Nachhaltige Softwareentwicklung für die Digitalisierung der Wissenschaft

Prof. Dr. Wilhelm (Willi) Hasselbring Software Engineering Group

http://se.informatik.uni-kiel.de/

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ozean der zukunft













Thema hier: Digitalisierung der Wissenschaft und Reproduzierbarkeit

https://doi.org/10.1109/MCSE.2018.108162940

[Johanson & Hasselbring 2018]



Software Engineering for Computational Science:

Past, Present, Future

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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.

With the constantly increasing capabilities of modern computers, in silico experiments are becoming more complex and playing a more important role in the scientific discovery process. As a consequence, the complexity and lifespan of scientific software are growing, as well as the necessity for its output to be reproducible and verifiable. This increases the importance of employing sound software engineering practices in the development of scientific software to guarantee reliable and accurate scientific results. However, surveys show that state-of-the-art software engineering methods are rarely adopted in computational science. ^{2,3} To understand the underlying causes for this and to identify ways to improve the current situation, in this article, we survey literature on software engineering in computational science and identify key characteristics that are unique to scientific software development.

To provide a basis for our survey, we outline the historical development of the relationship between the disciplines of software engineering and computational science. This relationship is, to a large extent, characterized by an isolation between the two disciplines that has resulted in

Computing in Science & Engineering March/April 2018

Copublished by the IEEE CS and the AIP 1521-9615/18/\$33 @2018 IEEE Genome Biology 2016 17:177 **DOI:** 10.1186/s13059-016-1044-7

Gene name errors are widespread in the scientific literature

Mark Ziemann¹, Yotam Eren^{1,2} and Assam El-Osta^{1,3*}

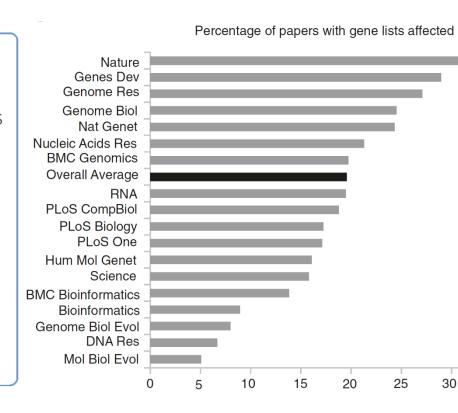
Abstract

The spreadsheet software Microsoft Excel, when used with default settings, is known to convert gene names to dates and floating-point numbers. A programmatic scan of leading genomics journals reveals that approximately one-fifth of papers with supplementary Excel gene lists contain erroneous gene name conversions.

Keywords: Microsoft Excel, Gene symbol, Supplementary data

Abbreviations: GEO, Gene Expression Omnibus;

JIF, journal impact factor



A Challenge for Arne's PhD research

Helmholtz Ocean System Science and Technology











Marine Biology Research

Publication details, including instructions for authors and subscription information: http://www.tandfonline.com/loi/smar20

Estimating the horizontal and temporal overlap of pelagic fish distribution in the Norwegian Sea using individual-based modelling

Kjell Rong Utne a & Geir Huse a

^a Institute of Marine Research, Bergen, Norway Version of record first published: 25 Apr 2012.

http://dx.doi.org/10.1080/17451000.2011.639781

- Utne & Huse provide an abstract (in part mathematical) description of their individual-based model, but:
 - We cannot reconstruct the implementation from the provided information
 - Sources for calibration data are named (some are unpublished) but again we cannot reconstruct the specific input data and parameters used.
- Without releasing the source code and the input/configuration data of the model, reproducibility of the results is hard or even impossible.

Science 2 December 2011:

Vol. 334 no. 6060 pp. 1226-1227

DOI: 10.1126/science.1213847

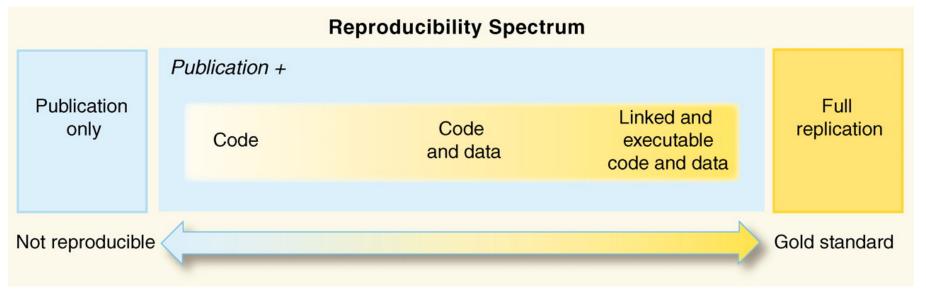


PERSPECTIVE

Reproducible Research in Computational Science

Roger D. Peng

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



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."

At least Repeatability, not necessarily reproducibility

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



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Artifact Review and Badging:

A variety of research communities have embraced the goal of reproducibility in experimental science. [more information]

Artifacts Evaluated - Functional



The artifacts associated with the research are found to be documented, consistent, complete, exercisable, and include appropriate evidence of verification and validation.

٩

Artifacts Evaluated - Reusable

The artifacts associated with the paper are of a quality that significantly exceeds minimal functionality.

Artifacts Available



Author-created artifacts relevant to this paper have been placed on a publically accessible archival repository.

Results Replicated



The main results of the paper have been obtained in a subsequent study by a person or team other than the authors, using, in part, artifacts provided by the author.

Results Reproduced



The main results of the paper have been independently obtained in a subsequent study by a person or team other than the authors, without the use of author-supplied artifacts.

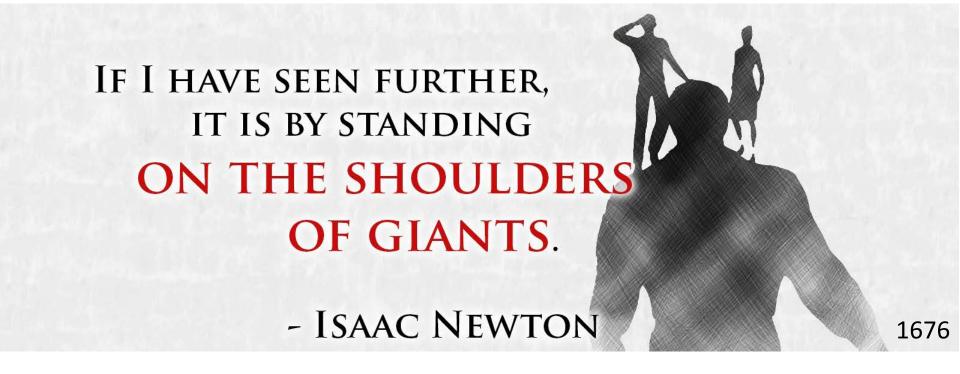
Artifact Evaluation Track

Chairs: Wilhelm Hasselbring (Kiel University) & Petr Tuma (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

Is it worth making the effort?



"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

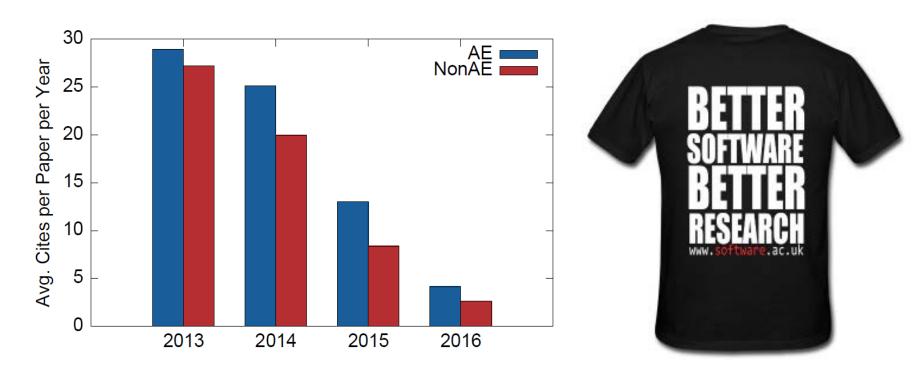


Fig. 1. Average citation counts of AE and non-AE papers for conferences that used AE in 2013 to 2016 (conferences: VISSOFT, PPoPP, POPL, PLDI, PACT, OOPSLA, ISSTA, FSE, ECRTS, ECOOP, CGO, CAV).



[Childers & Chrysanthis 2017]

What are we doing?

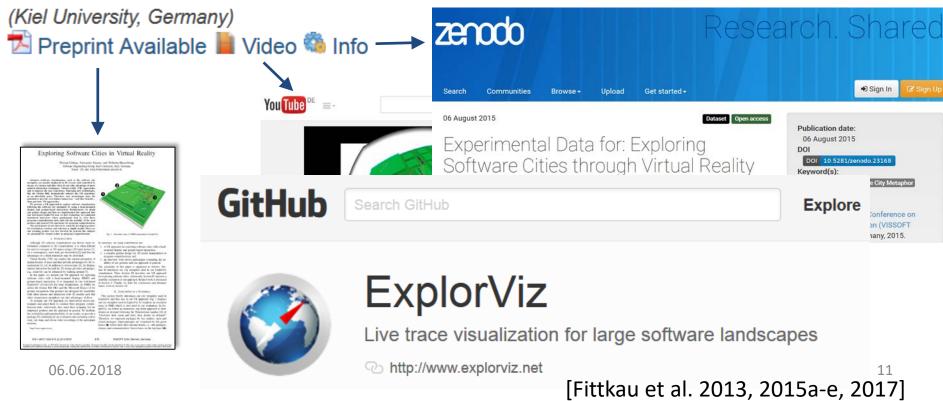
Hierarchical Software Landscape Visualization for System Comprehension: A Controlled Experiment

Florian Fittkau, Alexander Krause, and Wilhelm Hasselbring Software Engineering Group, Kiel University, Kiel, Germany Email: {ffi, akr, wha}@informatik.uni-kiel.de



Exploring Software Cities in Virtual Reality

Florian Fittkau, Alexander Krause, and Wilhelm Hasselbring

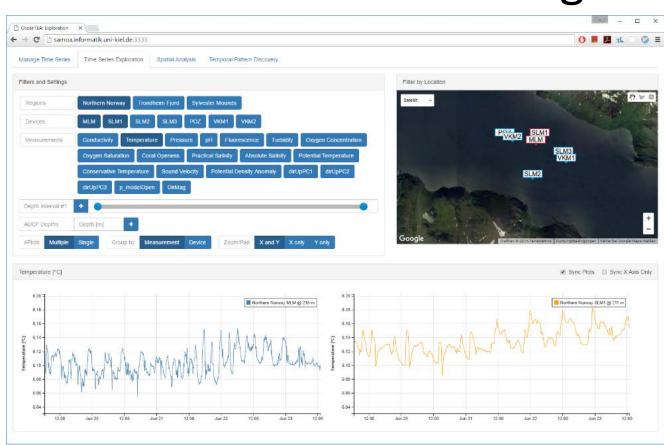


Cloud-Based Platform for Repeatable Ocean Observation Data Processing

OceanTEA

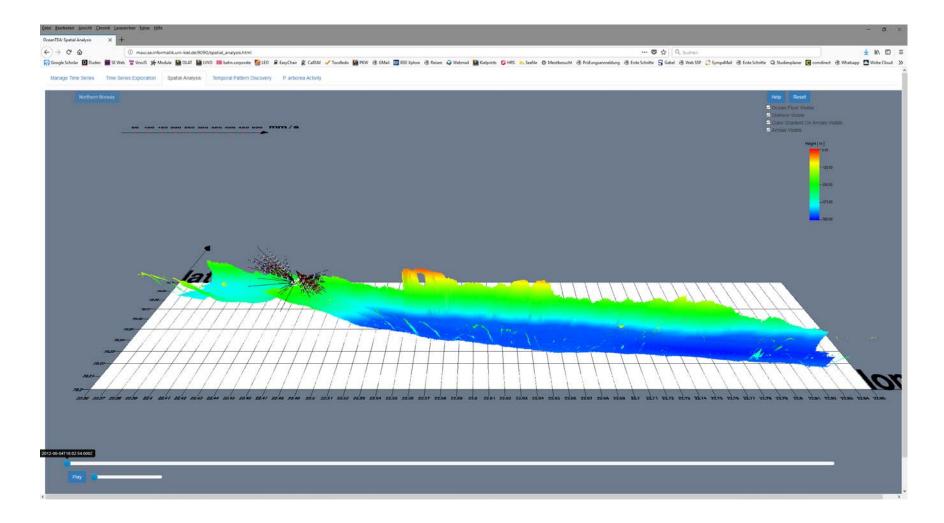






[Johanson et al. 2016a]

4D Spatial Analysis with OceanTEA

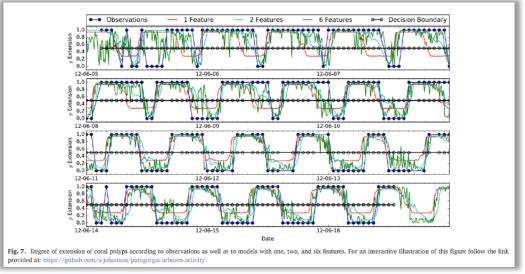


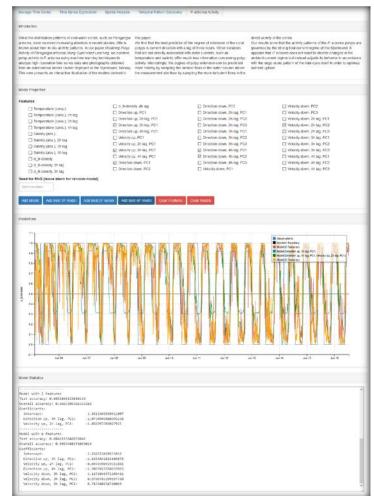


Machine Learning on Ocean Observation Data with OceanTEA

- Paper: http://dx.doi.org/10.1016/j.ecoinf.2017.02.007
- Source code: https://github.com/a-johanson/oceantea
- Software service with data: http://maui.se.informatik.uni-kiel.de:9090/
 (URL will change, refer to the GitHub repository for updates)



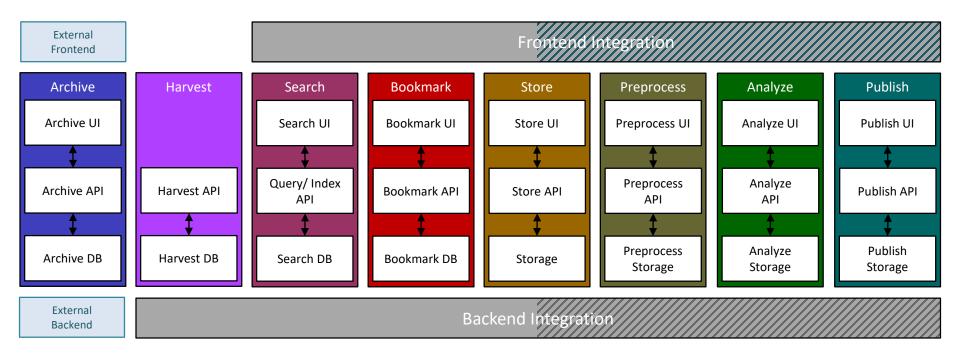








Generic Research Data Infrastructure







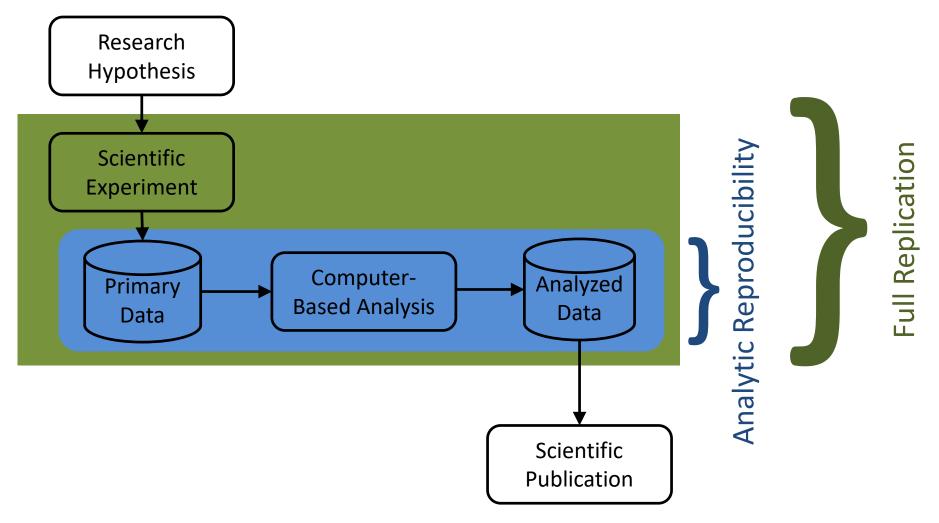






http://www.gerdi-project.de/ [Tavares de Sousa et al. 2018]

Analytic Reproducibility vs. Full Replication



Ausblick: Digtal Ocean 2018

https://digitalewochekiel.de/

digitale woche 2018





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