

Data Analysis Group: – Alun Ashton

Data Acquisition Group: – Rob Walton

Beamline Controls Group: - Nick Rees

Scientific Computing Team: - Greg Matthews

.....  
Beamline Groups





UK Atomic  
Energy  
Authority

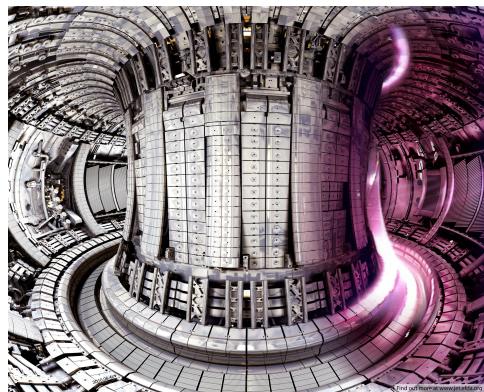
## Team leader - 7 RSEs

- Data systems & tools
- Consultancy
- Permanent staff

## Internal software committee

- Policy
- Training
- Lifecycle / QA
- Tools

# Alys Brett



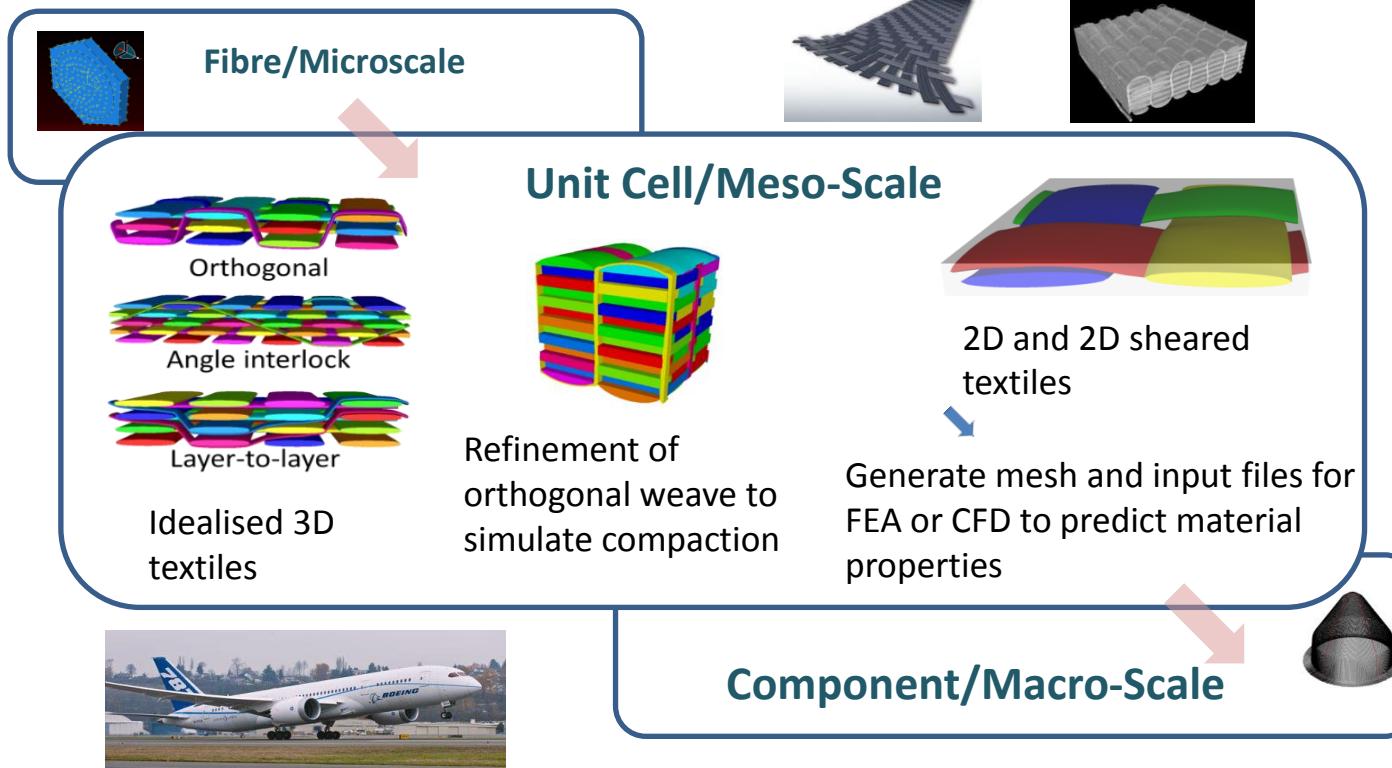
JET: world's largest  
fusion experiment  
Running since 1983



Background in physics  
9 years - developer  
1 year - team leader  
  
RSE network co-investigator

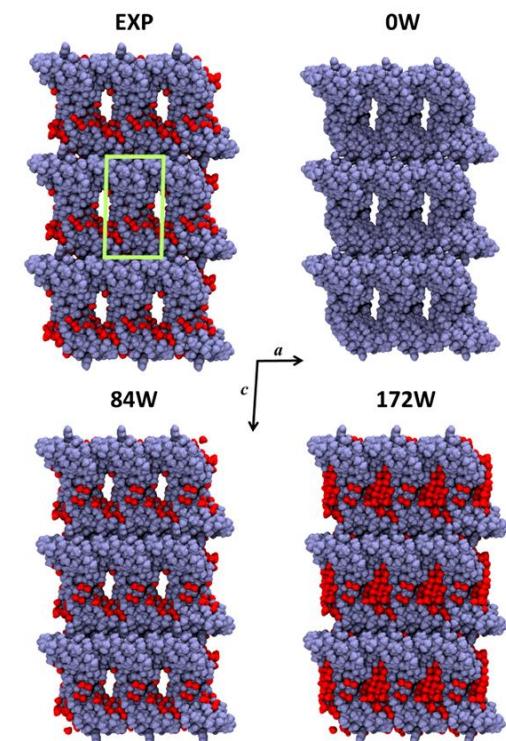
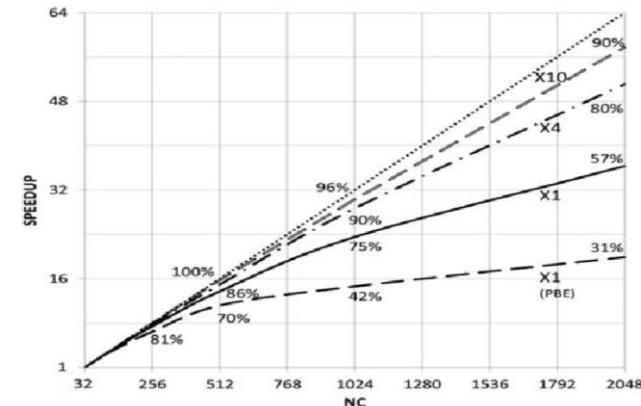


- Research Fellow – Composites Research Group, Faculty of Engineering at the University of Nottingham
- Returned to academia in December 2009
- Run the TexGen project for modelling of textiles and textile composites



# Ian Bush – 30 Years in 1 Slide

- Background – HPC for atomistic modelling
  - DL\_POLY, CRYSTAL, CASTEP, VASP ...
  - Enabling science studying large systems at large core counts
- RSE Fellowship at OeRC, Oxford
  - CRYSTAL/CRYSCOR – Turin, RAL, IC
  - DL\_POLY – Daresbury, Bristol
  - GS 2 – Culham, Oxford, York
  - Training



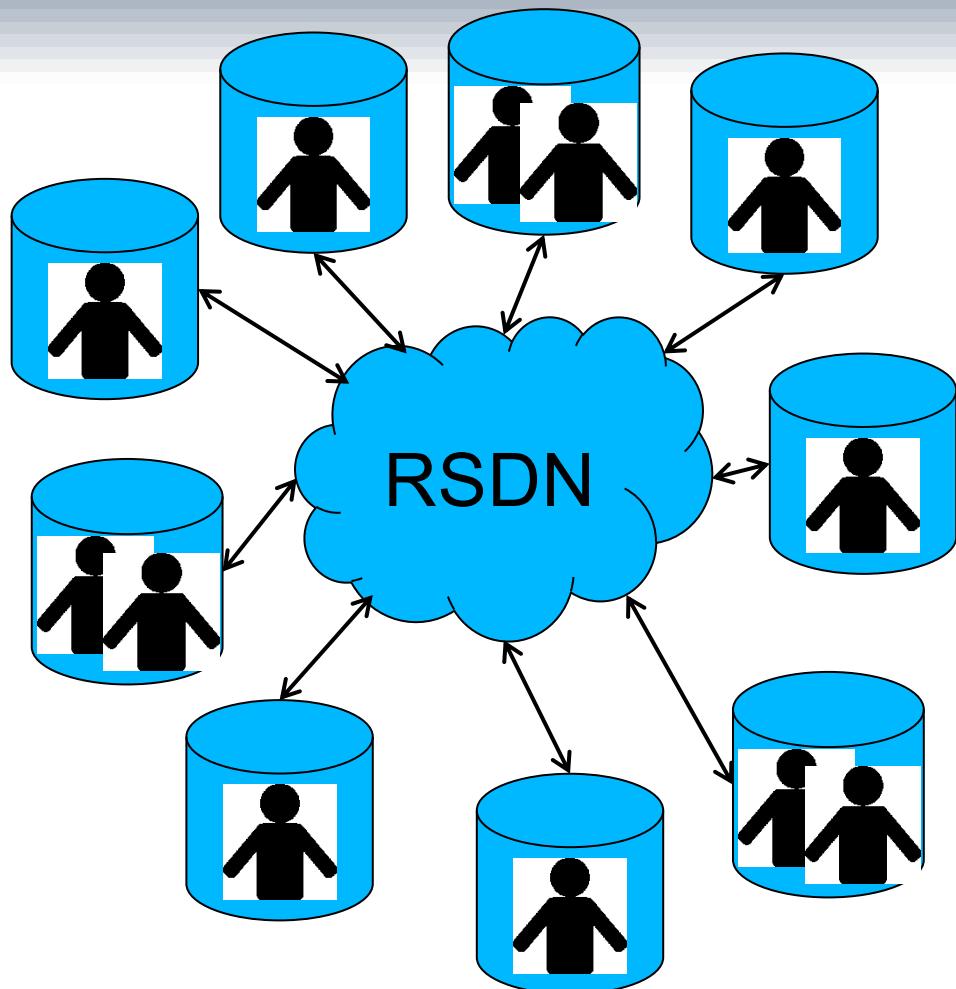
# Jonathan Cooper

- Leader, Research Software Developers Network
- 50% Research Fellow, 2020 Science project
- 50% Co-Director, Systems Biology Doctoral

Training Centre

# Research Software Developers Network

- The RSDN provides a community and support structure
- Share experiences and expertise among RSDs
- Better RSD staff recruitment and retention
- Training & mentoring for RSDs (and researchers)
- Better research!



# RSE for the long tail researcher



Mike Croucher

<http://www.walkingrandomly.com>

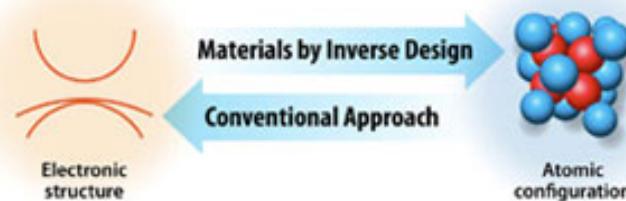
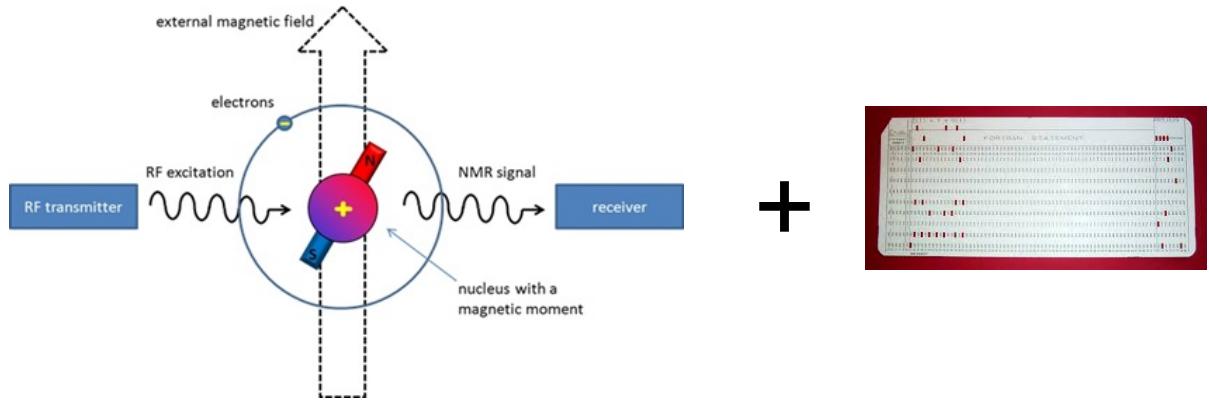
EPSRC RSE Fellow

@walkingrandomly

# Mayeul d'Avezac

## RSD at UCL

Before 

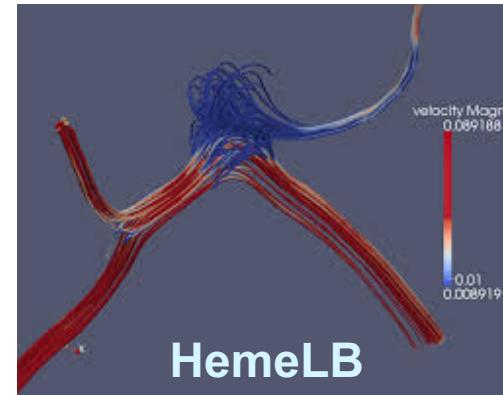


Center for  
Inverse Design

Put



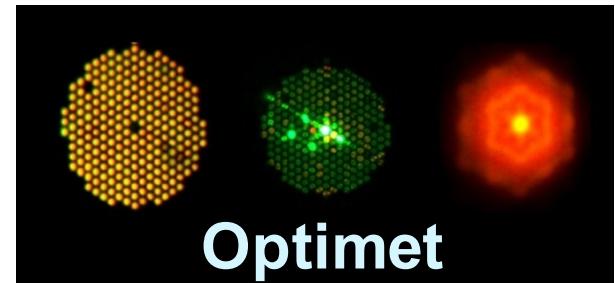
into



Put



into



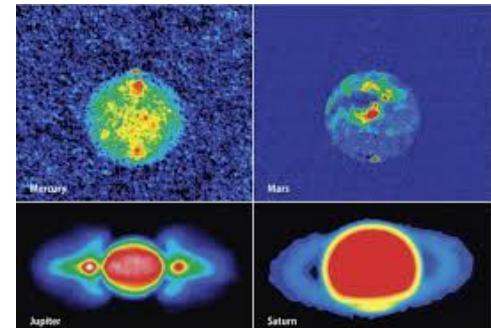
Put

```

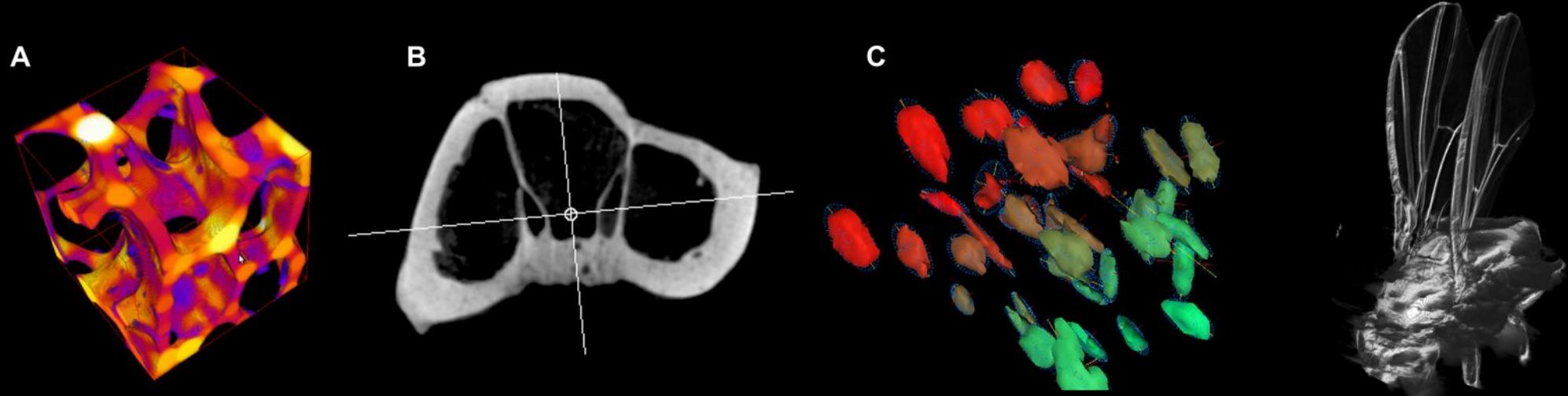
11 template<class SCALAR>
12 void ProximalADMM<SCALAR>::initialization_step(
13     t_Vector const & input, t_Vector& out, t_Vector & residual,
14     out = Phi().adjoint() * input / nu();
15     residual = Phi() * out - input;
16 }
17 template<class SCALAR>
18 void ProximalADMM<SCALAR>::iteration_step(
19     t_Vector const & input, t_Vector &out, t_Vector &residual,
20     t_Vector &lambda, t_Vector &z) const
21 {
22     g_proximal(z, gamma(), -lambda - residual);
23     f_proximal(out, gamma() / nu(), out - Phi().adjoint() * (residual + z));
24     residual = Phi() * out - input;
25     lambda += lagrange_update_scale() * (residual + z);
26 }
27

```

into



# Michael Doube



- Lecturer, Royal Veterinary College (Skeletal Biology Group)
- Imaging and bioimage informatics
- BoneJ (Java plugin for ImageJ)

# Robert Haines

## University of Manchester



- Research Software Engineering Manager
  - Team of six developers – recruiting more soon
  - We work on research projects across whole University
    - Pre-award and post-award funding model
      - Day rate, not subject to FEC, “too good to be true”
    - Different levels of engagement
      - “Go away and build this for me” – rare
      - “Let’s build this together” – common and preferred
      - “Give me a software engineer and leave me alone” – legacy
  - We provide software engineering consultancy
    - Interview panels, advice, prototype exploration, &c
  - Coming soon
    - Research Applications Support
    - Training
- Honorary Lecturer in Computer Science
  - Agile and Test-Driven Development – MSc Programme
  - Software Engineering – BSc programme
- SSI Fellow, UKRSE committee, RSE Leaders, RSE Network Co-I

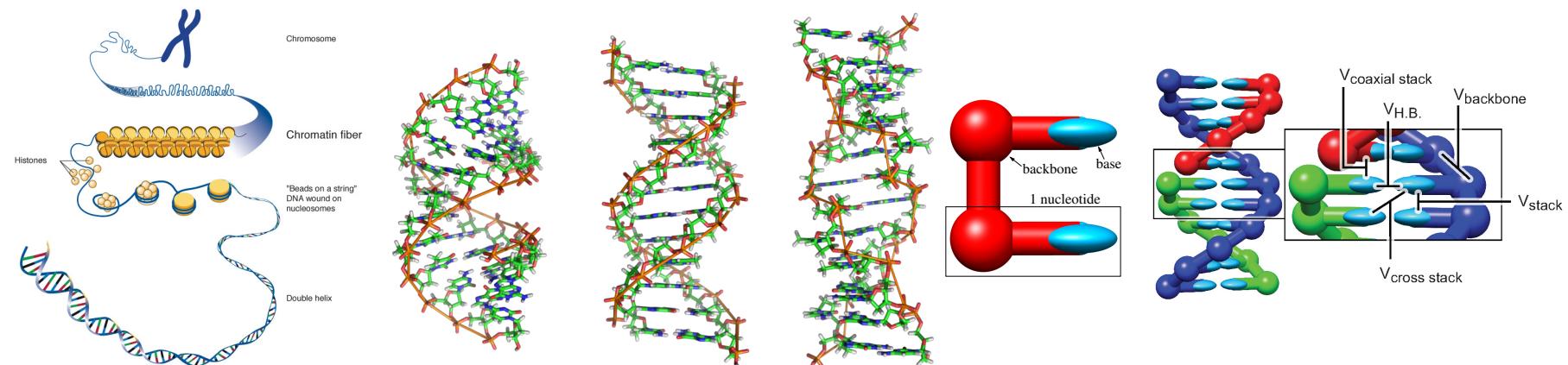
Name: Oliver Henrich

Address: EPCC, School of Physics & Astronomy, University of Edinburgh

Email: ohenrich@epcc.ed.ac.uk

## Background:

- Soft condensed matter physics: complex fluids, liquid crystals, active matter, biophysics
- Graduated physicist (PhD, U Konstanz), postdoctoral simulator (UoE, UCL), RSE (EPCC)
- Discrete simulation methods of fluid dynamics (lattice Boltzmann, particle-based methods): various HPC codes
- Coarse-grained models of DNA and RNA: LAMMPS (Sandia National Lab)



- *Coarse-grained DNA models* must deliver correct persistence length, electrostatics, if sequence-specific correct melting temperature, elastic constants ...
- Epigenetics: not (only) sequence, but also 3D structure and dynamics matter

2D still  $\longleftrightarrow$  3D movie !

# UCL Research Software Development



StartDate: 20120901

## Team:

- [James Hetherington, Mayeul D'Avezac, Jens Nielsen, Gary MacIndoe, Raquel Alegre, Sinan Shi, David Perez-Suarez, Ben Laken]

## Purpose:

### Scientific software:

- Readable
- Reliable
- Efficient

### Researchers who code:

- Community
- Skills
- Good Practice

## Free projects:

- Selected by Academic Review
- Including:
  - Whodunnit DNA
  - 30 year-old FORTRAN by FRS
  - Brain ultrasound physics
  - Square kilometer array Python
  - Maternal DNA chromosome analysis

Grant funded projects ~1M since start

### Sources:

- EPCC Software for the Future
- ARCHER eCSE programme
- Post-award money

### Topics:

- Ancient Mesopotamian writing
- Protein bioinformatics
- Graph theoretical catalysis
- Aneurysm fluid dynamics
- Intensive care data

### Infrastructure:

- UCL GitHub
- Testing Server (Jenkins)

### Training:

- [Python, C++, Engineering, Supercomputing, Data]
- Software Carpentry

### Social:

Twitter: @uclrcsoftdev

Blog: blogs.ucl.ac.uk/research-software-development

# Who am I?

- Software Sustainability Institute
- Southampton Research Software Group
- RSE Network
- UKRSE Committee

# Catherine Jones – Software Engineering Group Leader, SCD, STFC

- Computing degree & qualified librarian: <https://uk.linkedin.com/in/jonescm>
- **Group Activities:**
  - Team of 6, 5 are developers – Java, C/C++, Fortran
  - EPSRC Software Engineering Support Centre
  - EPSRC funded projects – mostly CFD focussed
  - Development of publication & data repositories and plans for overarching search system
- **Personal interests**
  - Software and data management & curation
  - Software identification and citation <http://rrr.cs.st-andrews.ac.uk/>
- **Claim to Computing Fame** – I heard Cmdr Grace Hopper speak when I was a student ☺

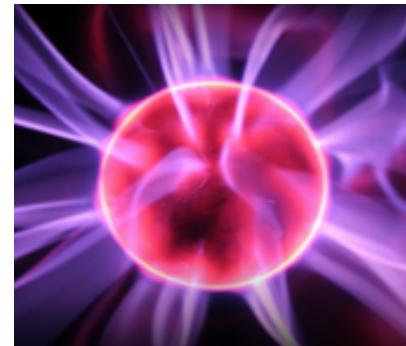


Science & Technology  
Facilities Council

# Anders Markvardsen

- Background:
  - University of Aarhus (Denmark) Physics/Chemistry
  - University of Oxford Physics
  - Postdoc ISIS facility, Data Analysis
  - Senior scientists and software engineer ISIS facility
- Scientific software projects:
  - Crystal field calculation program
  - Maximum entropy program to handle PND data
  - Robotics vs molecular constraints
  - ExtSym (Extinction Symbol) program for powder data
  - Hybrid Monte Carlo global optimisation algorithm
  - MDME, Molecular Dynamics Monte Carlo
  - Jpowder, small footprint visualisation tool for powder data
  - Mantid

# Physics & Astronomy – Research Software



**DiRAC**



# Chris Richardson (chris@bpi.cam.ac.uk)



## FEnICS Project

Chicago, Cambridge, Oslo,  
Gothenburg, Prague



**Open Source:** github / bitbucket

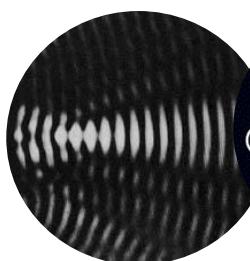
**Automatic testing:** buildbot / Jenkins / bamboo



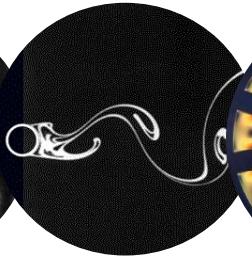
## docker

**HPC:** FEniCS on ARCHER

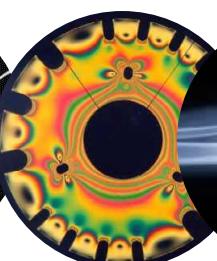
**Containerisation:** docker



acoustics



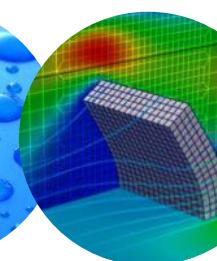
fluid mechanics



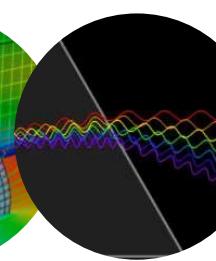
solid mechanics



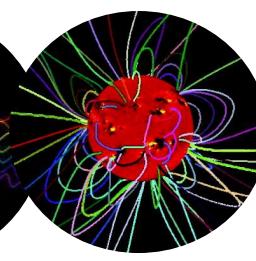
surface tension



FSI

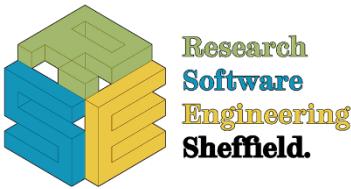


electromagnetics

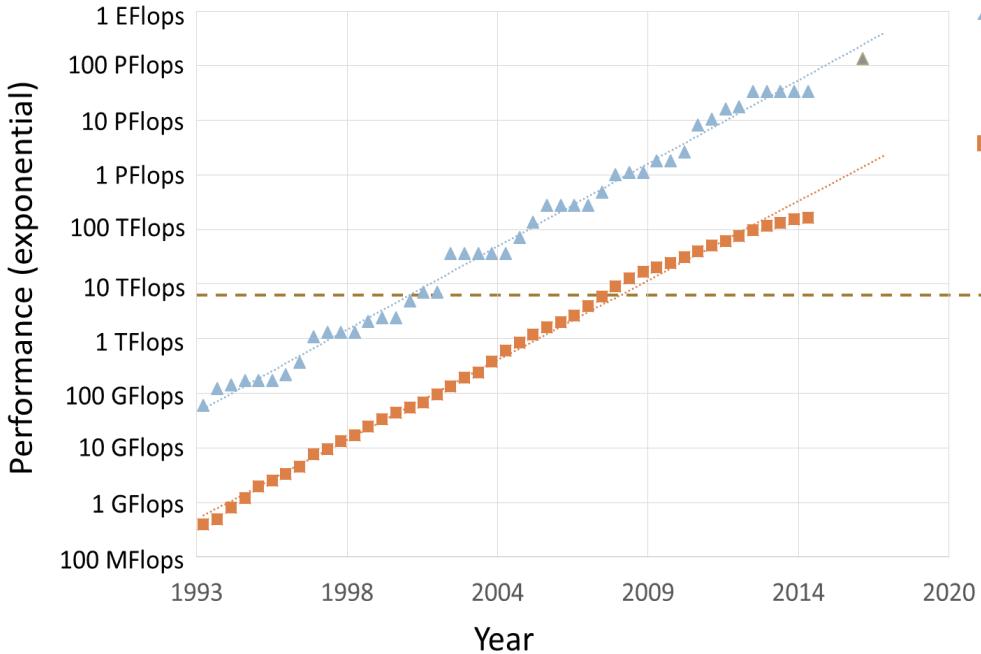


MHD

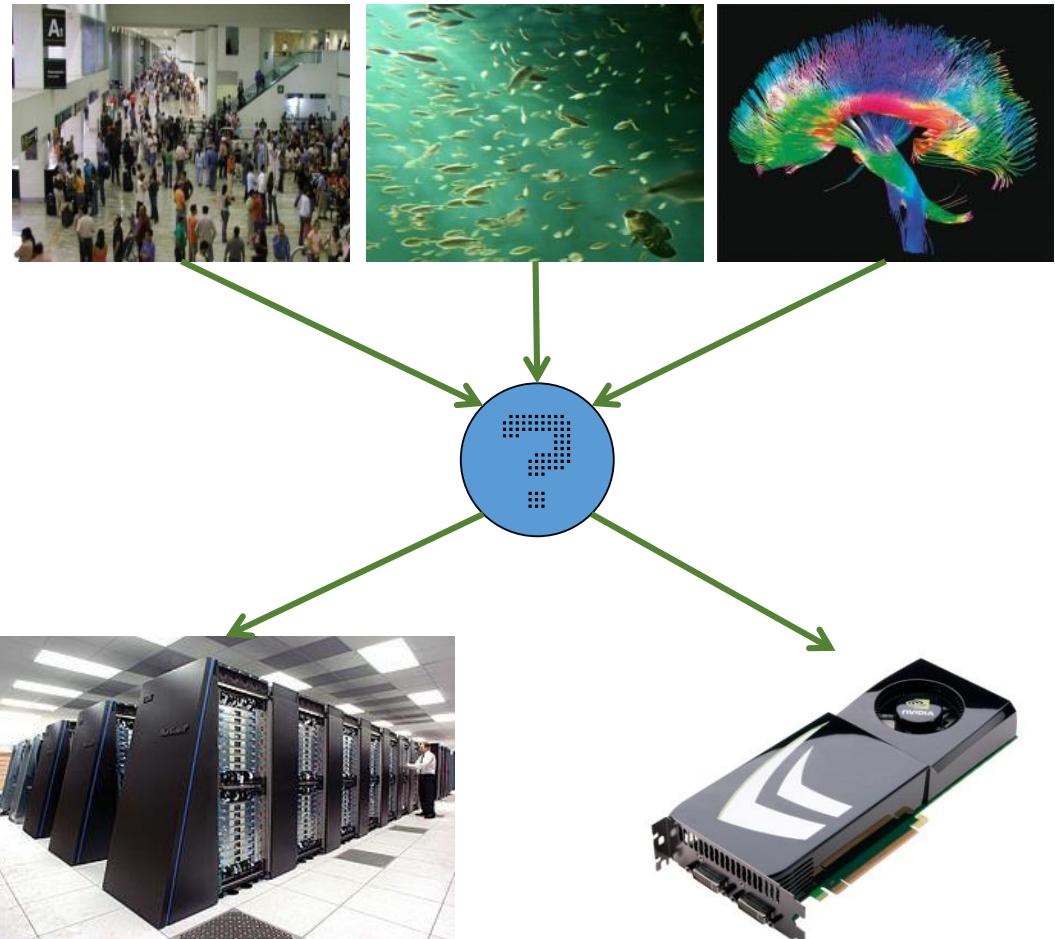
# Dr Paul Richmond Accelerating Science with Accelerated Computing



<http://paulrichmond.shef.ac.uk>  
[p.richmond@Sheffield.ac.uk](mailto:p.richmond@Sheffield.ac.uk)



- ▲ Top Supercomputer
- Number 500 on list



# John Robinson

- Research Software Group
- University of Southampton
- [rsg.soton.ac.uk](http://rsg.soton.ac.uk)
- [@RSGSoton](https://twitter.com/RSGSoton)

UNIVERSITY OF  
Southampton

RESEARCH  
SOFTWARE  
GROUP

# Research Software Engineering @ Cambridge

- RSE team is part of *Research and Institutional Services (RIS)*, within *University Information Services (UIS)* department
- RSE team officially created November 2015 (after division restructuring)
- Currently 3 people (me included) paid on an industrial project, aim to grow to 6~7 in total (mix permanent and fixed-term)
- Funding from CHEST soon to be approved for 2~3 full permanent FTE
- RSE services similar to “UCL model” plus specialized training
- Starting advertise service offer around June 2016
- Two new positions to be created (RSE “classic” and “GPU Specialist”), one currently advertised (RSE “Data Specialist”)

RSE Cambridge contact: [fs395@cam.ac.uk](mailto:fs395@cam.ac.uk)

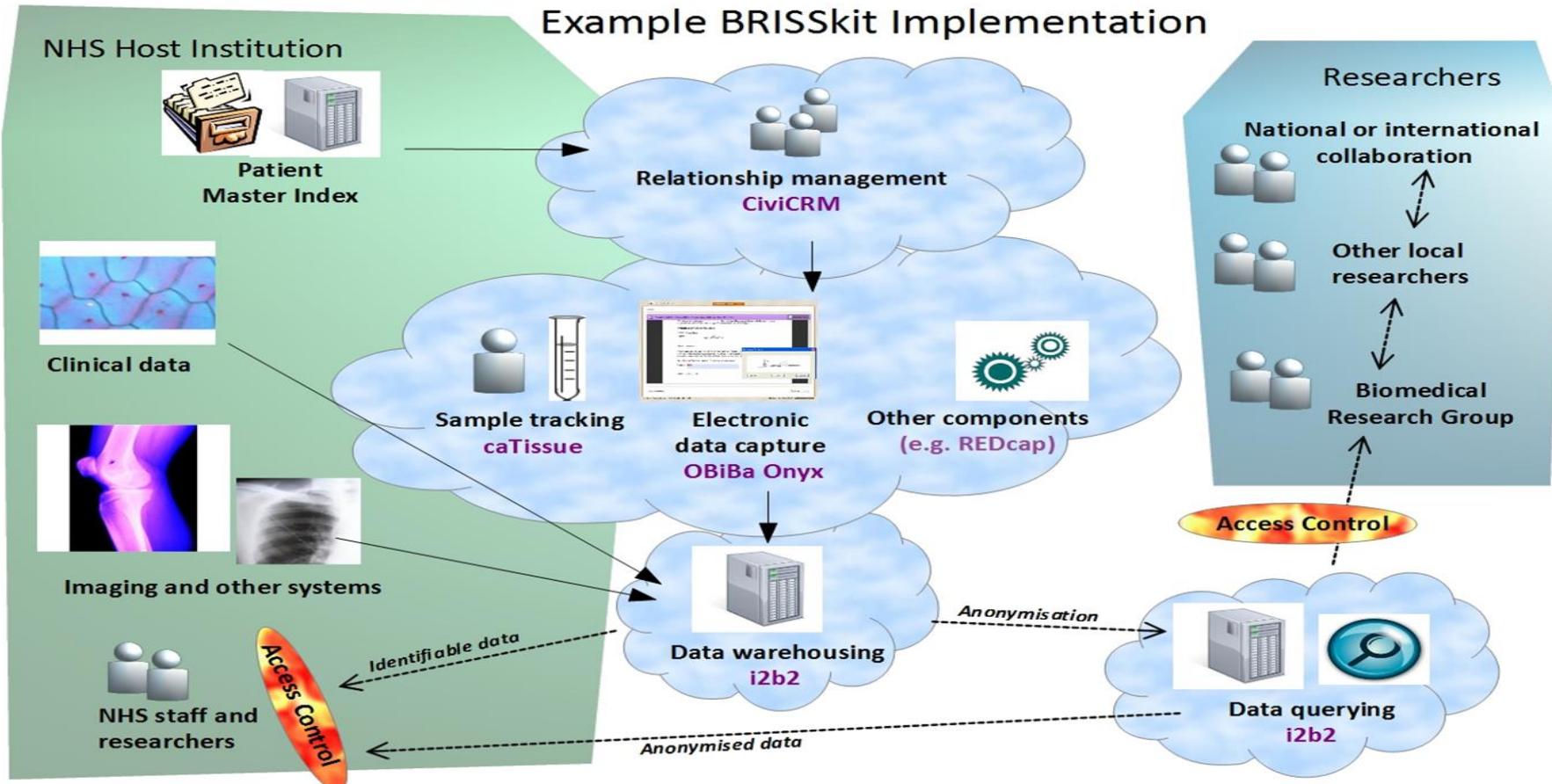
- ▶ Co-chair, UKRSE
- ▶ Software Carpentry certified instructor
  - ▶ organized one workshop last year
  - ▶ volunteered at two others
- ▶ Co-Organizer, Reproducibility in Parallel Computing workshop
  - ▶ [reppar.org](http://reppar.org)
- ▶ Research Associate, Imperial College London
  - ▶ distributed job scheduling
  - ▶ cloud computing
  - ▶ in transition at the moment...

Dr Jonathan Tedds [jat26@le.ac.uk](mailto:jat26@le.ac.uk) @jtedds

Senior Research Fellow, Health Sciences, PI BRISSKit <http://www.brisskit.le.ac.uk>

+ Recomputation project (Gent, Jones) + Editor-in-Chief Open Health Data +

RDA Publishing Data IG + Astrophysics 20+ yrs researcher incl Virtual Observatory



+ Mark Wilkinson (Physics & Astronomy) - Dirac, NEW RSE POSITION!

+ Jon Wakelin (Research IT Lead, ITS) - HPC support, LAMP Service

## **St George's, University of London**

- Medical School and UK's only dedicated health sciences University
- Co-located with St George's University Hospitals, Tooting, SW London
- Research Institutes of Infection and Immunity, Cardiovascular and Cell Sciences, Population Health

## **Adam Witney, Research Fellow, Infection and Immunity**

- Originally a lab based scientist working on drug resistance in Malaria
- Computational genomic analysis of infectious disease e.g. Tuberculosis, MRSA, gonorrhoeae
- Web interface and database development
  - Research databases e.g. tracking European neonatal infections
  - Patient databases e.g. Infection control
- Ad hoc, anything else people ask me to do!
- BSc, MSc, PhD student teaching e.g. DNA sequence analysis, genomics

# **Christopher Woods**

Advanced Computing Research Centre  
University of Bristol

## **Software Developer**

Monte Carlo / Molecular Dynamics / Particle Modelling

Electrons ↔ Atoms ↔ Molecules ↔ Proteins ↔ Bacteria

<http://github.com/chryswoods>

## **RSE Fellow / RSE Group at Bristol**

RSE Co-Coding Projects (3+6+3 months)

Graduate Accelerator Program

Workshops on Coding and Software Carpentry

<http://chryswoods.com>