IBERGRID 2024 28-30 OCT UNIVERSITY OF PORTO software better science

SQAaaS platform as the quality gate for Digital Twins

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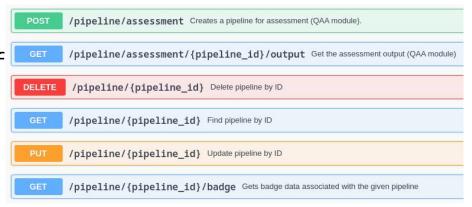




SQAaaS: the QA building block for Digital Twins

■ SQAaaS features:

- Programmatic QA assessment (RESTful API) and awarding of digital research content
 - SQA characteristics on code and (web) services (custom)
 - FAIR principles on data (RDA maturity model)
- Adhoc composition of CI/CD pipelines
- ..besides providing clients (web portal, CLI) to streamline usage
- ☑ Digital Twins orchestrate and operate computational end-to-end data analysis workflows
- Workflow steps consume/execute/produce such research content:
 - Input and output data
 - Software/code and/or services



















your badge in popular code and data repository platforms using Markdow







SQAaaS role in Digital Twin projects (EC-funded)

- SQAaaS fits in as the QA building block during the development and operation phases of a Digital Twin
 - QA+FAIR assessment of individual digital assets
 - Integration with Workflow Management Systems (WfMSs)
 - Integration with Scientific Data Management technologies
- SQAaaS is already an architectural component within projects developing Digital Twin solutions:
 - InterTwin: developing an engine (DTE) for building, validating and deploy multidisciplinary digital twins
 - o DT-GEO: building a complex prototype digital twin on geophysical extremes













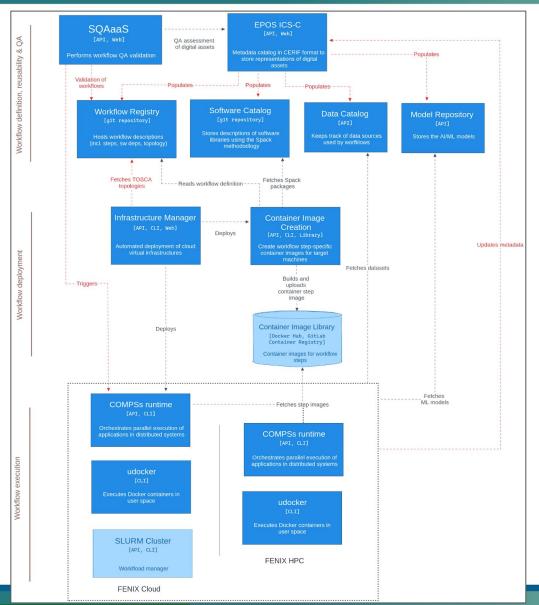




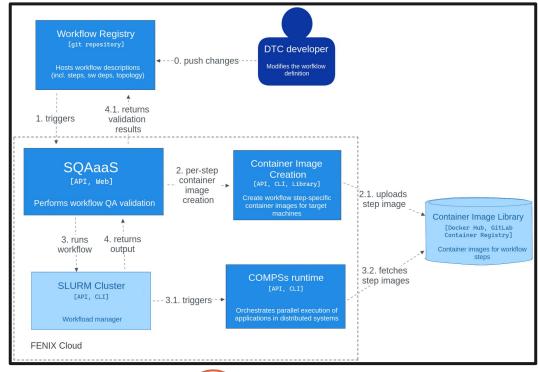








Role of SQAaaS in Digital Twin projects: **DT-GEO**

















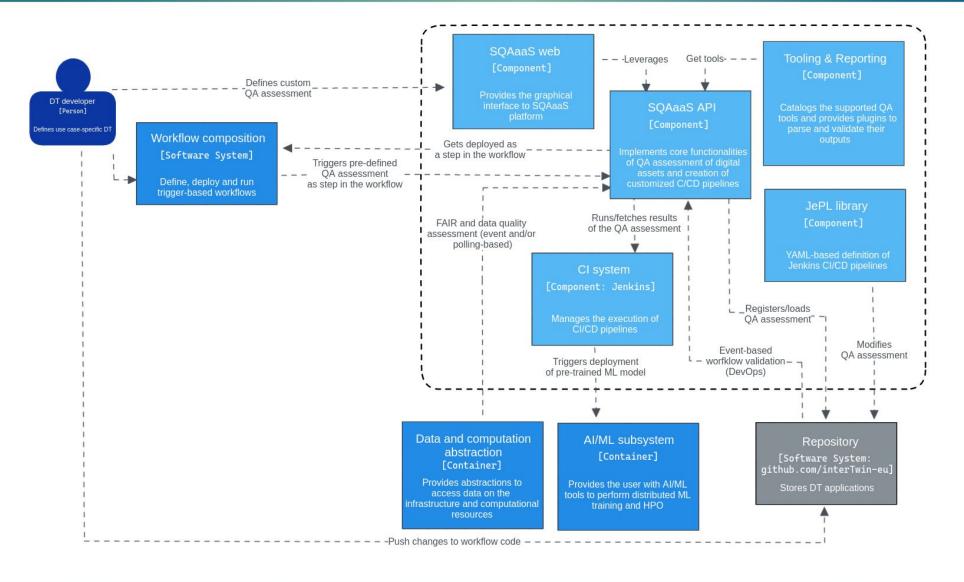






Role of SQAaaS in Digital Twin projects: InterTwin

























- Suitable for: QA work done at development time, in the platform where the code is maintained
- Target/s: source code (incl. workflow code)
- Automation: reacts to events triggered by the hosting platform (push, change request, releases, etc.)
- Platform/s: GitHub and GitLab





Features:

- #1. Leverages already existent CI technologies: GitHub Actions & GitLab CI
- #2. **Reporting summary** for each build
- #3. **Dynamic badging**, updated as SQAaaS assessment progresses





















Feature #1: Leverages already existent CI technologies: GitHub Actions & GitLab CI

Marketplace / Actions / SQAaaS source code assessment



Baseline evaluation

uses: eosc-synergy/sqaaas-assessment-action@v2

GitHub



Extended evaluation

uses: eosc-synergy/sqaaas-assessment-action@v2 with: qc_uni_steps: model_validation_step

SQAaaS tutorial at Ibergrid 2024 conference @ Mon 28







assessment in the SQAaaS platform















Feature #1: Leverages already existent CI technologies: GitHub Actions & GitLab CI





Following the approach of GitHub, a 2nd CI component has been implemented to define an additional step in the SQAaaS assessment

SQAaaS tutorial at Ibergrid 2024 conference @ Mon 28

Baseline evaluation

include: - component: gitlab.com/dtgeo/sqa-assessment-ci-template/SQA.gitlab-ci@1.0.0

Extended evaluation

```
variables:
  INPUT_NAME: pycompss-step
  INPUT TOOL: commands
 INPUT_COMMANDS: echo 'Here we will execute PyCOMPSs'
 INPUT_QC_UNI_STEPS: pycompss-step
stages:
  - SQA
include:
  - component: $CI_SERVER_FQDN/dtgeo/metadata/sqa-assessment-ci-template/SQA-step.gitlab-ci@1.0.0
  - component: gitlab.com/dtgeo/sqa-assessment-ci-template/SQA.gitlab-ci@1.0.0
```













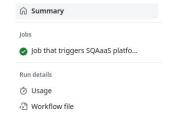








Feature #2: Reporting summary for each build



- Displayed in GitHub Actions' job view
- Provides link to full report in SQAaaS platform

Result	Assertion	Subcriterion ID	Criterion II
V	Source code uses Git for version control	QC.Acc01	QC.Acc
V	A README file is present in the code repository	QC.Doc06.1	QC.Doc
V	A CODE_OF_CONDUCT file is present in the code repository	QC.Doc06.3	QC.Doc
V	A CONTRIBUTING file is present in the code repository	QC.Doc06.2	QC.Doc
~	Documentation resides in the same repository as code	QC.Doc01.1	QC.Doc
•	Docs are not fully compliant with markdownlint standard	QC.Doc02.X	QC.Doc
V	An Open Source license found in the code repository: GPL-3.0	QC.Lic01	QC.Lic
V	LICENSE file is visible at the root path of the code repository: LICENSE	QC.Lic01.1	QC.Lic
V	License GPL-3.0 is approved by the Open Source Initiative	QC.Lic02	QC.Lic
~	License GPL-3.0 is listed under the Open Source Initiative popular category	QC.Lic02.1	QC.Lic
V	JSON files are compliant with jsonlint standard	QC.Sty01	QC.Sty
V	The code repository uses tags for releasing new software versions	QC.Ver01.0	QC.Ver
~	Latest release tag 2.9.1 is SemVer compliant	QC.Ver01	QC.Ver
V	All release tags are SemVer compliant	QC.Ver02	QC.Ver
0	No matching files found for language <i>CodeMeta</i> in repository searching by extensions or filenames No matching files found for language <i>Citation File Format</i> in repository searching by extensions or filenames	QC.Met01	QC.Met
•	No matching files found for language <i>Python</i> in repository searching by extensions or filenames No matching files found for language <i>Go</i> in repository searching by extensions or filenames	QC.Sec02	QC.Sec





















Feature #3: **Dynamic badging** (powered by shields.io), updated as the SQAaaS assessment progresses



More on SQAaaS badging docs.sqaaas.eosc-synergy.eu

















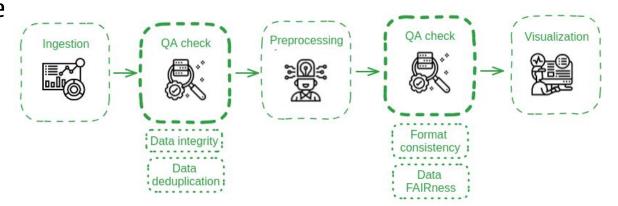




Further Integrations & features (in the making)

Workflow Management Systems (WfMSs)

- Suitable for: individual QA work during the execution of a workflow
- Target/s: components of a workflow
- Automation: not through events, coded in the workflow specification
- Tool/s: PyOphidia & CWL (InterTwin)



Data Management Systems

- Suitable for:
 - QA work on data (FAIR, quality dimensions)
 - React to CRUD operations on data repositories/lakes
- Target/s: data
- Automation: notifications sent by the data management system on CRUD operations
- Tool/s (potential): Rucio (InterTwin)















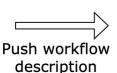




Use cases: InterTwin's Climate Change (PyOphidia+SQAaaS)



Use case repository







pytest

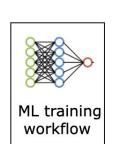
SQAaaS

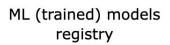
✓ Main integration leveraging <u>SQAaaS GitHub actions</u>:

- Validation of (PyOphidia) workflow description document
- 2. **Test trained models statically** with small test set

☑ Further potential integrations (adhoc support into Workflow and Data Management Systems): Stronger scientific validation of the model with statistically relevant (larger) test set

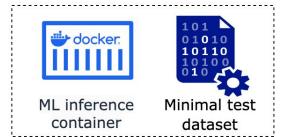
 Data quality and ML model FAIRness (to be better explored)

























CONDA

PyOphidia (validate workflow)





Use cases: **DTC development in #1** Builds Docker images DT-GEO image_creation workflow-registry Triggers **Pushes** CI\CD GitLab CI workflow #2 Triggers pipeline code **SOAaaS** #3 Triggers assessment **е** ру **сомр**ѕѕ workflow execution

- Offloads work to GitLab CI
- SQAaaS GitLab CI component performs the workflow validation (PyCOMPSs execution) in an HPC-like ecosystem in the Cloud

Potential integrations with:

- PyCOMPSs WfMS: define QA work within workflow steps (e.g. data FAIRness)
- Software and data registries: react to changes

















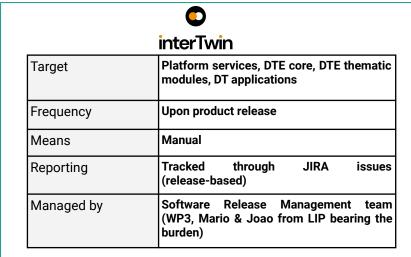


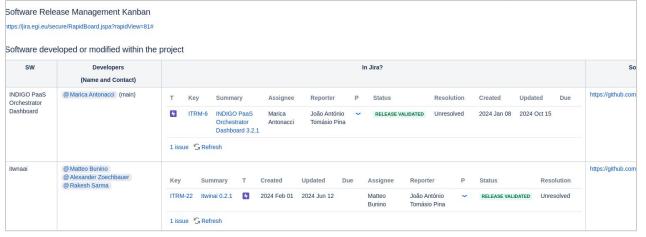
Jenkins

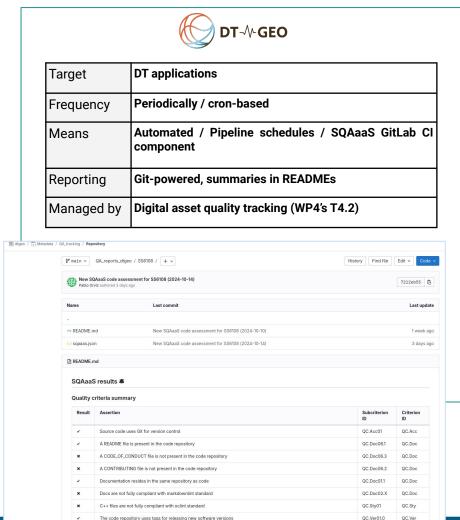
COMPSs



Further uses of SQAaaS platform: QA tracker















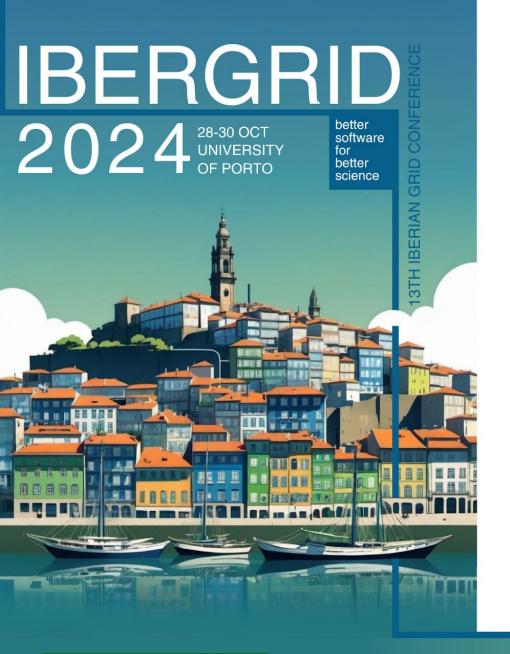












Q&A

Thanks for your attention

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