Parallel Programming 101

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What is High-Performance Computing (HPC)?

- Not a real definition, depends from the prospective:
  - HPC is when I care how fast I get an answer
  - HPC is when I foresee my problem to get bigger and bigger

Not just exploiting resources, u even need to know what u need

- Thus HPC can happen on:
  - A workstation, desktop, laptop, smartphone!
  - A supercomputer
  - A Linux Cluster
  - A grid or a cloud
  - Cyberinfrastructure = any combination of the above

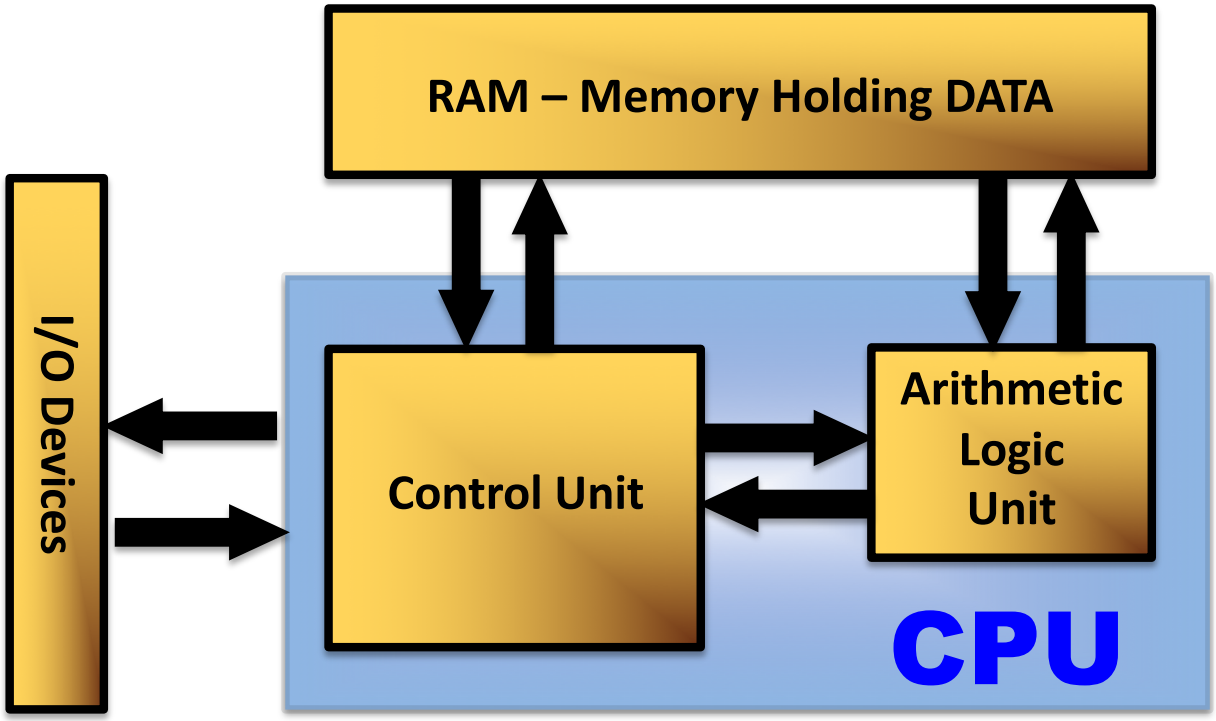
Cluster: made of multiple computers made by commodity hardwareSupercor

- HPC means also High-Productivity Computing

The Classical Model

John Von Neumann

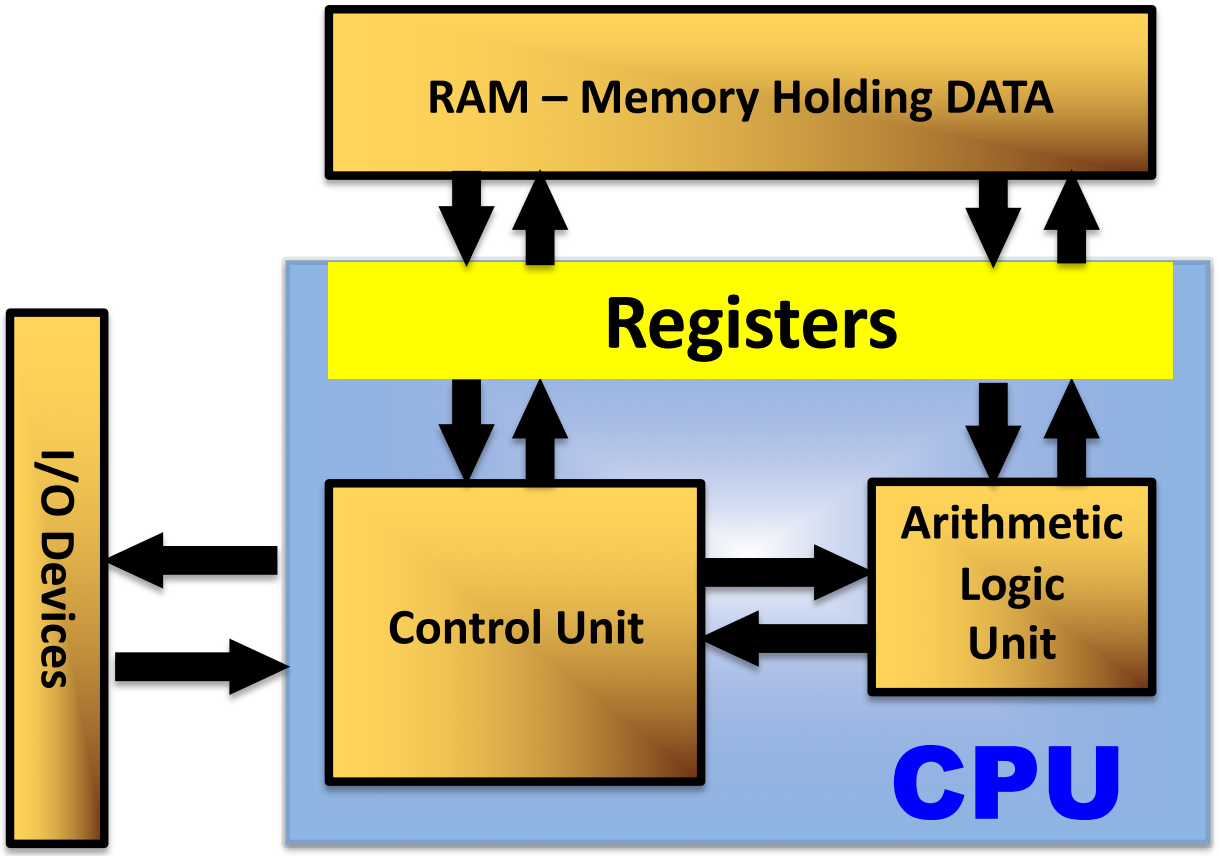
Program stored in disk, when executed move from disk to RAM along with data.Cod



The Classical Model

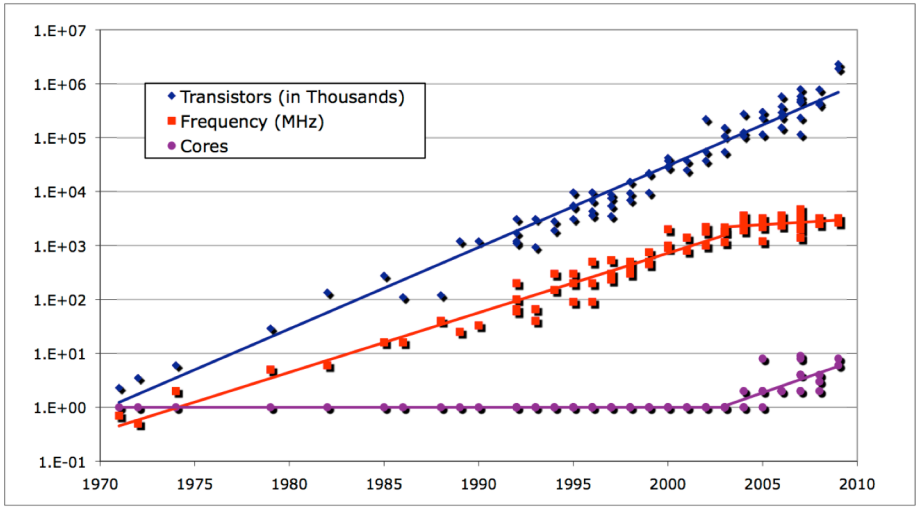
John Von Neumann

Actually the ALU can only work on data on registers:A+=1 provoke LOAD, ADD and STO



Evolution of Computers (in a nutshell)

- Higher capability is achieved by increasing computer complexity

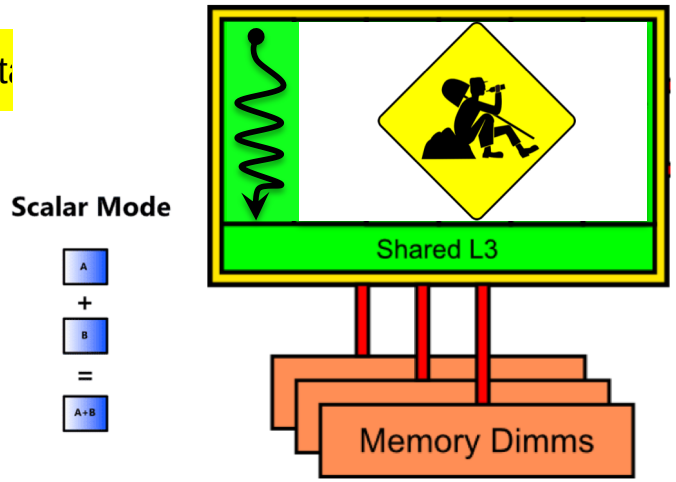


at some point (2004ish) no more adva

- CPU power is measured in number of floating point operations x second (FLOPs)
  - FLOPS = #cores x clock freq. x (FLOP/cycle)

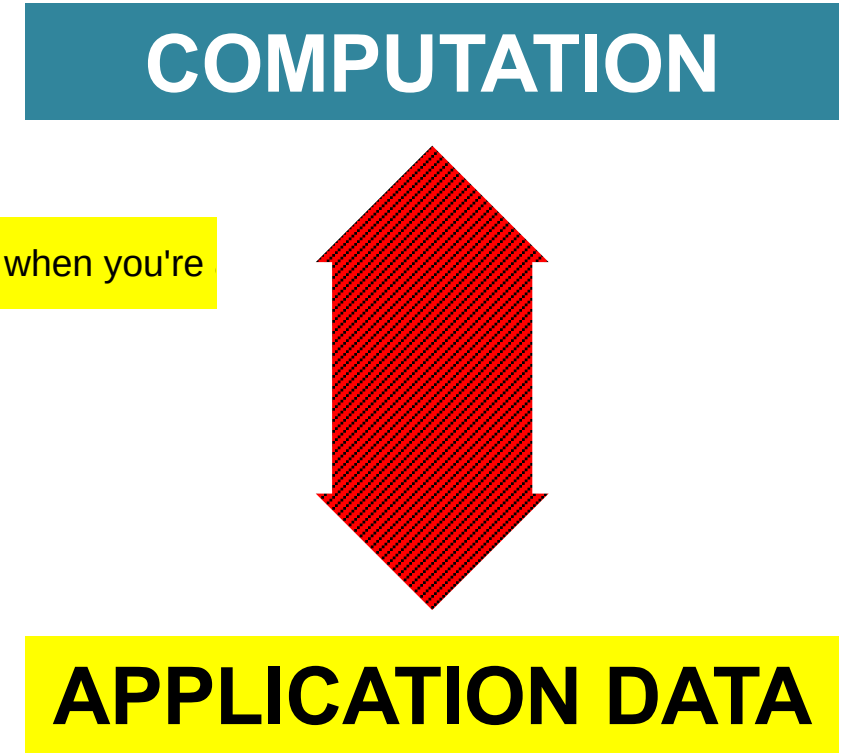
we even have vector units ->SIMD: Single instructions Multiple Data

#cores	Vector Length	Freq. (GHz)	GFLOPs
1	1	1.0	1
1	16	1.0	16
10	1	1.0	10
10	16	1.0	160

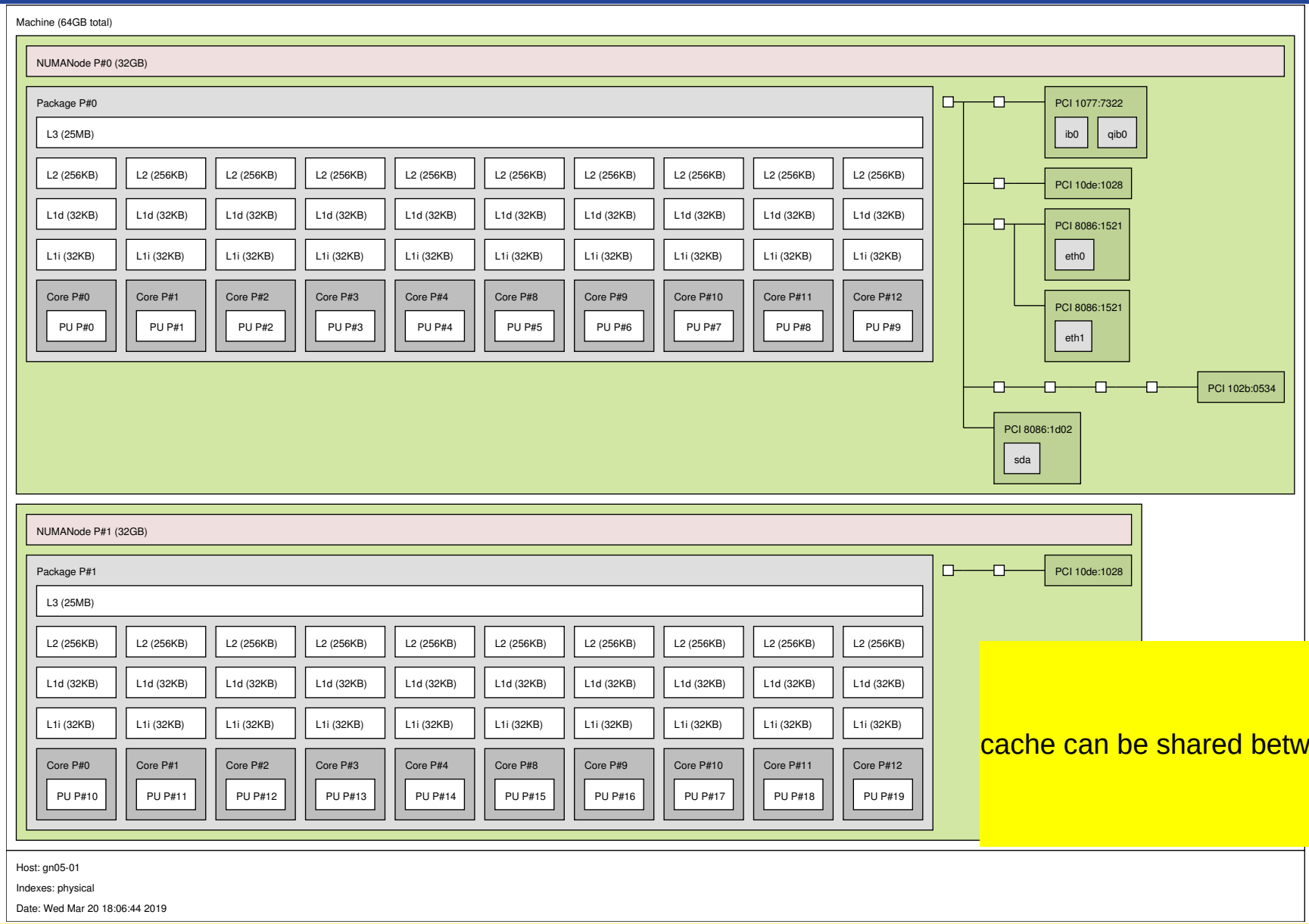


Key Aspect towards Real Performances

- When all CPU component work at maximum speed that is called *peak of performance*
  - Tech-spec normally describe the theoretical peak
  - Benchmarks measure the real peak
  - Applications show the real performance value 6-7-8% of Theoretical peak when you're
- CPU performance is measured FLOP/s
- But the real performance is in many cases mostly related to the memory bandwidth (Bytes/s)
- The way data are stored in memory is a key-aspect for high performance



Intel(R) Xeon(R) CPU E5-2680 v2 @ 2.80GHz

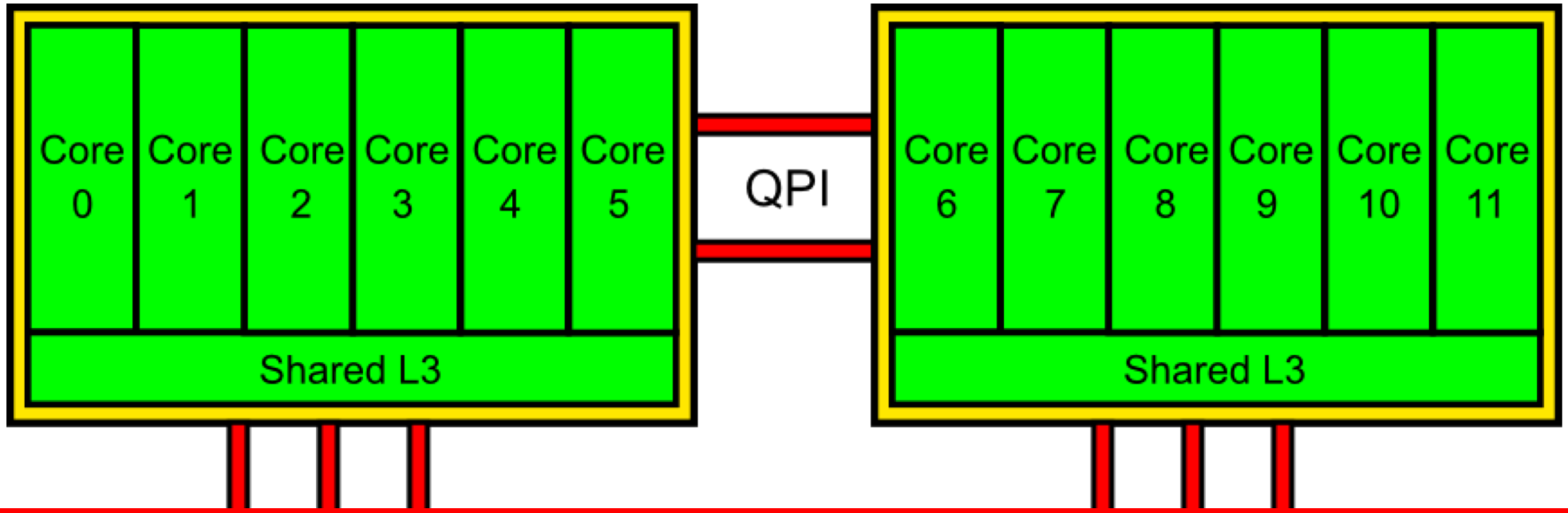


cache can be shared between cores a

Picture obtained on Ulysses compute node using the following commands:

```
$ module load hwloc/1.11.0
$ lstopo --output-format pdf output.pdf
```

Real World NUMA Nodes

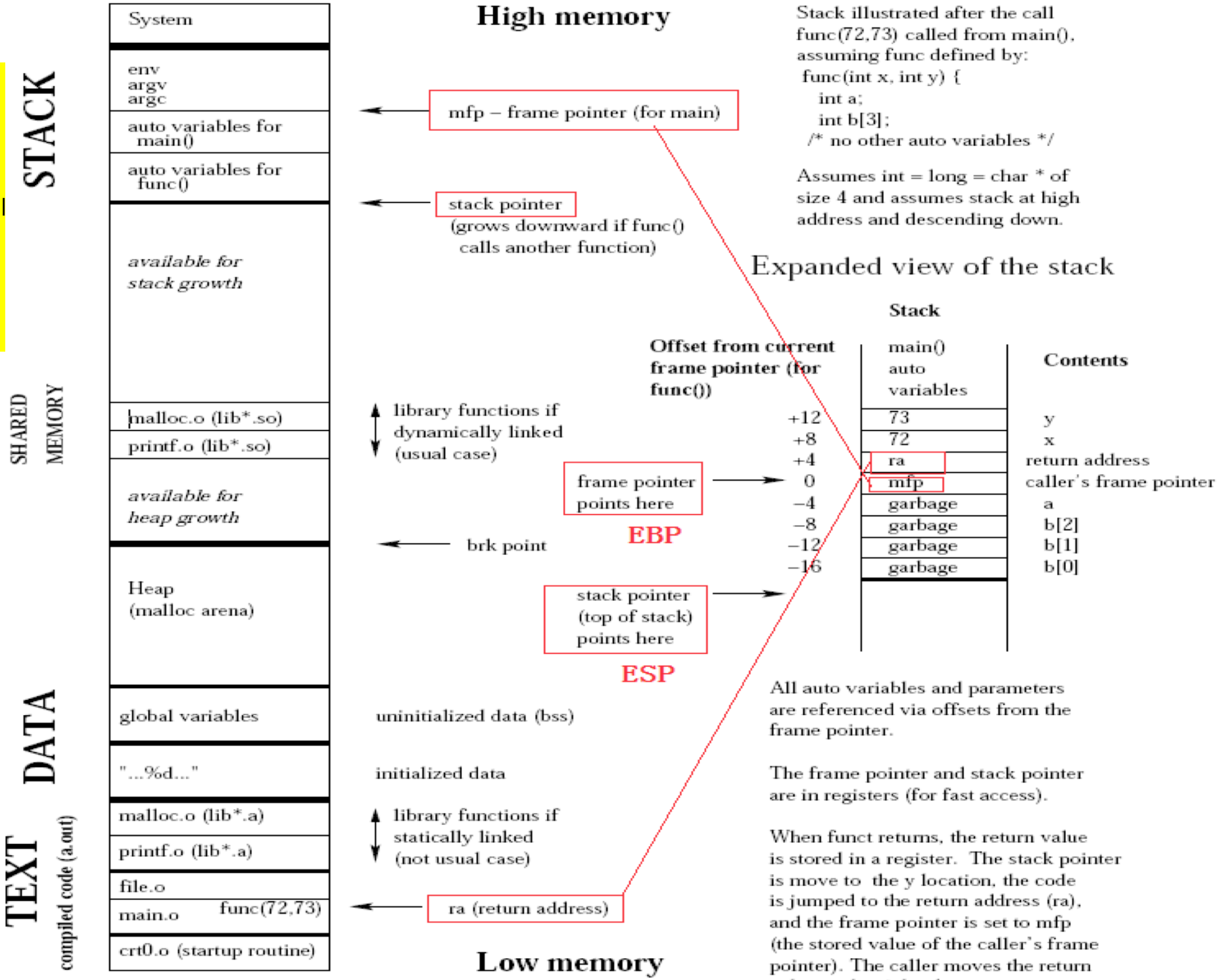


Main Memory

Dual Socket - 64GB RAM

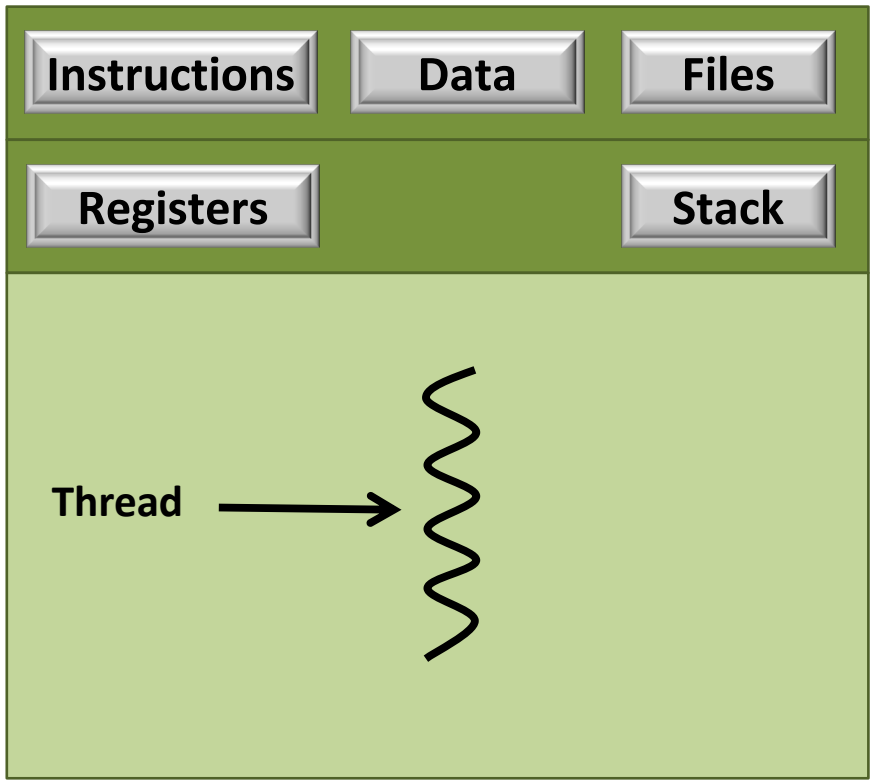
```
[igirotto@gn05-01 ~]$ free -g -o
             total       used       free     shared    buffers     cached
Mem:            62          1         61          0          0          0
Swap:            0          0          0
```

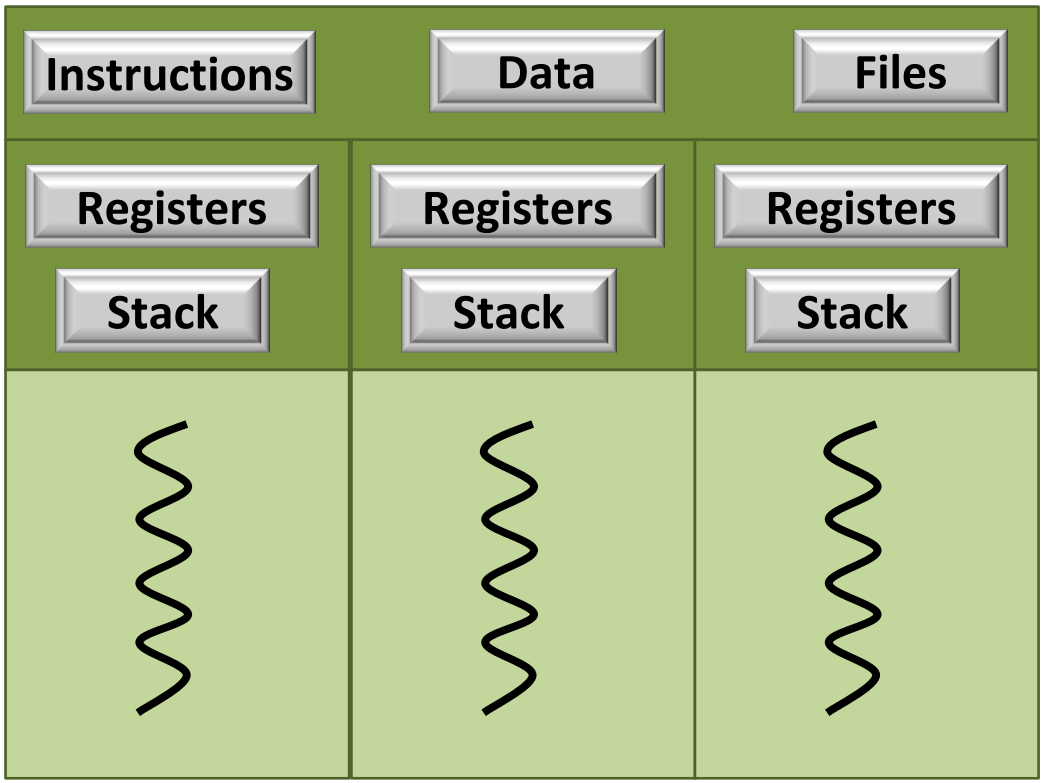
Stack vs H


STACK
SHARED MEMORY
DATA
TEXT
compiled code (a.out)
System
env
argv
argc
auto variables for main()
auto variables for func()
available for stack growth
malloc.o (lib*.so)
printf.o (lib*.so)
available for heap growth
Heap
(malloc arena)
global variables
"...%d..."
malloc.o (lib*.a)
printf.o (lib*.a)
file.o
main.o
func(72,73)
crt0.o (startup routine)
High memory
Low memory
mfp – frame pointer (for main)
stack pointer
(grows downward if func() calls another function)
library functions if dynamically linked (usual case)
frame pointer points here
EBP
brk point
stack pointer (top of stack) points here
ESP
uninitialized data (bss)
initialized data
library functions if statically linked (not usual case)
ra (return address)
Stack illustrated after the call func(72,73) called from main(), assuming func defined by:
func(int x, int y) {
int a;
int b[3];
/* no other auto variables */
Assumes int = long = char * of size 4 and assumes stack at high address and descending down.
Expanded view of the stack
Stack
Offset from current frame pointer (for func())
main() auto variables
Contents
+12
+8
+4
0
−4
−8
−12
−16
73
72
ra
mfp
garbage
garbage
garbage
garbage
y
x
return address
caller's frame pointer
a
b[2]
b[1]
b[0]
All auto variables and parameters are referenced via offsets from the frame pointer.
The frame pointer and stack pointer are in registers (for fast access).
When funct returns, the return value is stored in a register. The stack pointer is move to the y location, the code is jumped to the return address (ra), and the frame pointer is set to mfp (the stored value of the caller's frame pointer). The caller moves the return value to the right place.

Processes and Threads

Threads vs processesThreads: processing element part of a process. It execute the computation and in order to do that.





Multi-threading - Recap

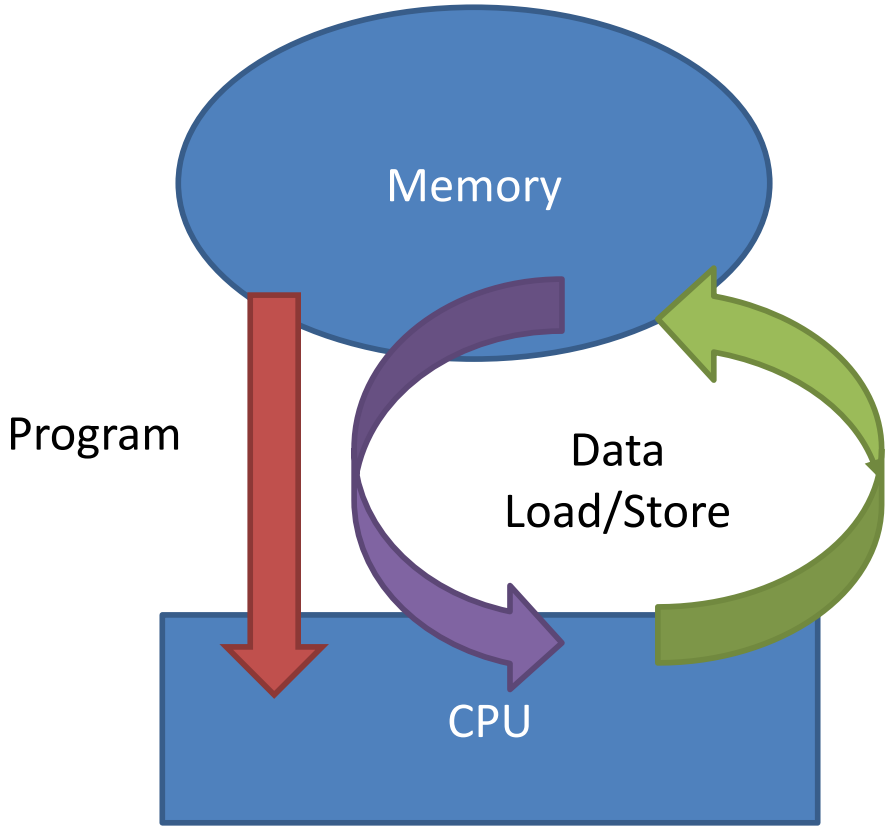
- A thread is a (lightweight) process - an instance of a program plus its own data (private memory)

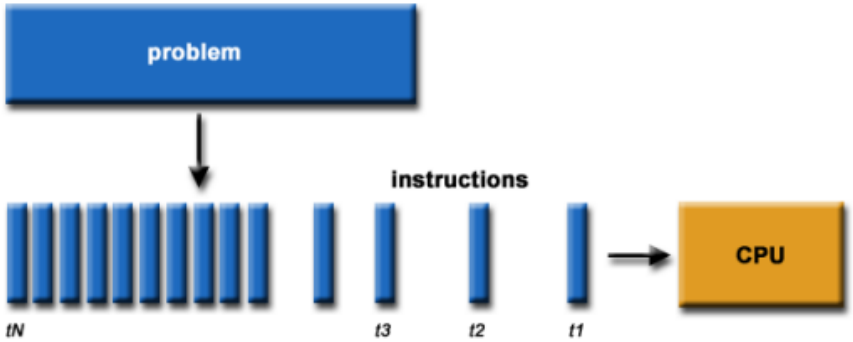
no other thread can access another thread private memory, but they can share data through heap.Sharin

- Each thread can follow its own flow of control through a program
- Threads can share data with other threads, but also have private data
- Threads communicate with each other via the shared data.
- A *master thread* is responsible for co-ordinating the threads group

Serial Programming

- A problem is broken into a discrete series of instructions
- Instructions are executed one after another
- Only one instruction may execute at any moment in time

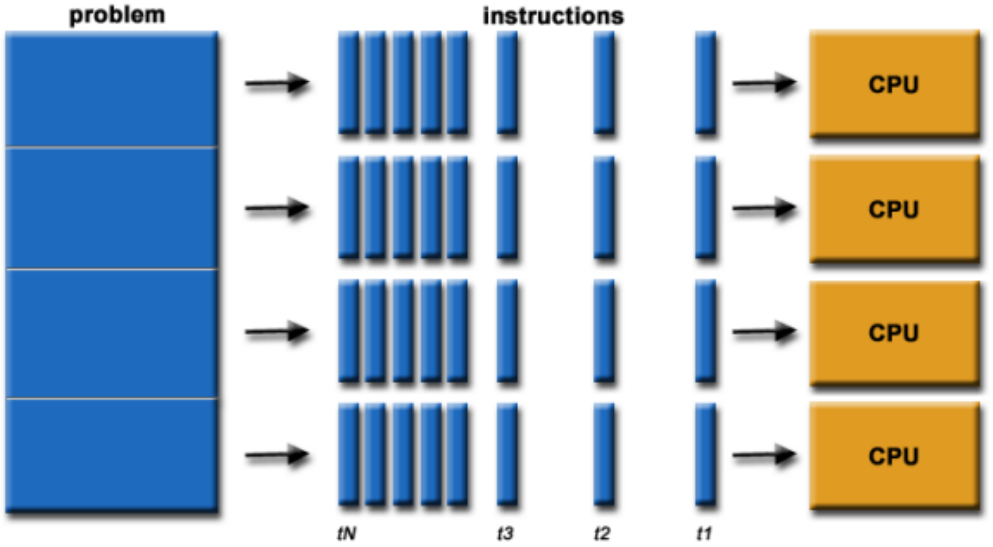




Parallel Programming

The first step in developing a parallel algorithm is to decompose the problem into tasks that can be executed concurrently

First: u have to identify all of the parts of the code that can be executed indipendently->PARALLELIZATION. This is decomposing



- A problem is broken into discrete parts that can be solved concurrently
- Each part is further broken down to a series of instructions
- Instructions from each part execute simultaneously on different processors
- An overall control / coordination mechanism is employed

Fundamental Steps of Parallel Design

- Identify portions of the work that can be performed concurrently
- Mapping the concurrent pieces of work onto multiple processes running in parallel
- Distributing the input, output and intermediate data associated within the program
- Managing accesses to data shared by multiple processors AVOID OVERHEAD: newtime=SerialTime/Numb_ofthreac

overhead time makes graph N_pel vs time a parabula: after a certain number, overhead stops the decrease(p_el=processing element)

- Synchronizing the processors at various stages of the parallel program execution

Granularity

- Granularity is determined by the decomposition level (number of task) on which we want divide the problem
- The degree to which task/data can be subdivided is limit to concurrency and parallel execution
- Parallelization has to become “topology aware”
  - coarse grain and fine grained parallelization has to be mapped to the topology to reduce memory and I/O contention
  - make your code modularized to enhance different levels of granularity and consequently to become more “platform adaptable”

coarse grain: small number of processing element-> less pieces and big chunksFine grain: huge number of p_elem so u divide

Type of Parallelism

u can have different problems to be parallelized or u can have the same problem/task to

- **Functional (or task) parallelism**: different people are performing different task at the same time

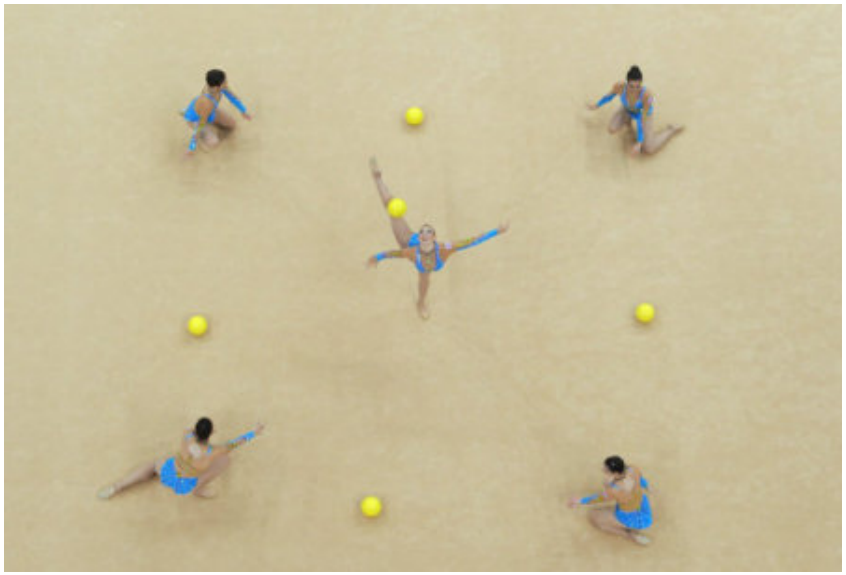
- **Data Parallelism**: different people are performing the same task, but on different equivalent and independent objects

most used in SC is Data Parallelism: u have a domain of data to process, and u try to divide the pro

Tasks Interactions

- The effective speed-up obtained by the parallelization depend by the amount of overhead we introduce making the algorithm parallel
- There are mainly two key sources of overhead:
  1. Time spent in inter-process interactions (**communication**)
  2. Time some process may spent being idle (**synchronization**)

     waiting someone else to do something (synchronization)



Load Balancing

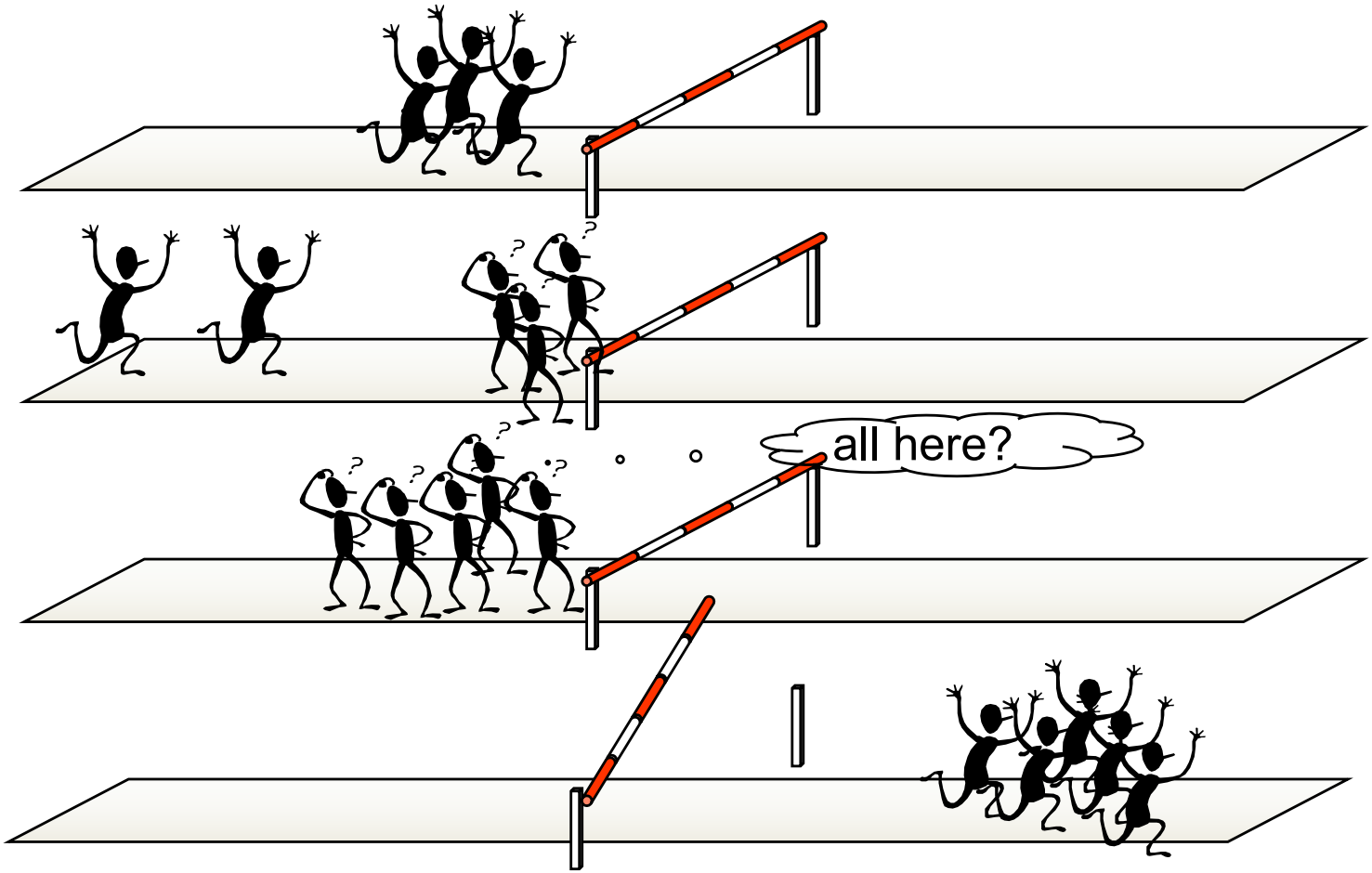
- Equally divide the work among the available resource: processors, memory, network bandwidth, I/O, ...

I'll always be bounded by the slowest processing element: so LOAD BALANCING

- This is usually a simple task for the problem decomposition model
- It is a difficult task for the functional decomposition model

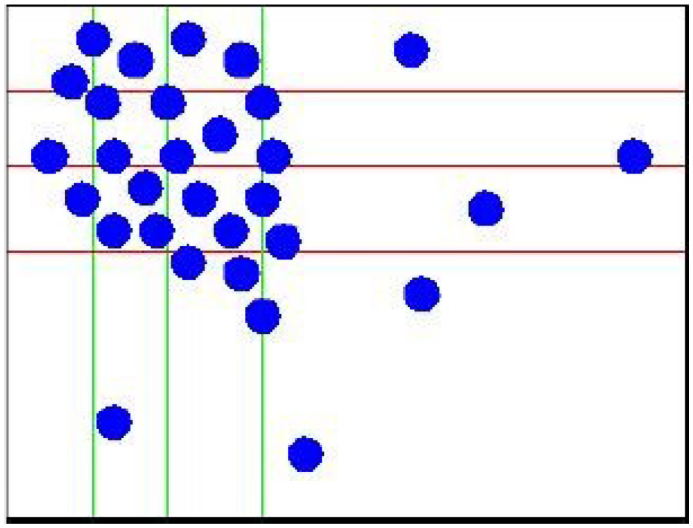
problem decomposition model: p_el are doing all the same thing, so it's easy usually to divide workloadFunctional decom

Effect of Load Unbalancing



Limitations of Parallel Computing

- Fraction of serial code limits parallel speedup
- Degree to which tasks/data can be subdivided is limit to concurrency and parallel execution
- Load imbalance:
  - parallel tasks have a different amount of work
  - CPUs are partially idle
  - redistributing work helps but has limitations
  - communication and synchronization overhead

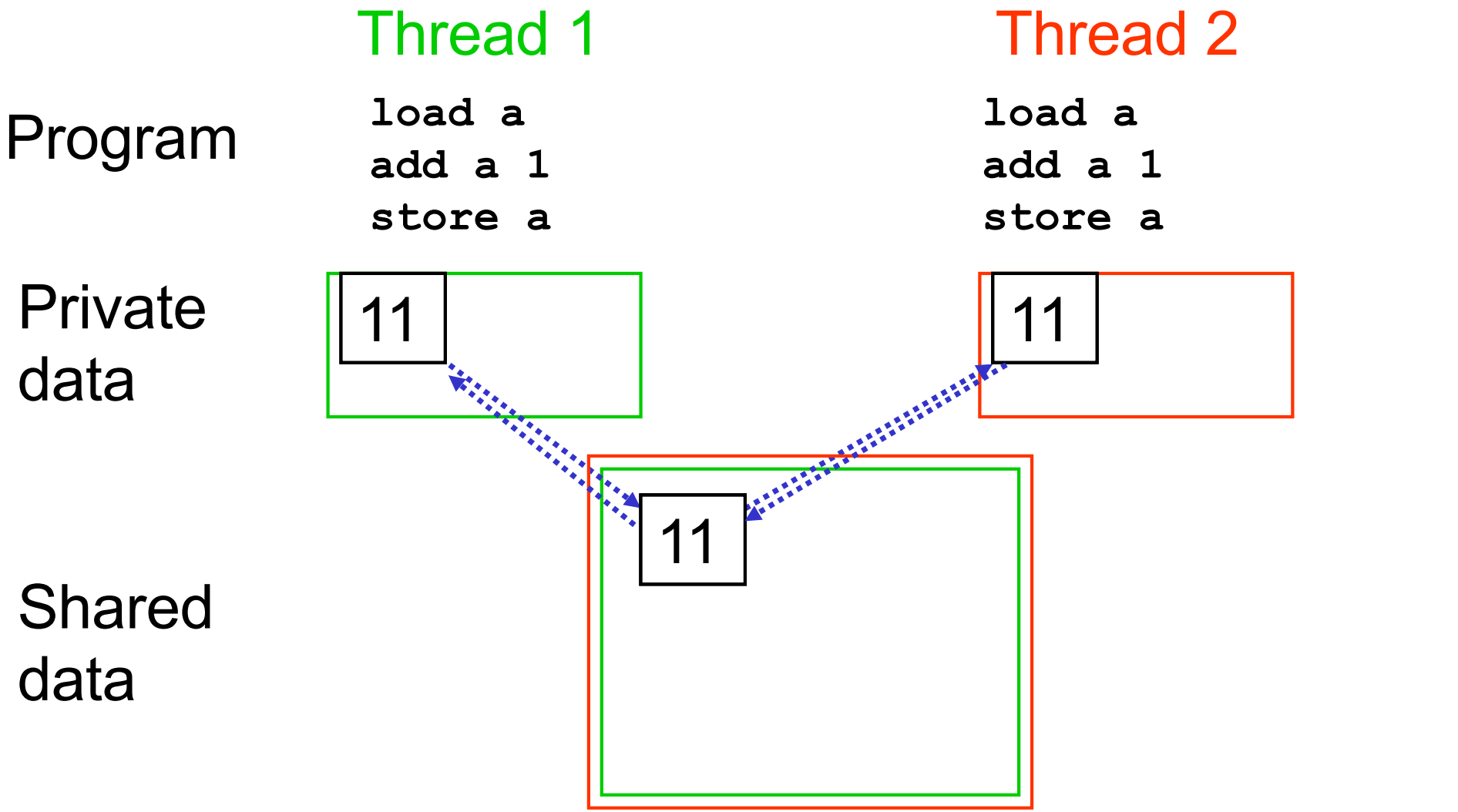


Shared Resources

- In parallel programming, developers must manage exclusive access to shared resources
  avoid concurring access
- Resources are in different forms:
  - concurrent read/write (including parallel write) to shared memory locations
  - concurrent read/write (including parallel write) to shared devices
  - a message that must be send and received

Shared Resources

a+=1. if I dont order the operations of the threads, or do any c



Fundamental Tools of Parallel Programming

understand how the memory is working, how the data is flowing and order of instructions

Timing

- Time measurement becomes a relevant issue:
  - MPI_WTIME()
  - Clock
  - Seconds()

How do we evaluate the improvement?

- We want estimate the amount of the introduced overhead => $T_o = n_{pes}T_P - T_S$
- But to quantify the improvement we use the term **Speedup**:

$$S_P = \frac{T_S}{T_P}$$

Scalability Limits

- Amdahl's law (there is a serial part which is not effected) linear speedup is never achieved: u have the parabula because of message passing and unav
- Parallelism introduces overhead due to communication, synchronization, additional operations (I/O, memory copies, reordering, etc...)
- Sometimes the limit of scalability can be somehow predicted:
  - is there enough work for any process?
- When considering complex problem not all part of the problem scale equally

OpenMP

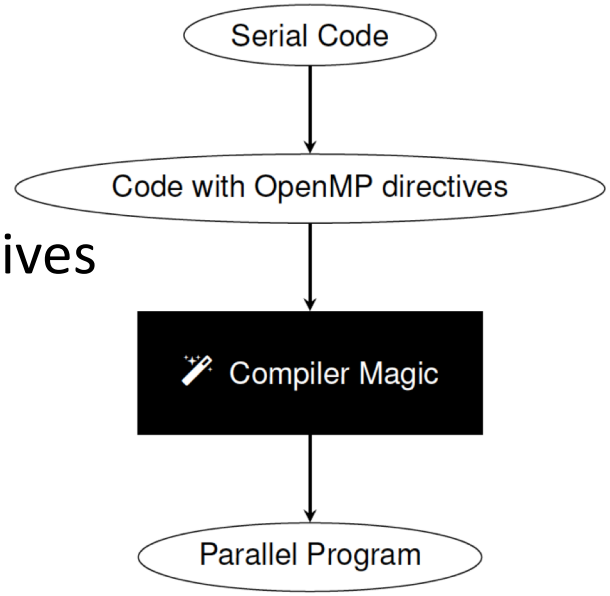
OpenMP (Open specifications for Multi Processing)

- OpenMP is not a programming language
  - Rather it works in conjunction with existing languages such as standard Fortran or C/C++
- A high-level application programming interface (API) used to write multi-threaded, portable shared-memory applications
- Application Programming Interface (API)
  - that provides a portable model for parallel applications
  - Three main components:
    - Compiler directives
    - Runtime library routines
    - Environment variables

incremental parallel approach: u can apply it on serial code. U pass pragma to the compiler, and the compiler will transform your pro

OpenMP Parallelization

- OpenMP is directive based
  - code (can) work without them
  - you annotate your code with OpenMP directives
- OpenMP can be added incrementally
- OpenMP only works in shared memory
  - multi-socket nodes, multi-core processors
- OpenMP hides the calls to a threads library
  - less flexible, but much less programming
- **Caution**: write access to shared data can easily lead to race conditions and incorrect data



so limited to node, no multinode? Actually

Directives Format

- A directive is a special line of source code with meaning only to certain compilers.
- A directive is distinguished by a sentinel at the start of the line.
- OpenMP sentinels are:
  - Fortran:

    !$OMP (or **C$OMP** or ***$OMP**) ***directive [clause [clause]…]***

  - C/C++:

    #include <omp.h>

    #pragma omp *directive [clause [clause]…]*

Hello World!

```c
#include <stdio.h>

int main() {
    printf("Hello World!\n");

    return 0;
}
```

Output:

```
Hello World!
```

Hello World!

```
#include <stdio.h>

int main() {
    #pragma omp parallel
    printf("Hello OpenMP!\n");

    return 0;
}
```

Hello World!

```
#include <stdio.h>

int main() {
    printf("Starting!\n");

    #pragma omp parallel
    printf("Hello OpenMP!\n");

    printf("Done!\n");

    return 0;
}
```

Output:

```
Starting!
Hello OpenMP!
Hello OpenMP!
Hello OpenMP!
Hello OpenMP!
Done!
```

Compiling

GCC

```
gcc -fopenmp -o omp_hello omp_hello.c
```

```
g++ -fopenmp -o omp_hello omp_hello.cpp
```

Intel

```
icc -qopenmp -o omp_hello omp_hello.c
```

```
icpc -qopenmp -o omp_hello omp_hello.cpp
```

Running

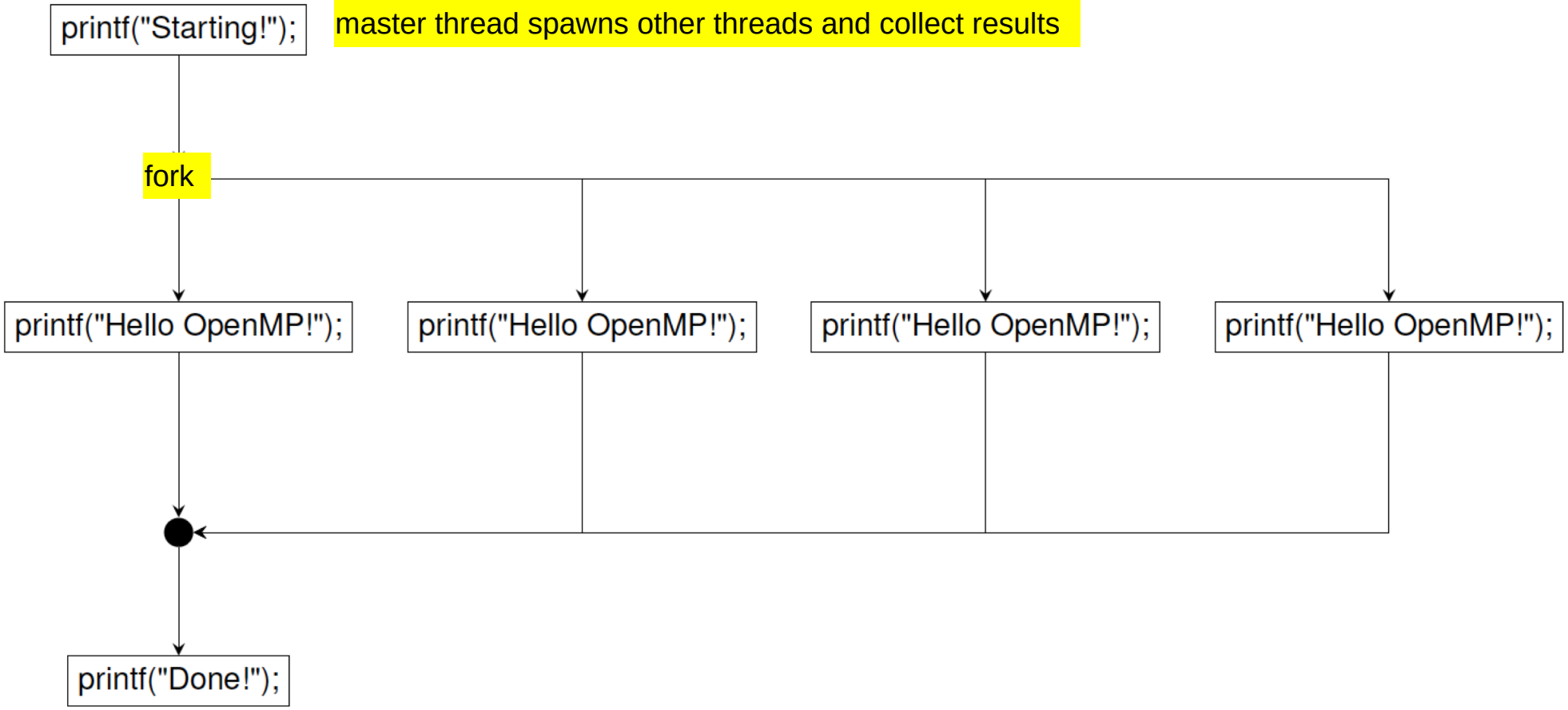
```
# default: number of threads equals number of cores
./omp_hello
```

```
# set environment variable OMP_NUM_THREADS to limit default
$ OMP_NUM_THREADS=4 ./omp_hello

# or

$ export OMP_NUM_THREADS=4
$ ./omp_hello
```

The Fork/Join Model



- Each thread executes the structured block independently
- The end of a parallel region acts as a **barrier** before rejoining all threads all tasks must have
- All threads must reach this barrier, before the main thread can continue.

How many threads?

1. At the `parallel` directive

```
#pragma omp parallel num_threads(4)
{
    ...
}
```

2. Setting a default via the `omp_set_num_threads(n)` library function

Set the number of threads that should be used by the **next** `parallel` region

3. Setting a default with the `OMP_NUM_THREADS` environment variable

number of threads that should be spawned in a parallel region if there is no other specification. By default, OpenMP will use all available cores.

Threads are numbered from 0 (master thread) to N-1

Library Functions

- Requires the inclusion of the `omp.h` header!

`omp_get_num_threads()`

Returns the number of threads in current team

`omp_set_num_threads(n)`

Set the number of threads that should be used by the **next** `parallel` region

`omp_get_thread_num()`

Returns the current thread's ID number

`omp_get_wtime()`

Return walltime in seconds

Parallel Region

Launches a team of threads to execute a block of structured code in parallel.

```
#pragma omp parallel
statement; // this is executed by a team of threads

// implicit barrier: execution only continues when all
// threads are complete
```

```
#pragma omp parallel
{
    // this is executed by a team of threads
}
// implicit barrier: execution only continues when all
// threads are complete
```

SPMD (Single Process Multiple Data)

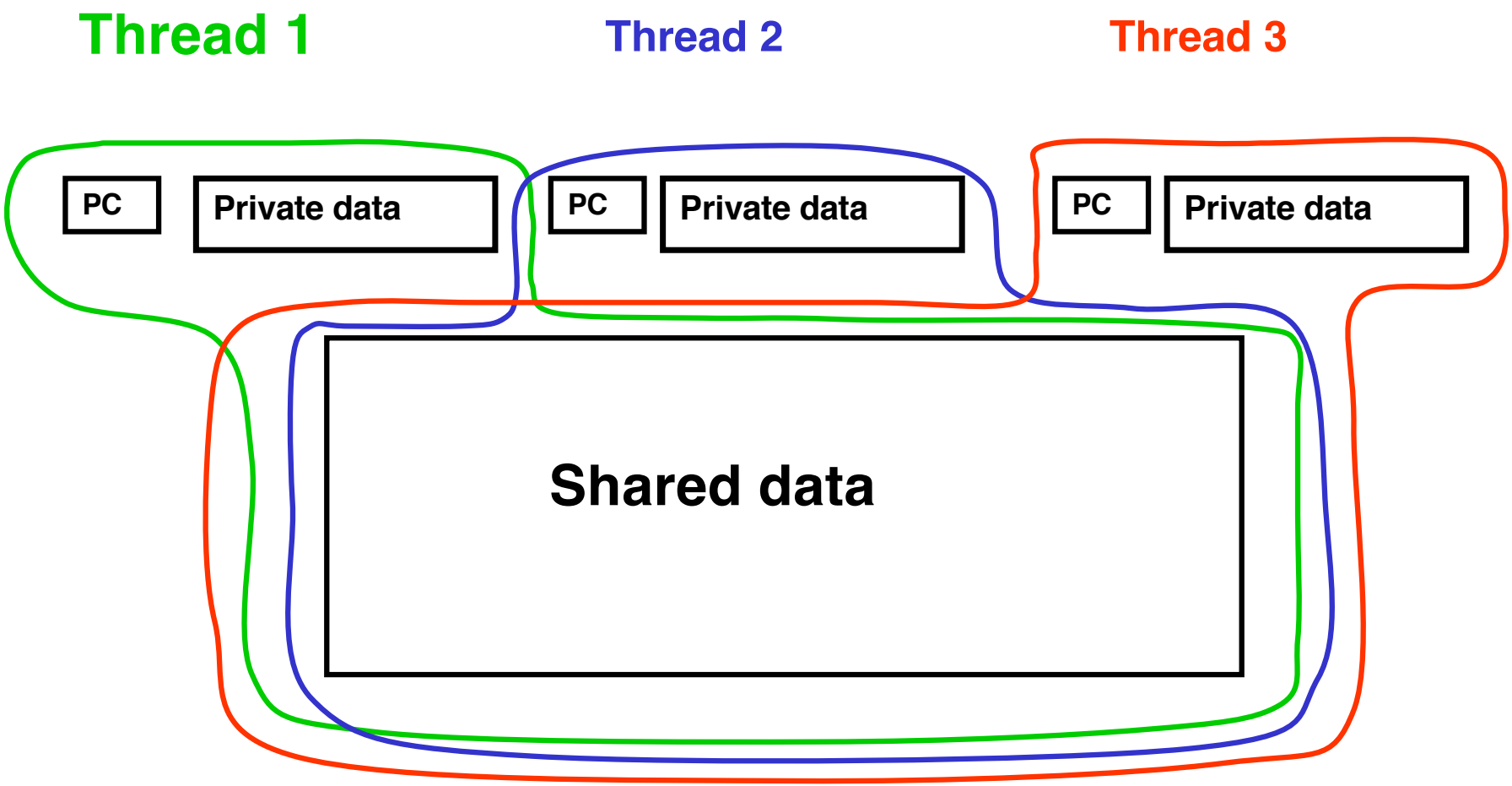
```
#include <stdio.h>
#include <omp.h>

int main() {
    #pragma omp parallel
    { same instruction for all the threads. First function will return 4 for everyone. Even the second one generates t
        int tid = omp_get_thread_num();
        int nthreads = omp_get_num_threads();
        printf("Hello from thread %d/%d!\n", tid, nthreads);
    }
    return 0;
}
```

```
Hello from thread 2/4!
Hello from thread 1/4!
Hello from thread 0/4!
Hello from thread 3/4!
```

we'll do single program multiple data: every thread has the same instructions but acts on different data

OpenMP Data Environment



Variable Scope /1

- by default all variables which are visible in the parent scope of a parallel region are **shared**
- variables declared inside of the parallel region are by definition of the scoping rules of C/C++ only visible in that scope. Each thread has a **private** copy of these variables

```
int a; // shared

#pragma omp parallel
{
    int b; // private
    ...
    // both a and b are visible
    // a is shared among all threads
    // each thread has a private copy of b
    ...
} // end of scope, b is no longer visible
```

Variable Scope /2

- a variable's scope can be modified at the beginning of a parallel region using clauses
- useful for legacy code where all variables are declared at the beginning of a function. E.g. in Legacy Fortran an C code you need to declare all variables at the beginning of a function.

```
int a = 1.0;
int b = 3.0;
int c = 5.0;

#pragma omp parallel shared(a) private(b,c)
{
    // a is shared among all threads (a = 1.0)
    // each thread has a private copy of b and c
    // b = uninitialized
    // c = uninitialized
    // outside b and C are not visible
    ...
}
```

Variable Scope /3

- a variable's scope can be modified at the beginning of a parallel region using clauses
- useful for legacy code where all variables are declared at the beginning of a function. E.g. in Legacy Fortran an C code you need to declare all variables at the beginning of a function.

```
int a = 1.0;
int b = 3.0;
int c = 5.0;

#pragma omp parallel shared(a)
{
    // a is shared among all threads (a = 1.0)
    // each thread has a private copy of b and c
    int b, c;
    // outside b and c are not visible
    ...
}
```

global scope b and c are not passed-> are not seen by threads

an array allocated on the heap (malloc) is global, if u pass it as private u have to reallocate space in the stack, otherwise segm

Variable Scope /3

- the `firstprivate` clause does the same as **`private`**, but initializes each copy with the value of the parent thread.

```
int a = 1.0;
int b = 3.0;
int c = 5.0;

#pragma omp parallel firstprivate(b) private(c)
{
    // a is shared
    // the value of the private b is 3.0
    // the value of the private c is uninitialized
    ...
}
```

Variable Scope /4

Let’s make some examples …

Work-Sharing: loop

- Divides the execution of the enclosed code region among the members of the team that encounter it.
- Work-sharing constructs **do not** launch new threads.
- No implied barrier upon entry to a work sharing construct.
- However, there is an implied barrier at the end of the work sharing construct (unless nowait is used).

Work-Sharing: loop

Sequential code

```
for( i = 0; i < N; i++ ) {
        a[ i ] = a[ i ] + b[ i ];
}
```

OpenMP // Region

```
#pragma omp parallel
{
    int id, i, Nthrds, istart, iend;
    id = omp_get_thread_num();
    Nthrds = omp_get_num_threads();
    istart = id * N / Nthrds;
    iend = ( id + 1 ) * N / Nthrds;
    for(i = istart; i < iend; i++ ) {
        a[ i ] = a[ i ]+ b[ i ];
    }
}
```

OpenMP Parallel Region and a work-sharing for construct

```
#pragma omp parallel for schedule(static) private(i)
for(i = 0;i < N; i++ ) {
      a[ i ] = a[ i ] + b[ i ];
}
```

Work-Sharing: loop

Sequential code

```
for( i = 0; i < N; i++ ) {
        a[ i ] = a[ i ] + b[ i ];
}
```

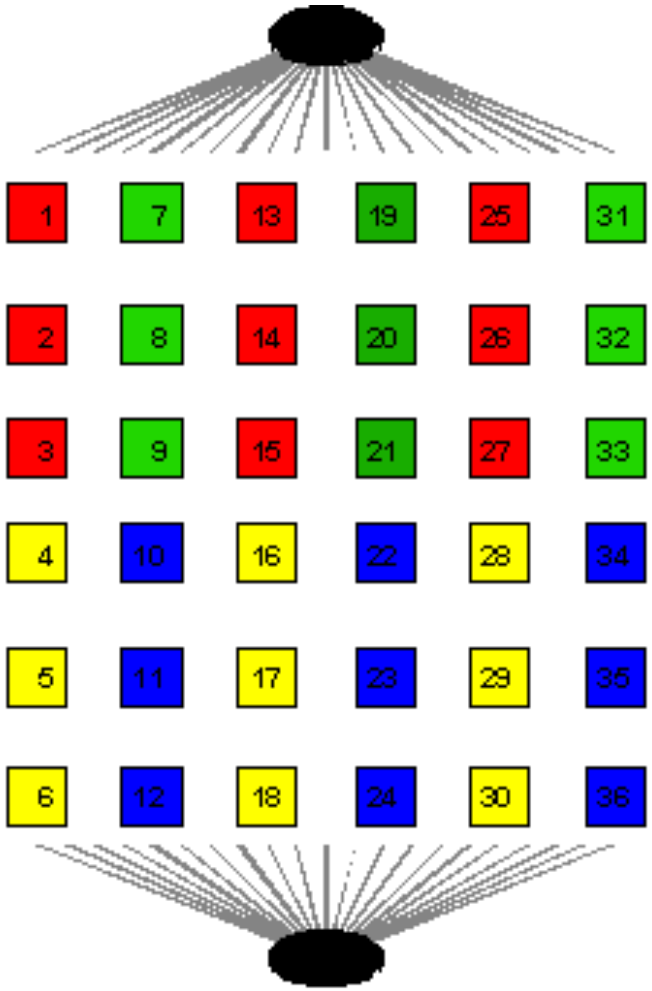
OpenMP // Region

```
#pragma omp parallel
{
    int id, i, Nthrds, istart, iend;
    id = omp_get_thread_num();
    Nthrds = omp_get_num_threads();
    istart = id * N / Nthrds;
    iend = ( id + 1 ) * N / Nthrds;
    for(i = istart; i < iend; i++ ) {
        a[ i ] = a[ i ]+ b[ i ];
    }
}
```

OpenMP Parallel Region and a work-sharing for construct

```
#pragma omp parallel
#pragma omp for schedule(static) private(i)
for(i = 0;i < N; i++ ) {
      a[ i ] = a[ i ] + b[ i ];
}
```

schedule(static [,chunk])



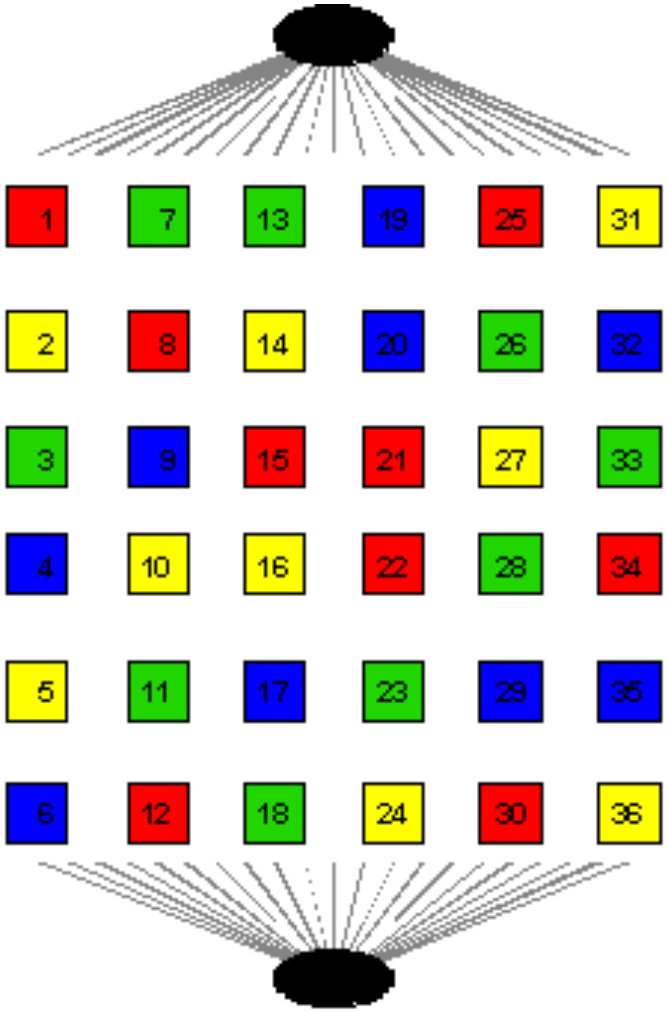
- Deal-out blocks of iterations of size "chunk" to each thread
- Iterations are divided evenly among threads
- If chunk is specified, divides the work into chunk sized parcels
- If there are N threads, each thread does every N^{th} chunk of work.

```
!$OMP PARALLEL DO &
!$OMP SCHEDULE(STATIC,3)

DO J = 1, 36
Work (j)
END DO

!$OMP END DO
```

schedule(dynamic [,chunk])



- Each thread grabs "chunk" iterations off a queue until all iterations have been handled
- Divides the workload into chunk sized parcels.
- As a thread finishes one chunk, it grabs the next available chunk.
- Default value for chunk is one.
- More overhead, but potentially better load balancing.

```
!$OMP PARALLEL DO &
!$OMPSCHEDULE(DYNAMIC,1)

DO J = 1, 36
Work (j)
END DO

!$OMP END DO
```

Variable Scope /4

Let’s make some examples …