#### Pulling everything together

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# Reusing this material



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http://www.archer.ac.uk support@archer.ac.uk







# Best practices for scientific computing

- Write programs for people, not computers
- Let the computer do the work
- Make incremental changes
- Don't repeat yourself (or others)
- Plan for mistakes
- Optimize software only after it works correctly
- Document design and purpose, not mechanics
- Collaborate

Wilson G, Aruliah DA, Brown CT, Chue Hong NP, Davis M, et al. (2014) Best Practices for Scientific Computing. PLoS Biol 12(1): e1001745. doi:10.1371/journal.pbio.1001745. http://dx.doi.org/10.1371/journal.pbio.1001745.







## Ten simple rules for reproducible computational research

- For every result, keep track of how it was produced
- Avoid manual data manipulation steps
- Archive the exact versions of all external programs used
- Version control all custom scripts
- Record all intermediate results, when possible in standardized formats 5.
- For analyses that include randomness, note underlying random seeds
- Always store raw data behind plots
- Generate hierarchical analysis output, allowing layers of increasing detail to be inspected
- Connect textual statements to underlying results
- Provide public access to scripts, runs, and results

Sandve GK, Nekrutenko A, Taylor J, Hovig E (2013) Ten Simple Rules for Reproducible Computational Research. PLoS Comput Biol 9(10): e1003285. doi:10.1371/journal.pcbi.1003285. http://dx.doi.org/10.1371/journal.pcbi.1003285.







## Why bother?

- Poor organizational choices can lead to significantly slower research progress
- Help someone unfamiliar with your project look at your files and understand in detail what you did and why
  - Researchers, collaborators, students, research supervisors, Pls
  - You!
- Help yourself do things over and over again
  - Correct flaws in the initial preparation of the data being analysed
  - Update when you get access to new data
  - Broaden parameterizations of a particular model

Noble WS (2009) A Quick Guide to Organizing Computational Biology Projects. PLoS Comput Biol 5(7): e1000424. doi:10.1371/journal.pcbi.1000424. http://dx.doi.org/10.1371/journal.pcbi.1000424.







#### Iterative development

What did you think of this bootcamp?

- http://www.archer.ac.uk/training/feedback/
- Sticky Notes:
  - One good point on green learned, enjoyed
  - One bad point on red confused, bothered
- Optional post-course questionnaire:
  - http://tinyurl.com/2014-09-16-imperial-post







### Getting access to ARCHER

- Standard research grant
  - Request Technical Assessment using form on ARCHER website
  - Submit completed TA with notional cost in Je-S
  - Apply for time for maximum of 2 years
- ARCHER Resource Allocation Panel (RAP)
  - Request Technical Assessment using form on ARCHER website
  - Submit completed TA with RAP form
  - Every 4 months
- Application for computer time only
  - Instant Access Pump-Priming Time
  - Request Technical Assessment using form on ARCHER website
  - Submit completed TA with 2 page description of work







#### Support and Documentation

- Helpdesk
  - Email <u>support@archer.ac.uk</u>
  - via ARCHER SAFE <a href="http://www.archer.ac.uk/safe">http://www.archer.ac.uk/safe</a>
  - phone: +44 (0)131 650 5000
  - By post, to: Liz Sim EPCC, University of Edinburgh JCMB, The King's Buildings Mayfield Road, EDINBURGH, EH9 3JZ
- http://www.archer.ac.uk/community/techforum/
- http://www.archer.ac.uk/documentation/







## Training opportunities

- ARCHER Training (free to academics)
  - http://www.archer.ac.uk/training/
- Online sessions (using Blackboard Collaborate)
  - Technical Forum meetings (normally15:00 last Wednesday of month)
    - technical presentations of interest to ARCHER users
    - http://www.archer.ac.uk/community/techforum/
  - Virtual tutorials (normally 15:00 second Wednesday of month)
    - opportunity for discussion with ARCHER staff on any topic
    - usually starts with a presentation of general interest
    - http://www.archer.ac.uk/training/virtual/
- EPCC MSc in HPC (scholarships available)
  - http://www.epcc.ed.ac.uk/msc/







# Funding calls

- Embedded CSE support
  - Through a series of regular calls, Embedded CSE (eCSE) support provides funding to the ARCHER user community to develop software in a sustainable manner for running on ARCHER. Funding will enable the employment of a researcher or code developer to work specifically on the relevant software to enable new features or improve the performance of the code
  - Apply for funding for development effort
  - Planned every 4 months
  - Third call opens Tuesday 5th August, 2014 and closes at 4pm on Tuesday 16th September, 2014 (to be confirmed)
- See http://www.archer.ac.uk/community/eCSE/ for details



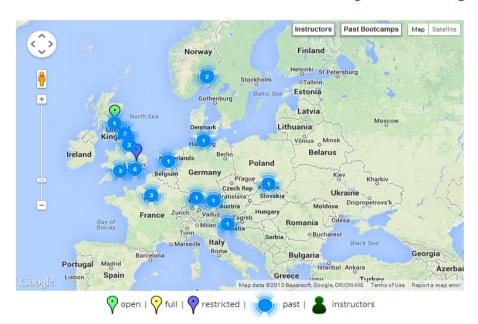


#### Getting involved in Software Carpentry









admin-uk@software-carpentry.org http://software-carpentry.org/bootcamps http://software-carpentry.org/lessons.html







#### Software Sustainability Institute



#### We want the research community to

- Recognise software as a fundamental research output
- Recognise the value of research software engineers
- Receive better software training
- Recognise the role of software in reproducibility

#### What we do

- **Fellowship**: we find and nurture researchers with combined talents in research and software
- **Software Carpentry**: teaching basic software skills to researchers from all disciplines
- **Consultancy**: providing software expertise to advance research software
- **Campaigning**: raising the profile of software in research and highlighting the issues it faces



#### Thank you!







