INNOVATING AT THE INTERSECTION SOFTWARE ENGINEERING RESEARCH FOR SCIENCE AND INDUSTRY

Prof. Dr. Michael Felderer





DLR Research Areas

11,000 Employees

54
Institutes and Facilities

35
Locations and
Offices

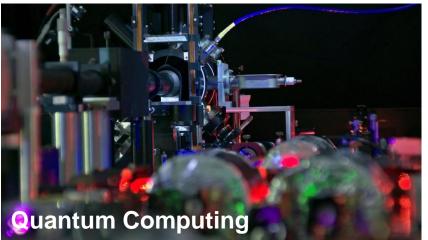


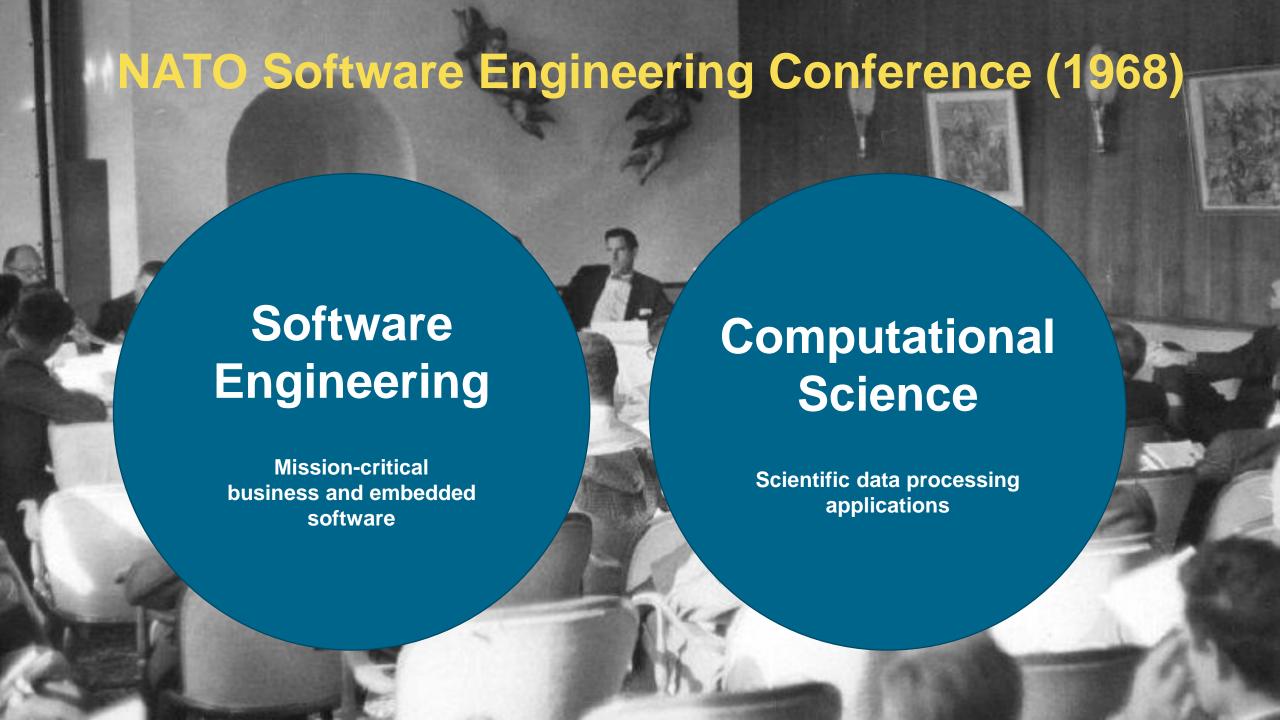






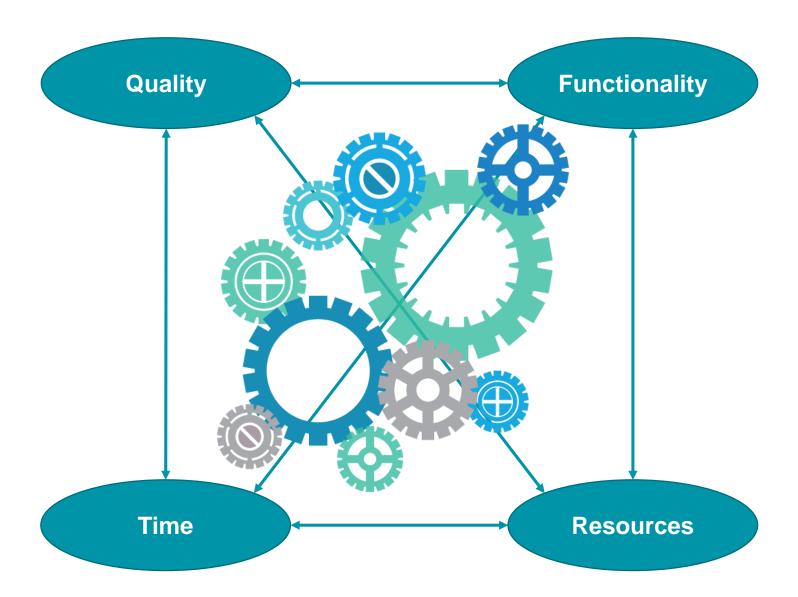
Security





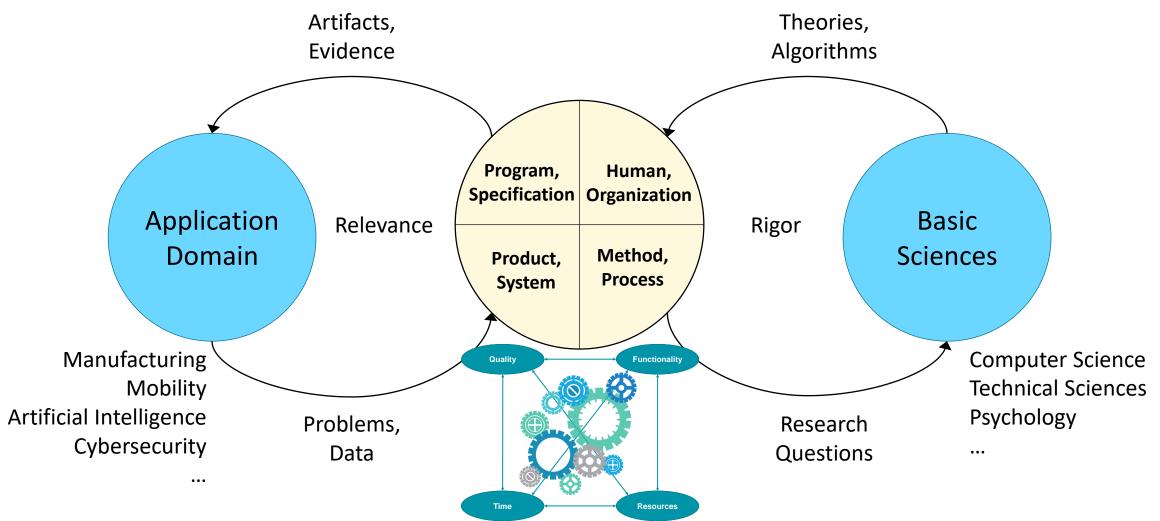
Trade Off in Software Engineering





Software Engineering Research



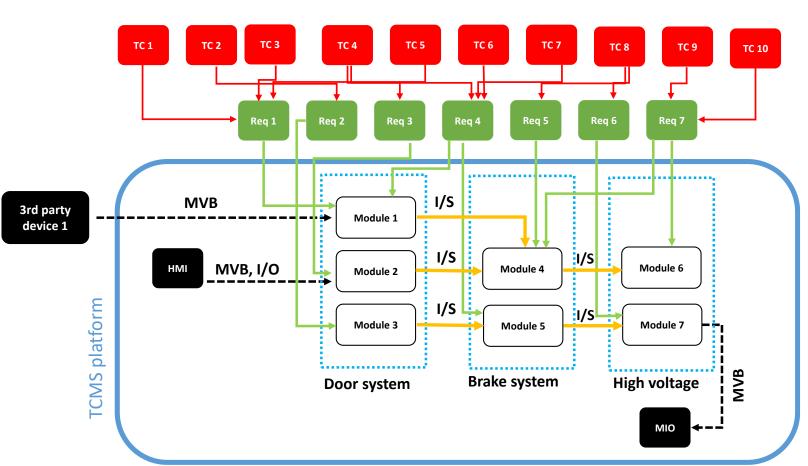


Application Domain: Mobility





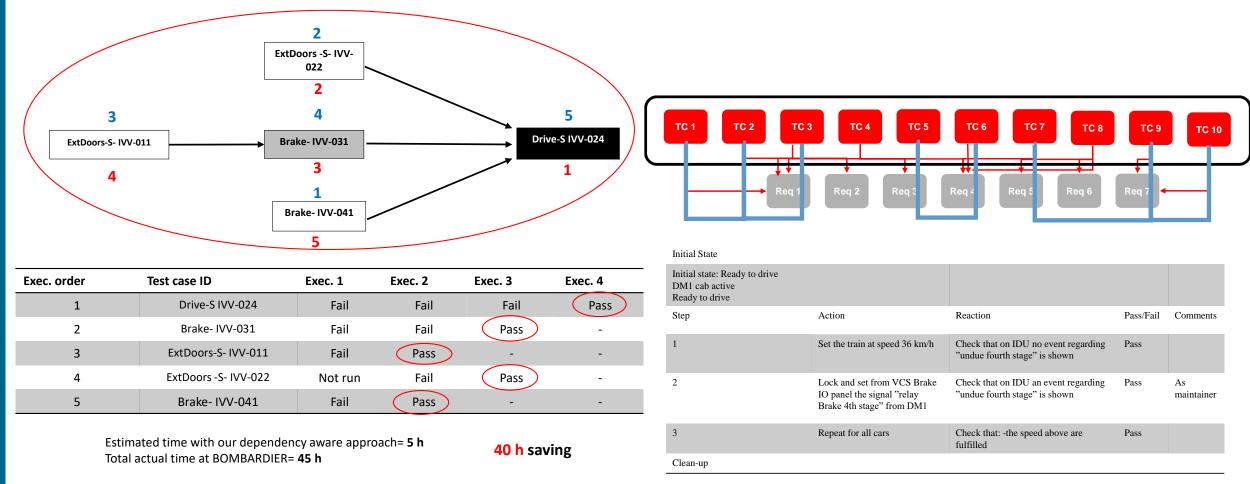
Bombardier BR 490 S-Bahn Hamburg



Established System and Software Development Processes and Artifacts

Problem: Automated Test Case Dependency Detection

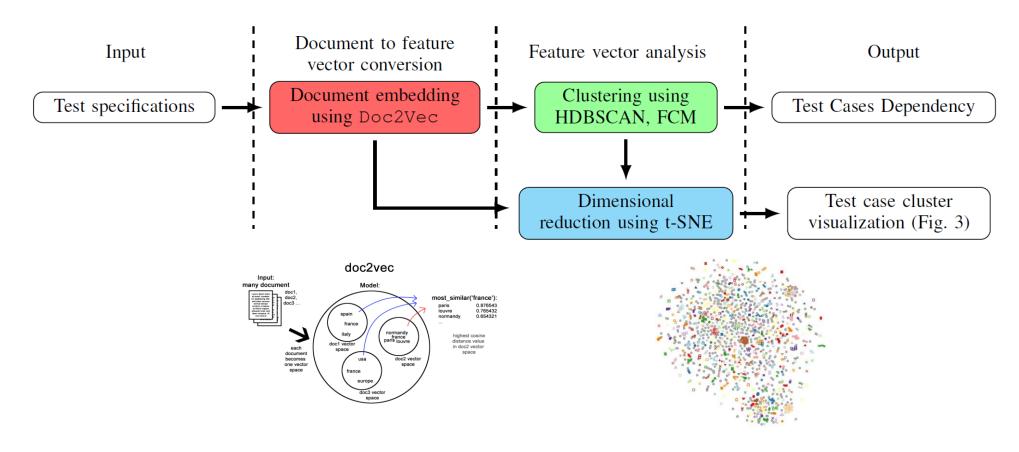




Improving Efficiency (Time) taking Quality and Resources into account

Approach: ML-Based Test Case Dependency Detection



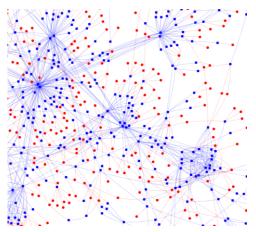


Tahvili, S., Hatvani, L., Felderer, M., Afzal, W., Bohlin, M. (2019) Automated Functional Dependency Detection Between Test Cases Using Doc2Vec and Clustering. AITest 2019.

Application of timely ML approaches to develop an automated test case dependency detection method

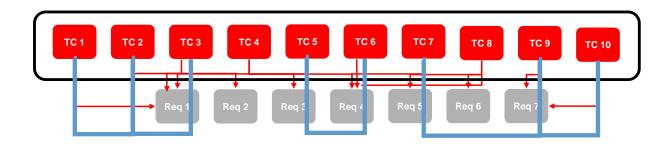
Evaluation and Implementation





Functional dependencies between approx. 4000 regs (blue) and approx.2000 tests (red) via artifact analysis and survey

	HDBSCAN				FCM				
\overline{D}	Precision	Recall	Accuracy	F1 Score	Precision	Recall	Accuracy	F1 Score	
2	0.9981	0.6113	0.8050	0.7582	0.8789	0.3871	0.6668	0.5375	
3	0.9959	0.2781	0.6385	0.4348	0.8275	0.2534	0.6002	0.3879	
4	0.9891	0.0958	0.5474	0.1747	0.8021	0.2127	0.5801	0.3363	
5	0.9804	0.0535	0.5262	0.1015	0.7845	0.1913	0.5694	0.3076	
6	0.9628	0.0286	0.5137	0.0555	0.7727	0.1772	0.5625	0.2883	
7	0.9476	0.0203	0.5096	0.0397	0.7653	0.1672	0.5580	0.2745	
8	0.9287	0.0139	0.5064	0.0273	0.7583	0.1589	0.5541	0.2627	
9	0.9104	0.0111	0.5050	0.0220	0.7477	0.1490	0.5494	0.2485	
10	0.8913	0.0089	0.5039	0.0176	0.7340	0.1373	0.5438	0.2313	



Empirically Evaluated Method is implemented in Industrial System Development Process

and fancy



Research software is a critical artifact that requires software engineering



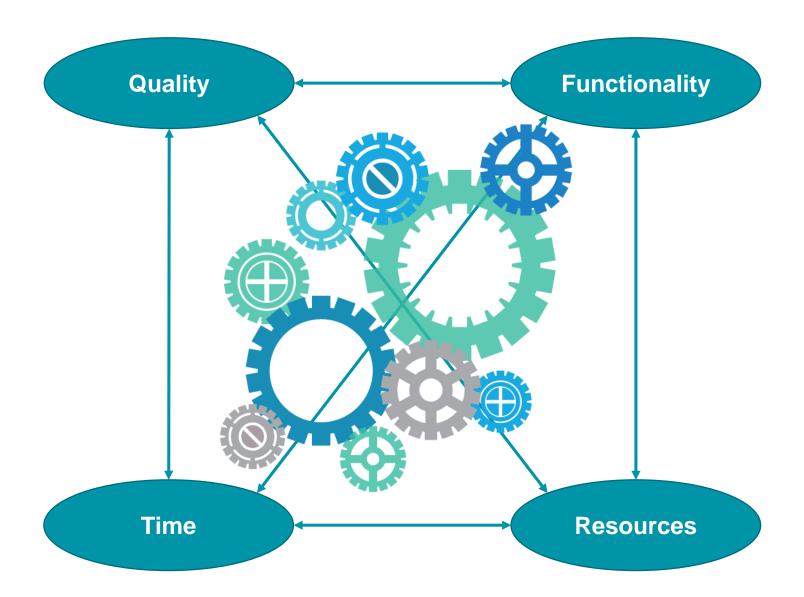


Well, just apply software engineering techniques ...



Guide to the Software Engineering Body of Knowledge



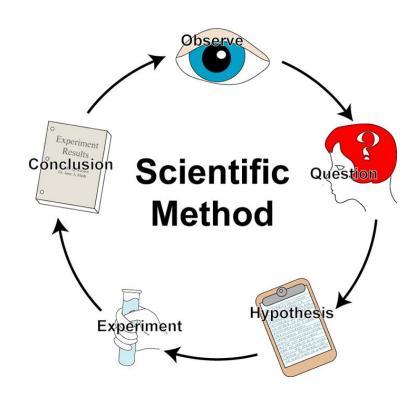




Functionality

Requirements Unknown

Research Related



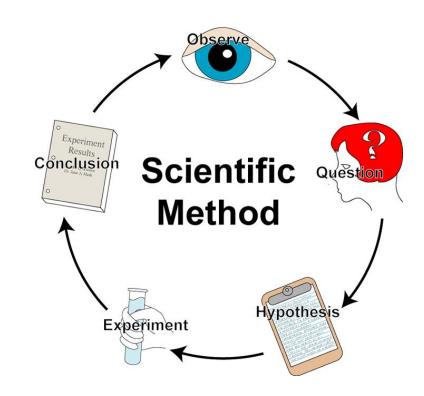
$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \hat{H} |\Psi\rangle$$



Verification is Difficult

FAIR Principles

Quality









Time-Limited Contracts

Dev Processes Restrict

Time



Practice

Training

Infrastructure

RSE Praxis

Bewährte Praktiken für die Entwicklung von Software im Forschungsalltag

RSE Training

Entwicklung von (R)SE-Fähigkeiten bei Forschenden und von R(SE)-Fähigkeiten bei Softwareentwickler/-innen

RSE Infrastruktur

Unterstützung bei Entwicklung, Betrieb und Wartung von Forschungssoftware



RSE Community



RSE Karrierepfade

Entwicklung von RSE als eigenes Berufsprofil und Karrierewegen für RSEs

Career Path

RSE Interessenvertretung

für institutionelle Unterstützung, Finanzierung und Anerkennung von RSE und RSEs

Advocacy

RSE Forschung

Analyse und Verbesserung (des Entwicklungsprozesses) von Forschungssoftware

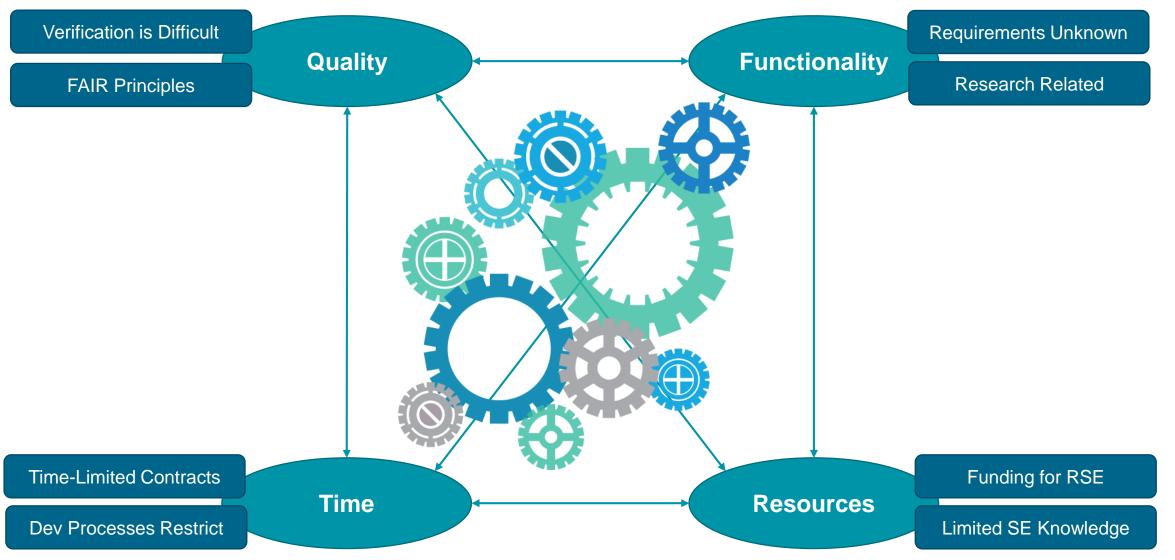
Research

Resources

Funding for RSE

Limited SE Knowledge





Always a Problem:

Joint Goals, Knowledge Gaps, Mutual Understanding





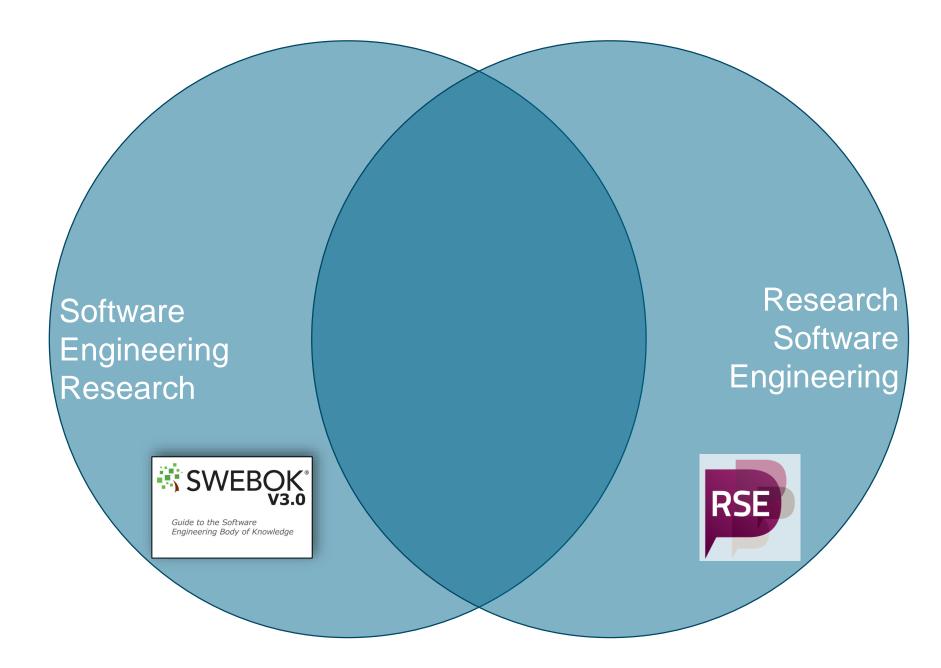
Patterns:

- Proper and active knowledge management (PAKM)
- Ensuring engagement and managing commitment (ENMC)
- Considering and understanding industry's needs, and giving explicit industry benefits (<u>CUIN</u>)
- Having mutual respect, understanding and appreciation (HMRU)
- Being Agile (BA)
- Working in (as) a team and involving the "right" practitioners (WTI)
- Considering and manage risks and limitations (CMRL)
- Researcher's on-site presence and access (ROSP)
- Following a proper research/data collection method (FPRM)
- Managing funding/recruiting/partnerships and contracting privacy (MFRP)
- Understanding the context, constraints and language (UCCL)
- Efficient research project management (ERPM)
- Conducting measurement/ assessment (CMA)
- Testing pilot solutions before using them in industry (TPS)
- Providing tool support for solutions (PTS)

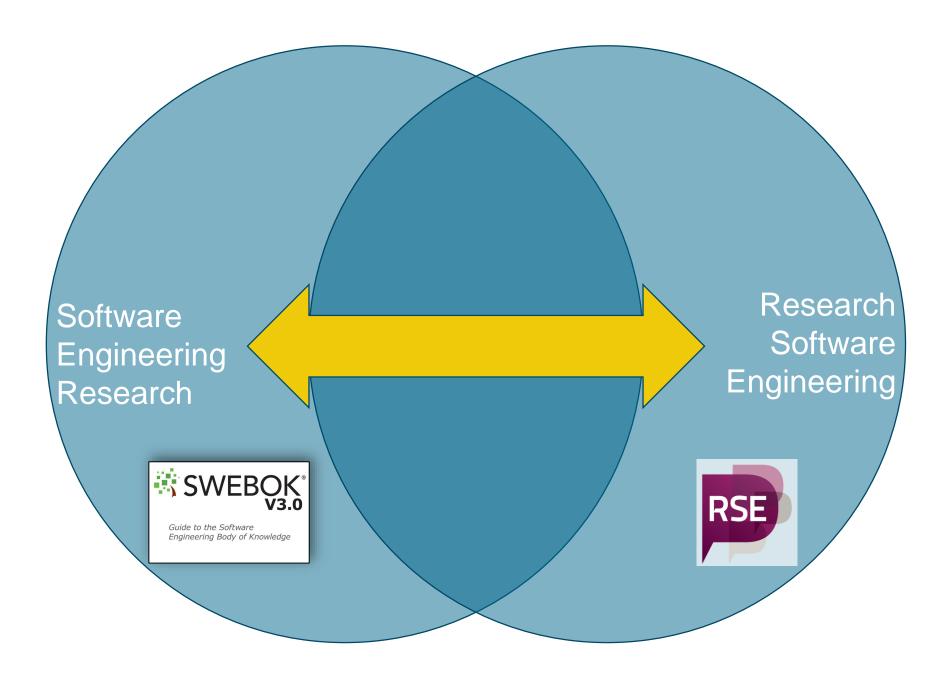
Anti-patterns:

- (Anti-pattern): Following self-centric approach (FSCA)
- Unstructured decision structures (UDS)
- Poor change management (PCM)
- Ignoring project, organizational, or product characteristics (IPOP)









The Most Important Thing: Talking To Each Other

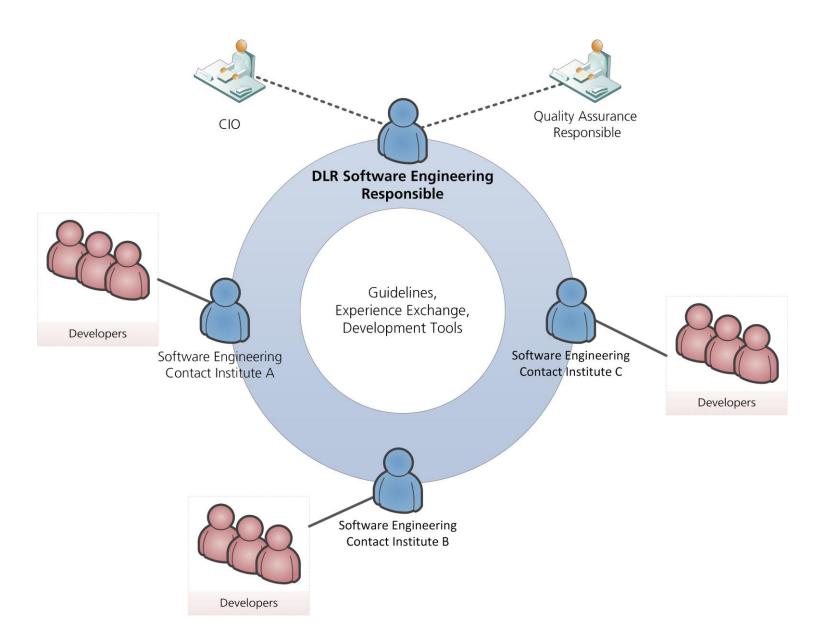




11:00	A short introduction to Nextflow: Bring your data science pipelines to the next level Marie	Large Language Models(LLMs in RSE Felipe Donose Aguirre	Schaarscl	lines	Researd Softwar working Medical Frank Lo	e Jon Data Deffler	BoFs Rese		SE: Architectures Sven Peldszus	SE: Reproducibil Matthias Tichy Vortragsraum 3. OG, Building
12:00	Latar et al.	Audimax-1, Building 30.95	SR A+B, Building 3	0.95	TBD, Bu 30.70		Semi	narroom, ing 30.96	Audimax-2, Building 30.95	30.51 (Bibliothek)
		11:00 - 12:30	11:00 - 12	:30	11:00 - 1	12:30	11:00	- 12:30	11:00 - 12:30	11:00 - 12:30
14:00	Aspects of Usability in RSE Jan Bernoth et al.	ML-assisted and more general data workflows Joerg Schaarschmi	Software arou Rese Software HPC Software Inga Martone		Commo around Resear Softwa Inga Uli	ch re usoy om	together software engineering researchers and research software engineers		SE: Testing Timo Kehrer	SE: Quality Assurance
15.00	Seminarroom, Building 30.96 14:00 - 15:30	Audimax-1, Building 30.9 14:00 - 15:30	5 Building 3	SR A+B, Building 30.95 14:00 - 15:30				Science @ SE25)	Audimax-2, Building 30.95 14:00 - 15:30	Bibliothek, Building 30.51 14:00 - 15:30
16:00	Joa Lower Sem 16:00 - 16 How to ac Nitai	Community in NFDI Stephan Janosch Audimax-1, Building 30.95	Open Source Community Building Inga Ulusoy SR A+B, Building 30.95	and Disco Resea Softw Berna Fritzso	are dette ch	BoFs: Challeng for RSEs Upper Seminari Building 30.96	S	SE: Softwa Evolution Wilhelm Hasselbring Audimax-2, Building 30.95	Requireme Andreas Vogelsang Vortragsraum Bibliothek, Building 30.51	Competition: Presentati Dr Hamideh Hajiabadi
		16:00 - 17:30	16:00 - 17:30		oom - 17	16:00 - 17:30		16:00 - 17:30	16:00 - 17:30	Seminar ro 16:00 - 17

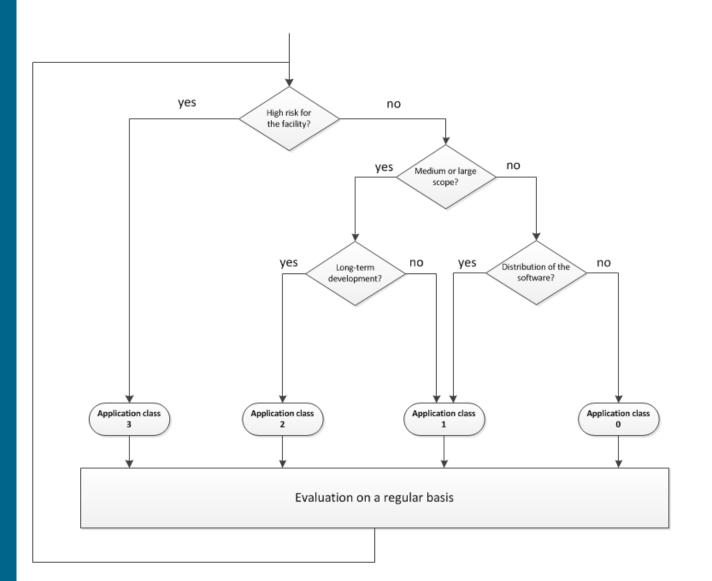
DLR Software Engineering Network





DLR Software Engineering Guidelines





Recommendation	from AC	Explanation
EAM.1: The problem definition is coordinated with all parties involved and documented. It describes the objectives, the purpose of the software, the essential requirements and the desired application class in a concise, understandable way.	1	It is important that the problem definition is early coordinated between the parties involved to prevent misunderstandings and incorrect developments. The problem definition also provides important hints for later use and further development.
EAM.2: Functional requirements are documented at least including a unique identifier, a description, the priority, the origin and the contact person.	2	Requirements must be clearly identifiable to refer to them during development and to trace them back to software changes (see the Change Management section). In addition, prioritisation helps to determine the order of implementation. Finally, information about the contact person and the origin is essential in case of questions.
EAM.3: The constraints are documented.	1	The relevant constraints (e.g., mandatory programming languages and frameworks, the opera-

Guidelines "Efficient Development of Research Software"





- 1. Executive Summary (for Decision Makers)
- 2. Introduction
- 3. Guidelines for Software Development
 - Categories of research software
 - Minimum requirements for core competencies
 - Development processes
 - Projekt planning
 - Methodical Foundations
- 4. Licensing and usage (Legal safeguarding)
- 5. Support Services
 - Technical (Git, Overleaf, FDM-Tools)
 - Personel through trained RSEs

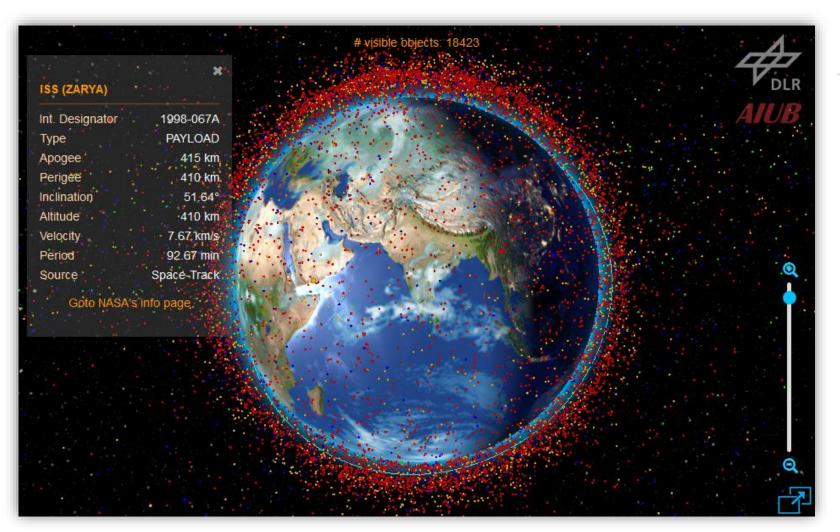
Research software is created during the research process or for a research purpose

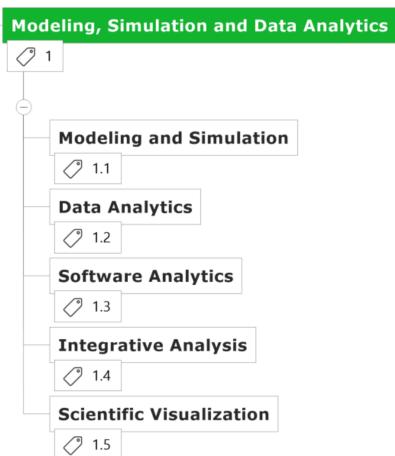




Modeling, Simulation and Data Analytics

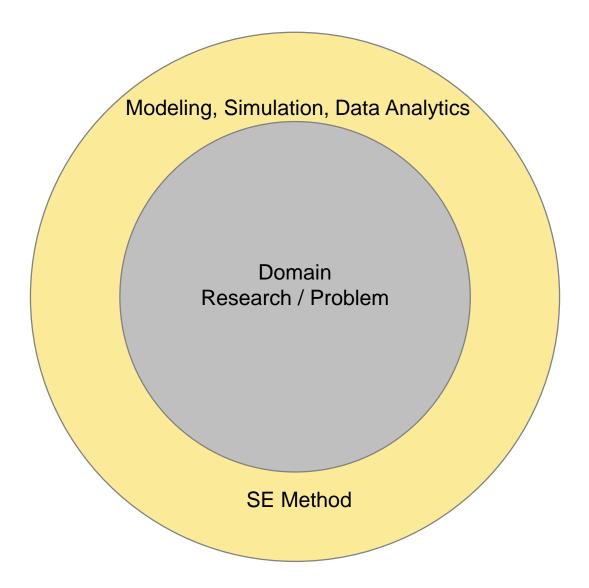


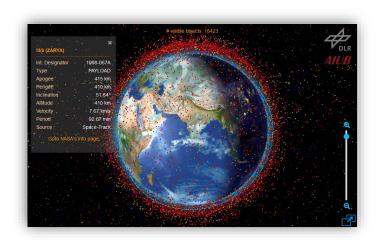


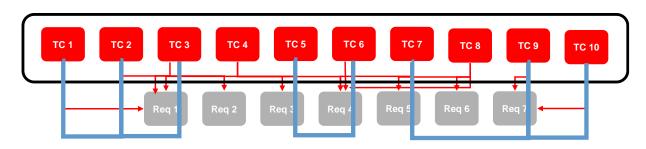


Software in Research and SE





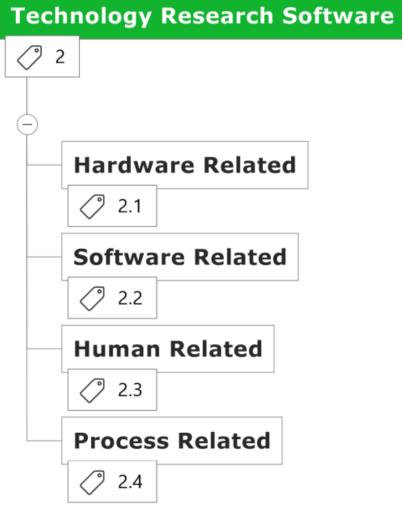




Technology Research Software (1/2)







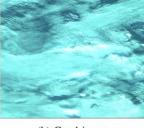
Technology Research Software (2/2)







(a) Good image



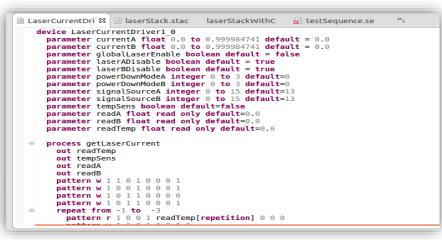
(b) Good image



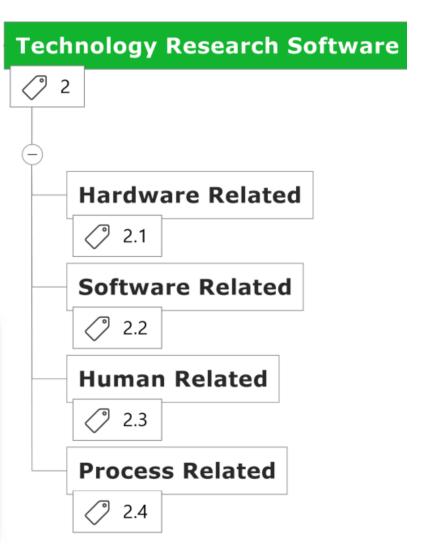
(c) Bad image (high exposure)



(d) Bad image (too dark)

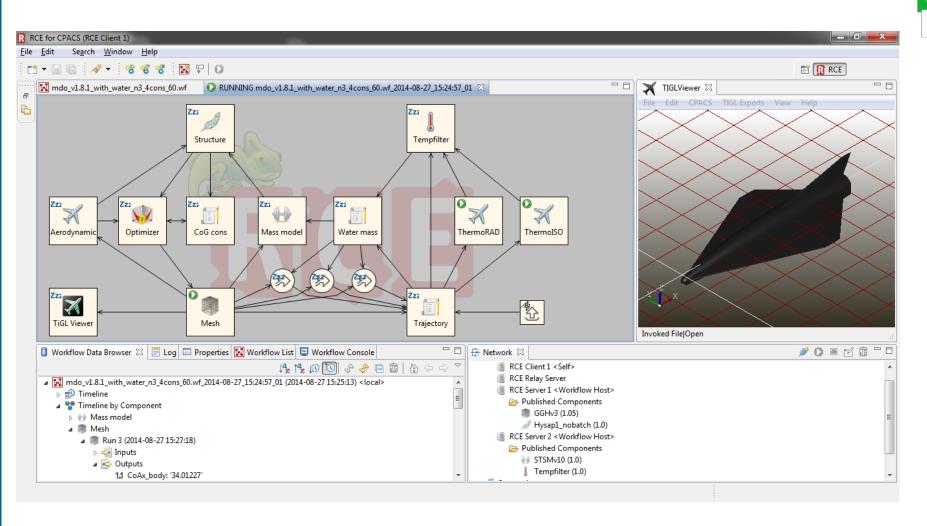


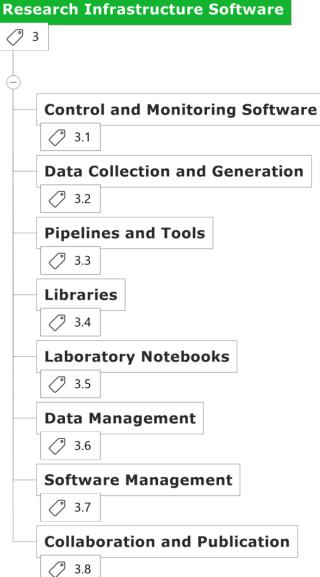
ScOSA (Scalable On-board Computing for Space Avionics)
https://www.dlr.de/en/sc/research-transfer/projects/scosa-flight-experiment



Research Infrastructure Software (1/2)

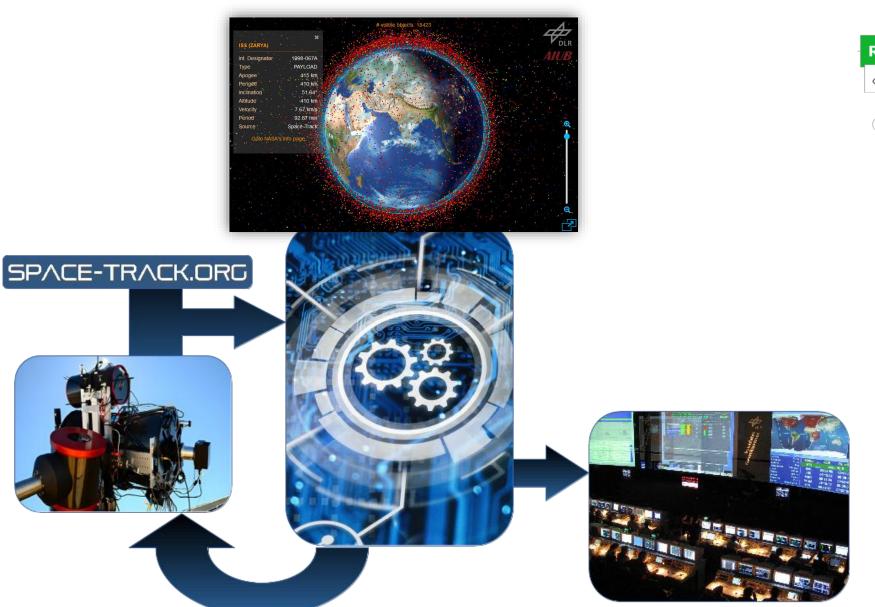


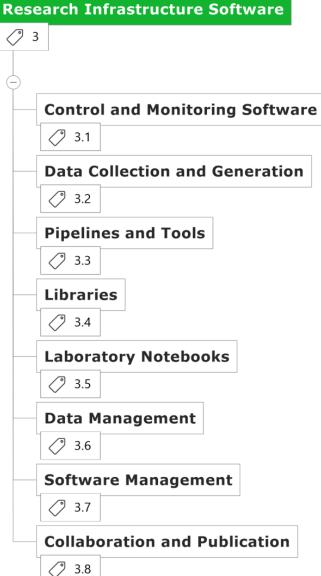




Research Infrastructure Software (2/2)

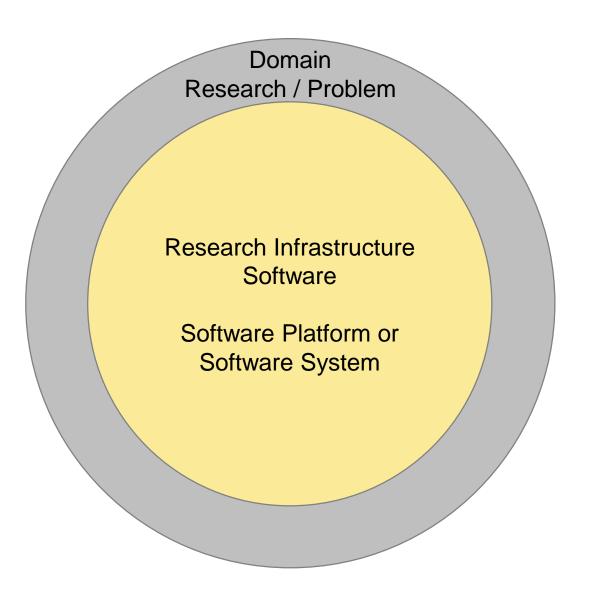


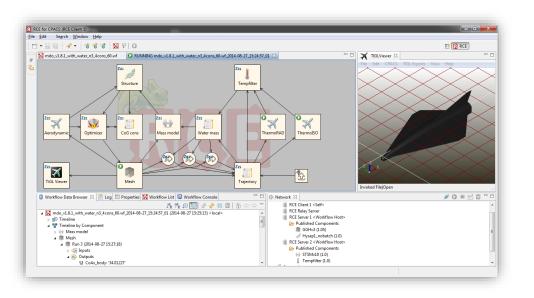




Software in Research and SE







Research Software in Space (TRL 9)













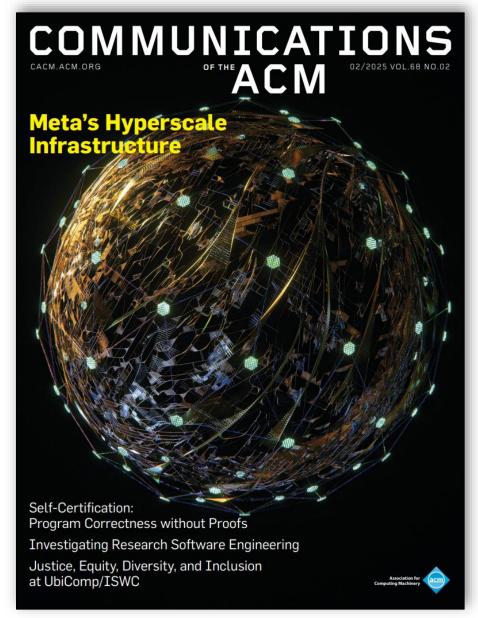


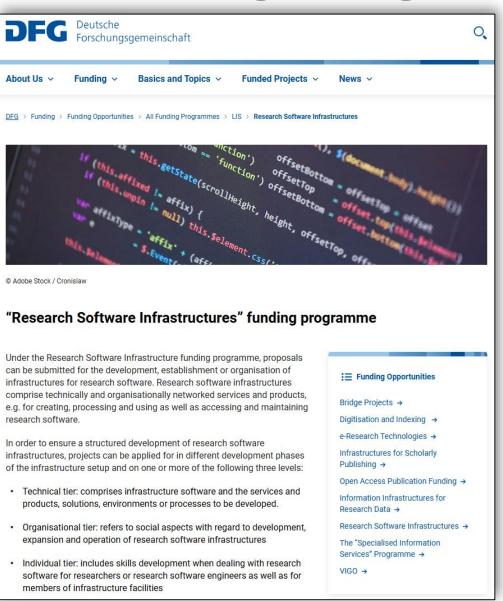
Research Software can also be successful outside research ...



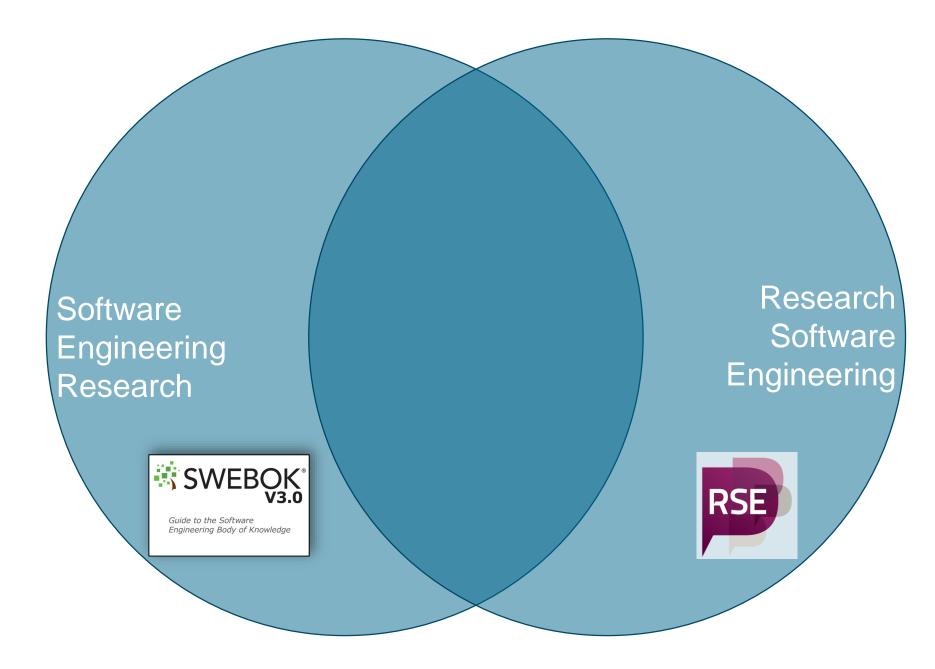
Momentum of the Area Research Software Engineering



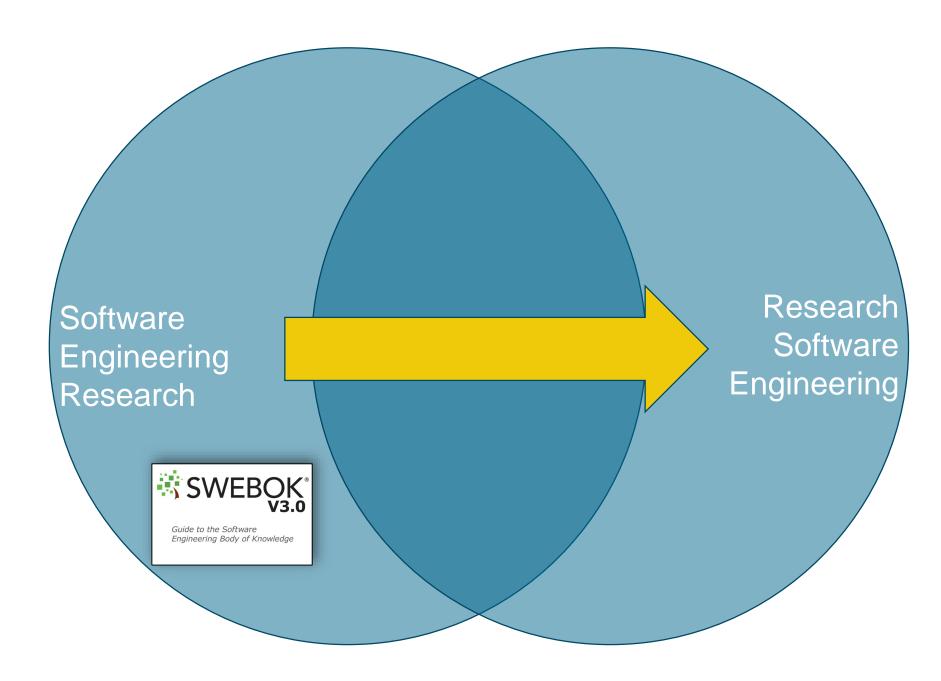






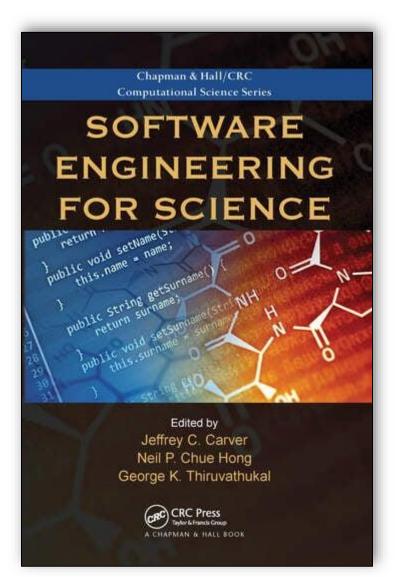






SE Practices for Research Software Engineering





Automated Metamorphic Testing of Scientific Software (Kanewala et al.)

Evaluating Hierachical Domain-Specific Languages for Computational Science (Johanson et al.)

Metamorphic Testing



 $R_{
m g}^2 \stackrel{
m def}{=} rac{1}{2N^2} \sum_{i
eq j} \left| {f r}_i - {f r}_j
ight|^2$

Figure 7.1: Function from the SAXS project described in Section 7.5.1 used for calculating the radius of gyration of a molecule.

Describes the distribution of atoms of a molecule around its axis

Metamorphic Testing

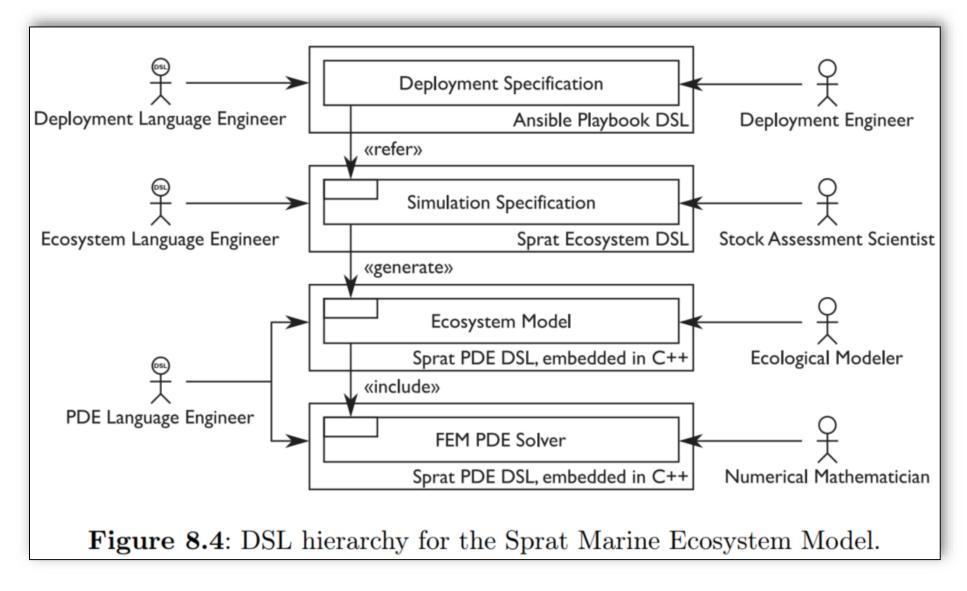


```
@Test
public void findGyrationRadiusRandTest() {
Random rand=new Random();
int arrLen=rand.nextInt(MAXSIZE)+1;
//initial test cases
  double [] iX=new double [arrLen];
  double [] iY=new double [arrLen];
  double [] iZ=new double [arrLen];
   for (int k=0; k=0; k=1)
      iX[k]=rand.nextDouble();
      iX[k]=rand.nextDouble();
      iX[k]=rand.nextDouble();
   //Executing the initial test case on the function under test
   double intialOutput=SAXSFunctions.findGyrationRadius(iX, iY, iZ);
   //create follow-up test cases by randomly permuting the array
     elements
   double [] fX=permuteElements(iX);
  double [] fY=permuteElements(iY);
  double [ ] fZ=permuteElements(iZ);
   //Executing the follow-up test case on the function under test
  double followUpOutput=SAXSFunctions.findGyrationRadius(fX, fY, fZ);
   assertEquals (intialOutput, followUpOutput, eps);}
```

Figure 7.2: JUnit test case that uses the permutative MR to test the function in Figure 7.1.

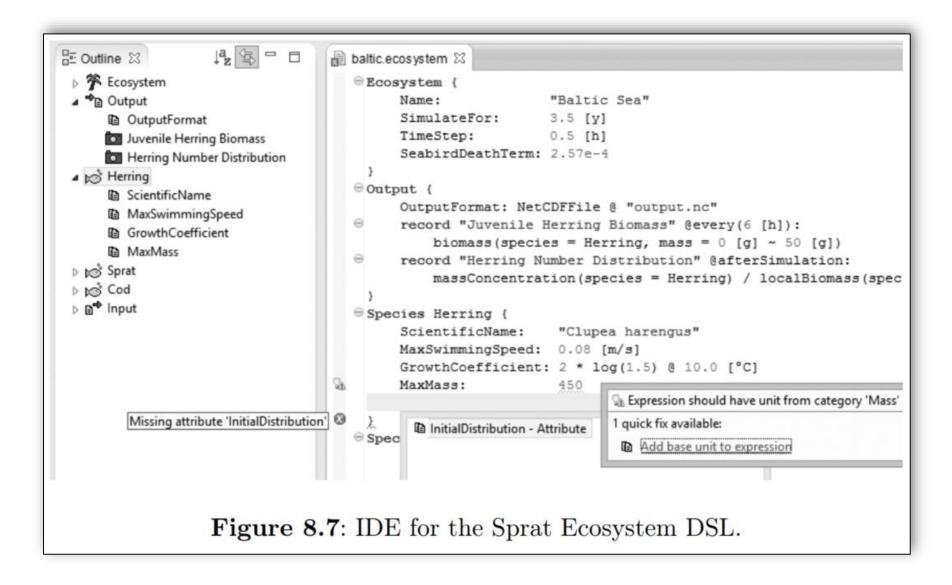
Domain-Specific Languages in Computational Sciences





Domain-Specific Languages in Computational Sciences



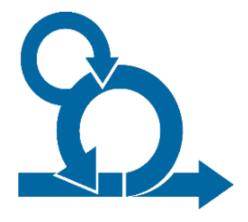


Many other relevant topics ...

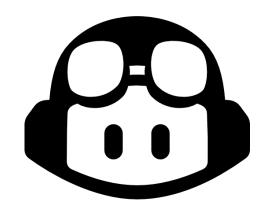


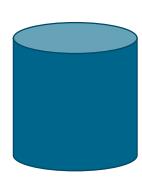
Agile Software Development
DevOps Practices
Software Security

GenAl for Software Development Repository Mining

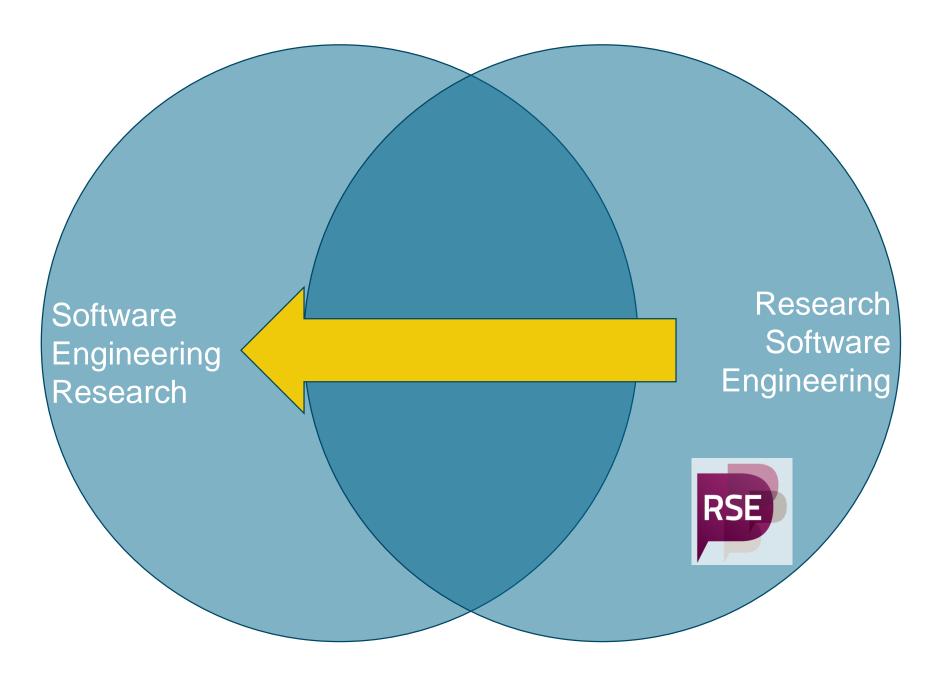














Open Science in Software Engineering

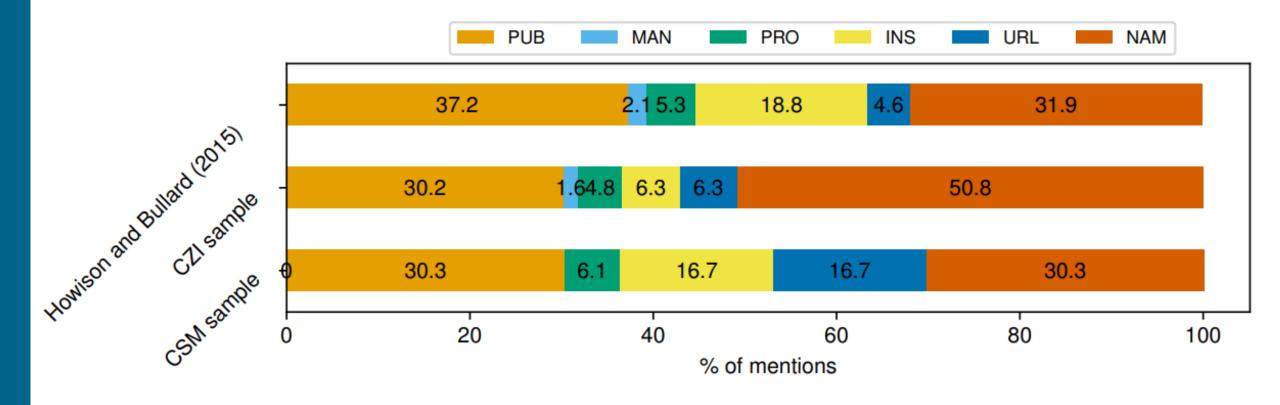


Daniel Mendez (5), Daniel Graziotin (5), Stefan Wagner, and Heidi Seibold

Abstract Open science describes the movement of making any research artifact available to the public and includes, but is not limited to, open access, open data, and open source. While open science is becoming generally accepted as a norm in other scientific disciplines, in software engineering, we are still struggling in adapting open science to the particularities of our discipline, rendering progress in our scientific community cumbersome. In this chapter, we reflect upon the essentials in open science for software engineering including what open science is, why we should engage in it, and how we should do it. We particularly draw from our

Software is currently mentioned, not cited ...





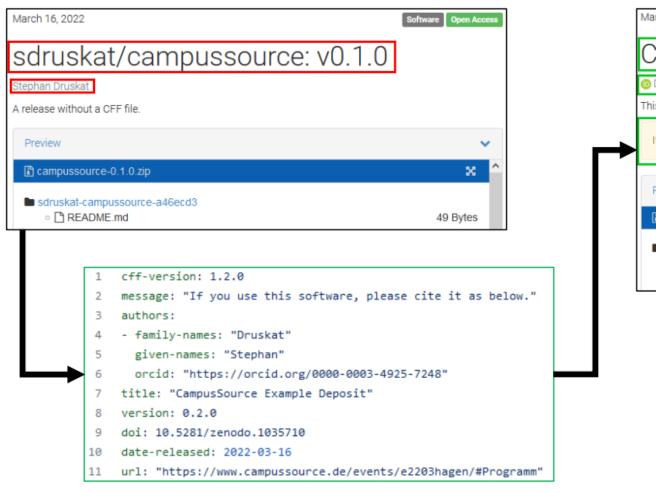
PUB: cites publication

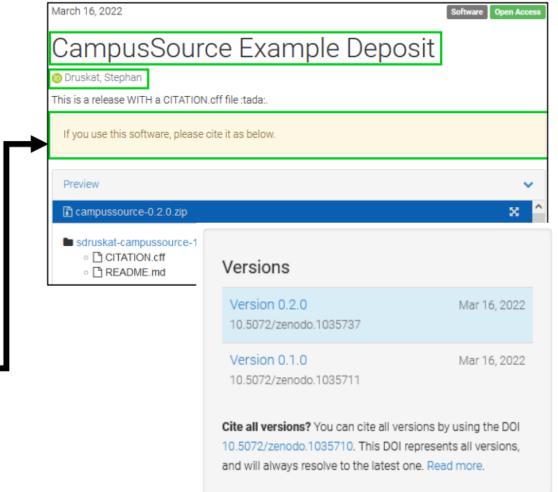
PRO: cites project name/website

INS: instrument-like URL: URL in text NAM: in-text name only

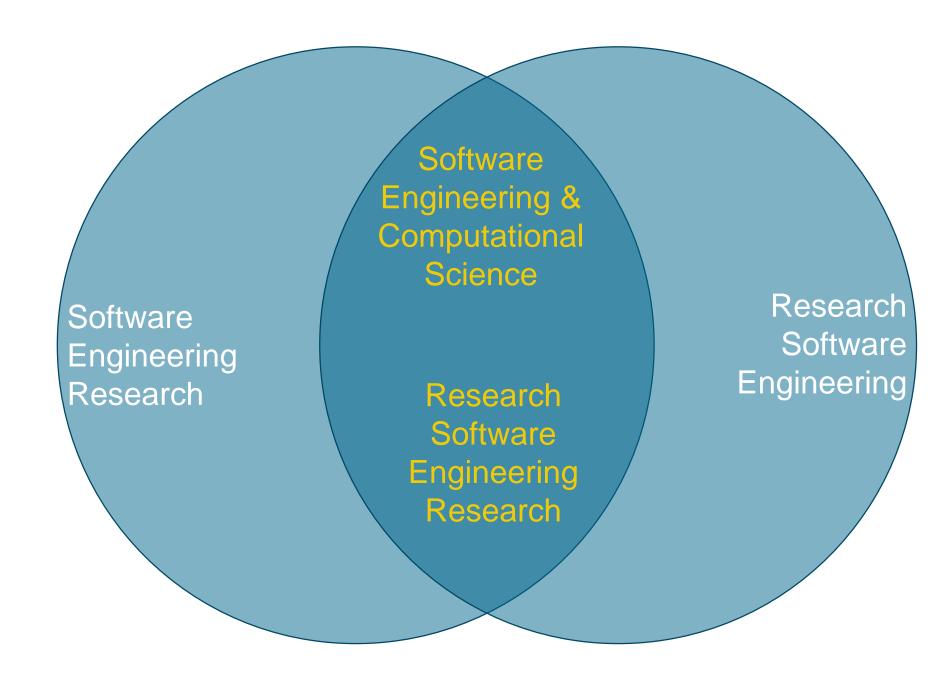
Citation File Format (CFF)















Software
Engineering &
Computational
Science

Research
Software
Engineering
Research

Research Software Engineering

Quantum Computing

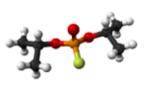


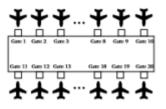
Quantum computing is a multidisciplinary field comprising aspects of computer science and physics that utilizes quantum mechanics to solve complex problems faster than on classical computers

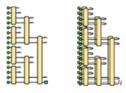
Quantum Simulation Combinatorial Optimisation

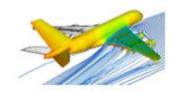
Quantum Enhanced Machine Learning

Classical Simulation





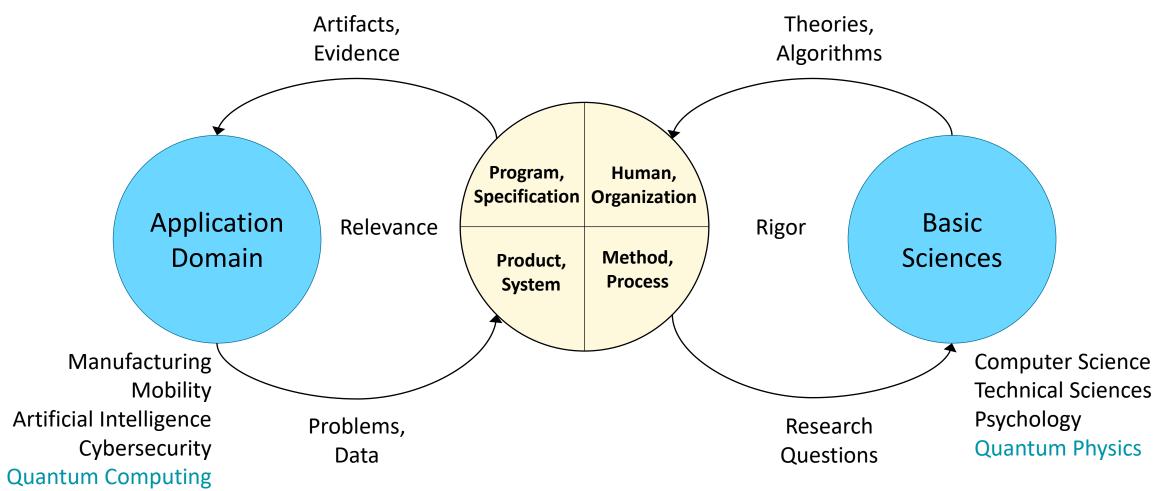




Required Error Correction

SE Research Process for Quantum Computing





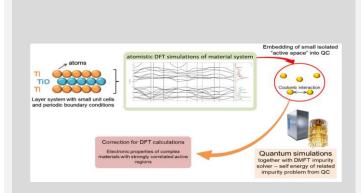
Project ELEVATE: Use Case Discovery @DLR

ENHANCED PROBLEM SOLVING WITH QUANTUM COMPUTERS



ELEVATE: Investigation of DLR use cases in 42 voucher studies

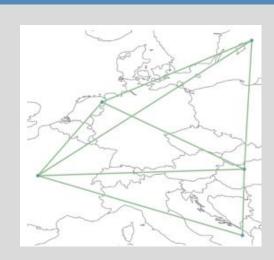
Atomistic simulation of engineering alloys



Topic: Improving the prediction of material properties with quantum computing.

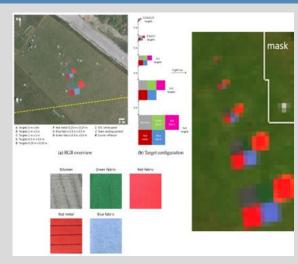
(Material Design)

Transmission Expansion Problem



Topic: Development of a hybrid quantum algorithm for transmission network expansion planning. **(Optimization)**

Hyperspectral Data Unmixing

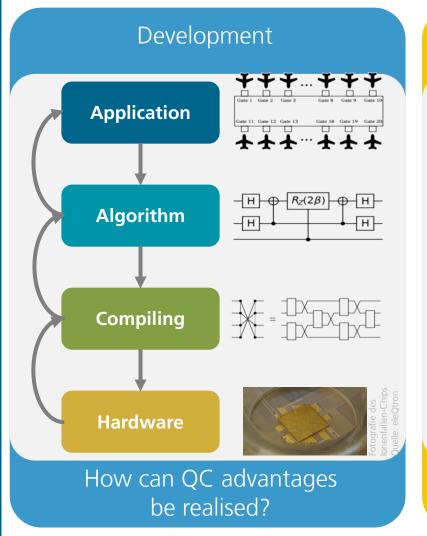


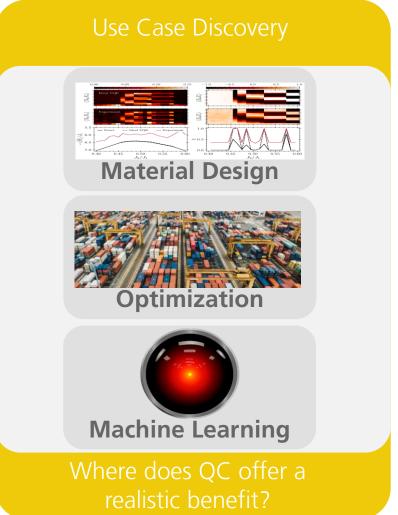
Topic: QML for analysing multimodal spectral data from satellite observations.

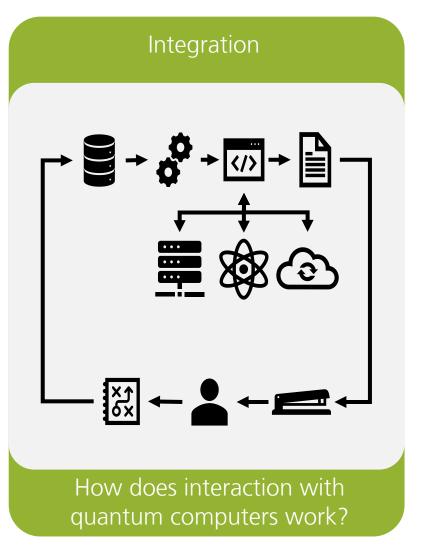
(Quantum Machine Learning)

Key Challenges



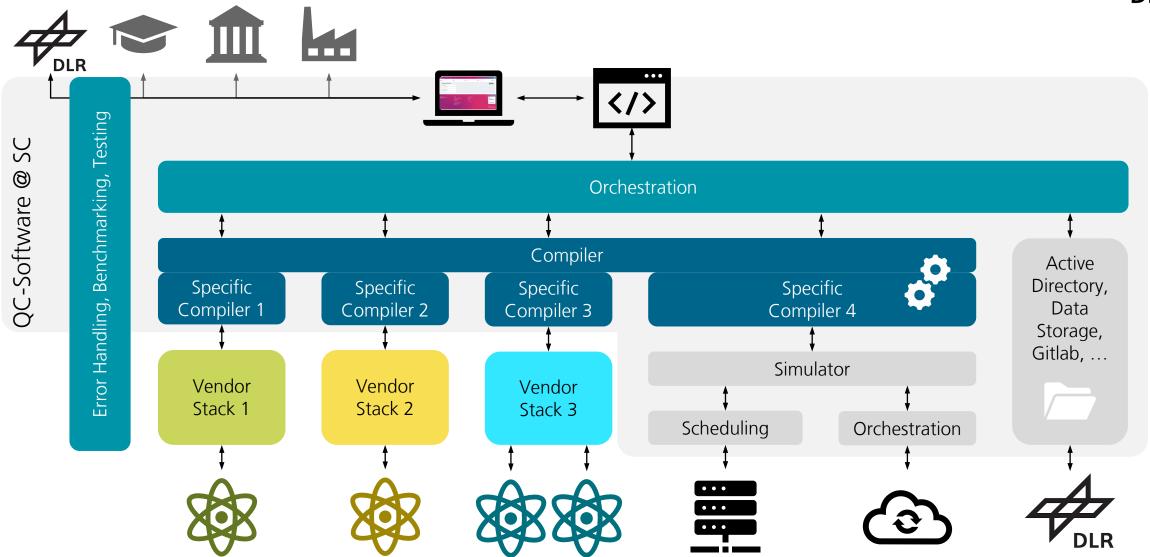






Quantum software as a bridge-builder and research area



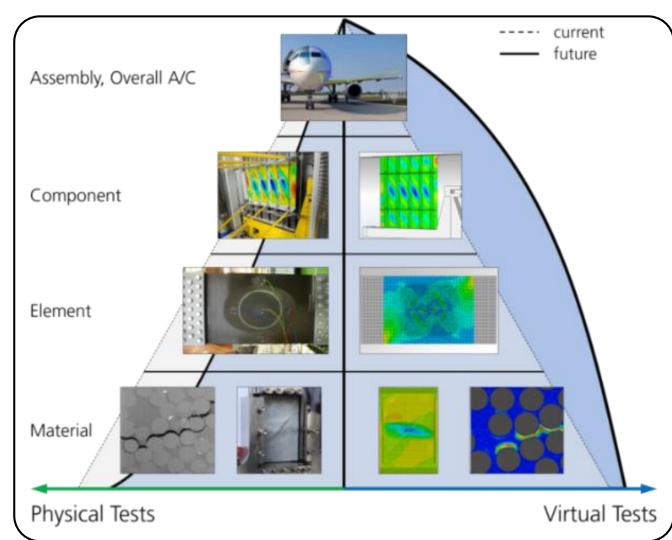


Virtual Product House (VPH): Overview



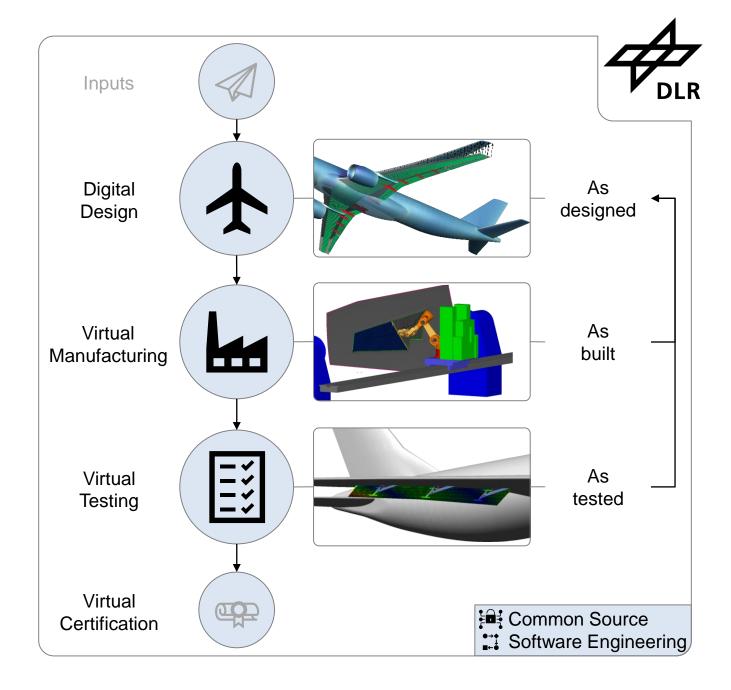
- Objectives
 - Virtual Aircraft Development & Evaluation
 - Reduce physical tests
 - Improvements in aircraft emissions
 - Virtual Certification
- Digital Twins are key





VPH: Phases Considered

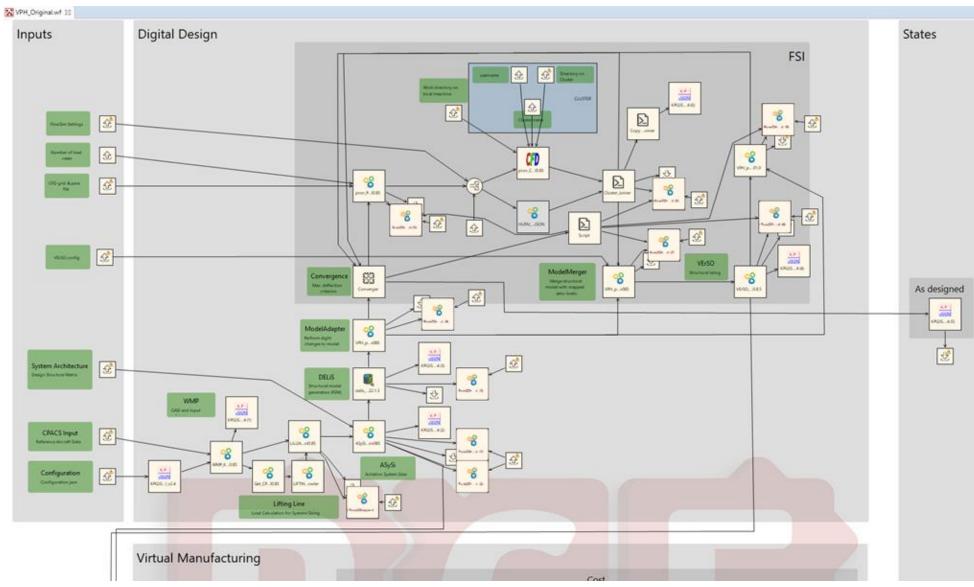
- Key phases are
 - Digital Design
 - Virtual Manufacturing
 - Virtual Testing
- Virtual Certification as vision
- Software platform key enabler and research topic



Virtual Product House Virtual Design

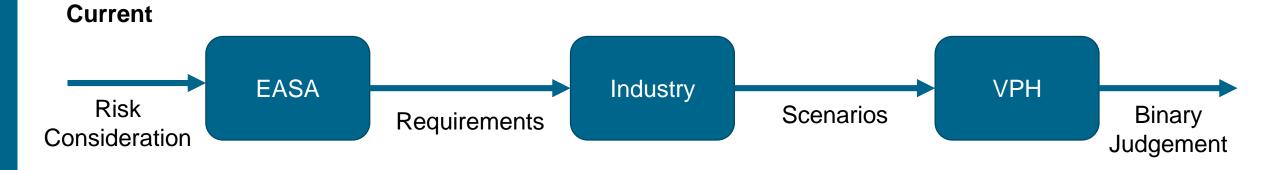
- Digital aircraft (component) design process
- Input: Initial design of aircraft component
- Output: sized component structure ("As designed")

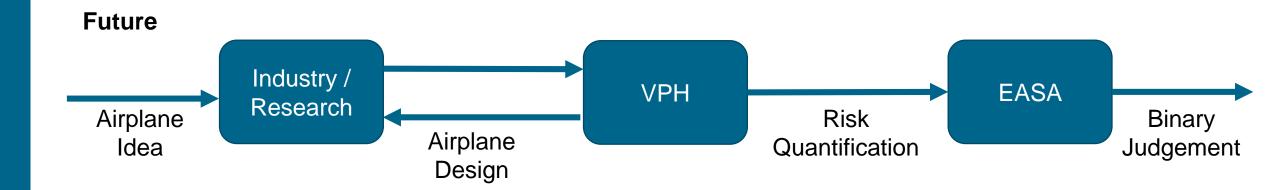




Current and Future Certification Process







Now: Conservative Airplane Design driven by Top-Down Waterfall Process Future: Risk-Driven Agile Airplane Design

- Judgement currently based solely on experience of Subject Matter Expert (SME)
- Automated testing support required that takes
 - Provides fast feedback
 - Takes parameter space (length, width, shape, no. of flaps, ...) into account
 - Takes massive amounts of data into account
 - Provides suitable oracles
 - Considers human-in-the-loop



Software
Engineering &
Computational
Science

Research
Software
Engineering
Research

Research Software Engineering

Software Engineering Research

Research software engineering provides an interesting application context for empirical software engineering



Dealing with vast configuration spaces

Dealing with highly dynamic requirements and complex domains

Dealing with simulations, digital twins and big data

Dealing with long-lived software artifacts and reuse

Dealing with development under resource constraints

Dealing with software development by domain experts

Research Questions for RSE



There is little knowledge about the relation between Software Engineering and Research Software Engineering

How to organize

What are suitable lifecycle models for research software?

software-centric scientific processes?

What is specific about RSE compared to other SE specializations?

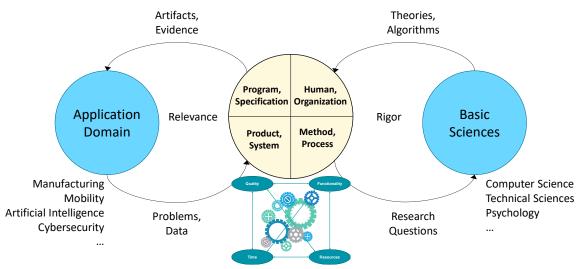
Which skills and educational formats are required for RSE practitioners?

How to integrate SE techniques into research software development?

Is research software of poorer quality than industry software?

Software Engineering Research

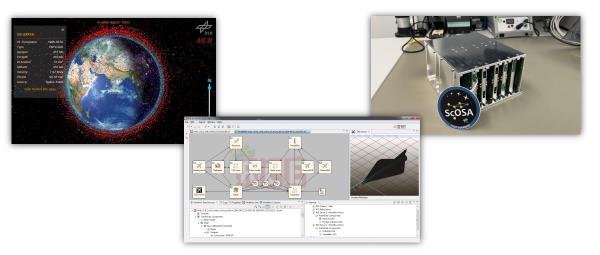




Felderer, M., Reussner, R., Rumpe, B. (2021) Software Engineering und Software Engineering Forschung im Zeitalter der Digitalisierung. Informatik Spektrum.

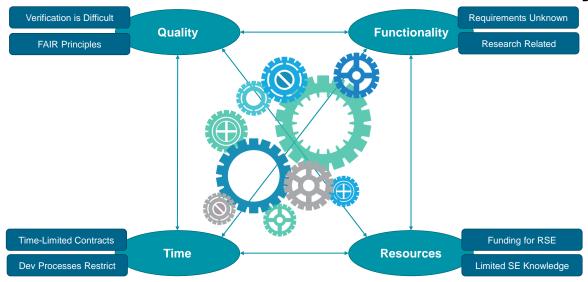
Research software is created during the research process or for a research purpose

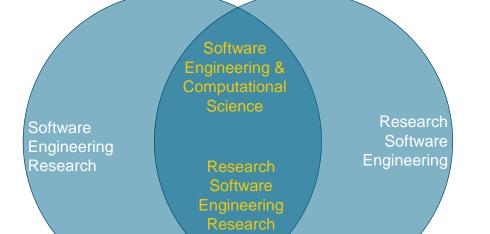




Trade Off in Software Engineering: Specifics of RSE





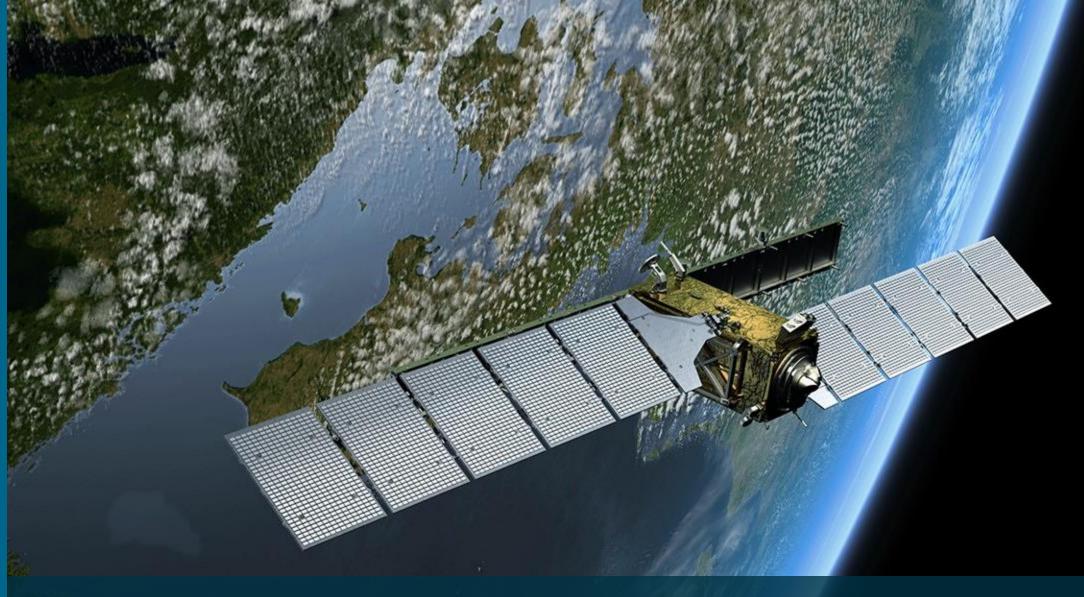




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