ARCHER Software Carpentry bootcamp

Mike Jackson, Arno Proeme, ARCHER CSE Team
michaelj@epcc.ed.ac.uk
aproeme@epcc.ed.ac.uk

Reusing this material

This work is licensed under a Creative Commons Attribution-NonCommercial-ShareAlike 4.0 International License.

http://creativecommons.org/licenses/by-nc-sa/4.0/deed.en_US

This means you are free to copy and redistribute the material and adapt and build on the material under the following terms: You must give appropriate credit, provide a link to the license and indicate if changes were made. If you adapt or build on the material you must distribute your work under the same license as the original.

Note that this presentation contains images owned by others. Please seek their permission before reusing these images.

archer software carpentry | epcc | THE UNIVERSITY OF EDINBURGH

http://www.archer.ac.uk

support@archer.ac.uk

ARCHER in a nutshell

- UK National Supercomputing Service
  - Replacement for HECToR (they overlap by ~4 months)
- Cray XC30 Hardware
  - Nodes based on 2×Intel Ivy Bridge 12-core processors
  - 64GB (or 128GB) memory per node
  - 3008 nodes in total (72162 cores)
  - Linked by Cray Aries interconnect (dragonfly topology)
- Cray Application Development Environment
  - Cray, Intel, GNU Compilers
  - Cray Parallel Libraries (MPI, SHMEM, PGAS)
  - DDT Debugger, Cray Performance Analysis Tools

Performance

- HECToR #50 in top 500 with 830 TFlop/s
- ARCHER
  - Designed to provide 3-4 times scientific throughput of HECToR
  - #19 in November 2013 top 500 list with 1.65 PFlop/s
  - Fastest (known) computer in the UK
- Extract the best performance possible from the hardware

Optimization

- “More computing sins are committed in the name of efficiency (without necessarily achieving it) than for any other single reason ..
- …Including blind stupidity” (Wulf)
- "We should forget about small efficiencies, say about 97% of the time:
- …Premature optimization is the root of all evil.“ (Knuth 1974)
- “performance variability that derives from differences among programmers of the same language … is on average as large or larger than the variability found among the different languages.” (Prechelt 2000)

Three rules of optimization

- Don't – optimised code is not readable or maintainable code
- Don't....yet – designing code is not the same as optimising code
- Profile first – anything else is just a guess!

- How do we prevent ourselves introducing bugs when we're optimizing and parallelizing?
- Isn't our time more valuable than a computer's time?
- Hardware life < software life < our life

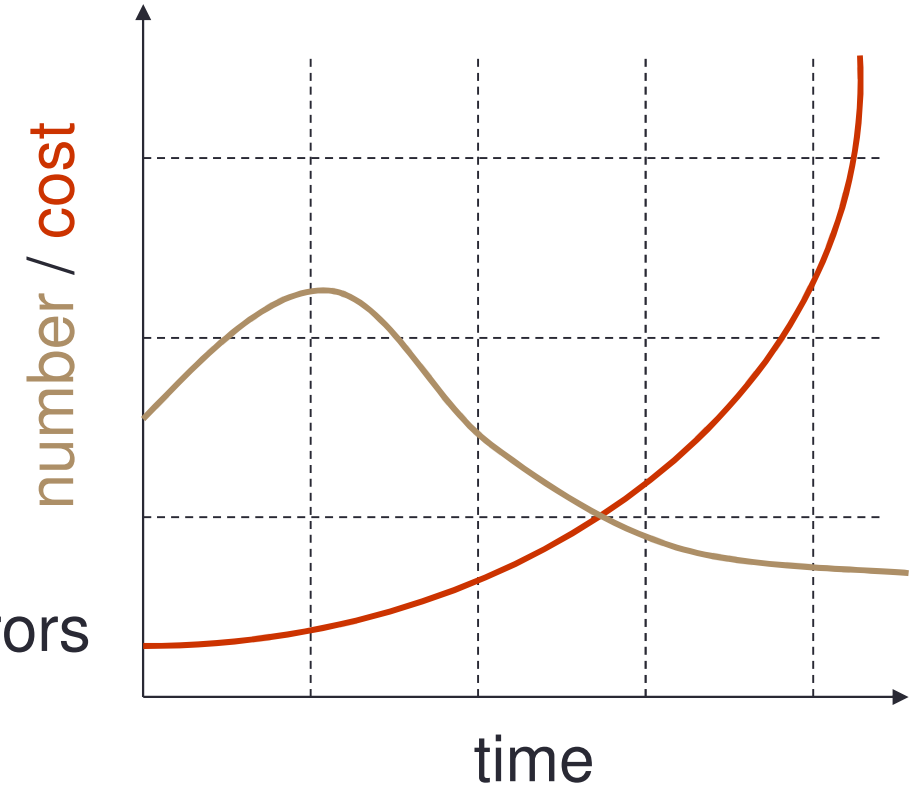
Optimize ourselves

50%-80% of errors
in
15%-20% of modules
(Davis 1995 quoting Endres 1975, Weinberg 1992)

50% of modules are error free
(Boehm and Basili 2001)

design errors >> # coding errors
(Boehm et al. 1975)

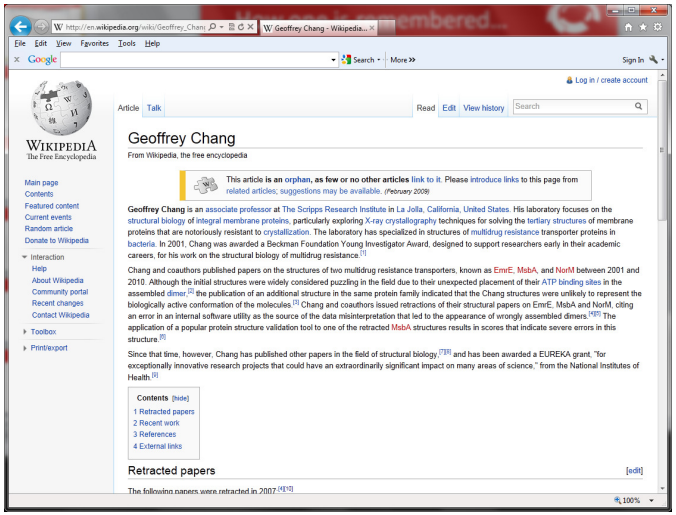
Technical debt
1-10-100 rule



archer | software carpentry | epcc | The University of Edinburgh

What about correctness?

We wish to retract our research article … and both of our Reports...
An **in-house data reduction program** introduced a change in sign for anomalous differences…
Unfortunately, the use of the multicopy refinement procedure still allowed us to obtain reasonable refinement values for the **wrong** structures.

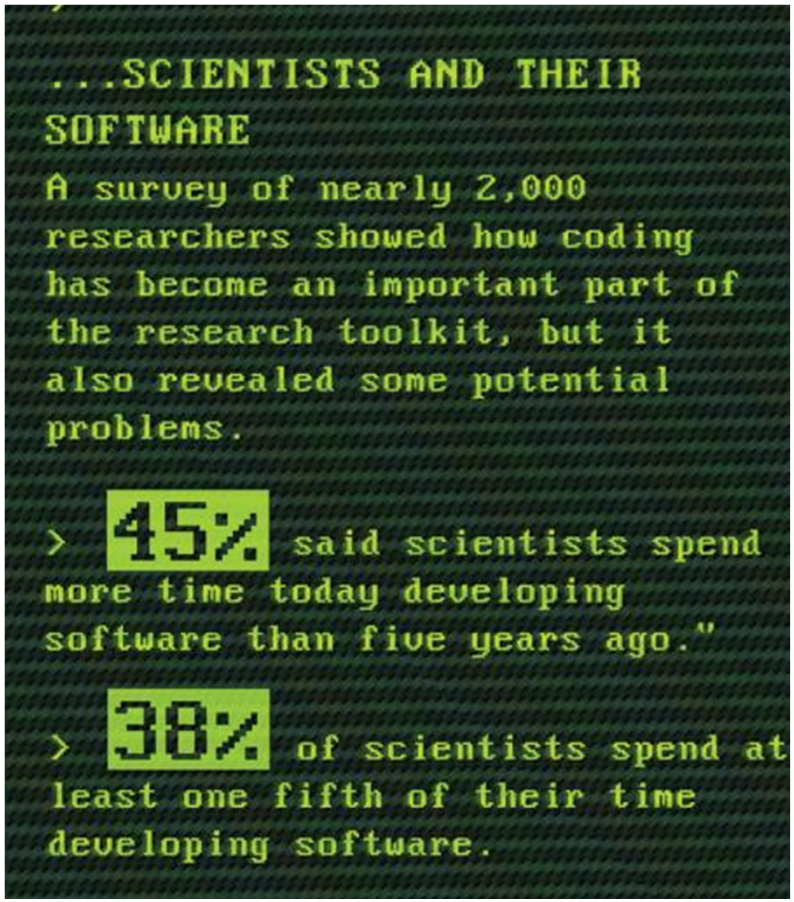


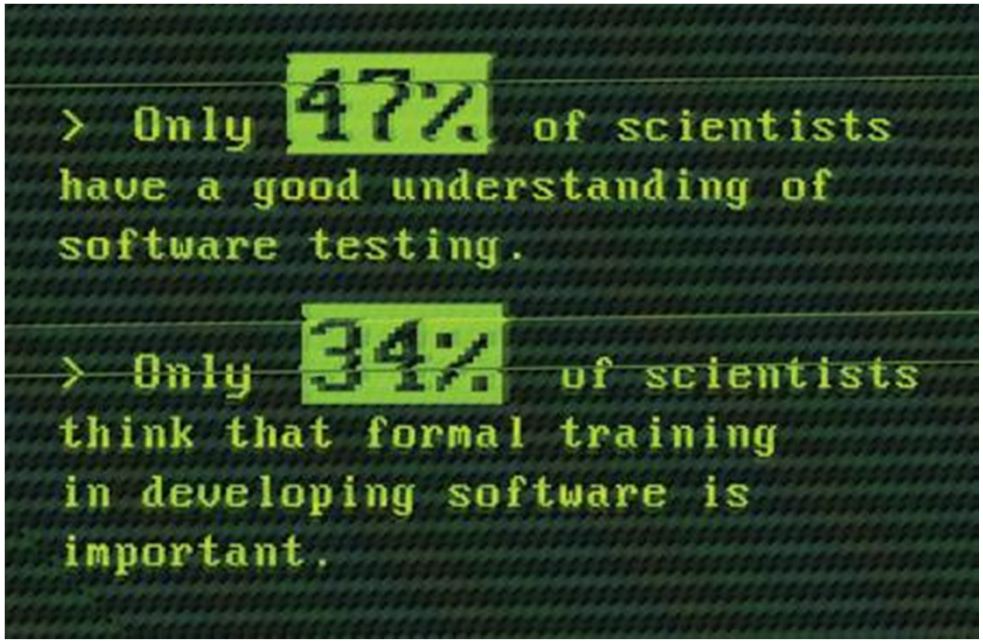
archer

epcc

THE UNIVERSITY OF EDINBURGH

A skills gap



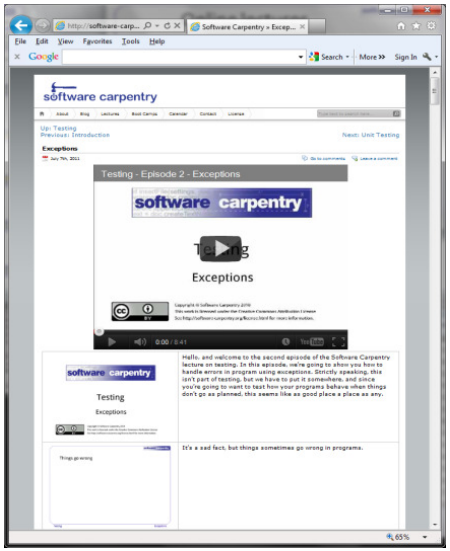


Hannay et al, "How Do Scientists Develop and Use Scientific Software?
SECSE '09 Proceedings of the 2009 ICSE Workshop on Software Engineering for Computational Science and Engineering, IEEE Computer Society, 2009. DOI: 10.1109/SECSE.2009.5069155
Images courtesy of Greg Wilson and Neil Chue Hong

archer | software carpentry | epcc | The University of Edinburgh

Filling the gap

Software Sustainability Institute



DiRAC

mozilla Science Lab

DTC

RESEARCH COUNCILS UK

Centre for Doctoral Training

archer

software carpentry

epcc

THE UNIVERSITY OF EDINBURGH

Important stuff

Images courtesy of (clockwise from top-left) oneVillage initiative, Bobbymond, Dajanda, Anton Novojilov

archer | software carpentry | epcc | The University of Edinburgh

How to ask for help

- Flag down a helper

- Stick up your sticky note
  - Red – I'm stuck, help!
  - Green – I'm fine