Introduction to profiling and optimisation

Stewart Martin-Haugh, Nikos Konstantinidis (UCL), Tim Scanlon (UCL)

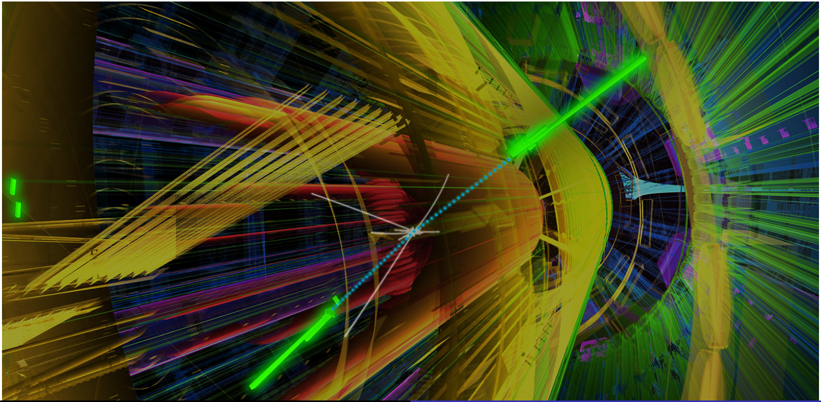
Data Intensive Science Centres for Doctoral Training Launch Event, Cardiff

27/28 October 2017

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) $\approx$ 1 megabyte
- $\approx$ 40 million collisions every second $\rightarrow$ 40 terabyte/second output rate
- Google data storage $\approx$ 15 exabytes = 15 $\times$ 10^18 bytes[1]

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

- Even if we fill up Google's data centres, we would only have 1/100th of the data we have now
  - Google would probably not agree to give up their data centres
- 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

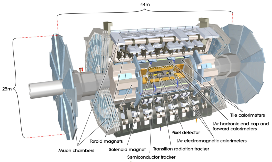
To summarise

- 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

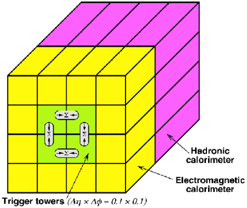
Trigger systems for particle physics

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



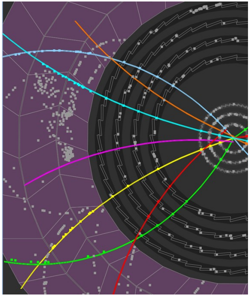
ATLAS detector

$\rightarrow$



Fast hardware - microsecond decision time

$\rightarrow$



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

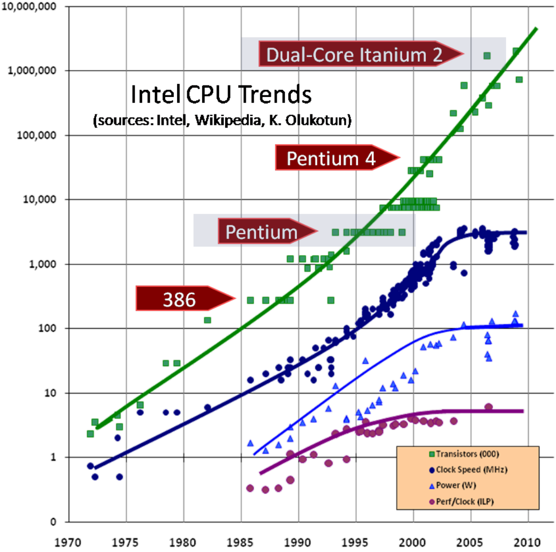
- Always implement something correct and readable (and save it to your version control system) first
- **Then** you can have fun optimising

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 ≈ 2006)
- Memory has fallen behind CPU - big bottleneck frequently memory access
- More processing power available through parallelisation - not covered here



Source: Herb Sutter

Pipelining

- Pipelining allows processors to execute multiple instructions per clock cycle

IF	ID	EX	MEM	WB				
	IF	ID	EX	MEM	WB			
		IF	ID	EX	MEM	WB		
			IF	ID	EX	MEM	WB	
				IF	ID	EX	MEM	WB

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
   1234567890987654321123456789876543211234567890
1234567890987654321123456789876543211234567890: 3 3 3 3 3
    7 300239 122516477 13357815735863 14771126268510
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
```

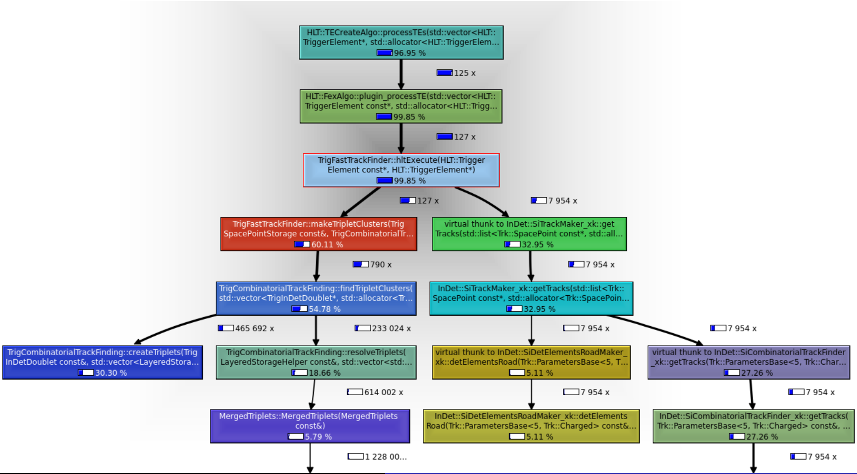
Exercise 1

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

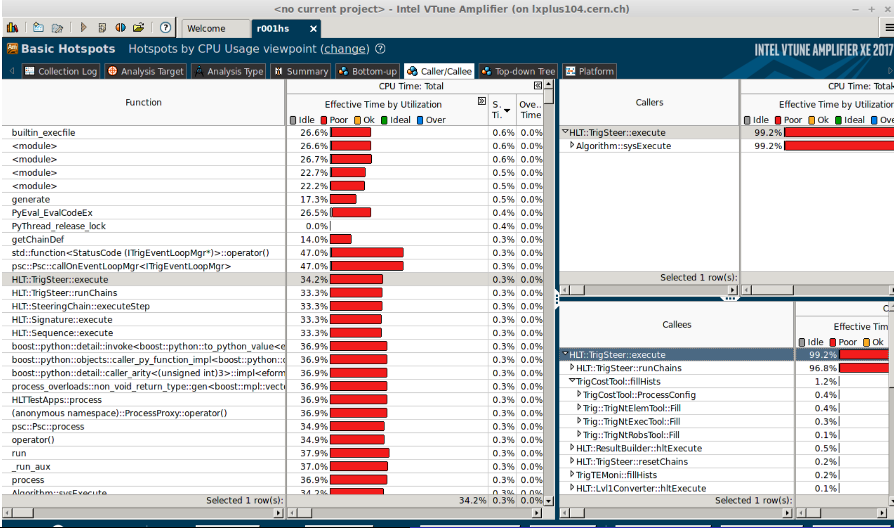
Sampling profilers

- 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 Valgrind[2])
- 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

[2] Very 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
- 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
  - -03 = 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

Optimisation example

- GCC and Clang compilers can reduce square example[3] down to something sensible

```
int square(int n)
{
  int k = 0;
  while (true)
  {
    if(k == n*n)
    {
      return k;
    }
    k++;
  }
}
```

→

```
int square2(int n)
{
    return n*n;
}
```

- Optimising compilers are amazing - you only need to care when optimisation fails

[3] NB: Don't write a square function, just square numbers in the code

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

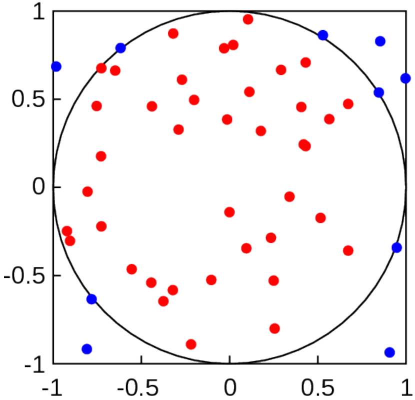
- Profiling and reasoning about code cannot tell you if you're using the wrong algorithm for your problem
- Writing your own implementation of something is an excellent way to learn, even if you never use it
- Correctness must come before optimisation

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
}
```

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

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

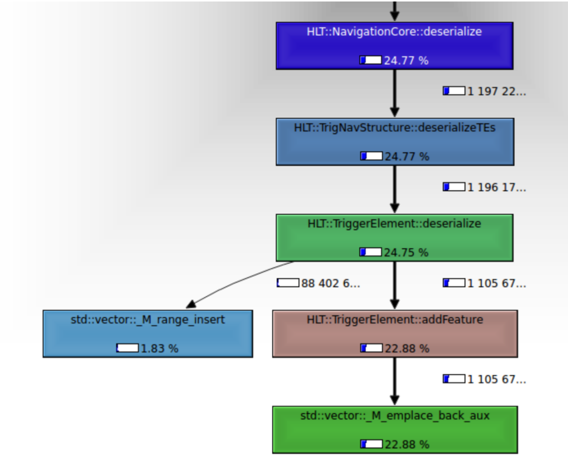
- Scenario: your program is running out of memory
- How to track down large (e.g. 1 GB) allocations?
- **`tcmalloc`** provides a printout when this happens

```
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

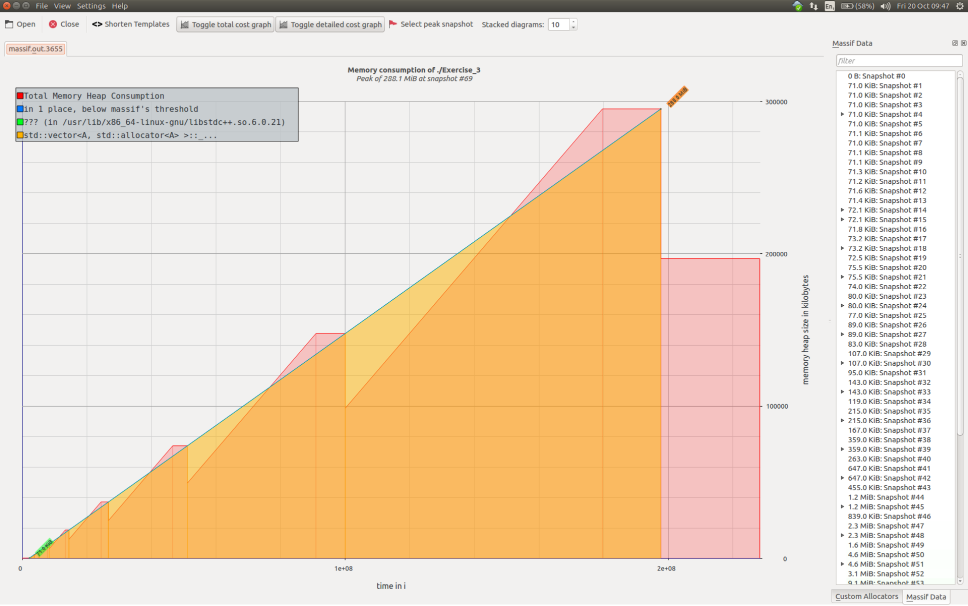
- Exercise 3 is a program that creates a C++ vector and fills it with some data
- Vectors are dynamically allocated - once you get to the end it asks for 2x as much storage space
- Better to pre-reserve data: **`vec.reserve(maxlen)`** so it only asks for as much space as needed
- Measure effect using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

Exercise 3: the memory hog

```
ms_print massif.out.3655
--------------------------------------------------------------------------------

Command:              ./Exercise_3 --detailed-freq
Massif arguments:     (none)
ms_print arguments: massif.out.3655
--------------------------------------------------------------------------------


    MB
288.1^                                                        :::::#
     |                                                        :    #
     |                                                        :    #
     |                                                        :    #
     |                                                        :    #
     |                                                        :    #
     |                                                        :    #
     |                                                        :    #:::::::::
     |                                                        :    #        :
     |                                                        :    #        :
     |                            :::@                        :    #        :
     |                            :  @                        :    #        :
     |                            :  @                        :    #        :
     |                            :  @                        :    #        :
     |                            :  @:::::::::::::::::::::::::    #        :
     |              ::@           :  @                        :    #        :
     |              : @           :  @                        :    #        :
     |              : @::::::::::::  @                        :    #        :
     |       :@     : @           :  @                        :    #        :
     |    @  :@:::::  @           :  @                        :    #        :
   0 +----------------------------------------------------------------------->Mi
     0                                                                   217.9
```


File View Settings Help
Fri 20 Oct 09:47
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
Total Memory Heap Consumption
in 1 place, below massif's threshold
??? (in /usr/lib/x86_64-linux-gnu/libstdc++.so.6.0.21)
std::vector<A, std::allocator<A> >::_...
288.6 MiB
71.0 KiB
300000
200000
100000
0
memory heap size in kilobytes
0
1e+08
2e+08
time in i
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
73.2 KiB: Snapshot #18
72.5 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
Custom Allocators
Massif Data

Memory profiling thoughts

- Memory profiling is more difficult than CPU profiling - tools less advanced/convenient
  - But improving all the time
- Can make a big difference if you're using a lot of memory

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