

Introduction to profiling and optimisation

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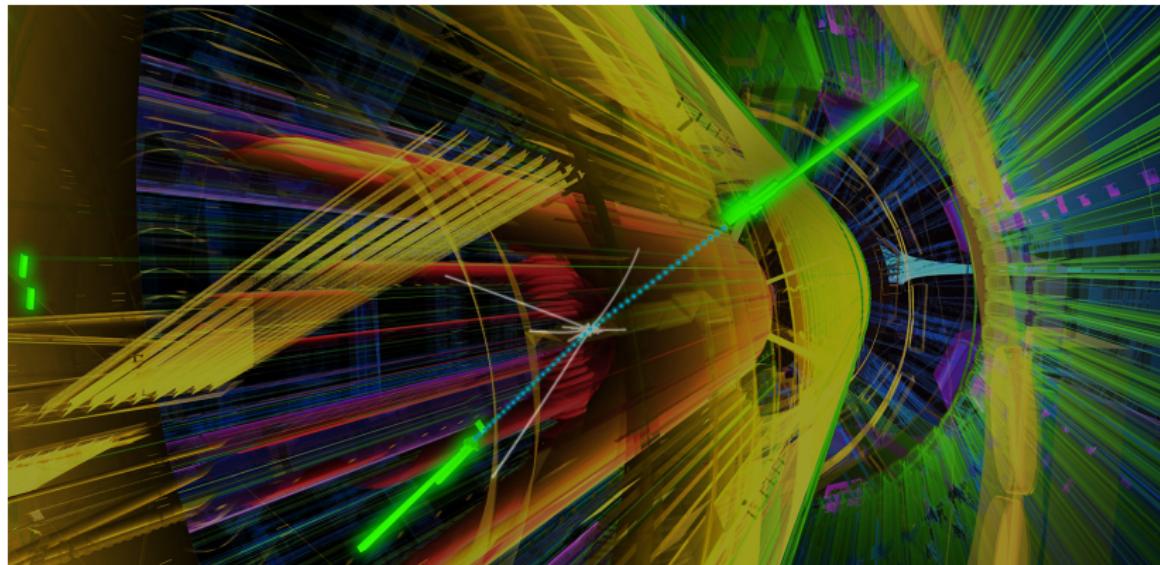
**Data Intensive Science Centres for Doctoral
Training Launch Event, Cardiff**

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Particle collider experiments

Large Hadron Collider is the best-known collider experiment, but there are others

- ▶ Collide protons together at high energy
- ▶ Measure fragments of proton-proton collision in specialised detectors
- ▶ Most collisions are low-energy - really interesting physics happens only 1 in a billion collisions



Data at collider detectors

Take e.g. ATLAS detector at LHC

- ▶ Each proton-proton collision record (output from all sub-detectors) ≈ 1 megabyte
- ▶ ≈ 40 million collisions every second $\rightarrow 40$ terabyte/second output rate
- ▶ Google data storage ≈ 15 exabytes¹

$$\frac{15 \text{ exabytes}}{40 \text{ terabytes/second}} = 4.34 \text{ days}$$

- ▶ Even if we fill up Google's data centres, we only produce ≈ 1000 Higgs boson events, and not many in "golden channels"
- ▶ In any case, we cannot read out the detector at 40 terabytes per second!

¹<https://what-if.xkcd.com/63/>

Data at collider detectors

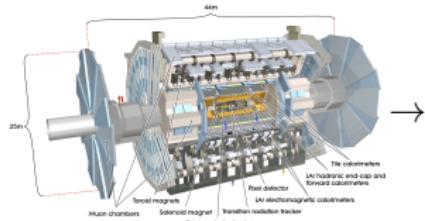
To summarise

- ▶ We physically **cannot** read out LHC data at the rate the LHC can provide
- ▶ If we could record all the data produced by the LHC, we would run out of worldwide disk space in a few days
- ▶ Once we filled up all the disk space worldwide, we still wouldn't have found the Higgs boson

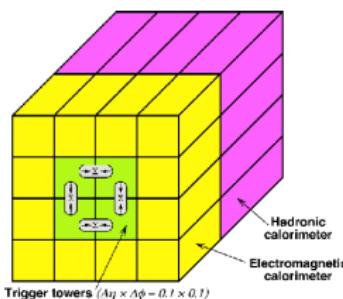
We need a **trigger** system - decide on the fly which collisions to accept and which to reject

Trigger systems for particle physics

- ▶ Goal: reduce the output data rate from 40 terabytes/second to e.g. ≈ 1 gigabyte/second
- ▶ Need hardware and software systems that read the detector output and decide whether the collision contains interesting physics



ATLAS detector



Fast hardware -
microsecond decision
time



Fast software -
millisecond decision
time

- ▶ For a more detailed introduction, see. e.g [here](#)

Software trigger systems for particle physics

- ▶ 40,000 CPU cores needed to read collisions and reduce the data rate to an acceptable output rate (1 gigabyte/second)
- ▶ Strong requirements for trigger software
 - ▶ Fast, smart pattern recognition algorithms - excellent rejection
 - ▶ Robust software - rare/no crashes
 - ▶ Reproducible/correct software - free/mostly free of bugs, no spurious rejection of interesting physics
- ▶ Trigger systems at LHC are **the** canonical data intensive science system!
- ▶ Focus on CPU and RAM performance today
- ▶ But feel free to ask me about robustness/reproducibility later on

This workshop

- ▶ You have an algorithm you want to use for a data intensive science application
- ▶ But you want the algorithm to run faster or use less RAM
 - ▶ Allow for more refined selection
 - ▶ Reduce computing requirements
- ▶ Need to measure and improve speed
- ▶ Focus on Linux, C++ applications

Warning

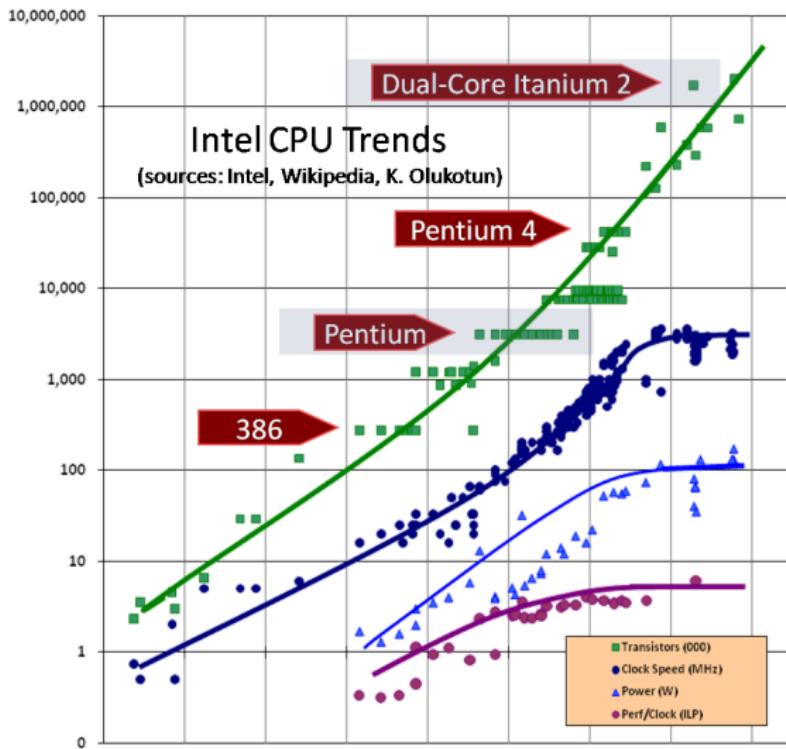
- ▶ Always implement something correct and readable (and save it to your version control system) first
- ▶ **Then** you can have fun optimising

Courtesy of reddit

```
//I don't know what I did but it works
//Please don't modify it
private int square(int n)
{
    int k = 0;
    while (true)
    {
        if (k == n*n)
        {
            return k;
        }
        k++;
    }
}
```

CPUs 101

- ▶ Moore's Law no longer holding for CPU clock speed (since \approx 2006)
 - ▶ Before then, could reasonably expect code to run faster on newer machines
- ▶ Memory has fallen behind CPU - big bottleneck frequently memory access
- ▶ More processing



Memory profiling

- ▶ Using too much memory is bad for two reasons
 - ▶ Eventually you run out (e.g. memory leak)
 - ▶ Allocating memory has a significant CPU cost - higher if your data doesn't fit in e.g. L1 cache
 - ▶ A single large allocation is cheaper than several small allocations
- ▶ Better to access memory in order - data-locality
 - ▶ Appropriate data structures help with this

Pipelining

- ▶ Pipelining allows processors to execute multiple instructions per clock cycle

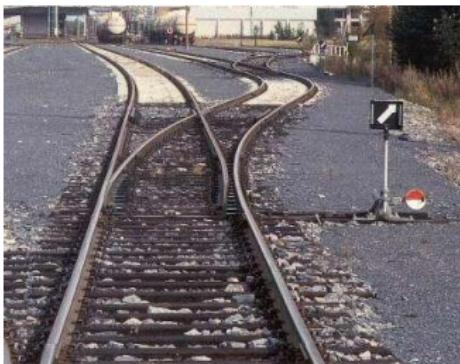


Five stage Instruction pipeline

- ▶ Only works for linear code
- ▶ Branching (e.g. `if` and `else`) is a problem
- ▶ Naively, can only execute one instruction to test branch

Branch prediction

- ▶ Module within CPU decides which branch to take (details [here](#))
- ▶ Allows CPU to pipeline code with branches
- ▶ Significant penalty if you take an unexpected branch - CPU has to load new code into pipeline



- ▶ Solution: remove branches if possible
- ▶ Unbalance your branches - 50/50 **if else** is harder to predict than e.g. 90/10 **if else**

Measuring runtimes

- ▶ Basic solution: time command
- ▶ user = time spent in your code
- ▶ sys = time spent in (Linux) kernel code
- ▶ real = sum of user + sys = **Walltime**

```
>time factor
 123456789098765432112345678987654321123456789
123456789098765432112345678987654321123456789: 3 3 3 3 3
    7 300239 122516477 13357815735863 147711262685101
real  0m1.172s
user  0m1.162s
sys  0m0.011s
```

- ▶ You (probably) only care about user
- ▶ If you're worried about system calls, you can use strace to see which ones are used (see e.g. [Julia Evans strace zine](#))

Walltime

- ▶ Walltime is the most important number for profiling, but also the most difficult to measure accurately
 - ▶ Varies with CPU
 - ▶ Some variation from operating system
 - ▶ Penalty for running in a virtual machine



Measuring runtimes

- ▶ Next level in complication: debugger
- ▶ Start your program, then randomly interrupt it a few times and see which function it's in

```
^C
Program received signal SIGINT, Interrupt.
0x00007f8d81f09b55 in SiSpacePointsSeedMaker_ATLxk::
    production3Sp() ()
    from libSiSpacePointsSeedTool_xk.so
(gdb) bt
#0  0x00007f8d81f09b55 in production3Sp() ()
    from libSiSpacePointsSeedTool_xk.so
#1  0x00007f8d81f0baaa in production3Sp() ()
    from libSiSpacePointsSeedTool_xk.so
#2  0x00007f8d81f0bc0b in find3Sp() ()
    from libSiSpacePointsSeedTool_xk.so
```

- ▶ This is the **callstack**
- ▶ If your program spends 90% of its time in function X, you have a 90% chance of catching it

Sampling profilers

- ▶ Congratulations, you've made a basic sampling profiler!
- ▶ Sample = interrupt, look at the call stack

```
^C
Program received signal SIGINT, Interrupt.
0x00007f8d81f09b55 in costlyFunction() ()
    from costlyNumerics.so
(gdb) bt
#0  0x00007f8d81f09b55 in costlyFunction() ()
    from costlyNumerics.so
#1  0x00007f8d81f0baaa in frameworkCode() ()
    from frameworkCode.so
#2  0x00007f8d81f0bc0b in main() ()
    from program.so
```

Cost

- ▶ costlyFunction() (top of the stack trace): where program was when halted
 - ▶ “Self cost”
- ▶ frameworkCall(), main(): call the function doing the work
 - ▶ “Total cost”
- ▶ Self cost \leq total cost
- ▶ Focus optimisation efforts on functions with highest self-cost

```
#0 0x00007f8d81f09b55 in costlyFunction() ()  
from costlyNumerics.so  
#1 0x00007f8d81f0baaa in frameworkCall() ()  
from frameworkCode.so  
#2 0x00007f8d81f0bc0b in main() ()  
from program.so
```

- ▶ Some would argue this is the one true profiler

Exercise 1: basic gdb

- ▶ Find number of primes below 1 million

```
gdb ./Exercise_1
...
(gdb) run
*Press Ctrl-C*
(gdb) backtrace
#0  0x00007f8d81f09b55 in costlyFunction()  ()
   from costlyNumerics.so
#1  0x00007f8d81f0baaa in frameworkCode()  ()
   from frameworkCode.so
(gdb) continue
*Press Ctrl-C*
(gdb) backtrace
#0  0x00007f8d81f09b55 in costlyFunction()  ()
   from costlyNumerics.so
#1  0x00007f8d81f0baaa in frameworkCode()  ()
   from frameworkCode.so
```

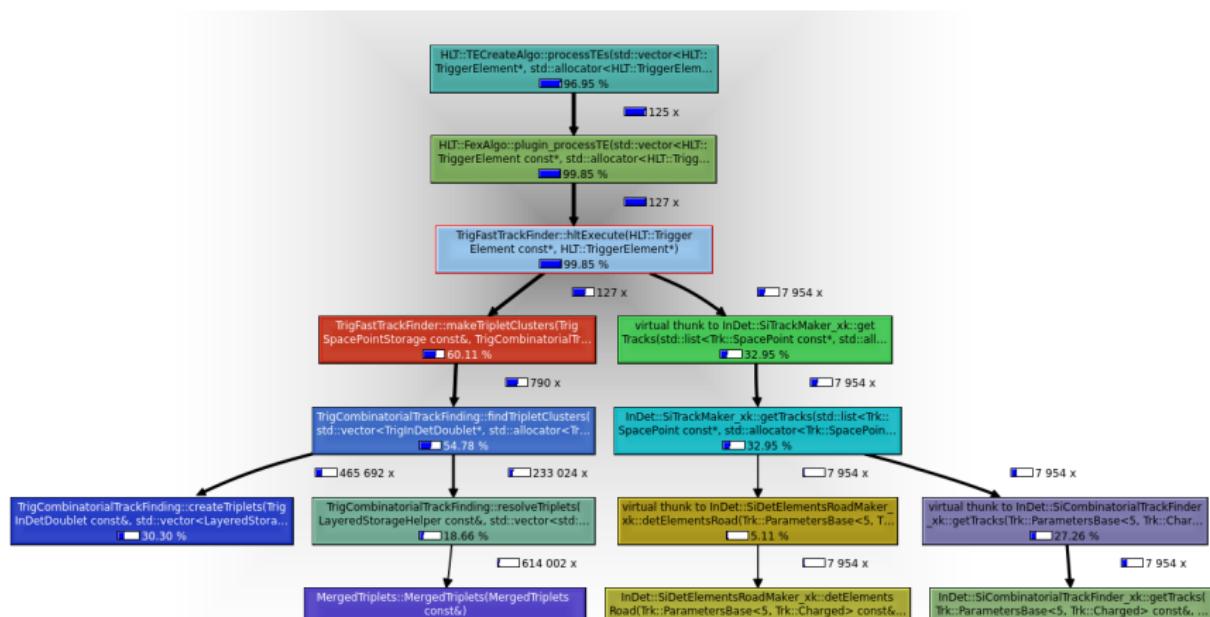
Exercise 1

Things to try

- ▶ Compare python and C++ speed
- ▶ Change optimisation flags -O0, -O1, -O2, -O3
- ▶ Swap clang for g++
- ▶ Keep code the same for now (even if you think/know you can improve it)
- ▶ Time code, interrupt in gdb

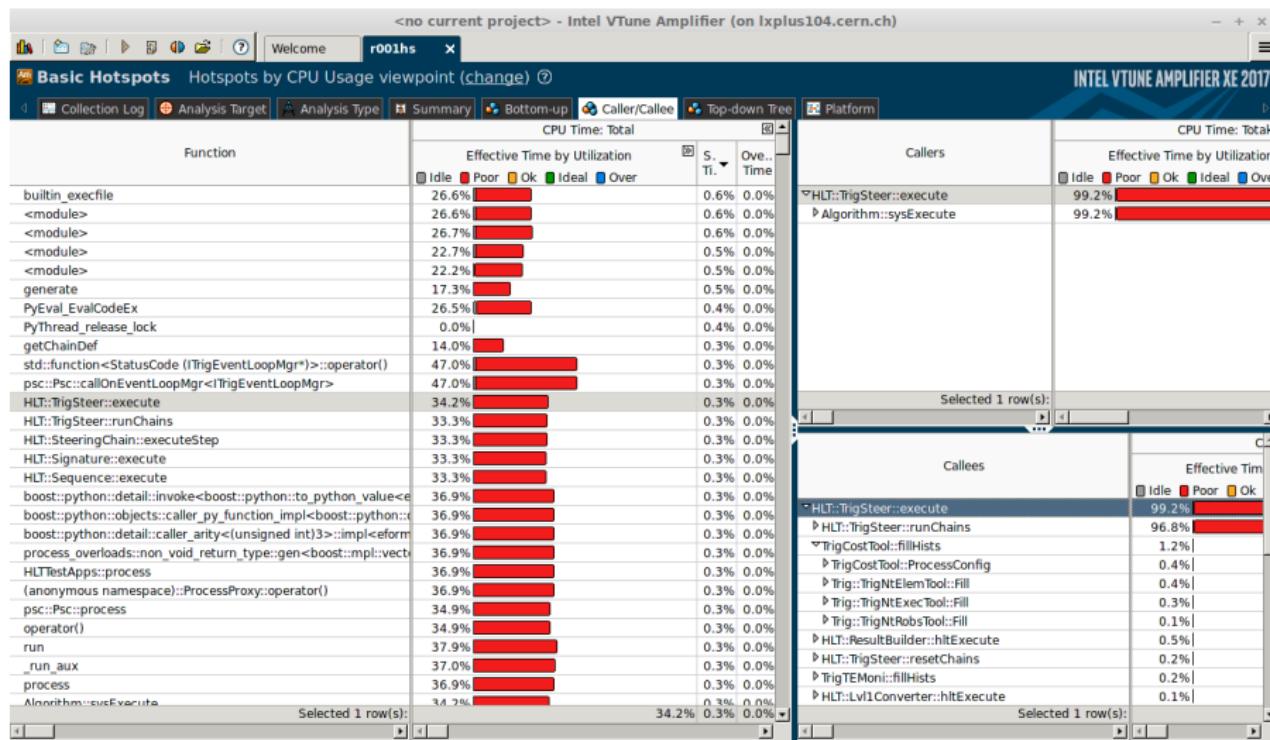
Sampling profilers

- ▶ Automate the call stack sampling procedure, generate a call graph (can be nicely explored in KCacheGrind)
- ▶ gperftools, Intel VTune, igprof
- ▶ Can also assign cost to lines of code (but take with a pinch of salt)



VTune

- ▶ Intel VTune is an excellent (but proprietary) tool
- ▶ Access possible through e.g. CERN



Emulation

- ▶ Callgrind tool (part of Valgrind²)
- ▶ Emulates a basic modern CPU, with level 1, level 2 caches,
branch prediction (somewhat configurable)
- ▶ Runs slowly
- ▶ Information about cache misses and branch misprediction
- ▶ Produces output suitable for KCacheGrind

²Very useful suite of tools for debugging and profiling

Instrumentation

- ▶ **perf** is now the gold standard - sampling and instrumenting
- ▶ Part of Linux kernel (best results with new kernels)
- ▶ Monitor performance monitoring counters (PMCs)
- ▶ VTune also has access to these
 - ▶ Some features require root access

```
perf stat -d program
      10 152 172 182      cycles:u          #
          3,451 GHz          (49,86%)
      14 584 154 073      instructions:u     #
          1,44  insn per cycle    (62,43%)
      2 318 605 154      branches:u        #
          788,130 M/sec       (74,93%)
      44 768 463      branch-misses:u     #
          1,93% of all branches   (75,00%)
      4 116 170 377      L1-dcache-loads:u   #
          1399,150 M/sec      (74,18%)
      167 821 302      L1-dcache-load-misses:u #
          4,08% of all L1-dcache hits   (25,06%)
      45 252 042      LLC-loads:u        #
          15,382 M/sec       (24,89%)
      8 794 669      LLC-load-misses:u    #
          
```

Profiling thoughts

- ▶ It's a cliche, but the biggest improvements usually come from changing algorithm, not minor changes to code
- ▶ Compiler Explorer is a great tool to get a feel for what the compiler is doing to your code
- ▶ Don't second-guess modern compilers
- ▶ Many profilers available
- ▶ Measure and benchmark

Compiler optimisation

- ▶ Standard compilers (GCC, clang) can do a lot of optimising for you!
 - ▶ -O0 = no optimisations applied
 - ▶ -O1, -O2 = basic, safe optimisations applied
 - ▶ -O3 = more experimental optimisations applied (for the brave)
- ▶ O2 is a good optimisation reference level
- ▶ Measure at O2/O3 **before** optimising by hand
- ▶ Fine-tuned optimisation options available - check GCC/clang documentation for details

CPU optimisation

- ▶ Once you've identified which part of your code takes the most time, you can start optimising
- ▶ Strategies are somewhat language-dependent, but some general points always true
- ▶ Compiled languages (C++, Fortran) faster than interpreted (Python, Ruby)
- ▶ Standard libraries (FFTW, BLAS, Eigen) likely faster than your own code - don't reinvent the wheel!

Floating-point operations

- ▶ Avoid square root if possible
- ▶ Avoid division if possible

```
y=x/5.0; //Bad  
y=x*0.2; //Good
```

- ▶ Rearrange calculations to minimise number of operations
- ▶ Compiler won't necessarily do this for you (floating point rules)

```
y = d*x*x*x + c*x*x + b*x + a; //Bad  
y = x*(x*(x*d+c)+b) + a; //Good
```

Higher mathematical functions

- ▶ Trigonometric functions are slow
 - ▶ Consider using an optimised library (see e.g. [VDT](#))
 - ▶ Trigonometric identities can help you
- ▶ For linear algebra, definitely use a library (e.g. [Eigen](#))

Loops

- ▶ Don't recalculate within loops: move code outside
- ▶ Consider storing frequently calculated values

```
for (i = 0; i < 50; i++) {  
    for (j = 0; j < 50; j++) {  
        x = sin(5*i) + cos(6*j);  
        //Can move sin() into earlier loop  
    }  
}
```

Putting it all together

- Sometimes you can remove branches and reduce number of operations all at once

```
//OLD
if ( h >= 0.) {
    h = min( max( 0.25*h, pow((x / y), 0.25)*h), 4.*h);
} else {
    h = max( min( 0.25*h, pow((x / y), 0.25)*h), 4.*h);
}
//NEW
h = h*min( max( 0.25, pow((x / y), 0.25)), 4.);
```

Algorithmic complexity

- ▶ If possible, stick to standard algorithms (e.g. C++ `std::sort`) instead of writing your own
- ▶ If the algorithm is a hotspot, consider trying out different algorithms (note, flashing lights)

Data structures

- ▶ Worth thinking about which data format fits your problem
- ▶ In C++, `std::vector` is probably a good fit

Points to remember

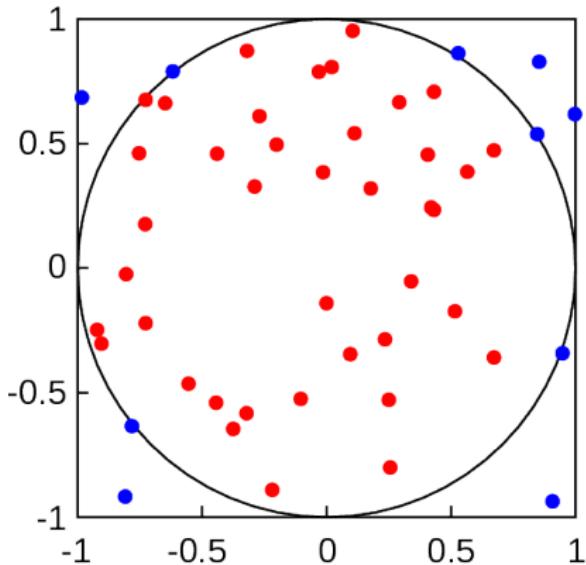
- ▶ Profiling and reasoning about code cannot tell you if you're using the wrong algorithm for your problem
- ▶ Writing your own implementation of something is an excellent way to learn, even if you never use it
- ▶ Correctness must come before optimisation

Back to exercise 1

- ▶ Fix identified bottleneck
- ▶ Measure result

Exercise 2

- ▶ Classic demonstration of Monte Carlo integration
- ▶ Throw darts at a circle inscribed in a square
- ▶ Ratio of darts hitting the blackboard tends to $(\pi r^2)/(4r^2) = \pi/4$
- ▶ Big difference in O0 vs. O2 runtime - where is the bottleneck?



Memory 101

Programs have access to two pools of memory: stack and heap

- ▶ Stack:

- ▶ Small amount of memory associated with program
- ▶ Fast to access - can be e.g. in CPU L1 cache
- ▶ E.g. variables in a function

```
int f(int x) {  
    int i = 55;  
    return x + i;  
}
```

- ▶ Heap:

- ▶ Slower to access than stack
- ▶ Can be **dynamically** allocated
- ▶ If you don't free up memory, this is where it leaks
- ▶ All the RAM available on the machine (if it runs out, it will use hard drive - v slow!)

```
int g(int x) {  
    int* i = new int(55); //On heap  
    return x + *i;  
    //Memory for i not given back to OS - leak  
}
```

Different allocators

- ▶ Your program will not just receive the memory it asks for when it asks for it
- ▶ Allocator decides how much to request at a time and how much should be contiguous
- ▶ **glibc** used by default
- ▶ Others available, particularly **jemalloc** (Facebook) and **tcmalloc** (Google)
- ▶ No need to recompile, just preload
- ▶ May work better for your memory access pattern than glibc - free speedup!

```
LD_PRELOAD=/usr/lib/libtcmalloc.so.4 ./my_program
```

Finding big allocations

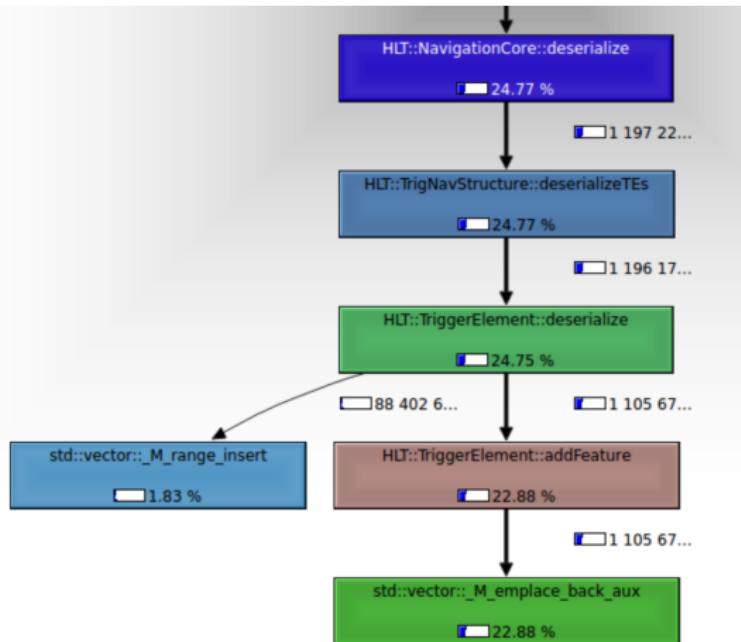
- ▶ Scenario: your program is running out of memory
- ▶ How to track down large (e.g. 1 GB) allocations?
- ▶ `tcmalloc` provides a printout when this happens

```
tcmalloc: large alloc 2720276480 bytes == 0x73eda000 @  
tcmalloc: large alloc 2720276480 bytes == 0x2a96f0000 @  
tcmalloc: large alloc 2720276480 bytes == 0x34b932000 @
```

- ▶ Add a breakpoint at `ReportLargeAlloc`

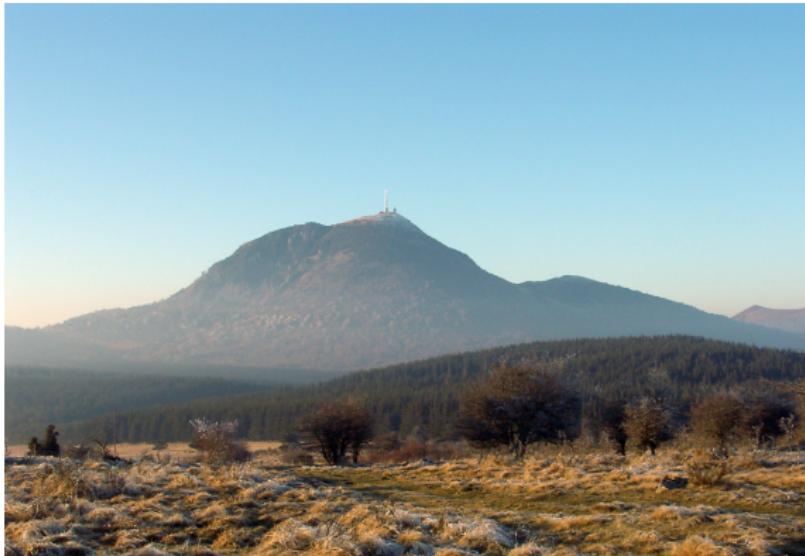
Heap profilers

- ▶ `jemalloc` and `tcmalloc` both come with low-overhead profilers to analyse which functions allocate most memory
- ▶ Output can be interpreted much as with a call-graph



Exercise 3: the memory hog

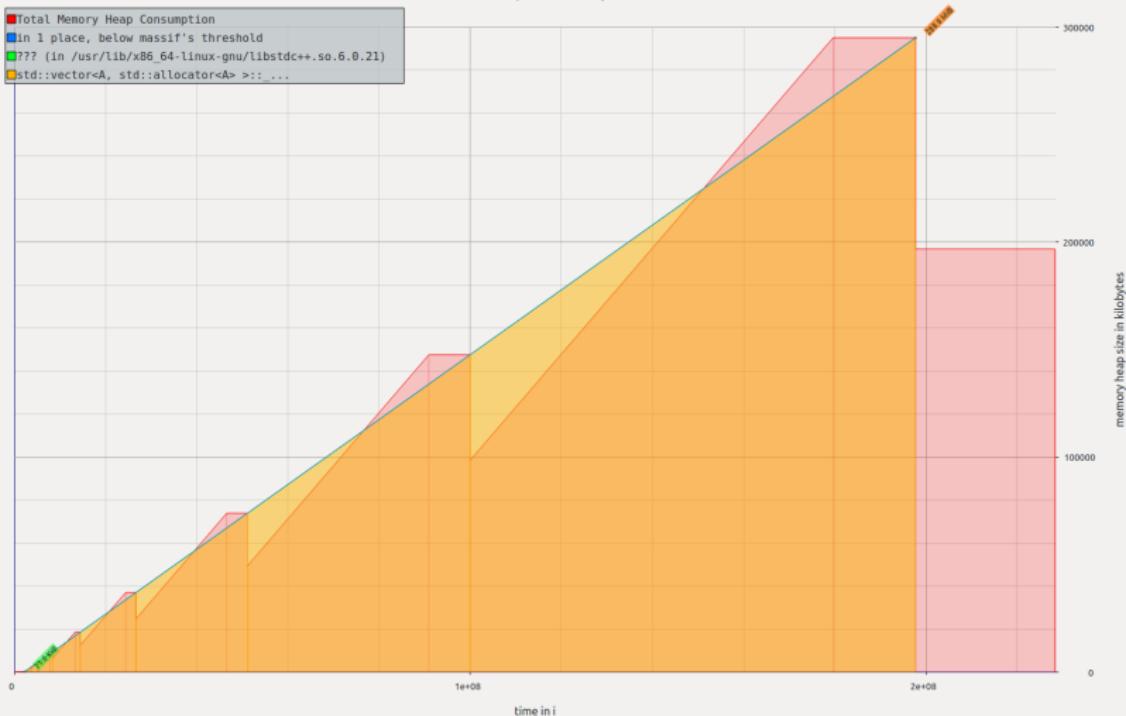
- ▶ Exercise 3 is a program that creates a C++ vector and fills it with some data
- ▶ Vectors are dynamically allocated - once you get to the end it asks for 2x as much storage space
- ▶ Better to pre-reserve data: `vec.reserve(maxlen)` so it only asks for as much space as needed
- ▶ Measure effect using Valgrind massif tool



Open Close <> Shorten Templates Toggle total cost graph Toggle detailed cost graph Select peak snapshot Stacked diagrams: 10

massif.out.3655

Memory consumption of ./Exercise_3
Peak of 288.1 MiB at snapshot #69



Massif Data

filter	
0 B: Snapshot #0	
71.0 KiB: Snapshot #1	
71.0 KiB: Snapshot #2	
71.0 KiB: Snapshot #3	
► 71.0 KiB: Snapshot #4	
71.0 KiB: Snapshot #5	
71.1 KiB: Snapshot #6	
71.0 KiB: Snapshot #7	
71.1 KiB: Snapshot #8	
71.1 KiB: Snapshot #9	
71.3 KiB: Snapshot #10	
71.2 KiB: Snapshot #11	
71.6 KiB: Snapshot #12	
71.4 KiB: Snapshot #13	
► 72.1 KiB: Snapshot #14	
► 72.1 KiB: Snapshot #15	
71.8 KiB: Snapshot #16	
73.2 KiB: Snapshot #17	
72.5 KiB: Snapshot #18	
75.5 KiB: Snapshot #19	
75.5 KiB: Snapshot #20	
► 75.5 KiB: Snapshot #21	
74.0 KiB: Snapshot #22	
80.0 KiB: Snapshot #23	
80.0 KiB: Snapshot #24	
77.0 KiB: Snapshot #25	
89.0 KiB: Snapshot #26	
► 89.0 KiB: Snapshot #27	
83.0 KiB: Snapshot #28	
107.0 KiB: Snapshot #29	
► 107.0 KiB: Snapshot #30	
95.0 KiB: Snapshot #31	
143.0 KiB: Snapshot #32	
► 143.0 KiB: Snapshot #33	
119.0 KiB: Snapshot #34	
215.0 KiB: Snapshot #35	
► 215.0 KiB: Snapshot #36	
167.0 KiB: Snapshot #37	
359.0 KiB: Snapshot #38	
► 359.0 KiB: Snapshot #39	
263.0 KiB: Snapshot #40	
647.0 KiB: Snapshot #41	
► 647.0 KiB: Snapshot #42	
455.0 KiB: Snapshot #43	
1.2 MiB: Snapshot #44	
► 1.2 MiB: Snapshot #45	
839.0 KiB: Snapshot #46	
2.3 MiB: Snapshot #47	
► 2.3 MiB: Snapshot #48	
1.6 MiB: Snapshot #49	
4.6 MiB: Snapshot #50	
► 4.6 MiB: Snapshot #51	
3.1 MiB: Snapshot #52	
► 3.1 MiB: Snapshot #53	

Custom Allocators Massif Data

Conclusions

- ▶ A small amount of profiling/optimisation knowledge can dramatically improve your application performance
 - ▶ Profiling is more important than optimisation
- ▶ Advanced techniques useful once you've done the easy bits

Useful references

- ▶ Numerical Recipes in C++, Second Edition, Press, Teukolsky, Vetterling and Flannery
- ▶ Brendan Gregg [Linux performance resources](#)
- ▶ Agner Fog [optimisation resources](#) (C++ focused)
- ▶ Ulrich Drepper
[What Every Programmer Should Know About Memory](#)