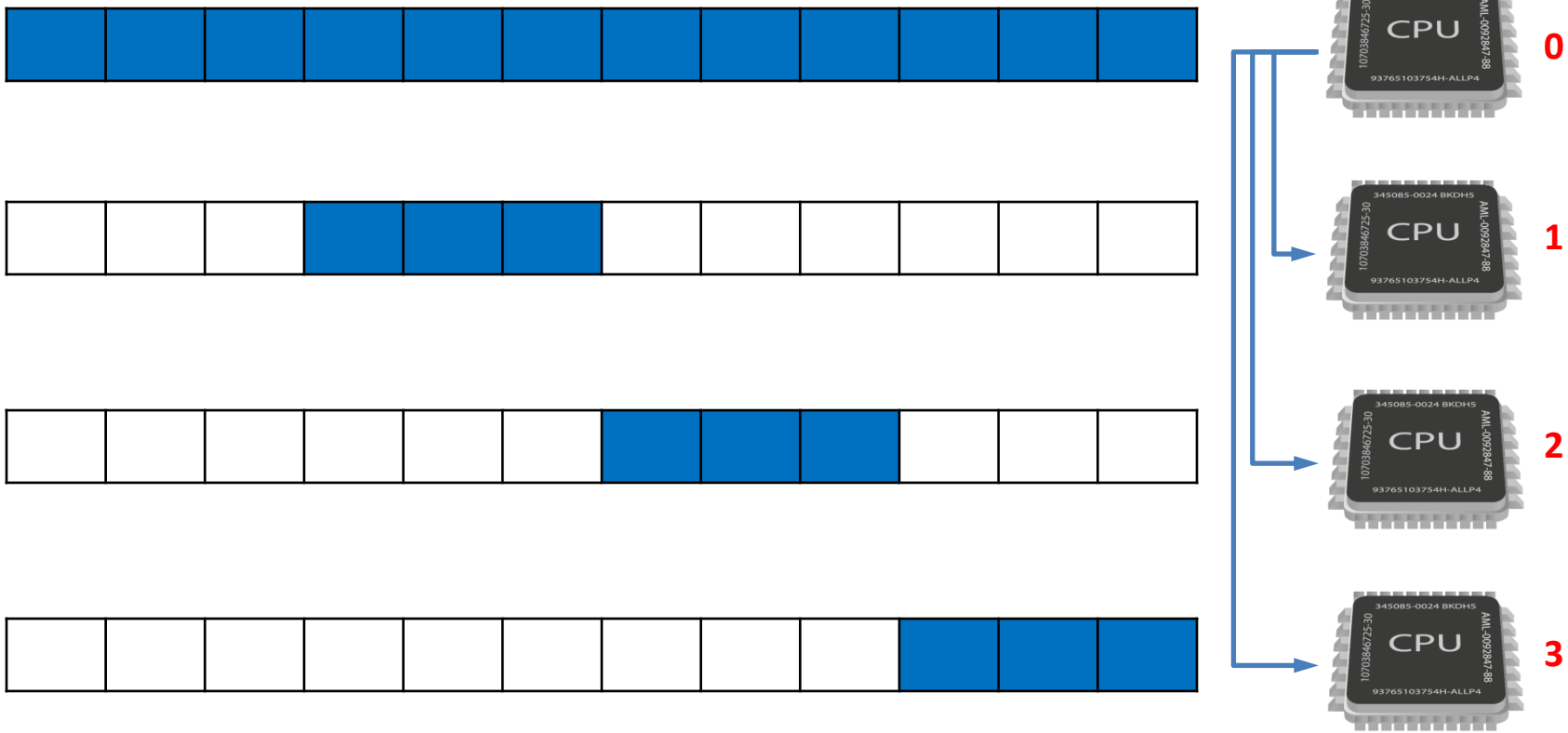
Only process 0 has the correct values!




```
call MPI_REDUCE(arr,result,arraysize,<type>,<operation>,<dest_id>,MPI_WORLD_COMM,ierr)
call MPI_REDUCE(arr,result,12,MPI_INT,MPI_SUM,0,MPI_WORLD_COMM,ierr)
```

Open MPI

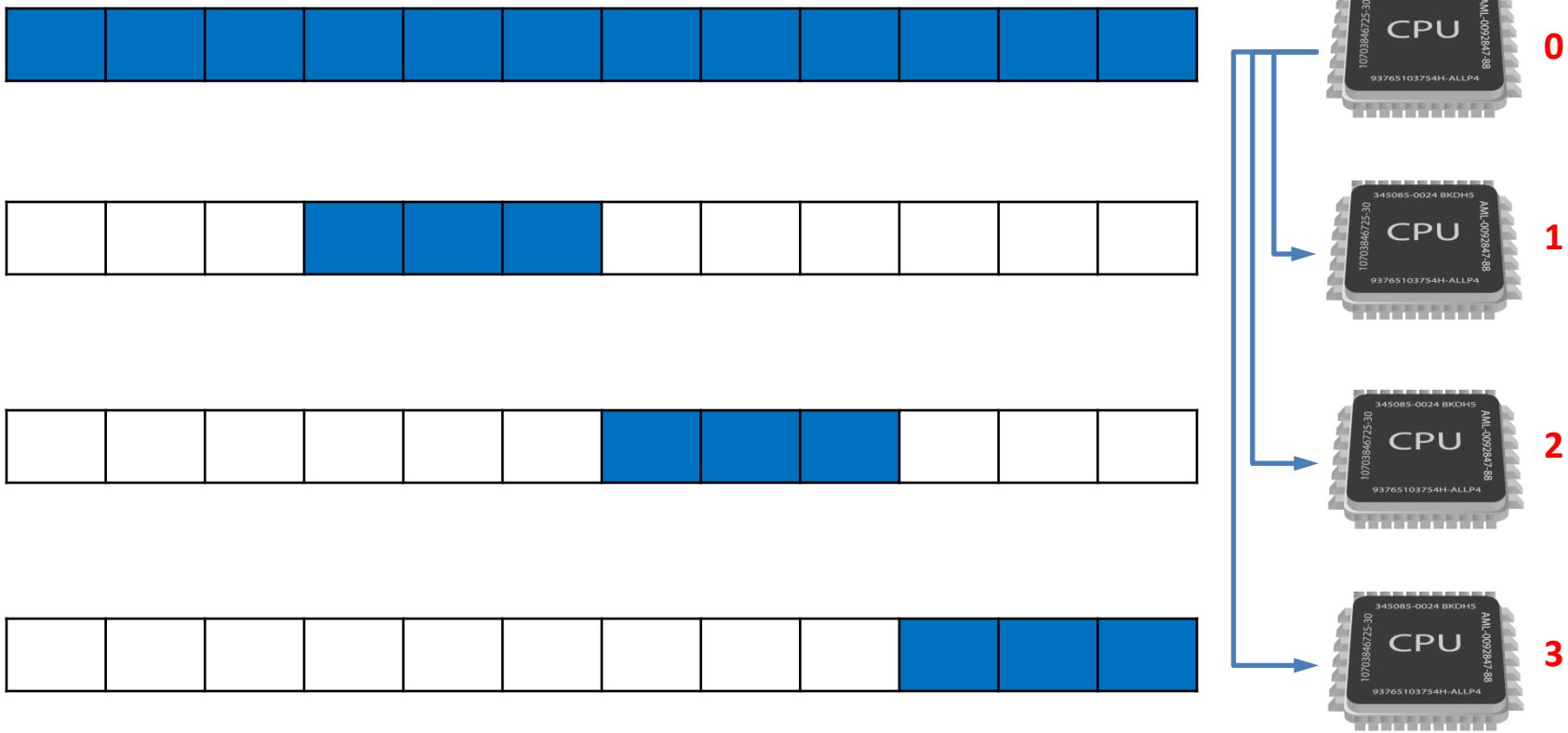
Only process 0 has the correct values!




```
call MPI_REDUCE(arr,result,arraysize,<type>,<operation>,<dest_id>,MPI_WORLD_COMM,ierr)
call MPI_REDUCE(arr,result,12,MPI_INT,MPI_SUM,0,MPI_WORLD_COMM,ierr)
```

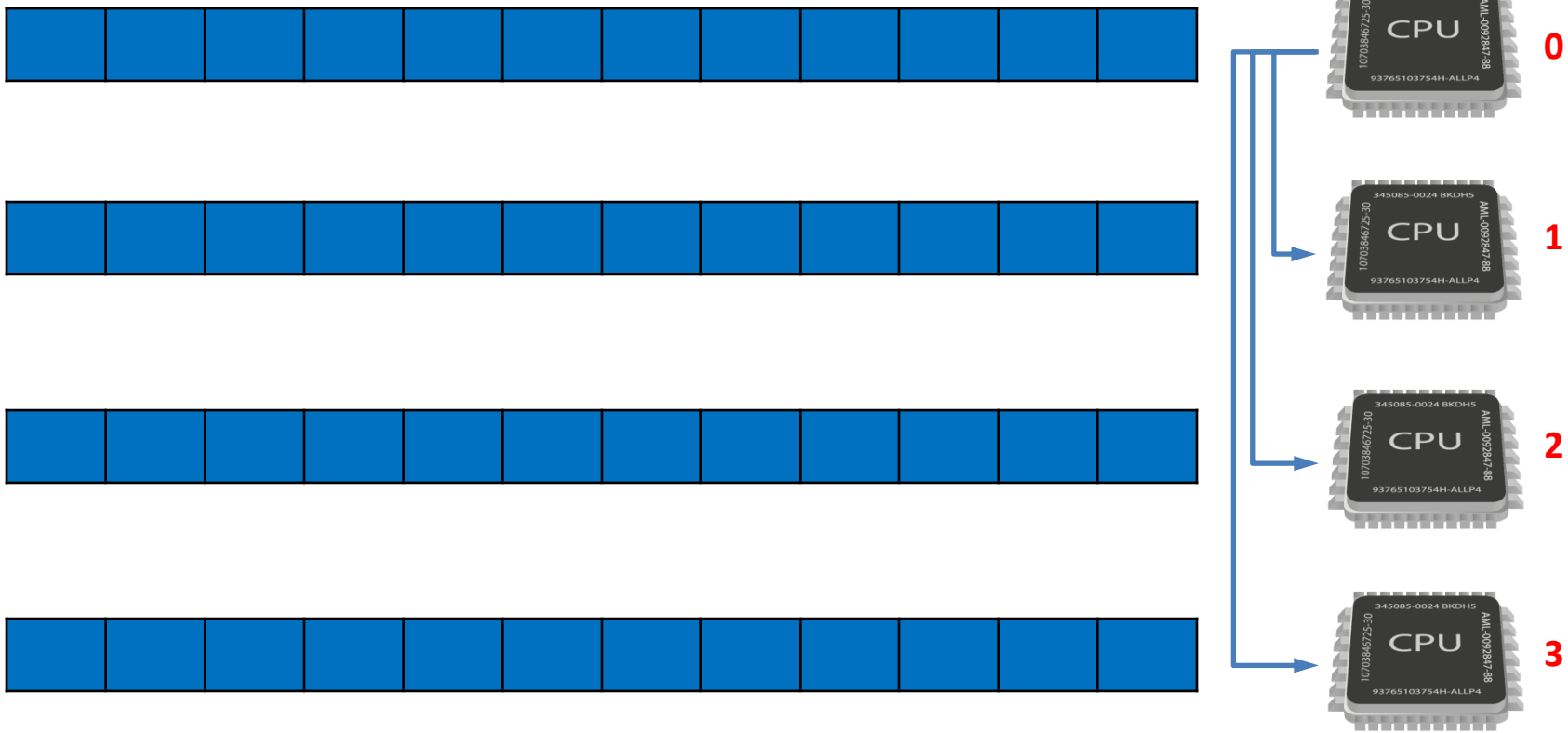
Open MPI

Only process 0 has the correct values!

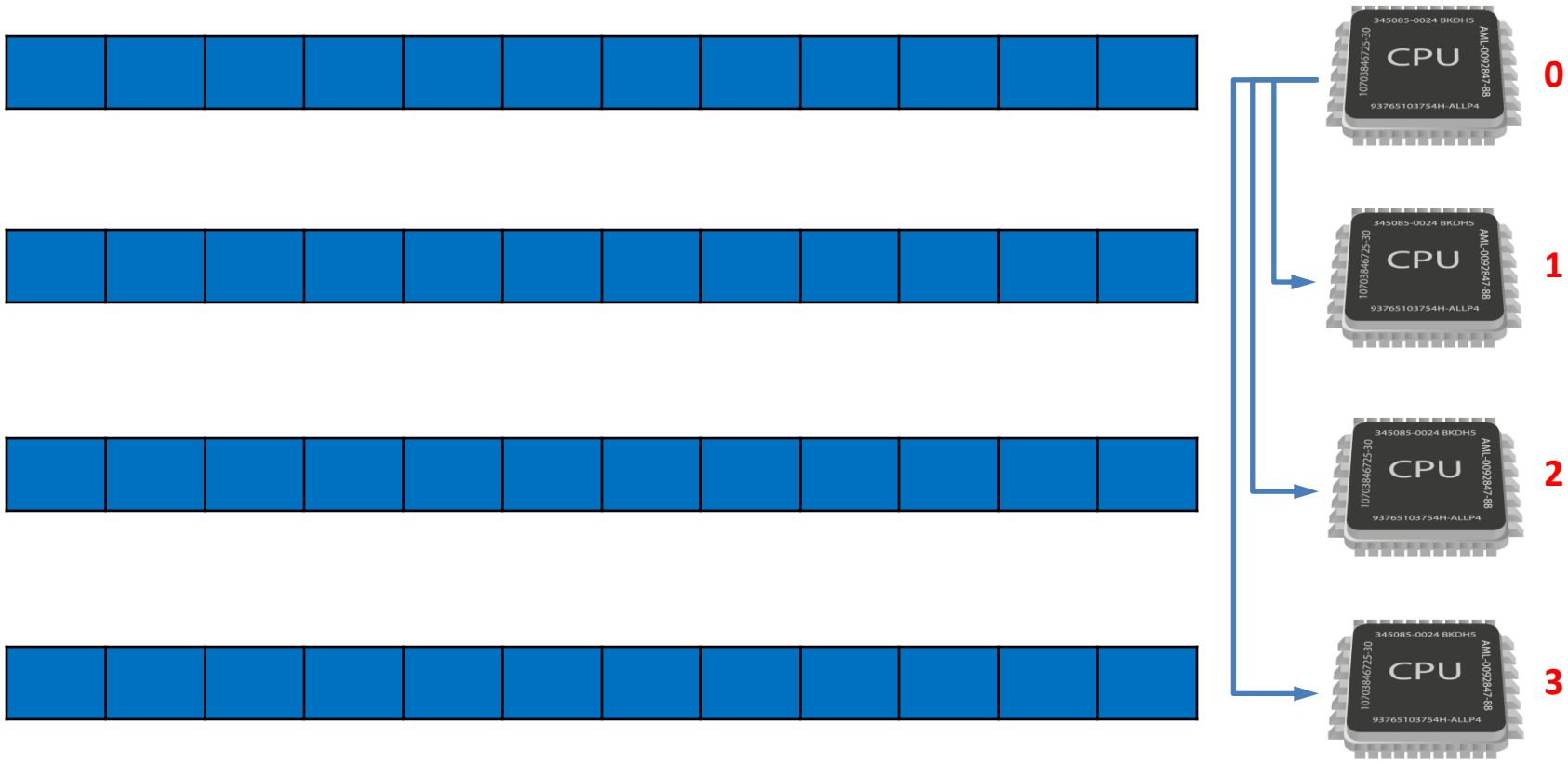



```
call MPI_REDUCE(arr,result,arraysize,<type>,<operation>,<dest_id>,MPI_WORLD_COMM,ierr)
call MPI_REDUCE(arr,result,12,MPI_INT,MPI_SUM,0,MPI_WORLD_COMM,ierr)
call MPI_BCAST(result,12,MPI_INT,0,MPI_WORLD,COMM,ierr)
```

Only process 0 has the correct values!




```
call MPI_REDUCE(arr,result,arraysize,<type>,<operation>,<dest_id>,MPI_WORLD_COMM,ierr)
call MPI_REDUCE(arr,result,12,MPI_INT,MPI_SUM,0,MPI_WORLD_COMM,ierr)
call MPI_BCAST(result,12,MPI_INT,0,MPI_WORLD,COMM,ierr)
```




```
call MPI_ALLREDUCE(arr,result,12,MPI_INT,MPI_SUM,MPI_WORLD_COMM,ierr)
```

Open MPI

Example: Numerical integration

```
include 'mpif.h'

call MPI_INIT(ierr); comm = MPI_COMM_WORLD
call MPI_COMM_RANK(comm, rank, ierr)
call MPI_COMM_SIZE(comm, size, ierr)
```

Initialize MPI

FORTRAN

Example: Numerical integration

```
include 'mpif.h'

call MPI_INIT(ierr); comm = MPI_COMM_WORLD
call MPI_COMM_RANK(comm, rank, ierr)
call MPI_COMM_SIZE(comm, size, ierr)

totalsteps = 1000000
steps = totalsteps/size

ini = rank * steps
fin = (rank+1) * steps

if(fin.ge.totalsteps) then
    fin = totalsteps
endif
```

Initialize MPI

Define the range

FORTRAN

Example: Numerical integration

```
include 'mpif.h'

call MPI_INIT(ierr); comm = MPI_COMM_WORLD
call MPI_COMM_RANK(comm, rank, ierr)
call MPI_COMM_SIZE(comm, size, ierr)

totalsteps = 1000000
steps = totalsteps/size

ini = rank * steps
fin = (rank+1) * steps

if(fin.ge.totalsteps) then
    fin = totalsteps
endif

dx = 1.d0 / totalsteps
x = -0.5d0 * dx

localSum = 0.d0
do i = ini, fin
    x = (i-0.5d0)*dx
    localSum = localSum + 4.d0 / (1.d0 + x*x)
enddo
localSum = localSum * dx
```

Initialize MPI

Define the range

FORTRAN

Do the computation

Example: Numerical integration

```
include 'mpif.h'

call MPI_INIT(ierr); comm = MPI_COMM_WORLD
call MPI_COMM_RANK(comm, rank, ierr)
call MPI_COMM_SIZE(comm, size, ierr)

totalsteps = 1000000
steps = totalsteps/size

ini = rank * steps
fin = (rank+1) * steps

if(fin.ge.totalsteps) then
    fin = totalsteps
endif

dx = 1.d0 / totalsteps
x = -0.5d0 * dx

localSum = 0.d0
do i = ini, fin
    x = (i-0.5d0)*dx
    localSum = localSum + 4.d0 / (1.d0 + x*x)
enddo
localSum = localSum * dx

call MPI_ALLREDUCE(localSum,globalSum,1,MPI_DOUBLE_PRECISION,MPI_SUM,comm,ierr)

write(*,*) localSum, globalSum
```

Initialize MPI

Define the range

FORTRAN

Do the computation

Sum the data across nodes

Example: Numerical integration

```
include 'mpif.h'

call MPI_INIT(ierr); comm = MPI_COMM_WORLD
call MPI_COMM_RANK(comm, rank, ierr)
call MPI_COMM_SIZE(comm, size, ierr)

totalsteps = 1000000
steps = totalsteps/size

ini = rank * steps
fin = (rank+1) * steps

if(fin.ge.totalsteps) then
    fin = totalsteps
endif

dx = 1.d0 / totalsteps
x = -0.5d0 * dx

localSum = 0.d0
do i = ini, fin
    x = (i-0.5d0)*dx
    localSum = localSum + 4.d0 / (1.d0 + x*x)
enddo
localSum = localSum * dx

call MPI_ALLREDUCE(localSum,globalSum,1,MPI_DOUBLE_PRECISION,MPI_SUM,comm,ierr)

write(*,*) localSum, globalSum

call MPI_FINALIZE(ierr)
```

Initialize MPI

Define the range

FORTRAN

Do the computation

Sum the data across nodes

Don’t forget to Finalize MPI

Example: Numerical integration

```
from mpi4py import MPI
import numpy

comm = MPI.COMM_WORLD
rank = comm.Get_rank()
size = comm.Get_size()

totalsteps = 1000000
steps = totalsteps/size

ini = rank * steps
fin = (rank+1) * steps

if fin > totalsteps:
      fin = totalsteps

dx = 1./totalsteps
x = -0.5*dx

localSum = 0.
for i in range(int(ini), int(fin)):
      x = (i-0.5)*dx
      localSum = localSum + 4./(1. + x*x)

localSum = localSum * dx

globalSum = comm.allreduce(localSum, op=MPI.SUM)

print(localSum, globalSum)
```

Initialize MPI

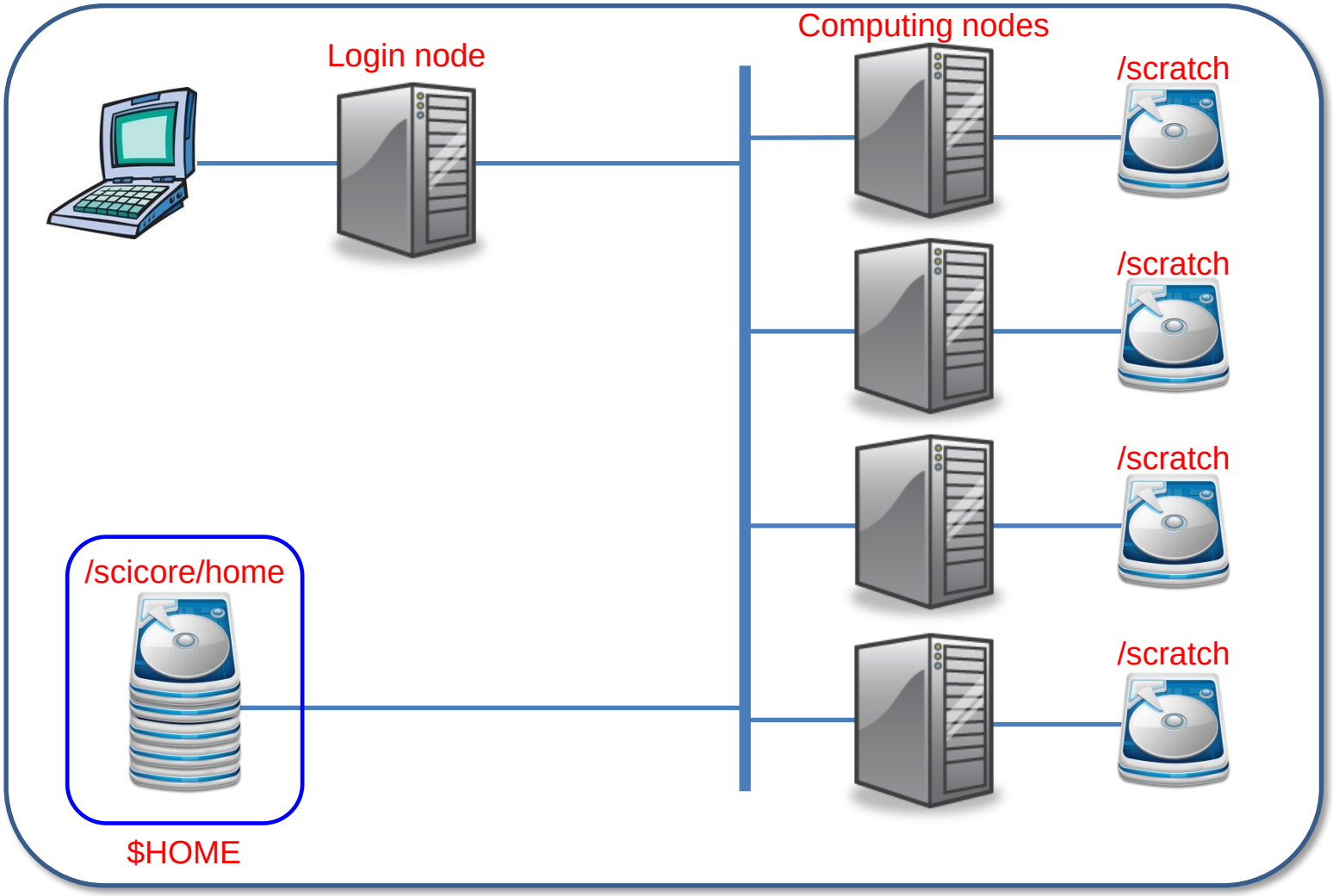
Define the range

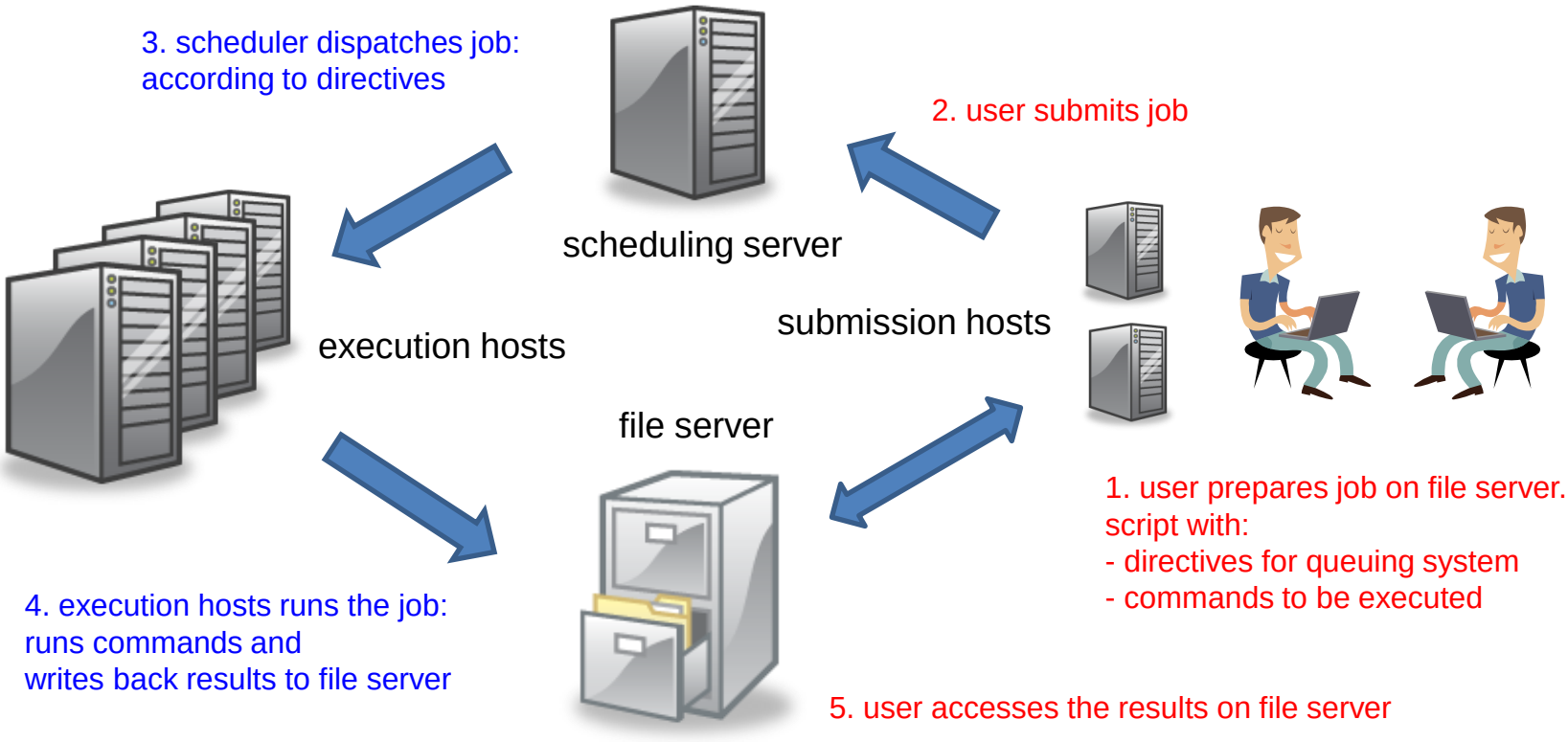
Python

Do the computation

Sum the data across nodes

Mpi4py tutorial at: https://mpi4py.readthedocs.io/en/stable/tutorial.html


Computing nodes
Login node
/scratch
/scratch
/scratch
/scratch
/scicore/home
$HOME



User takes care

Cluster takes care

Lest’s play “Spot the Differences”

Lest's play "Spot the Differences"

Which script launches an OpenMP job and which one an MPI?

```
#!/bin/bash

#SBATCH --job-name=myJob
#SBATCH --cpus-per-task=8
#SBATCH --mem=3.5G
#SBATCH --time=05:00:00
#SBATCH --qos=6hour
#SBATCH --output=/path/to/stdout/folder
#SBATCH --error=/path/to/stderr/folder
#SBATCH --mail-type=END,FAIL,TIME_LIMIT
#SBATCH --mail-user=mailaddress@unibas.ch

# Tell OpenMP how many threads to use
##########################
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

# load your required modules
########################
module load <module name>
…

# and here goes your command line
./my_openmp_program

# Some third party programs include a threading
# option, configuration or environment variable
```

```
#!/bin/bash

#SBATCH --job-name=myJob
#SBATCH --ntasks=8
#SBATCH --mem=3.5G
#SBATCH --time=05:00:00
#SBATCH --qos=6hour
#SBATCH --output=/path/to/stdout/folder
#SBATCH --error=/path/to/stderr/folder
#SBATCH --mail-type=END,FAIL,TIME_LIMIT
#SBATCH --mail-user=mailaddress@unibas.ch

# Tell OpenMP how many threads to use
##########################
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

# load your required modules
########################
module load <module name>
…

# and here goes your command line
srun ./my_openmp_program

# Some third party programs include a threading
# option, configuration or environment variable
```

How do I launch an hybrid job?

```
#!/bin/bash

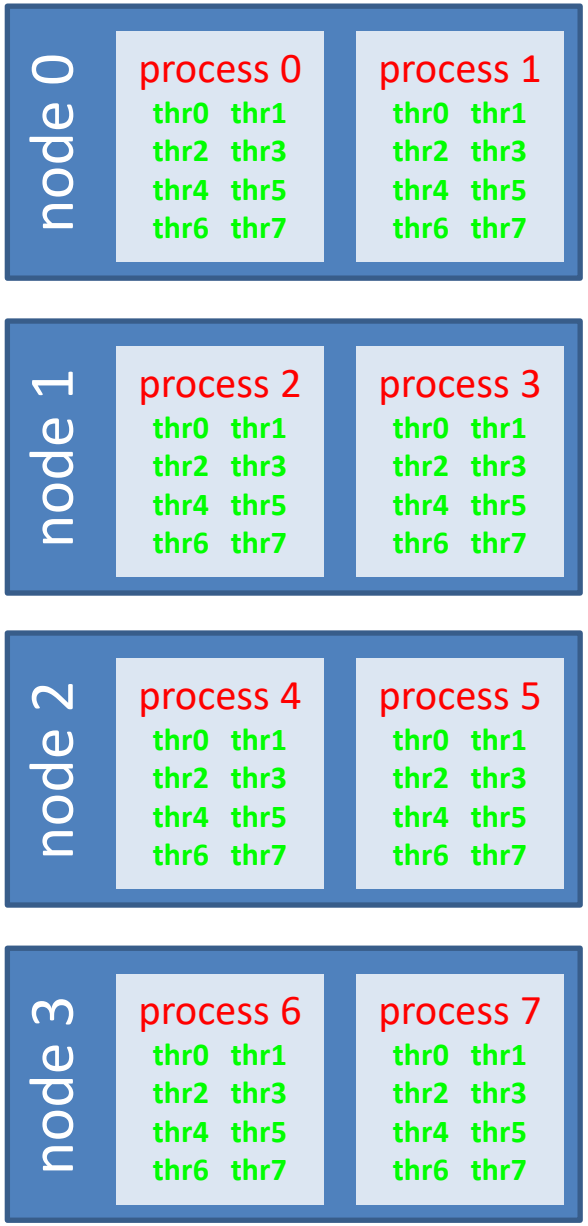
#SBATCH --job-name=myJob
#SBATCH --ntasks=?
#SBATCH --tasks-per-node=?
#SBATCH --cpus-per-task=?
#SBATCH --mem=3.5G
#SBATCH --time=05:00:00
#SBATCH --qos=6hour
#SBATCH --output=/path/to/stdout/folder
#SBATCH --error=/path/to/stderr/folder
#SBATCH --mail-type=END,FAIL,TIME_LIMIT
#SBATCH --mail-user=mailaddress@unibas.ch

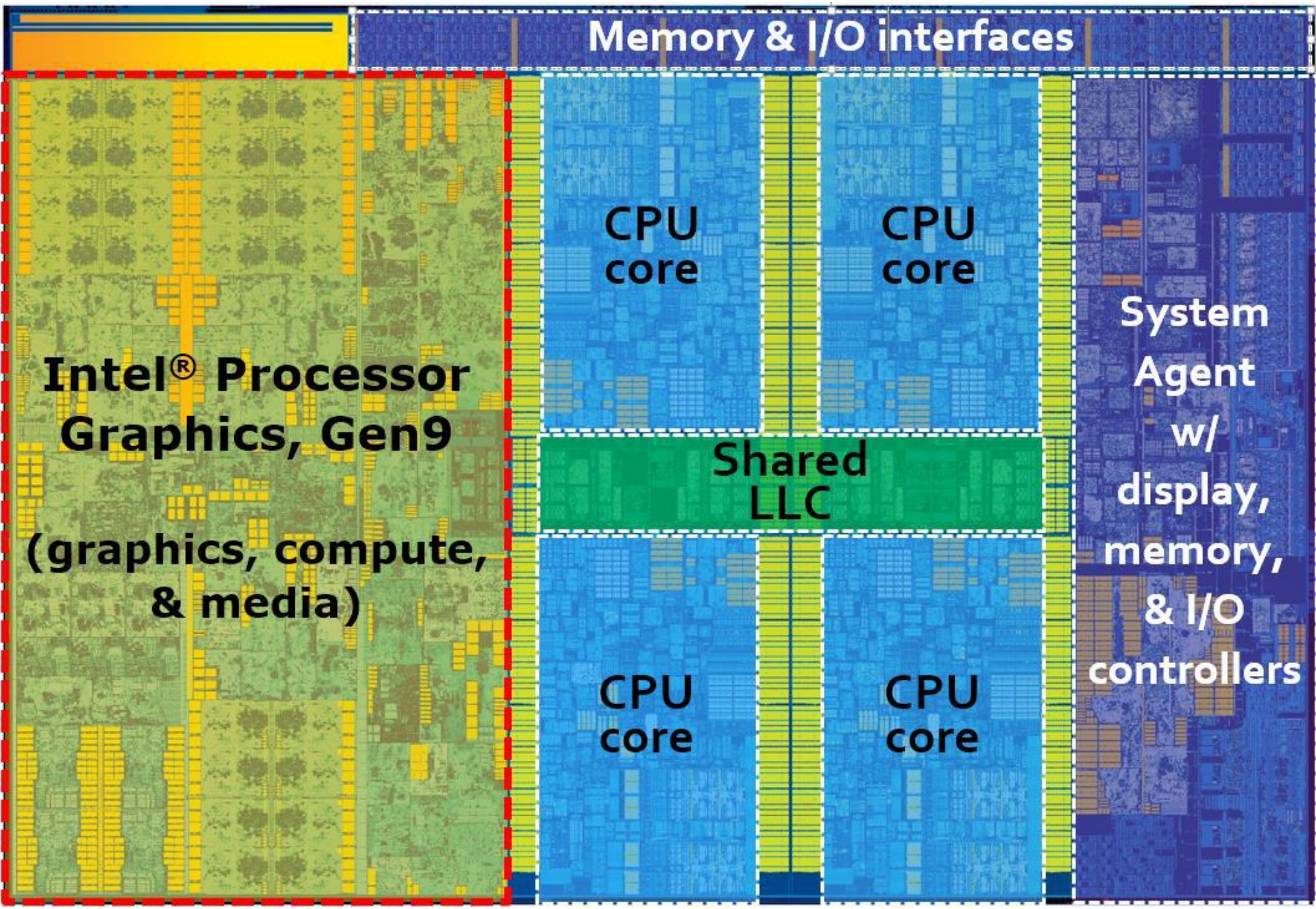
# Tell OpenMP how many threads to use
##########################
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

# load your required modules
########################
module load <module name>
…

# and here goes your command line
srun my_openmp_program

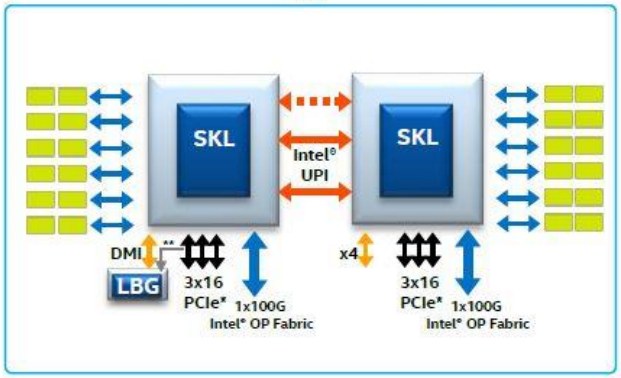
# Some third party programs include a threading
# option, configuration or environment variable
```




Memory & I/O interfaces
Intel® Processor Graphics, Gen9
(graphics, compute, & media)
CPU core
CPU core
Shared LLC
CPU core
CPU core
System Agent w/ display, memory, & I/O controllers

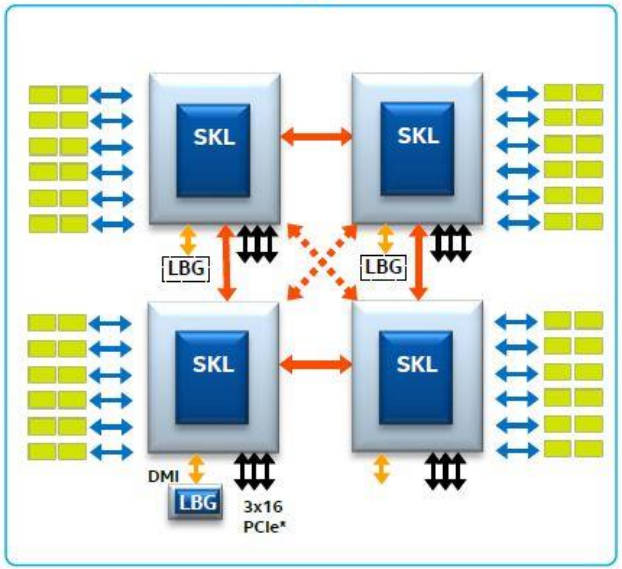
Platform Topologies

2S Configurations



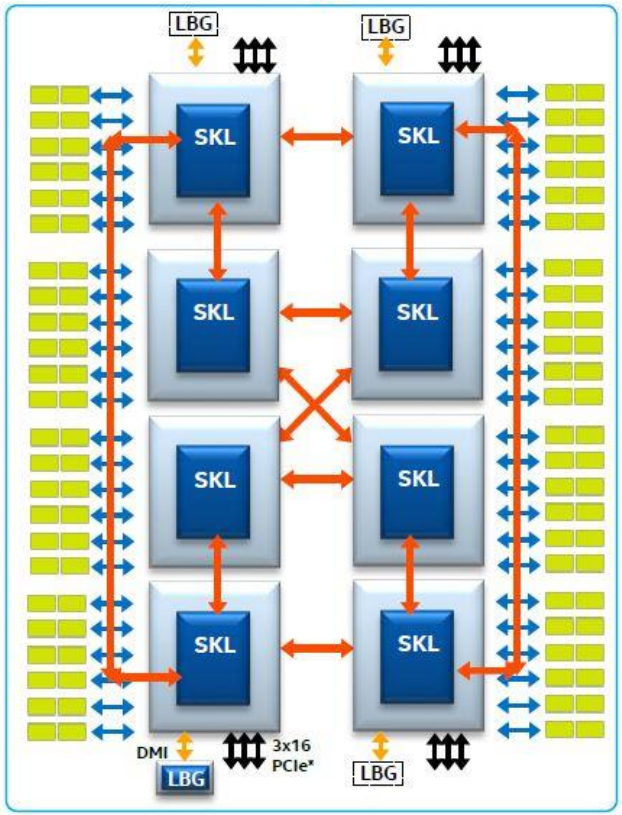
(2S-2UPI & 2S-3UPI shown)

4S Configurations



(4S-2UPI & 4S-3UPI shown)

8S Configuration



INTEL® XEON® SCALABLE PROCESSOR SUPPORTS CONFIGURATIONS RANGING FROM 2S-2UPI TO 8S

When using parallel programs you must be more aware of the hardware topology!

numactl --hardware

```
[cabezon@login10 ~]$ numactl --hardware
available: 2 nodes (0-1)
node 0 cpus: 0 1 2 3 4 5 6 7
node 0 size: 32742 MB
node 0 free: 188 MB
node 1 cpus: 8 9 10 11 12 13 14 15
node 1 size: 32768 MB
node 1 free: 10518 MB
node distances:
node   0   1
  0:  10  11
  1:  11  10
```

← Relative distances

lscpu

```
[cabezon@login10 ~]$ lscpu
Architecture:          x86_64
CPU op-mode(s):        32-bit, 64-bit
Byte Order:            Little Endian
CPU(s):                16
On-line CPU(s) list:   0-15
Thread(s) per core:    1
Core(s) per socket:    8
Socket(s):             2
NUMA node(s):          2
Vendor ID:             GenuineIntel
CPU family:            6
Model:                 45
Model name:            Intel(R) Xeon(R) CPU E5-2670 0 @ 2.60GHz
Stepping:              7
CPU MHz:               1298.578
BogoMIPS:              5205.23
Virtualization:        VT-x
L1d cache:             32K
L1i cache:             32K
L2 cache:              256K
L3 cache:              20480K
NUMA node0 CPU(s):     0-7
NUMA node1 CPU(s):     8-15
```

Two sockets!

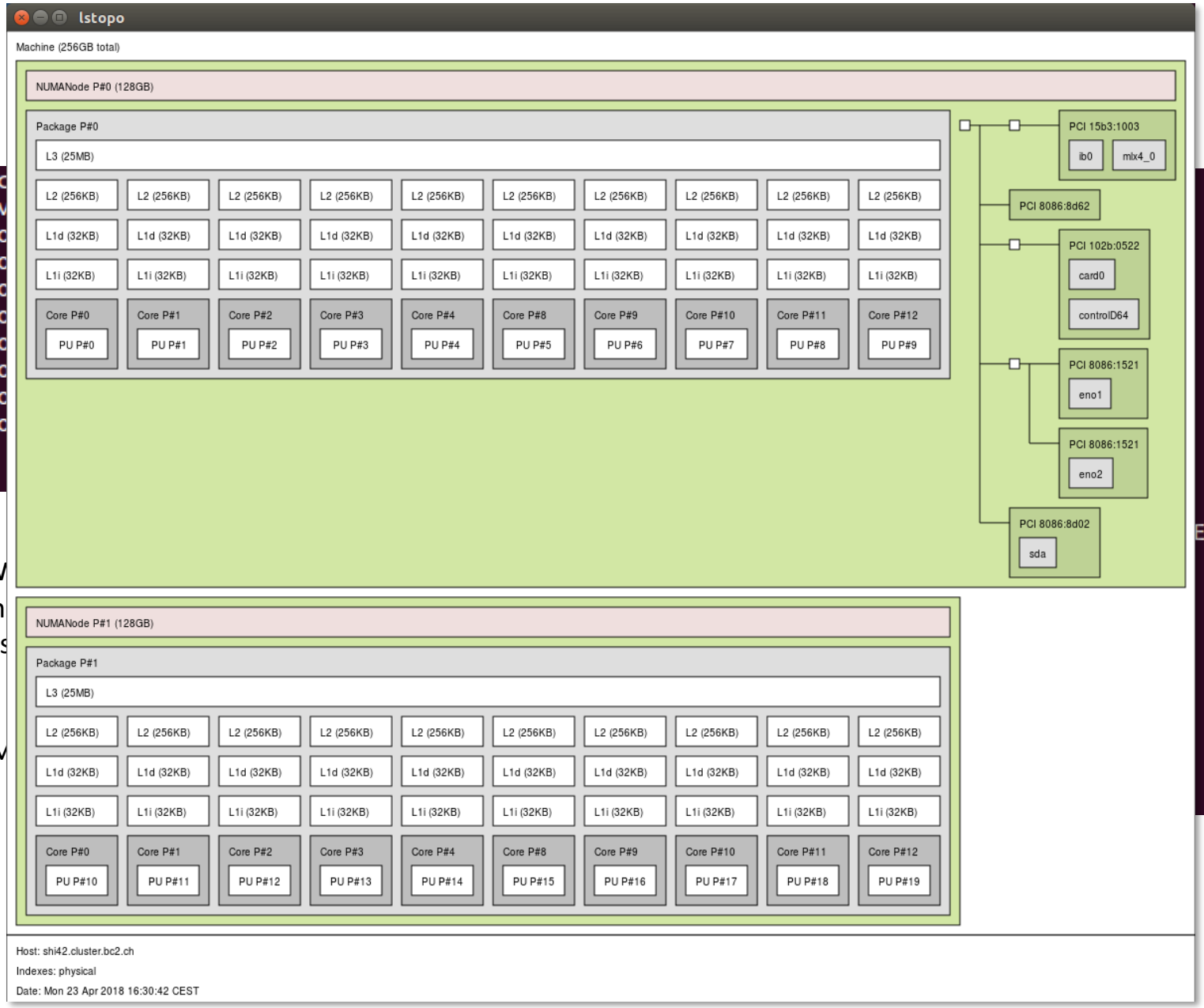
This is a NUMA (non-uniform memory access) system.

vs.

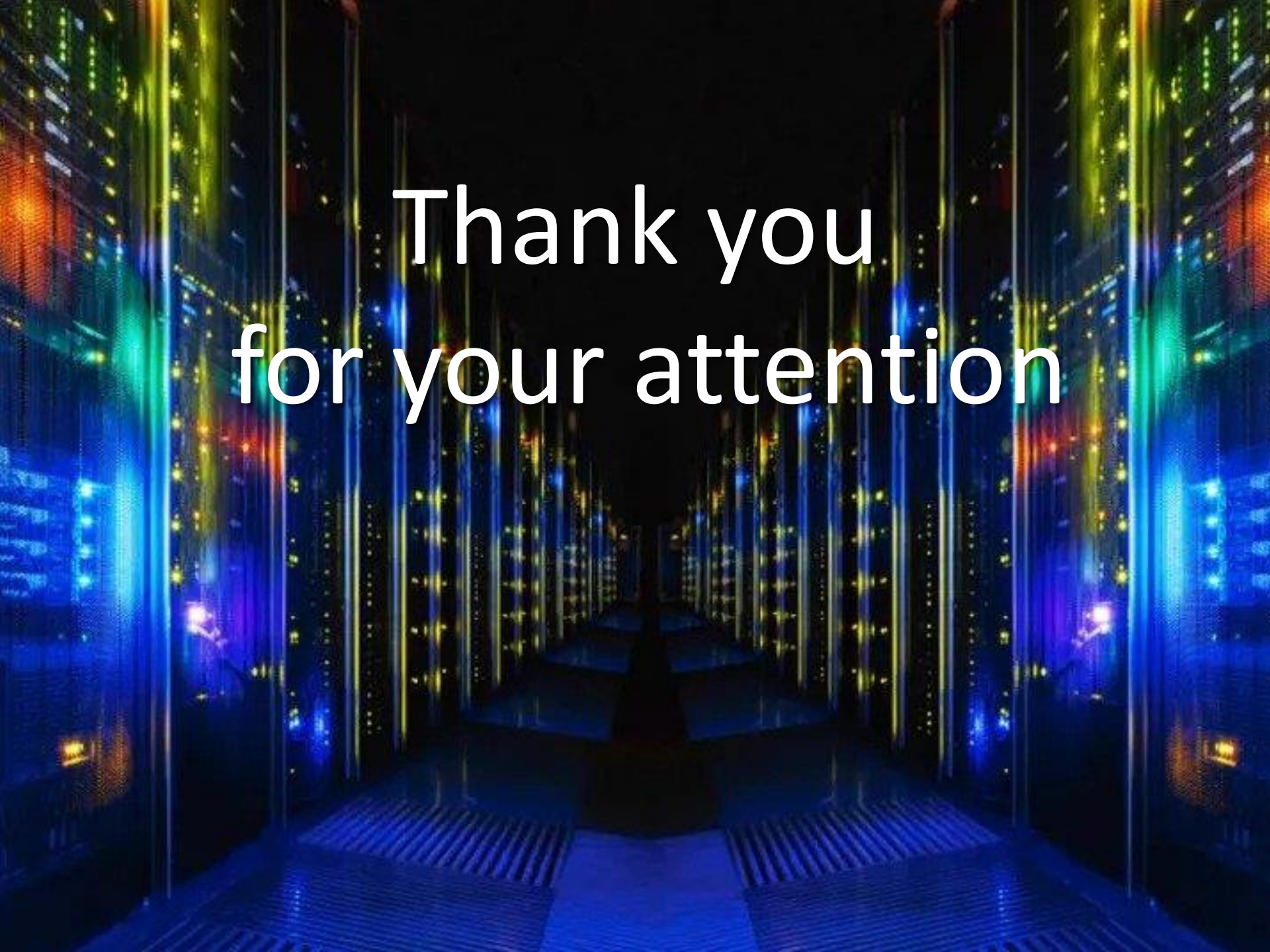
SMP (symmetric multi-processor):

```
ruben@jarvis:~$ numactl --hardware
available: 1 nodes (0)
node 0 cpus: 0 1 2 3 4 5 6 7
node 0 size: 7885 MB
node 0 free: 252 MB
node distances:
node   0
  0:  10
```

lstopo
(from hwloc package)



E5-2670 0 @ 2.60GHz


Thank you
for your attention


Resume at:
13:30


Coffee
break