



From source code to software as a service, how to make software more accessible?

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www.helmholtz.de

Motivation

Modern <u>Software is used as a Service</u> (SaaS) in the cloud, also in science. What are the **advantages**?

- The software is visible and accessible and supports the work in large teams.
- It is scalable and enables the use of large storage and computing resources.
- It offers high availability, trustworthiness and latest releases.
- SaaS platforms support workflows connecting different applications.
- Usually help and support is provided

But what are implications for the software development and engineering?

- The talk addresses these questions.
- The illustrative examples relate to the <u>helmholtz.cloud</u> platform.

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Approaches of a software development

There are **different approaches** to software development

- A SW solution for a specific **project** or a research task
- A SW **product** is to be developed for a market.
- A SW service is to be created for a cloud platform. ٠

The approaches define certain **conditions** for a project, illustrated by a maturity diagram.

A SW service:

- can achieve increased visibility and recognition
- requires continuous funding and a larger team
- high quality: mature, reproducible development and engineering processes
- Active user community, open source: incremental, distributed development

Team, Recognition Budget Project Community Maturity Product **Reproducibility**, Quality

Market, Cost

Visibility,

Openness,

Project

Service

Fig. 1: Exemplary maturity diagram

The Software Development Lifecycle

Specific features of SaaS in the software development lifecycle:



Helmholtz Research Field Earth and Environment DataHub







Fig. 4: Helmholtz Datahub Earth-and-Environment see <u>DataHub</u> and <u>Helmholtz RF Earth and Environment</u> websites

- -> Establish an interoperable digital ecosystem for Earth System Science supporting the holistic research perspective
- Digitalization of data acquisition, workflows and pipelines address digital needs in science
- Interaction with incubator activities and use of services
- Guiding principles are Open Science and FAIR Data
- Use cases defined within the program research
- Implementation provides added value for research and the public
- Connection to national and international data infrastructure, e.g. NFDI and EOSC

SaQC – System for automated Quality Control



What is SaQC?

- A Python module, a command line application and, increasingly, a Software Service
- An framework to quality control of timeseries data
- A collection of **methods and algorithms to**:
 - process (resampling, interpolation, smoothing)
 - quality control (breaks-, constants-, outlier-, noise-, drift-detection) and
 - annotate timeseries data

SaQC as Software Development Project:

- Small team of 3 to 5 part time SW developers and data scientists from the UFZ HELMHOLTZ Centre for Environmental Research
- Initial commit 03.2019, first 'stable' release in 11.2021
- Open Source, License GPL 3



SaQC – System for automated Quality Control

What do we use it for?

- Quality control of timeseries data from terrestrial observatories
- As part of fully automatized data workflows from sensors into databases

Use cases of TERENO

- <u>Bode Hydrolgical Observatory</u>
 - 912 Sensors, 42 Dataloggers
 - > 185 mio. observations and growing
- Intensive Test Site Hohes Holz
 - 2114 sensors, 87 loggers
 - > 775 mio. data values and growing







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The long way from product to SaaS

- 2019: Source distributed, locally deployed CLI Application
- 2020: Package distributed Python API
- 2022: <u>Configuration App</u> as an centrally hosted, graphical user interface
- 2022: SaQC is <u>Helmholtz Software Spotlight</u>
- 2023: GitLab CI/CD deployed quality control pipelines:
 - Reduce the entry barrier for non/less technical staff
 - Build pipelines to run project specific SaQC setups on cloud infrastructure
- 2024: Planned integration into a fully-fledged Timeseries Management System:
 - Deploy SaQC as a service within a larger scale system to manage data flows from source to sink
 - Integrate SaQC into an ecosystem of community research data management tools



SaOC

HIFIS – Helmholtz Digital Services for Science



How does a Cloud Platform (HIFIS) help with that?



Trusted Data Center Infrastructure

Fig. 7: hifis.net

Services Platform Complexity





Fig. 8: hifis.net

Services Platform Complexity



and Access Management (Helmbring) Authentication, Identity



Mastering Complexity

Mastering complexity through using re-usable and generic solutions

- Building services on top of community standards, e.g. Ansible, HELM
- Provide reusable service provisioning recipes: <u>https://galaxy.ansible.com/hifis</u>, <u>https://github.com/hifis-net</u>

Allow scientists to build their own portable cloud-ready applications which can be embedded in research workflows!

- Testdrive community driven applications on federal cloud platforms
- Scientific communities provide test-instances and usable applications
- a SW platform can be a market place of ideas and solutions





Research Field Earth and Environment



HIFIS – Helmholtz Digital Services for Science





Fig. 9: helmholz.cloud

HIFIS – Helmholtz Digital Services for Science



Facts & Figures

>13.000 individual users in AAI >2.000 non-Helmholtz users

All Centres

One Login using Helmholtz AAI!



collaborating groups (VO)

27

active cloud services of 8 providers

5 service categories: Infrastructure, Storage, HPC, Collaboration and Science

>900

processed support tickets in 2022

Providing Software as a Service on a Research Cloud Platforms helps to

- enable a new quality of collaborative, data-centred research
- achieve greater impact and sustainability
- deploy cutting-edge technology based on a new technological paradigm



RESEARCH FOR

GRAND CHALLENGES

Visit us @:

- <u>https://hifis.net</u>
- <u>https://helmholtz.cloud</u>
- <u>https://datahub.erde-und-umwelt.de</u>
- <u>https://helmholtz.software/software/saqc</u>



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