Pulling everything together

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Reusing this material

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Partnership for Advanced Computing in Europe

http://www.training.prace-ri.eu

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Best practices for scientific computing

1. Write programs for people, not computers
    A. A program should not require its readers to hold more than a handful of facts in memory at once
    B. Make names consistent, distinctive, and meaningful
    C. Make code style and formatting consistent

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.

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Best practices for scientific computing

1. Write programs for people, not computers
2. Let the computer do the work
   A. Make the computer repeat tasks
   B. Save recent commands in a file for re-use
   C. Use a build tool to automate workflows

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.

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Best practices for scientific computing

1. Write programs for people, not computers
2. Let the computer do the work
3. Make incremental changes
   A. Work in small steps with frequent feedback and course correction
   B. Use a version control system
   C. Put everything that has been created manually in version control

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Best practices for scientific computing

1. Write programs for people, not computers
2. Let the computer do the work
3. Make incremental changes
4. Don't repeat yourself (or others)
   A. Every piece of data must have a single authoritative representation in the system
   B. Modularise code rather than copying and pasting
   C. Re-use code instead of rewriting it

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3. Make incremental changes
4. Don't repeat yourself (or others)
5. Plan for mistakes
   A. Add assertions to programs to check their operation
   B. Use an off-the-shelf unit testing library
   C. Turn bugs into test cases
   D. Use a symbolic debugger

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3. Make incremental changes
4. Don't repeat yourself (or others)
5. Plan for mistakes
6. Optimise software only after it works correctly
   A. Use a profiler to identify bottlenecks
   B. Write code in the highest-level language possible

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4. Don't repeat yourself (or others)
5. Plan for mistakes
6. Optimise software only after it works correctly
7. Document design and purpose, not mechanics
   A. Document interfaces and reasons, not implementations
   B. Refactor code in preference to explaining how it works
   C. Embed the documentation for a piece of software in that software

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5. Plan for mistakes
6. Optimise software only after it works correctly
7. Document design and purpose, not mechanics
8. Collaborate
   A. Use pre-merge code reviews
   B. Use pair programming when bringing someone new up to speed and when tackling particularly tricky problems
   C. Use an issue tracking tool

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10 rules for reproducible computational research

1. For every result, keep track of how it was produced
2. Avoid manual data manipulation steps
3. Archive the exact versions of all external programs used
4. Version control all custom scripts
5. Record all intermediate results, when possible in standardized formats
6. For analyses that include randomness, note underlying random seeds
7. Always store raw data behind plots
8. Generate hierarchical analysis output, allowing layers of increasing detail to be inspected.
9. Connect textual statements to underlying results
10. 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.

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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**

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Funding Calls

- **Embedded SCE 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**

- **See http://www.archer.ac.uk/community/eCSE/ for details**

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Support and Documentation

- **Helpdesk**
  - **Email support@archer.ac.uk**
  - **via ARCHER SAFE http://www.archer.ac.uk/safe**
  - **Phone: +44 (0) 131 650 5000**
  - **By post, to: Liz Sim**
    EPCC, University of Edinburgh
    JCMB, The King's Buildings
    Peter Guthrie Tait Road
    Edinburgh, EH9 3FD

- **http://www.archer.ac.uk/community/techforum**

- **http://www.archer.ac.uk/documentation/**

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Training opportunities

- **ARCHER Training (free to academics)**
  - **http://www.archer.ac.uk/training/**

- **Online sessions (using Blackboard Collaborate)**
  - **Technical Forum meetings (normally 15:00 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/**

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Ever used a supercomputer? Give it a go!

- **After completing an online course about how to use ARCHER, you should be able to attempt the ARCHER driving test. This is a set of 20 multiple-choice questions covering all aspects of the ARCHER service.**

On successful completion of the ARCHER Driving Test you will be invited to apply for an account on ARCHER with 1200 kAUs to use over 12 months, enabling you to put your skills into practice.

For more information go to:

- **http://www.archer.ac.uk/training/course-material/online/**

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Getting involved in Software Carpentry

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

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Looking back…

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Leaving here you will have learned to:

- Write robust code
- Minimize repetitive tasks
- Appreciate the value of “sharable” code
- Share your work
- Protect your work
- Collaborate on other people’s work

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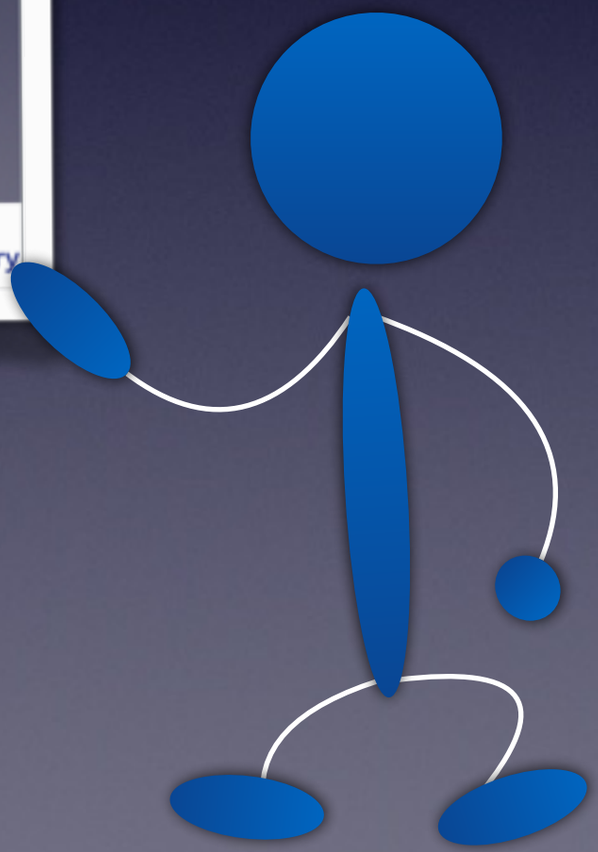

Thank you!


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