Practical Debugging & Performance Engineering for High Performance Computing

Xavier Besseron
LuXDEM Research Centre
University of Luxembourg

SC-Camp 2023
May 14-20, 2023
Cartagena, Colombia

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

Part I
Know Your Bugs: Weapons for Efficient Debugging

Why debugging?

Bugs are in every programs

- Industry Average:
  "*about 15 - 50 errors per 1000 lines of delivered code*" [1]

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

UNIVERSITÉ DU LUXEMBOURG

Outline

2. Tools for Debugging
   - 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

→ 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
C	`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

```
$ gcc -g -Wall program.c -o program
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 appears in
program.c:4:7: warning: unused variable 'z' [-Wunused-variable]
   int z = x + y;
       ^
```

GNU Debugger 1/2

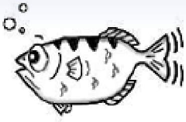
GDB is the GNU Debugger

- 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:

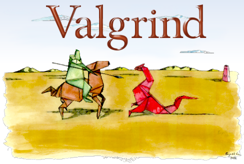
`http://sourceware.org/gdb/current/onlinedocs/gdb/`

`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

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
- `http://valgrind.org/docs/manual/cl-manual.html`

Valgrind 2/3

Example: memory errors with Memcheck

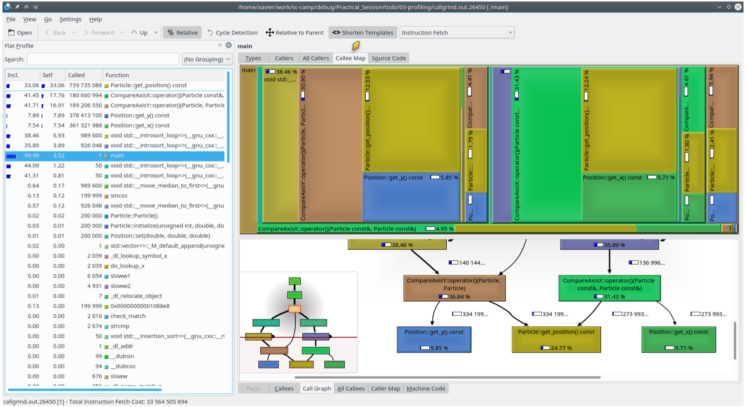
```
$ valgrind --tool=memcheck --leak-check=full --track-origins=yes ./program
[...]
==12534== Conditional jump or move depends on uninitialised value(s)
==12534==    at 0x40055E: main (program.c:11)
==12534==  Uninitialised value was created by a stack allocation
==12534==    at 0x400536: main (program.c:5)
==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)
[...]
```

Valgrind 3/3

Example: profiling with Callgrind

```
$ valgrind --tool=callgrind ./program
```

Example: Visualizing profile with KCachegrind



Outline

3 Common bugs
- 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

What to do?

- 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

```c
unsigned char A = 200;

unsigned char B =  60;

// Overflow!
unsigned char S = A + B;
```

		1	1	0	0	1	0	0	0	200
+		0	0	1	1	1	1	0	0	+ 60
=	~~1~~	0	0	0	0	0	1	0	0	= 4

→ No error at runtime!

What to do?

- 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:

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

Loss of precision

- The order of the operations matters:

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

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

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

What to do?

- 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

What to do?

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

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

What to do?

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

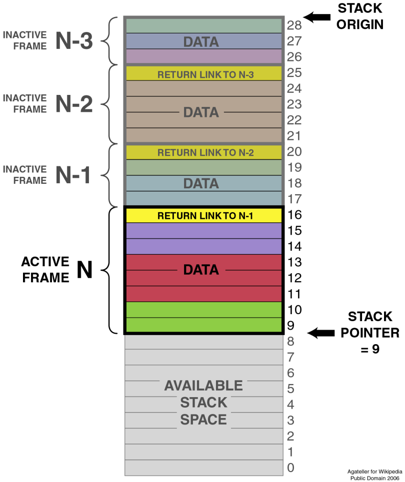
Stack overflow

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



Agateller for Wikipedia
Public Domain 2006

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

What to do?

- 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

What to do?

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

Race condition 1/3

"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

Race condition 2/3

Code example

```
void deposit(Account* account, double amount)
{

  account->balance += amount;

}
```

Race condition 2/3

Code example

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

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)
```

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)
```

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)
```

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)
```

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)
```

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)
```

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)
```

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)
```

Thread 2 calls `deposit(A,1000)`

```

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

Result: *balance* is 10 instead of 1010

Without protection, any interleave combination is possible!

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

What to do?

- Protect critical sections: Mutexes, Semaphores, etc.
- Use atomic instructions and memory barriers (low level)
- Use compiler builtin for atomic operations[2] (higher level)

[2] https://gcc.gnu.org/onlinedocs/gcc-5.1.0/gcc/_005f_005fatomic-Builtins.html

Deadlock 1/3

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."

Deadlock 2/3

Code example

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

```
void transfer(Account* accA,
              Account* accB,
              amount)
{
  lock(accA->mutex);
  lock(accB->mutex);
  accA->balance += amount;
  accB->balance -= amount;
  unlock(accA->mutex);
  unlock(accB->mutex);
}
```

Deadlock 3/3

Concurrent execution

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

```
lock(A->mutex);

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

...
```

Thread 2 calls `transfer(B,A,20)`

```
lock(B->mutex);

lock(A->mutex); // wait until
                   A is unlocked
...
```

What to do?

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

Deadlock 3/3

Concurrent execution

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

```
lock(A->mutex);

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

...
```

Thread 2 calls `transfer(B,A,20)`

```
lock(B->mutex);

lock(A->mutex); // wait until
                   A is unlocked
...
```

What to do?

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

Deadlock 3/3

Concurrent execution

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

```
lock(A->mutex);

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

...
```

Thread 2 calls `transfer(B,A,20)`

```
lock(B->mutex);

lock(A->mutex); // wait until
                   A is unlocked
...
```

What to do?

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

Deadlock 3/3

Concurrent execution

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

```
lock(A->mutex);

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

...
```

Thread 2 calls `transfer(B,A,20)`

```
lock(B->mutex);

lock(A->mutex); // wait until
                   A is unlocked
...
```

What to do?

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

Deadlock 3/3

Concurrent execution

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

```
lock(A->mutex);

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

...
```

Thread 2 calls `transfer(B,A,20)`

```
lock(B->mutex);

lock(A->mutex); // wait until
                   A is unlocked
...
```

What to do?

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

Deadlock 3/3

Concurrent execution

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

```
lock(A->mutex);

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

...
```

Thread 2 calls `transfer(B,A,20)`

```
lock(B->mutex);

lock(A->mutex); // wait until
                   A is unlocked
...
```

What to do?

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

Deadlock 3/3

Concurrent execution

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

```
lock(A->mutex);

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

...
```

Thread 2 calls `transfer(B,A,20)`

```
lock(B->mutex);

lock(A->mutex); // wait until
                   A is unlocked
...
```

We have a deadlock!

What to do?

- 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 $O(N^2)$, *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

What to do?

- 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

4 Good practices to catch bugs

Be a good programmer

Write good code

- Use explicit variable names, don't re-use variables
- 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

$\Rightarrow$ Catch more warnings and errors

$\Rightarrow$ 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`, 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

5 HPC Hardware & Performance Bottlenecks
- Processor bottleneck
- Memory Access bottleneck
- Memory Size bottleneck
- Storage Speed bottleneck
- Network bottleneck

6 Understanding CPU and Memory

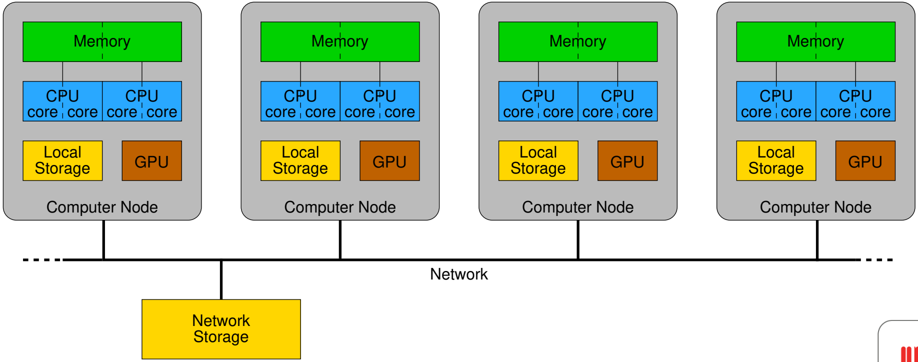
7 Tools for Performance Analysis

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

Getting faster: Identify performance bottlenecks

Know the hardware

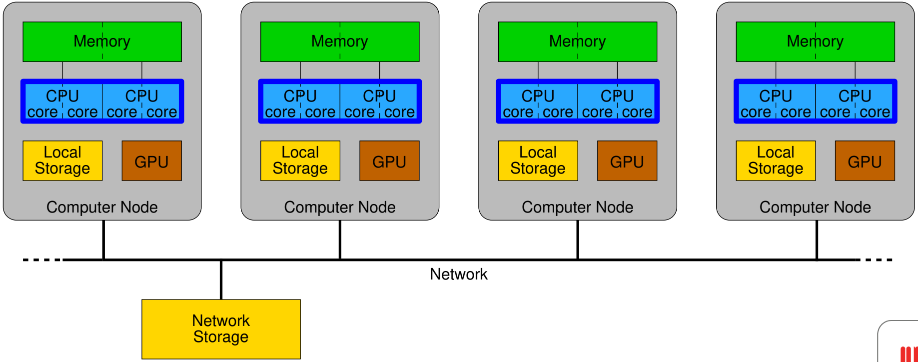
- Computer nodes are connected using a fast interconnect
- Different types of resources:
  Processors, GPU, Memory, Storage, Network



Getting faster: Identify performance bottlenecks

Know the hardware

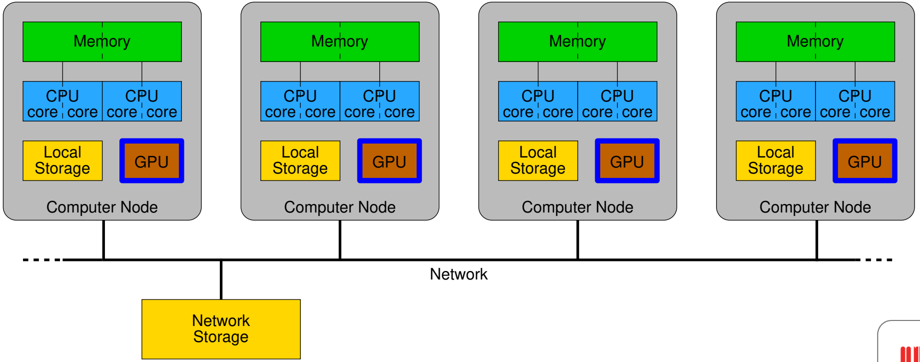
- Computer nodes are connected using a fast interconnect
- Different types of resources:
  Processors, GPU, Memory, Storage, Network



Getting faster: Identify performance bottlenecks

Know the hardware

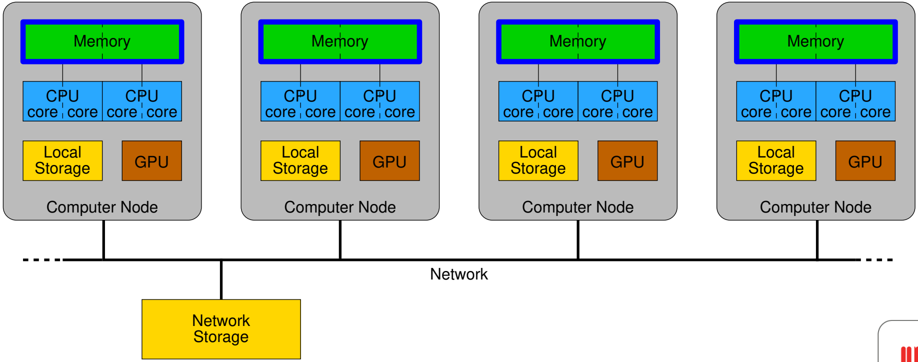
- Computer nodes are connected using a fast interconnect
- Different types of resources:
  Processors, GPU, Memory, Storage, Network



Getting faster: Identify performance bottlenecks

Know the hardware

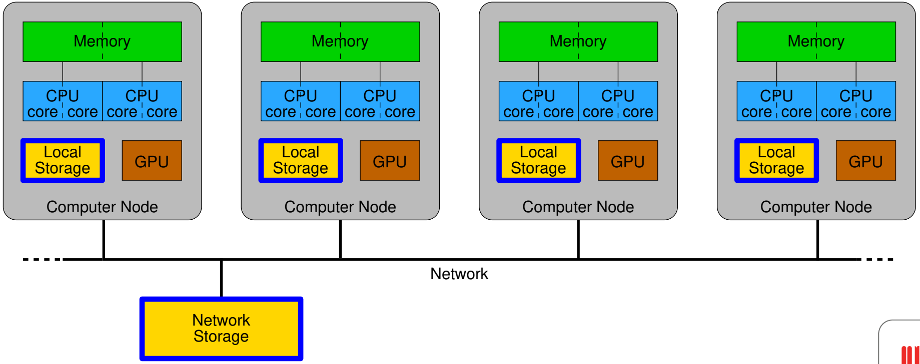
- Computer nodes are connected using a fast interconnect
- Different types of resources:
  Processors, GPU, Memory, Storage, Network



Getting faster: Identify performance bottlenecks

Know the hardware

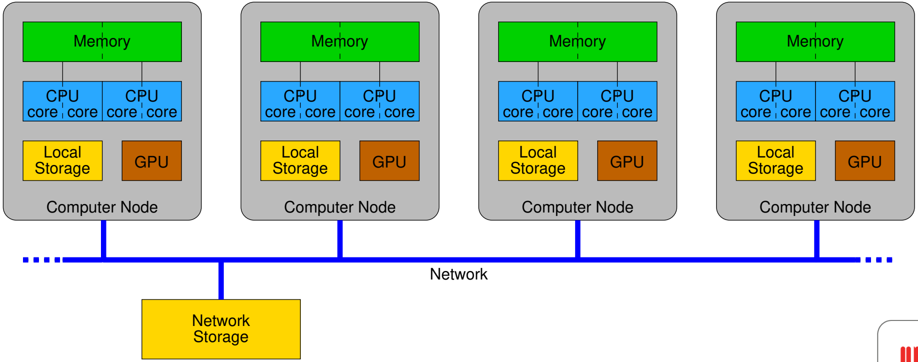
- Computer nodes are connected using a fast interconnect
- Different types of resources:
  Processors, GPU, Memory, Storage, Network



Getting faster: Identify performance bottlenecks

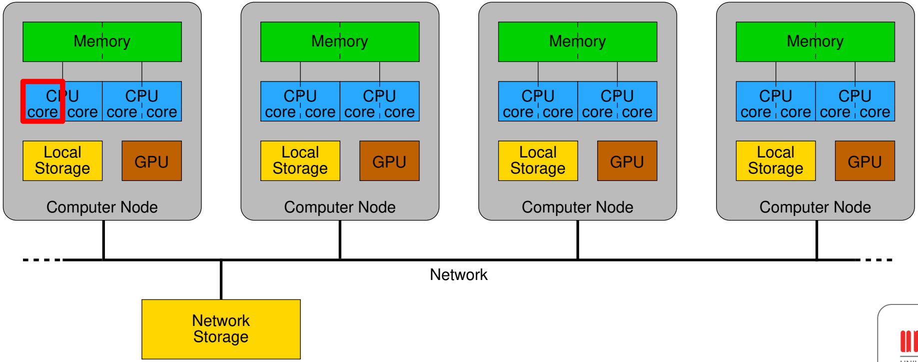
Know the hardware

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



Processor bottleneck

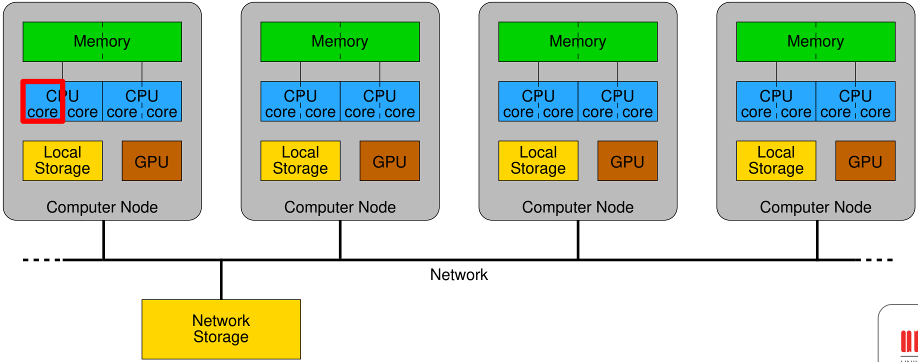
Application is limited by the speed of the processor



Processor bottleneck

Application is limited by the speed of the processor

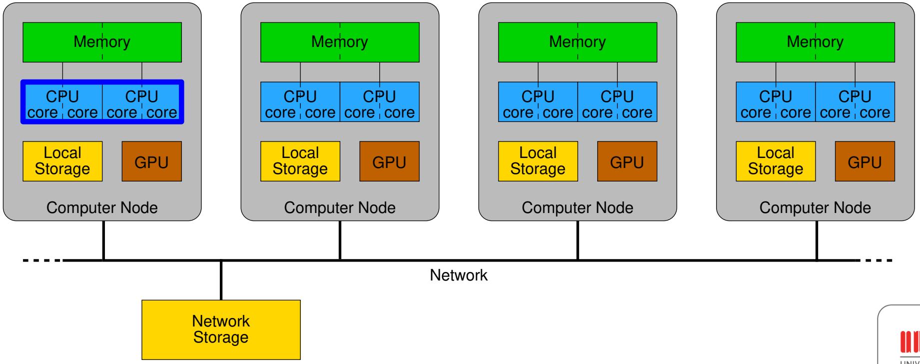
$\longrightarrow$ Optimize your code: better algorithm & implementation



Processor bottleneck

Application is limited by the speed of the processor

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



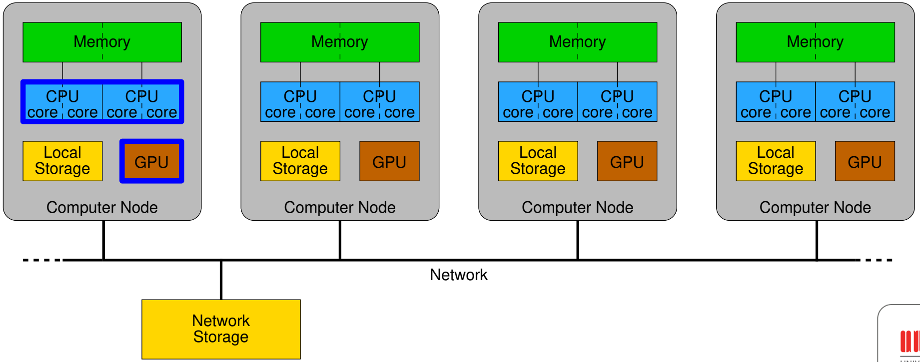
Processor bottleneck

Application is limited by the speed of the processor

→ Optimize your code: better algorithm & implementation

→ Parallel execution on a single node (pthread, OpenMP, Intel TBB)

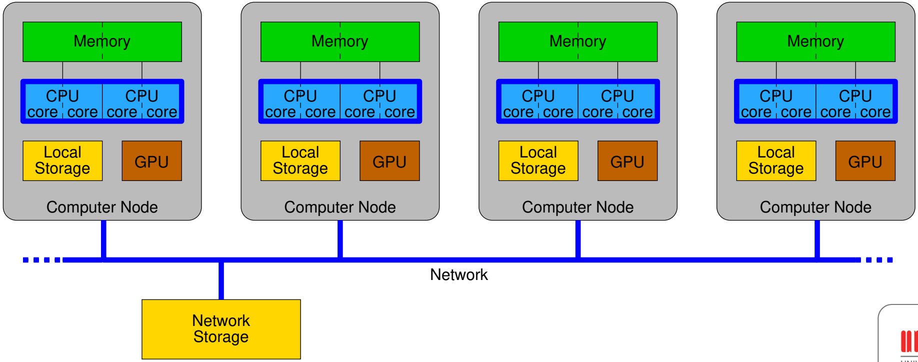
→ Use GPU accelerator (CUDA)



Processor bottleneck

Application is limited by the speed of the processor

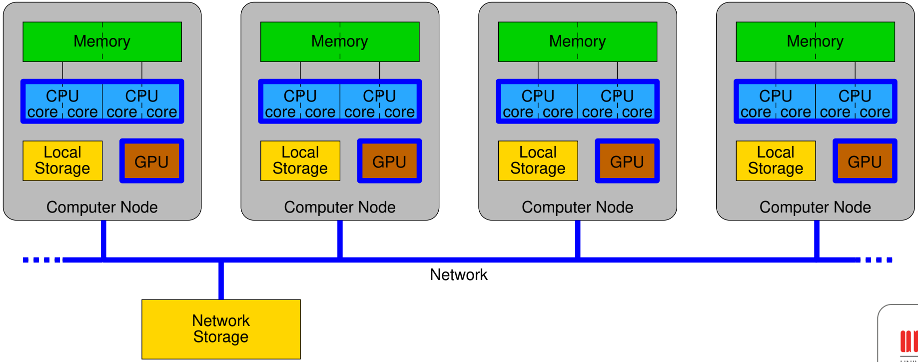
→ Optimize your code: better algorithm & implementation
→ Parallel execution on a single node (pthread, OpenMP, Intel TBB)
→ Use GPU accelerator (CUDA)
→ Parallel execution on multiple nodes (MPI)



Processor bottleneck

Application is limited by the speed of the processor

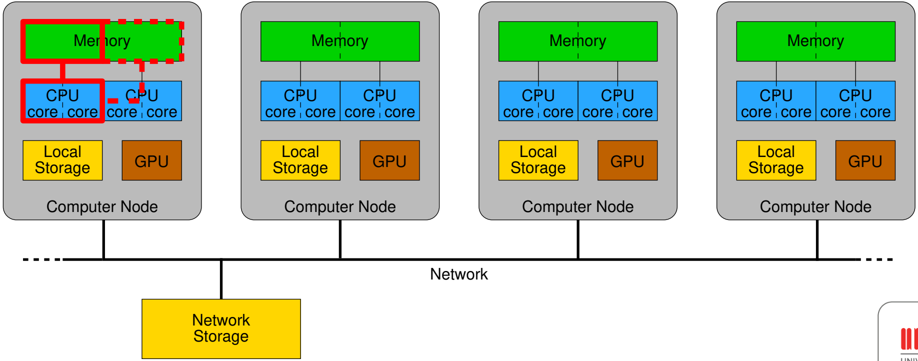
- → Optimize your code: better algorithm & implementation
- → Parallel execution on a single node (pthread, OpenMP, Intel TBB)
- → Use GPU accelerator (CUDA)
- → Parallel execution on multiple nodes (MPI)
- → Parallel execution on multiple nodes with GPUs (MPI+CUDA)



Memory Access bottleneck

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

- There is one memory bank attached to each CPU

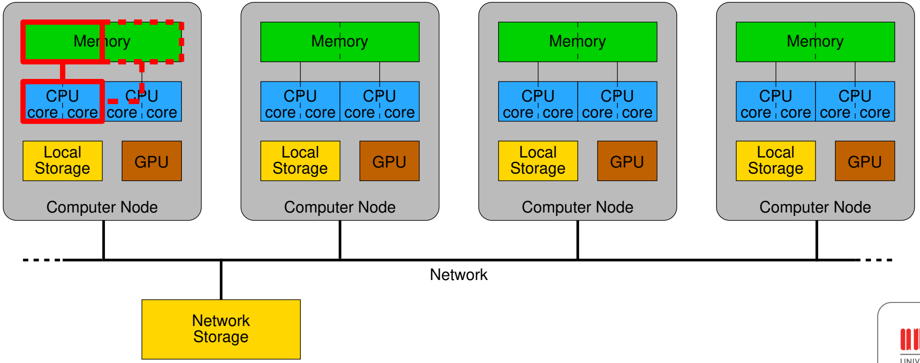


Memory Access bottleneck

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

- There is one memory bank attached to each CPU

→ Cache and memory access optimization



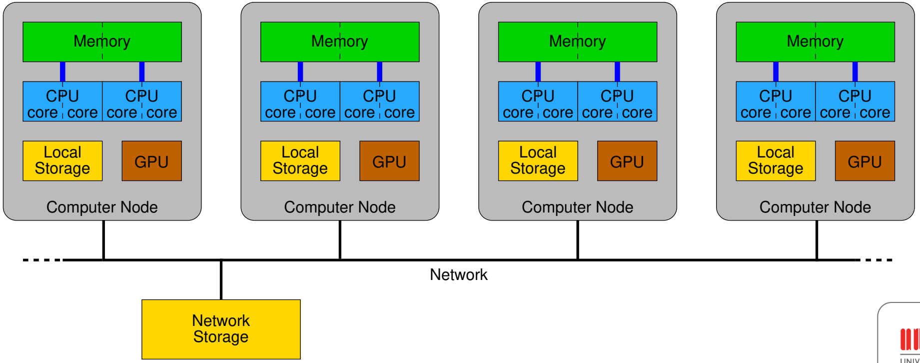
Memory Access bottleneck

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

- There is one memory bank attached to each CPU

→ Cache and memory access optimization

→ Use more memory banks to increase the memory bandwidth



Memory Access bottleneck

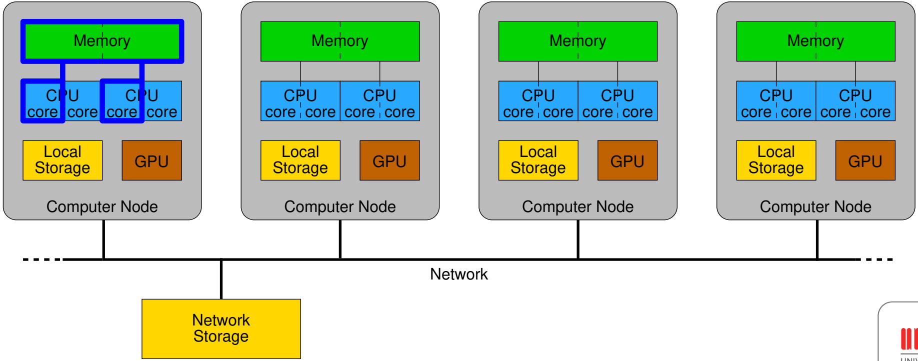
Application is limited by the **speed** of the memory

- 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, ...)



Memory Access bottleneck

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

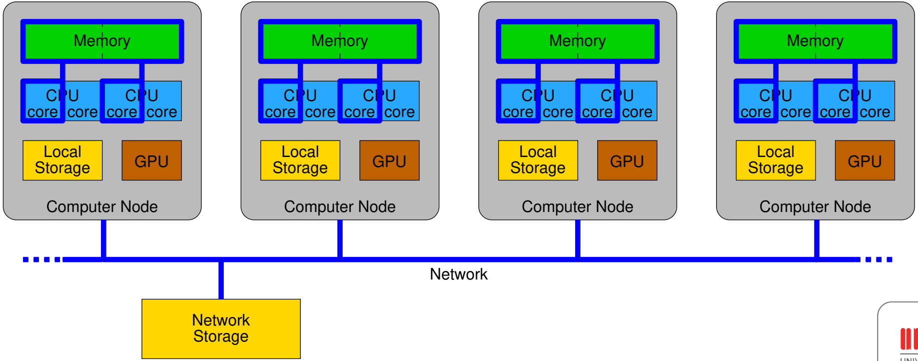
- There is one memory bank attached to each CPU

→ Cache and memory access optimization

→ Use more memory banks to increase the memory bandwidth

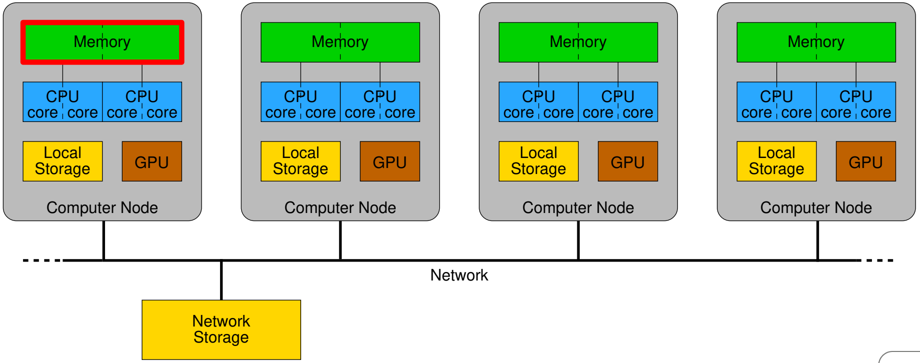
  → Use multiple CPUs inside one node (pthread, OpenMP, ...)

  → Distribute the memory access on multiple nodes (MPI)



Memory Size bottleneck

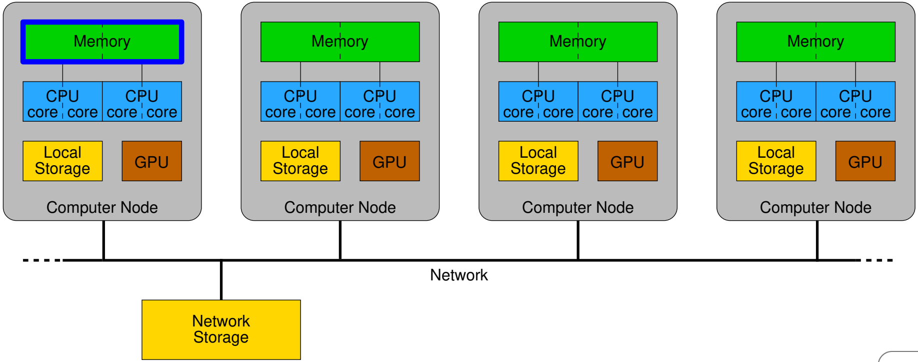
Application is limited by the **size** of the memory



Memory Size bottleneck

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

→ Use a node with a bigger memory

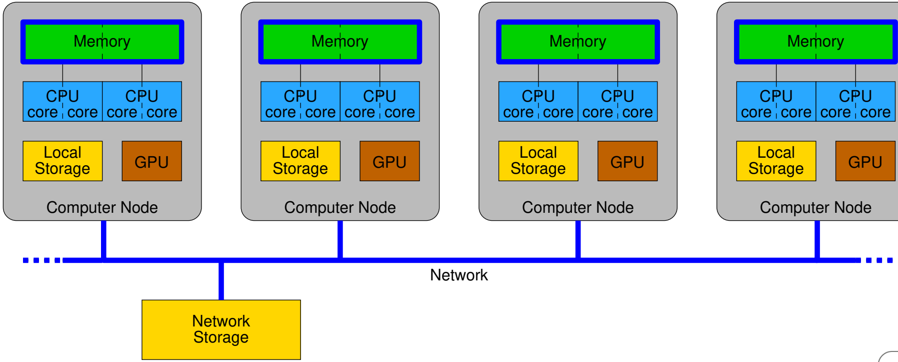


Memory Size bottleneck

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

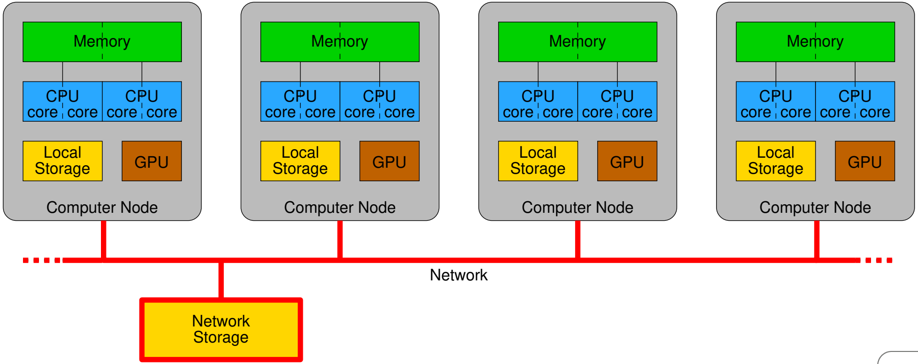
→ Use a node with a bigger memory

→ Distributed execution on multiple nodes (MPI)



Storage Speed bottleneck

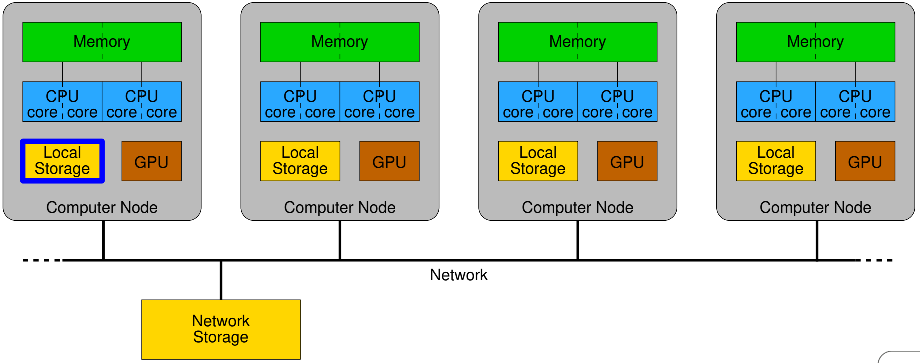
Application is limited by the speed of the storage



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)

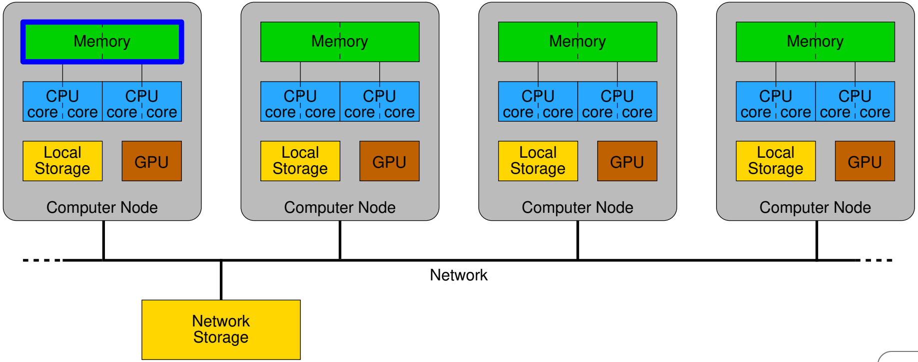


Storage Speed bottleneck

Application is limited by the speed of the storage

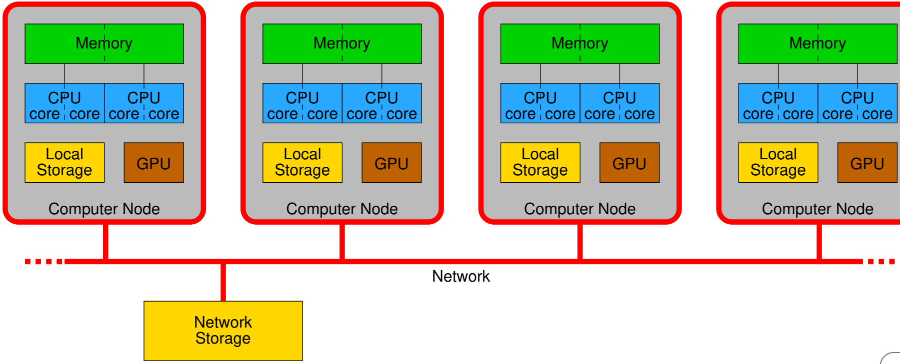
→ Use local storage instead of network storage
(copy data back to network storage after execution)

→ Use local memory, *eg* `/dev/shm` (space is limited!)



Network bottleneck

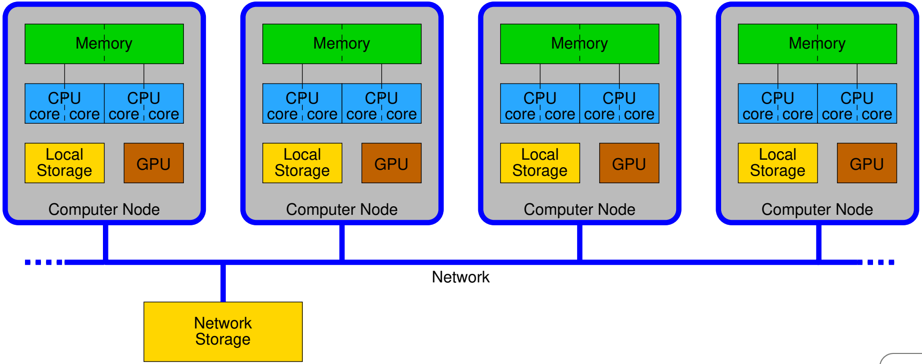
Application is limited by the speed of the network
(too many communications)



Network bottleneck

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

→ Use Infiniband network instead of Ethernet

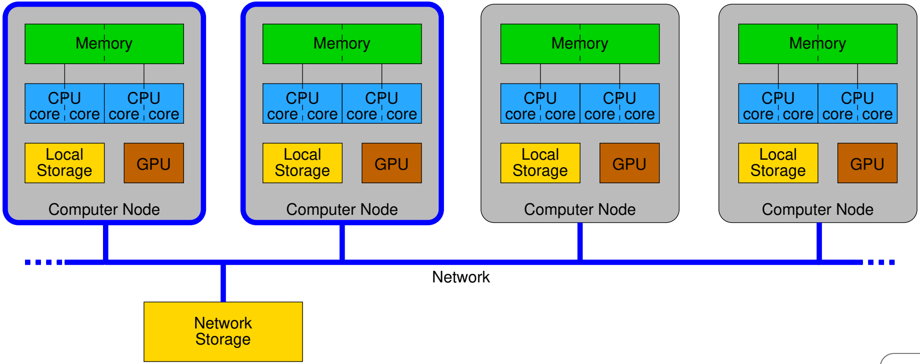


Network bottleneck

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

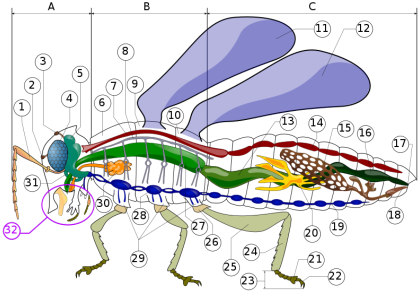
→ Use Infiniband network instead of Ethernet

→ Reduce the number of nodes



Outline

6 Understanding CPU and Memory

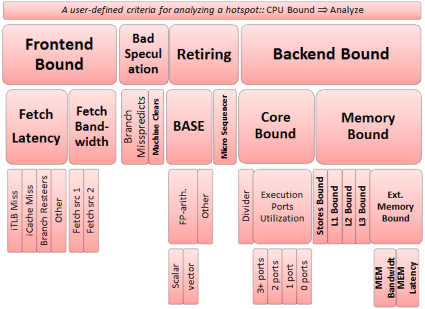


"Insect anatomy diagram" by Piotr Jaworski

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

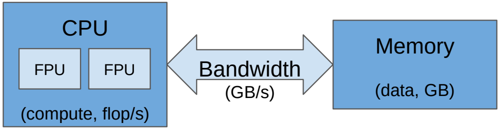
Model of the **CPU** + Model of the **algorithm** → Model of the **performance**

- 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

Roofline Model

Roofline Model

Model of a CPU

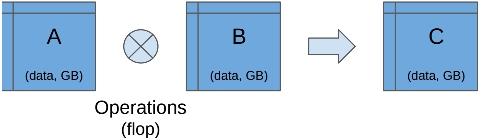


Peak performance limited by

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

Roofline Model

Model of an algorithm



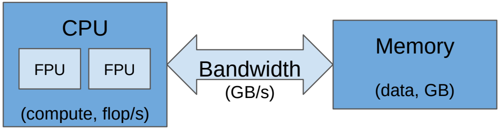
Algorithm characteristics

- Operations: Gflop
- Data: GB

Arithmetic Intensity

AI: flop / Byte

Model of a CPU

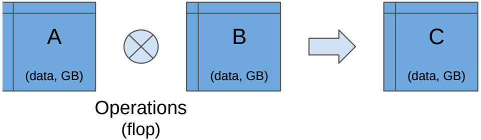


Peak performance limited by

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

Roofline Model

Model of an algorithm

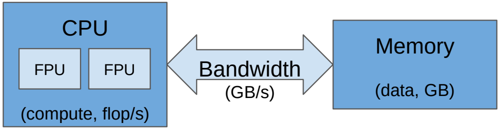


Algorithm characteristics

- Operations: Gflop
- Data: GB

Arithmetic Intensity
AI: flop / Byte

Model of a CPU



Peak performance limited by

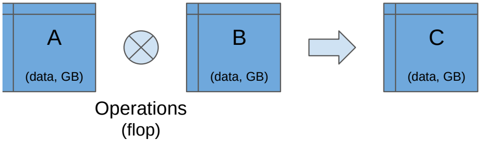
- Compute operations: Gflop/s
- Data bandwidth: GB/s

Attainable performance

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

Roofline Model

Model of an algorithm

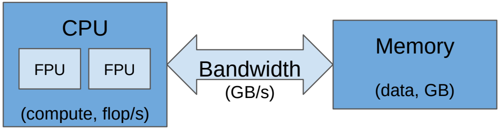


Algorithm characteristics

- Operations: Gflop
- Data: GB

Arithmetic Intensity
AI: flop / Byte

Model of a CPU



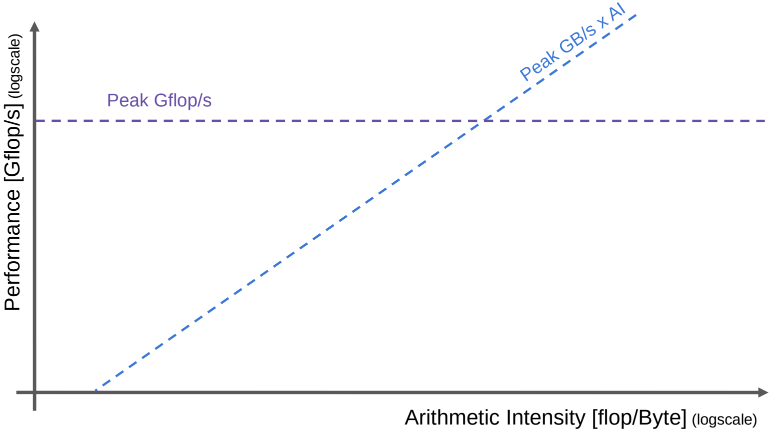
Peak performance limited by

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

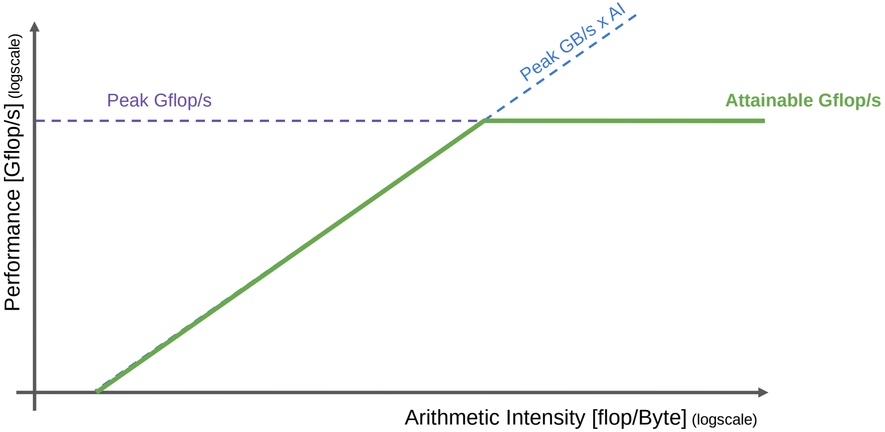
Attainable performance

$$\text{Gflop/s} = \min \begin{cases} \text{Peak Gflop/s} \\ \text{AI} \times \text{Peak GB/s} \end{cases}$$

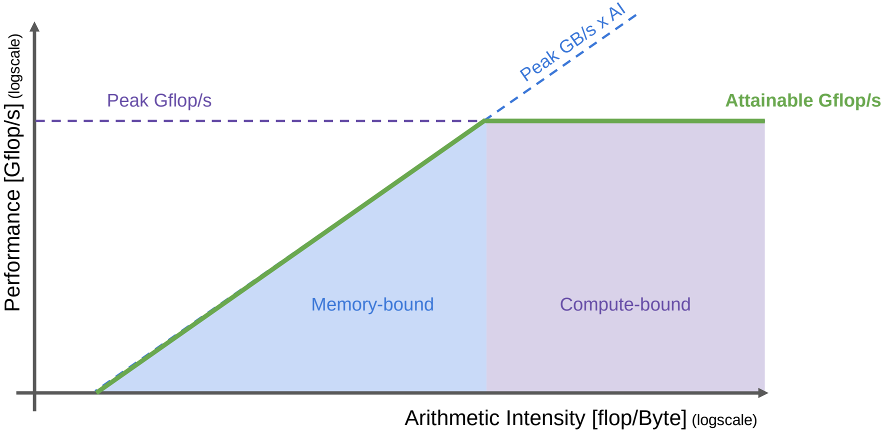
Roofline Plot



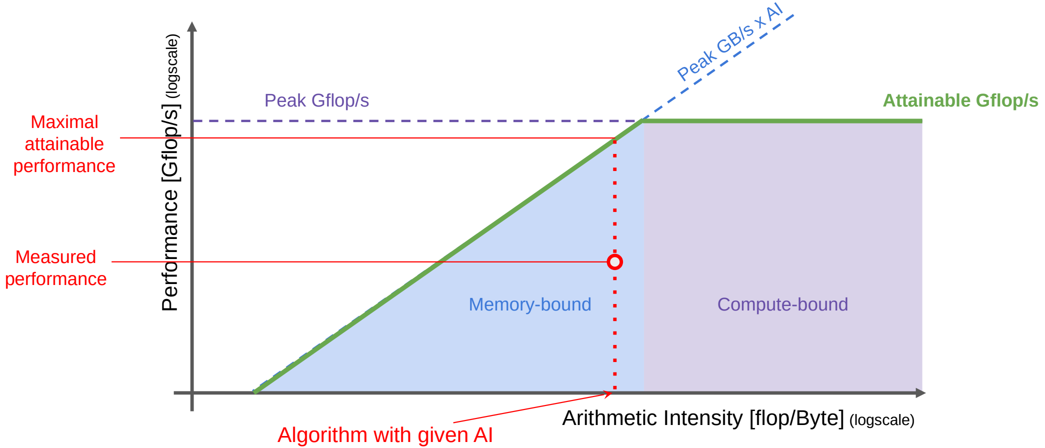
Roofline Plot



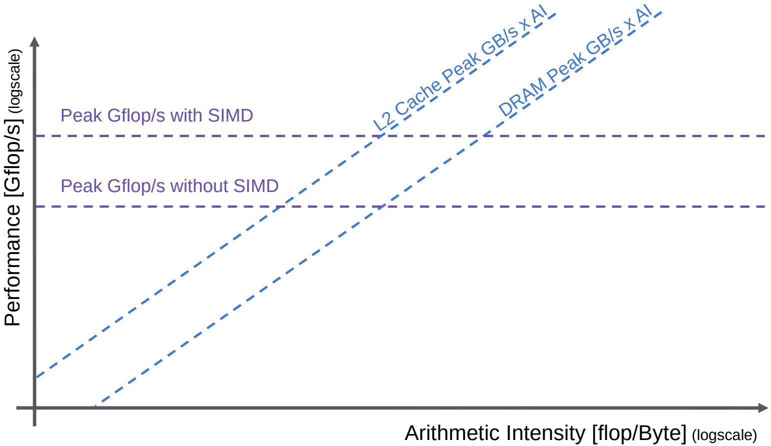
Roofline Plot



Roofline Plot

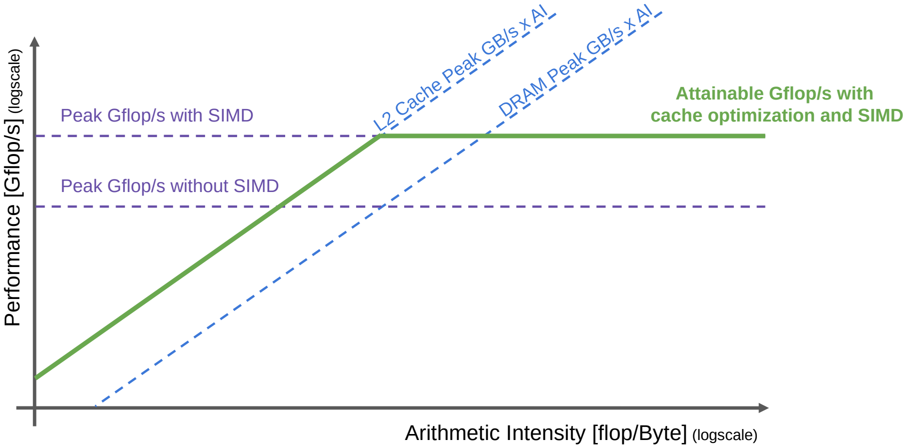


Advanced Roofline Plot



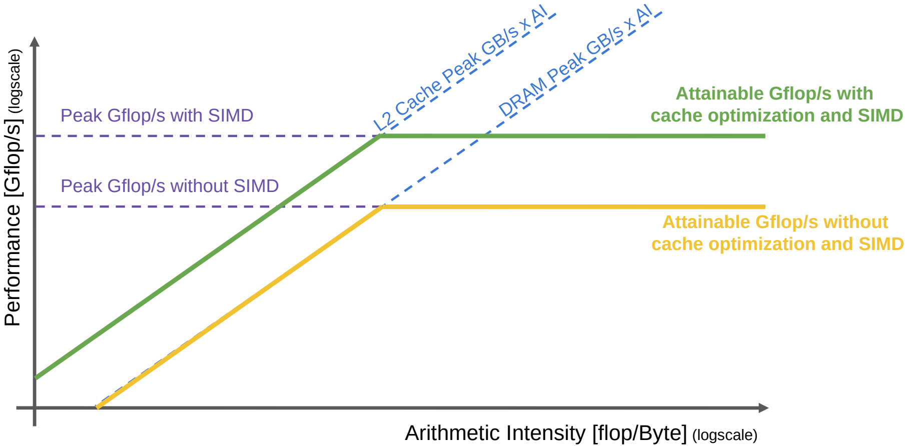
SIMD = Single Instruction, Multiple Data, ie vectorized instructions

Advanced Roofline Plot



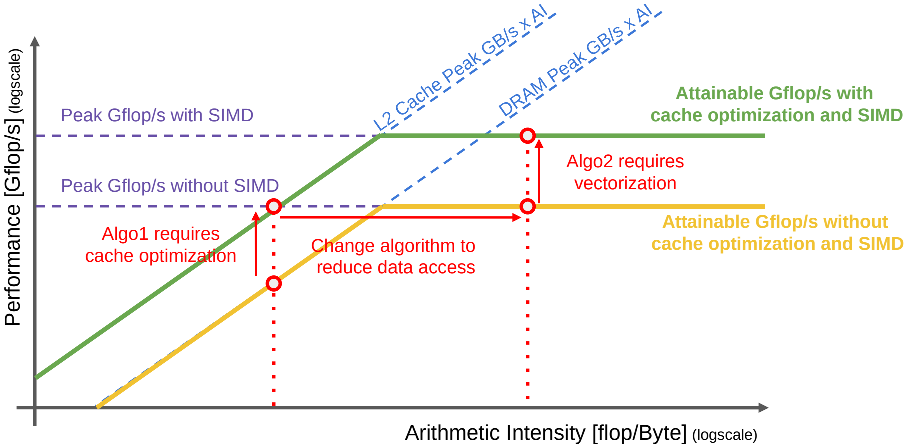
SIMD = Single Instruction, Multiple Data, ie vectorized instructions

Advanced Roofline Plot



SIMD = Single Instruction, Multiple Data, ie vectorized instructions

Advanced Roofline Plot



SIMD = Single Instruction, Multiple Data, ie vectorized instructions

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 $O(n^2)$ vs Quicksort $O(n \cdot log\ n)$

More about the Roofline Model

Tools

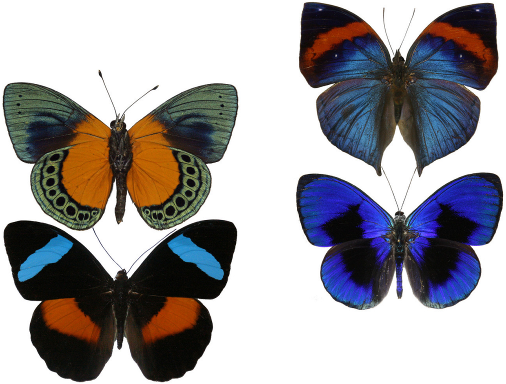
- CS Roofline Toolkit, Berkeley Lab
  `https://bitbucket.org/berkeleylab/cs-roofline-toolkit/`
- LIKWID, RRZE-HPC
  `https://github.com/RRZE-HPC/likwid`
- Intel Advisor, Intel
  `https://software.intel.com/en-us/advisor`

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

7 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