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Introduction to the Software Sustainability Institute

13 August 2014, CCP-SAS webinar

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Supported by EPSRC Pioneering research

Project funding from Jisc BBSRC NERC SCIENCE OF THE ENVIRONMENT

- Of course, we don't deliberately set out to create code that can't be used by others

  Right?

Pleiotropic loci – diabetes and Parkinson's disease

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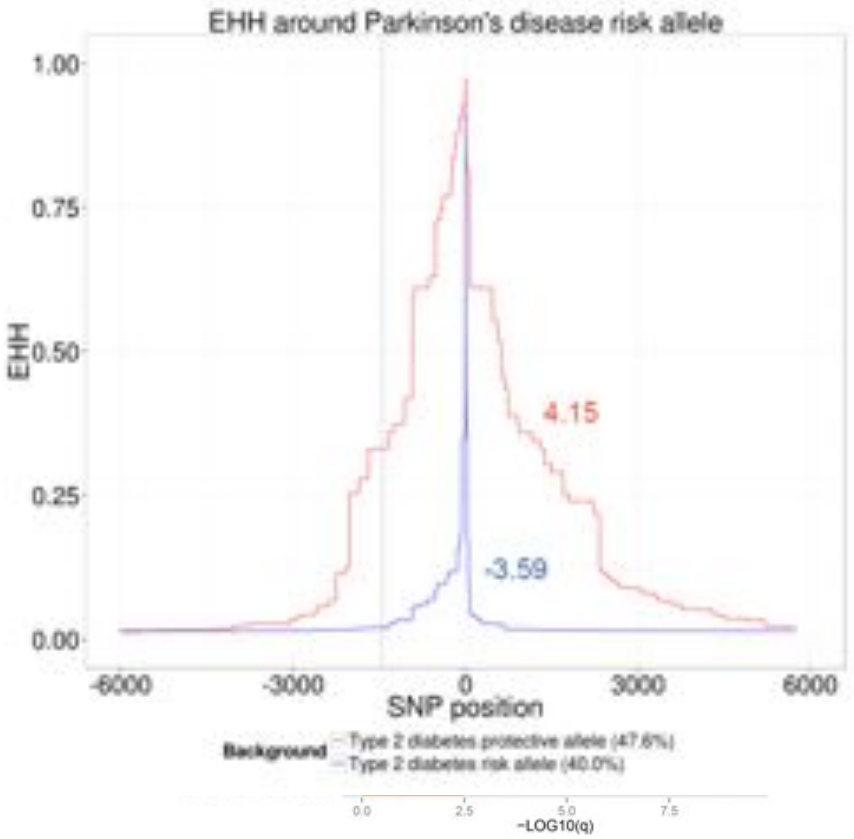

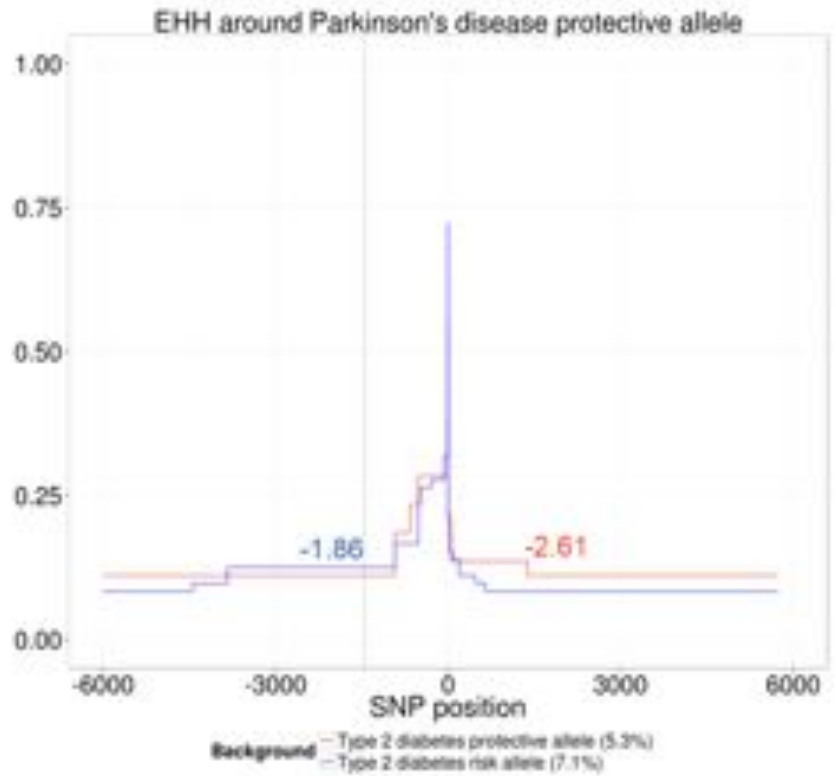

ROSLIN

Software Sustainability Institute

Selection at pleiotropic loci underlies disease co-occurrence in human populations.
Navarro, Haley, Karosas et al.
Submitted to Nature Genetics

Behind every great piece of science...


```
#go through each SNP of interest
for(my $x = 0; $x < scalar @pos; $x++)
{
    #and then each downstream SNP of interest
    for(my $y = $x+1; $y < scalar @pos; $y++)
    {
        #if SNPs within our chosen distance (500kb) and both present in the haplotypes file
        if((!($trait[$x] eq $trait[$y])) && (abs($pos[$x] - $pos[$y]) <= 500000) && (exists($legArrayPos{$po
        {
            my $snp1ArrayPos = "";
            my $snp2ArrayPos = "";
            my $snp1All = "";
            my $snp2All = "";

            #create output file for this SNP pair
            my $filename = "ConditionedResults2/$chr[$x].$pos[$x]-$pos[$y].EHH.GBR.2.txt";
            print "$filename\n";
            unless (-e $filename) {
                open(OUT, ">$filename");

                ######################CHANGE THESE IF NOT FOCUSING ON SECOND SNP#########################
                my $start = $pos[$y]-500000;
                if ($start < 1) {
                    $start = 1;
                }
                my $end = $pos[$y]+500000;
                if ($end > $chrLengths{$chr[$x]}) {
                    $end = $chrLengths{$chr[$x]};
                }
```

The modern researcher…

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Where do they learn how to do this?

Picture of Otto Stern courtesy of Emilio Segre Visual Archives

- … worries about:
  - Data management and analysis
  - Reproducible research
  - Scalable simulations
  - Integration of models and workflows
  - Collaboration

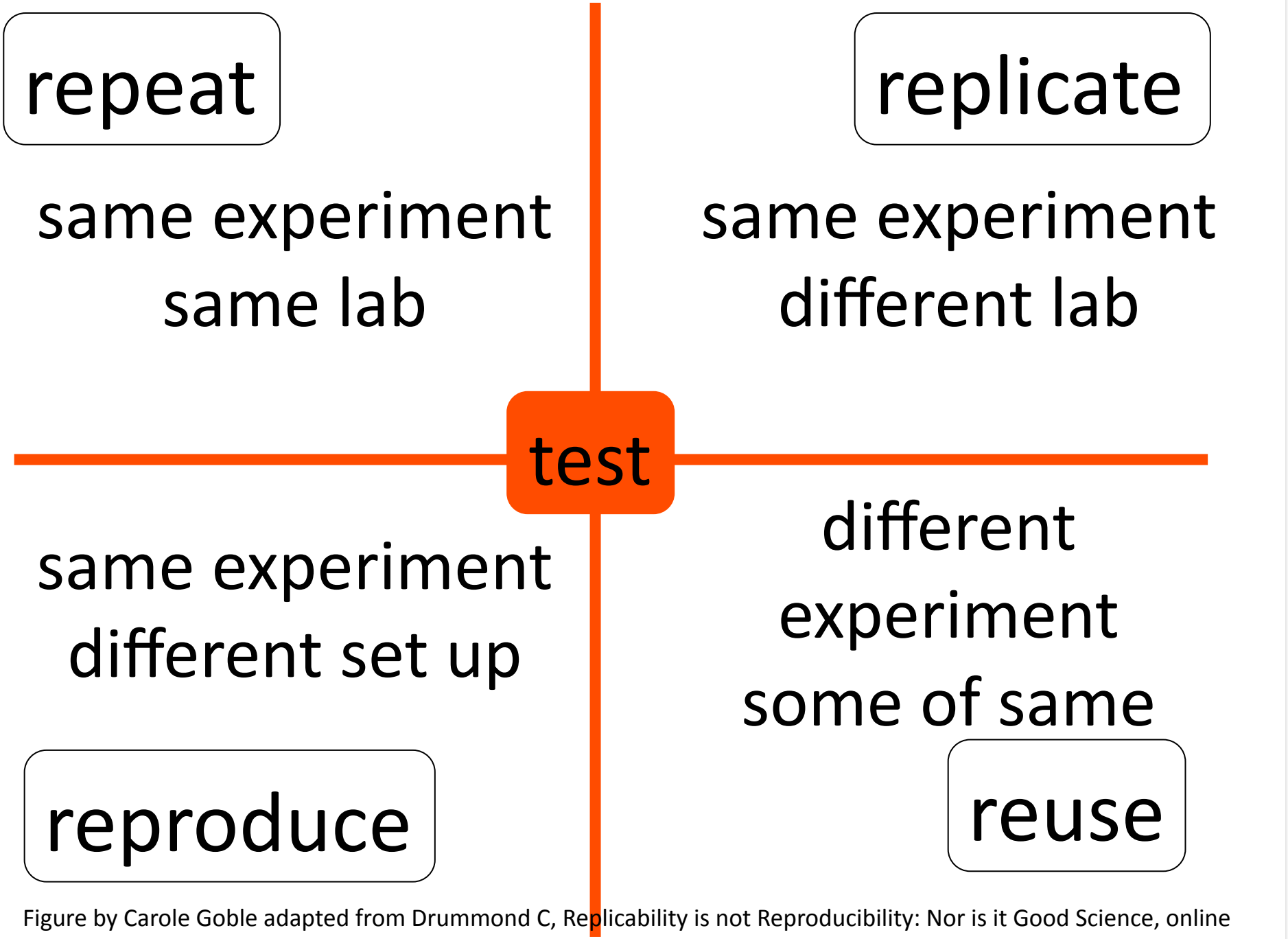

Figure by Carole Goble adapted from Drummond C, Replicability is not Reproducibility: Nor is it Good Science, online and Peng RD, Reproducible Research in Computational Science *Science 2 Dec 2011: 1226-1227.*

SIGMOD Reproducibility

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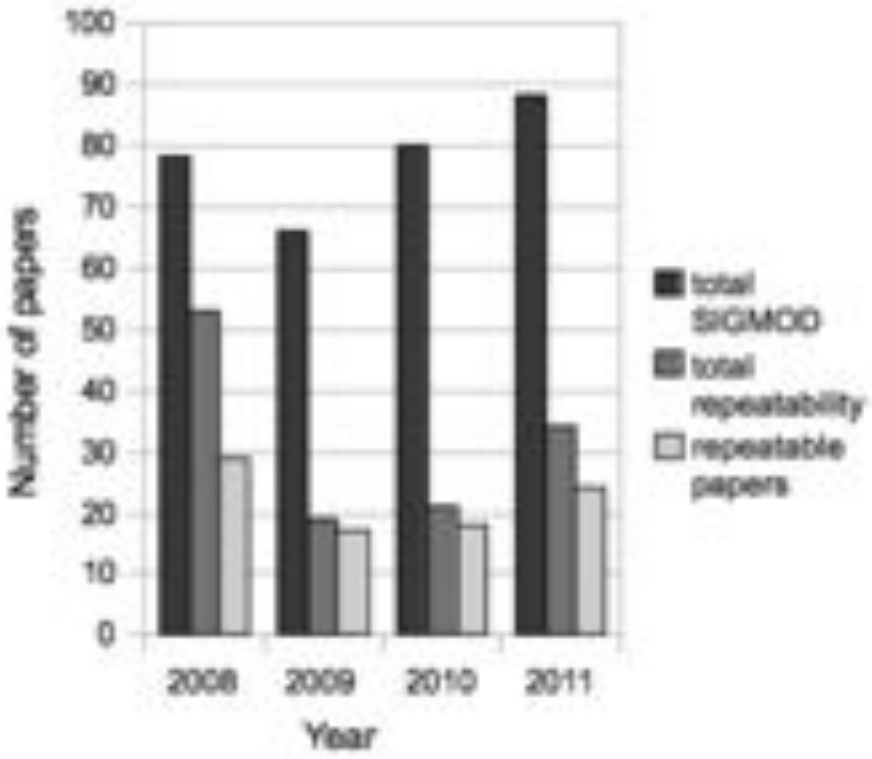

Bonnet et al, SIGMOD Record, June 2011 (Vol. 40, No. 2) doi: 10.1145/2034863.2034873

- SIGMOD conference offered to attempt to repeat/reproduce papers accepted at conference
  - 2008-2012
- "High burden on reviewers when setting up experiments"
  - Use of VMs advocated

SSI Drivers and Themes

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- Two key drivers which cause people to seek the SSI's advice:
  - They want to be more productive in their research
  - They don't want to be embarrassed by appearing worse than their peers

- Broadly, our work falls into a few key themes:
  - Developing the scientific computing / software development skill base
  - The role and reward of software in research
  - Recognition of software career paths
  - Re[peatable|producible|computable] research

The Software Sustainability Institute

www.software.ac.uk

EPSRC
Pioneering research and skills

A national facility for cultivating world-class research through software

- Better software enables better research
- Software reaches boundaries in its development cycle that prevent improvement, growth and adoption
- Providing the expertise and services needed to negotiate to the next stage
- Developing the policy and tools to support the community developing and using research software

Supported by EPSRC
Grant EP/H043160/1

UK Research Computing Ecosystem

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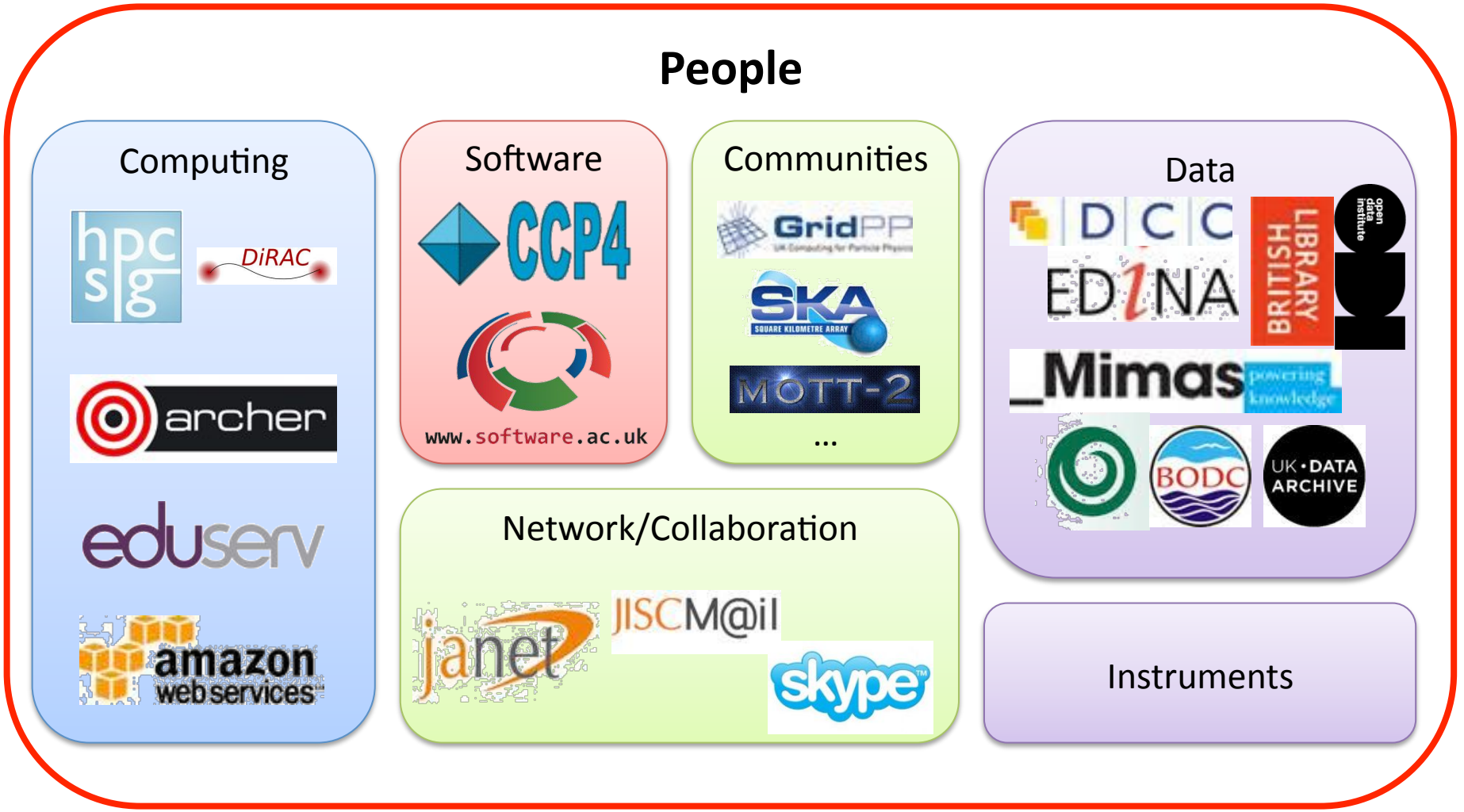

SSI Objectives

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1. Getting software on the research agenda
2. Supporting communities that want change
3. Increasing skills
4. Improving software

- Building a platform
- Engaging the community
- Being an authoritative voice

SSI Organisation

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- Community Engagement (Lead: Shoaib Sufi)
  - Fellowship Programme
  - Events and Roadshows
- Research Software (Lead: Steve Crouch)
  - Open Call for Consultancy Projects / Funded Collaborations
  - Software Evaluation
- Policy (Lead: Simon Hettrick)
  - Guides and Case Studies
  - Best Practice and Policy
- Training (Lead: Aleksandra Pawlik)
  - Software Carpentry
  - Software Surgeries

- Collaboration between universities of Edinburgh, Manchester, Oxford and Southampton.

EPSRC
Pioneering research and skills

THE UNIVERSITY OF EDINBURGH

MANCHESTER 1824

UNIVERSITY OF OXFORD

UNIVERSITY OF Southampton

Jisc

BBSRC

Water Swap Reaction Coordinate

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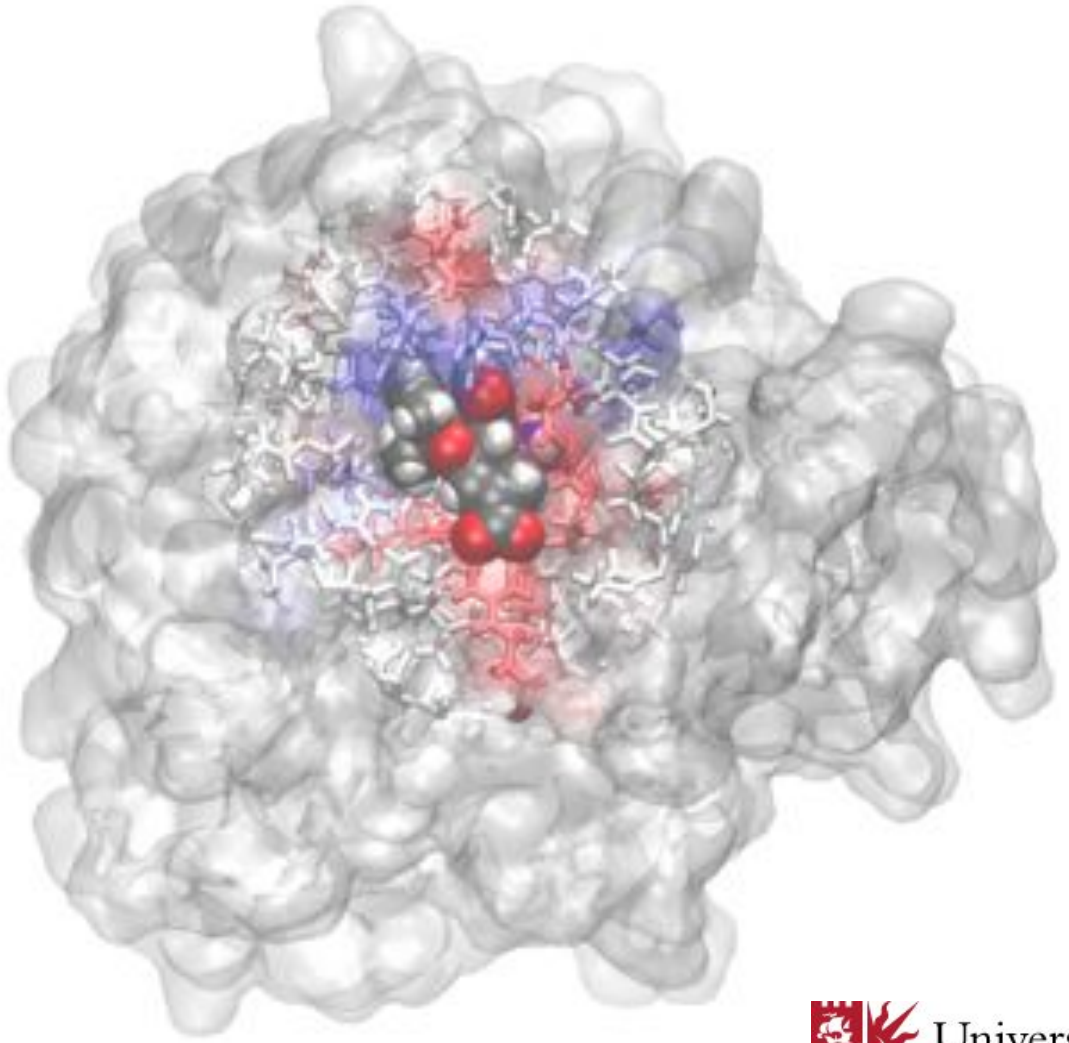

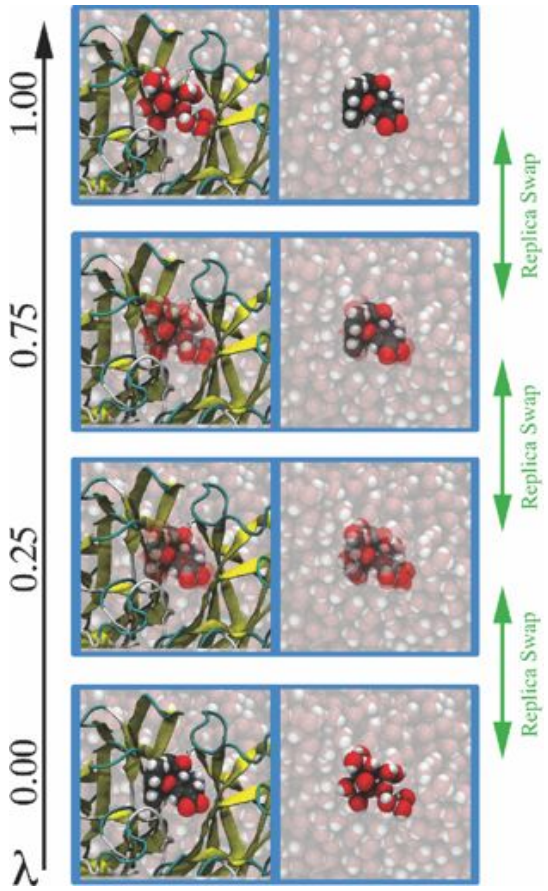

University of BRISTOL

A water-swap reaction coordinate for the calculation of absolute protein-ligand binding free energies
Woods CJ, Malaisree M, Hannongbua S, Mulholland AJ
J. Chem. Phys. (2011) vol. 134, pp. 054114
http://dx.doi.org/10.1063/1.3519057

Case Study: Ligand Binding

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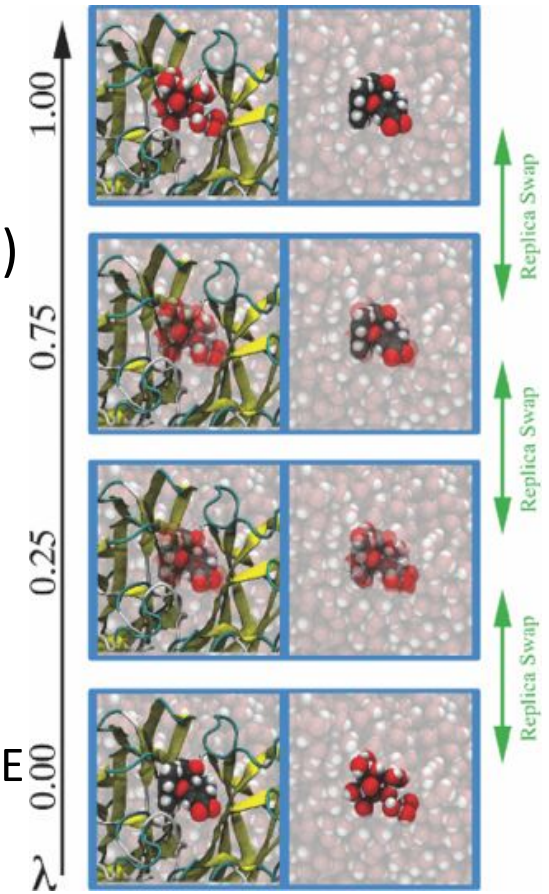
- Centre for Computational Chemistry, Bristol
  - New methods for rapid MC sampling of biomolecular systems modelled using QM/MM
  - Developed two codes ProtoMS (F77) + Sire (C++)
  - Water-Swap Reaction Coordinate method to calculate absolute protein-ligand binding free energies
- SSI's work is helping to scale development
  - ProtoMS and Sire both single developer codes
  - ASPIRE/ACQUIRE framework has multiple devs
    - Split architecture between ASPIRE (adaptive multiresolution hybrid MD simulation) and ACQUIRE (WorkPacket scheduling system with optimisation for time to result vs "green-ness"



- http://www.siremol.org/adaptive_dynamics

Case Study: ICAT

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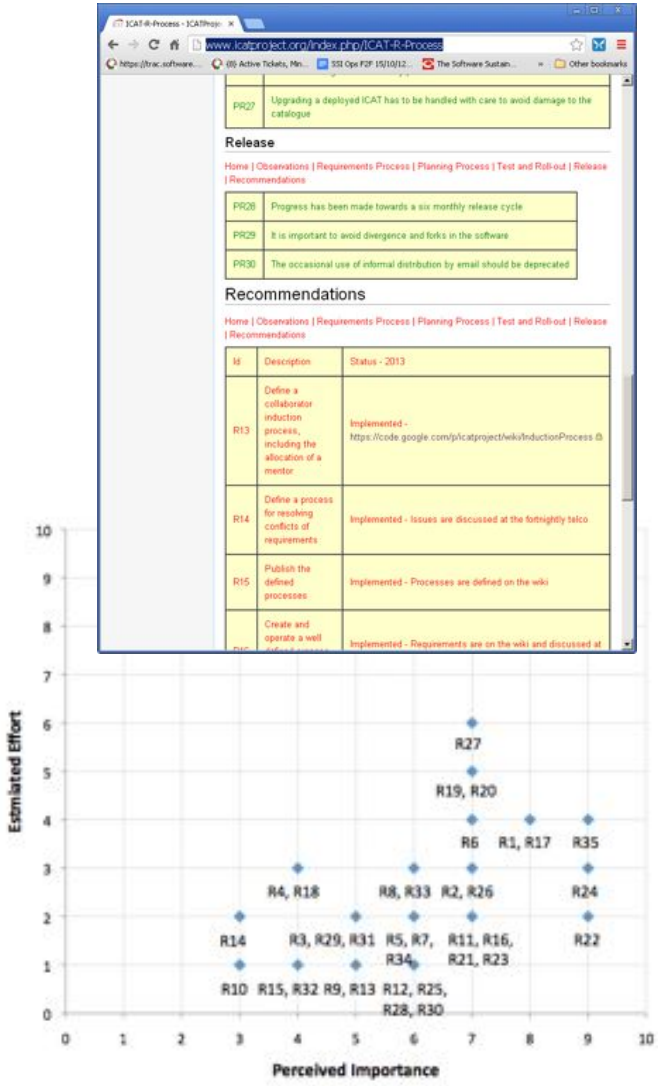
- ICAT metadata catalogue, STFC
  - Support experimental data linking at Large Facilities
  - RAL UK (ISIS, DIAMOND, CLF), SNS US, ELLETRA Italy
  - ICAT operationally critical at sites, other projects looking to use
  - Undertook interview-based organisational review
    - 92 observations, 32 recommendations
- SSI's work means the project has move forward
  - Taking forward: steering group, induction process, expanded roadmapping activity, technical workshops via Skype, involved with deployment
  - 1 year post-project
    - 25 (75%) recommendations implemented
    - Used by other major projects (PandataODI, CRISP)

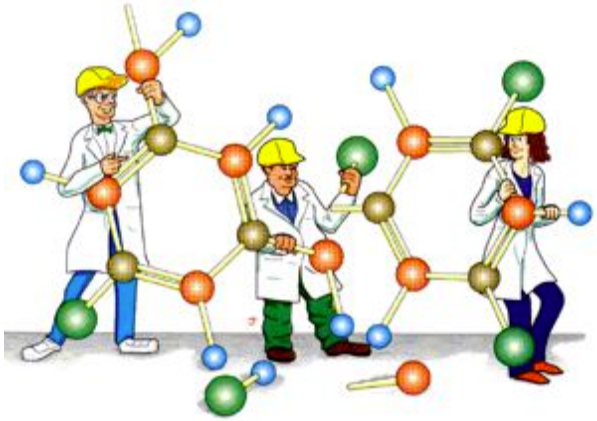


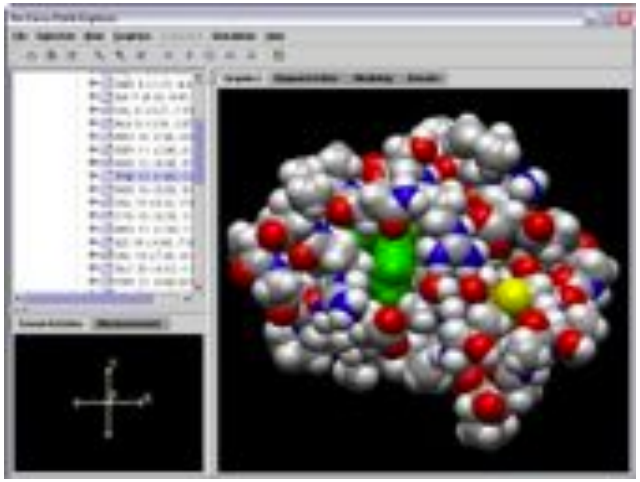
- http://www.software.ac.uk/blog/2012-02-17-evaluating-software-behind-some-worlds-large-experimental-facilities
- http://icatproject.org/

Case Study: Tinkering with APES

www.software.ac.uk

- NSF/EPSRC Funded
  - Polarisable empirical force fields (AMOEBA)
  - AMBER, Tinker, DL_POLY, ONETEP, Q-Chem
- SSI's work is helping to coordinate development across many packages and many people
  - Different languages, licenses, styles, teams





- http://apes-soft.github.io/

Current Consultancy (1)

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BoneJ

Royal Veterinary College, University of London

- *Trabecular geometry & whole bone shape analysis*
- Development review, community survey, CMS
- Assist future BBSRC BBR funding
  - 'SSI's involvement noted in a very positive light'

Lower Limb Model

Imperial College London

- *Musculoskeletal model for lower limbs*
- Wellcome Trust, EPSRC funded
- Development review, moving to Assembla
  - 'Institute's team were invaluable'

ForestGrowth-SRC

University of Southampton

- *Process-based tree growth model*
- NERC, Forestry Commission funded
- Run on IRIDIS cluster – take hours, not days
- Joint IfLS funding

Current Consultancy (2)

LabBook

Imperial College London

- *Fast, accurate, secure experiment recording/sharing*
- Wide domain potential
- Seeking funded development
- Infrastructure, outreach, roadmapping & feedback

DawnScience

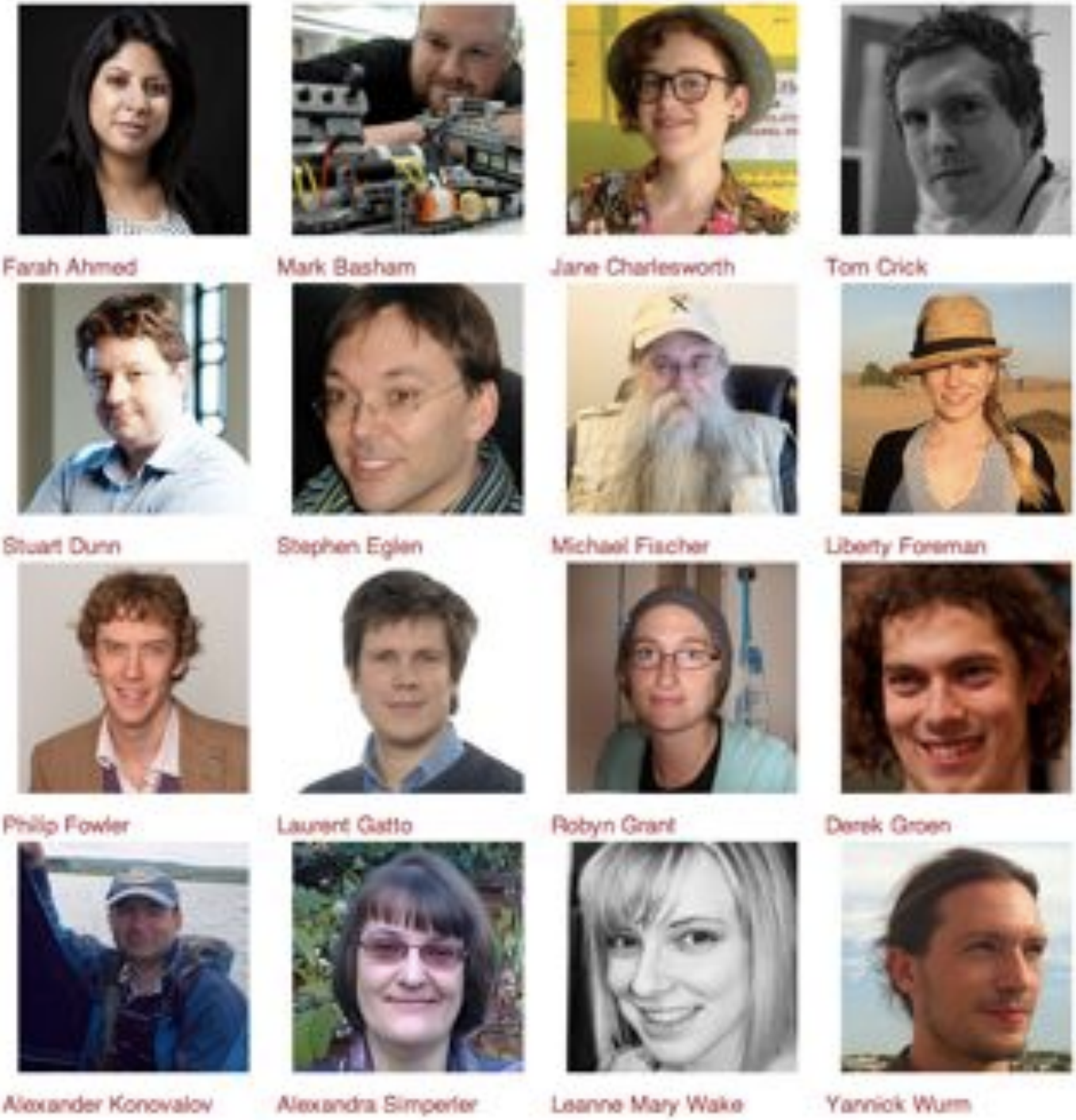
Science & Technology Facilities Council
Rutherford Appleton Laboratory

- *Eclipse-based workbench for scientific data analysis*
- STFC funded
- Collaboration review, community marketing
  - Uptake key measure of project success

BASIL/FABBER

UNIVERSITY OF OXFORD

- *Analysis tool library for FMRI, MRI, DTI brain imaging*
- Industry / EPSRC funded
- Architectural review, apply to new problems
- 10 groups outside Oxford using it



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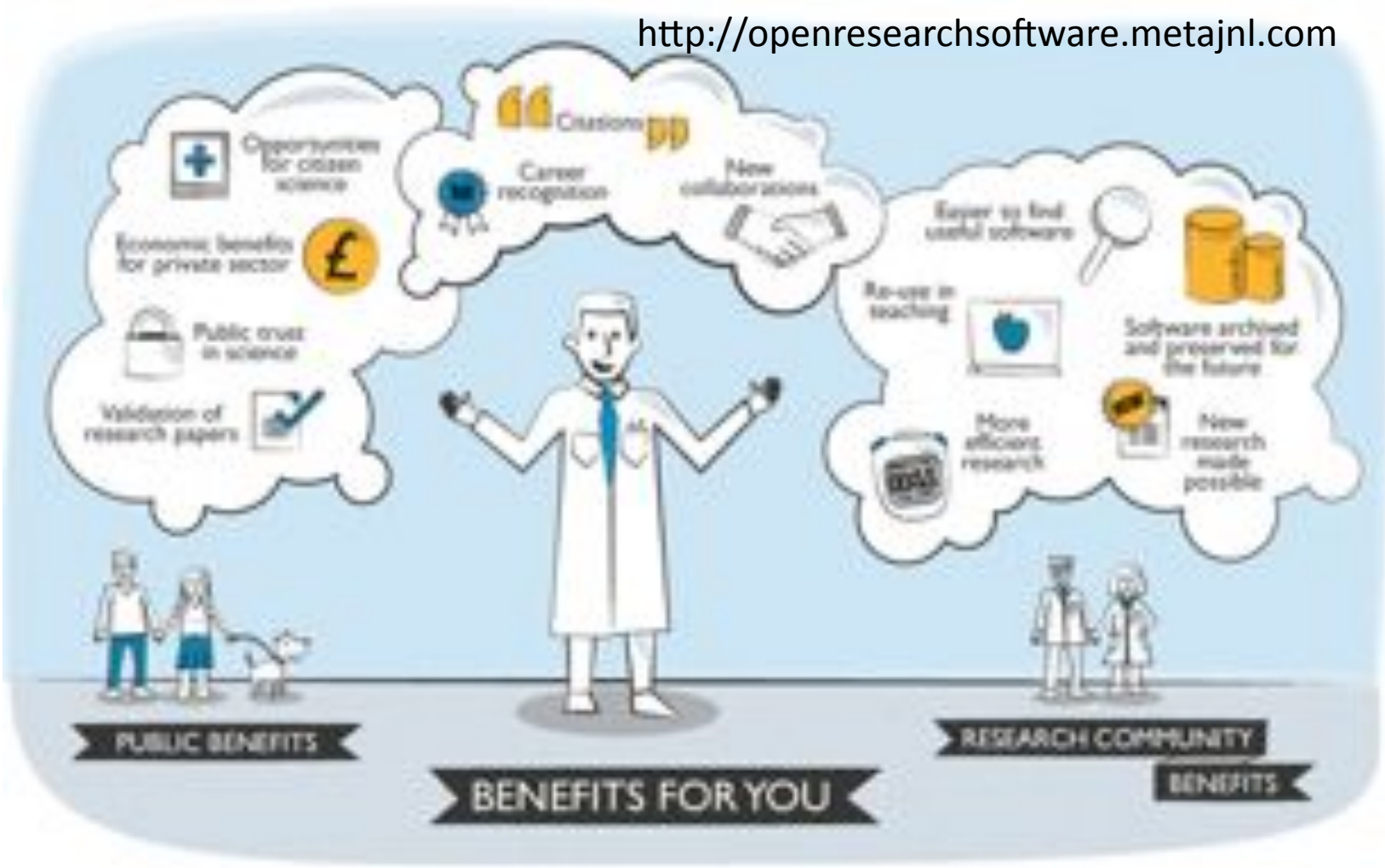
- 2014: 16 fellows
- 2013: 15 fellows
- 2012: 10 fellows
- Range of subjects, career stages

software.ac.uk/fellows

Journal of Open Research Software

www.software.ac.uk

http://openresearchsoftware.metajnl.com



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The Research Cycle

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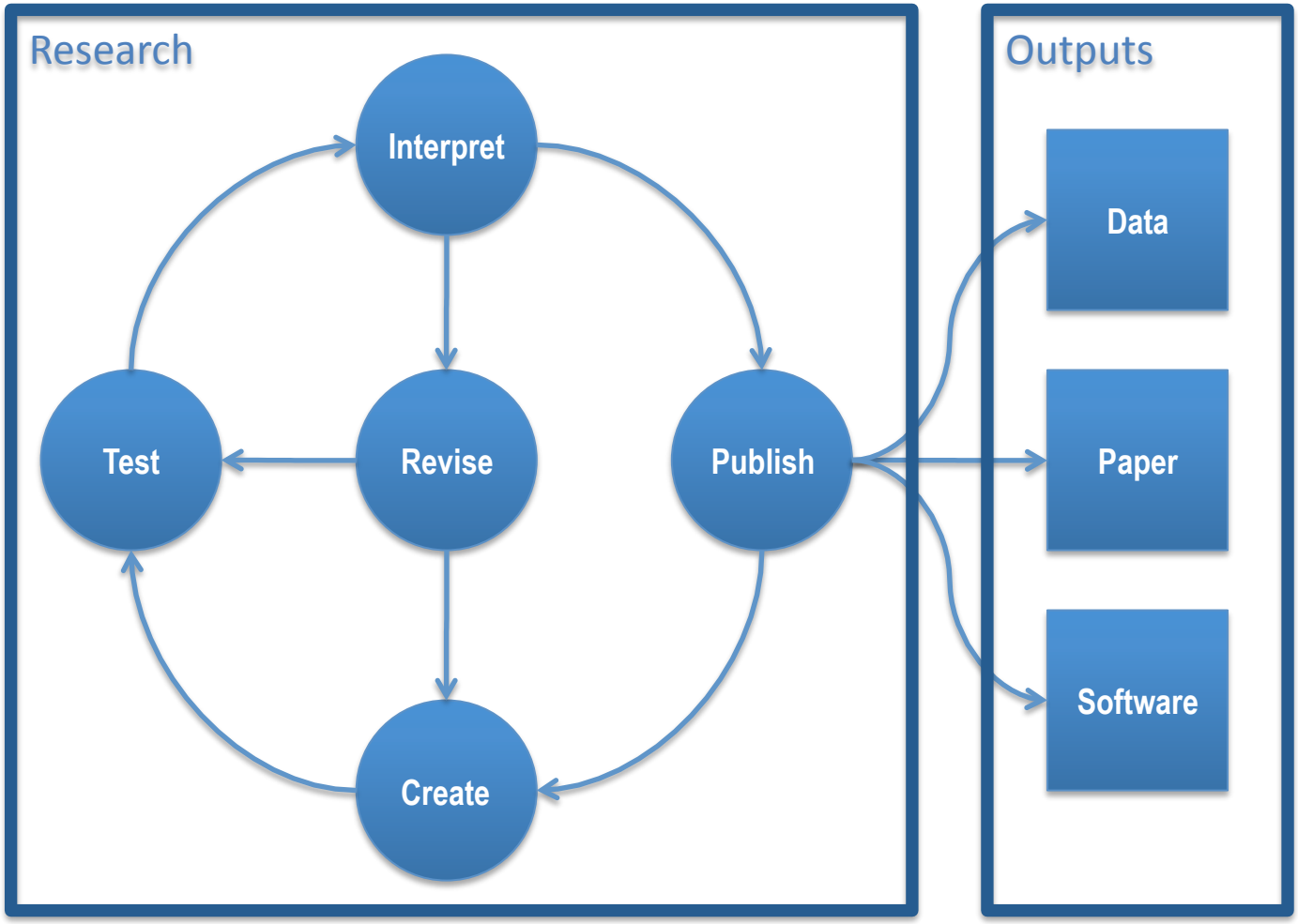

Research is a *continuous* cycle.

When we publish we are contributing to the body of knowledge.

Research/Reuse/Reward Cycle

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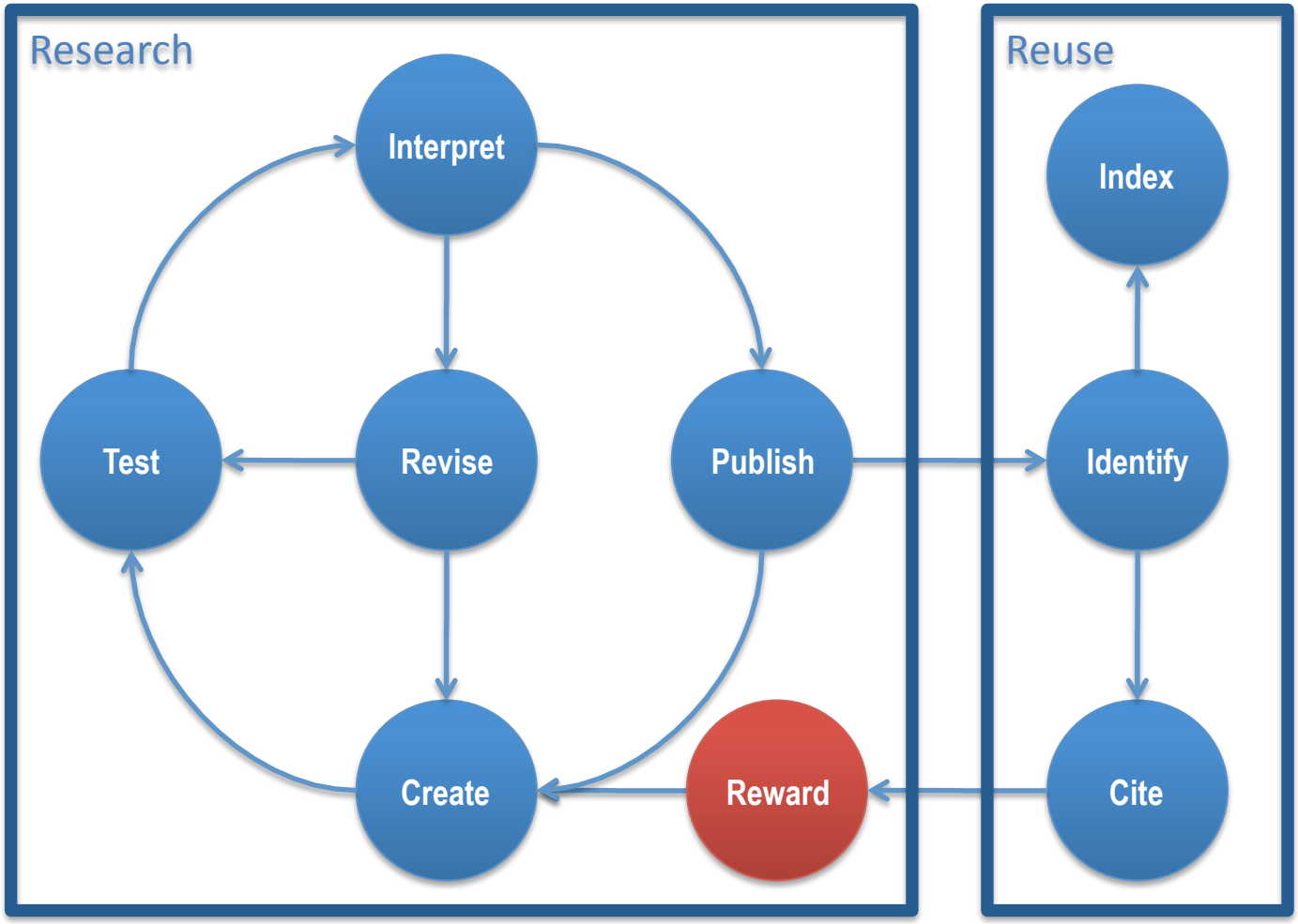

Reuse is also a cycle. We build our research on the work of others.

Reward mechanisms *should* encourage reuse.

The current process

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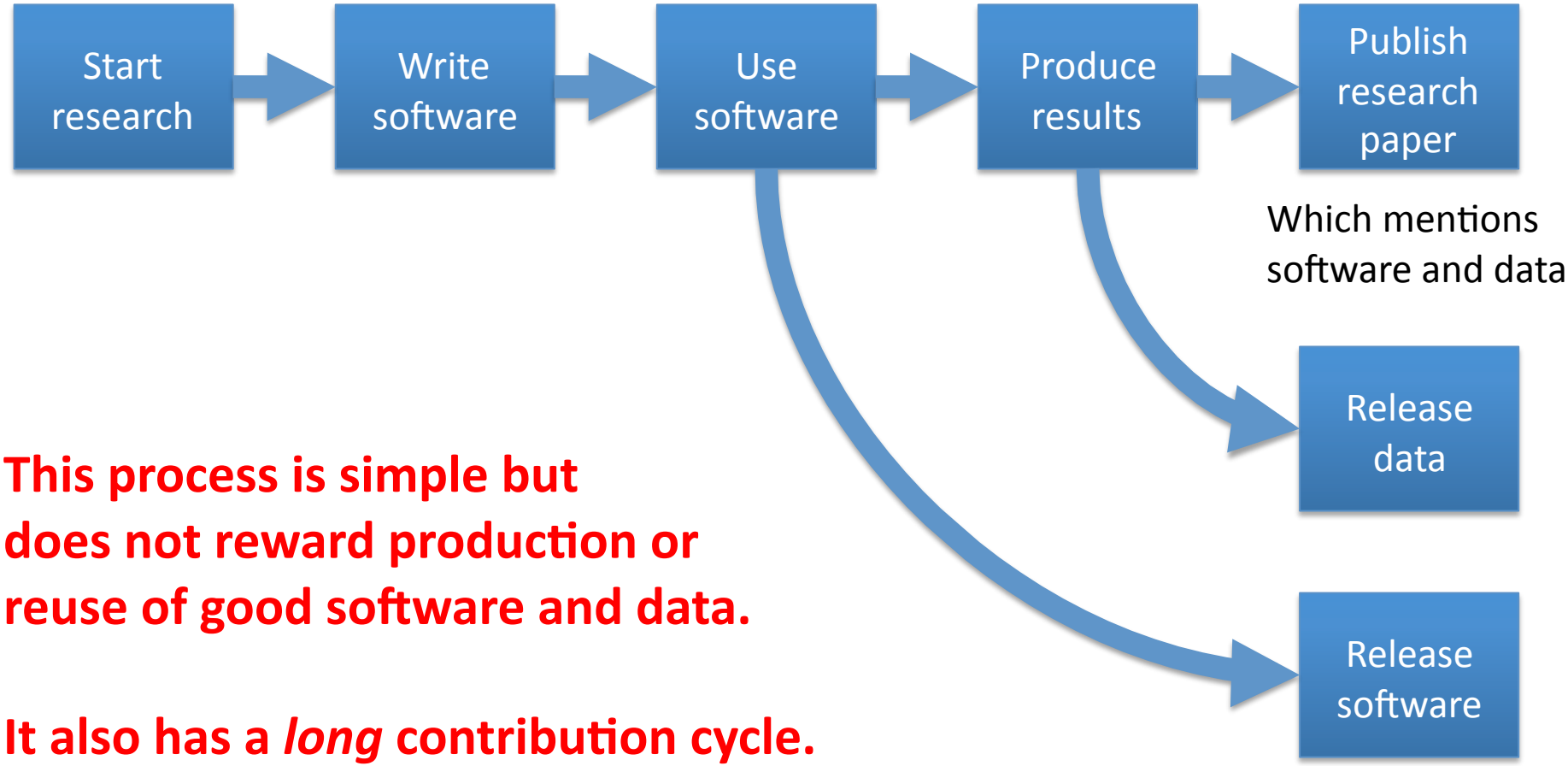

This process is simple but does not reward production or reuse of good software and data.

It also has a *long* contribution cycle.

A better process?

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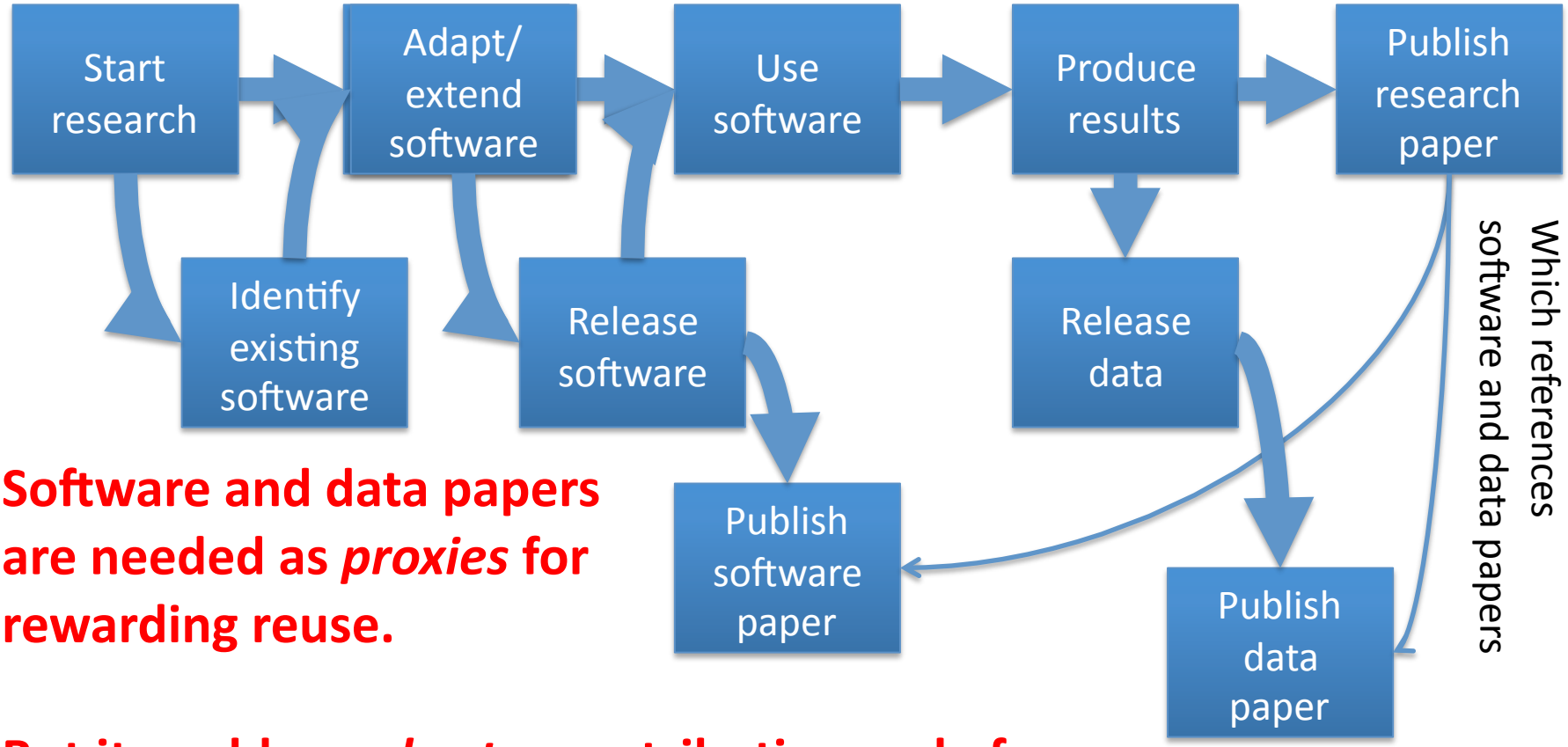


Software and data papers are needed as *proxies* for rewarding reuse.

But it enables a *shorter* contribution cycle for data and software.

SSI Website

www.software.ac.uk

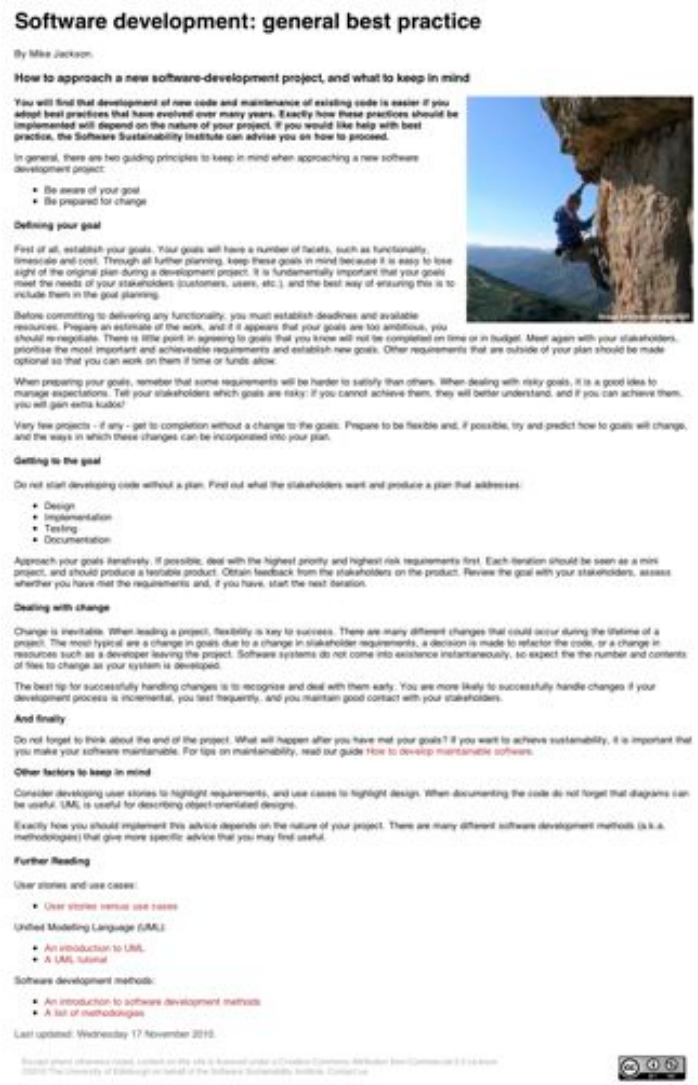
Disseminating best practice, gathering information

10,000+ unique visits/month

SSI Guides and Top Tips

www.software.ac.uk

- Guides provide in depth information
  - Licences
  - Software development
  - Project management
  - Repositories and project infrastructure
  - Open source
  - Community building
  - Publicising software
  - Policy
- Top Tips provide quick overviews
  - Software development
  - Repositories and project infrastructure
  - Software carpentry
  - Citing software
  - Data handling
  - Promoting and communicating your project
  - Community building and project management



Software development: general best practice

By Mike Jackson.

How to approach a new software-development project, and what to keep in mind

You will find that development of new code and maintenance of existing code is easier if you adopt best practices that have evolved over many years. Exactly how these practices should be implemented will depend on the nature of your project. If you would like help with best practice, the Software Sustainability Institute can advise you on how to proceed.

In general, there are two guiding principles to keep in mind when approaching a new software development project:

- Be aware of your goal
- Be prepared for change

Defining your goal

First of all, establish your goals. Your goals will have a number of facets, such as functionality, timescale and cost. Through all further planning, keep these goals in mind because it is easy to lose sight of the original plan during a development project. It is fundamentally important that your goals meet the needs of your stakeholders (customers, users, etc.), and the best way of ensuring this is to include them in the goal planning.

Before committing to delivering any functionality, you must establish deadlines and available resources. Prepare an estimate of the work, and if it appears that your goals are too ambitious, you should re-negotiate. There is little point in agreeing to goals that you know will not be completed on time or in budget. Meet again with your stakeholders, prioritise the most important and achievable requirements and establish new goals. Other requirements that are outside of your plan should be made optional so that you can work on them if time or funds allow.

When preparing your goals, remeber that some requirements will be harder to satisfy than others. When dealing with risky goals, it is a good idea to manage expectations. Tell your stakeholders which goals are risky: if you cannot achieve them, they will better understand, and if you can achieve them, you will gain extra kudos!

Very few projects - if any - get to completion without a change to the goals. Prepare to be flexible and, if possible, try and predict how to goals will change, and the ways in which these changes can be incorporated into your plan.

Getting to the goal

Do not start developing code without a plan. Find out what the stakeholders want and produce a plan that addresses:

- Design
- Implementation
- Testing
- Documentation

Approach your goals iteratively. If possible, deal with the highest priority and highest risk requirements first. Each iteration should be seen as a mini project, and should produce a testable product. Obtain feedback from the stakeholders on the product. Review the goal with your stakeholders, assess whether you have met the requirements and, if you have, start the next iteration.

Dealing with change

Change is inevitable. When leading a project, flexibility is key to success. There are many different changes that could occur during the lifetime of a project. The most typical are a change in goals due to a change in stakeholder requirements, a decision is made to refactor the code, or a change in resources such as a developer leaving the project. Software systems do not come into existence instantaneously, so expect the the number and contents of files to change as your system is developed.

The best tip for successfully handling changes is to recognise and deal with them early. You are more likely to successfully handle changes if your development process is incremental, you test frequently, and you maintain good contact with your stakeholders.

And finally

Do not forget to think about the end of the project. What will happen after you have met your goals? If you want to achieve sustainability, it is important that you make your software maintainable. For tips on maintainability, read our guide How to develop maintainable software.

Other factors to keep in mind

Consider developing user stories to highlight requirements, and use cases to highlight design. When documenting the code do not forget that diagrams can be useful. UML is useful for describing object-orientated designs.

Exactly how you should implement this advice depends on the nature of your project. There are many different software development methods (a.k.a. methodologies) that give more specific advice that you may find useful.

Further Reading

User stories and use cases:

- User stories versus use cases

Unified Modeling Language (UML):

- An introduction to UML
- A UML tutorial

Software development methods:

- An introduction to software development methods
- A list of methodologies

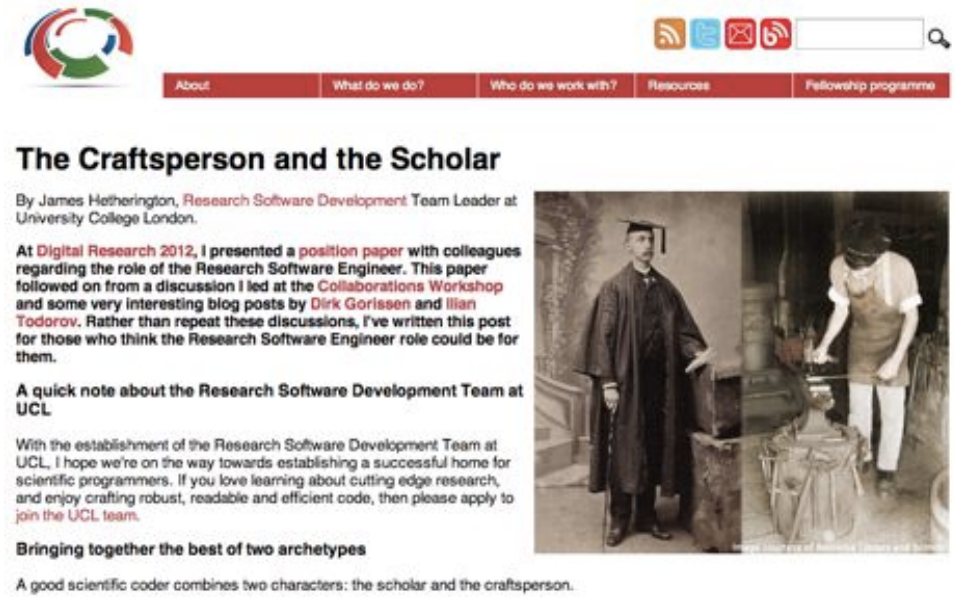
Last updated: Wednesday 17 November 2010.

Software Sustainability Instit

SSI Blog

www.software.ac.uk

- Articles on research software and related issues
  - Ask the Institute
  - A Day in the Software Life
  - Heroes of Software Engineering
  - Top Tips
  - Women in Software
- 150+ posts written by external contributors
  - 6,000+ unique pageviews/ month



SSI Training

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- Software Carpentry
  - http://software-carpentry.org
  - International initiative to teach basics of software engineering to computational researchers
    - The "why" more than the "how"
  - Phenomenally successful – 2x oversubscription
  - Cheap to run but budget for 3x the coffee!
  - SSI are UK Coordinators for SWC
  - We ran 13 workshops in 2013 to 600+ learners

- Software Sustainability Surgeries
  - "Bring your own code"
  - "What makes Good Code good?"
  - Run at existing conferences, and for software funding programmes
  - Offering bespoke advice as well as training

Creating a training community

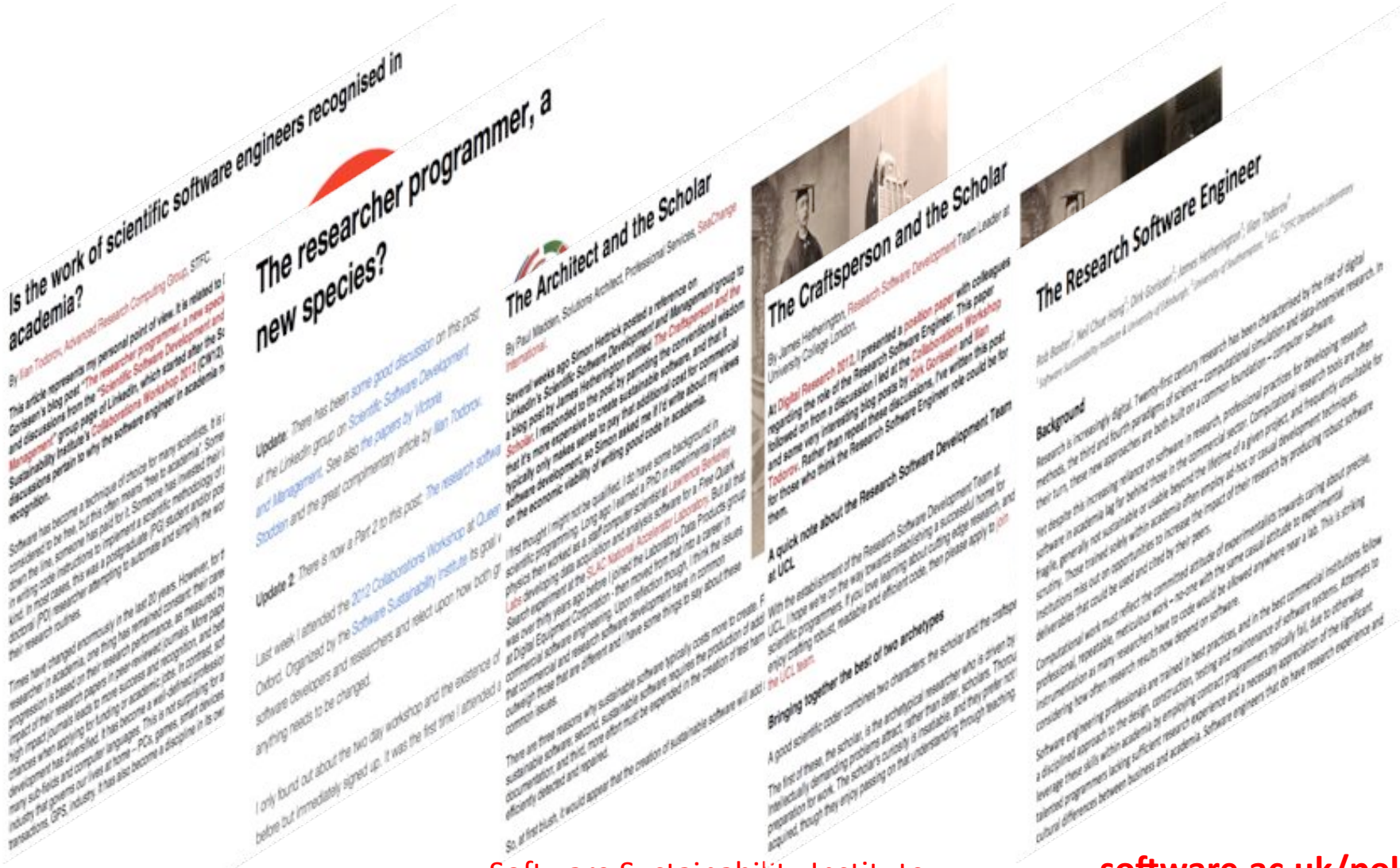
www.software.ac.uk

- Bringing together 39+ organisations with interest in e-Infrastructure training
- Raising issues and enablers with RCUK, BIS

software.ac.uk/policy

Campaigning for careers

www.software.ac.uk



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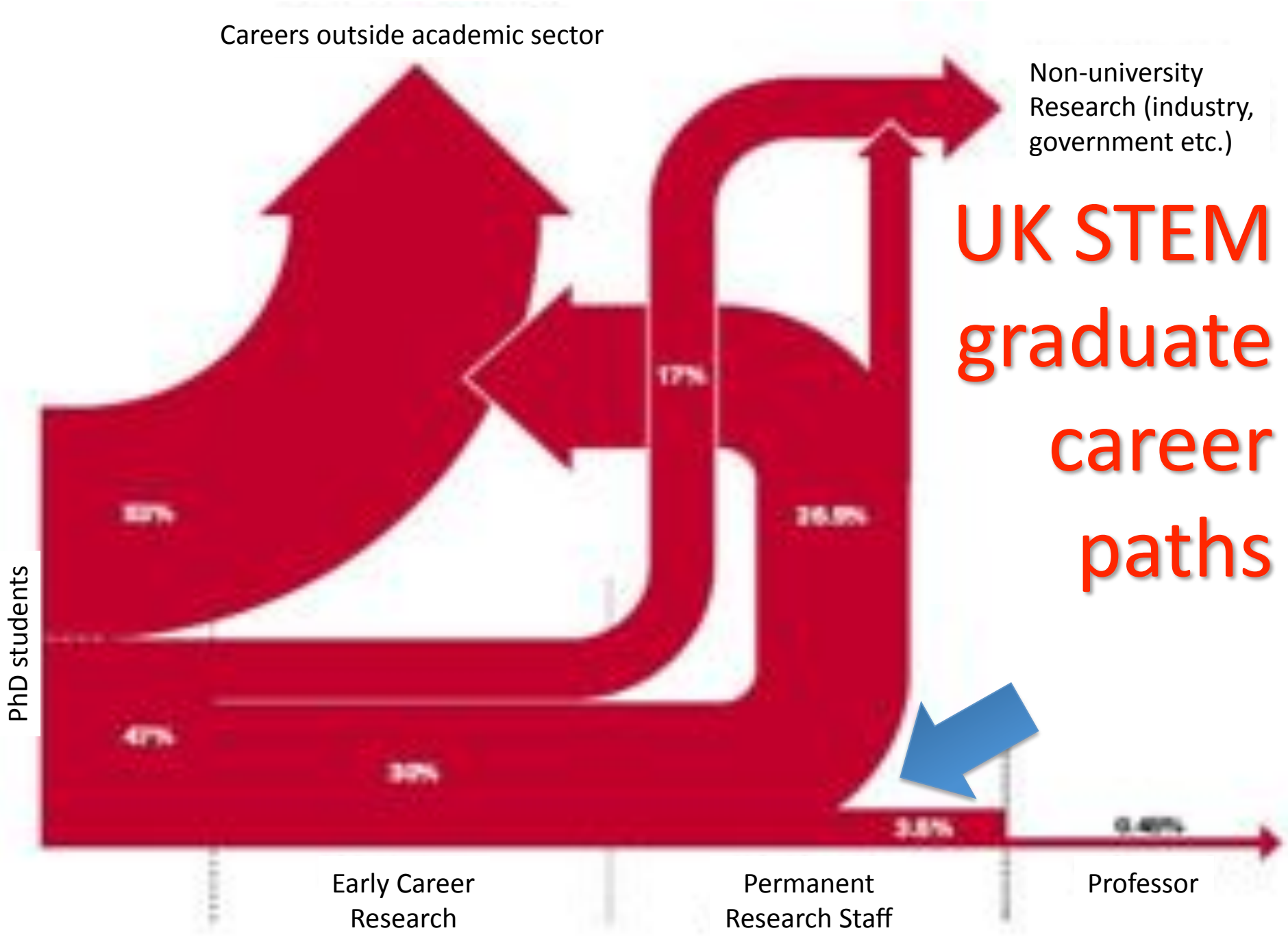

Source: The Scientific Century, Royal Society, 2010 (revised to reflect first stage clarification from "What Do PhD's Do?" study)

Shake up the system

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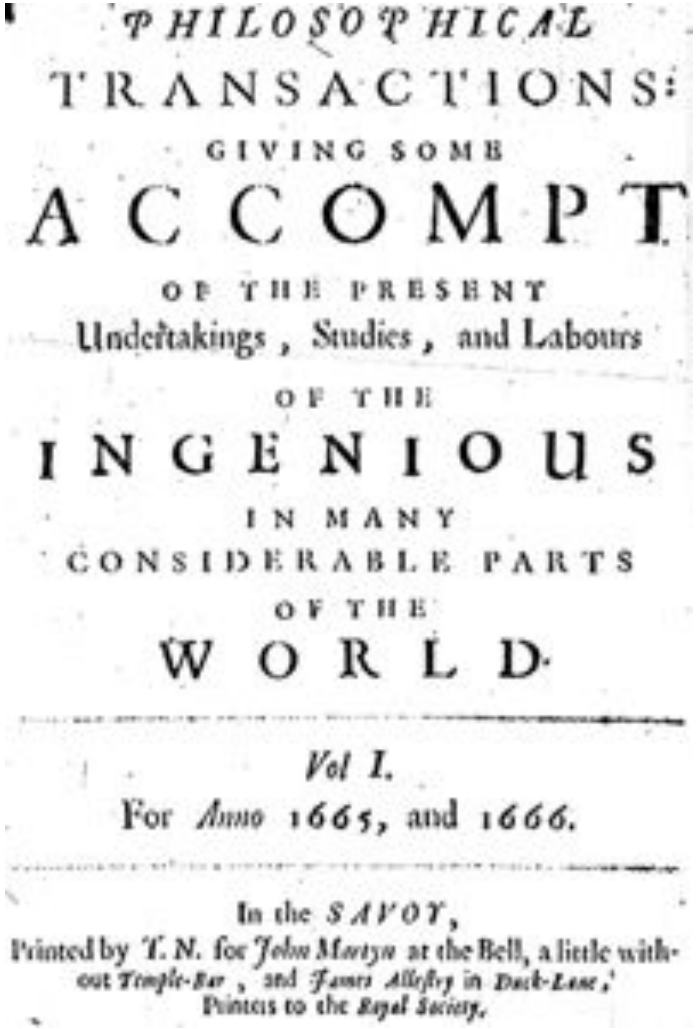
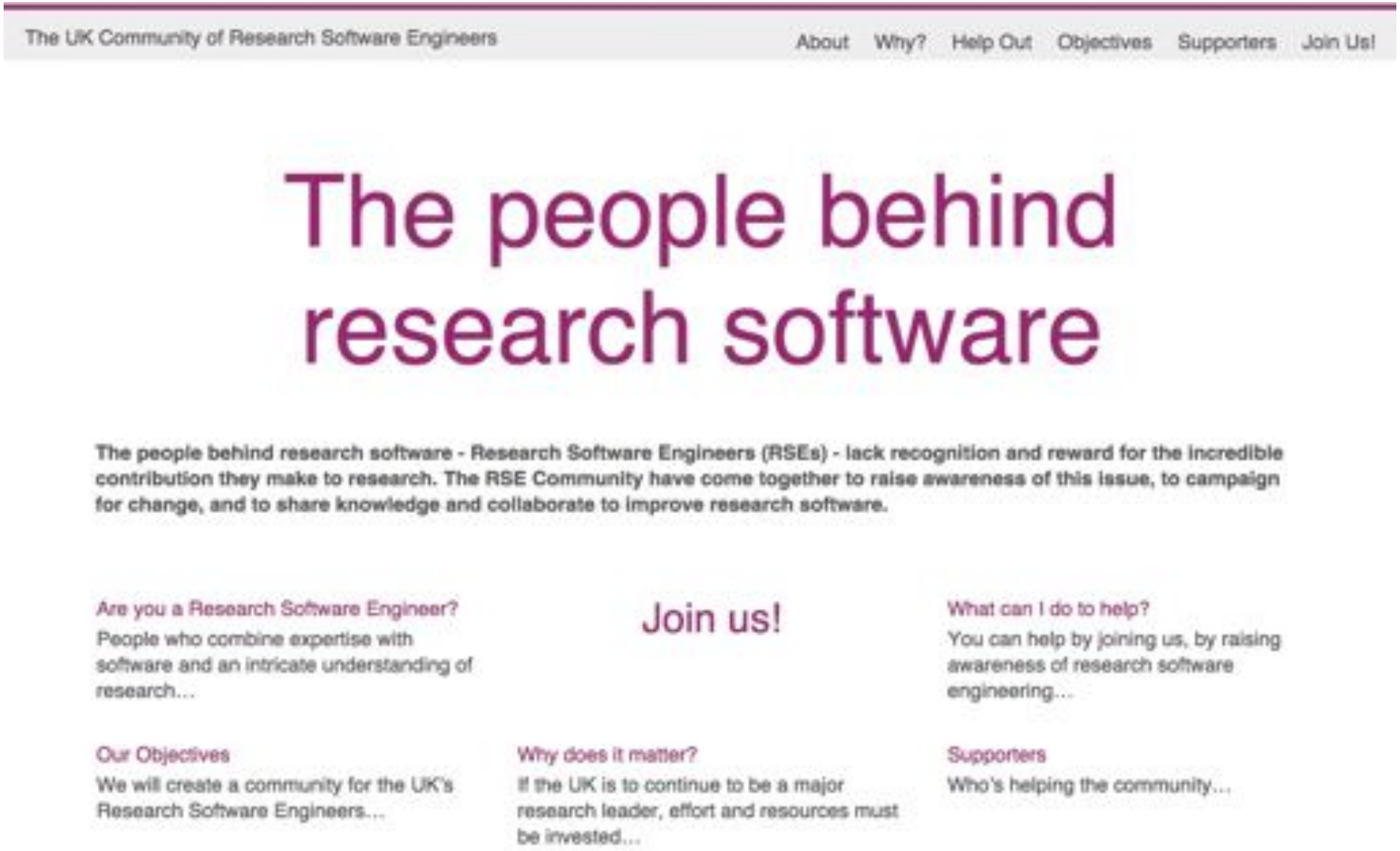
- *"Swim or drown"* is not an efficient learning method
- *"Publish or perish"* is not an effective reward mechanism
- *"Becoming a Professor"* is not a scalable career path
- *"I'll just have to do it myself"* is not a modern way of doing science



PHILOSOPHICAL
TRANSACTIONS:
GIVING SOME
ACCOMPT
OF THE PRESENT
Undertakings, Studies, and Labours
OF THE
INGENIOUS
IN MANY
CONSIDERABLE PARTS
OF THE
WORLD.

Vol I.
For Anno 1665, and 1666.

In the SAVOY,
Printed by T. N. for John Martyn at the Bell, a little without Temple-Bar, and James Allestry in Duck-Lane,
Printers to the Royal Society.


The UK Community of Research Software Engineers
About
Why?
Help Out
Objectives
Supporters
Join Us!
The people behind research software
The people behind research software - Research Software Engineers (RSEs) - lack recognition and reward for the incredible contribution they make to research. The RSE Community have come together to raise awareness of this issue, to campaign for change, and to share knowledge and collaborate to improve research software.
Are you a Research Software Engineer?
People who combine expertise with software and an intricate understanding of research...
Join us!
What can I do to help?
You can help by joining us, by raising awareness of research software engineering...
Our Objectives
We will create a community for the UK's Research Software Engineers...
Why does it matter?
If the UK is to continue to be a major research leader, effort and resources must be invested...
Supporters
Who's helping the community...
Join the RSE community at http://www.rse.ac.uk/
Academia must adapt to the fundamental role that software plays in today's research.

A national facility for cultivating world-class research through software

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Some of our collaborations

Become our next collaborators!

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Email: info@software.ac.uk

Twitter: twitter.com/SoftwareSaved

DEATH TO DECAY!
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