L2: C for High Performance

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Master Calcul Haute Performance et Simulation - GLHPC | UVSQ

- 1. C for High Performance
- 2. Managing Memory
- 3. Compilation & Assembly
- 4. Parallelism Basics

C for High Performance

Why C, C++, Python?

Programming occurs at several abstraction levels from the hardware

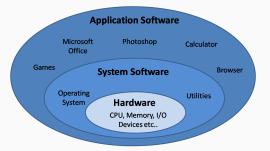


Figure 1: Hardware to Software layers (https://www.startertutorials.com/blog/basic-software-concepts.html)

Why C, C++, Python?

- · Layers close to metal are harder to program...
 - But they offer maximum control and performance
- High-level abstraction maximize productivity...
 - But have significant overhead, less control over performance

In practice; we often combine multiple languages

 C for performance critical sections, python for higher level APIs

	low level	mid/high level	high level	scripting
	Assembler	C/C++	Java/C#	Python
Development speed				*
Performance	-			
Low-level optimization	++	+	-	-
Meta programming	+	++	-/+	+
Cross-platform support	individual code for each platform	compiled everywhere	compiled once, run everywhere	interpreted on many platforms
Supporting OOP	-	+	+	+
Type of linking	mostly static	static/dynamic	dynamic only	n/a

Figure 2: Hardware to Software layers (Shershakov, Sergey. (2018). Enhancing Efficiency of Process Mining Algorithms with a Tailored Library: Design Principles and Performance Assessment Technical Report. 10.13140/RG.2.2.18320.46084.)

C Programming - Operations and Typing

C is a strongly typed imperative language:

```
int main() {
  int a = 5;
  int b = 10;

  int c = a + b;
  float d = c / a;
  float e = (float)c / a;

  int f = a * a * a * a;

  return 0;
}
```

main is the program entry point.

C Programming - Functions

```
#include <stdio.h> // For printf(...)
int sum_and_square(int a, int n) {
 int tmp = a + n;
 return tmp * tmp;
int main() {
 int a = 5;
 int b = 4:
  int c = sum_and_square(a, b);
  int d = sum and square(3, 9);
 // Print the result to the console
 printf("(5+4)**2: %d\n", c);
 printf("(3+9)**2: %d\n", d);
 return 0;
```

C Programming - Loops

Implementation C de $\sum_{i=1}^{100} i$

```
#include <stdio.h> // For printf(...)
int sum_range(const int start, const int end) {
  int sum = 0:
 // Consider start = 0: end = 100
 // For i starting at 0; while i <= 100; increment i by one
 for (int i = start: i <= end: i = i + 1) {
    sum += i:
 return sum;
int main() {
 printf("Result: %d\n", sum_range(1, 100));
 return 0;
```

const qualified variable cannot be modified. This may enable optimizations during compilation.

C Programming - Conditions

Numbers of multiple of 3 inside [0, 99] (i.e. $i \mod 3 = 0$)

```
void count_multiples_of_three() {
  unsigned int count = 0;
  // For i starting at 0; while i < 100; increment i by one
  for (unsigned int i = 0; i < 100; i++) {
    // if i % 3 (Remainder of the integer division) is equal to 0
    if (i % 3 == 0) {
      count++;
    }
  }
  printf("Result: %d\n", count);
}</pre>
```

Note

Here we could also do for (unsigned int i = 0; i < 100; i += 3)

C Programming - Basic Pointers

```
int a = 0;
int b = 5;
int* c = &a;
*c = *c + b;
printf("a: %d; b: %d; c: %d\n", a, b , *c);
```

c contains the address of a; so *c = *c + b write in a the sum of a and b.

Adress	Value	Variable
0x004	0	a
800x0	5	Ь
0x00c	0×004	С
	•••	

C Programming - Arrays

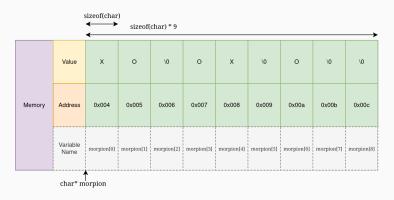


Figure 3: Morpion layout in memory

C Programming - Structures

Structures are user-defined composite types:

```
typedef struct {
  char* first_name;
  char* last_name;
  int age;
  float mean_grade;
  char gender;
} Student;
```

C has no concept of class, object, or method!

C programming - Structures 2

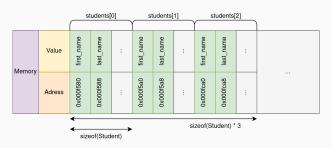


Figure 4: Array of Structure (AoS) layout

C Programming - Trading Abstraction for performance

In C, we must manually take care of very low level concepts

- We care about data layout, memory addresses, pointers, etc.
- The language doesn't provide linked lists, dynamic arrays, dictionaries, etc.
- · No basic algorithms like sorting

On the flip side, we can

- Manually lay out data to maximize efficiency
- Remove any abstractions and overhead to maximize performance
- Generate code that runs as close to the metal as possible
- Optimize our program for the hardware

C Programming - Trading Abstraction for performance (Example)

Consider the following python and C code:

```
sum = 0
for i in range(ub):
    sum += i
print(sum)
```

```
unsigned long long sum = 0;
for (unsigned int i = 0; i < ub; i++){
    sum += i;
}
printf("Sum of first %llu integers is: %llu\n", ub, sum);</pre>
```

Where ub is a very large number (100 Millions in this example). Which one is faster, and by how much?

C Programming - Trading Abstraction for performance (Example)

Results:

- c version: 0.024s
- Python version: 5.650s

That's a speedup of $\times 235$.

We will see later in this course how this is possible.

Numpy and other libraries

Note that we could use numpy or the sum python function: but those are actually implemented in c!

Managing Memory

Managing Memory - Concept

In High-level languages

- We operate on abstracted data structures (lists, dictionaries, etc.)
- Memory is managed automatically (allocation, resizing, deallocation)
- We don't care about memory alignment, stack vs. heap, page size, Numa effects, etc.

In C

- We perform directly with primitive data and raw memory
- We are responsible for allocation, layout, and cleanup
- We can only request chunks of raw memory, and fill it however we choose
- This is critical for performance

This low level control is critical for performance; hence we must understand how memory works under the hood!

Managing Memory - Memory Types

We can distinguish two types of memory

- Memory automatically allocated by the compiler on the stack.
 - Stores variables, functions arguments, etc.
 - Fast but limited in size
- Memory that is (manually) dynamically allocated on the heap
 - Must be allocated and freed by the developer!

The kernel (Linux / Windows) allocates **memory pages** and operates at a coarse grain level.

The standard library (11bc) manipulates pages on a finer scale and provides memory to the user.

```
#include <time.h> // for time
#include <stdlib.h> // For malloc, srand, rand
int do_the_thing(int n) {
 // We allocate n numbers
 float* numbers = malloc(sizeof(float) * n);
  // We seed the random number generator
  srand(time(NULL)):
 // We generate nsamples random numbers
  for (int i = 0; i < n; i++) {
   numbers[i] = (float) rand() / RAND_MAX; // Generate a number
    in [0, 1]
  ... // Do something complicated here
  free(numbers); // Release memory back to the kernel
 return 0;
```

Managing Memory - Allocation

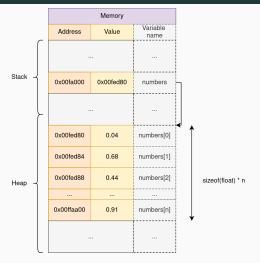


Figure 5: Results of memory allocation

malloc returns a pointer to the beginning of the allocated memory range

Managing Memory - Deallocation

Memory is not infinite!

In Python (and Java, C#, etc.); memory is managed by the garbage collector (GC):

- The runtime tracks all memory allocations; and all reference(s)
- When a memory block is not referenced by the program; the GC will release the memory back to the kernel.

In C/C++, the user must deallocate memory using free(ptr).

Memory leak

If memory is not freed (memory leak) the computer can run out:

- · The kernel can kill the program
- The OS can crash
- Other applications requesting memory can crash or fail

Virtual And Physical Memory - Problem

- How can the kernel guarantee that memory is always contiguous?
- Can I acess memory from another program and steal their data?
- How can multiple applications share the same memory?
 - · Some variables have hard-coded addresses!
- How to handle (Internal/External) fragmentation (Empty slot)?

Virtual And Physical Memory - Concept

We separate Physical Addresses (locations in memory) from Virtual Addresses (Logic locations) seen by each program!

- Physical memory is divided into small fixed-size blocks called pages (typically ~4KB).
- The CPU includes a **Memory Management Unit** (MMU) that translates virtual addresses into physical addresses.
- Each program is given its own isolated virtual address space.
- The kernel maintains a **page table** for each program that tells the MMU how to translate addresses.

The Illusion of contiguity

Each process believes it has acces to a large, contiguous block of memory; while it can be physically fragmented or shared.

Virtual And Physical Memory - Diagram

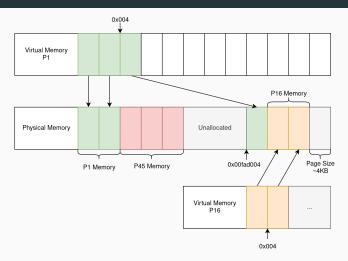


Figure 6: Virtual And Physical Memory

*Note that this is a simplified representation.

Memory Hierarchy

Which memory are we talking about?

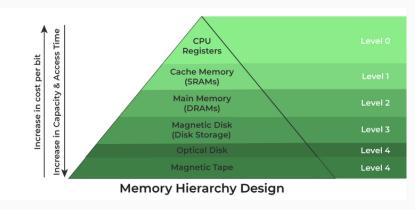


Figure 7: Memory Hierarchy (https://www.geeksforgeeks.org/memory-hierarchy-design-and-its-characteristics/)

Note that GPU(s) also have their own separate memory!

Memory Hierarchy

- CPU computations are extremely fast, and memory access can be a bottleneck
 - Registers have the lowest latency
 - CPU caches (L1, L2, L3) act as fast buffers for memory
- DRAM (main memory) is much slower, but cheaper and larger
 - Accessing DRAM causes significant delays compared to cache

To achieve high performance, we must maximize data reuse in registers or caches, and minimize DRAM access.

CPU Caches

Most CPU have 3 levels of cache

- L1d First Level Cache (Very fast)
- L2 Second Level Cache (Fast)
- L3 (Last Level Cache LLC) (Larger but slower than L1/L2)

Some cache level are per-core (L1, often L2) whereas others are shared between multiple cores (L3).

Instruction Cache

The assembly instructions are stored in a separate (L1i) instruction cache

CPU Caches

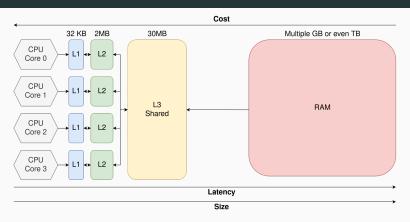


Figure 8: CPU Latency and Cache

We speak of **Heterogeneous Memory Hierarchy**: the same memory accesses can have different latency depending on where the data resides!

[Live example: LSTOPO]

CPU Caches - In practice

```
for (int i = 0; i < n; i++) {
  T[i] = A[i] * B[i];
}</pre>
```

- The cache controller looks-up the data inside the CPU cache (L1 -> L2 -> L3)
- 2. If available, data is sent to register for the ALU
- 3. Else, a memory request is emitted
 - This introduces latency and a bubble in the CPU pipeline
- 4. When the memory request is resolved; execution resumes
- 5. The results of $a \ast b$ is written to cache, and eventually back to main memory later on.

CPU Caches - In practice

In practice:

- The CPU fetches entire cache line (Often 64 Bytes) at once (If float: 64B/4B=16 values at once)
- The CPU can prefetch data: it learns data access patterns and anticipates future memory access.
- The CPU can execute **out-of-order**; independent instructions are executed while the memory request is in flight.

Caches CPU - Strided Access

Consider two NBody 3D implementations:

Array Of Structure (AoS)

```
// We allocate N tuples of (x, y, z) positions
float* positions = malloc(sizeof(float) * N * 3);
```

Structure Of Array (SoA)

```
// We allocate separate arrays for each components
float* x = malloc(sizeof(float) * N);
float* y = malloc(sizeof(float) * N);
float* z = malloc(sizeof(float) * N);
```

Caches CPU - Strided Access

We want to record the number of particles with $x \leq 0.5$

Array Of Structure (AoS)

```
for (int i = 0; i < N; i += 3)
  if (positions[i] < 0.5)
    count++;</pre>
```

Structure Of Array (SoA)

```
for (int i = 0; i < N; i++)
  if (x[i] < 0.5)
    count++;</pre>
```

Which one is faster; and why?

Which access pattern makes better use of cache lines?

Caches CPU - Strided Access

Perf results summed across 100 runs:

	Time	# Instr	# L1 Loads	# L1 Miss	# LLC Loads	# LLC Miss
AoS	~1.93s	~14 Billion	~3.5 Billion	~1 Million	~400k	~382k
SoA	~1.75s	~14 Billion	~3.5 Billion	~300k	~24k	~15k

	# Cache references (LLC)	# Cache miss
AoS	~158 Million	~151 Million
SoA	~52 Million	~35 Million

With AoS more load fail in the L1, leading to LLC accesses.

Most LLC loads still results in misses, leading to DRAM access.

Compilation & Assembly

Compilation & Assembly - Introduction

C is a compiled language: we must translate the source code to assembly for the CPU

```
gcc ./main.c -o main (<flags>)
```

- Python is interpreted
 - More flexible but significantly slower
- C# and Java are compiled to intermediary bytecode and then executed via a virtual machine (or JIT-ed)
 - Balances performance and productivity
- C/C++/Rust are compiled to assembly code
 - Poor portability, but no intermediary.

Compilation & Assembly - Simple Loop

```
int sum = 0;
for (int i = 0; i < 100000; i++){
   sum += i;
}</pre>
```

```
main:
.LFB6:
   pushq %rbp
                                 // We record the stack pointer
   movq %rsp, %rbp
   movl $0, -4(%rbp)
                                // Initialize sum
   movl $0, -8(%rbp)
                              // Initialize i
   jmp .L2
.L3:
   movl -8(%rbp), %eax // Load sum to a register
   addl %eax, -4(%rbp) // Add i and sum (from memory) addl $1, -8(%rbp) // Add 1 to i (from memory)
.1.2:
   cmpl $99999, -8(%rbp) // Check if i < 100 000
   jle .L3
                                 // Jump Less Equal
            $0, %eax
                                 // Set the return value of main
   movl
   popq %rbp
                                 // Return from main
   ret.
```

Compilation & Assembly

Assembly is as close to the metal we usually get, and is architecture dependant:

- Intel and AMD use the x86 Instruction Set
- x86 has multiple extensions (FMA, sse, avx, avx512, etc.)
- To maximize performance, we should compile our applications on each platform
 - Our binaries are not portable
 - But we can use dedicated instructions
- Other instructions set exists (ARM, Risc V, etc.)

Compilation & Assembly - Optimization passes

The compiler is not just a translator:

- The compiler can generate optimized instructions from our program
- Constant values can be propagated, unused values/code removed
- Operations can be reordered, inlined, vectorized using SIMD, etc.
- · Many, many more optimizations

Those optimizations are enable through flags such as -01, -02, -03 which are predefined sets of optimization passes.

The flag -march=native allows the compiler to target the current machine for compilation and use all the available ASM extensions.

Compilation & Assembly - Compiler Pipeline

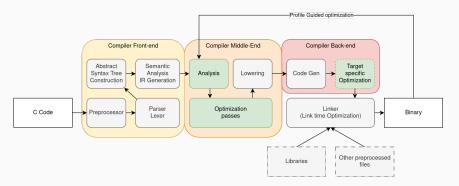


Figure 9: C Compiler Workflow

There are several compilers with varying performance and features:

- GCC and Clang-LLVM (The classics)
- MSVC (Microsoft), mingw-LLVM, arm-clang (For ARM) and many, many others.

Makefile Basics - Introduction

Make is a scripting tool to automate complex compilation workflows. It works by defining rules inside **Makefiles**.

```
CC := gcc
CFLAGS := -g

main: main.c my_library.c my_library.h
$(CC) -o $@ $^ $(CFLAGS)
```

- main is the target (What we want to build)
- main.c my_library.c my_library.h are the dependencies: rule reruns if any change
- \$(CC) -o \$@ \$< \$(CFLAGS) is the recipe
- \$@ expands to the target name
- \$^ expands to all dependency

Makefile Basics - Phony rules

Makefiles expects that a rule main produces a file called main. However, not all rules produce files:

```
.PHONY: all clean
all: main mylibrary
...
clean:
  rm -rf *.o
  rm -rf ./main
```

Here, make all will be an alias to build everything, while make clean is a custom rule to clean all build artifacts. Makefile has many, many other functionalities, outside the scope of this course.

Makefile Basics - Usage

The typical projects looks something like:

```
Project/
src/
main.c
my_library.c
include/
my_library.h
Makefile # We define the Make rules here
```

make will look for a file in the cwd named Makefile or makefile. You can directly call make all, make clean, etc.

Parallelism Basics

Parallelism Basics - Introduction

Compiler optimization is only one side of high peformance computing.

If you remember; we saw in LSTOPO that our CPU has many cores:

- Every core can perform computations independently of the other
- Multiple process (Google, vscode, firefox, excel) can run simultaneously on different cores.
- The kernel manages execution through thread scheduling and time-slicing

Main Thread

Every process has at least one "thread of execution", which is an ordered sequence of instructions executed by the CPU.

Parallelism Basics - Introduction

What if we could split our programs into multiple threads?

- If we have 1 thread only one computation happens at a time
- If we have 2 threads, we can potentially double throughput!

In practice, there is some overhead, we must handle dependencies between instructions, etc.

Parallelism Basics - Types of parallelism

We consider three main types of parallelism

- Single Instruction Multiple Data (SIMD): also called Vectorization
 - single instruction operates simultaneously on multiple data elements.
- Shared Memory: Multiple threads inside the same memory space
 - Threads share a memory space, enabling fast communication and synchronization.
- Distributed Memory: Multiple processes
 - Communications are slower, but this model enables scaling across multiple machines.

For this course, we will only focus on SIMD and Shared Memory parallelism.

Parallelism Basics - Shared Memory

Consider the following loop:

```
int sum = 0;
for (int i = 0; i < 100; i++)
   sum += i;</pre>
```

We can slice the iteration space in multiple chunks:

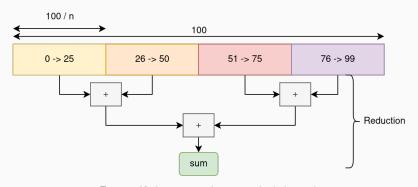


Figure 10: Iteration slicing with 4 threads

Parallelism Basics - Shared Memory

We split the program into multiple instruction sequences running in parallel.

- Every thread operates a sum on a subset of the data
- We synchronize every thread and combine the partial sums via a global reduction.

OpenMP is an HPC tool designed for scenarios like this!

It's a simple to use library/compiler pass to parallelize trivial loops.

```
int sum = 0;
#pragma omp parallel for reduction(sum: +)
for (int i = 0; i < 100; i++)
   sum += i;</pre>
```

```
gcc ./main.c -fopenmp -03 -march=native
```

This directive automatically distributes the loop iterations across all available CPU cores, performing a thread-safe reduction on sum.

Parallelism Basics - OpenMP details

OpenMP defines a set of clause which are operations followed by a set of modifiers.

- #pragma omp: is the start of all OpenMP clauses
- parallel: enable the creations of multiple threads
- for: toggle the automatic slicing of following loop
- reduction(sum: +): toggles a reductions clause for sum using the + operation.

This code will be enough for most cases; but OpenMP allows for significantly more complex operations.

Parallelism Basics - Advanced OpenMP Example

```
float global_min = FLT_MAX;
int global_min_index = -1;
#pragma omp parallel
  float min value = FLT MAX;
  int min_index = -1;
#pragma omp for nowait schedule(dynamic)
  for (int i = 0; i < N; i++) {</pre>
    if (T[i] < min value) {</pre>
      min_value = T[i];
      min_index = i;
#pragma omp critical
    if (min_value < global_min) {</pre>
      global_min = min_value;
      global_min_index = min_index;
```

Naive NBody 3D Strong Scaling - Setup

We increase the number of threads while keeping the work size constant.

```
OMP_PLACES={0,2,4,6,8,10,12,14} OMP_PROC_BIND=True
OMP_NUM_THREADS=8 ./nbody 10000
sudo cpupower frequency-set -g performance
```

5 Meta repetitions per run, 13th Gen Intel(R) Core(TM) i7-13850HX @5.30 GHz, 32KB/2MB/30MB:L1/L2/L3 15GB DDR5.

Naive NBody 3D Strong Scaling - Results

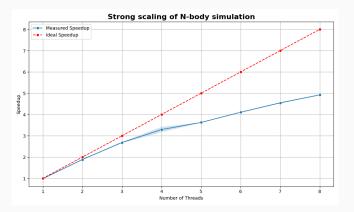


Figure 11: Speedup of Naive Gravitationnal NBody 3D

Speedup is limited by runtime overhead, concurrency, memory bandwidth, data size, etc.