Practical Debugging & Performance Engineering for High Performance Computing



Xavier Besseron LuXDEM Research Centre University of Luxembourg

SuperComputing Virtual Camp 2021





Overview

Part 1: Practical Debugging

- Tools for debugging
- List of common bugs
- Good practices to catch bugs

Part 2: Performance Engineering

- HPC hardware & performance bottlenecks
- Understanding CPU and memory
- Performance analysis and profiling tools

Practical Session

- Step-by-step tutorials
- Practical exercises



Part I

Know Your Bugs: Weapons for Efficient Debugging

- Introduction
- Tools for Debugging
 - Compilers
 - GNU Debugger
 - Valgrind
- Common bugs
 - Logic and syntax bugs
 - Arithmetic bugs
 - Memory related bugs
 - Multi-thread programming bugs
 - Performance bugs
- Good practices to catch bugs





Why debugging?

Bugs are in every programs

Industry Average:
 "about 15 - 50 errors per 1000 lines of delivered code"

Bugs in High Performance Computing

- Even more difficult due to concurrency
- Can crash super-computers
- Can waste large amount of CPU-time

Famous bugs and consequences

- Ariane 5 rocket destroyed in 1996: 1 billion US \$
- Power blackout in US in 2003: 45 million people affected
- Medtronic heart device vulnerable to remote attack in 2008
- ...



¹ Code Complete by Steve McConnell

Outline



- Compilers
- GNU Debugger
- Valgrind





Tools for debugging

Compilers

- It's the first program to check your code
- GCC, Intel Compiler, CLang, MS Compiler, ...

Static code analyzers

- Check the program without executing it
- Splint, Cppcheck, Coccinelle, ...

Debuggers

- Inspect/modify a program during its execution
- GDB: the GNU Project Debugger for serial and multi-thread programs
- Parallel debuggers (commercial): RogueWave Totalview, Allinea DDT

Dynamics code analyzers and profilers

- Check the program while executing it
- Valgrind, Gcov, Gprof, CLang sanitizers, ...
- Commercial software: Purify, Intel Parallel Inspector, ...



Compilers 1/2

What does a compiler do?

- Translate source code to machine code
- 3 phases:
 - Lexical analysis: recognize "words" or tokens
 - Syntax analysis: build syntax tree according to language grammar
 - Semantic analysis: check rules of the language, variable declaration, types, etc.
- With this knowledge, a compiler can find many bugs
- ightarrow Pay attention to compiler warnings and errors of a program

A compiler can find out if your program makes sense according to the language. However, it cannot guess what you are trying to do.



Compilers 2/2

How to use the compiler

Choose your compiler

	GCC	CLang	Intel Compiler
С	gcc	clang	icc
C++	g++	clang++	icpc
Fortran	gfortran		ifort

- Activate warning messages with the -Wall parameters
- Warnings can be enabled/disabled individually, cf documentation
- Compile with debug symbols with -g parameters

Example

```
program.c: In function 'main':
program.c:4:15: error: 'y' undeclared (first use in this function)
   int z = x + y;

program.c:4:15: note: each undeclared identifier is reported only once for each function it program.c:4:7: warning: unused variable 'z' [-Wunused-variable]
   int z = x + y;
```

\$ qcc -q -Wall program.c -o program

GNU Debugger 1/2

GDB is the GNU Debugger

- Allow to execute a program step by step
- Watch the value of variables
- Stop the execution on given condition
- Show the backtrace of an error
- Modify value of variables at runtime

Starting GDB

- Compile your program with the -g option
- Start program execution with GDB gdb --args myprogram arg1 arg2
- Or open a core file (generated after a crash) gdb myprogram corefile





GNU Debugger 2/2

Using GDB

- Command line tool
- Many graphical frontends available too: DDD, Qt Creator, ...
- Online documentation & tutorial:

http://sourceware.org/gdb/current/onlinedocs/gdb/ http://www.cs.swarthmore.edu/~newhall/unixhelp/howto_gdb.html

Main commands

- help <command>: get help about a command
- run: start execution
- continue: resume execute
- next: execute the next line
- break: set a breakpoint at a given line or function
- bracktrace: show the backtrace
- print: print the value of a variable
- quit: quit GDB





troduction Tools for Debugging Common bugs

Valgrind 1/3

Valgrind is a dynamic analysis tool

 Execute your program with dynamic checking tool: Memcheck, Callgrind, Helgrind, etc.

Memcheck: memory error detector

- Enable with --tool=memcheck (by default)
- Check for memory-related errors: unitialized values, out of bound access, stack overflow, memory leak, etc.
- For memory leaks, add option --leak-check=full
- http://valgrind.org/docs/manual/mc-manual.html

Callgrind: performance profiler

- Enable with --tool=callgrind
- Check the time you spend in each function of your code
- Visualize results with KCachegrind





Example: memory errors with Memcheck

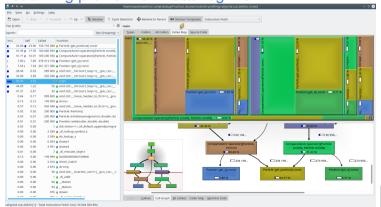
```
$ valgrind --tool=memcheck --leak-check=full --track-origins=ves ./program
[...]
==12534== Conditional jump or move depends on uninitialised value(s)
==12534==
             at 0x40055E: main (program.c:11)
==12534== Uninitialised value was created by a stack allocation
==12534==
             at 0x400536: main (program.c:5)
==12534==
==12534== Invalid write of size 8
==12534==
             at 0x4005CE: main (program.c:19)
==12534== Address 0x5203f80 is 0 bytes after a block of size 8,000 alloc'd
==12534==
             at 0x4C2BBA0: malloc (in /usr/lib/valgrind/vgpreload memcheck-amd64-linux.so)
==12534==
            by 0x400555: main (program.c:9)
==12534==
==12534==
==12534== HEAP SUMMARY:
==12534==
              in use at exit: 8,000 bytes in 1 blocks
==12534==
            total heap usage: 1 allocs. 0 frees. 8.000 bytes allocated
==12534==
==12534== 8,000 bytes in 1 blocks are definitely lost in loss record 1 of 1
==12534==
             at 0x4C2BBA0: malloc (in /usr/lib/valgrind/vgpreload memcheck-amd64-linux.so)
==12534==
            by 0x400555: main (program.c:9)
[ . . . 1
```

Example: profiling with Callgrind

\$ valgrind --tool=callgrind ./program



Example: Visualizing profile with KCachegrind





Outline



- Logic and syntax bugs
- Arithmetic bugs
- Memory related bugs
- Multi-thread programming bugs
- Performance bugs





Logic and syntax bugs

Due to careless programming

- Infinite loop / recursion
- Confusing syntax error,
 eg use of = (affectation) instead of == (equality)
- Hard to detect, because everything is correct in your mind

- Compile with warnings enabled
- Get some rest and/or an external advice



Integer overflow 1/2

Integer variables have limited size

	Size	Minimum	Maximum
signed short	16 bits	-2^{15}	2 ¹⁵ – 1
unsigned short	16 bits	0	$2^{16} - 1$
signed int	32 bits	-2^{31}	$2^{31}-1$
unsigned int	32 bits	0	$2^{32}-1$
signed long long int	64 bits	-2^{63}	$2^{63}-1$
unsigned long long int	64 bits	0	$2^{64} - 1$

If the result of an operation cannot fit in the variable, most-significant bits are discarded

 \Rightarrow we have an Integer Overflow



Integer overflow 2/2

Overflow example

→ No error at runtime!

- Use the right integer type for your data
- In C/C++/Fortran, overflow needs to be checked manually
- CLang and GCC 5.X offer builtin functions to check for overflow
 __builtin_add_overflow, __builtin_sub_overflow,
 __builtin_mul_overflow, ...



Floating-Point Number bugs 1/2

Floating-Point Exceptions (FPE)

Division by zero:

$$\frac{X}{0.0} = \infty$$

Invalid operation:

$$\sqrt{-1.0} = NaN (Not A Number)$$

Overflow / Underflow:

$$e^{1e30} = \infty$$
 $e^{-1e30} = 0.0$

Loss of precision

The order of the operations matters:

$$(10^{60} + 1.0) - 10^{60} = 0.0$$

 $(10^{60} - 10^{60}) + 1.0 = 1.0$



roduction Tools for Debugging Common bugs Good practices to catch bugs

Floating-Point Number bugs 2/2

Floating-Point Exceptions and Errors

- No error at runtime by default
- Errors can propagate through all the computation

What to do?

Enable errors at runtime in C/C++

```
#define _GNU_SOURCE
#include <fenv.h>
int main()
{
   feenableexcept(FE_DIVBYZERO|FE_INVALID| FE_OVERFLOW);
   ...
```

 Read "What Every Computer Scientist Should Know About Floating-Point Arithmetic" by David Goldberg

Memory allocation/deallocation

Dynamic memory management in C

- void *p = malloc(size) allocates memory
- free (p) de-allocates the corresponding memory
- In C++, equivalents are new and delete operations

Common mistakes

- Failed memory allocation
- Free non-allocated memory
- Free memory twice (double free error)

These mistakes might not trigger an error immediately Later on, they can cause crashes and undefined behavior

- Check return code (cf documentation)
- Use Valgrind with --leak-check=full to catch it



Memory leaks

Memory is allocated but never freed

- Allocated memory keeps growing until it fills the computer memory
- Can causes a crash of the program or of the full computer
- Very common is C program, almost impossible in Fortran, Java

- For each malloc(), there should be a corresponding free()
- Use Valgrind with --leak-check=full to catch it



oduction Tools for Debugging Common bugs Good practices to catch bugs

Using undefined values

Undefined values

- Uninitialized variable
- Not allocated or already freed memory

Can cause undefined/unpredictable behavior

- Difficult to track
- Error might not occur immediately
- It can compute incorrect result

- Compile with -Wuninitialized or -Wall
- Use Valgrind, it should show error
 Conditional jump or move depends on uninitialised value(s)



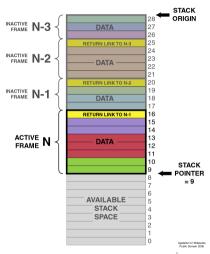
Stack overflow

Program stack

- Each function call create a new frame
- Function parameters and local variables are allocated in the frame

Stack overflow

- Too many function calls usually not-ending recursive calls
- Oversized local data



Buffer overflow

Buffer overflow

- Write data in a buffer with an insufficient size
- Overwrite other data (variable, function return address)
- Can be a major security issue
- Can make the stack trace unreadable

- Use functions that check the buffer size:
 strcpy() → strncpy(), sprintf() → snprintf(), etc.
- GCC option -fstack-protector checks buffer overflow



Out of bound access

Read/write outside of the bound of an array

- Mismatch in the bound of an array: [0, N-1] in C, [1, N] in Fortran
- Out of bound reading can cause undefined behavior
- Out of bound writing can cause memory corruption

What to do?

Use Valgrind, it should show error
 Invalid read/write of size X



Input/Output errors

Errors when reading/writing in files

- Usually have an external cause:
 - Disk full
 - Quota exceeded
 - Network interruption
- System call will return an error or hang

- Always can check the return code
- Usually stop execution with an explicit message



"Debugging programs containing race conditions is no fun at all." Andrew S. Tanenbaum, Modern Operating Systems

Race condition

- A timing dependent error involving shared state
- It runs fine most of the time, and from time to time, something weird and unexplained appears



Code example

```
void deposit(Account* account, double amount)
{
   account->balance += amount;
}
```



Code example

```
void deposit(Account* account, double amount)
{
   READ balance
   ADD amount
   WRITE balance
}
```



Code example

```
void deposit(Account* account, double amount)
{
   READ balance
   ADD amount
   WRITE balance
}
```

Concurrent execution

Thread 1 calls deposit (A, 10)

```
READ balance (0
```

Thread 2 calls deposit (A, 1000)

```
READ balance (0)
ADD 1000
WRITE balance (1000
```



Code example

```
void deposit(Account* account, double amount)
{
   READ balance
   ADD amount
   WRITE balance
}
```

Concurrent execution

```
Thread 1 calls deposit (A, 10)

READ balance (0)

ADD 10

WRITE balance (10)
```

Thread 2 calls deposit (A, 1000)

```
READ balance (0)
ADD 1000
WRITE balance (1000
```



Code example

```
void deposit(Account* account, double amount)
{
   READ balance
   ADD amount
   WRITE balance
}
```

```
Thread 1 calls deposit (A, 10)

READ balance (0)

ADD 10

WRITE balance (10)
```

```
Thread 2 calls deposit (A, 1000)
```

```
READ balance (0)
ADD 1000
WRITE balance (1000
```



Code example

```
void deposit(Account* account, double amount)
{
   READ balance
   ADD amount
   WRITE balance
}
```

```
Thread 1 calls deposit (A, 10)

READ balance (0)

ADD 10
```

```
Thread 2 calls deposit (A, 1000)
```

```
READ balance (0)
ADD 1000
WRITE balance (1000)
```



Code example

```
void deposit(Account* account, double amount)
{
   READ balance
   ADD amount
   WRITE balance
}
```

```
Thread 1 calls deposit (A, 10)

READ balance (0)

ADD 10

WRITE balance (10)
```

```
Thread 2 calls deposit (A, 1000)
```

```
READ balance (0)
ADD 1000
WRITE balance (1000)
```



Code example

```
void deposit(Account* account, double amount)
        balance
 READ
  ADD
        amount
  WRITE balance
```

```
Thread 1 calls deposit (A, 10)
  READ
        balance (0)
  ADD
         10
```

```
Thread 2 calls deposit (A, 1000)
  READ
        balance (0)
```

```
ADD
      1000
WRITE balance (1000)
```



Code example

```
void deposit(Account* account, double amount)
{
   READ balance
   ADD amount
   WRITE balance
}
```

```
Thread 1 calls deposit (A, 10)

READ balance (0)

ADD 10

WRITE balance (10)
```

```
Thread 2 calls deposit (A, 1000)
```

```
READ balance (0)
ADD 1000
WRITE balance (1000)
```



Race condition 2/3

Code example

```
void deposit(Account* account, double amount)
{
   READ balance
   ADD amount
   WRITE balance
}
```

Concurrent execution

```
Thread 1 calls deposit (A, 10)

READ balance (0)

ADD 10
WRITE balance (10)
```

```
Result: balance is 10 instead of 1010
```

Thread 2 calls deposit (A, 1000)

```
READ balance (0)
ADD 1000
WRITE balance (1000)
```



Race condition 3/3

Different kind of race conditions

- Data race: Concurrent accesses to a shared variable
- Atomicity bugs: Code does not enforce the atomicity for a group of memory accesses, eg Time of check to time of use
- Order bugs: Operations are not executed in order
 Compilers and processors can actually re-order instructions

- Protect critical sections: Mutexes, Semaphores, etc.
- Use atomic instructions and memory barriers (low level)
- Use compiler builtin for atomic operations² (higher level)





Deadlock, photograph by David Maitland

"I would love to have seen them go their separate ways, but I was exhausted. The frog was all the time trying to pull the snake off, but the snake just wouldn't let go."



Code example



Concurrent execution

Thread 1 calls transfer (A, B, 10)

Thread 2 calls transfer (B, A, 20)

- Think before writing multithread code
- Use high level programming model: Open MP, Intel TBB, MPI, etc.
- Theoretical analysis
- Software for thread safety analysis



Concurrent execution

```
Thread 1 calls transfer (A, B, 10)
```

Thread 2 calls transfer (B, A, 20)

- Think before writing multithread code
- Use high level programming model: Open MP, Intel TBB, MPI, etc.
- Theoretical analysis
- Software for thread safety analysis



Concurrent execution

```
Thread 1 calls transfer (A, B, 10)
```

- Think before writing multithread code
- Use high level programming model: Open MP, Intel TBB, MPI, etc.
- Theoretical analysis
- Software for thread safety analysis



Concurrent execution

```
Thread 1 calls transfer(A,B,10)

lock(A->mutex);

lock(B->mutex); // wait until

B is unlocked
```

- Think before writing multithread code
- Use high level programming model: Open MP, Intel TBB, MPI, etc.
- Theoretical analysis
- Software for thread safety analysis



Concurrent execution

```
Thread 1 calls transfer(A,B,10)

lock(A->mutex);

lock(B->mutex); // wait until

B is unlocked
```

- Think before writing multithread code
- Use high level programming model: Open MP, Intel TBB, MPI, etc.
- Theoretical analysis
- Software for thread safety analysis



Concurrent execution

```
Thread 1 calls transfer(A,B,10)

lock(A->mutex);

lock(B->mutex); // wait until

B is unlocked

...
```

- Think before writing multithread code
- Use high level programming model: Open MP, Intel TBB, MPI, etc.
- Theoretical analysis
- Software for thread safety analysis



Concurrent execution

```
Thread 1 calls transfer (A,B,10)

lock (A->mutex);

lock (B->mutex); // wait until

B is unlocked

...
```

We have a deadlock!

- Think before writing multithread code
- Use high level programming model: Open MP, Intel TBB, MPI, etc.
- Theoretical analysis
- Software for thread safety analysis



Performance bugs

Bad Performance can be seen as a bug

- Bad algorithm: too high computation complexity
 Example: Insertion Sort is O(N²), Quick Sort is O(N.log(N))
- Memory copies can be a problem, specially with Object Oriented languages
- Some memory allocator have issues: memory alignment constraints, multithread context

- Try use existing proven libraries when possible:
 eg Eigen library for linear algebra, C++ STL, Boost, etc.
- Use a profiler to see where your program spend most of its time Valgrind with Callgrind, GNU gprof, many commercial tools ...
- ...



Outline

Good practices to catch bugs





Be a good programmer

Write good code

- Use explicit variable names, don't re-use variable
- Avoid global variables (problematic in multi-threads)
- Comment and document your code
- Keep your code simple, don't try to over-optimize

Use defensive programming

- Add assertions, cf assert()
- Always check return codes, cf manpages and documentation

Re-use existing libraries

- Use existing libraries when available/possible
- Probably better optimized and tested than your code
- ⇒ Code easier to understand and maintain
- ⇒ Catch bugs as soon as possible



Compilers and Tests

Use your compilers

- Enable (all) warnings of the compiler
- Vary the compilers and configurations
 - Different compilers (GCC, CLang, Intel Compiler, MS Compiler)
 - Various architectures (Windows/Linux, x86/x86_64/ARM)

Testing and Code Checking

- Write unit tests and regression tests
- Use coverage analysis tools
- Use static and dynamic code analysis tools
- Continuous integration:
 - Frequent compilation, testing, execution
 - Different configurations and platforms
- ⇒ Catch more warnings and errors
- ⇒ Better portability



Know your tools

Know the error messages

- Look in the documentation / online
- Compiler errors/warnings
- Runtime errors:

Segmentation fault, Floating point exception, Double free, ${\it etc.}$

Valgrind errors:

```
Invalid read of size 4
Conditional jump or move depends on uninitialised value(s)
8 bytes in 1 blocks are definitely lost
...
```

Use the right tool

- Know your tools and when to use them
 - GDB: locate a crash
 - Valgrind: memory-related issue
 - .



Debug with methodology

Find a minimal case to reproduce the bug

- Some bugs are intermittent
- Easier to debug
- Help you to understand the cause
- Allow to check that the bug is really fixed
- Bonus: make a regression test

Use a Control Version System (GIT, SVN, ...)

- Keep history, serve as a backup, allow to go back in time
- GIT has a nice feature of code bisection in history to find when a bug has been introduced



Any question about debugging?





Part 2 Performance Engineering

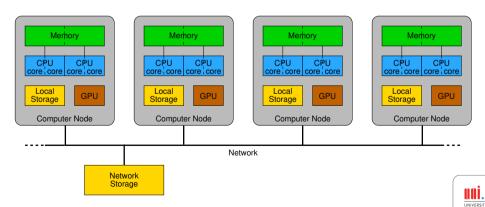
- 6 HPC Hardware & Performance Bottlenecks
 - Processor bottleneck
 - Memory Access bottleneck
 - Memory Size bottleneck
 - Storage Speed bottleneck
 - Network bottleneck
- Understanding CPU and Memory
- Tools for Performance Analysis



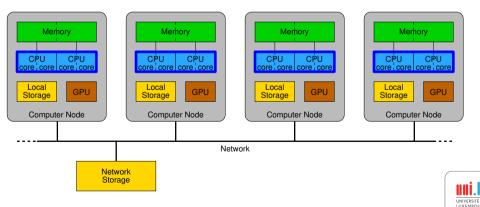
"Ruches Haute-Savoie" (CC BY-SA 3.0) by Myrabella



- Computer nodes are connected using a fast interconnect
- Different types of resources: Processors, GPU, Memory, Storage, Network

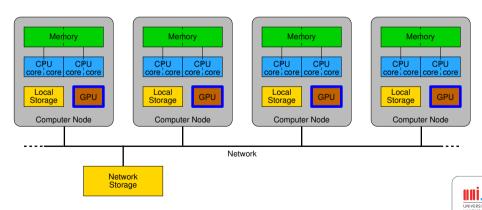


- Computer nodes are connected using a fast interconnect
- Different types of resources:
 Processors, GPU, Memory, Storage, Network

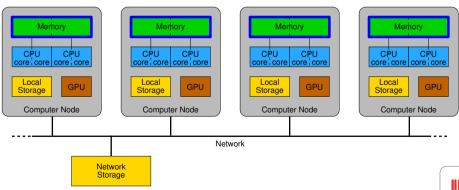


Getting faster: Identify performance bottlenecks

- Computer nodes are connected using a fast interconnect
- Different types of resources:
 Processors, GPU, Memory, Storage, Network

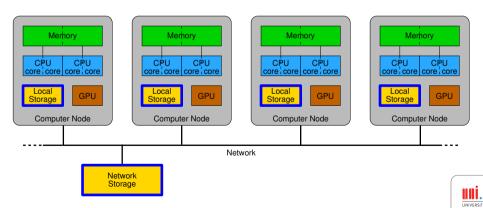


- Computer nodes are connected using a fast interconnect
- Different types of resources: Processors, GPU, Memory, Storage, Network



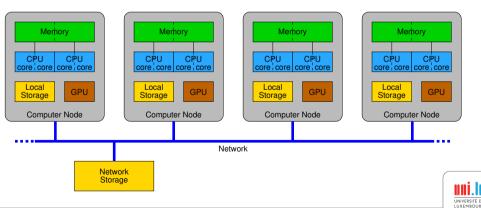
Getting faster: Identify performance bottlenecks

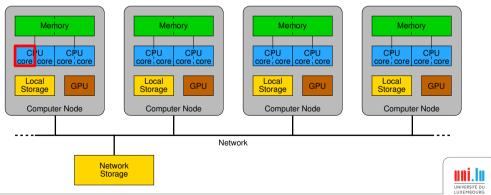
- Computer nodes are connected using a fast interconnect
- Different types of resources:
 Processors, GPU, Memory, Storage, Network



Getting faster: Identify performance bottlenecks

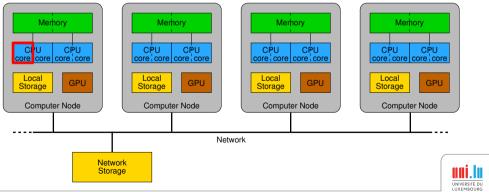
- Computer nodes are connected using a fast interconnect
- Different types of resources:
 Processors, GPU, Memory, Storage, Network



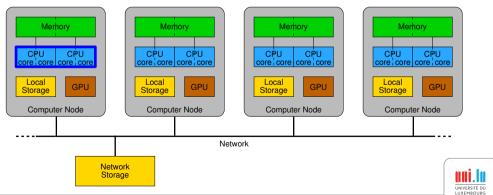


Application is limited by the speed of the processor

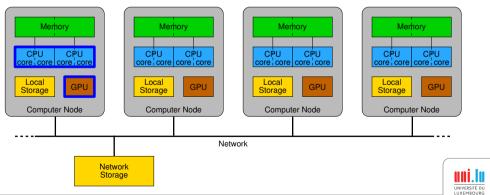
→ Optimize your code: better algorithm & implementation



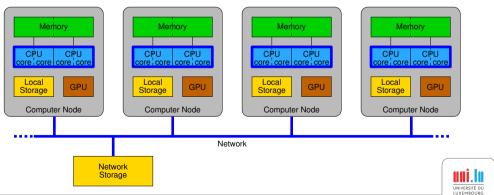
- → Optimize your code: better algorithm & implementation
- → Parallel execution on a single node (pthread, OpenMP, Intel TBB)



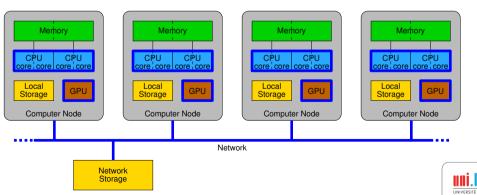
- → Optimize your code: better algorithm & implementation
- → Parallel execution on a single node (pthread, OpenMP, Intel TBB)
- → Use GPU accelerator (CUDA)



- → Optimize your code: better algorithm & implementation
- → Parallel execution on a single node (pthread, OpenMP, Intel TBB)
- → Use GPU accelerator (CUDA)
- → Parallel execution on multiple nodes (MPI)

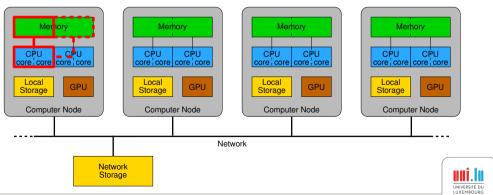


- → Optimize your code: better algorithm & implementation
- → Parallel execution on a single node (pthread, OpenMP, Intel TBB)
- → Use GPU accelerator (CUDA)
- → Parallel execution on multiple nodes (MPI)
- → Parallel execution on multiple nodes with GPUs (MPI+CUDA)

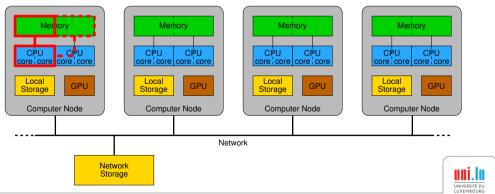


Application is limited by the **speed** of the memory

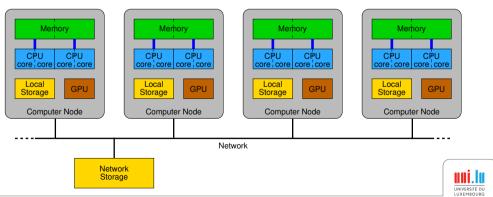
• There is one memory bank attached to each CPU



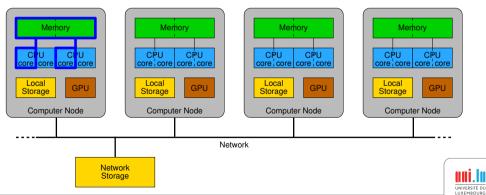
- There is one memory bank attached to each CPU
- → Cache and memory access optimization



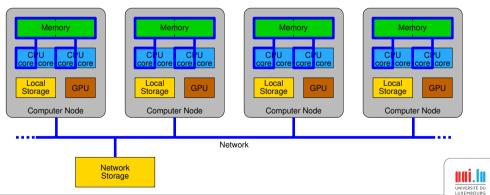
- There is one memory bank attached to each CPU
- Cache and memory access optimization
- Use more memory banks to increase the memory bandwidth



- There is one memory bank attached to each CPU
- Cache and memory access optimization
- Use more memory banks to increase the memory bandwidth
 - → Use multiple CPUs inside one node (pthread, OpenMP, ...)

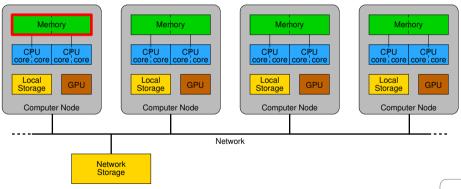


- There is one memory bank attached to each CPU
- → Cache and memory access optimization
- → Use more memory banks to increase the memory bandwidth
 - → Use multiple CPUs inside one node (pthread, OpenMP, ...)
 - → Distribute the memory access on multiple nodes (MPI)



Memory Size bottleneck

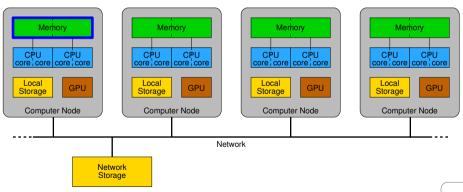
Application is limited by the size of the memory



Memory Size bottleneck

Application is limited by the size of the memory

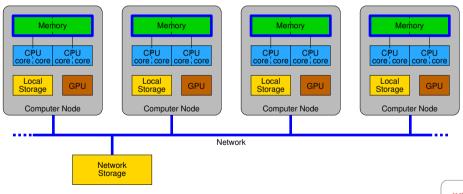
→ Use a node with a bigger memory



Memory Size bottleneck

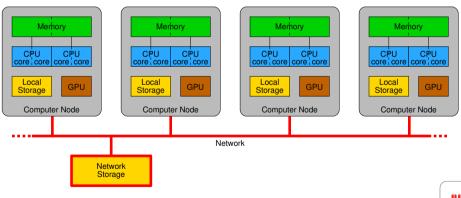
Application is limited by the **size** of the memory

- → Use a node with a bigger memory
- → Distributed execution on multiple nodes (MPI)



Storage Speed bottleneck

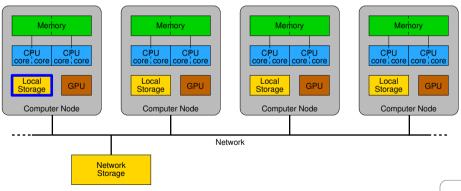
Application is limited by the speed of the storage



Storage Speed bottleneck

Application is limited by the speed of the storage

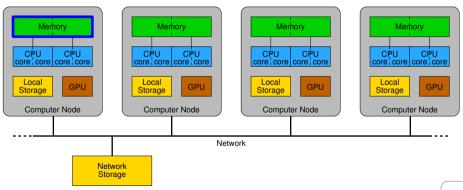
→ Use local storage instead of network storage (copy data back to network storage after execution)



Storage Speed bottleneck

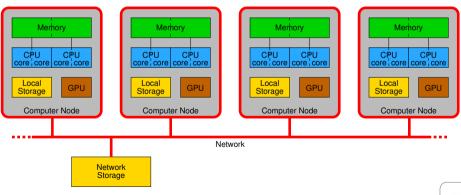
Application is limited by the speed of the storage

- → Use local storage instead of network storage (copy data back to network storage after execution)
- → Use local memory, eg /dev/shm (space is limited!)



Network bottleneck

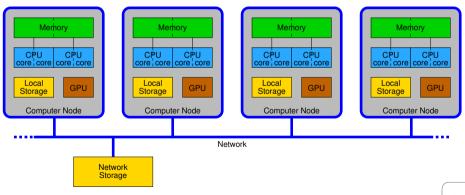
Application is limited by the speed of the network (too many communications)



Network bottleneck

Application is limited by the speed of the network (too many communications)

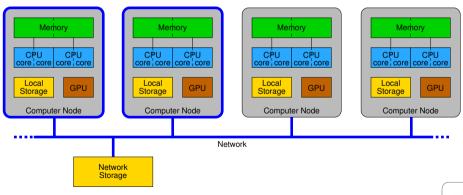
→ Use Infiniband network instead of Ethernet



Network bottleneck

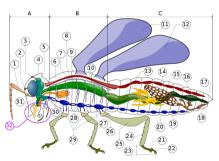
Application is limited by the speed of the network (too many communications)

- → Use Infiniband network instead of Ethernet
- → Reduce the number of nodes



Outline

6 Understanding CPU and Memory



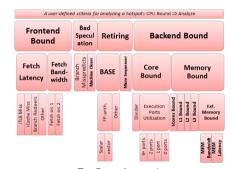
"Insect anatomy diagram" by Piotr Jaworski



Finding the bottlenecks

Models, Methodologies and Tools

- Methodology: Top-Down Approach
 - → identifies the cause of the bottleneck in the CPU
 - → implemented in Intel VTune
- Model: Roofline Model
 - → model the performance of an algorithm
 - → implemented in Intel Advisor
- Tools: Many performance profilers
 - → Arm Forge, Intel Toolsuite, Valgrind, etc.



Top-Down Approach 10.1109/ISPASS.2014.6844459



Roofline Model Overview

Model of the **CPU**



Model of the **algorithm**



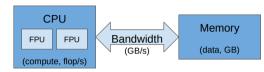
Model of the **performance**

- Estimate the performance of an algorithm on a given CPU
 - Also applies to GPUs, TPUs, etc.
- Throughput oriented model
- Identify the bottleneck
- Allow to improve the implementation of an algorithm





Model of a CPU

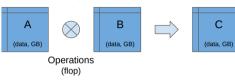


Peak performance limited by

- Compute operations: Gflop/s
- Data bandwidth: GB/s



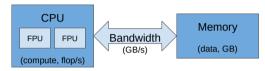
Model of an algorithm



Algorithm characteristics

Operations: Gflop
 Data: GB
 Arithmetic Intensity
 AI: flop / Byte

Model of a CPU

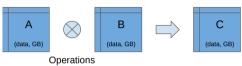


Peak performance limited by

- Compute operations: Gflop/s
- Data bandwidth: GB/s



Model of an algorithm

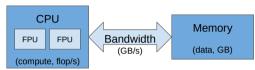


Algorithm characteristics

(flop)

Operations: Gflop
 Data: GB
 Arithmetic Intensity
 AI: flop / Byte

Model of a CPU



Peak performance limited by

- Compute operations: Gflop/s
- Data bandwidth: GB/s

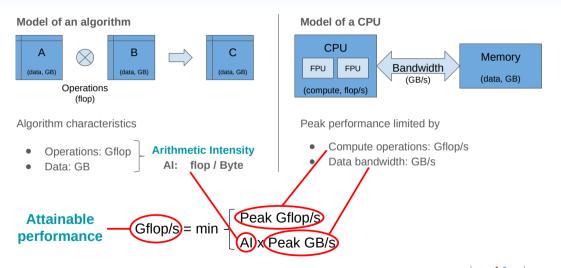
Attainable performance

Gflop/s = min
$$\begin{cases} Peak Gflop/s \\ Al x Peak GB/s \end{cases}$$

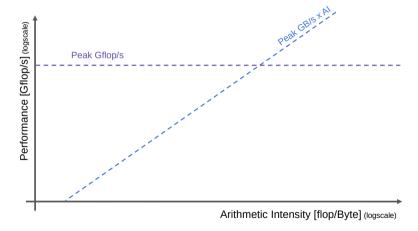


Xavier Resseron

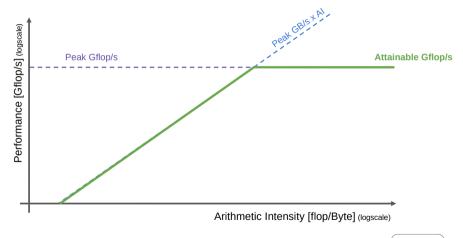
Roofline Model



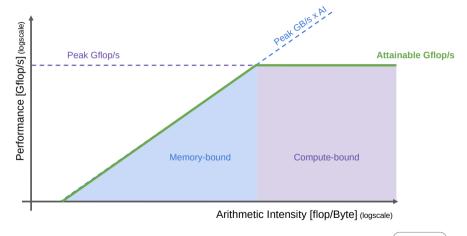




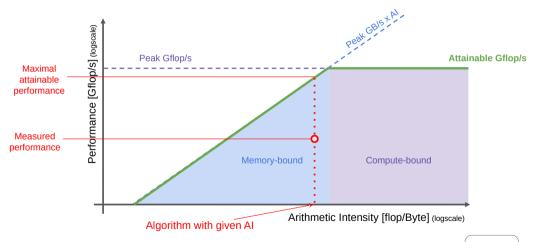




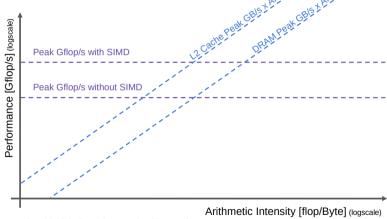




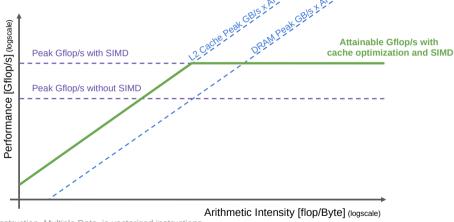




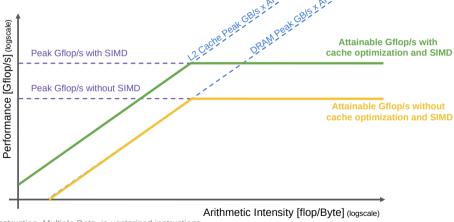




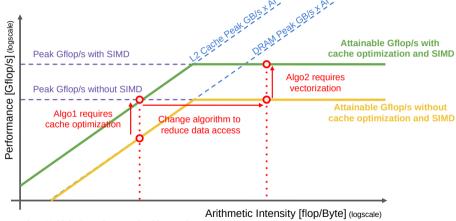














Comments about the Roofline Model

In theory

- Gives good insight of the bottleneck of a given algorithm
- Guides and gives an upperbound/objective for optimization

In practice, use automatic tools

- CPU model can be hard to find
- Algorithm characterization is hard for complex algorithm or loops

Warnings

- The Roofline Model tells if an algorithm performs well,
- not if the algorithm is the best for your problem e.g. Bubble sort O(n²) vs Quicksort O(n · log n)



More about the Roofline Model

Tools

- CS Roofline Toolkit, Berkeley Lab https://bitbucket.org/berkeleylab/cs-roofline-toolkit/
- LIKWID, RRZE-HPC
 https://github.com/RRZE-HPC/likwid
- Intel Advisor, Intel https://software.intel.com/en-us/advisor

References

- Roofline: An Insightful Visual Performance Model for Multicore Architectures, Williams et al., CACM, 2009 https://people.eecs.berkeley.edu/~kubitron/cs252/handouts/papers/RooflineVyNoYellow.pdf
- Performance Tuning of Scientific Codes with the Roofline Model, Williams et al., SC'18 Tutorial, 2018 https://crd.lbl.gov/assets/Uploads/SC18-Roofline-1-intro.pdf
- Applying the roofline model, Ofenbeck et al., ISPASS, 2014
 http://spiral.ece.cmu.edu:8080/pub-spiral/pubfile/ispass-2013_177.pdf



Outline

Tools for Performance Analysis







Tools for Performance Analysis 1/3

HPC specific tools - Arm (prev. Allinea)

- Arm DDT (part of Arm Forge)
 - Visual debugger for C, C++, Fortran & Python // code
- Arm MAP (part of Arm Forge)
 - Visual profiler for C, C++, Fortran & Python
- Arm Performance Reports
 - Application characterization tool

Arm tools are commercial tools that require a license!



Tools for Performance Analysis 2/3

HPC specific tools - Intel

- Intel Advisor
 - Vectorization + threading advisor: check blockers and opport.
- Intel Inspector
 - Memory and thread debugger: check leaks/corrupt., data races
- Intel Trace Analyzer and Collector
 - MPI communications profiler and analyzer: evaluate patterns
- Intel VTune Amplifier
 - Performance profiler: CPU/FPU data, mem. + storage accesses



Tools for Performance Analysis 3/3

Generic profilers

gprof, Valgrind, perf, gperftools

HPC specific tools - Scalasca & friends

- Scalasca
 - Study behavior of // apps. & identify optimization opport.
- Score-P
 - Instrumentation tool for profiling, event tracing, online analysis.

Extra-P

Automatic performance modeling tool for // apps.

Free and Open Source!
See other awesome tools at http://www.vi-hps.org/tools



Summary

Know the hardware

Know your application

Identify the bottleneck: monitoring & profiling

Optimize your code

- Work on the algorithm
- Parallelization: pick the right approach
- Use quantitative measures of the performance
 - e.g. FLOPS, bandwidth usage, unbalance, etc.
 - measure effect of optimization
 - identify when optimization is over



Any question about performance engineering?



"Question Mark caterpillar" (CC BY-NC-SA 2.0) by Keith Roragen



Practical Session

Instructions

https://gitlab.uni.lu/SC-Camp/2021/debugging-and-profiling

Objectives

- Short GDB Tutorial
 - Get familiar with basic usage
- Short Valgrind Tutorial
 - Try Memcheck on a small example
- Profiling with Callgrind
 - Profile a small example
 - Try to improve the performance
- Bug hunting
 - Examples of different kinds of bugs
 - Try to fix them





