Case Studies of Research Software Development & Management in Universities

Daniel S. Katz

d.katz@ieee.org, http://danielskatz.org, @danielskatz

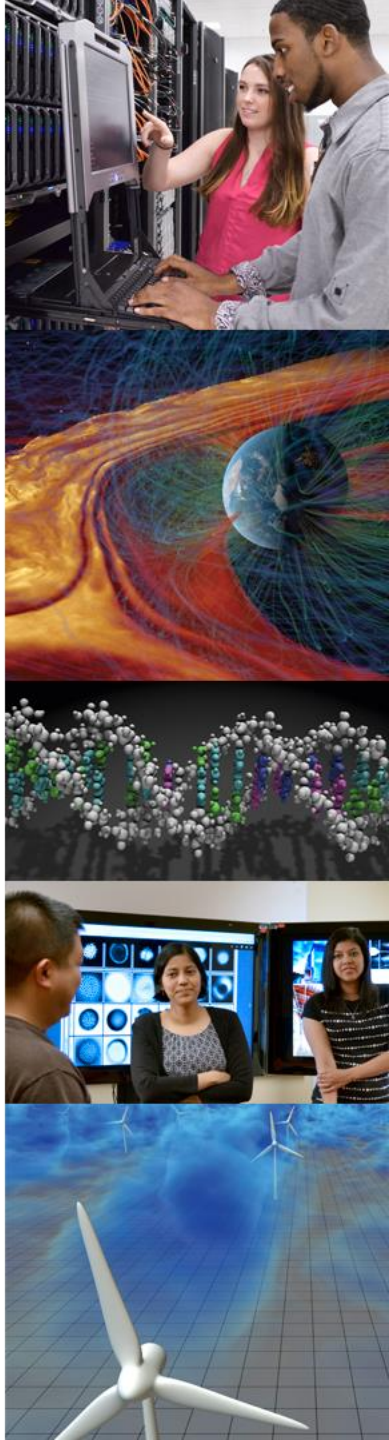
NITRD MAGIC, 2 September 2020

ILLINOIS

NCSA | National Center for Supercomputing Applications

Credit to Rob Haines for the original slides for our paper (10.1109/SE4Science.2019.00009 & https://arxiv.org/abs/1903.00732)

Research Software and Research Software Engineers



ILLINOIS NCSA

Why do we care about research software?

Why do we care about research software?

- Funding
  - ~20% of NSF projects over 11 years topically discuss software in their abstracts ($10b)
  - 2 of 3 main ECP areas are research software (~$4b)

Why do we care about research software?

- Funding
  - ~20% of NSF projects over 11 years topically discuss software in their abstracts ($10b)
  - 2 of 3 main ECP areas are research software (~$4b)
- Publications
  - Software intensive projects are a majority of current publications
  - Most-cited papers are methods and software

Why do we care about research software?

- Funding
  - ~20% of NSF projects over 11 years topically discuss software in their abstracts ($10b)
  - 2 of 3 main ECP areas are research software (~$4b)
- Publications
  - Software intensive projects are a majority of current publications
  - Most-cited papers are methods and software
- Researchers
  - >90% of US/UK researchers use research software
  - ~65% would not be able to do their research without it
  - ~50% develop software as part of their research

Software as a strategic advantage

Software as a strategic advantage

- Both direct (software itself) and indirect (things enabled by software and by professional software developers)

Software as a strategic advantage

- Both direct (software itself) and indirect (things enabled by software and by professional software developers)
- Competition between institutions
  - E.g. for faculty who want to go where they can be successful and are supported by resources including start up funding, facilities (computing, data, software, etc.) and staff
  - E.g. for projects that build or rely on software

Software as a strategic advantage

- Both direct (software itself) and indirect (things enabled by software and by professional software developers)
- Competition between institutions
  - E.g. for faculty who want to go where they can be successful and are supported by resources including start up funding, facilities (computing, data, software, etc.) and staff
  - E.g. for projects that build or rely on software
- UK Research Excellence Framework (REF)
  - System for assessing quality of research in UK higher education institutions, tied to university funding, includes software as an output and research that relies on software

How do we develop better research software?

How do we develop better research software?

There are two hard problems in Software Engineering:

How do we develop better research software?

There are two hard problems in Software Engineering:

1. People

How do we develop better research software?

There are two hard problems in Software Engineering:

1. People
2. Convincing others that “people” is a hard problem

https://martinfowler.com/bliki/TwoHardThings.html;
https://twitter.com/holman/status/776291833336979456

How do we develop better research software?

There are two hard problems in Software Engineering:

1. People
2. Convincing others that “people” is a hard problem

So, lets talk about people…

https://martinfowler.com/bliki/TwoHardThings.html;
https://twitter.com/holman/status/776291833336979456

How do we develop better research software?

There are two hard problems in Software Engineering:

1. People
2. Convincing others that “people” is a hard problem

So, lets talk about people…

Really:

https://martinfowler.com/bliki/TwoHardThings.html;
https://twitter.com/holman/status/776291833336979456

How do we develop better research software?

There are two hard problems in Software Engineering:

1. People
2. Convincing others that “people” is a hard problem

So, lets talk about people…

Really:

- Culture problems (hardest)

https://martinfowler.com/bliki/TwoHardThings.html;
https://twitter.com/holman/status/776291833336979456

How do we develop better research software?

There are two hard problems in Software Engineering:

1. People
2. Convincing others that “people” is a hard problem

So, lets talk about people…

Really:

- Culture problems (hardest)
- Management problems

https://martinfowler.com/bliki/TwoHardThings.html;
https://twitter.com/holman/status/776291833336979456

How do we develop better research software?

There are two hard problems in Software Engineering:

1. People
2. Convincing others that “people” is a hard problem

So, lets talk about people…

Really:

- Culture problems (hardest)
- Management problems
- Software problems (easiest)

https://martinfowler.com/bliki/TwoHardThings.html;
https://twitter.com/holman/status/776291833336979456

The Craftsperson and the Scholar

The Craftsperson and the Scholar

- Scholar: archetypical researcher driven to understand things to their fullest capability
  - Find intellectually-demanding problems
  - Curiosity-driven, work on a topic until understanding has been acquired, pass on that understanding through teaching

http://www.software.ac.uk/blog/2012-11-09-craftsperson-and-scholar

The Craftsperson and the Scholar

- Scholar: archetypical researcher driven to understand things to their fullest capability
  - Find intellectually-demanding problems
  - Curiosity-driven, work on a topic until understanding has been acquired, pass on that understanding through teaching
- Craftsperson: driven to create and leave behind an artifact that reifies their efforts in a field
  - Feels pain when things they make are fragile or ugly
  - Prefer to make things that explain themselves
  - Work requires patience, and pride in doing a job well

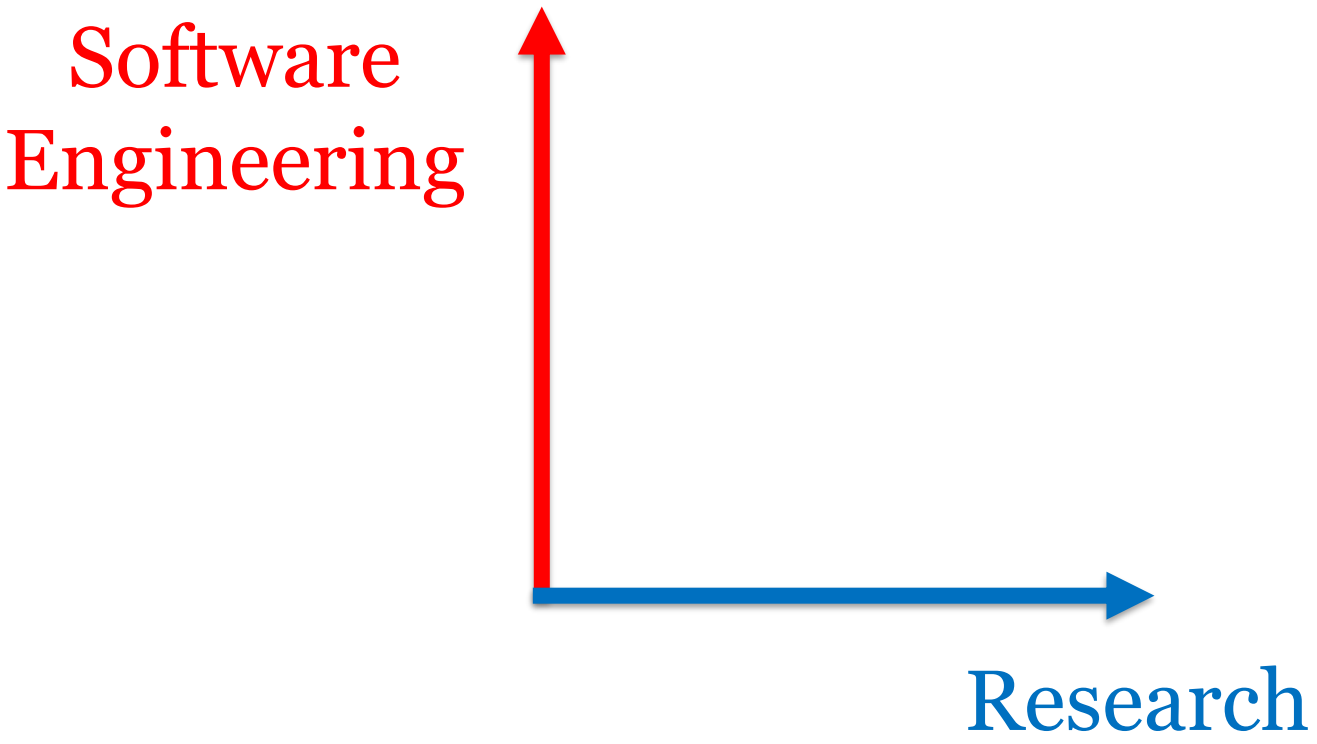
http://www.software.ac.uk/blog/2012-11-09-craftsperson-and-scholar

The Craftsperson and the Scholar

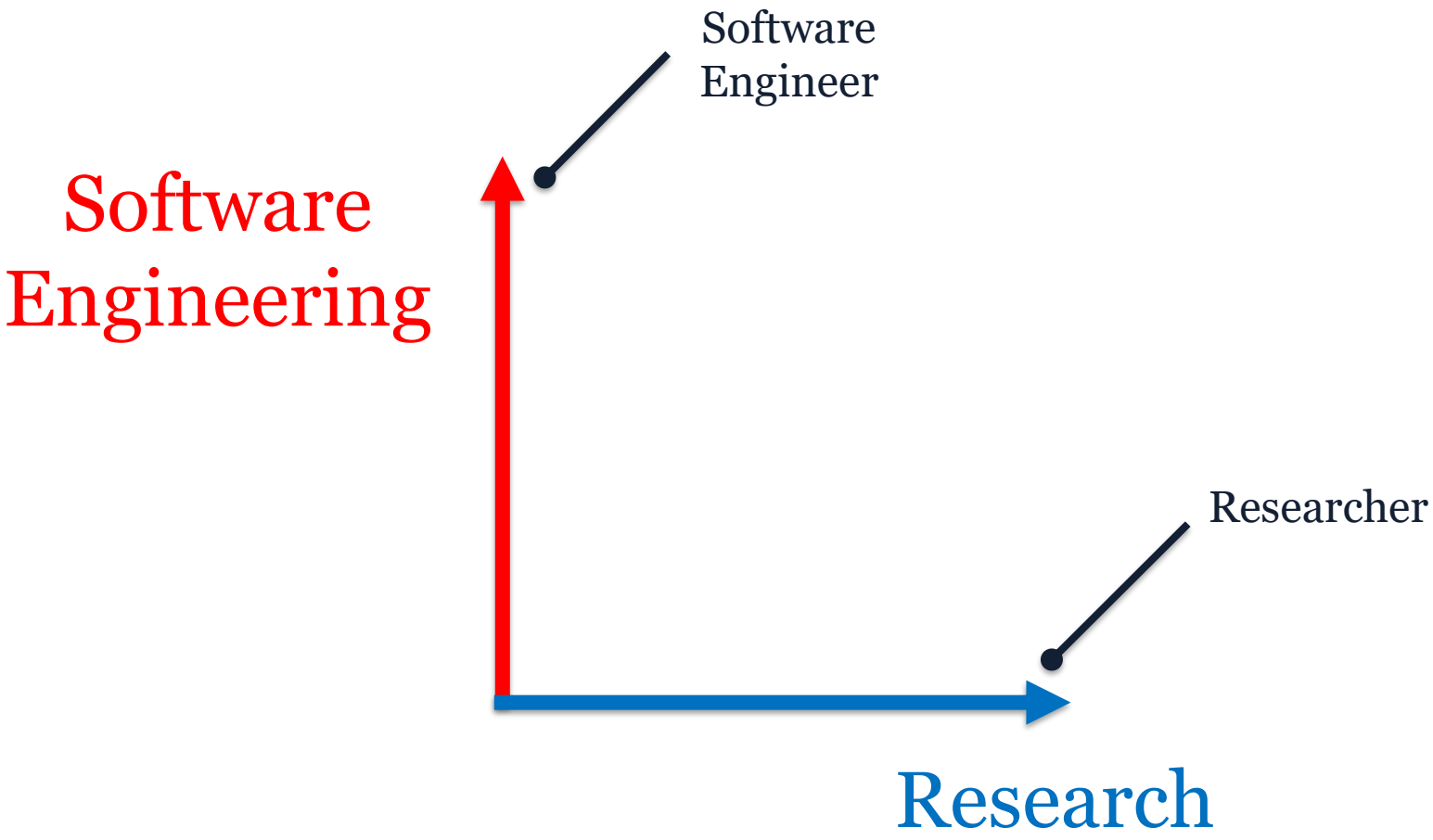
- Scholar: archetypical researcher driven to understand things to their fullest capability
  - Find intellectually-demanding problems
  - Curiosity-driven, work on a topic until understanding has been acquired, pass on that understanding through teaching
- Craftsperson: driven to create and leave behind an artifact that reifies their efforts in a field
  - Feels pain when things they make are fragile or ugly
  - Prefer to make things that explain themselves
  - Work requires patience, and pride in doing a job well
- Scientific software requires individuals who combine the best of both roles.

http://www.software.ac.uk/blog/2012-11-09-craftsperson-and-scholar

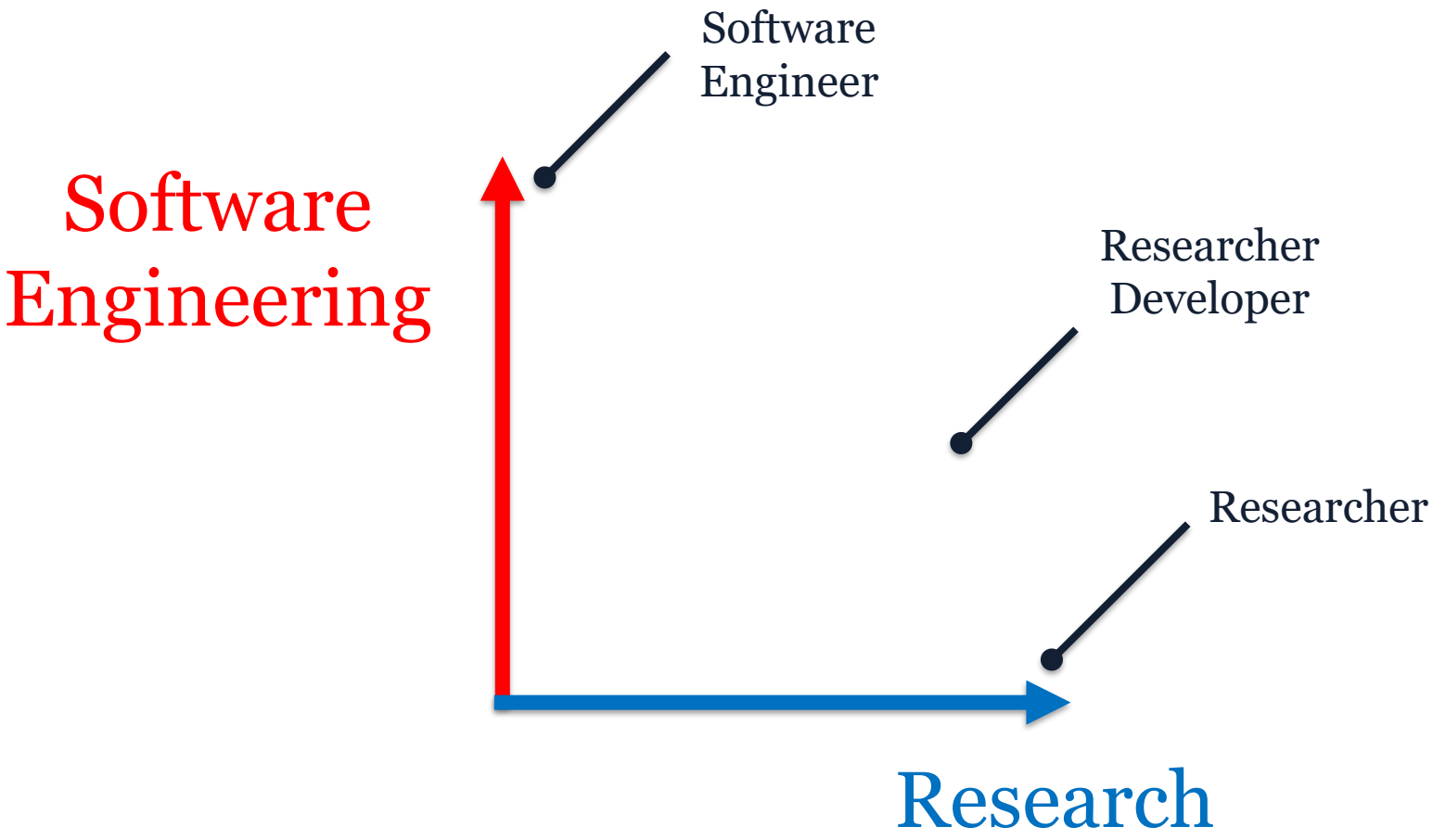
What is a Research Software Engineer?



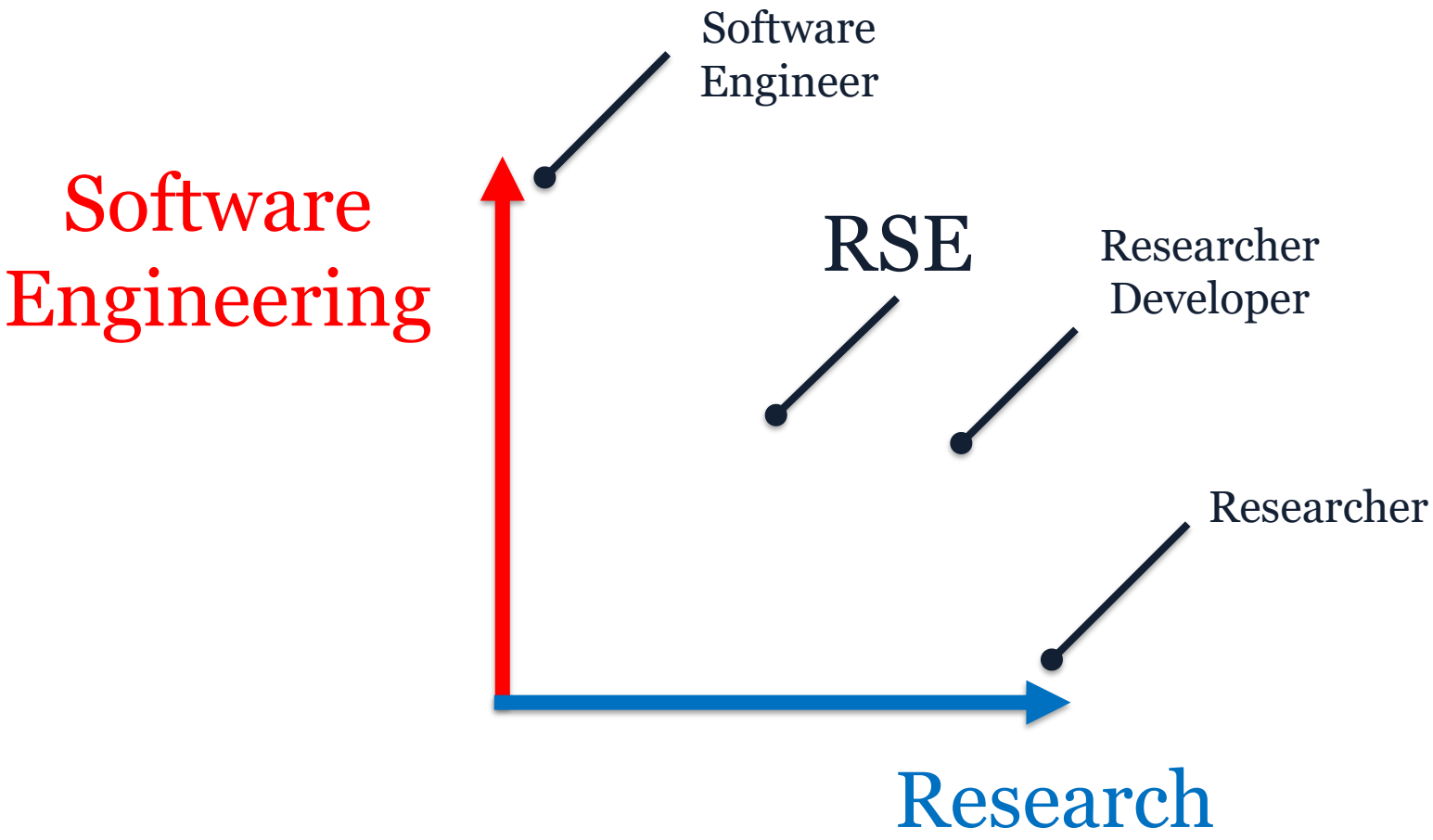
What is a Research Software Engineer?



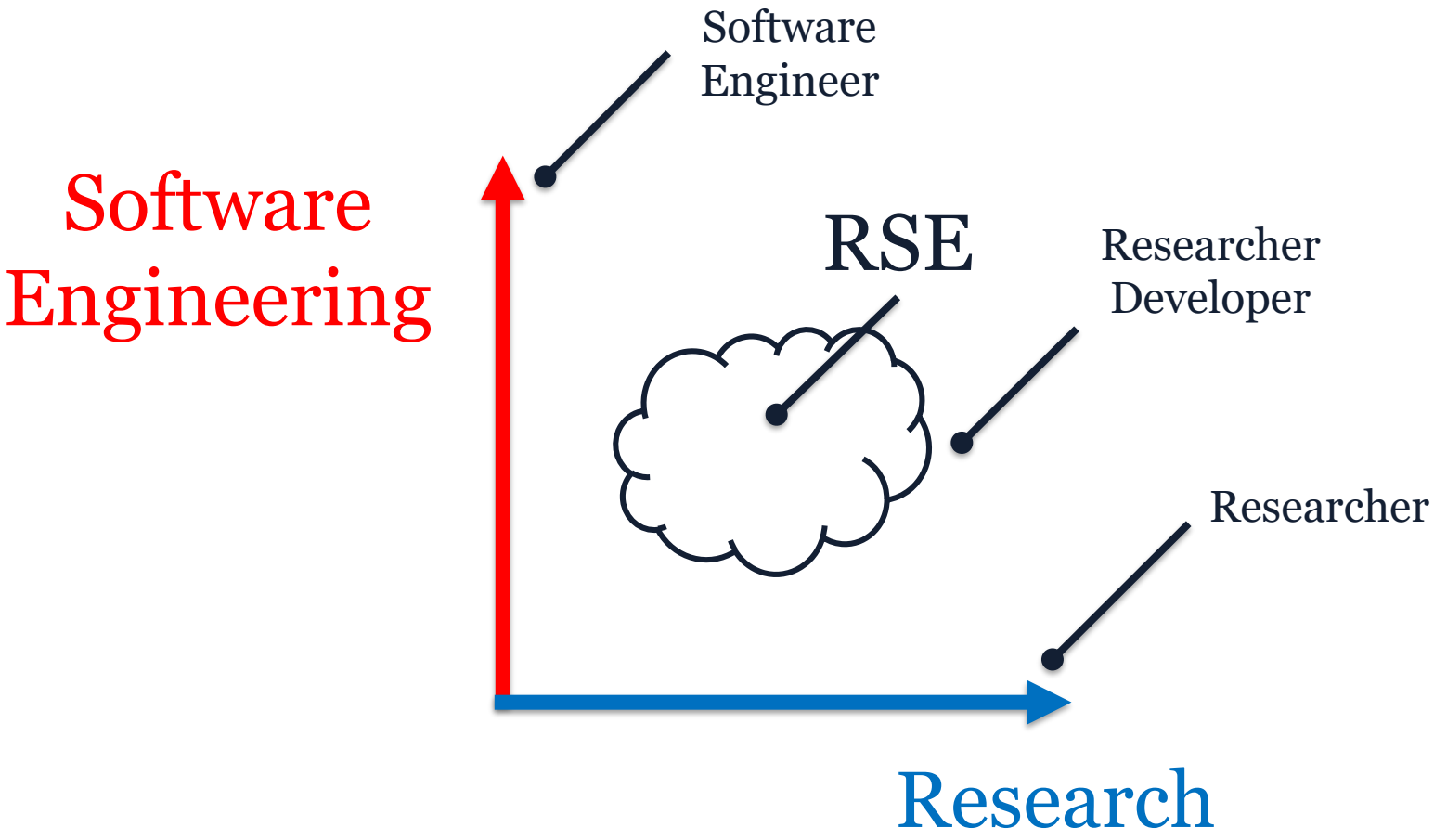
What is a Research Software Engineer?



What is a Research Software Engineer?



What is a Research Software Engineer?



https://danielskatzblog.wordpress.com/2019/07/12/super-rses-combining-research-and-service-in-three-dimensions-of-research-software-engineering/

Society of Research Software Engineering

An independent organization for the RSE movement

- Membership
- Voting rights
- International

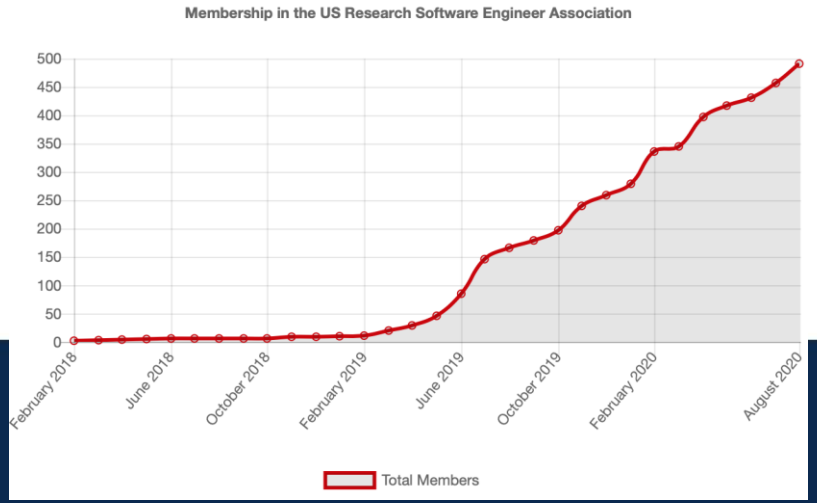
UK Registered Charity Number 1182455

- Same model as Royal Society of Chemistry and Institute of Physics, etc.

- https://www.society-rse.org/

US RSE Association

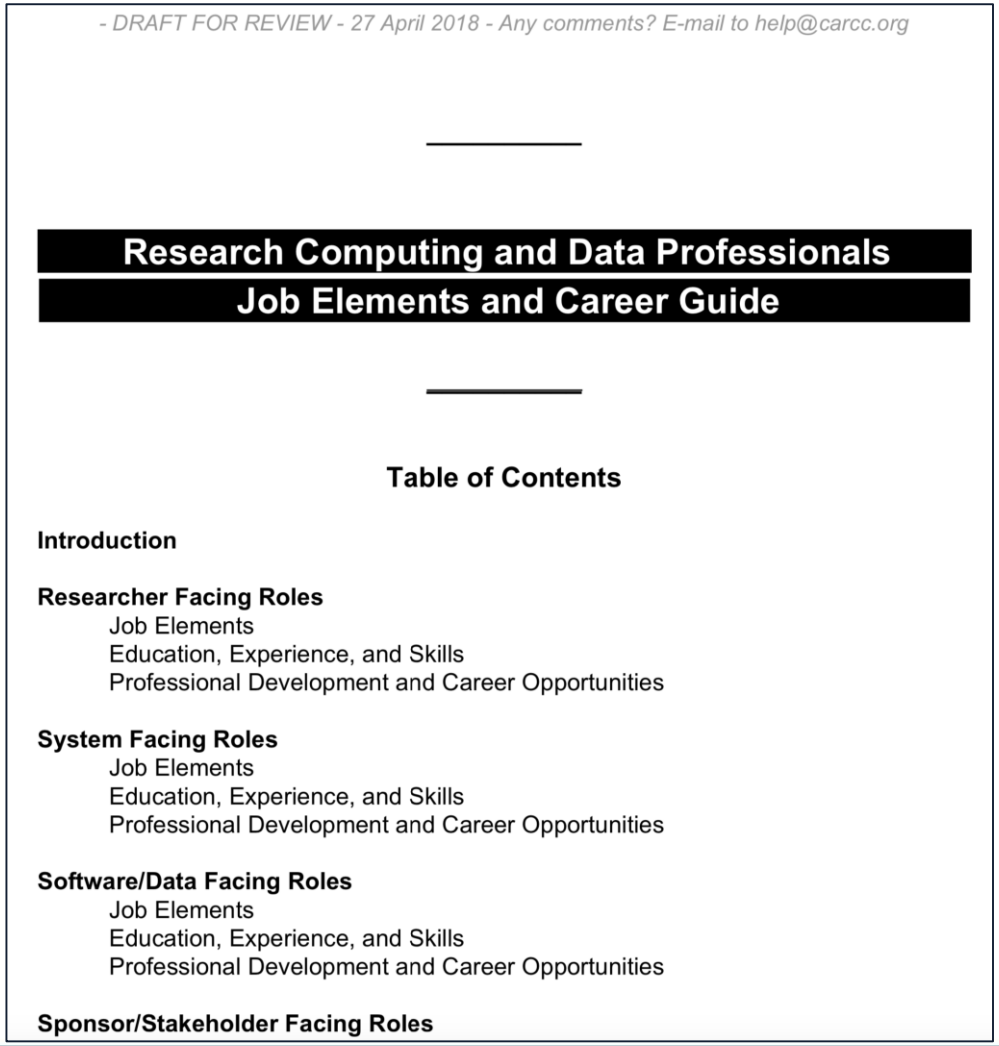
- Created with inspiration and support from Society of Research Software Engineering
- Focused on US members and US issues
  - Networking, jobs, careers, events, …
  - In academia, labs, industry, …
- Started in 2018, publicized in 2019
- BOF at PEARC 2019, panels & BOF at SC19, workshops at PEARC 2020 & SC20
- About 500 members
- https://us-rse.org



US RESEARCH SOFTWARE ENGINEER ASSOCIATION

Career paths in US universities

- Campus Research Computing Consortium (CaRCC)'s CI Workforce Development/Professionalization Committee held 2018 CI Professionalization Workshop
- One outcome: draft Research Computing and Data Professionals Job Elements and Career Guide
- Organized around "four facings" roles: researcher-facing, system-facing, software/data-facing, sponsor/stakeholder-facing
- For RSEs and data scientists (software/data facing), similar to the NCSA descriptions
- Now publicizing, aim to get universities to support and implement

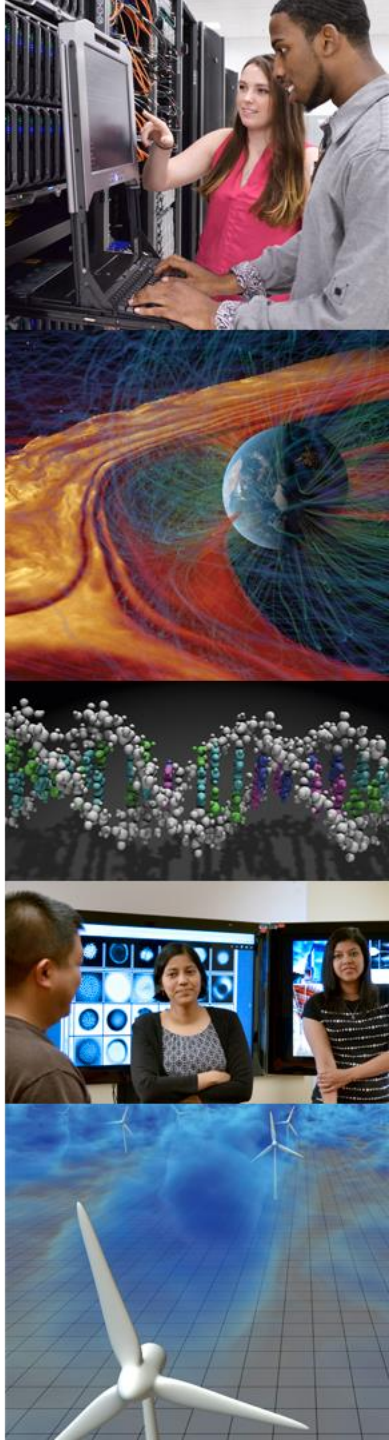


- DRAFT FOR REVIEW - 27 April 2018 - Any comments? E-mail to help@carcc.org

Research Computing and Data Professionals
Job Elements and Career Guide

Table of Contents

Research Software Group Models



ILLINOIS NCSA

Illinois NCSA: Software Directorate

ILLINOIS NCSA

- Organizational context
  - Research institute hosted at a university, outside of academic departments
- Team size
  - ~40
- Remit
  - Support individual needs; generalize those needs across projects; build software frameworks in response
- Funding model
  - Research grants (soft funding)
- Job security; career progression
  - Staff hired on indefinite contracts
  - Five grades of research programmer (RP): assistant, RP, senior, lead, principal

Notre Dame: Center for Research Computing

- Organizational context
  - Part of the broader Notre Dame Research organization at the university
- Team size
  - 24
- Remit
  - Provide software development support and services to researchers
- Funding model
  - Grants, contracts, and collaborations (soft funding)
- Job security; career progression
  - Staff hired on fixed term contracts
  - Three grades of Research Programmer, roughly equivalent to first three NCSA grades

Manchester: Research Software and Data Science

- Organizational context
  - IT Services, external to the Faculties
- Team size
  - 25
- Remit
  - Application support; training; short projects (weeks); research projects (months-years)
- Funding model
  - Application support and training: baseline funded (hard funding)
  - Projects: cost recovery from grants (soft funding), but underwritten by IT Services
- Job security; career progression
  - Staff hired on permanent contracts
  - Three grades of RSE: ~ graduate, postdoc, lecturer

MANCHESTER 1824
The University of Manchester

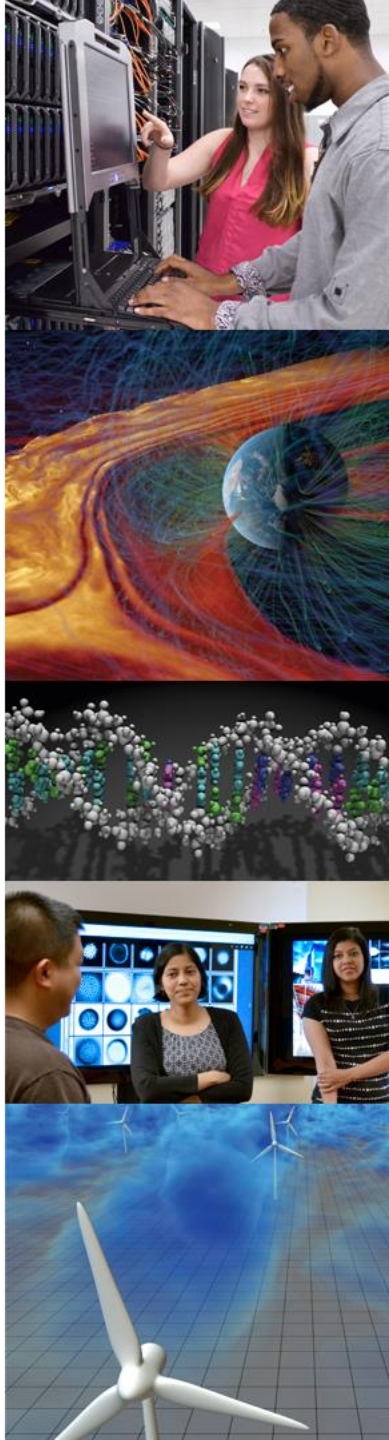
Agility

- Notre Dame is the most “agile”
  - Group divided into 4 teams, each with research programmers, a product owner, and a scrum master (shared across each two teams)
  - A team works on 1-6 projects, generally using 2-week sprints
- Illinois uses some agile methods for overall group
  - Staff work on multiple projects and in multiple teams, so twice weekly team standups help keep everyone focused on tasks and share knowledge
  - Projects can adapt some agile methods while recognizing staff are shared
- Manchester uses some agile processes within faculty-focused teams
  - Staff work on multiple projects in multiple teams; informal sprint model with regular feedback from PIs
  - Coordination between the faculty teams is via a weekly leaders' meeting

Line management & mentoring

- Manchester
  - Head & 6 area leads line-manage & mentor staff
  - 0.5 FTE institutional support for each
- Illinois
  - 2 co-leads and 6 group leaders manage and mentor staff
  - 0.2 FTE institutional support for each
  - Each project also has a senior developer, supported ~0.1 FTE on that project to mentor staff in that project
- Notre Dame
  - Line management provided by dual Scrum Master/Manager role within teams (~8:1 dev to manager ratio, 2:1 team to manager), then above, Assoc. Director of Cyberinfrastructure (head of software group)
  - Mentoring through technical leadership team composed of senior developers, with representation from each scrum team

Supporting
Research Software Development



ILLINOIS NCSA

High-level comparison

	Effect	Manchester	Illinois	Notre Dame
Institutional memory spanning projects, domains, time	+	✓	✓	✓
Flexible workforce with flexible skills	+	✓	✓	
Can support varying levels of effort, in particular portions of staff members	+	✓	✓	✓
Supports mentoring/coaching	+	✓	✓	✓
Reduced bus factor with regards to project core knowledge	+	✓		✓
Enables scalable growth to more rapidly take on new/large efforts	+			✓
Fosters reuse and sustainability of built software	+	✓	✓	
Costlier staff, however, better more maintainable code	±	✓	✓	✓
Perpetual precarious staffing allocations when solely reliant on grants	−	✓	✓	✓
Difference from status quo makes model hard to describe to funding agencies/PIs	−	✓	✓	✓
Not possible to fund permanent staff under some agencies	−	✓		
Risk of siloed staff after prolonged embedding in projects	−	✓	✓	
Lack of assimilation into domain if project is too short	−			✓
Projects today too often do not consider/reward reuse	−			✓

Overcoming varying finite duration funding streams

Overcoming varying finite duration funding streams

- We want to retain professional software development staff

Overcoming varying finite duration funding streams

- We want to retain professional software development staff
- Grant funding
  - Often less than 1 RSE FTE
    - And at NCSA and Manchester, a project's 1 RSE FTE should be split across 2 staff members to lower project risk and reduce project capture of staff
  - Shorter duration than staff careers

Overcoming varying finite duration funding streams

- We want to retain professional software development staff
- Grant funding
  - Often less than 1 RSE FTE
    - And at NCSA and Manchester, a project's 1 RSE FTE should be split across 2 staff members to lower project risk and reduce project capture of staff
  - Shorter duration than staff careers
- RSE groups tend towards a form of "Matrix Management"
  - Principle Investigator axis: changes over time
  - RSE group manager axis: fixed

Overcoming varying finite duration funding streams

- We want to retain professional software development staff
- Grant funding
  - Often less than 1 RSE FTE
    - And at NCSA and Manchester, a project's 1 RSE FTE should be split across 2 staff members to lower project risk and reduce project capture of staff
  - Shorter duration than staff careers
- RSE groups tend towards a form of "Matrix Management"
  - Principle Investigator axis: changes over time
    - Funded by research projects
  - RSE group manager axis: fixed

Overcoming varying finite duration funding streams

- We want to retain professional software development staff
- Grant funding
  - Often less than 1 RSE FTE
    - And at NCSA and Manchester, a project's 1 RSE FTE should be split across 2 staff members to lower project risk and reduce project capture of staff
  - Shorter duration than staff careers
- RSE groups tend towards a form of "Matrix Management"
  - Principle Investigator axis: changes over time
    - Funded by research projects
  - RSE group manager axis: fixed
    - Funded by … ? Overhead? Tax on projects? Institution?

Overcoming varying finite duration funding streams

- We want to retain professional software development staff
- Grant funding
  - Often less than 1 RSE FTE
    - And at NCSA and Manchester, a project's 1 RSE FTE should be split across 2 staff members to lower project risk and reduce project capture of staff
  - Shorter duration than staff careers
- RSE groups tend towards a form of "Matrix Management"
  - Principle Investigator axis: changes over time
    - Funded by research projects
  - RSE group manager axis: fixed
    - Funded by … ? Overhead? Tax on projects? Institution?
- How do we fund RSE groups to set aside time for growth?

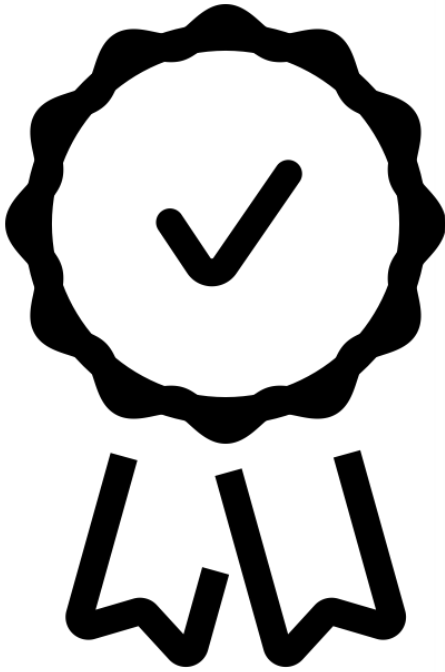
Overcoming varying finite duration funding streams

- We want to retain professional software development staff
- Grant funding
  - Often less than 1 RSE FTE
    - And at NCSA and Manchester, a project's 1 RSE FTE should be split across 2 staff members to lower project risk and reduce project capture of staff
  - Shorter duration than staff careers
- RSE groups tend towards a form of "Matrix Management"
  - Principle Investigator axis: changes over time
    - Funded by research projects
  - RSE group manager axis: fixed
    - Funded by … ? Overhead? Tax on projects? Institution?
- How do we fund RSE groups to set aside time for growth?
  - E.g., skill development, technology exploration, grant writing

Career paths (NCSA)

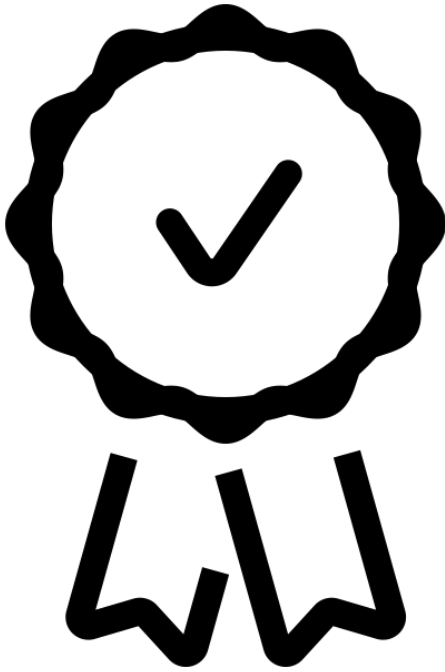
Title	Assistant Research Programmer	Research Programmer	Senior Research Programmer	Lead Research Programmer	Principal Research Programmer
Major Function	Develop software and tools to address scientific and other real world problems		Lead development activites and oversee/mentor groups of developers as a "player coach"		
Key Responsibilities	**Develop** novel software or **contribute** to existing software, both independently and/or in collaboration with team members, in support of a project's goals **Interact** with people in a wide range of educational, scientific, and engineering disciplines to create advanced software **Represent** the group at meetings, give presentations at conferences or other venues, and contribute to publications and grant proposals **Carry development** and **contribute** significantly towards the **reporting** on one or more projects **Track** technologies changes/research activity in relevant fields **Evaluate** the strengths and weaknesses between varieties of novel approaches to problems and communicate these to colleagues **Design** new approaches and techniques in resolving project specific problems using independent judgement **Oversee** and **develop** on a number of projects: **assist** in ensuring deliverables/deadlines are met, **contribute** to proposals, and **teach** others **Lead** and assume responsibility for activities of a project's development team/sub-team, ensure team/project goals and deadlines are met Oversee/steward **design** and development of several significant software code bases **Steward** funded projects				Leading the building, maintaining, and growth of a broad **active and sustainable community** around one or more codebases Unwavering **conflict resolution** towards maintaining teams/efforts Estabilishing **non-grant funded sources** for one or more codebases (e.g. service cost models, industry partnerships)
Decision Making Authority		Project developers and students			
Supervision	Senior/Lead/Principal Research Programmer, Group/Division Leads, Project Leads		Group/Division Leads, Project Leads		
Required Education, Training, and Experience	BA/BS in computer science. Alternative degree fields will be considered/accepted if accompanied by equivalent experience Some course level soft. dev. Experience	1-3 years software development experience	5+ years software development experience	10+ years software development experience	Demonstrated ability to create/lead sub-teams
	Knowledge of **programming,** ability to **follow research** publications, an ability to **write,** and an ability to be creative towards **open ended software development**				
Preferred Experience	Subject matter experts on one or more technologies Ability to establish a software development effort from the ground up (create software from scratch) Programming in one or more programming languages (e.g. Java, C++, Python, Scala, FORTRAN, Ruby, Javascript) Proficient in 3 or more programming languages with an ability to explain/decide why one would be utilized over another Web development (e.g. Server side scripting, client side frameworks, HTML5, CSS, REST) Databases (e.g. MySQL, MongoDB, PostgreSQL) Contributions towards research publications Experience in one or more of the following: Machine learning or data mining, Natural language processing, Geospatial data management and programming, Computer vision or graphics, HPC environments, cloud computing, and/or systems administration				

Best practices



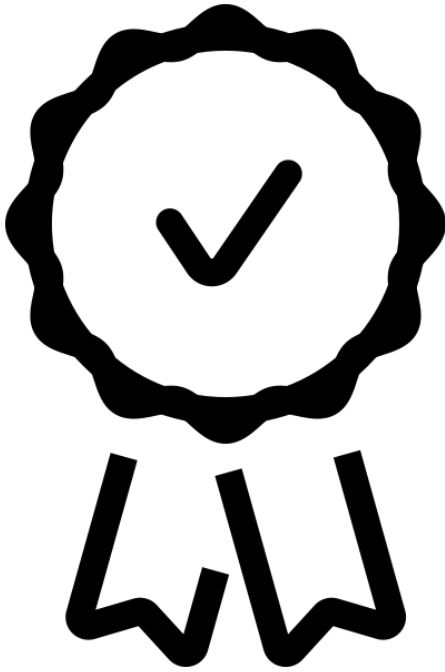
Best practices

- Research is a team endeavor; larger & more complex projects need a wider range of skills



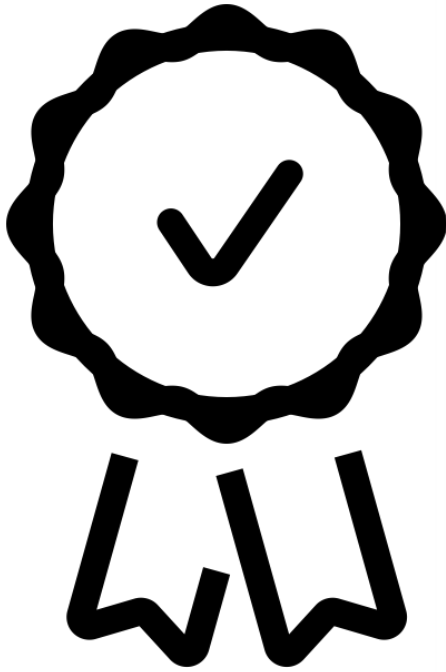
Best practices

- Research is a team endeavor; larger & more complex projects need a wider range of skills
- Professionals who write software & analyze data are essential
  - Can’t push these activities to students & post-docs, but need to work with them



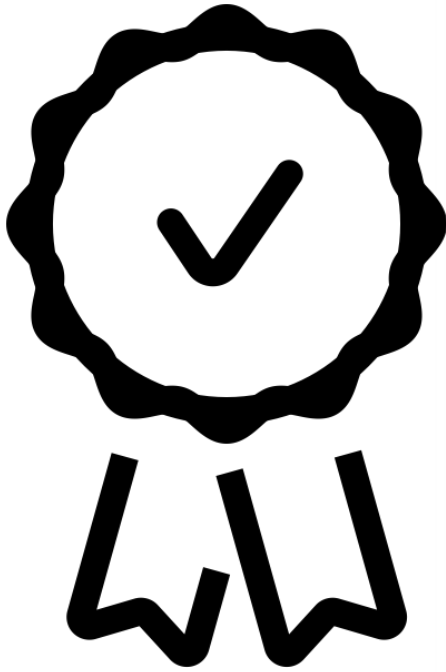
Best practices

- Research is a team endeavor; larger & more complex projects need a wider range of skills
- Professionals who write software & analyze data are essential
  - Can't push these activities to students & post-docs, but need to work with them
- RSE group members (senior developers and/or project managers) can bring more mature project management aspect/structure
  - Team organization (roles, responsibilities)
  - Work organization (WBS & timelines for deliverables)
  - Software organization (code repositories, issue trackers, wikis, messaging)
  - Coding practices (sprints, code reviews, TDD, integration testing, autobuilds)
  - → better, more sustainable code & more efficient group coordination

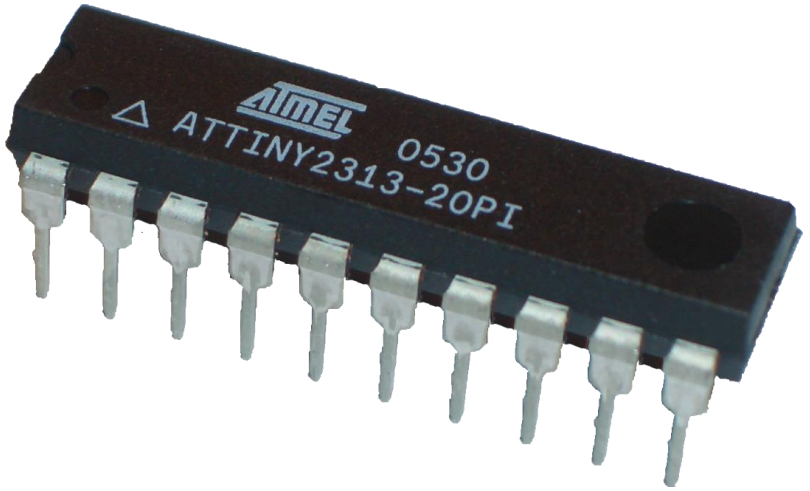


Best practices

- Research is a team endeavor; larger & more complex projects need a wider range of skills
- Professionals who write software & analyze data are essential
  - Can't push these activities to students & post-docs, but need to work with them
- RSE group members (senior developers and/or project managers) can bring more mature project management aspect/structure
  - Team organization (roles, responsibilities)
  - Work organization (WBS & timelines for deliverables)
  - Software organization (code repositories, issue trackers, wikis, messaging)
  - Coding practices (sprints, code reviews, TDD, integration testing, autobuilds)
  - → better, more sustainable code & more efficient group coordination
- These can be barriers in projects that focus on science questions

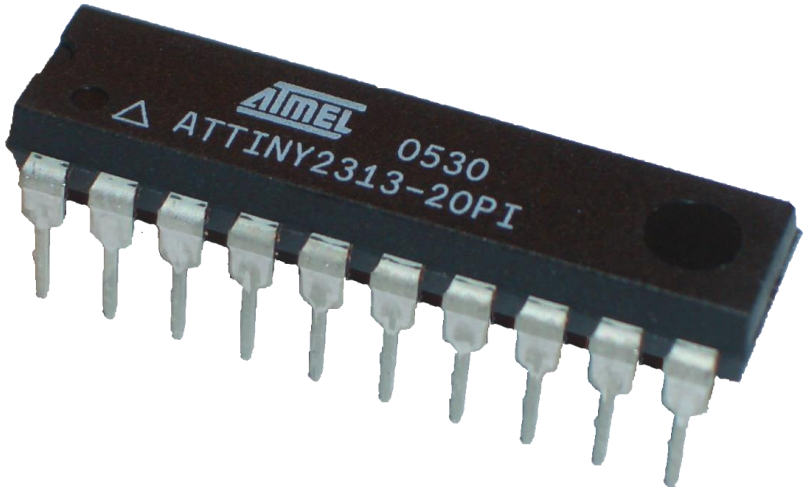


Institutional memory



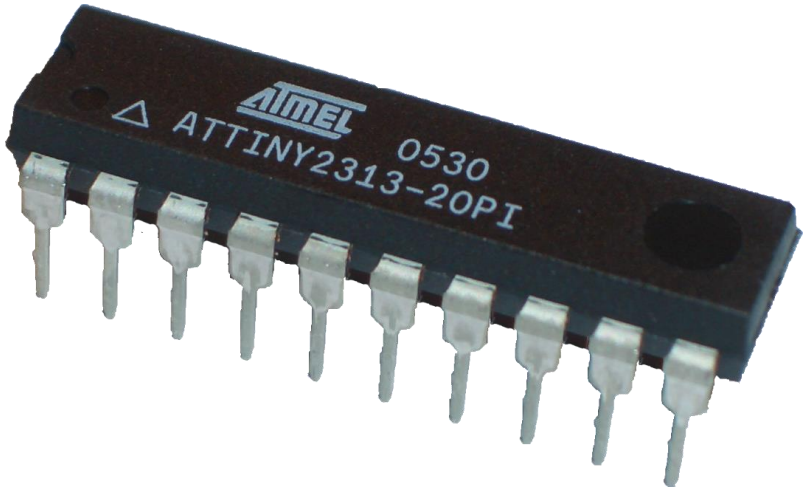
Institutional memory

- Research software is becoming more important, complex, and costly



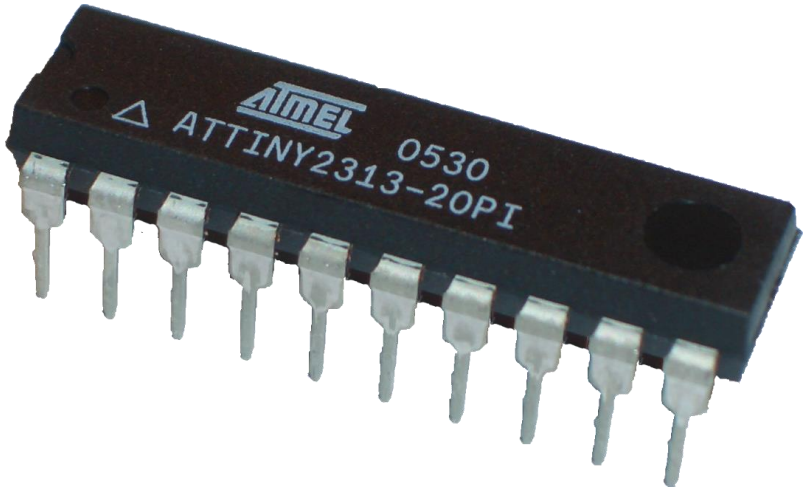
Institutional memory

- Research software is becoming more important, complex, and costly
- Expertise is valuable



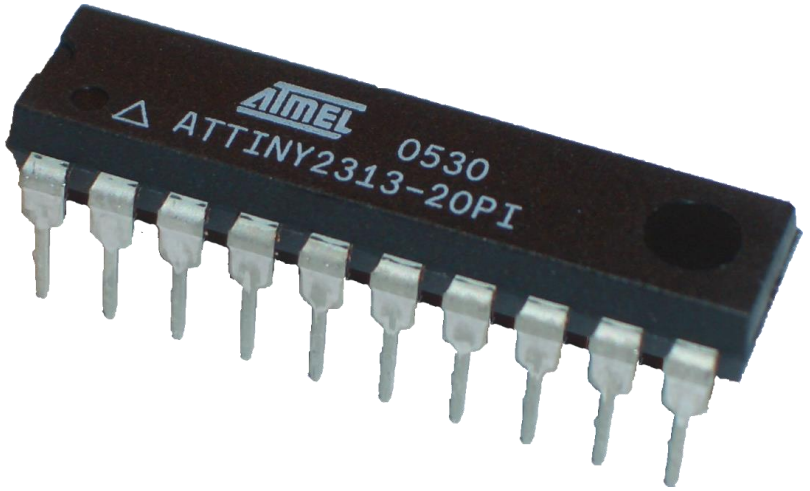
Institutional memory

- Research software is becoming more important, complex, and costly
- Expertise is valuable
- Students and postdocs pack up and move on



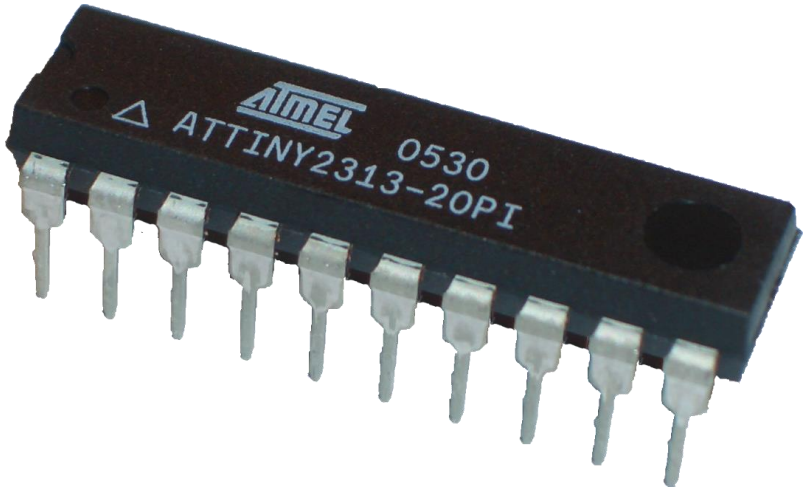
Institutional memory

- Research software is becoming more important, complex, and costly
- Expertise is valuable
- Students and postdocs pack up and move on
- RSE groups with longevity beyond any individual project, can act as “institutional memory”
  - Long-term/permanent contracts
  - Contracts not aligned to projects



Institutional memory

- Research software is becoming more important, complex, and costly
- Expertise is valuable
- Students and postdocs pack up and move on
- RSE groups with longevity beyond any individual project, can act as “institutional memory”
  - Long-term/permanent contracts
  - Contracts not aligned to projects



- RSEs are generally more mobile across domains than other research staff
  - Opportunities for translation of knowledge/artifacts across more users/communities

Changing scientific culture

Changing scientific culture

- Scientific research is about scientific discovery first and foremost

Changing scientific culture

- Scientific research is about scientific discovery first and foremost
- There's a long and deep culture as to what this means
  - Scientific method, students, paper publications, …

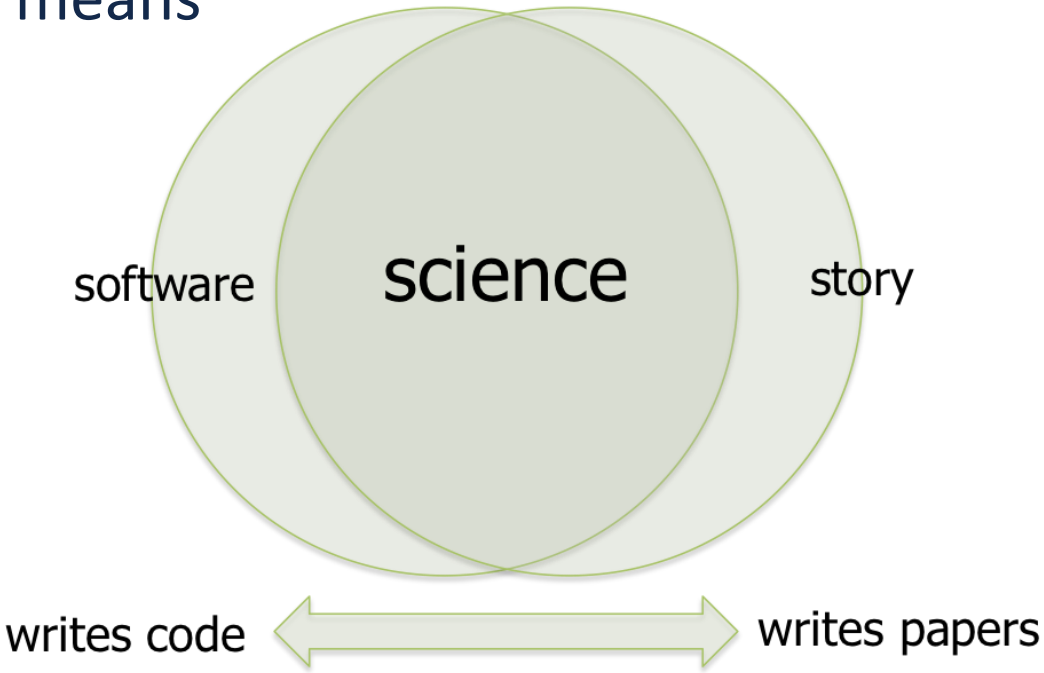
Changing scientific culture

- Scientific research is about scientific discovery first and foremost
- There's a long and deep culture as to what this means
  - Scientific method, students, paper publications, …
- We're trying to change that culture
  - Or at least adapt it to include technical aspects required by modern day science

Changing scientific culture

- Scientific research is about scientific discovery first and foremost
- There's a long and deep culture as to what this means
  - Scientific method, students, paper publications, …
- We're trying to change that culture
  - Or at least adapt it to include technical aspects required by modern day science

- Research is increasingly a team endeavor
  - As projects become larger and more complex, a wider range of skills is required

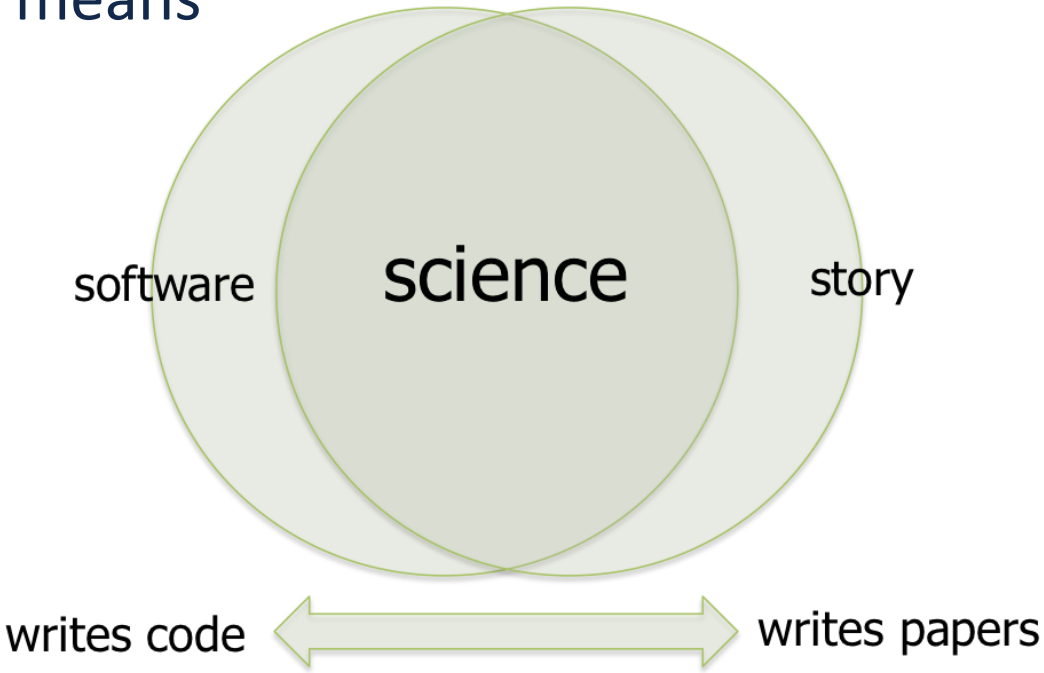


Jay, *et al*; Identifying the challenges of code/theory translation; 2017; 10.3897/rio.3.e13236

Changing scientific culture

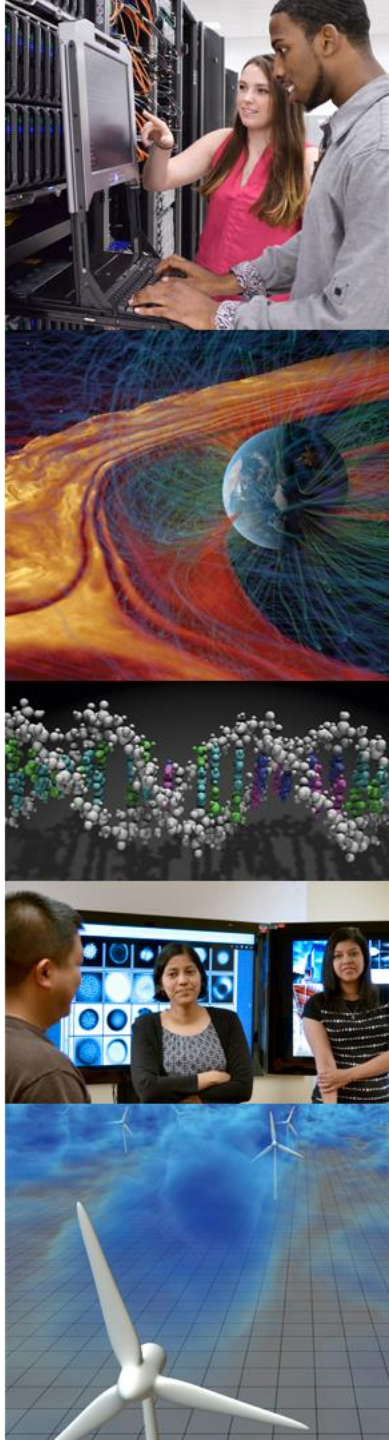
- Scientific research is about scientific discovery first and foremost
- There's a long and deep culture as to what this means
  - Scientific method, students, paper publications, …
- We're trying to change that culture
  - Or at least adapt it to include technical aspects required by modern day science

- Research is increasingly a team endeavor
  - As projects become larger and more complex, a wider range of skills is required
- Whether we write software or papers, ***we are all researchers***



Jay, *et al*; Identifying the challenges of code/theory translation; 2017; 10.3897/rio.3.e13236

Summary



ILLINOIS NCSA

Conclusions

Conclusions

- Software is becoming recognized as an *essential* part of research

Conclusions

- Software is becoming recognized as an *essential* part of research
- Support aspects of such software are not … yet
  - RSE staff, RSE groups
  - Models for sustaining, citing and crediting software

Conclusions

- Software is becoming recognized as an *essential* part of research
- Support aspects of such software are not … yet
  - RSE staff, RSE groups
  - Models for sustaining, citing and crediting software
- RSE-type groups are emerging globally to address these needs

Conclusions

- Software is becoming recognized as an *essential* part of research
- Support aspects of such software are not … yet
  - RSE staff, RSE groups
  - Models for sustaining, citing and crediting software
- RSE-type groups are emerging globally to address these needs
- RSEs and data scientists do not work in a vacuum
  - They are key to common research activities, such as hypothesis generation, study design, data analysis, and interpretation of results

Conclusions

- Software is becoming recognized as an *essential* part of research
- Support aspects of such software are not … yet
  - RSE staff, RSE groups
  - Models for sustaining, citing and crediting software
- RSE-type groups are emerging globally to address these needs
- RSEs and data scientists do not work in a vacuum
  - They are key to common research activities, such as hypothesis generation, study design, data analysis, and interpretation of results
- Efforts to make this well understood and accepted by the scientific community at large are ongoing

Acknowledgments

Acknowledgments

Paper: 10.1109/SE4Science.2019.00009

Acknowledgments

Paper: 10.1109/SE4Science.2019.00009

Preprint: https://arxiv.org/abs/1903.00732

The University of Manchester

Acknowledgments

Paper: 10.1109/SE4Science.2019.00009

Preprint: https://arxiv.org/abs/1903.00732

Thanks:

– Rob Haines, Kenton McHenry, Caleb Reinking

Acknowledgments

Paper: 10.1109/SE4Science.2019.00009

Preprint: https://arxiv.org/abs/1903.00732

Thanks:

- Rob Haines, Kenton McHenry, Caleb Reinking
- Caroline Jay, Carole Goble, Jeff Carver, Sandra Gesing, Ian Cosden, Ian Cottam, James Howison, Simon Hettrick, Neil Chue Hong, Jeremy Cohen, James Hetherington, Mark Turner, Alys Brett, Catherine Jones, Christopher Woods, Andy Turner, Claire Wyatt

"Any opinions, findings, conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the Networking and Information Technology Research and Development Program."

The Networking and Information Technology Research and Development (NITRD) Program

Mailing Address: NCO/NITRD, 2415 Eisenhower Avenue, Alexandria, VA 22314

Physical Address: 490 L'Enfant Plaza SW, Suite 8001, Washington, DC 20024, USA Tel: 202-459-9674, Fax: 202-459-9673, Email: nco@nitrd.gov, Website: https://www.nitrd.gov