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THE GREEK AI FACTORY

OpenMP

A gentle introduction to OpenMP

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Outline

1. Motivation for OpenMP
   - Simplicity and Portability
2. Introduction
   - Shared Memory Systems
   - Threaded Programming Model
   - Thread Sharing Data Example
   - Synchronisation
   - Parallel Loops
   - Synchronisation Example
3. OpenMP Basics
   - Parallel Regions
   - Data Sharing
   - Work Sharing
   - Reductions
   - Synchronisation
   - Utilities
4. Wrap-Up

Why OpenMP?

- Simplicity and Portability
- Avoid low-level threading (e.g., pthreads)

First example from https://people.math.sc.edu/burkardt/cpp_src/openmp/openmp.html

Simplicity and Portability

- A de-facto standard API to write shared memory parallel applications in C, C++ and Fortran
- Compiler directives
- Runtime routines
- Environment variables
- Very mature (around since 1997)
- Version 6.0 has been released (11/2024)

Simplicity and Portability

- Portable: supported by GNU, Intel, NVIDIA/PGI, SUN Studio, others
- Portable: supported on many (all important ones) Hardware platforms
- Allows incremental parallelisation (see next slide)
- You can revert to your serial application with a flick of a switch (either set OPENMP_NUM_THREADS to 1 or don't link with libopenmp)
- Supports tasks
- Supports other architectures (offloading to accelerators)
- Can be used with MPI for hybrid parallelism

Incremental Approach

Parallelism added incrementally until performance goals are met:

- Start with a serial application
- Benchmark
- Identify hotspots
- Parallelise that section
- Repeat

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Introduction

- OpenMP stands for Open Multi-Processing.
- It is an API for shared-memory parallel programming.
- Supports C, C++, and Fortran.

C/C++

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

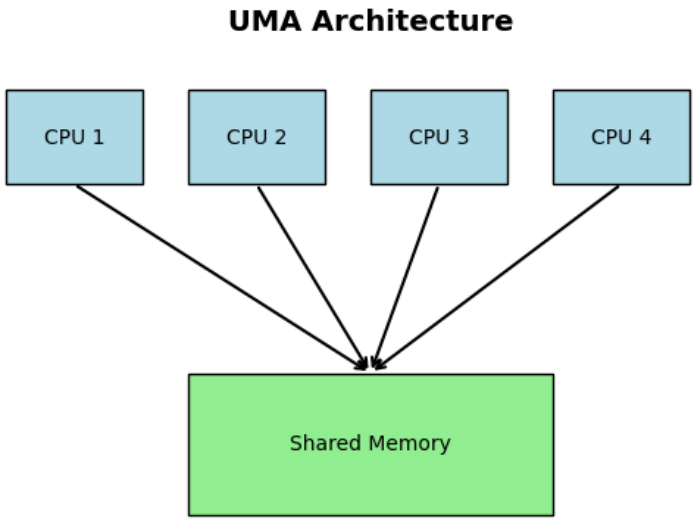
Fortran

```
!$omp parallel do
do i = 1, N
   a(i) = b(i) + c(i)
end do
!$omp end parallel do
```

Shared Memory Systems

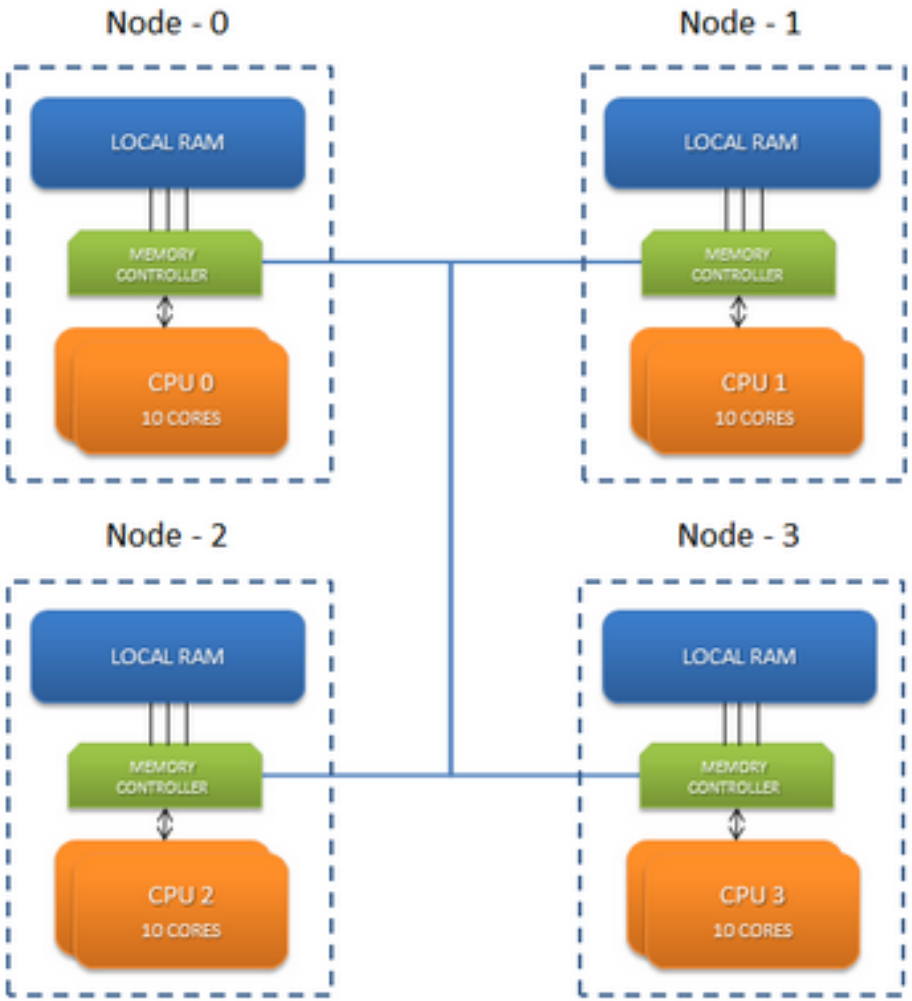
- A shared memory system has processing units (CPUs/cores) and memory
- Memory is accessible by every CPU/core
- There is one and only one memory (address) space

Uniform Memory Access



- All CPUs share the same memory.
- Equal access time for all processors.
- Simpler programming model.
- Common in small-scale systems like desktops or basic servers.

Non-Uniform Memory Access



a

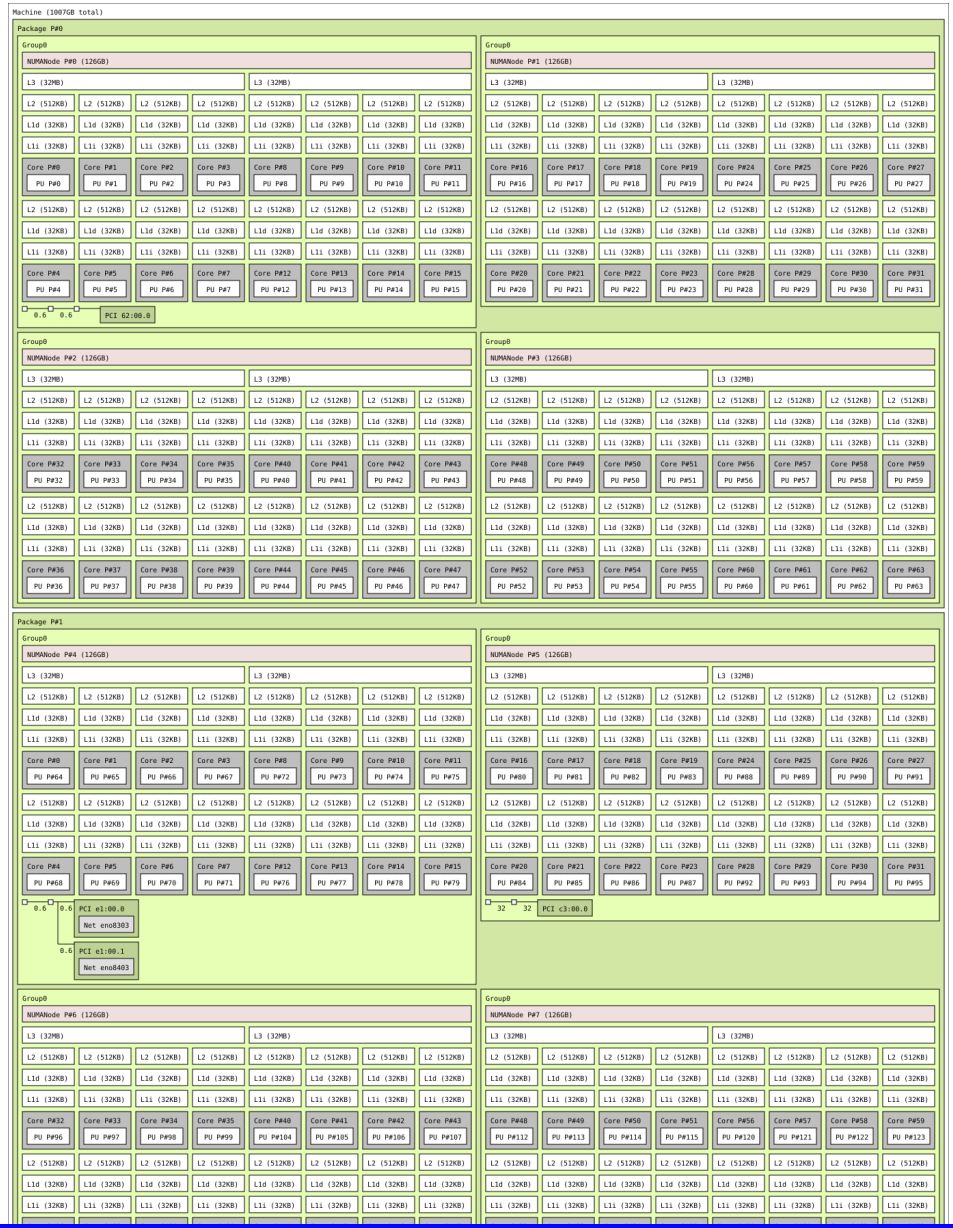
- Each processor has its own local memory, but can also access other CPUs' memory.
- Faster access to local memory, slower to remote memory.
- More complex but scales better for large systems.
- Common in modern HPC nodes and multi-socket servers.

[a] Image source: What is NUMA

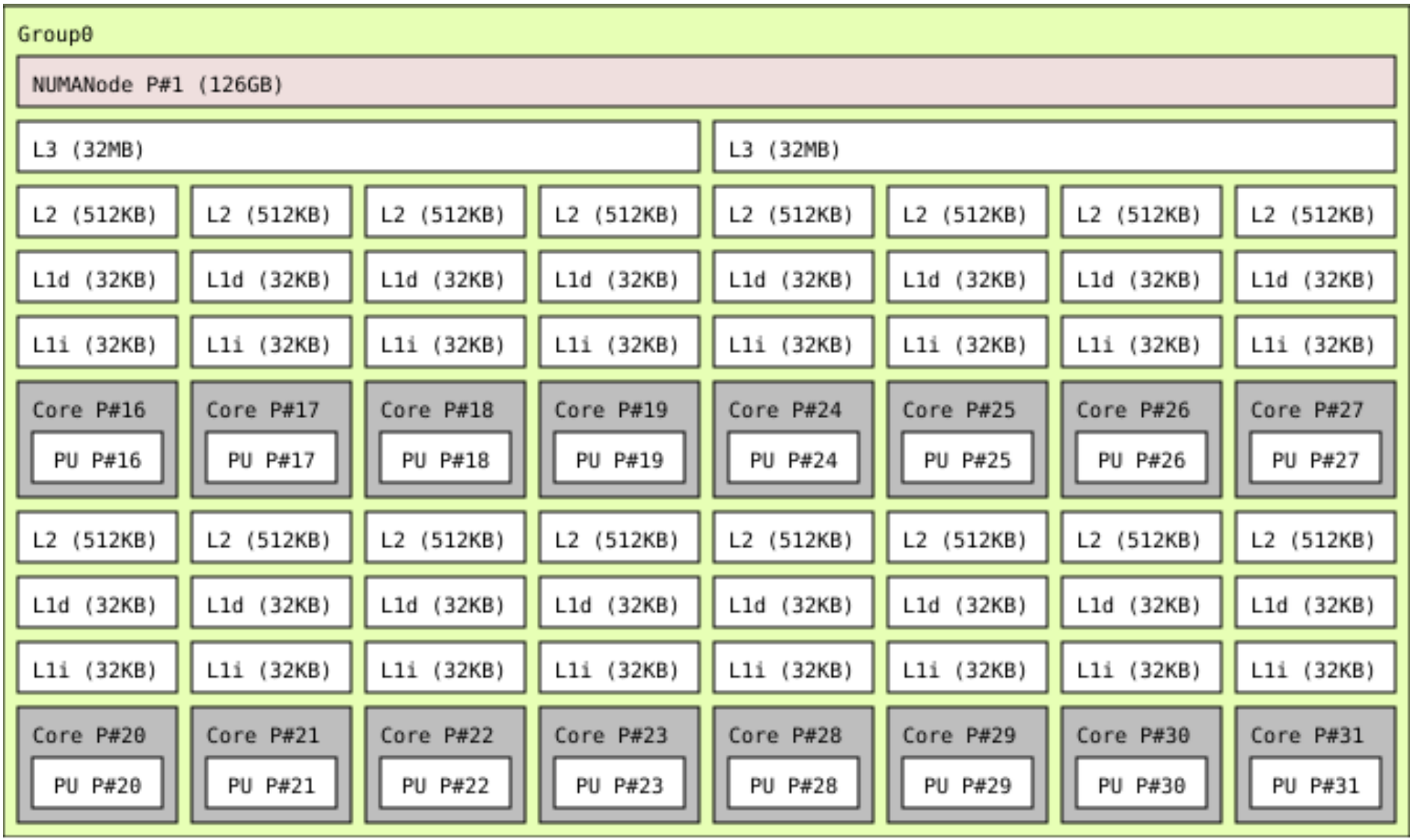
Reality

This is how a Real System looks like. (ARIS expansion)

- Multiple levels of Cache(s)
- Memory could be split/fragmented across CPUs/Sockets
- Sharing of hardware resources across CPUs/Sockets (L3 caches)



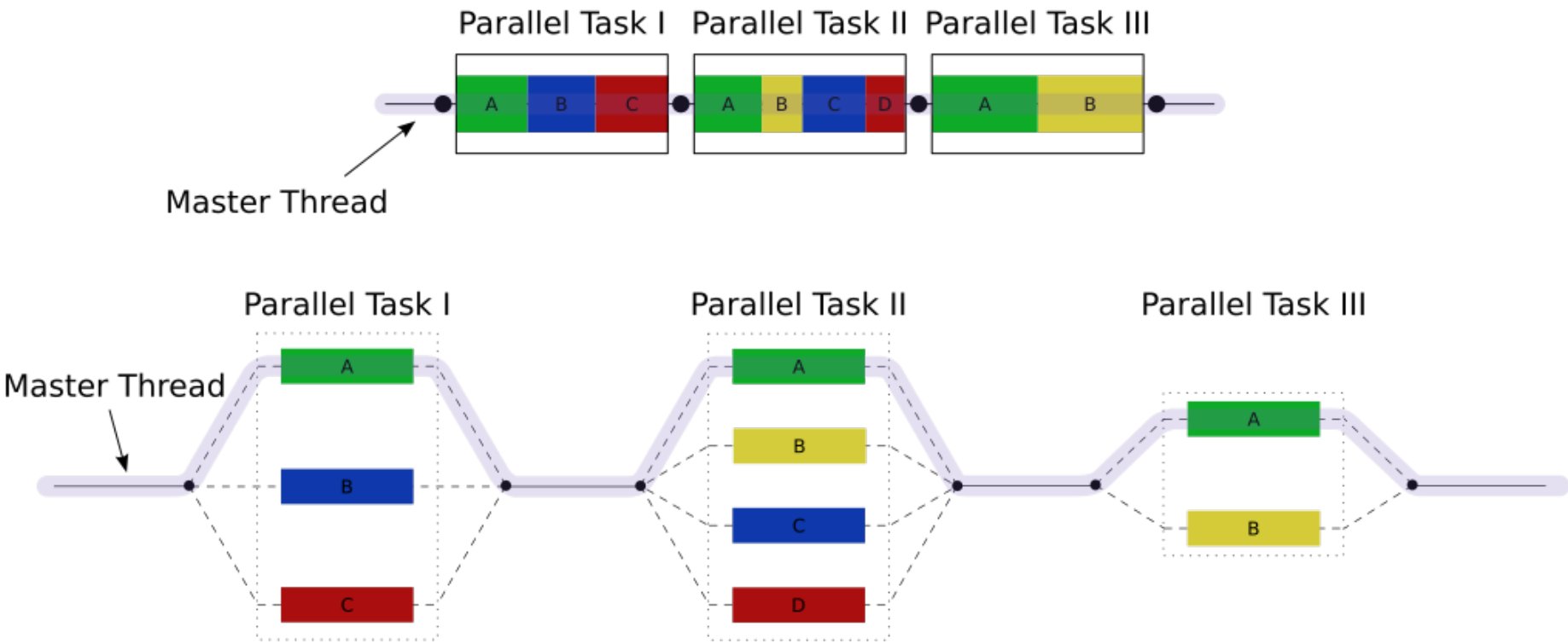
Reality / Closeup



Threaded Programming Model

- OpenMP uses threads.
- A thread is the smallest unit of processing that can be scheduled by an operating system.
- Threads are very light-weight processes; but threads can share memory with other threads.
- However, each Thread has it's own stack and stack pointers.
- Threads are part of a process. Without a process, threads do not exist.
- Threads can access Shared Data.
- Threads can have Private Data.
- Threads are unique and have their own state (regardless of the other threads).

Fork - Join Model



[1]

[1] Image source: By Wikipedia user A1 - w:en:File:Fork_join.svg, CC BY 3.0

Hello World C/C++

C/C++

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

int main()
{
  #pragma omp parallel
  {
    printf("Hello from process: %d \n",
        omp_get_thread_num());
  }
}
```

```
gcc -g3 -O2 -Wall -Wextra 01.c -o 01.exe -fopenmp
```

Hello World Fortran

Fortran

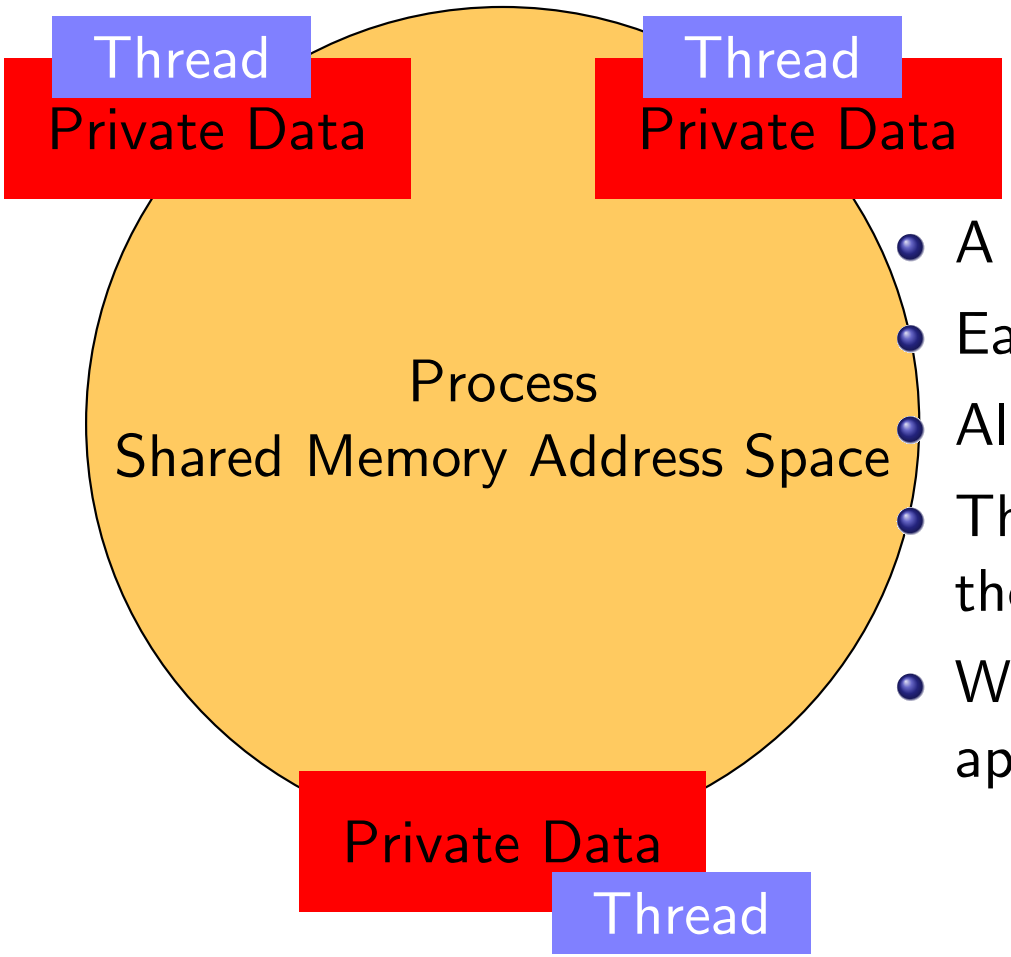
```
PROGRAM Parallel_Hello_World
USE OMP_LIB

!$OMP PARALLEL

PRINT *, "Hello from process: ", OMP_GET_THREAD_NUM()

!$OMP END PARALLEL

END
```

```
gfortran -g3 -O2 -Wall -Wextra 01.f90 -o 01_f.exe -
    fopenmp
```

Shared Data Model

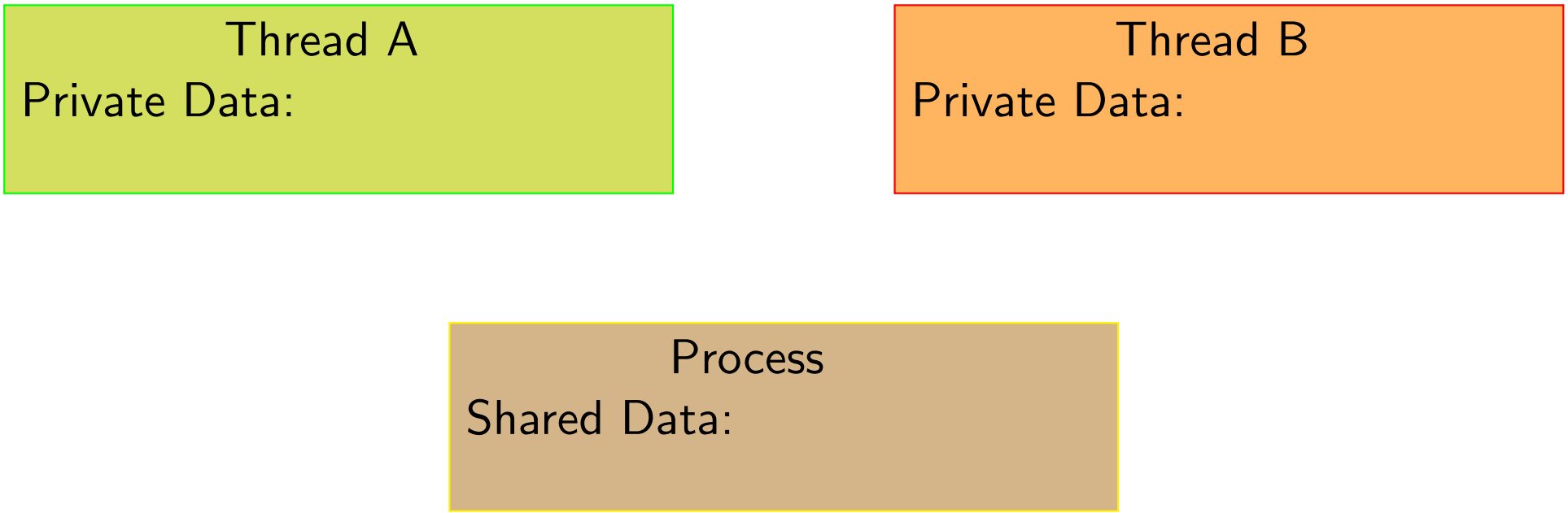
- Threads can (for non-trivial problems they must) exchange data.
- Shared Data constructs are used to exchange data.
  - Thread A writes to a shared variable.
  - Thread B reads the shared variable.
- No implicit synchronisation
- No implicit barriers (on entry)
- No implicit checks

Thread Sharing Data



- A single Process; with many Threads
- Each Thread has it's own Private Data
- All Threads share Shared Data
- The OS is responsible for scheduling the Process/Threads
- Without synchronisation, things fall apart.

Thread Sharing Data Example



Thread Sharing Data Example

Thread A

Private Data:

p_answer=42

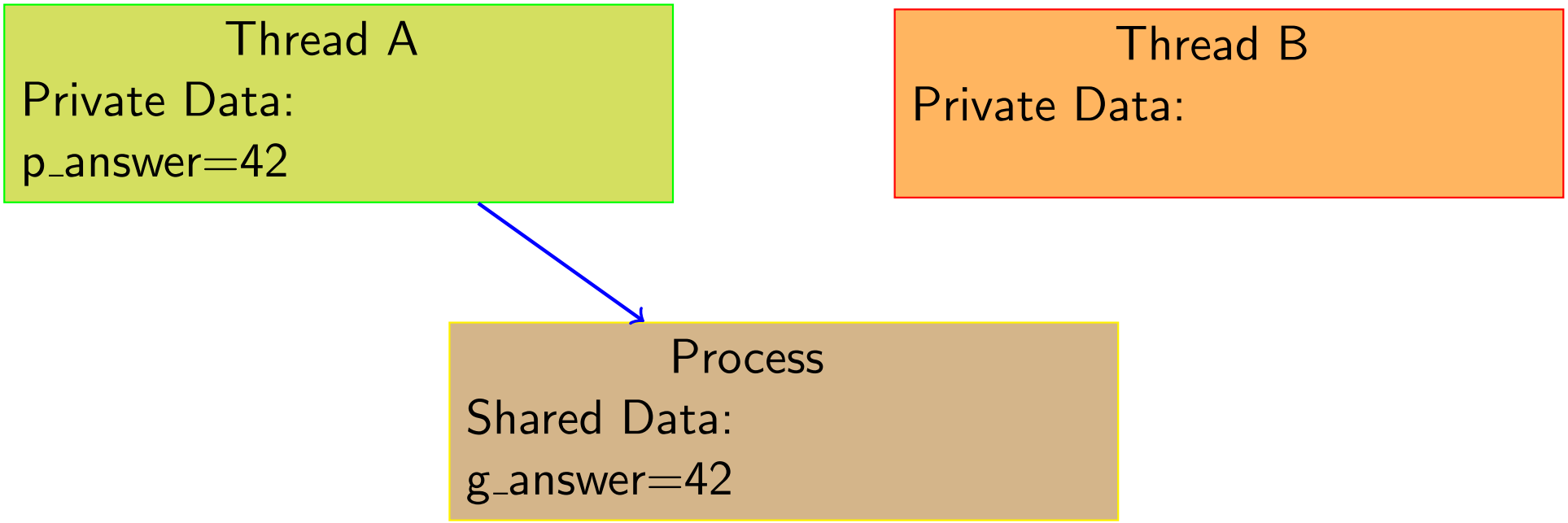
Thread B

Private Data:

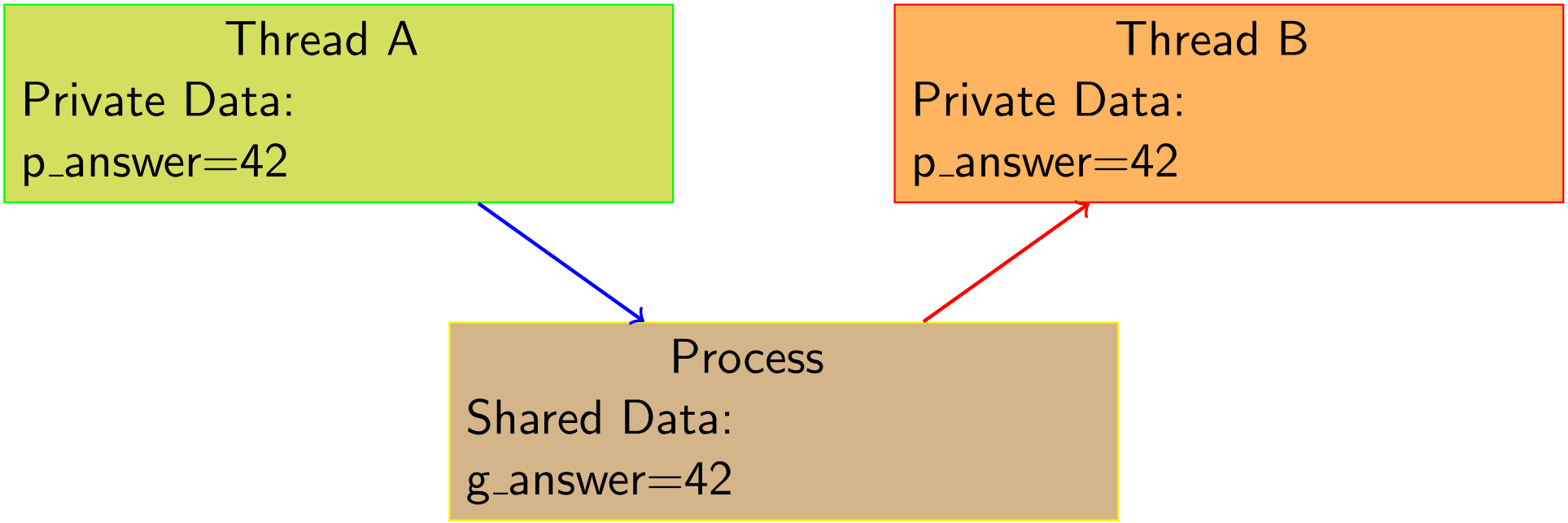
Process

Shared Data:

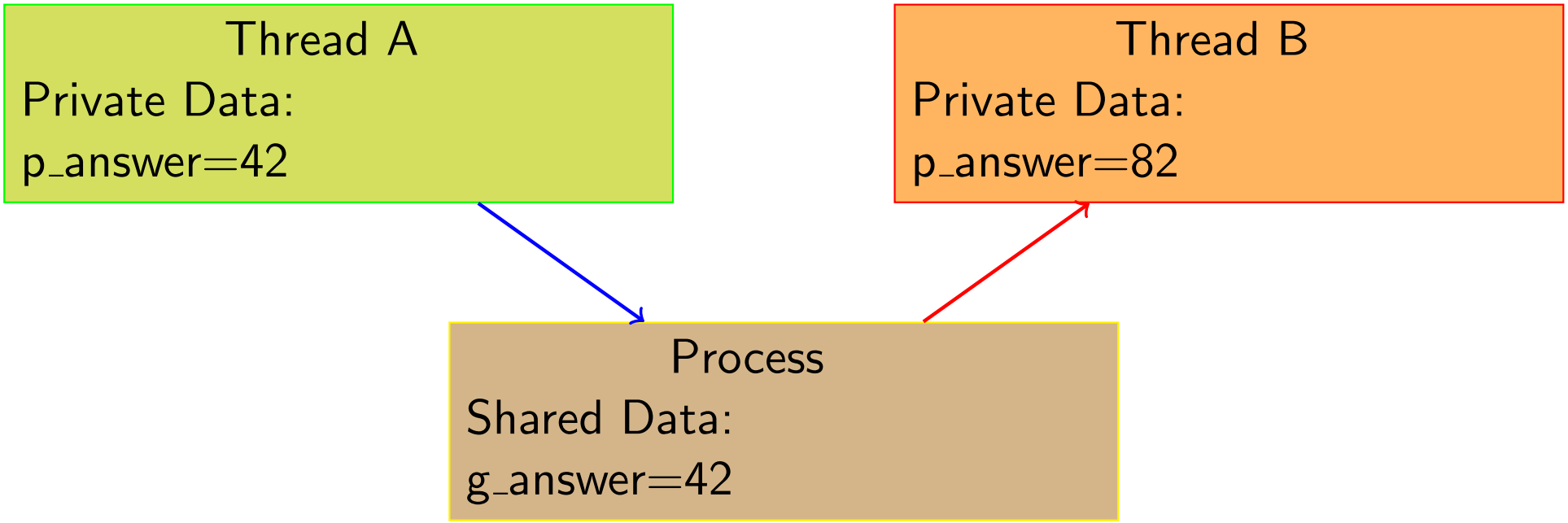
Thread Sharing Data Example



Thread Sharing Data Example



Thread Sharing Data Example



Synchronisation

Simple Example, yet:

- We don't control the Threads (unless we block them) [DONT]
- The OS controls thread execution and scheduling
- Threads run at their own pace
- Even in this very simple example, we need to guard that Thread B doesn't read an unitialised value from g_answer.
- Even though it takes one line of source code to modify a value; in reality this is a multi-step process (at least three instructions are issued).
- If multiple threads try to modify a shared variable at the same time ...

Synchronisation Example

Simple Example:

- We want to add 8 to 0.
- This is a computationally expensive problem; so we will use OpenMP.
- Since we are adding 8; we will use 8 Threads.
- Each Thread will add 1.
- At the end we will print the result.
- We are expecting to dramatically improve the performance of our application.

Synchronisation Example Single Threaded (C/C++)

C/C++

```c
#include <stdio.h>

#define NUM_TIMES 8

int main()
{
  int VALUE = 0;

  for (int i = 0; i < NUM_TIMES; ++i)
  {
    VALUE += 1;
  }

  printf("Result:%d \n", VALUE);
}
```

Synchronisation Example Single Threaded (Fortran)

Fortran

```
PROGRAM Training
implicit none

integer :: NUM_TIMES = 8, VALUE = 0, n

do n = 1, NUM_TIMES
  VALUE = VALUE + 1
end do

PRINT *, "Result: ", VALUE

END PROGRAM Training
```

Synchronisation Example Single Threaded (Fortran)

C/C++

```
gcc -g3 -O2 -Wall -Wextra -fsanitize=address,undefined
    02.c -o 02.exe

./02.exe
Result:8
```

Fortran

```
gfortran -g3 -O2 -Wall -Wextra -fsanitize=address,
   undefined 02.f90 -o 02_f.exe

./02_f.exe
Result:                8
```

Parallel Loops

- In most applications; runtime is spent in loops.
- Loops are the first place that we will want to parallelise.
- If a loop is independent then it can be trivially parallelised.
- A loop from 0-99 can be run on one thread running all iterations; or 4 threads can run iterations 0-24/25-49/50-74/75-99.

Synchronisation Example Single Threaded (C/C++)

C/C++

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

#define NUM_TIMES 8

int main()
{
  int VALUE = 0;

#pragma omp parallel for              <================
  for (int i = 0; i < NUM_TIMES; ++i)
  {
    VALUE += 1;
  }

  printf("Result:%d \n", VALUE);
```

Synchronisation Example Single Threaded (Fortran)

Fortran

```
PROGRAM Training
USE OMP_LIB                    <================
  implicit none

  integer :: NUM_TIMES = 8, VALUE = 0, n

!$OMP PARALLEL DO               <================
  do n = 1, NUM_TIMES
    VALUE = VALUE + 1
  end do

  PRINT *, "Result: ", VALUE

END PROGRAM Training
```

Synchronisation Example Single Threaded (Fortran)

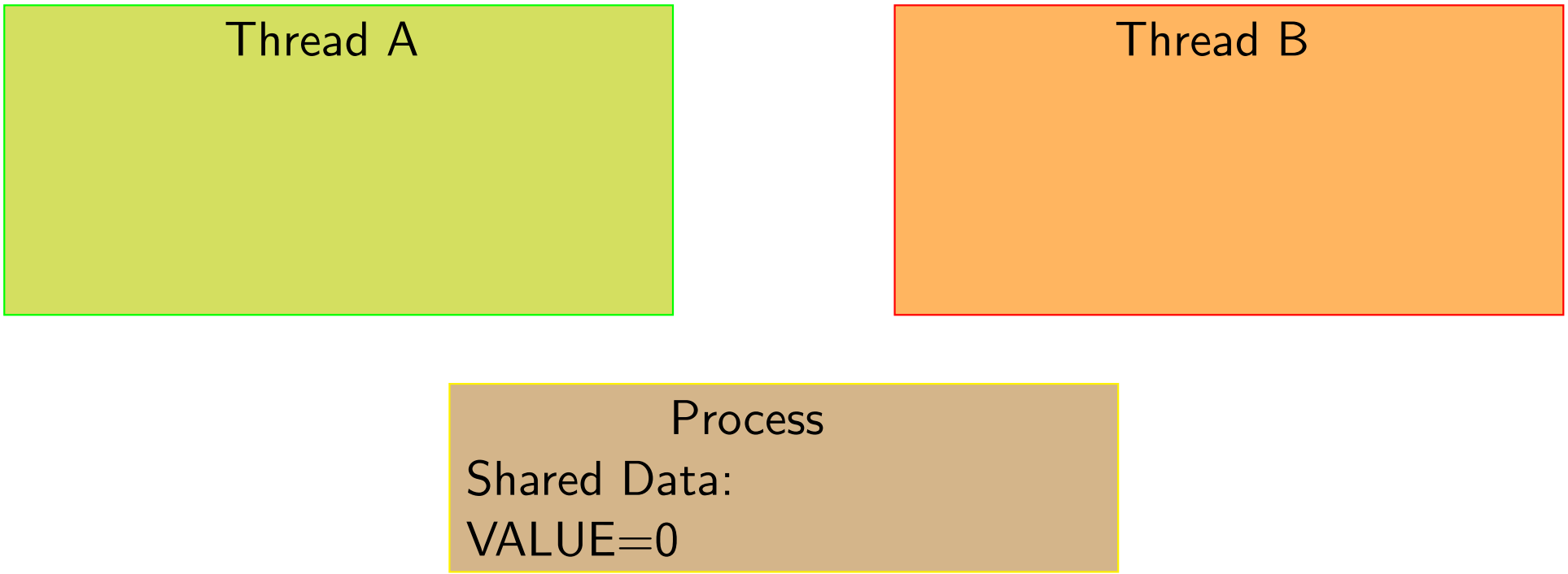
C/C++

```
gcc -g3 -O2 -Wall -Wextra -fsanitize=address,undefined
    02.c -o 02.exe -fopenmp

./02.exe
Result:X
```

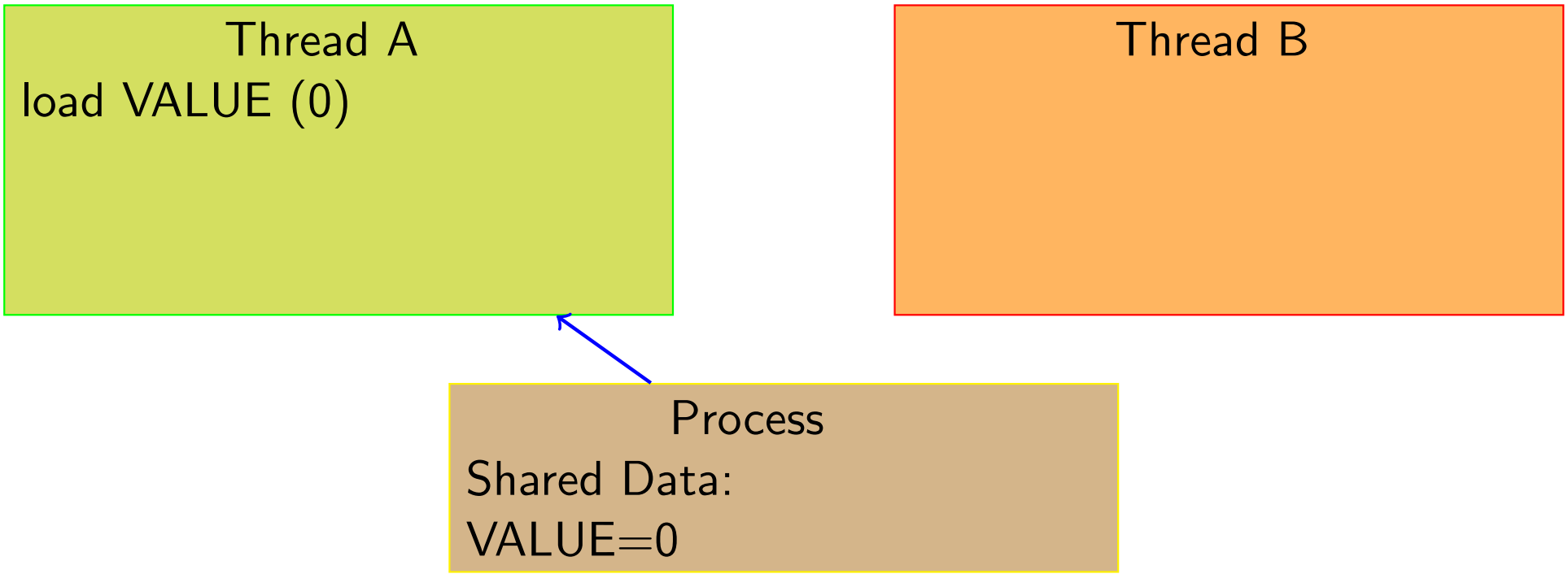
Fortran

```
gfortran -g3 -O2 -Wall -Wextra -fsanitize=address,
   undefined 02.f90 -o 02_f.exe -fopenmp

./02_f.exe
Result:                X
```

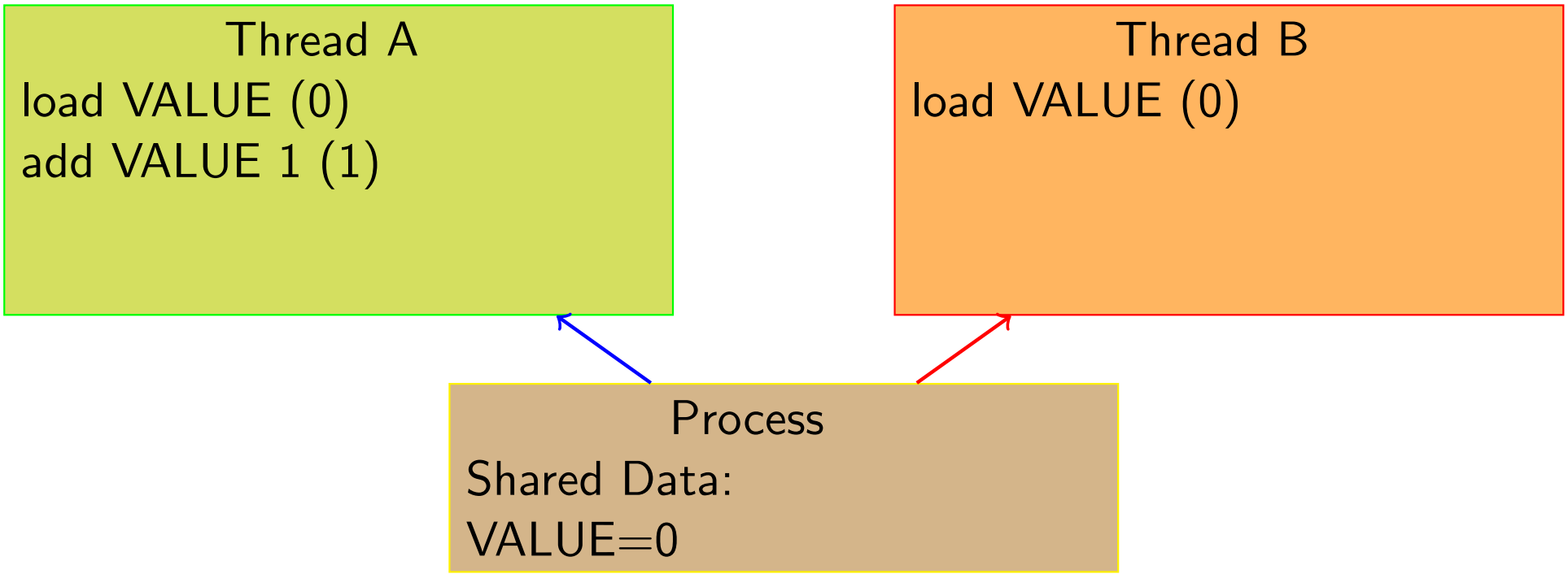
Synchronisation Example



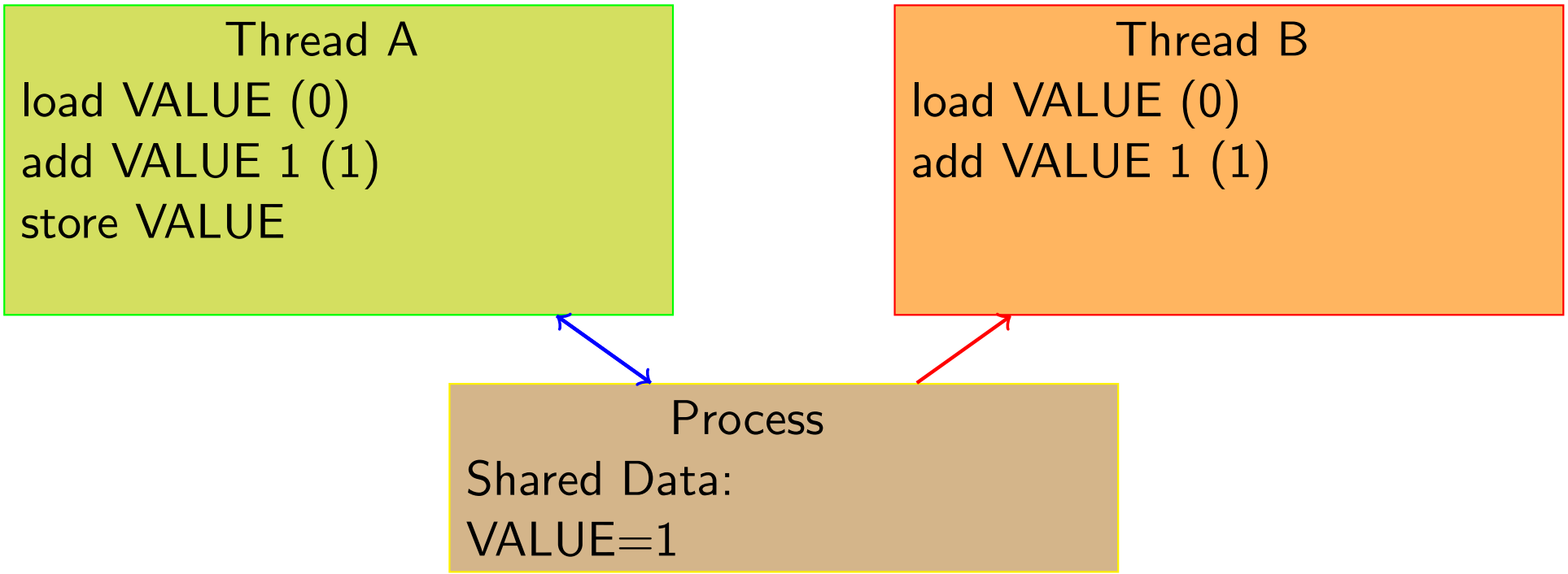
Synchronisation Example



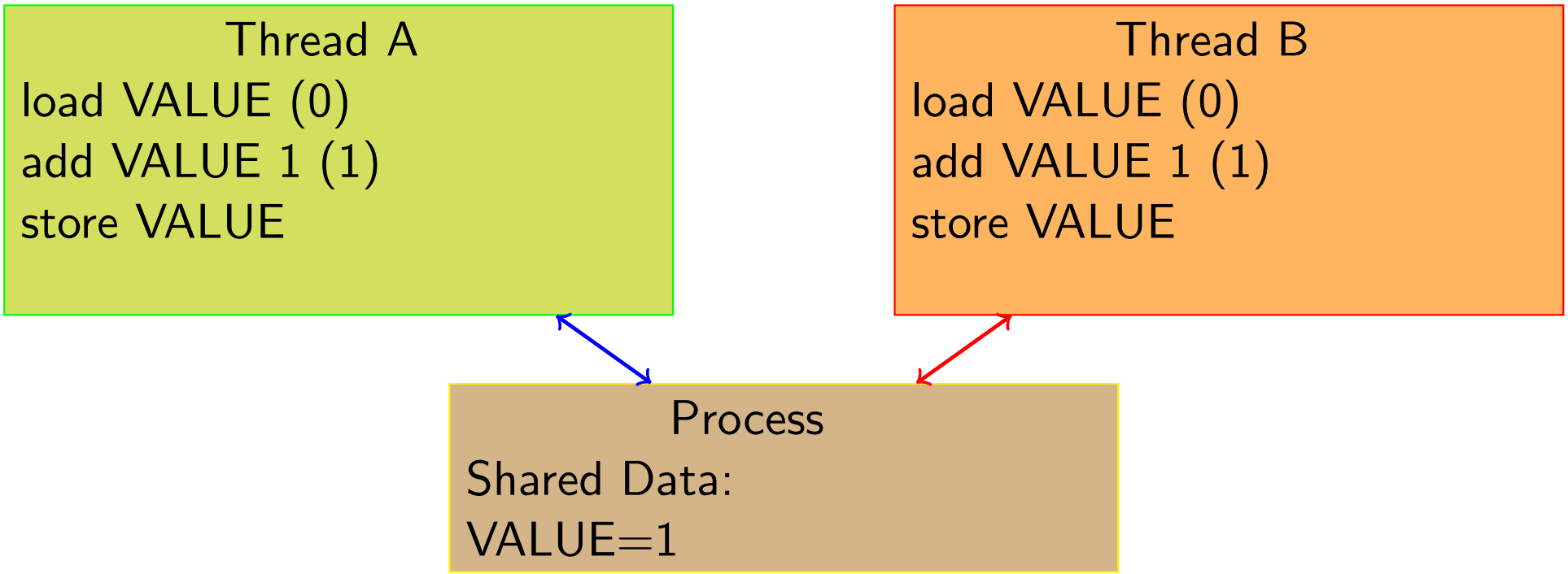
Synchronisation Example



Synchronisation Example



Synchronisation Example



Race Condition

- If you run the example code (in Linux or WSL) you will see that the result is not always 8.
- Why?? Sometimes the threads run one after another. Other times they overlap.
- If they overlap and at least one (in our case all of them) writes/updates a shared value; we can have a race condition.
- Race conditions are hard to debug
- Sometimes they can be detected by run-time debuggers

See example 02.c

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OpenMP Basics

- Parallel Regions
- Data sharing & scoping: shared, private, firstprivate, lastprivate, default(shared or none)
- Worksharing: for / do, sections, schedule
- Reductions & loop shaping: reduction, collapse
- Synchronization: barrier, critical, atomic, ordered (loop order), master / masked
- Utilities: omp_get_num_threads(), omp_get_thread_num(), timing via omp_get_wtime()
- Good practices

Parallel Regions

- This one is simple. Any code inside an OMP pragma is executed by **all** threads
- Don't assume that OpenMP will handle special cases for you
- If you have code that writes data to the file system inside an OMP pragma; then you will write the data OMP_NUM_THREAD times.
- Same for functions. A function called from inside an OMP pragma will be called OMP_NUM_THREAD times.

Parallel Regions

C/C++

```
#pragma omp parallel
{
  CODE
}
```

Fortran

```
!$omp parallel

CODE

!$omp end parallel
```

C/C++

```
#pragma omp parallel
{
  FUNCTION  <== NUM_THREAD
}
```

Fortran

```
!$omp parallel

FUNCTION  <== NUM_THREAD

!$omp end parallel
```

Parallel Regions

- Parallel Regions can also use clauses
- #pragma omp parallel num_threads(4) : Use 4 threads
- #pragma omp parallel for if(condition) : Only start extra threads if condition is TRUE. For example, if the size of an array is less than 10000 run serially. If not, start X number of Threads

Data Sharing

The most important clauses in any Parallel Region are:

- default(shared | none)
- private(list)
- firstprivate(list)
- shared(list)

Data Sharing

Reminder about variables (single variables, arrays, etc):

- SHARED: All threads see the same copy (careful when reading/writing)
- PRIVATE: Every thread sees it's own copy.

Data Sharing

SHARED and PRIVATE variables important caveats:

- When entering any PARALLEL section, PRIVATE variables are uninitialised.
- When exiting any PARALLEL section (even when you have another one starting immediately after) private copies/variables are lost.
- Any variable declared **inside** a PARALLEL section is PRIVATE.
- Always, always, **always** use DEFAULT(none). It will save you time and money.

Data Sharing

SHARED and PRIVATE variables important caveats:

- By default, global and static variables are SHARED, and loop indices are private.
- firstprivate: Like PRIVATE, but each thread's copy is initialized with the value of the original variable at entry
- lastprivate: Like private, but after the parallel region finishes, the variable in the original context is updated with the value from the last iteration (or section) in the region

Data Sharing

C/C++

```
int a, b=10;

#pragma omp parallel \
  private(a) firstprivate(b)
{
// 'a' is uninitialized
// private per thread;

// 'b' is private per thread
// each initialized to 10.
}
```

Fortran

```
integer :: a, b

b = 10

!$omp parallel private(a
   ) &
!$omp&  firstprivate(b)
! 'a' is uninitialized
!     private per thread

! 'b' is private per
   thread
!     each initialized
   to 10

!$omp end parallel
```

Worksharing

- Loops (for / do)
- Schedules
- Sections
- Single
- Master

Loops (for / do)

Loops (for / do): Divides loop iterations among threads in a parallel region

C/C++

```
int N = 1000
#pragma omp parallel for
for (int i = 0; i < N; i++)
{
        a[i] = b[i] + c[i];
}
```

Loops (for / do)

Loops (for / do): Divides loop iterations among threads in a parallel region

Fortran

```
integer, parameter :: N = 1000
real :: a(N), b(N), c(N)
integer :: i

!$omp parallel do
do i = 1, N
  a(i) = b(i) + c(i)
end do
!$omp end parallel do
```

Schedules

Loops (for / do) support the following schedule types:

- static: assigns fixed chunks in advance
- dynamic: hands out chunks on the fly as threads finish
- guided: starts with large chunks that shrink over time to balance workload.
- auto: the compiler/runtime decides.
- runtime: use OMP_SCHEDULE environment variable or a call to set it.
- chunk: we can define the size of the chunks.

Schedules

- If we know exactly what is going on; static is the fastest.
- If we don't know; but we know that there is variability, use dynamic. But your data locality (if important) will disappear.
- If we know nothing; then start with guided. More overhead.
- We can also set the chunk size to help the compiler.

Loops (for / do)

Use a dynamic schedule. Each thread will get 4 iterations. The first thread that finishes, will get the next 4; until the end of the loop.

C/C++

```
int N = 1000
#pragma omp parallel for schedule(dynamic,4)
for (int i = 0; i < N; i++)
{
  a[i] = b[i] + c[i];
}
```

Loops (for / do)

Use a dynamic schedule. Each thread will get 4 iterations. The first thread that finishes, will get the next 4; until the end of the loop.

Fortran

```
integer, parameter :: N = 1000
real :: a(N), b(N), c(N)
integer :: i

!$omp parallel do schedule(dynamic,4)
do i = 1, N
  a(i) = b(i) + c(i)
end do
!$omp end parallel do
```

Sections

- Not all code runs in loops.
- Allows different code blocks to run in parallel.
- Each section block is executed by one thread.
- When all sections complete, threads synchronize (unless nowait is used).

Sections

The two functions will run on two different threads. There is a block at the end of the parallel section; waiting for both threads to finish.

C/C++

```
#pragma omp parallel sections
{
  #pragma omp section
  something_interesting_A();
  #pragma omp section
  something_interesting_B();
}
```

Sections

The two functions will run on two different threads. There is a block at the end of the parallel section; waiting for both threads to finish.

Fortran

```
!$omp parallel sections

!$omp section
call somethinginterestingA()

!$omp section
call somethinginterestingB()

!$omp end parallel sections
```

Sections

- Pure Sections only allow running 1 Thread per section.
- If somethinginterestingA() needs 10x more CPU; then you are out of luck
- (until the advanced Session which talks about Tasks and Nested Parallelism)

Single

- Single: Ensures a block is executed by only one thread (unspecified which)
- All other threads wait at an implicit barrier at the end of the single region
- Unless nowait is specified.
- You can still use PRIVATE and FIRSTPRIVATE clauses.

See example 03_single.c

Single

C/C++

```c
#pragma omp single
{
  something_only_for_one();
}
```

Fortran

```fortran
!$omp single

call something_only_for_one()

!$omp end single
```

Master

- The Master directive specifies that the enclosed code block is executed only by the master thread (thread 0).
- Unlike single, it has no implicit barrier at entry or exit, so other threads skip it and continue without waiting.
- It's often used for setup, I/O, or coordination work that must be done once without pausing the other threads.

Reduction operations

- Reduction operations
- Collapse

Reduction operations

- Performs a parallel reduction on a variable across threads.
- Each thread gets a private copy of var
- Updates it with
- At the end all copies are combined (reduced) into a single result.
- Common operators include +, *, max:, min:, etc.
- Why use a reduction?? Performance!

See example 04_reduction.c

Reduction operations

C/C++

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

Reduction operations

Fortran

```
integer, parameter :: N = 100
integer :: i, sum
integer :: data(N)

!$omp parallel do reduction(+:sum)
do i = 1, N
  sum = sum + data(i)
end do
!$omp end parallel do
```

Collapse

- When you use an omp parallel do/for you only parallelise the **outer** loop.
- With **COLLAPSE** we can tell the OpenMP library to treat the next 2, 3, 4 loops as one big loop and divide it to the available threads.

Collapse

In this example OpenMP will create 3 threads to parallelise the outer loop. This is obviously inefficient (in a machine with 128 cores; 125 will sit IDLE).

C/C++

```
int i, j;

#pragma omp parallel for
for (i = 1; i <= 3; i++) {
  for (j = 1; j <= 400; j++) {
    printf("Thread %d: i=%d, j=%d\n",
        omp_get_thread_num(), i, j);
  }
}
```

Collapse

Fortran

```
integer :: i, j
!$omp parallel do
do i = 1, 3
  do j = 1, 400
    print *, 'Thread', omp_get_thread_num(), 'i=', i,
        'j=', j
  end do
end do
```

Collapse

In this example OpenMP will divide the 1200 iterations to all available threads. Better usage of the 128 cores.

C/C++

```
int i, j;

#pragma omp parallel for collapse(2)
for (i = 1; i <= 3; i++) {
  for (j = 1; j <= 400; j++) {
    printf("Thread %d: i=%d, j=%d\n",
        omp_get_thread_num(), i, j);
  }
}
```

Collapse

Fortran

```
integer :: i, j
!$omp parallel do collapse(2)
do i = 1, 3
  do j = 1, 4
    print *, 'Thread', omp_get_thread_num(), 'i=', i,
        'j=', j
  end do
end do
```

Synchronisation

- barrier: makes all threads in a team wait until every thread has reached the barrier.
- critical: ensures the enclosed code block is executed by only one thread at a time.
- atomic: makes a simple memory update (e.g. count++) atomic at the hardware level.
- lock: creates user managed lock(s)
- ordered: Enforces the enclosed block to execute in sequential loop order.
- master: Specifies that only the master thread (thread 0) of the team executes the block.
- masked (OpenMP 5.0+): Runs a block on a subset of threads. Without a filter, it behaves like master (only thread 0 executes).

Barrier

#pragma omp barrier

- All threads stop at this point until every thread in the team reaches it.
- It ensures that no thread proceeds past the barrier before the others have caught up.
- Useful for synchronizing phases of work across threads.

Barrier

The second function will only be called once all threads have finished executing the first one.

C/C++

```
#pragma omp parallel
{
  calculate_critical_mass();
  #pragma omp barrier
  simulate_explosion();
}
```

Barrier

The second function will only be called once all threads have finished executing the first one.

Fortran

```
!$omp parallel
call calculate_critical_mass()
!$omp barrier
call simulate_explosion()
!$omp end parallel
```

Critical

#pragma omp critical [(name)]

- Only one thread at a time can execute the block of code marked critical.
- Threads wait their turn to enter, preventing race conditions on shared data.
- This is straightforward but can become a bottleneck if the protected code is slow.
- Use this to protect updates to shared data when atomic cannot be used.

Critical

Sum will be updated correctly. DO NOT DO THIS. USE A REDUCTION!!

C/C++

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

Critical

Sum will be updated correctly. DO NOT DO THIS. USE A REDUCTION!!

Fortran

```
!$omp parallel do
do i = 1, Ni
!$omp critical
  sum = sum + array(i)
!$omp end critical
end do
!$omp end parallel do
```

Atomic

#pragma omp atomic

- Protects a single memory update so it happens without interference from other threads.
- It's lighter weight than critical because it's limited to simple operations (e.g., increments, sums).
- Ideal for fine-grained synchronization on shared variables

Atomic

Sum will be updated correctly. DO NOT DO THIS. USE A REDUCTION!!

C/C++

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

See example 04_reduction.c

Atomic

Sum will be updated correctly. DO NOT DO THIS. USE A REDUCTION!!

Fortran

```
!$omp parallel do
do i = 1, Ni
!$omp atomic
  sum = sum + array(i)
!$omp end critical
end do
!$omp end parallel do
```

See example 04_reduction.c

Critical vs Atomic

- Atomic uses hardware instructions
- Atomic does not use lock/unlock on entering/exiting the line of code
- Lower overhead

Lock

- You explicitly create and control a lock object with omp_init_lock(), omp_set_lock(), and omp_unset_lock().
- Locks give you more control over when and where mutual exclusion happens.
- They can protect complex or multiple code regions, but require careful pairing of set/unset to avoid deadlocks.
- Same functionality as a mutex/semaphore.

Lock

C/C++

```
omp_lock_t myLock;

(void) omp_init_lock(&myLock);
#pragma omp parallel
{
  (void) omp_set_lock(&myLock); // acquire lock
  important_function();
  (void) omp_unset_lock(&myLock); // release lock
} // End of parallel region
(void) omp_destroy_lock(&myLock);
```

Lock

Fortran

```
integer(kind=OMP_LOCK_KIND) :: myLock

call omp_init_lock(myLock)

!$omp parallel
  call omp_set_lock(myLock)       ! acquire lock
  call important_function()
  call omp_unset_lock(myLock)     ! release lock
!$omp end parallel

call omp_destroy_lock(myLock)
```

Reality Check: Locks, Critical, Atomic

- Critical sections serialise execution. They **destroy** scalability.
- Locks serialise execution. They **destroy** scalability.
- Atomic uses hardware instructions: CAS instructions.
- CAS instructions still need to fetch data (sometimes from another NUMA node)
- CAS: Compare-and-swap
- Fetching needs time.
- Atomic sooner (or later) **destroy** scalability.
- It's better to re-think/re-write the algorithm to allow **parallelisation**.

Ordered

- For use inside a parallel for, it forces the enclosed code to run in loop-iteration order.
- Only one thread executes the ordered block at a time, and in the correct sequence.
- Handy when most work is parallel but a small part must happen in strict order.

Ordered

C/C++

```
#pragma omp for ordered
for (i=0; i<n; i++) {
  #pragma omp ordered
  work(i);
}
```

Lock

Fortran

```
!$OMP    DO ORDERED
DO I = 1,N
  !$OMP         ORDERED
  CALL WORK(I)
  !$OMP         END ORDERED
END DO
!$omp end parallel do
```

Master

#pragma omp master

- The enclosed code is executed only by the master thread (thread 0).
- Unlike single, it has no implicit barrier before or after, so other threads skip it and keep going.
- Useful for setup, teardown, or I/O handled by a single designated thread.
- Or for MPI operations. Usually, the MPI library requires the Master thread to make MPI calls.

Masked

#pragma omp masked

- Similar to master, but lets you specify which thread(s) should execute the region via a filter expression.
- For example, filter(omp_get_thread_num()==1) would make only thread 1 run the block.
- Other threads skip the block and can continue without waiting.
- Gives more flexibility than master for designating work to a specific thread in the team

Utilities

- omp_get_num_threads() : How many threads we are using
- Careful; will always return 1 if run **outside** a parallel section
- omp_get_thread_num() : Returns our Thread number

Utilities

C/C++

```
#pragma omp parallel
{
  CODE
}
```

Fortran

```
!$omp parallel

CODE

!$omp end parallel
```

C/C++

```
#pragma omp parallel
{
  FUNCTION  <== NUM_THREAD
}
```

Fortran

```
!$omp parallel

FUNCTION  <== NUM_THREAD

!$omp end parallel
```

Outline

1. Motivation for OpenMP
   - Simplicity and Portability
2. Introduction
   - Shared Memory Systems
   - Threaded Programming Model
   - Thread Sharing Data Example
   - Synchronisation
   - Parallel Loops
   - Synchronisation Example
3. OpenMP Basics
   - Parallel Regions
   - Data Sharing
   - Work Sharing
   - Reductions
   - Synchronisation
   - Utilities
4. Wrap-Up

Summary

- Tips and Tricks
- Performance
- Resources

Tips and Tricks

- Creating and starting a Parallel section takes time.
- The optimised code must be worth it (it must runs for at least for a couple of seconds).
- If the optimised code doesn't always run long enough all the time; use the IF clause.
- NOWAIT can help; however, it can cause also cause race conditions.
- CHUNKSIZE is important. It should be tuned. It can be changed at RUNTIME (which is always helpful).

Tips and Tricks

- MASTER, SINGLE and MASKED are useful. However, MASTER is the one with lowest overhead. SINGLE and MASKED require some synchronisation.
- However, if you don't know beforehand which THREAD will reach the directive first; best to use SINGLE. Most of the time this will be quicker than waiting for the MASTER thread to arrive.

Tips and Tricks

- Never, ever, ever use default(shared).
- Never, ever, ever have a parallel section without a default (most implementations default to shared).

Tips and Tricks

- I found the section of my code that takes up most of the runtime ...
- ... but it's a FOR/DO loop with hundreds lines of code!!!
- How do I set the PRIVATE and SHARED variables??
- You said to never use default(shared)!!

Tips and Tricks

- You need to put that code into a function.
- Use the SCOPE attributes of C/C++ and Fortran and pass everything as an argument to the function.
- Everything else can be a local variable inside the function.
- Test.
- If everything works; start adding PARALLEL sections.

Tips and Tricks

- Sometimes; you will need to refactor your code. Either because it's on the verge of the standards or because it has already fallen off and it compiles/works with a specific compiler and runs on a specific hardware.

Tips and Tricks

Handy and useful environment variables:

- OMP_WAIT_POLICY=active : Tell the OpenMP runtime to spin IDLE threads; instead of putting them to sleep.
- OMP_DYNAMIC=false : Tell the OpenMP runtime to allocate exactly the number of threads you asked for.
- OMP_PROC_BIND=true : Stop threads from migrating and destroying data locality.

Tips and Tricks

- Modern debuggers support OpenMP (gdb, DDT, TotalView).
- For Race Conditions you need other tools.
- SUN Studio, Intel Inspector (or the Intel Studio), Valgrind DRD, Clang ThreadSanitizer

Tips and Tricks

Timers:

- Don't use clock() or other system timers. They don't work well with OpenMP.
- "srun time myapplication.exe" will give you the correct overall duration of your application.
- Use omp_get_time(). It works perfectly with OpenMP.

Performance

I've gone through your excellent training and optimised my code using OpenMP. I got a 2% speedup!!

- Sequential Code
- Synchronisation
- Scheduling / Idle Threads
- Communication
- Hardware resources

Performance: Sequential Code

- Anything that is not parallelised (outside PARALLEL section, inside MASTER, SINGLE sections) runs sequentially.
- Amdahl's law[2] states that the maximum speedup is limited by the unparallelised code.
- If exactly 50% of the work can be parallelized, the best possible speedup is 2 times.
- If 95% of the work can be parallelized, the best possible speedup is 20 times.

[2] `https://en.wikipedia.org/wiki/Amdahllaw`

Performance: Sequential Code

Solutions:

- Try to parallelise everything :-)
- If you can't, then understand the limitations of your code.

Performance: Synchronisation

- Whenever we synchronise; there is implicit communication between the Threads.
- Communication uses hardware resources (next slides); uses CPU time; sometimes destroys data locality.
- CRITICAL, ATOMIC, LOCKS are points where we lose performance.

Performance: Synchronisation

Solutions:

- Minimise barriers. You may need to refactor your code.
- Use NOWAIT; but be careful.
- Use ATOMIC rather than CRITICAL or LOCKS. But know that every time you use it; you lose performance.

Performance: Scheduling / Idle Threads

- More often than not (always); some threads finish first and wait for the others.
- When they wait; they are IDLE. They are not doing anything helpful.
- When multiple Threads reach a CRITICAL section; they start to wait.
- Even worse, they have to talk to each other to pass through the CRITICAL section one at a time.
- Not only they wait and do nothing; they are actually using Hardware Resource to talk to each other!!!

Performance: Scheduling / Idle Threads

- The wrong scheduling type or chunksize can have very bad effects.

C/C++

```
#pragma omp parallel for schedule(dynamic, 1)
for(int i=0; i < 50000000; i++) {
  CODE
}
```

- The OpenMP runtime will not be very happy about our choice of scheduler and chunksize.

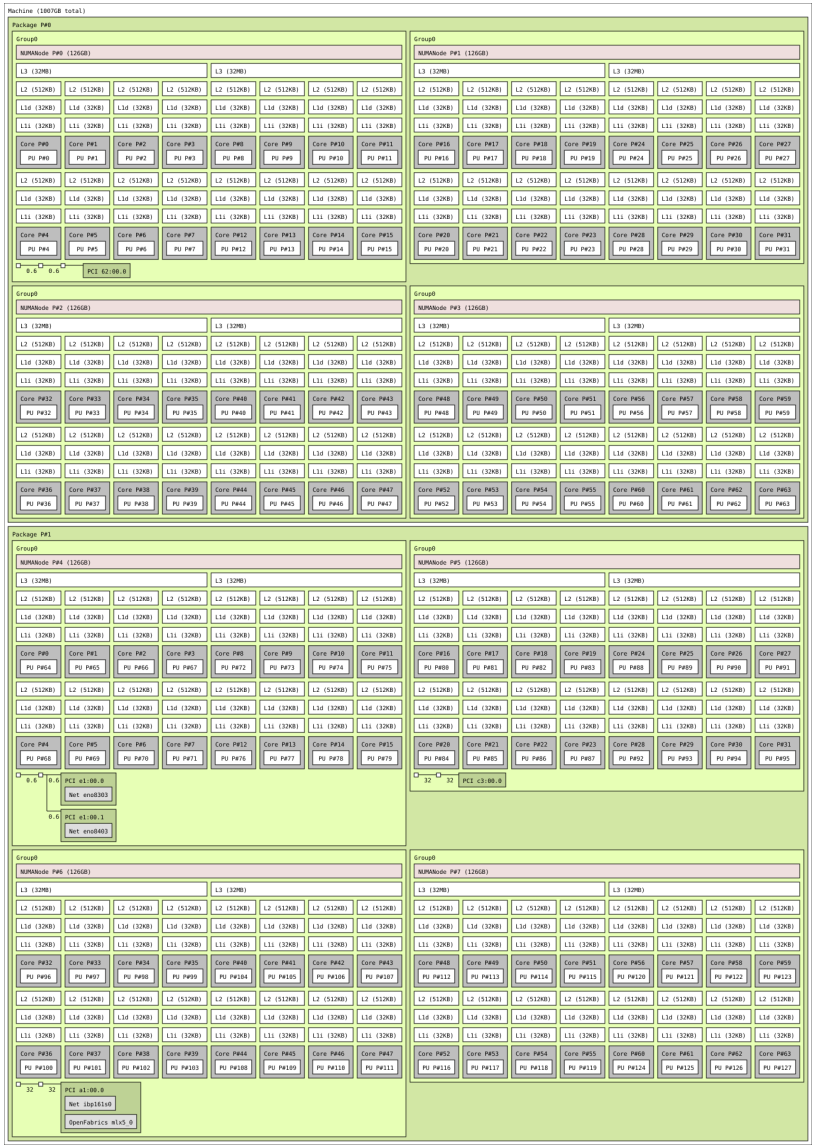
See example 05_scheduler_atomic.c

Performance: Scheduling / Idle Threads

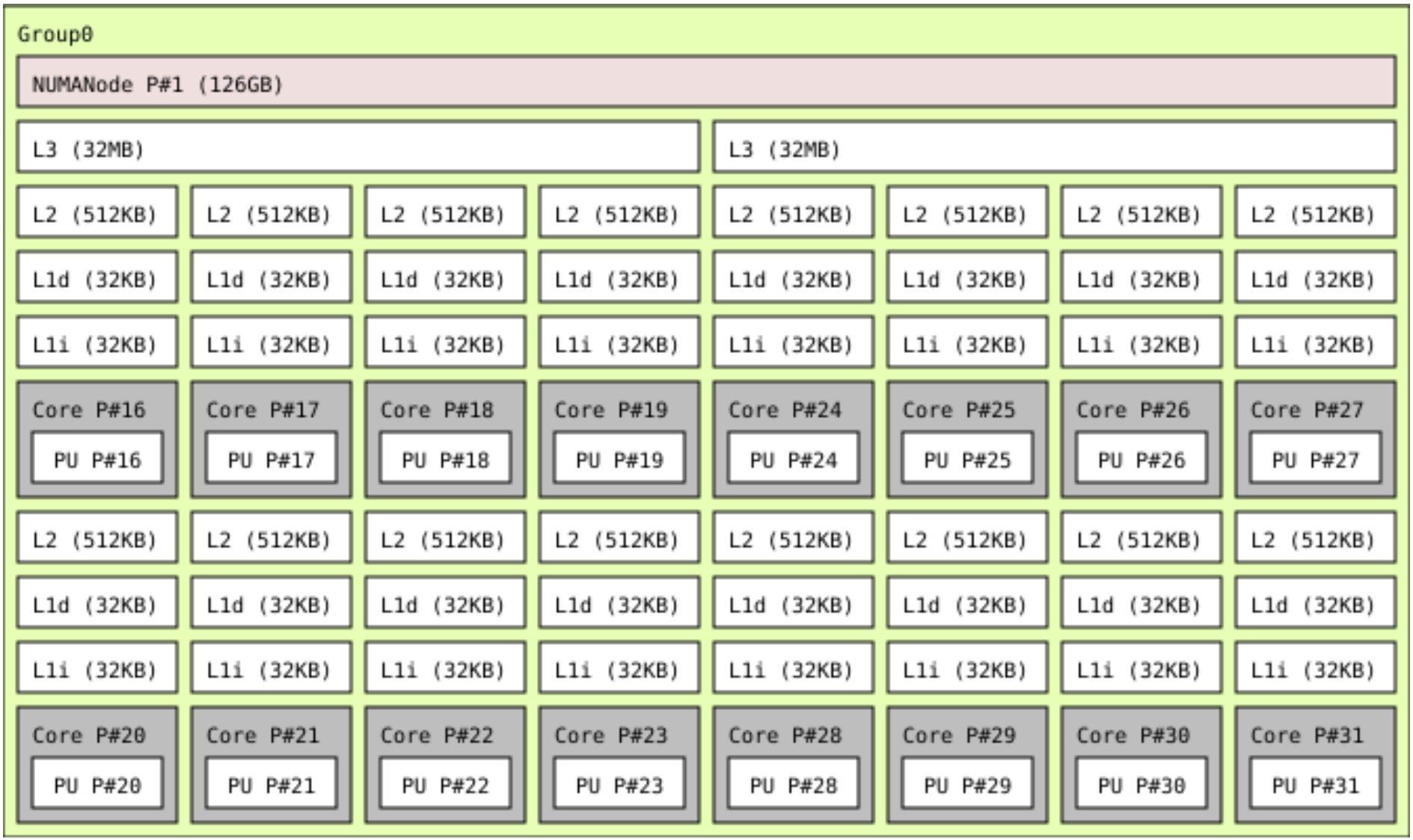
Solutions:

- Use sensible SCHEDULE parameters. Experiment with different schedulers.
- Use sensible CHUNKSIZE values. Experiment with different values.
- Too big CHUNKSIZE and you risk some THREADS finishing early and wait.
- Too small CHUNKSIZE and you will cause scheduling overheads and synchronisation bottlenecks in the OpenMP runtime.
- Ideally, we want all threads to finish at the same time.

Performance: Communication



Performance: Communication



Performance: Communication

- Accessing DATA from Memory is really slow (compared to CACHE).
- Really slow means hundreds to thousand times slower.
- If we need to access memory from a remote NUMA node; that's even worse.
- And that's only about reading.
- Every READ (and WRITE) operation goes through the Cache Coherency Mechanism.

Performance: Communication

When we write (modify) data; things become really expensive. When a THREAD (running on CPU#1) writes some data:

- The Cache Coherency fetches the data (from wherever) and brings it to the local CACHE (L3, L2 or L1).
- **All** other copies of that memory are invalidated on all the other CACHEs of all the other CPUs (to avoid reading stale data).
- If another Thread on another CPU wants to read the same data; the Cache Coherency Mechanism needs to fetch and propagate that Memory location to the local CACHE (L3, L2 or L1) of that CPU.
- Imagine if our Threads write to some memory that other Threads need to read. Say goodbye to any performance improvements.

Performance: Communication

Solutions (kind of):

- We need to use Data Affinity!
- This means that we should (as much as possible) access (READ/WRITE) the same data with the same THREAD
- Try to use large contiguous memory areas (don't update single INT8)
- We can then use CACHEd data (ten to hundred times faster than local memory)
- Use OMP_PROC_BIND=true to help pin the threads.

Performance: Communication

More problems with NUMA (most systems):

- Most Operating Systems employ the first touch policy.
- The first touch policy essentially tells the Memory Subsystem to place memory closest to the THREAD (or PROCESS) that asked for the memory.
- That makes sense for sequential applications. The memory is now in the local NUMA node and hopefully in the CACHE as well.
- It doesn't work for parallel applications.
- Especially if initialisation is done by the MASTER thread. Everything is now in the MASTER thread NUMA node; and everyone else have to wait for the data to trickle across.

Performance: Communication

Solutions (kind of):

- For OpenMP (and parallel applications in general); it's better to initialise in a parallel section.
- Try to keep the data local. Try not to change the loop iteration forcing data to migrate to other CPUs (or even worse other NUMA nodes).
- Use numactl (on Linux) to change the NUMA policy.

Performance: Communication

More problems:

- Memory is written in 4KB and 16KB pages.
- Some (most) systems use huge pages (2MB, 4MB, 1GB).
- Operating Systems like larger pages because they have to handle less pages overall.
- Less TLB (Translation Lookaside Buffer) misses, mean higher memory access.
- However, if our stride is more than the page size; we will go through the huge pages like a knife through butter.

Performance: Communication

We write an int8 at i*2MB+1byte :

- The TLB updates the mapping of the virtual page to the physical memory frame.
- The CPU fetches the 64 bytes cache line containing the target byte into L1 (read-for-ownership), modifies 1 byte, and later evicts the dirty line.
- For a 1 byte update; we get a 64 bytes read traffic and 64 bytes write traffic (assuming that each CACHE line size is 64 bytes).
- If the same CACHE line was in any other CPU; it needs to get invalidated.
- Since we never use this line again; we don't get the benefits of the CACHE system.
- Soon we start incurring extra costs; because the TLB misses will start to increase.
- Imagine this scenario with tens or hundreds of THREADs running at the same time.

Performance: Communication

- And to give a name to this problem: False Sharing.
- We discussed how CACHEs, CACHE line size Memory and the Cache Coherency Mechanism work.
- If we have THREADs updating a single int8, the whole CACHE line get's invalidated.
- What if we have a SHARED array of int8 counters and each THREAD updates it's own index.

C/C++

```
counter_array[omp_get_thread_num()]++;
```

Performance: Communication

- The previous code looks innocent enough.
- However, each update of an index; will invalidate the surrounding 64 bytes.
- The surrounding 64 bytes are 64 entries which will need to start their journey around the NUMA node(s).
- Invalidating all copies. And fetching the new value from the THREAD that did the original update.
- The next THREAD comes along and updates it's copy (which has been just fetched from who knows where).
- Once the update takes place, **all** the other copies will get invalidated again.
- Say a big goodbye to your memory bandwidth and to performance.

See example false_sharing.c

Performance: Hardware resources

Memory bandwidth / Caches:

- As we have seen; memory bandwidth (which is limited) can be exhausted really easily.
- False sharing.
- Not using Data Locality.
- Not using Data Affinity.
- Most systems share a level of CACHE (usually L3)
- Using multithreaded applications, CPUs fight for the same resource. Sometimes, using the whole resource for themselves.

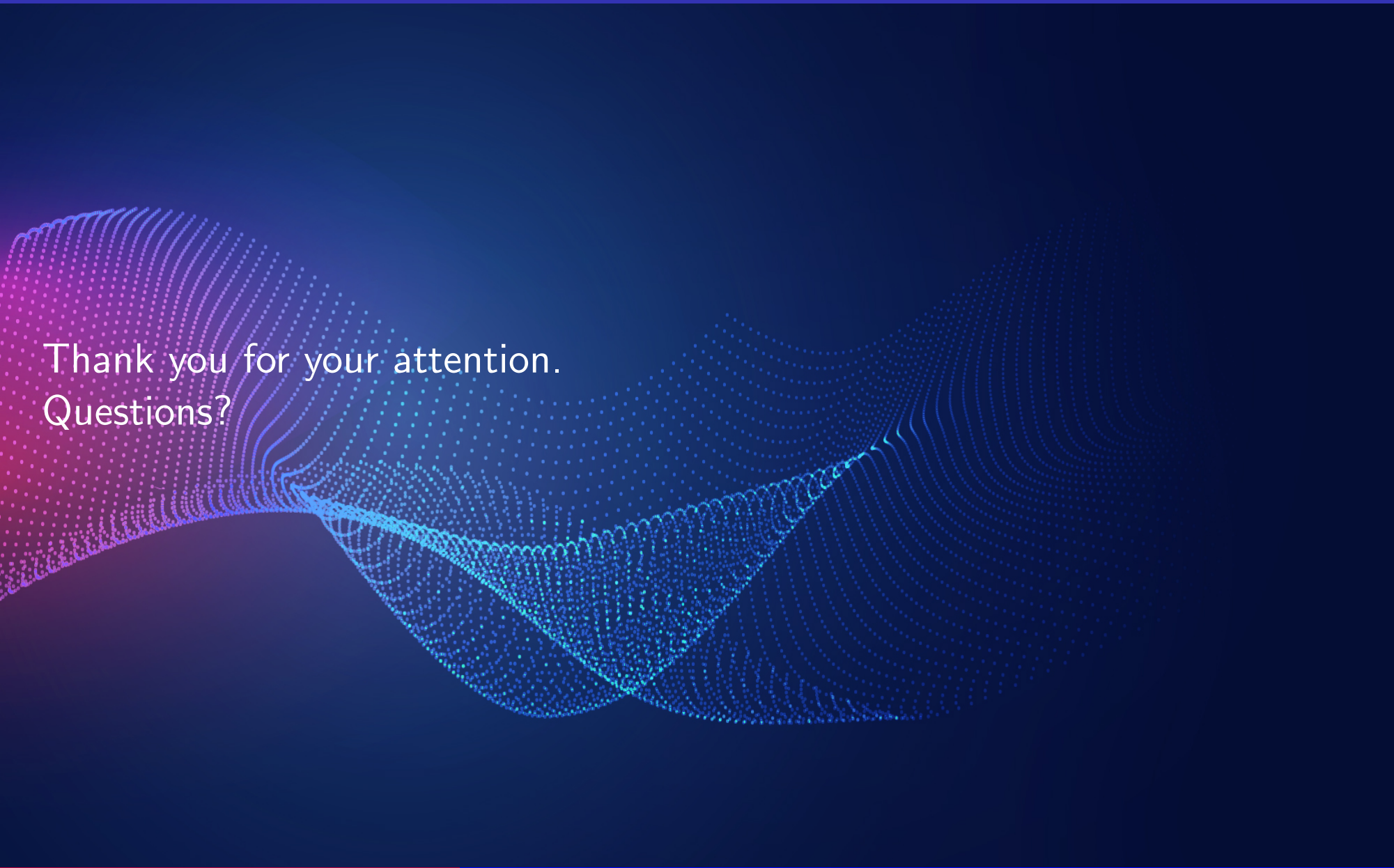
Performance: Hardware resources

- CPU instructions and instructions CACHEs are not infinite.
- For compute intensive codes; they can run out and THREADs have to wait.
- On the other hand, when THREADs wait for memory resources; even compute intensive codes can run happily.
- Don't oversubscribe (unless you are testing).
- Using more THREADs than COREs destroys data locality and is really slow.
- Using more THREADs than COREs is a nice test for your implementation. Sometimes, it makes hard to detect race conditions more prominent.

Resources

- OpenMP: `https://openmp.org`
- OpenMP: `https://www.openmp.org/resources/openmp-presentations/`
- Varis HPC centers and documentation (EPCC, HLRS, LLNL, others)

Questions



Thank you for your attention.
Questions?