:: Excellence in Research through Software Development & Leadership

:: A Brief History of UK's Research Software Engineers Movement/Association/Society

:: Sustainable Software Creation in Academia
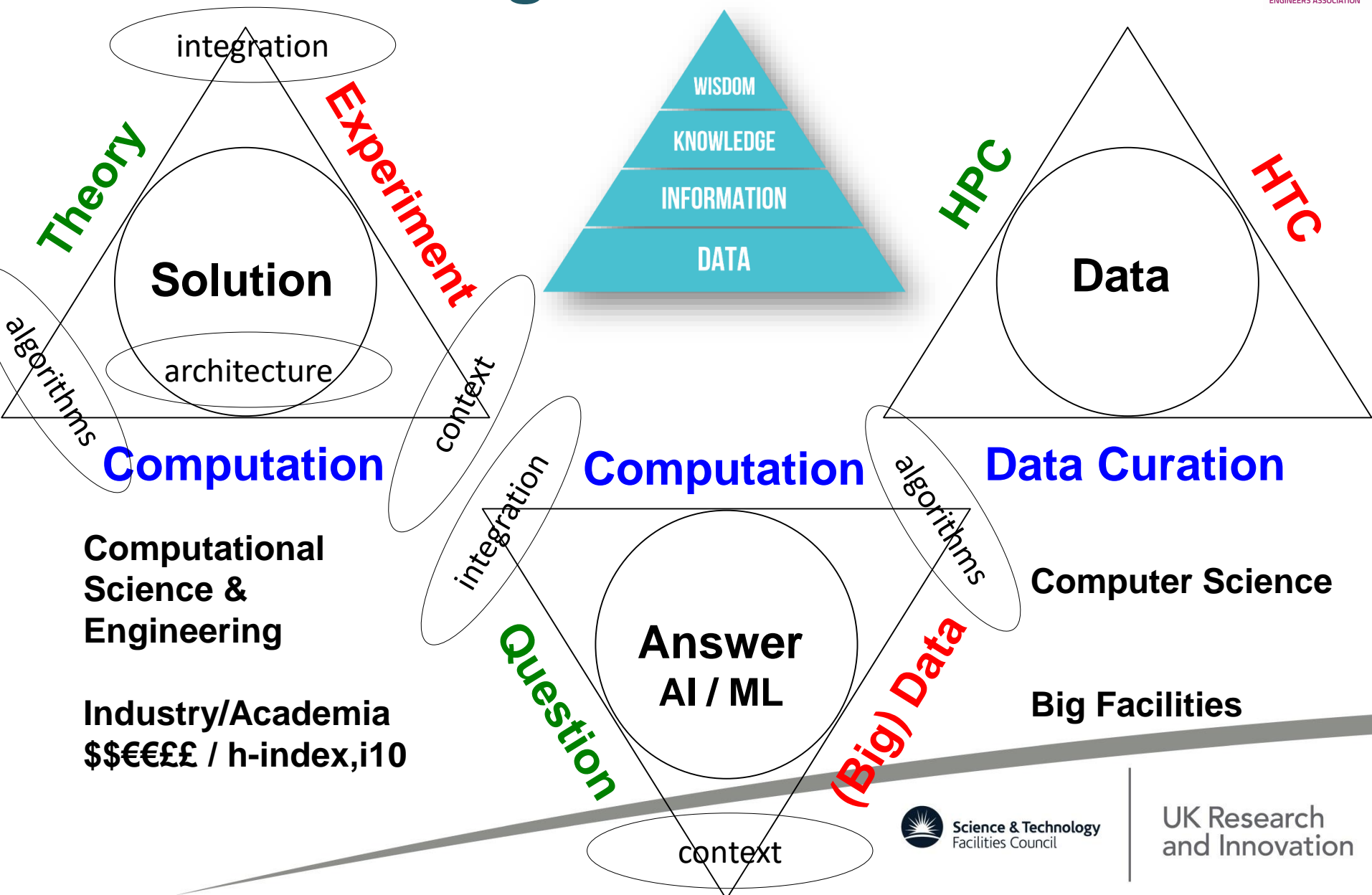
ILIAN TODOROV

Daresbury Laboratory

Alice's Wonderland (1865)

Lewis Carroll (Charles Lutwidge Dodgson)
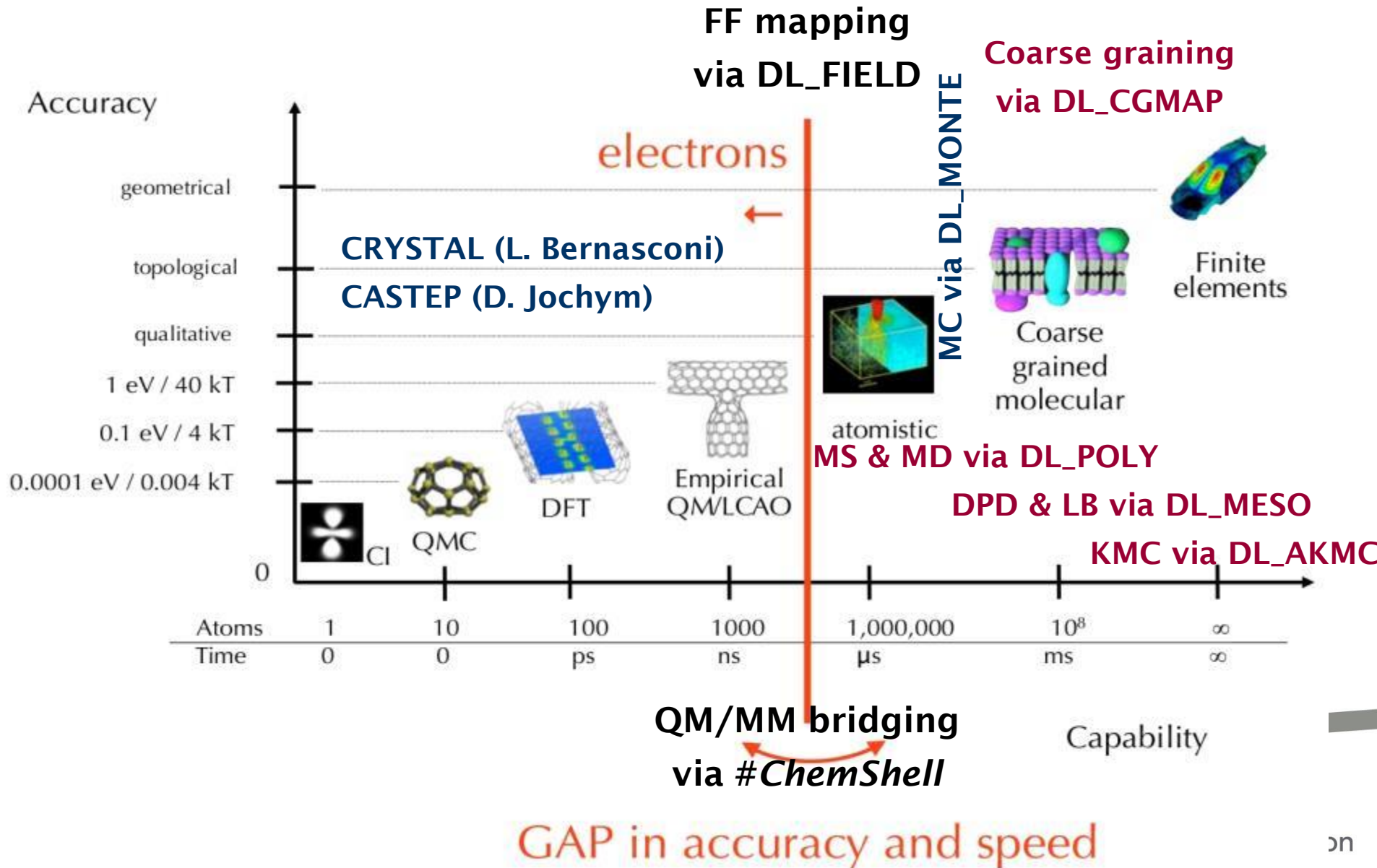
The CECAM/CCP Path to Software

Triangles of Research

integration

Theory

Experiment

algorithms

Solution

architecture

context

Computation

WISDOM

KNOWLEDGE

INFORMATION

DATA

HPC

HTC

Data

Data Curation

**Computational
Science &
Engineering**

**Industry/Academia
$$€€££ / h-index,i10**

integration

Computation

algorithms

Computer Science

**Answer
AI / ML**

Question

(Big) Data

context

Big Facilities

Science & Technology
Facilities Council

UK Research
and Innovation

Multiple Scales of Materials Modelling

FF mapping via DL_FIELD

Coarse graining via DL_CGMAP

MC via DL_MONTE

Accuracy

electrons

geometrical

CRYSTAL (L. Bernasconi)

topological

CASTEP (D. Jochym)

qualitative

1 eV / 40 kT

0.1 eV / 4 kT

0.0001 eV / 0.004 kT

CI   QMC   DFT   Empirical QM/LCAO   atomistic   Coarse grained molecular   Finite elements

MS & MD via DL_POLY

DPD & LB via DL_MESO

KMC via DL_AKMC

Atoms	1	10	100	1000	1,000,000	10^8	∞
Time	0	0	ps	ns	μs	ms	∞

QM/MM bridging via *#ChemShell*

Capability

GAP in accuracy and speed

RoMM VI

What makes a material function?
Let me compute the ways...
Modeling in H2020 NMBP Programme Materials projects

Modelling in
H2020 LEIT-NMBP Programme
Materials and Nanotechnology projects

One reality with four veridical views each at a different level of granularity.

This is true for observations and for simulations.

ELECTRONS

ELECTRONIC MODEL
Physics Based Model using a Physics Equation and Material Relation describing the behaviour of electrons quasi particles either as waves, particles or distributions.

ATOMS

ATOMISTIC MODELS
Physics Based Model using a Physics Equation and Material Relation describing the behaviour of atoms either as waves, particles or distributions.

BEADS

MESOSCOPIC MODELS
Physics Based Model using a Physics Equation and Material Relation describing the behaviour of Beads either as particles or distributions.

CONTINUUM VOLUME ELEMENT

CONTINUUM MODELS
Physics Based Model using a Physics Equation and Material Relation describing the behaviour of Continuum Volume.

MODA DEFINITION

RoMM VI

a first step in the direction of a standardised description of modelling has been taken by the EC

MODA (MOdelling DAta)

is a **template** for the **standardised description** of **materials models**
(https://emmc.info/moda-workflow-templates/)

The **MODA** is meant to **guide users** towards a complete **high-level documentation** of material models, starting from the **end-user case** via the **computational details** to the **results**.

It provides all necessary aspects for: **description, reproducibility, curation** and **interfacing** with other models and databases.

The MODA uses **core model concepts**

PHYSICS ENTITY

EQUATIONS (physics- or data-based)

What makes a material function?
Let me compute the ways...
Modeling in H2020 NMBP Programme Materials projects

Review of Materials Modelling VI
RoMM

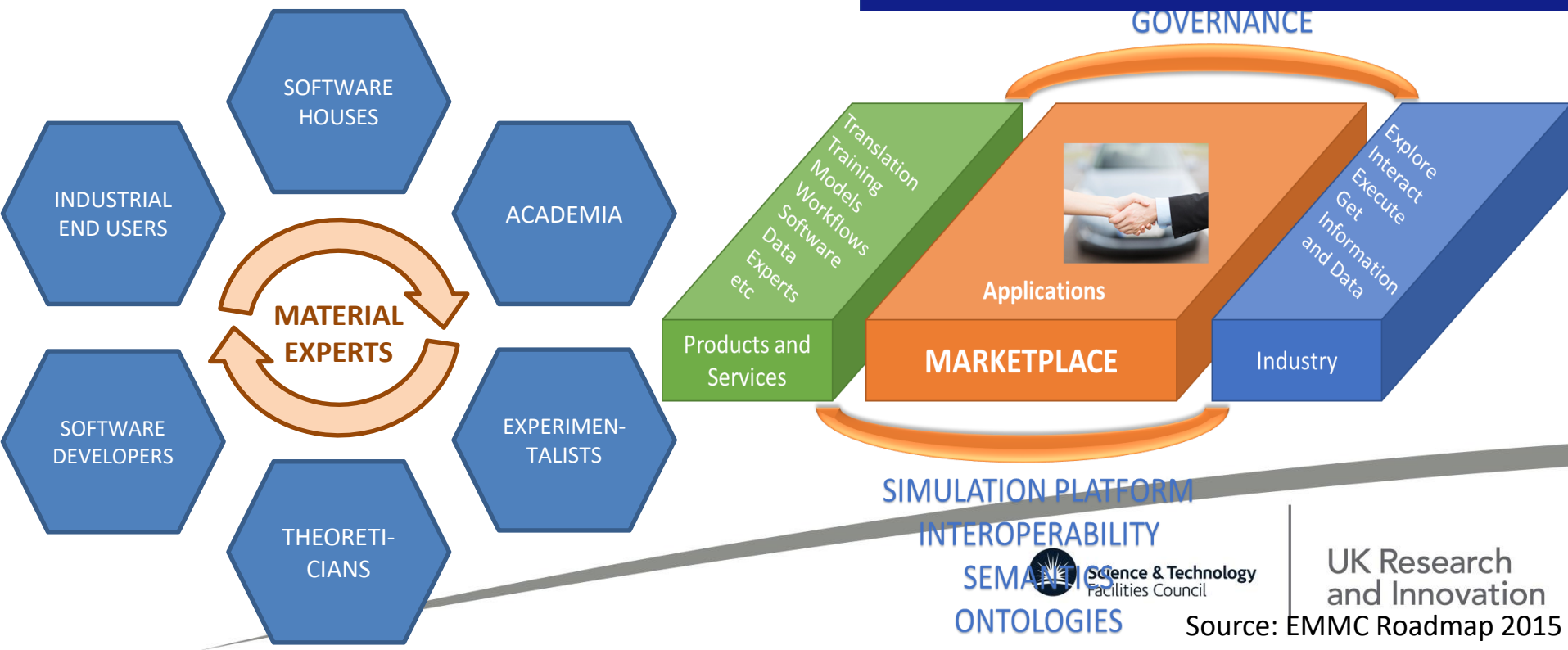Vocabulary, classification and metadata for materials modelling (130 FP7 and H2020 projects)

https://bookshop.europa.eu/en/what-makes-a-material-function--pbKI0616197/

GOVERNANCE

Translation
Training
Models
Workflows
Software
Data
Experts
etc

Products and Services

Applications

MARKETPLACE

Explore
Interact
Execute
Get
Information
and Data

Industry

SIMULATION PLATFORM
INTEROPERABILITY
SEMANTICS
ONTOLOGIES

SOFTWARE HOUSES

INDUSTRIAL END USERS

ACADEMIA

MATERIAL EXPERTS

SOFTWARE DEVELOPERS

EXPERIMEN-TALISTS

THEORETI-CIANS

Science & Technology Facilities Council

UK Research and Innovation

Source: EMMC Roadmap 2015

Software Creation in Academia

Issues & Topics (academia):

- Recognition
- Identification
- Identity
- Appreciation
- Credit
- Satisfaction
- Sustainability & Job Security
- Personal Development & Career Progression

Software is a critical part of modern research...

SOFTWARE CITATION PRINCIPLES

IMPORTANCE

Software should be considered a legitimate and citable product of research. Software citations should be accorded the same importance in the scholarly record as citations of other research products; they should be included in the metadata of the citing work, such as a reference list. Software should be cited on the same basis as any other research product such as a paper or a book.

UNIQUE IDENTIFICATION

A software citation should include a method for identification that is machine actionable, globally unique, interoperable, and recognized by at least a community of the corresponding domain experts, and preferably by general public researchers.

ACCESSIBILITY

Software citations should facilitate access to the software itself and to its associated metadata, documentation, data, and other materials necessary for both humans and machines to make informed use of the referenced software.

PERSISTENCE

Unique identifiers and metadata describing the software and its disposition should persist —even beyond the lifespan of the software they describe.

CREDIT AND ATTRIBUTION

Software citations should facilitate giving scholarly credit and normative, legal attribution to all contributors to the software, recognizing that a single style or mechanism of attribution may not be applicable to all software.

SPECIFICITY

Software citations should facilitate identification of, and access to, the specific version of software that was used. Software identification should be as specific as necessary, such as using version numbers, revision numbers, or variants such as platforms.

... yet there is little support for its acknowledgement and citation

History Line - 2009

2009: **EPSRC** Pioneering research and skills

There appears to be a lot of software out there…

…someone should really do something about it

Q: Is Software Important?

A: "*Witnesses struggled to point to a sector of the economy that was unaffected by digital technologies*"

- Make or Break: The UK's Digital Future, Select Committee on Digital Skills

Is Software Important for Research?

Study at: https://goo.gl/gmHwGm

What is Software?
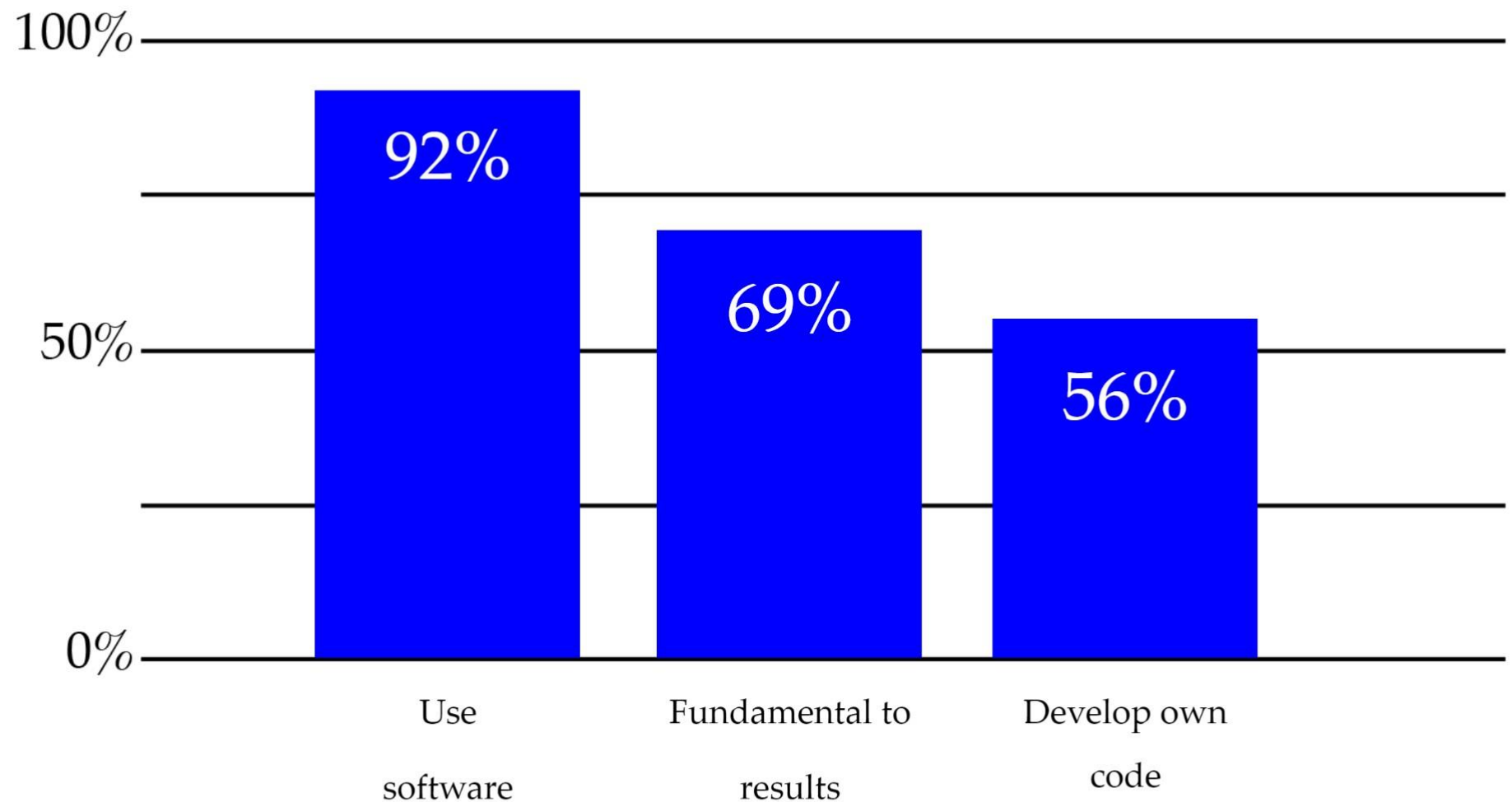
UK Research
and Innovation
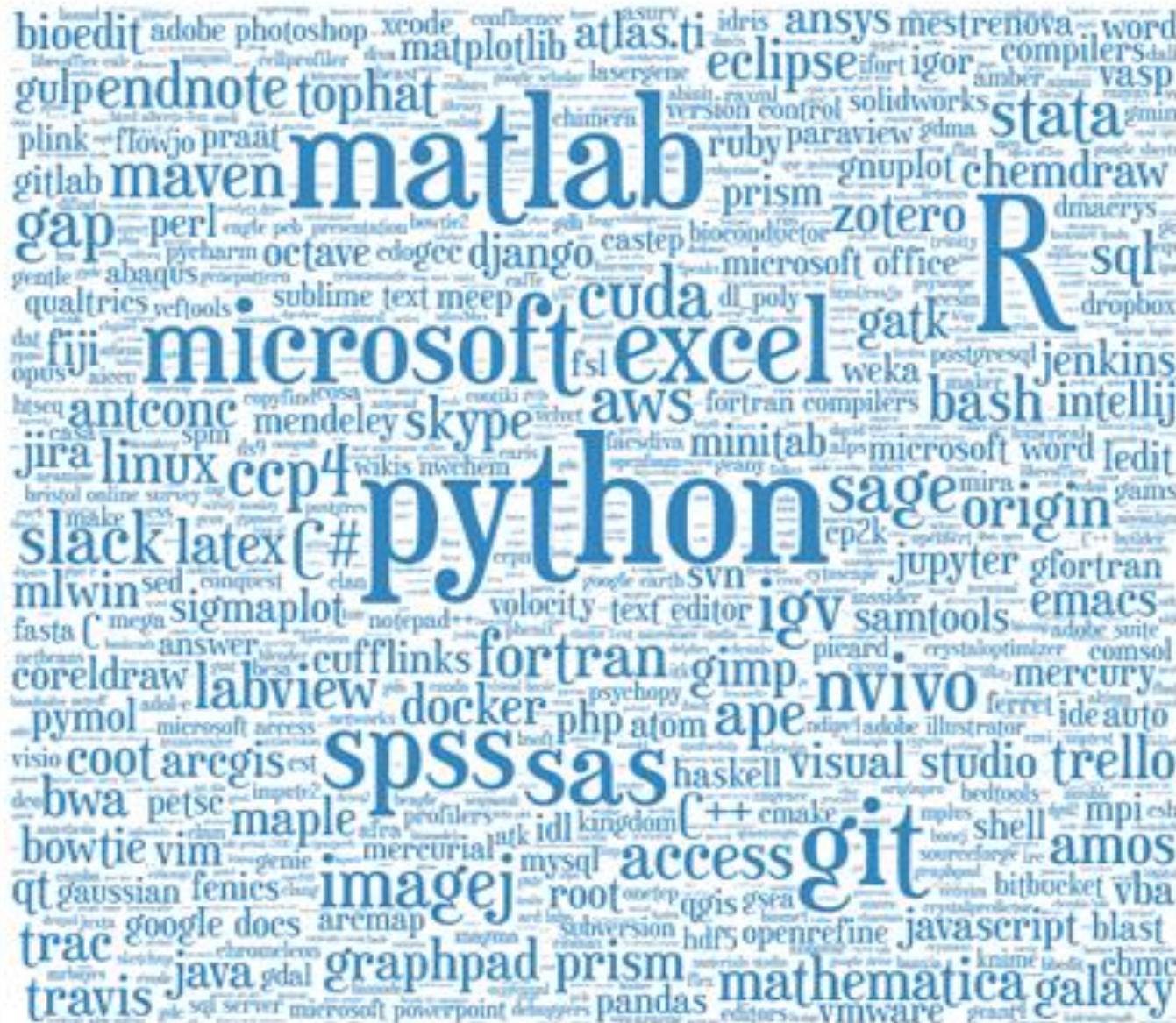
UKRI Survey

44,000 research grants (~£3bn) over 7 Research Councils

38% of total spend invested into software-reliant research in 2017
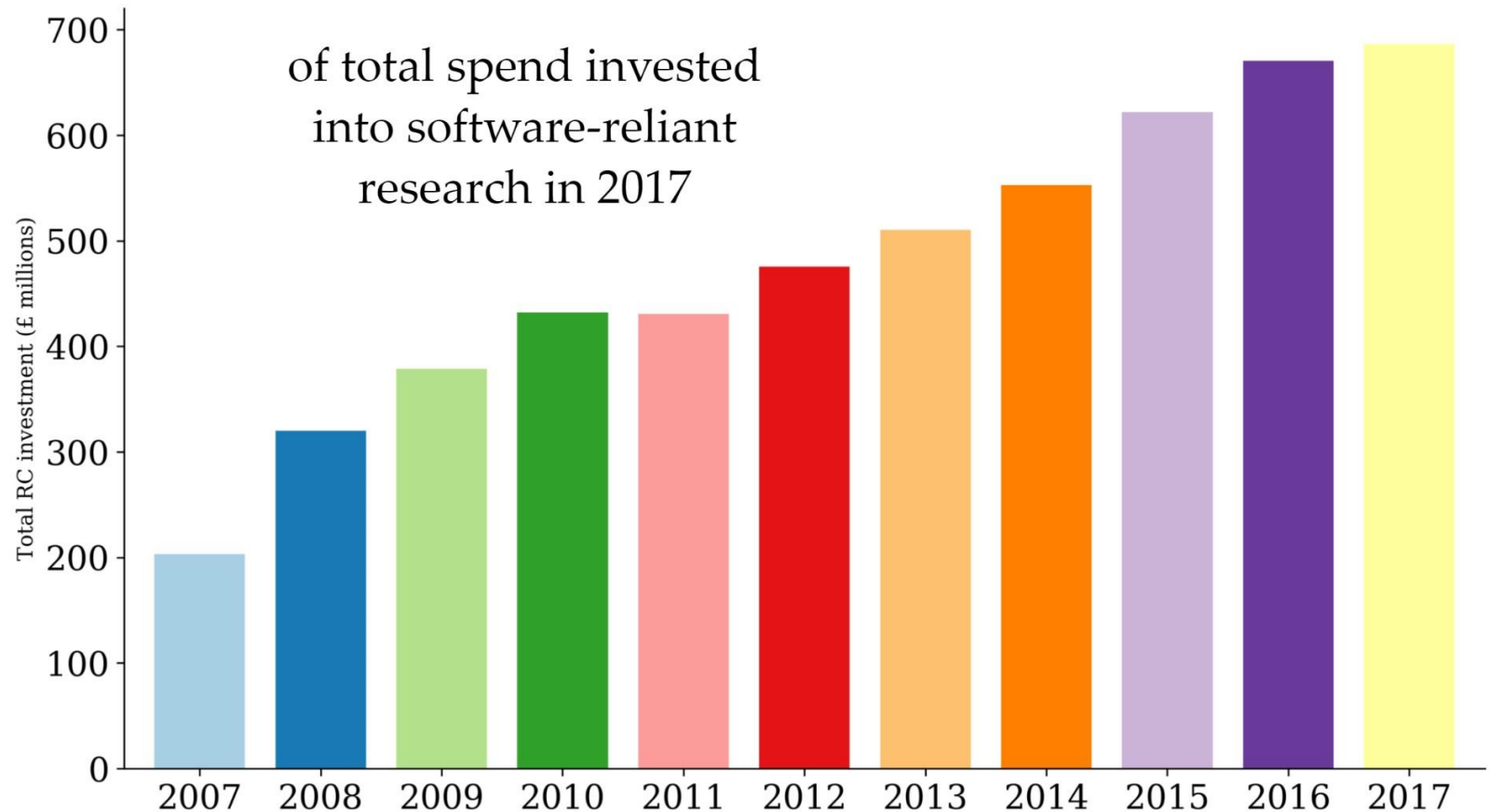
ePrints Repository Software

31 repositories

~600,000 papers

UK Academia Publications

2/3rds

of papers indicate software reliance in 2017
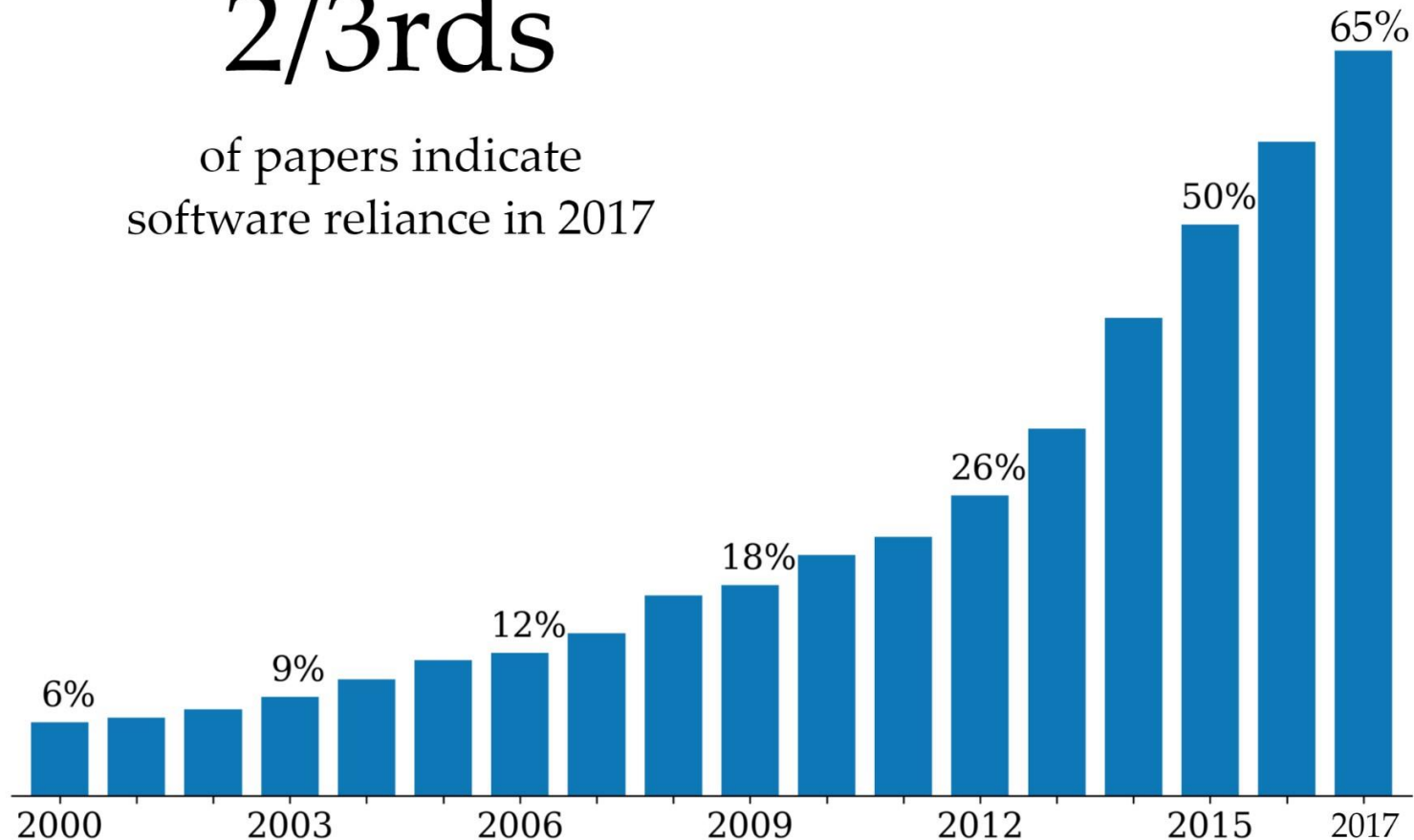
Evidence of Issues

24% of researchers who develop code have no training

50% of group leaders looking to commercialise code would not feel comfortable sharing their code

3% of REF 2014 case studies mention software

120 fold more paper outcomes registered in ResearchFish® than software outcomes

Evidence of Issues
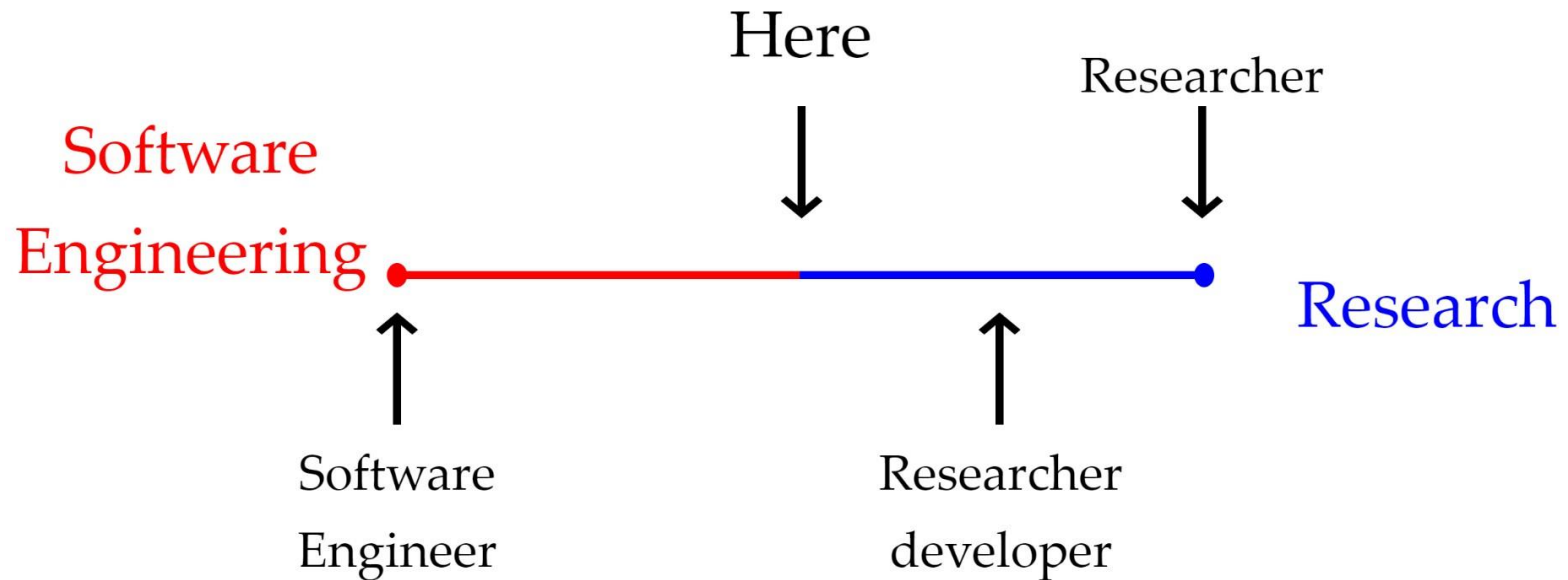
No career path for software experts in academia

History Line – 2010

2010:

Software
Sustainability
Institute

Cultivating better, more sustainable research software to enable world-class research

Software

29 projects
All 7 Research Councils

Training

Over 4500 learners
137 trainers
80 guides, 50000 views

Outreach

20,000+ monthly visits
Vibrant Twitter community

112 Fellows across domains
Over 20 workshops

RSE campaign
Demographic studies
Finance and career studies

Community

Policy

23 staff (assoc.) catering for *210,000* UK researchers

- Networking
- Events
- Publicity
- Money
- Links to funders
- Research, policy, evidence

Enabled the RSE movement to get off the ground

Science & Technology
Facilities Council

UK Research
and Innovation

History Line – 2012

2012: Collaborative Workshop @ Oxford

"Developing the profession of a scientific software engineer and the career track of software developers in academia"

- James Hetherington

"It is not **the naming of the new species** that defines the problem, *but the lack of recognition and appreciation of the work, role and skill of the scientific software engineer in both academia and industry*."

- Ilian Todorov

devcsi.ukoln.ac.uk/2012/04/20/career-progression-for-software-developers-in-the-uk-academia/
software.ac.uk/blog/2016-10-06-work-scientific-software-engineers-recognised-academia

2012 – RSE Term Coined

2012: Collaborative Workshop @ Oxford

jobs.ac.uk

10,000 jobs assessed

~400 related to software development (4%)

~194 different job titles for for RSE roles within UK academia

Research
Software
Engineer

Researcher

Software
Engineering

Research

Software
Engineer

Researcher
developer

2013 – RSE Publicity

2013 – First Meeting

Workshop for RSEs
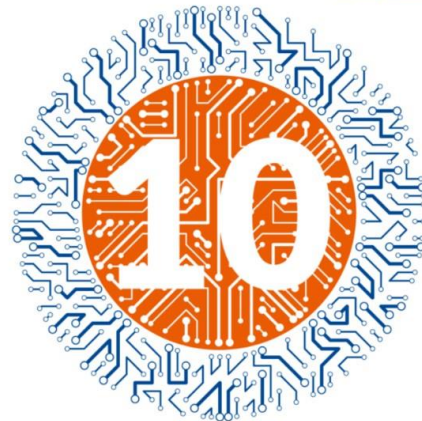
11 September 2013

160 members in first 3 months

"Should we create a community to represent RSEs?"

Outcome: Aim for identity & inclusiveness "UKRSE Association" www.rse.ac.uk @ResearchSoftEng

2014 – RSE Association Founded

2010	Mar 2012	Late 2012	Early 2014
SSI	Term coined	First RSG	UK RSE
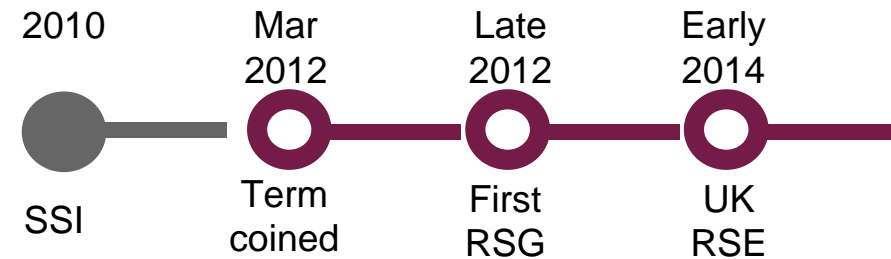
- A common name is powerful and a symbol of self-recognition
- There are pre-existing roles and teams, and history…
- Job titles and group names may vary, e.g. "engineer" is often a protected term (preventing RSE identification)…
- But the community is inclusive and encourages diversity

Science & Technology Facilities Council

UK Research and Innovation

2015 – RSE Fellowships

Timeline:

2010	Mar 2012	Late 2012	Early 2014	Late 2014	June 2015
SSI	Term coined	First RSG	UK RSE	Democratic	RSE fellows
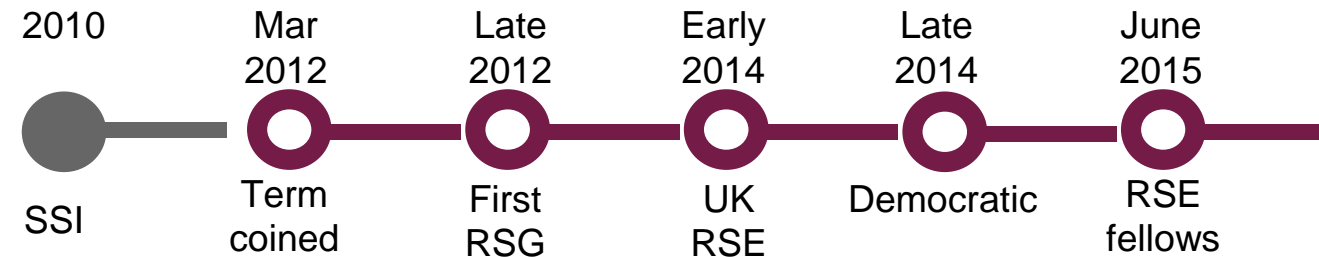
EPSRC

Funding body creates dedicated **RSE Fellowships** (5 years duration)

211 applicants – 6 fellowships awarded
2nd round in 2017 – 4 fellowship awarded

RSE Networks & groups
- RSE network coordinator: Claire Wyatt
- RSE leaders networking group & forum for networking, help & moral support for people setting up or running RSE Groups
- Expansion of more RSE groups around the country

2016/18 – Expansion & Society

Term RSE Coined	First RSE Group	First RSE Workshop	UK RSE founded	RSE fellowships	RSE Conferences	Society of RSE

2012 — **2013** — **2014** — **2015** — **2016-17-18**

Establishing a professional society
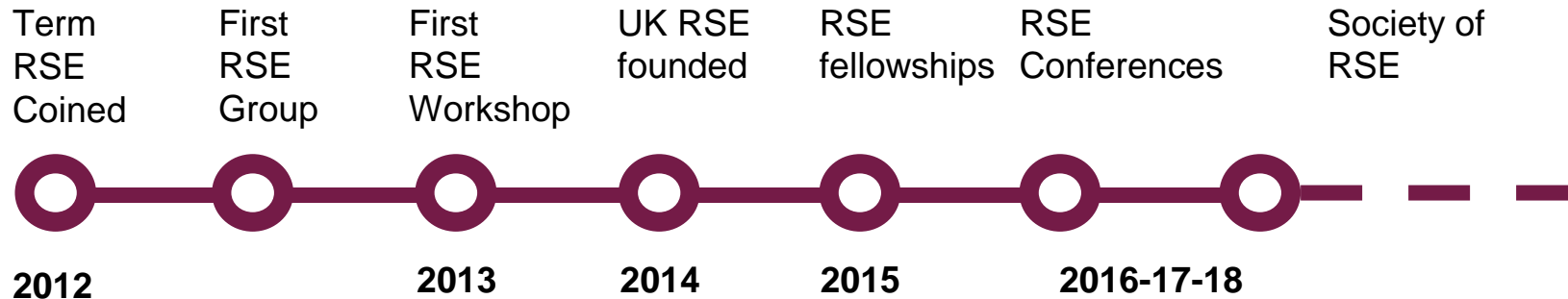
Recognition by funding bodies:

"RSE State of the Nation Report 2017"
doi.org/10.5281/zenodo.495360
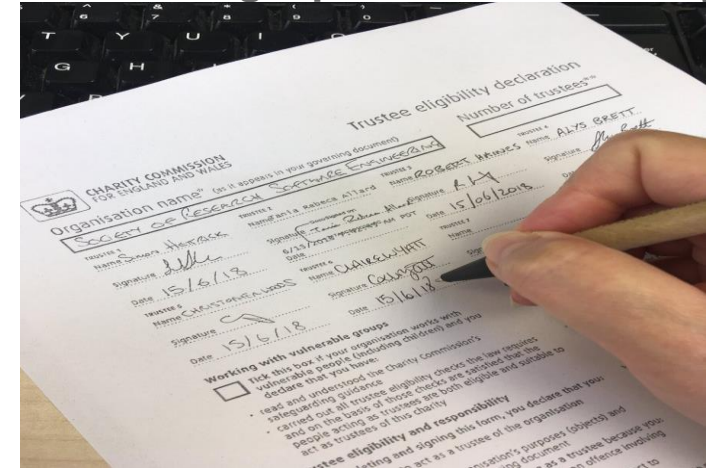
Community Growth

#RSE16
Manchester
200 attendees!

#RSE17
Manchester
224 attendees!

#RSE18
Birmingham
>320 attendees!!!

1294 members
In Aug'18!

160 members
Jan-Mar'14!

1000

500

0

1 Jan 2015   1 Jan 2016   1 Jan 2017   1 Jan 2018

RSE
RESEARCH SOFTWARE
ENGINEERS ASSOCIATION
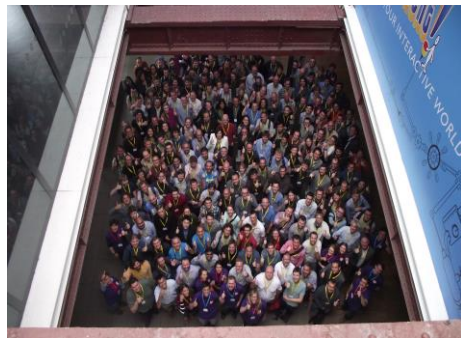
Communication Growth

823 active members

~**3000** messages per month

~**44,000** in total

> **200** members active per week

@ResearchSoftEng

100s of jobs advertised on the mailing list and #jobs every year

>**1700** followers

UK Groups Expansion

- Alan Turing Institute
- University of Bath
- University of Birmingham
- University of Bristol
- University of Cambridge
- University of Cardiff
- UKAEA
- Imperial College London
- Francis Crick Institute
- Kings College London
- University of Leeds
- University of Leicester
- The University of Manchester
- Newcastle University
- Open University
- The University of Sheffield
- University of Southampton
- University College London
- University of Warwick
- Queen Mary University
- EPCC
- Daresbury Laboratory
- Oxford eResearch Centre
- Software Engineering Suppo...

International Follow Up

Germany: DE-RSE

www.de-rse.org

Netherlands: NL-RSE

nl-rse.org

Nordic Countries: NORDIC-RSE

www.nordic-rse.org

Conferences

RSE17

▸ Int. workshop
▸ WSSSPE co-located

Sessions / talks in several national & international conferences

RSE Surveys

Comparative data from:

▸ Germany
▸ Netherlands
▸ UK
▸ USA
▸ South Africa
▸ Canada

Networks & Groups

Name and concept being adopted, eg

▸ Princeton, ORNL, USA
▸ Radboud, Netherlands

First International Workshop

International RSE leaders workshop 2018

RSE leaders met to collaborate on running RSE groups & initiatives

Read more at **researchsoftware.org**

11 Countries
41 People

RSE Research Software Engineers International

Research Software Engineers

This is the website of the international research software engineering community.

Research Software Engineers are people who combine professional software expertise with an understanding of research. They work in many contexts and may have various job titles but the term Research Software Engineer (RSE) is fast gaining international recognition.

National RSE Associations

RSE associations exist now in several countries:

✚ UK RSE - UK Research Software Engineers Association

● DE-RSE - Society for Research Software in Germany

━ NL-RSE - The community of Research Software Engineers in the Netherlands

✚✚✚✚ NORDIC-RSE - Nordic Research Software Engineers Community

EPSRC

Engineering and Physical Sciences Research Council

Science & Technology Facilities Council

UK Research and Innovation

Promotion & Outreach

Case studies **rse.ac.uk/resources**

Career case studies

"With the RSE title, everyone knows what it means"

"What's great about it is that I learn new things every day"

RSE group case studies

- University of Bath
- University of Birmingham
- University of Bristol
- Imperial College London
- University of Leicester
- University of Manchester
- Norwegian University of Science and Technology
- Oak Ridge National Laboratory
- Princeton University
- University of Sheffield
- University of Southampton
- St George's, University of London
- UCL
- UK Atomic Energy Authority

Describing how RSE leaders successfully made the case to set up their group.

An Average RSE (UK)

- **12%** called Research Associate
- **67%** holds a PhD
- **27%** Computer Scientist or Physicist
- **13 years** of experience on average
- **58%** consider themselves professional software developer
- **84%** are male
- **40%** are 35-44 year's old
- **47%** earn between £32-43k
- **61%** use Linux
- **15%** use Python
- **28%** are 7/10 satisfied with their current position
- **25%** are 7/10 satisfied with their career

1. **Wants to work in a research environment**

2. **Wants to advance research**

3. **Wants to develop software**

An Average RSE (worldwide)

Country	Gender	PhDs	Background	Reason to work
Canada	n/a	45%	IT	n/a
Germany	83% male	48%	Physics	Research environment
Netherlands	63% male	56%	Comp. sci.	N/A
UK	84% male	67%	Comp. sci./physics	Research environment
USA	82% male	60%	Comp. sci.	Advance research
South Africa	92% male	68%	Physics	Research environment

UKRSE Committees
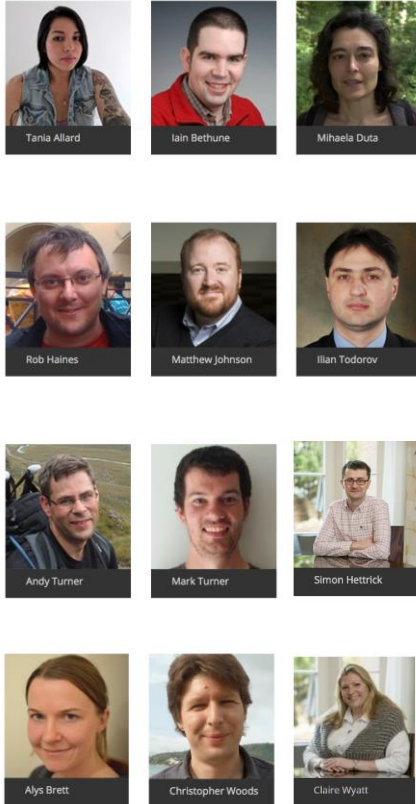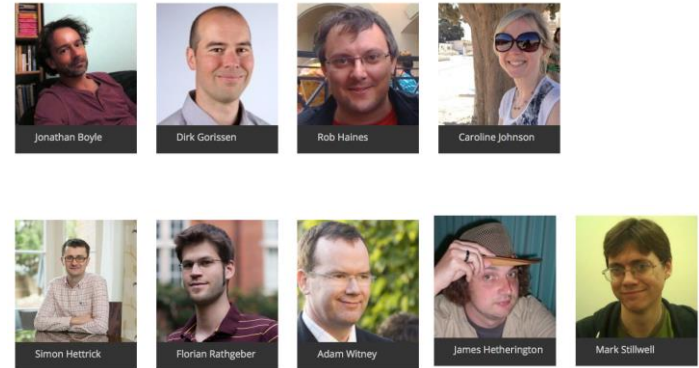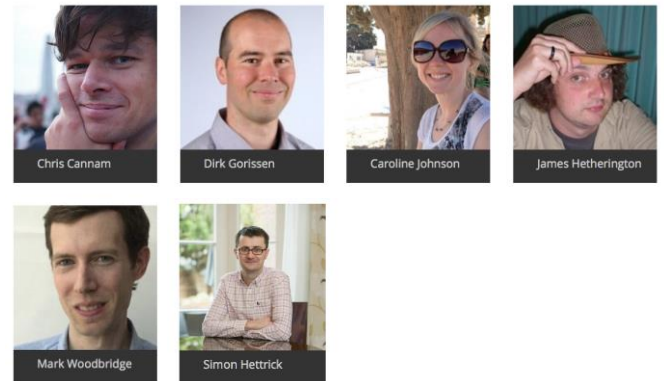
What have We Achieved?

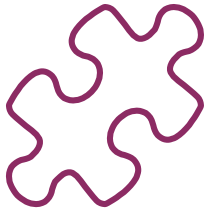"It's a noble goal and all, but you won't change anything"
- Anonymous

"Genius is one percent inspiration, ninety-nine percent perspiration"
- Thomas Edison

- Identity & Recognition
- A career path, albeit still informal
- A growth in the number of software experts
- Greater access to RSE skills for researchers

PICK WHAT FITS

Action can be taken on all scales
You know your context best

CHANGE IS
HARD

COMMUNITIES
ARE POWERFUL

BIG GOAL
SMALL STEPS

Keep going and small changes add up

MAKE IT
HAPPEN!