FAIR and Open Research Software

Based on: W. Hasselbring, L. Carr, S. Hettrick, H. Packer, T. Tiropanis: "From FAIR Research Data toward FAIR and Open Research Software", it - Information Technology, 2020. DOI <u>https://doi.org/10.1515/itit-2019-0040</u>

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Software Sustainability Institute

Research Software

- Research software is software
 - that is employed in the scientific discovery process or
 - a research object itself.
- Computational science (also scientific computing) involves the development of research software
 - for model simulations and
 - data analytics

to understand natural systems answering questions that neither theory nor experiment alone are equipped to answer.



RSE

Agenda

1. Research Software

- Characteristics
- Mutual ignorance
- 2. Research Software Publishing
- 3. Open Science
 - For Computational Science
 - For Computer Science / Software Engineering: Artifact Evaluation
- 4. FAIR and Open Research Software
- 5. Summary & Outlook

Characteristics of Research Software

- Functional Requirements are not known up front
 - And often hard to comprehend without some PhD in science
- Verification and validation are difficult,
 - and strictly scientific
- Overly formal software **processes** restrict research



[Johanson & Hasselbring 2018]

Characteristics of Research Software

• Software quality requirements

- Jeffrey Carver and colleagues found that scientific software developers rank the following characteristics as the most important, in descending order [Carver et al. 2007]:
 - 1. functional (scientific) correctness,
 - 2. performance,
 - 3. portability, and
 - 4. maintainability.
- Research software in itself has no value
 - Not really true for community software
- Few scientists are **trained** in software engineering
 - Disregard of most modern software engineering methods and tools

SE for Computational Science ?

SOFTWARE ENGINEERING

Report on a conference sponsored by the NATO SCIENCE COMMITTEE Garmisch, Germany, 7th to 11th October 1968

Chairman: Professor Dr. F. L. Bauer Co-chairmen: Professor L. Bolliet, Dr. H. J. Helms

Editors: Peter Naur and Brian Randell

January 1969

Although much of the discussions were of a detailed technical nature, the report also contains sections reporting on discussions which will be of interest to a much wider audience. This holds for subjects like

- the problems of achieving sufficient reliability in the data systems which are becoming increasingly integrated into the central activities of modern society
- the difficulties of meeting schedules and specifications on large software projects
- the education of software (or data systems) engineers
- the highly controversial question of whether software should be priced separately from hardware.

Thus, while the report is of particular concern to the immediate users of computers and to computer manufacturers, many points may serve to enlighten and warn policy makers at all levels. Readers from the wider audience should note, however, that the conference was concentrating on the basic issues and key problems in the critical areas of software engineering. It therefore did not attempt to provide a balanced review of the total state of software, and tends to understress the achievements of the field.



In fact, a tremendously excited and enthusiastic atmosphere developed at the conference as participants came to realize the degree of common concern about what some were even willing to term the *"software crisis"*, and general agreement arose about the importance of trying to convince not just other colleagues, but also policy makers at all levels, of the seriousness of the problems that were being discussed.

[Randell 2018]

http://homepages.cs.ncl.ac.uk/brian.randell/NATO/index.html

Mutual Ignorance: Software Engineering

Software Engineering and Computer Science for Generality [Randell 2018]:

- "That **NATO** was the sponsor of this conference marks the relative **distance** of software engineering from computation in the academic context.
- The perception was that while **errors** in scientific data processing applications might be a 'hassle,' they are all in all **tolerable**.
- In contrast, failures in **mission-critical** military systems might cost lives and substantial amounts of money.
- Based on this attitude, software engineering—like computer science as a whole— aimed for generality in its methods, techniques, and processes and focused almost exclusively on **business** and **embedded** software.
- Because of this ideal of generality, the question of how specifically computational scientists should develop their software in a well-engineered way would probably have perplexed a software engineer, whose answer might have been:
 - 'Well, just like any other application software.' "

Mutual Ignorance: Computational Science

The Productivity Crisis in Computational Science

 As early scientific software was developed by small teams of scientists primarily for their own research, modularity, maintainability, and team coordination could often be neglected without a large impact.

The **Credibility Crisis** in Computational Science:

- **Climategate.** The scandal erupted after hackers leaked the email correspondence of scientists just before the 2009 United Nations Climate Change Conference.
- While the accusations that data was forged for this conference turned out to be unfounded, the emails uncovered a lack of programming skills among the researchers and exposed to a large public audience the widely applied practice in climate science of not releasing simulation code and data together with corresponding publications [Merali 2010].
- This in itself was, of course, enough to undermine the scientists' work, as the predictive capabilities of simulations are only as good as their code quality and their code was not even available for peer review—not to mention public review [Fuller and Millett 2011].

Modular Scientific Code



Contents lists available at ScienceDirect

Software Impacts

journal homepage: www.journals.elsevier.com/software-impacts

Eulerian-Lagrangian fluid dynamics platform: The ch4-project

Enrico Calzavarini

Highlights

- Ch4-project is a fluid dynamics code used in academia for the study of fundamental problems in fluid mechanics.
- It has contributed to the understanding of global scaling laws in non-ideal turbulent thermal convection.
- It has been used for the characterisation of statistical properties of bubbles and particles in developed turbulence.
- It is currently employed for a variety for research projects on inertial particle dynamics and convective melting.
- Its modular code structure allows for a low learning threshold and to easily implement new features.



Modular Scientific Code

[Calzavarini 2019]:

"A dream for principal investigators in this field is to not have to deal with different (and soon mutually incompatible) code versions for each project and junior researcher in his/her own group.

- In this respect an **object-oriented modular** code structure would be the ideal one,
 - but this makes the code less prone to modifications by the less experienced users.
- The choice made here is to rely on a systematic use of C language preprocessing directives and on a hierarchical naming convention in order to configure the desired simulation setting in a module-like fashion at compiling time."

So, SE for Computational Science

[Johanson & Hasselbring 2018]:

- Among the methods and techniques that software engineering can offer to computational science are
 - testing without test oracles,
 - modular software architectures, and
 - model-driven software engineering with domain-specific languages.
- This way, computational science may achieve maintainable, long-living software [Goltz et al., 2015; Reussner et al. 2019],
 - in particular for community software.

Software Engineering for Computational Science:

Past, Present, Future

Arne N. Johanson XING Marketing Solutions GmbH

Wilhelm Hasselbring Kiel University

Editors: Jeffrey Carver, carver@cs.ua.edu; Damian Rouson, damian@sourceryinstitute.org Despite the increasing importance of in silico experiments to the scientific discovery process, state-of-the-art software engineering practices are rarely adopted in computational science. To understand the underlying causes for this situation and to identify ways to improve it, we conducted a literature survey on software engineering practices in computational science. We identified 13 recurring key characteristics of scientific software

development that are the result of the nature of scientific challenges, the limitations of computers, and the cultural environment of scientific software development. Our findings allow us to point out shortcomings of existing approaches for bridging the gap between software engineering and computational science and to provide an outlook on promising research directions that could contribute to improving the current situation.



Teaching basic lab skills for research computing

- Programming / Coding
 - Fortran, C++, Python, R, etc
 - Using compilers, interpreters, editors, etc
- Using version control (git etc)
- Team coordination (GitHub, Gitlab, etc)
- Continuous integration (Jenkins, etc)
- https://software-carpentry.org/

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Computer



SOCIETY

COMPUTER

IEEE

Open Source Research Software

Wilhelm Hasselbring, Kiel University

Leslie Carr, University of Southampton

Simon Hettrick, Software Sustainability Institute and University of Southampton

Heather Packer and Thanassis Tiropanis, University of Southampton

For good scientific practice, research software should be open source. It should be both archived for reproducibility and actively maintained for reusability. are reused. To study the state of the art in this field, we analyzed research software publishing practices in computer and computational science and observed significant differences: computational science emphasizes reproducibility, while computer science emphasizes reuse.

SOFTWARE ENGINEERING FOR SUSTAINABLE RESEARCH SOFTWARE

Research Software Publishing

• Relating research software to research publications:



Research software is identified either by

- research publications that cite software repositories or
- software repositories that cite research publications.

Research Software Publishing Practices



[Hasselbring et al. 2020a]

Research Software Publishing Practices



[Hasselbring et al. 2020a]

Covered Research Areas

A first interesting observation is that our three data sets cover quite different research areas:

- The GitHub research software set is drawn mainly from the computational sciences, particularly the life sciences.
- The ACM research software set is dominated by software engineering, information systems, social and professional topics and human-centered computing.
- The arXiv research software set is dominated by computer science topics,
 - which is mainly composed of **AI topics** (computer vision, machine learning, computational linguistics, Figure 2d).

Sustainability of Research Software

- Research software publishing practices in computer science and in computational science show significant differences:
 - computational science emphasizes reproducibility,
 - computer science emphasizes reuse.

computer science publications



computational science publications

[Hasselbring et al. 2020a]

Sustainability of Research Software

- The **computer science** software repositories' lifespan is distributed with a median of 5 years.
 - Our hypothesis is that in computer science research, often commercial open-source software frameworks are employed.
 - These software frameworks are maintained over long times by employees of the associated companies.
- The **computational science** software repositories' lifespan has a distribution with a median lifespan of 15 days. A third of these repositories are live for less than 1 day.
 - Our hypothesis is that in computational science research, often the research software is only published when the corresponding paper has been published. The software is then not further maintained at GitHub, but at some private place as before (if it is further maintained at all).
- The arXiv repositories are somewhere in between with a median of 8 months lifespan. Furthermore, 75% of the arXiv repositories are live.
 - Our hypothesis is that the attitude of publishing as early as possible in parts of the artificial intelligence community also motivates the researchers to develop their research software openly from the start of research projects.

Categories of Research Software

We observe different categories and relationships between research publications and research software:

- Software as an output of research, collaboratively constructed and maintained through an active open source community.
- Software as an output of research, privately developed but published openly and abandoned after publication.
- Software itself as an **object** of study or analysis.
- Software that then leads to a **fork** (in GitHub) that is independently developed as a research output and published openly (if successful, it may be fed back into the original project via pull requests).
- Software used as a **tool or framework** to do the research.

Besides these relationships, software is cited as related work, background, or example.

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Reproducible Research in Computational Science

"Replication is the ultimate standard by which scientific claims are judged."





[Peng 2011]

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COMMUNICATIONS OF THE ACM | MARCH 2015 | VOL. 58 | NO. 3

DOI:10.1145/2658987

Shriram Krishnamurthi and Jan Vitek

Viewpoint The Real Software Crisis: Repeatability as a Core Value

Sharing experiences running artifact evaluation committees for five major conferences.

"Science advances faster when we can build on existing results, and when new ideas can easily be measured against the state of the art."

Repeatability, replicability & reproducibility

Several ACM SIGMOD, SIGPLAN, and SIGSOFT conferences have initiated **artifact evaluation** processes.

Example Experimental "Reproducibility Data" in Software Engineering

A Comparison of the Influence of Different Multi-Core Processors on the Runtime Overhead for Application-Level Monitoring

Jan Waller¹ and Wilhelm Hasselbring^{1,2}

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² SPEC Research Group, Steering Committee, Gainesville, VA, USA



[Waller and Hasselbring 2012]



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[Eichelberger et al. 2016]





²⁷ https://www.acm.org/publications/artifacts



Report: Artifact Evaluation Track

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CHARLES UNIVERSITY

Some numbers for ICPE 2018

- 59 submitted full research papers
- 14 accepted full research papers
- 6 submitted artifacts
- 2 accepted artifacts, evaluated as functional
- 0 accepted artifacts, evaluated as reusable
- It seems that repeatability and reproducibility of **performance** research results brings specific challenges
- However, it is also of particular importance to this field
- Is it worth making the effort?

IF I HAVE SEEN FURTHER, IT IS BY STANDING **ON THE SHOULDERS OF GIANTS**.

- ISAAC NEWTON

"Science advances faster when we can build on existing results, and when new ideas can easily be measured against the state of the art."

[Krishnamurthi & Vitek 2015]

Impact of Artifact Evaluation





Fig. 1. Average citation counts of AE and non-AE papers for conferences that used AE in 2013 to 2016 (conferences: VISSOFT, PPoPP, POPL, PLDI, PACT, OOPSLA, ISSTA, FSE, ECRTS, ECOOP, CGO, CAV).

[Childers & Chrysanthis 2017]

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Open Science for Research Software

- 1. Findable
 - Software citation
 - Domain-specific Metadata
- 2. Accessible
 - GitHub etc. for use and involvement
 - Zenodo etc. for archival
- 3. Interoperable
 - Obey to standards.
 - Proper interfaces in modular software
- 4. Reusable
 - Artifact evaluations support this.
 - Domain-specific languages may help with comprehensibility
 - Modular software architecture allow for reusing parts

Recommendations for FAIR Research Software [Hasselbring et al. 2020b]

FAIR Principle	Recommended Measure
Findability	Provide software metadata to improve software retrieval Use software citation to allow for proper reference and reward Employ research software observatories which may serve as retrieval service
Accessibility	Use software development platforms such as GitHub for code cloning Use repositories such as Zenodo to access archived software versions Use research software observatories as dedicated repository services
Interoperability	Provide proper interface definitions in modular software architectures Conform to established software standards Use software virtualization techniques for portability Participate in artifact evaluation processes to evaluate interoperability
Reusability	Use software development platforms such as GitHub for active involvement Build modular software architectures to allow for reusing parts of research software Use domain-specific languages for comprehensibility and modularity of research software Follow good software engineering practices to achieve high software quality Use software virtualization techniques such as Docker to support reusability across platforms Use software-as-a-service platforms such as BinderHub for immediate execution Use research software observatories for online analytics Participate in artifact evaluation processes to evaluate reusability

Modularization of Earth-system simulation software



Software Modularization





How to

- improve maintainability, stability, reusability, reproducibility, ... ?
- enable scalable execution in the Cloud?
- parallelize for high performance and exascale computing?
- test for higher quality?
- achieve higher flexibility?

Live Trace Visualization Tool ExplorViz

- Program- and system comprehension for software engineers
- Started as a Ph.D project in 2012
- Open Source from the beginning (Apache License, Version 2.0)
- Continuously extended over the years
- [Fittkau et al. 2013, 2015a-d, 2017; Krause et al. 2018, 2020; Zirkelbach et al. 2019, 2020; Hasselbring et al. 2020c]
- <u>https://ExplorViz.dev</u> <u>https://github.com/ExplorViz</u>
- See also Kieker [Hasselbring et al. 2020d] https://www.performance-symposium.org/2022/



3D Application Visualization with Exp|srViz



37

Summary & Outlook

- On the basis of an examination of the historical development of the relationship between software engineering and computational science (the **past**),
 - we identified key characteristics of scientific software development (the **present**).
- We examined attempts to bridge the gap in order to reveal the shortcomings of existing solutions and indicate further research directions (the possible **future**),
 - such as the use of domain-specific software engineering methods (OceanDSL project).
- Modularity is essential for maintainability, scalability and agility
 - also for reusability
 - also for testability
- Open Science also for Computer Science / Software Engineering research itself
 - "Eat your own dog food"
 - Follow the FAIR principles and publish research software open source



deRSE23 - Conference for Research Software Engineering in Germany

20-21 Feb 2023 Paderborn (Germany)

https://de-rse23.sciencesconf.org/

Contribution Deadline: Nov. 21st 2022

Associated to:



https://se-2023.gi.de/

Bionotes



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40

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Thanks!

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