OpenEBench: the ELIXIR benchmarking platform

Laura Portell (laura.portell@bsc.es)

Asier Gonzalez (asier.gonzalez@bsc.es)

Jose Maria Fernandez (jose.m.fernandez@bsc.es)

Laura Rodriguez-Navas (laura.rodriguez@bsc.es)

Barcelona Supercomputing Center (BSC), ELIXIR-ES

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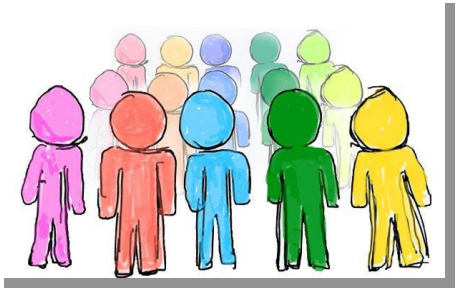
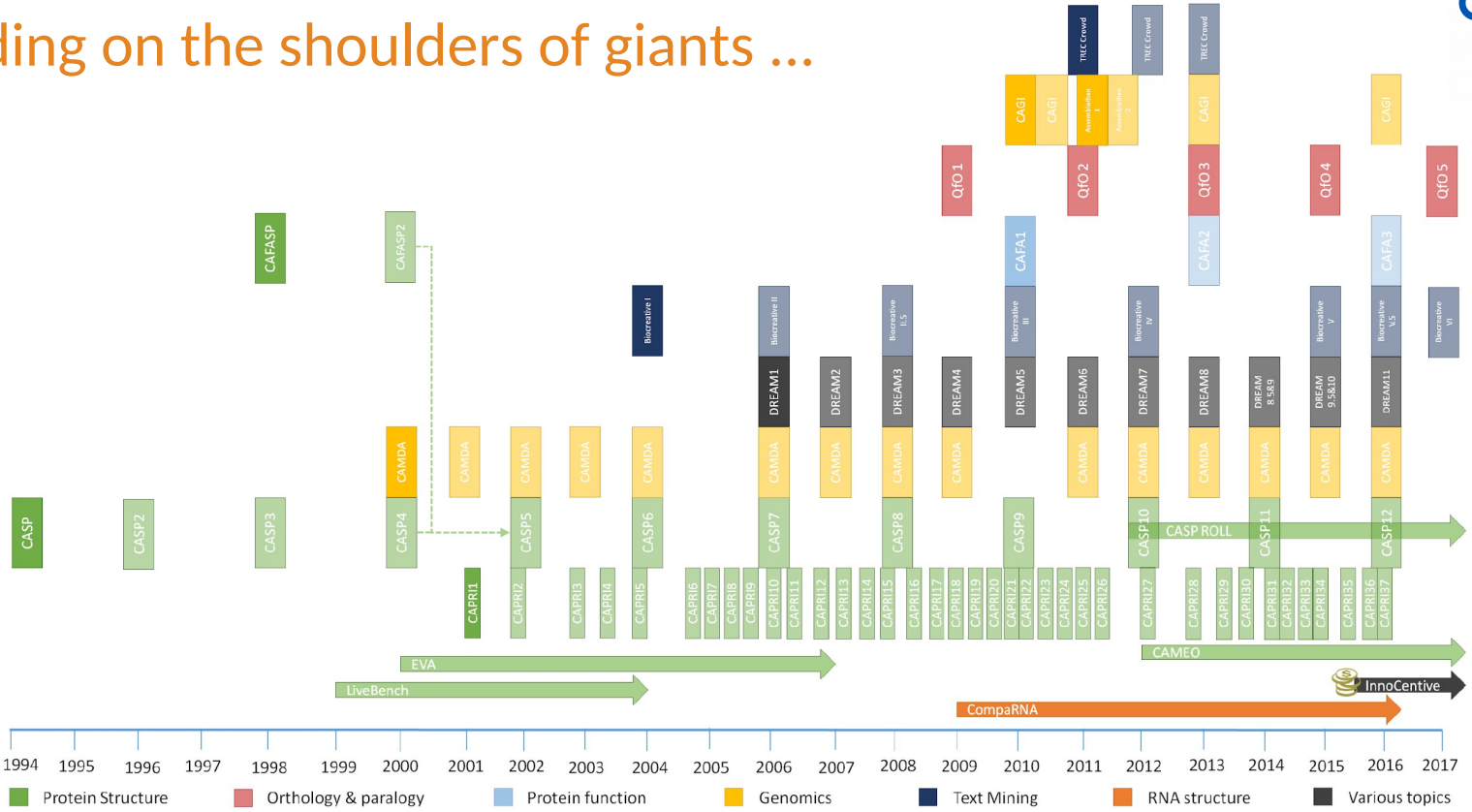
INDICATOR
METRICS
OPERATIONAL
COST
PLAN
STRATEGIC
EVALUATION
METHODOLOGY
TECHNICAL
COMPARE
PRODUCT
FUNCTIONAL
BEST PRACTICES
TARGET
SPECIFIC
IDENTIFY
BENCHMARKING
UNIT
FINANCIAL
MANAGEMENT
SURVEY
TOOLS
PROCESS
BUSINESS
PERFORMANCE
INFORMATION
TIME
ENERGY
INDUSTRY
IMPROVEMENT
QUALITY
ASPECT
RESULT
PROCEDURE

Community-driven benchmarking

- Face similar challenges and want to collaborate for advancing in the understanding of specific scientific problems.
- Guarantees a more complete benchmarking.
- Useful for a wider group of people: software developers and users.
- Follows the principles of ***Open Science*** to foster reproducibility, data sharing…



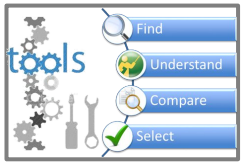
Standing on the shoulders of giants …



Lessons Learned: Recommendations for Establishing Critical Periodic Scientific Benchmarking.
Capella-Gutierrez S … Gelpi JL, Valencia A. bioRxiv 181677; 10.1101/181677

The ELIXIR Tools Platform

To support efforts around software packaging & containers, *e.g.* Bioconda/ BioContainers, and support sustainable integration into *bio.tools* and OpenEBench



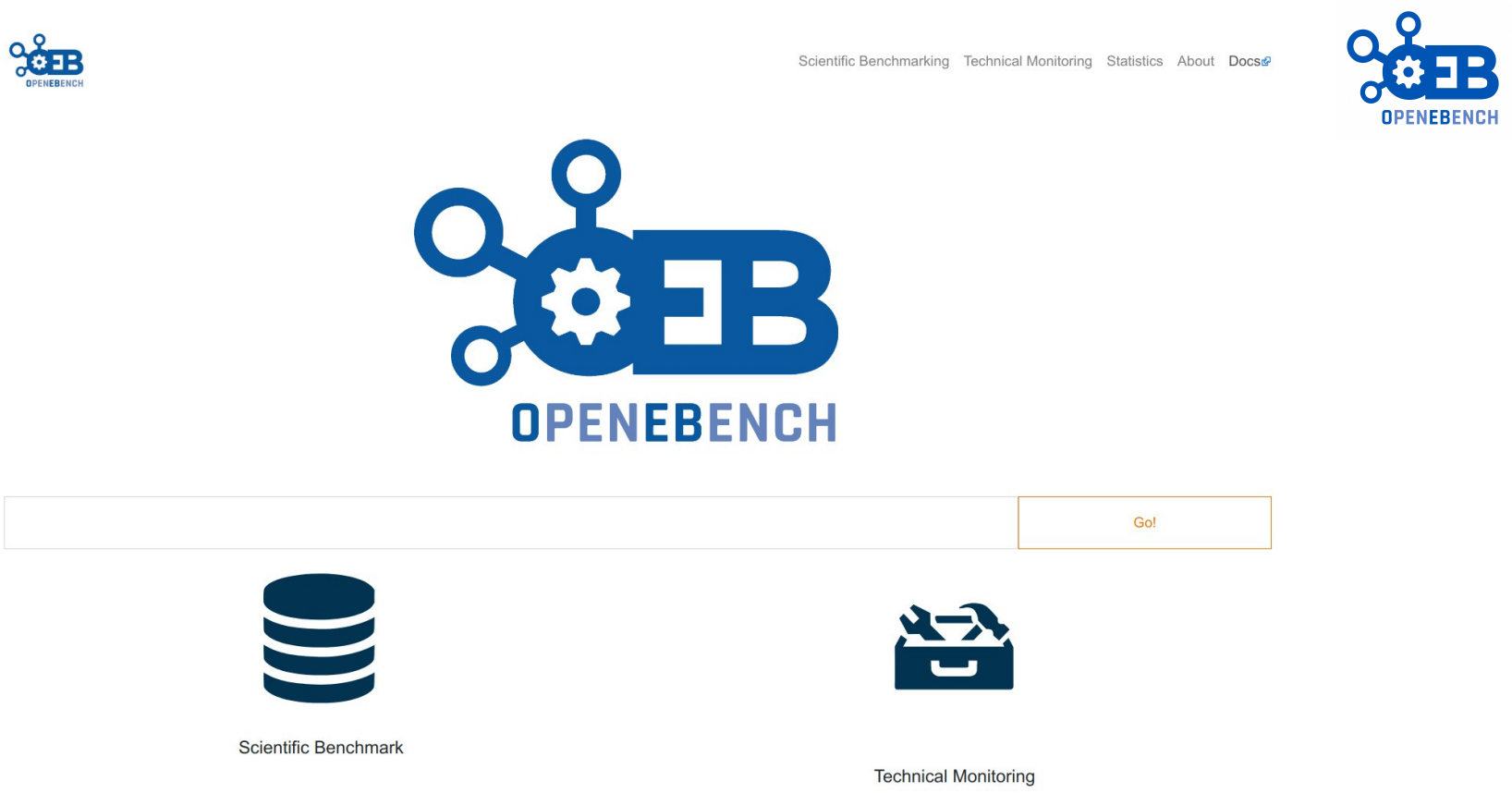
bio.tools, a discovery portal for bioinformatics software information, providing curated description of tools and data services

OpenEBench, an infrastructure providing services for hosting scientific benchmark activities and technical monitoring of bioinformatics tools and services

To drive the development of execution platforms (*e.g.* Galaxy) and ensure integration with *bio.tools*, OpenEBench, and workflows using CWL

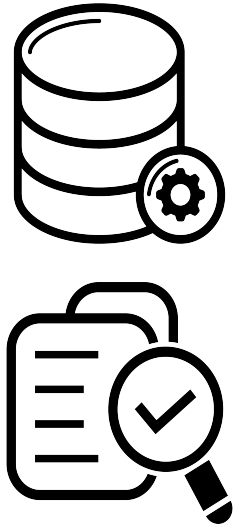
Raise software quality and sustainability, by producing and promoting software best practices and developing training activities

Tools Interoperability, guidelines and resources for guaranteeing Platforms integration within the ELIXIR Tools Platform Ecosystem, with other Platforms in ELIXIR and beyond.

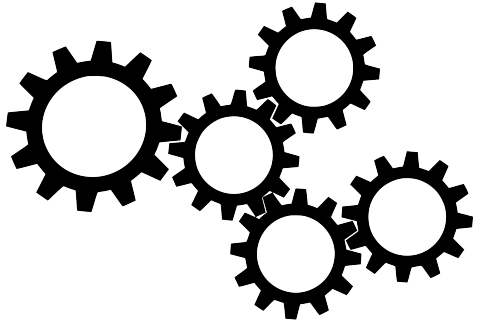


https://openebench.bsc.es

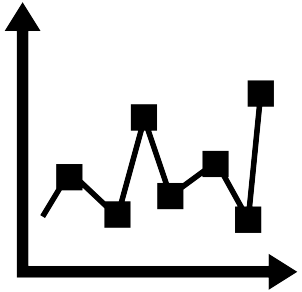
Scientific benchmarking in **OpenEBench**



Datasets



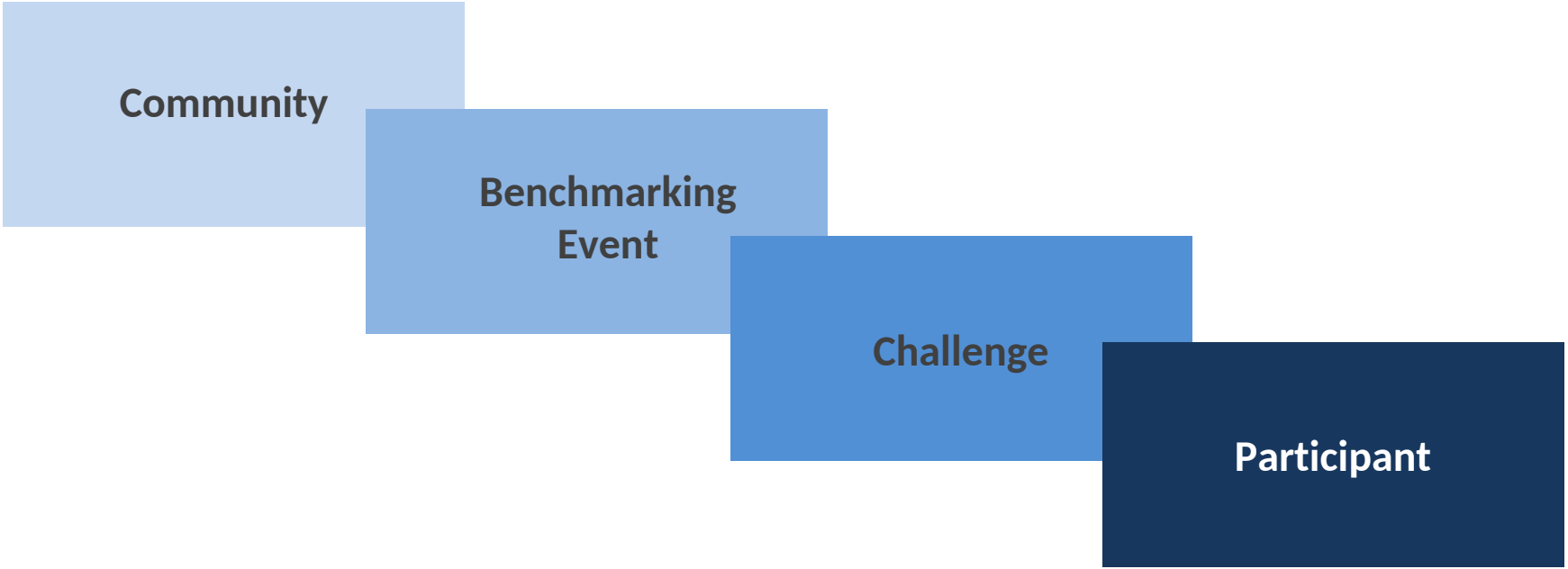
Evaluation Metrics



Results Interpretation

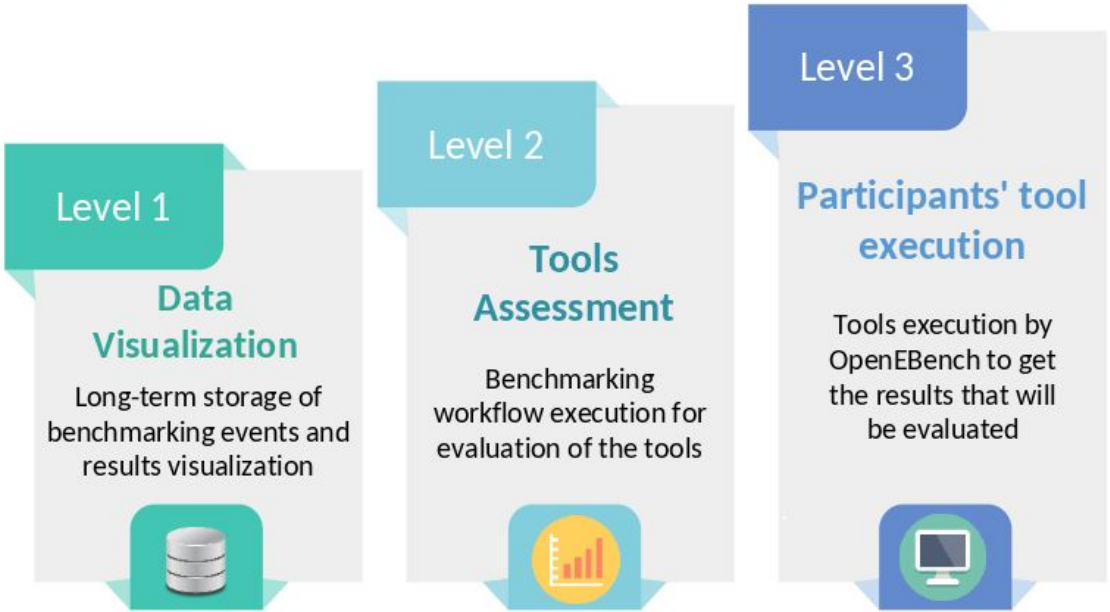
Scientific benchmarking in **OpenEBench**

How OpenEBench is organized



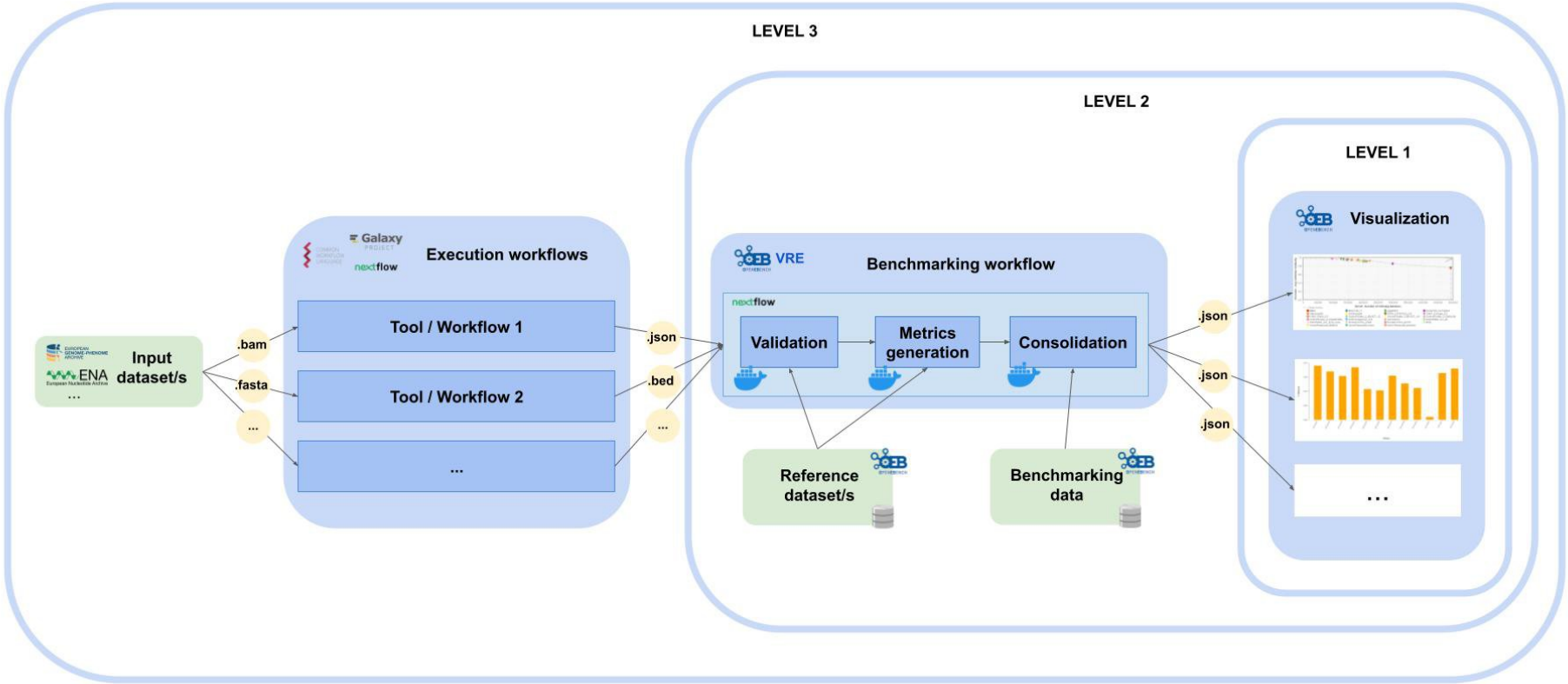
Scientific benchmarking in **OpenEBench**

Levels of engagement



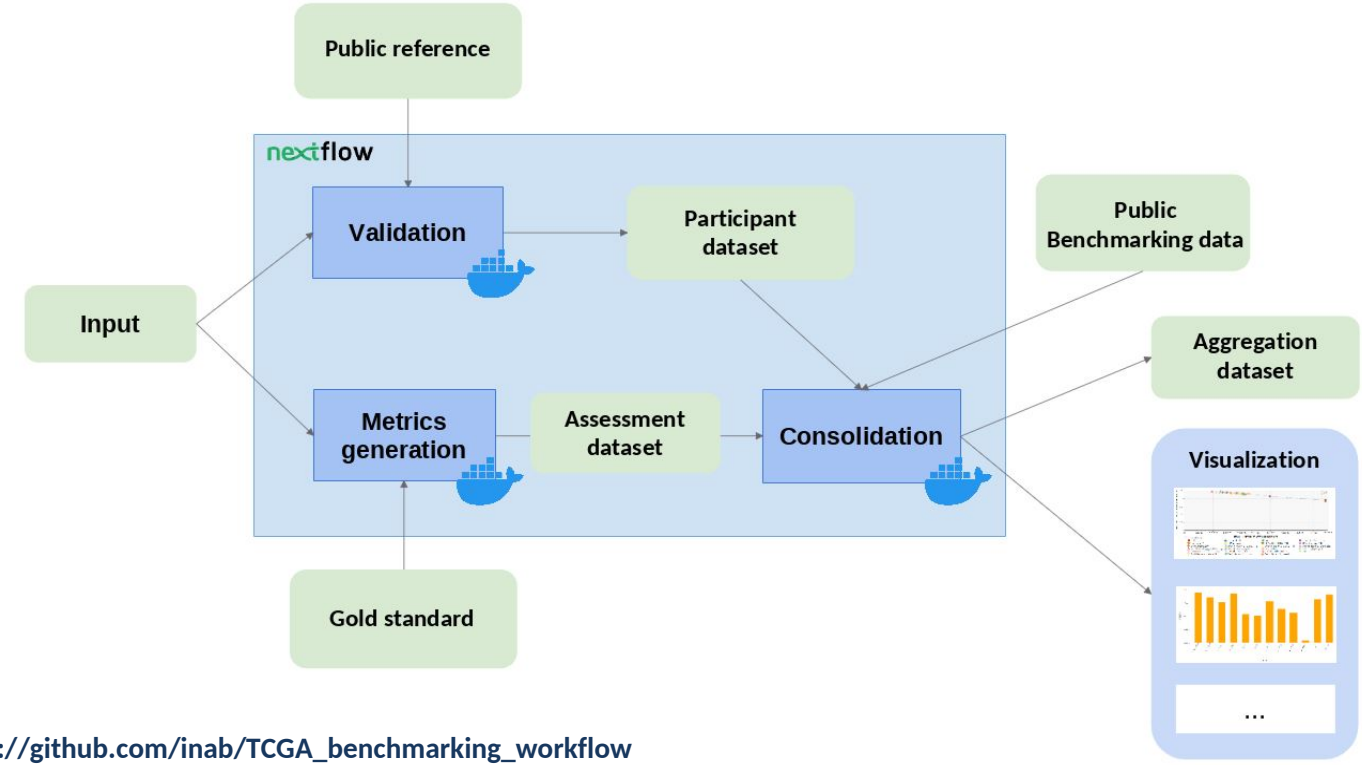
Scientific benchmarking in **OpenEBench**

Benchmarking process



Scientific benchmarking in **OpenEBench**

Benchmarking workflow



https://github.com/inab/TCGA_benchmarking_workflow
https://github.com/inab/TCGA_benchmarking_dockers

HANDS-ON EXERCISE 1

Running the TCGA benchmarking workflow

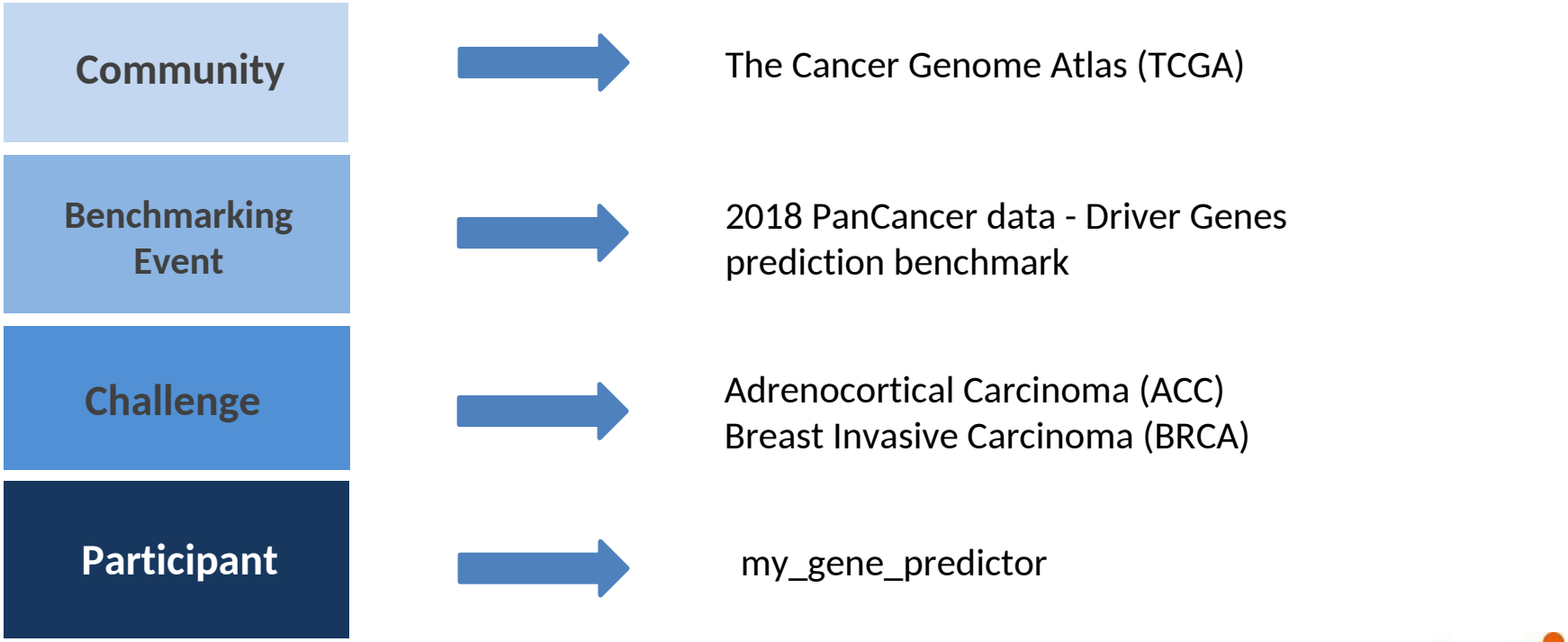
TCGA Cancer Driver Genes benchmarking description

- The Cancer Genome Atlas consortium organized a benchmarking event to compare the performance of cancer driver gene identification tools in 33 cancer types [see Bailey et al, 2018 for more info]

- 8 tools have published their results in OpenEBench [OEBC001]

- You have a tool called “my gene predictor” and want to compare the results against the public ones

TCGA Cancer Driver Genes benchmarking organization



Running the workflow from the CLI

For detailed information please refer to the README in the workflow's GitHub repository

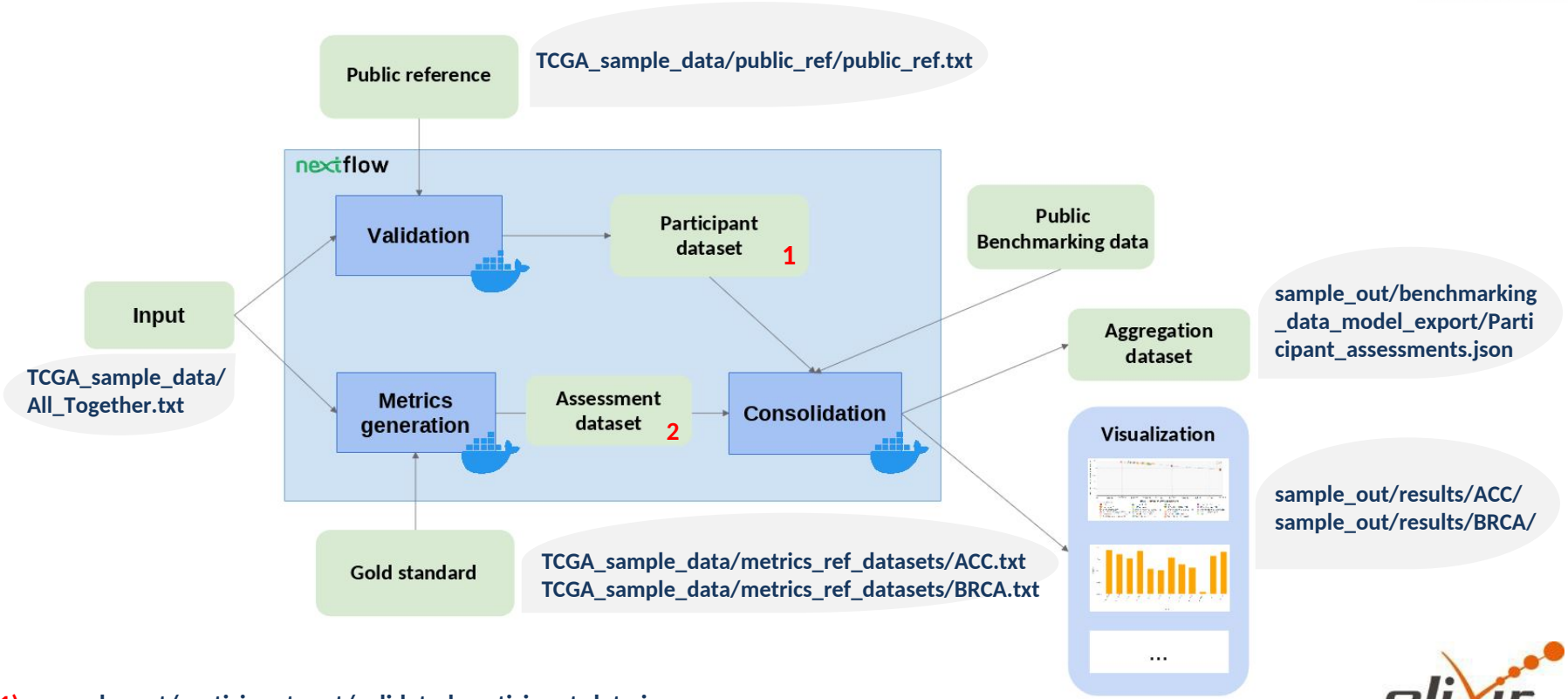
Requirements:

- Git
- Docker
- Nextflow ≥ 19.10.0 (it requires Bash ≥ 3.2 and Java ≥ 8 and ≤ 17)

Download version 1.0,8 of the workflow from GitHub:

```
> git clone https://github.com/inab/TCGA_benchmarking_workflow.git
> cd TCGA_benchmarking_workflow/
> git checkout 1.0.8 -b 1.0.8
```

TCGA Cancer Driver Genes benchmarking workflow



1) sample_out/participant_out/validated-participant-data.json
2) sample_out/assessment_out/Assessment_datasets.json

Running the workflow from the CLI

Let’s do the magic!

```
> nextflow run main.nf -profile docker
```

Now it’s time to explore the results

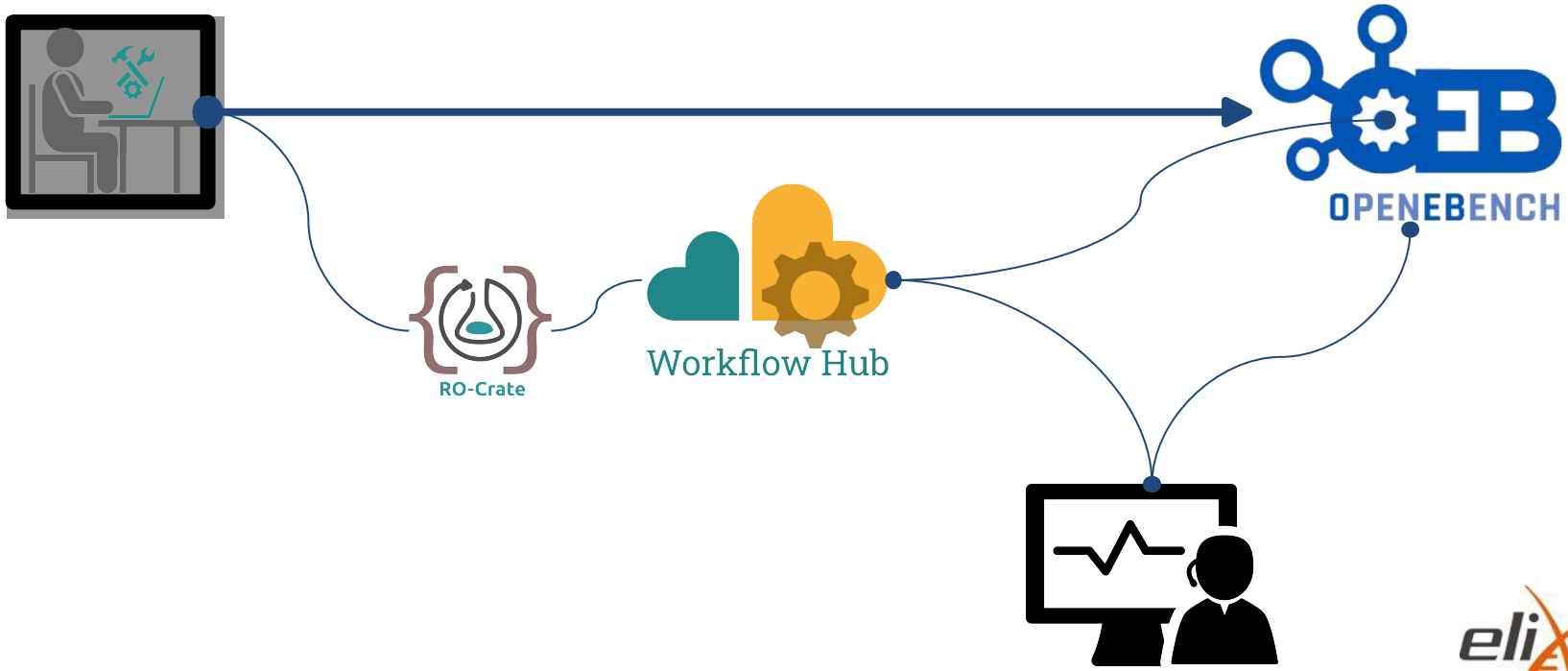
Running the benchmarking in the **OpenEBench Virtual Research Environment (VRE)**

Run same workflow in OpenEBench VRE

https://openebench.bsc.es/vre

Scientific benchmarking in **OpenEBench**

Engagement level 3: Participants' tools execution



Scientific benchmarking in **OpenEBench**

Engagement level 3: Participants' tools execution

The **W**ork**f**low **Ex**ecution **S**ervice backend engine aims to fetch a workflow from a TRS-enabled WorkflowHub instance, fetch the inputs (which should be reachable through URLs) and workflow execution engine, and execute the workflow in a secure way.

Scientific benchmarking in **OpenEBench**

Engagement level 3: Participants' tools execution

The **W**ork**f**low **Ex**ecution **S**ervice backend engine aims to fetch a workflow from a TRS-enabled WorkflowHub instance, fetch the inputs and workflow execution engine, and execute the workflow in a secure way.

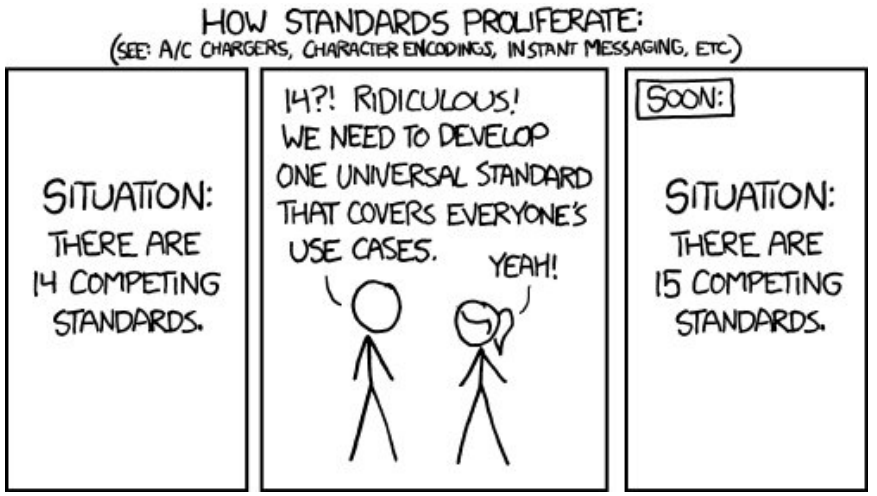
Compatible with **RO-Crate** and GA4GH cloud workstream specifications (TRS/WES/TES):

- Materialize **Nextflow** and **CWL** workflows from WorkflowHub.
- Materialize remote repositories that contain the materialized workflows.
- Materialize inputs and reference data to launch workflows.
- Setup **Nextflow** and **CWL** engines (currently working with Nextflow and cwltool).
- Validate workflows and materialize their containers (Docker and Singularity).
- Launch the workflows in an execution environment.
- Create execution provenance.
- Generate **RO-Crate** from execution provenance.

Scientific benchmarking in **OpenEBench**

Engagement level 3: Participants' tools execution

… still, we need a back-end engine that be able to interpret RO-Crate and execute any workflow contained within.



… we are not developing (or proposing to develop) the 300th workflow manager.

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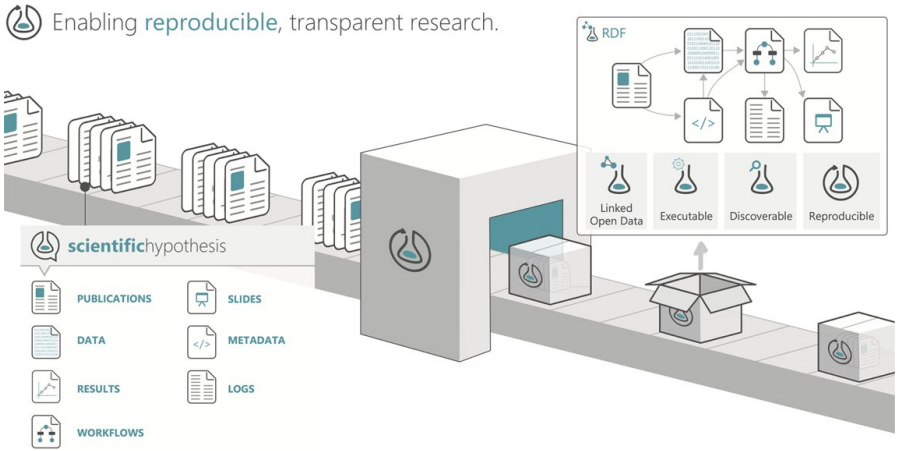
Engagement level 3: Participants' tools execution



RO-Crate is a mechanism to bundle digital objects semantic metadata.
It offers the flexibility of being a single digital object that encapsulates relevant metadata and data (or link to them). The target for workflow executions are the workflow and execution provenance: software containers, input and output datasets (along with their public ids), etc...

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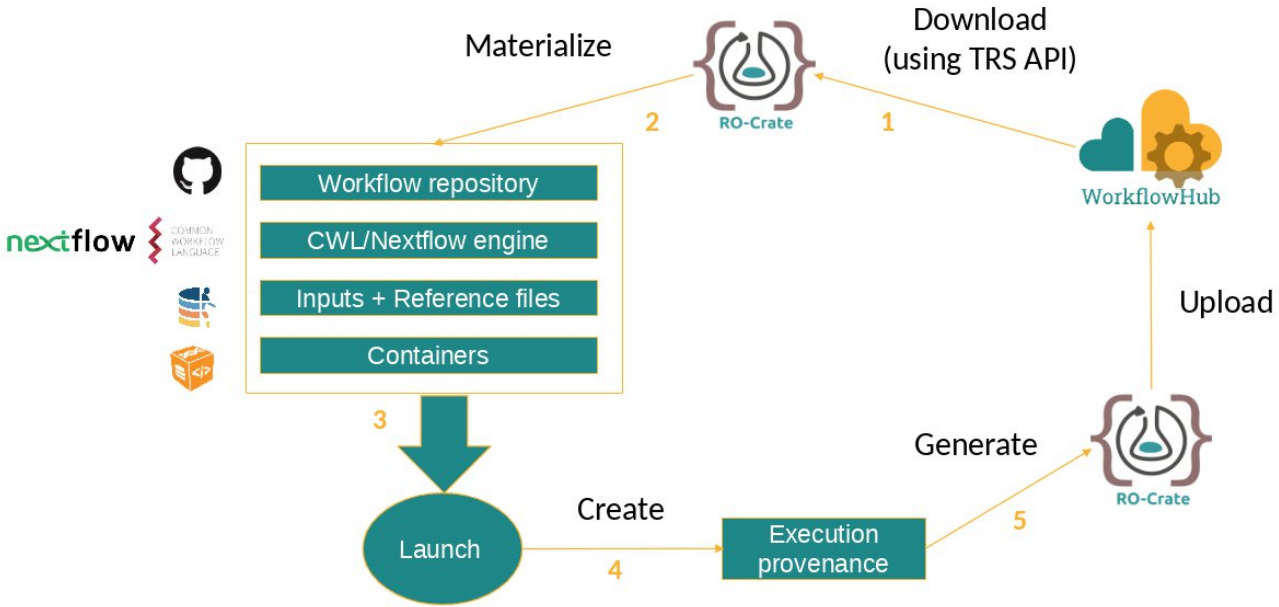
Engagement level 3: Participants' tools execution

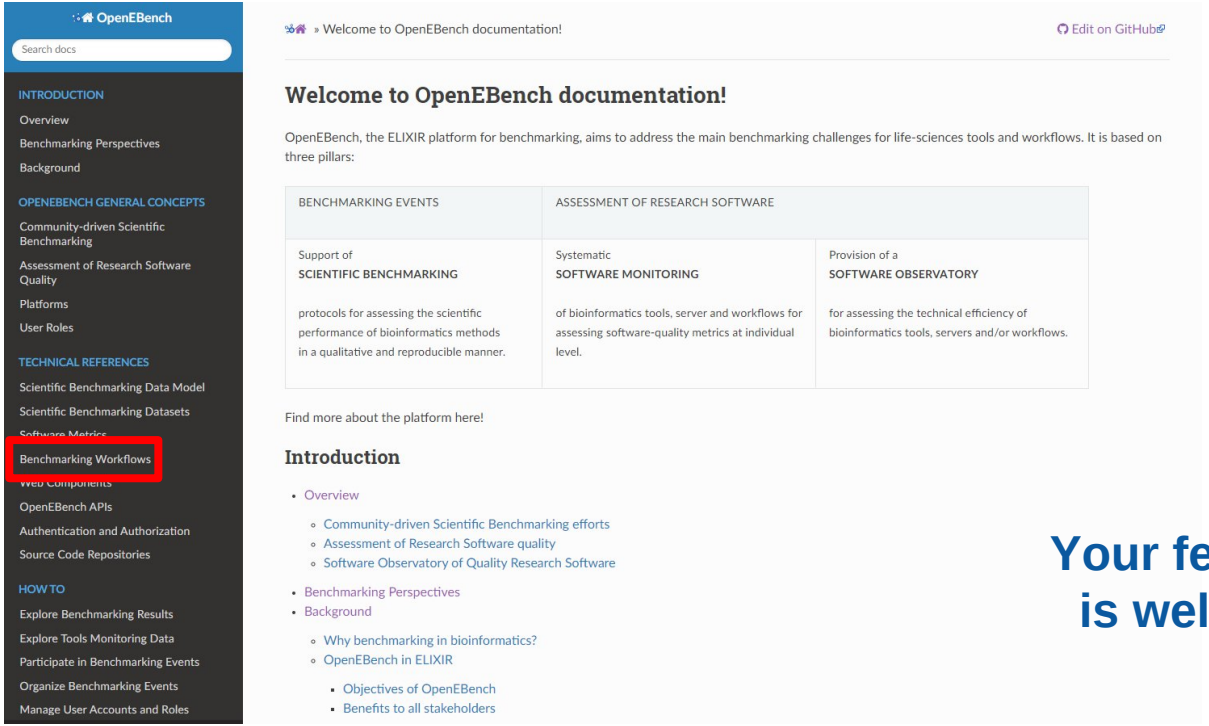


Demo case on the execution of the selected workflow https://asciinema.org/a/452404
Back-end engine installation https://asciinema.org/a/452311
Rootless singularity (advanced) https://asciinema.org/a/452320
Workflow execution files (old) https://asciinema.org/a/385268

HANDS-ON EXERCISE 2

Running TCGA workflow with WfExS

Want to know more about OpenEBench?



Your feedback is welcome!

https://openebench.readthedocs.io/en/latest/

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INB/ELIXIR-ES Coordination Team
INB/ELIXIR-ES Computational Team

Reach out to us at openebench-support@bsc.es

Thank you