



# OpenEBench: the ELIXIR benchmarking platform



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# Index

- **Why benchmarking?**
- **OpenEBench approach to reproducible benchmarking**
  - OpenEBench platform
  - Levels of engagement
  - OpenEBench benchmarking process
  - Hands-on exercise 1
- **WfExS: A workflow execution service**
  - How does WfExS fit in OpenEBench?
  - RO-Crate and WorkflowHub
  - Hands-on exercise 2

EVALUATION METRICS INDICATOR OPERATIONAL

TECHNICAL COMPARE SPECIFIC IDENTIFY

UNIT FINANCIAL MANAGEMENT SURVEY TOOLS

PROCESS RESULT

BUSINESS PERFORMANCE INDUSTRY PROCEDURE IMPROVEMENT

COST PLAN METHODOLOGY

BEST PRACTICES TARGET

STRATEGIC

# BENCHMARKING

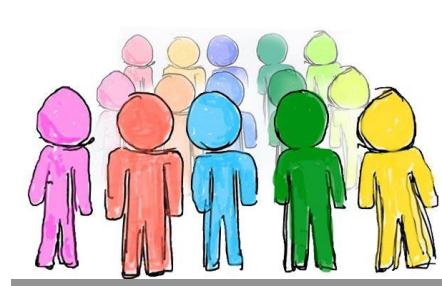
INFORMATION ENERGY TIME ASPECT

QUALITY

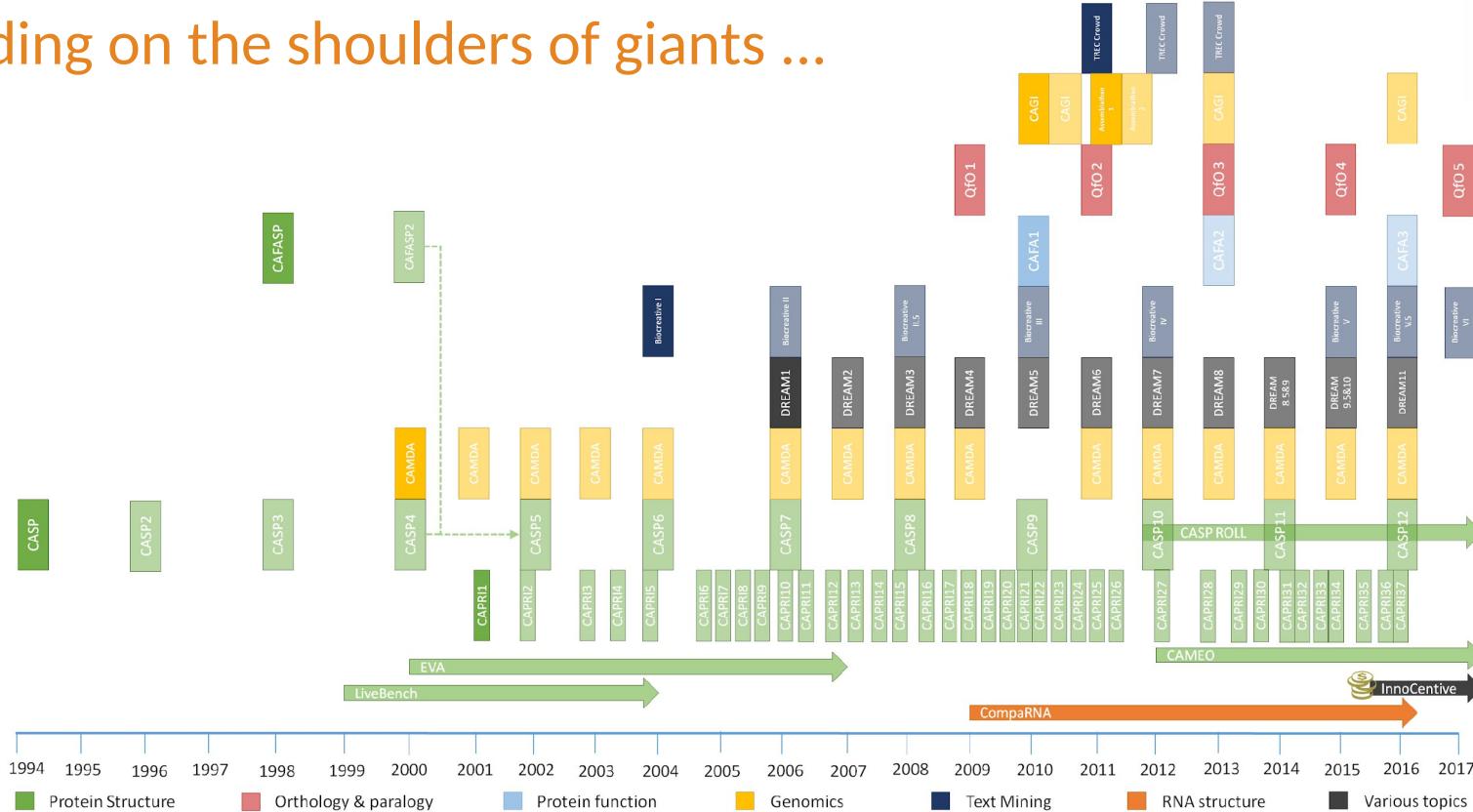
The logo for elair, featuring the word "elair" in a stylized orange font with a red swoosh graphic above it.

## 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

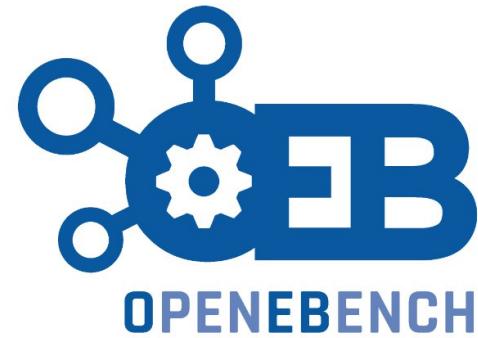


To drive the development of execution platforms (e.g. Galaxy) and ensure integration with *bio.tools*, OpenEBench, and workflows using CWL



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.



Scientific Benchmark

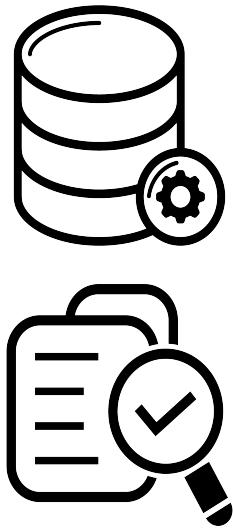


Technical Monitoring

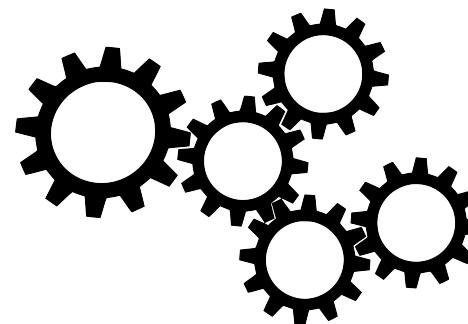
<https://openebench.bsc.es>



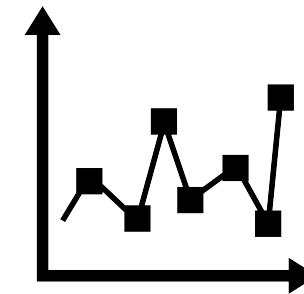
# Scientific benchmarking in OpenEBench



Datasets



Evaluation  
Metrics

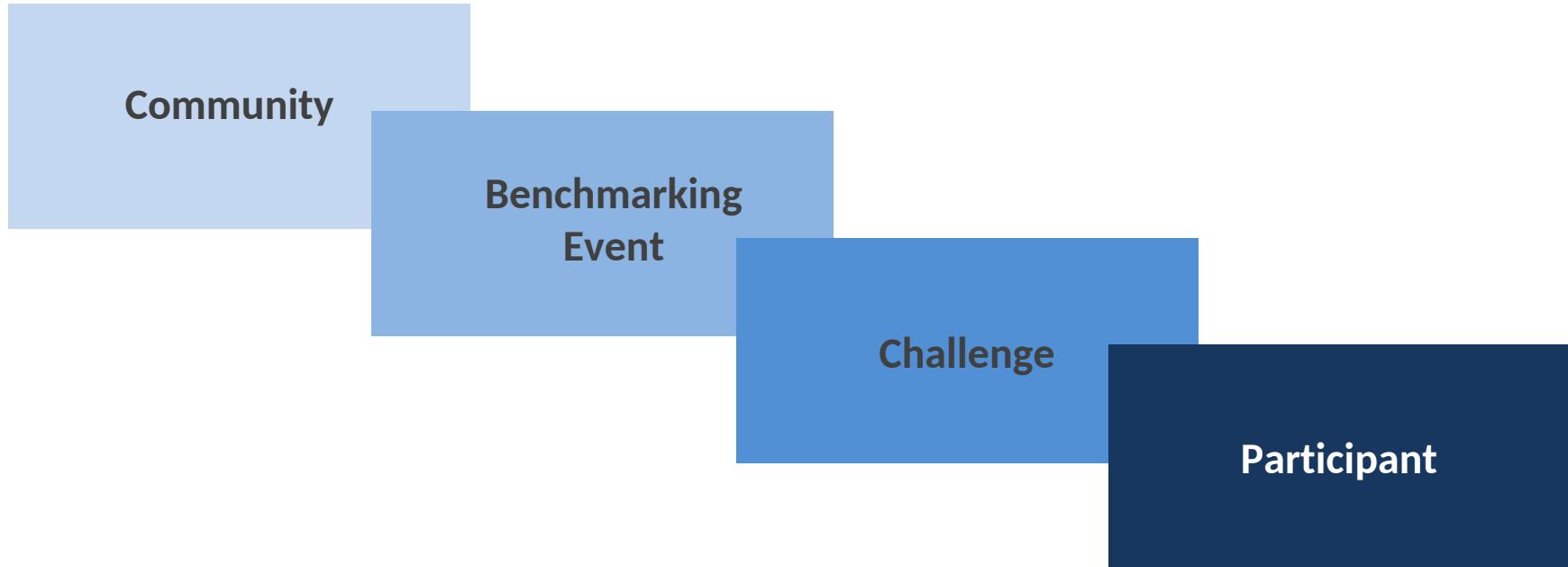


Results  
Interpretation



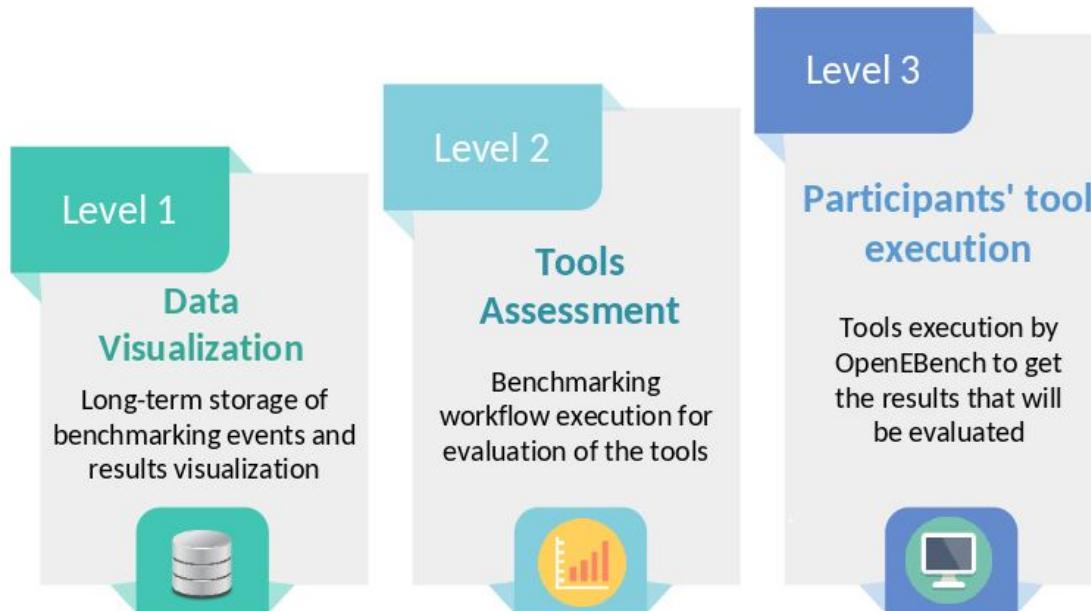
# Scientific benchmarking in OpenEBench

## How OpenEBench is organized



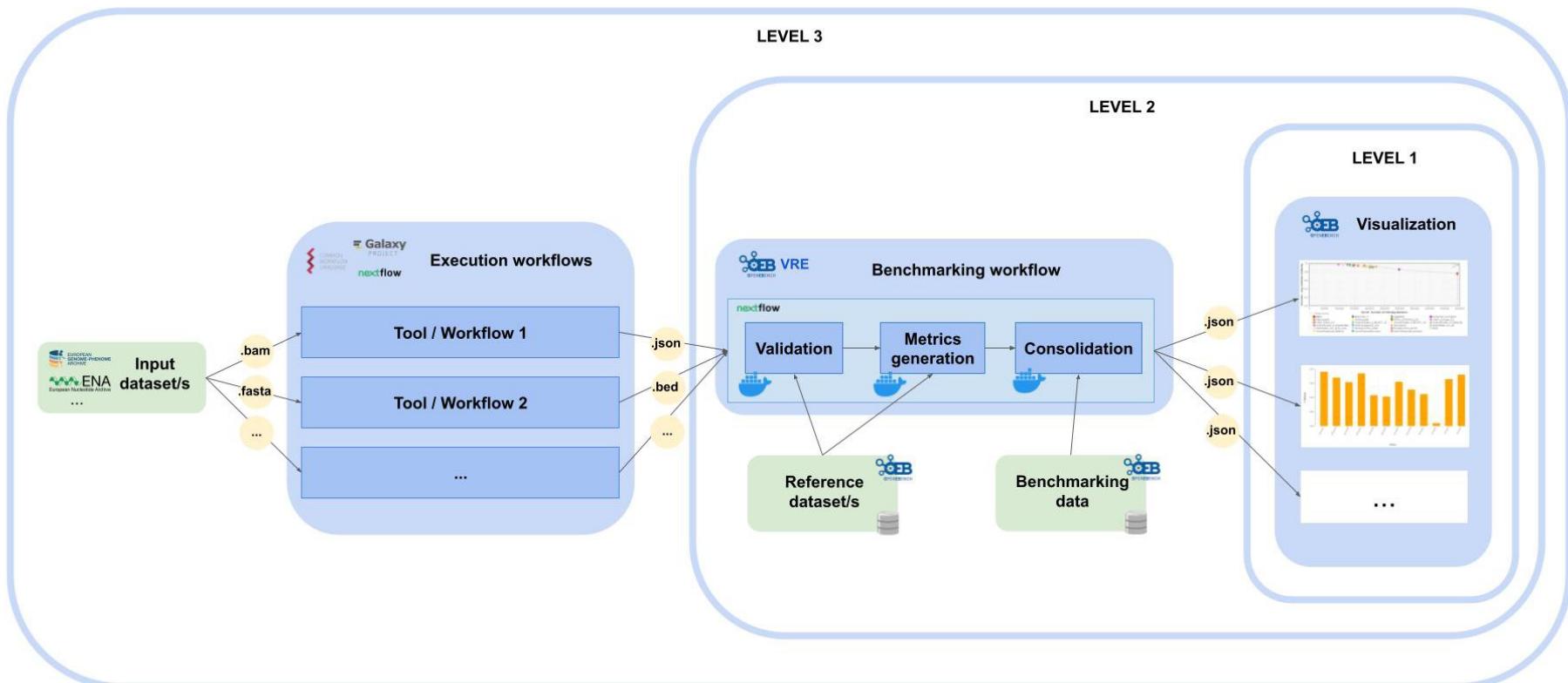
# Scientific benchmarking in OpenEBench

## Levels of engagement



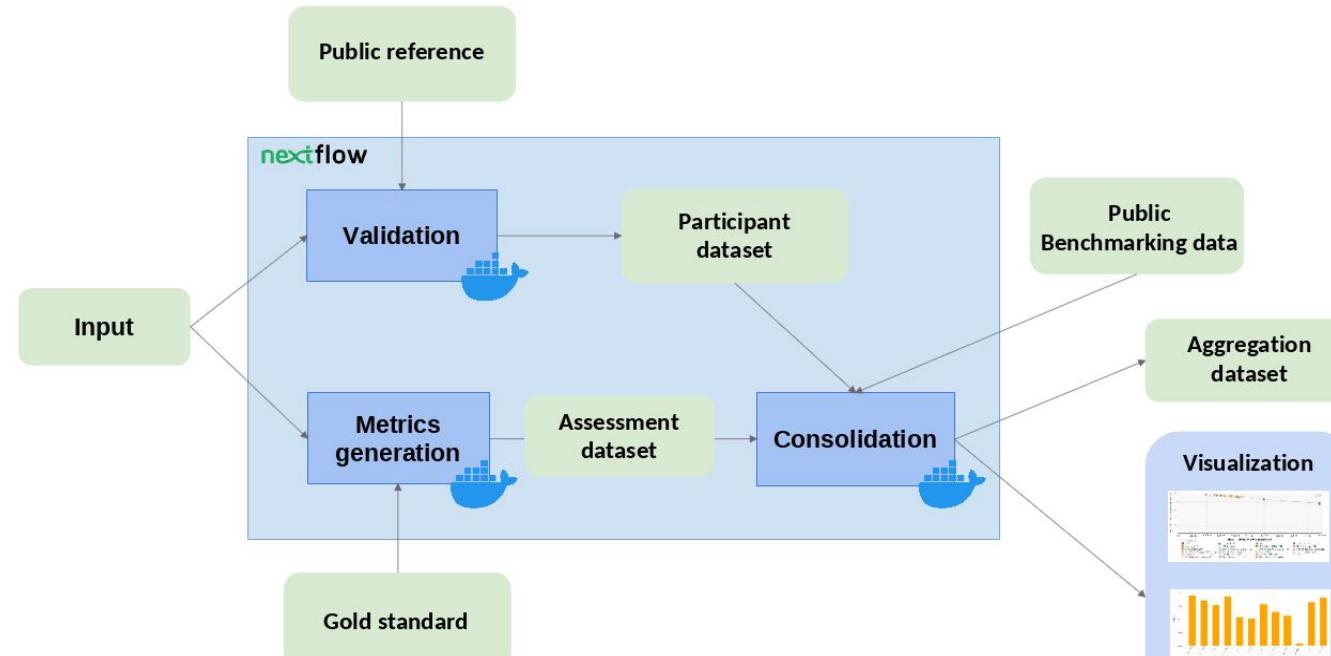
# Scientific benchmarking in OpenEBench

## Benchmarking process



# Scientific benchmarking in OpenEBench

## Benchmarking workflow



[https://github.com/inab/TCGA\\_benchmarking\\_workflow](https://github.com/inab/TCGA_benchmarking_workflow)  
[https://github.com/inab/TCGA\\_benchmarking\\_dockers](https://github.com/inab/TCGA_benchmarking_dockers)

## HANDS-ON EXERCISE 1

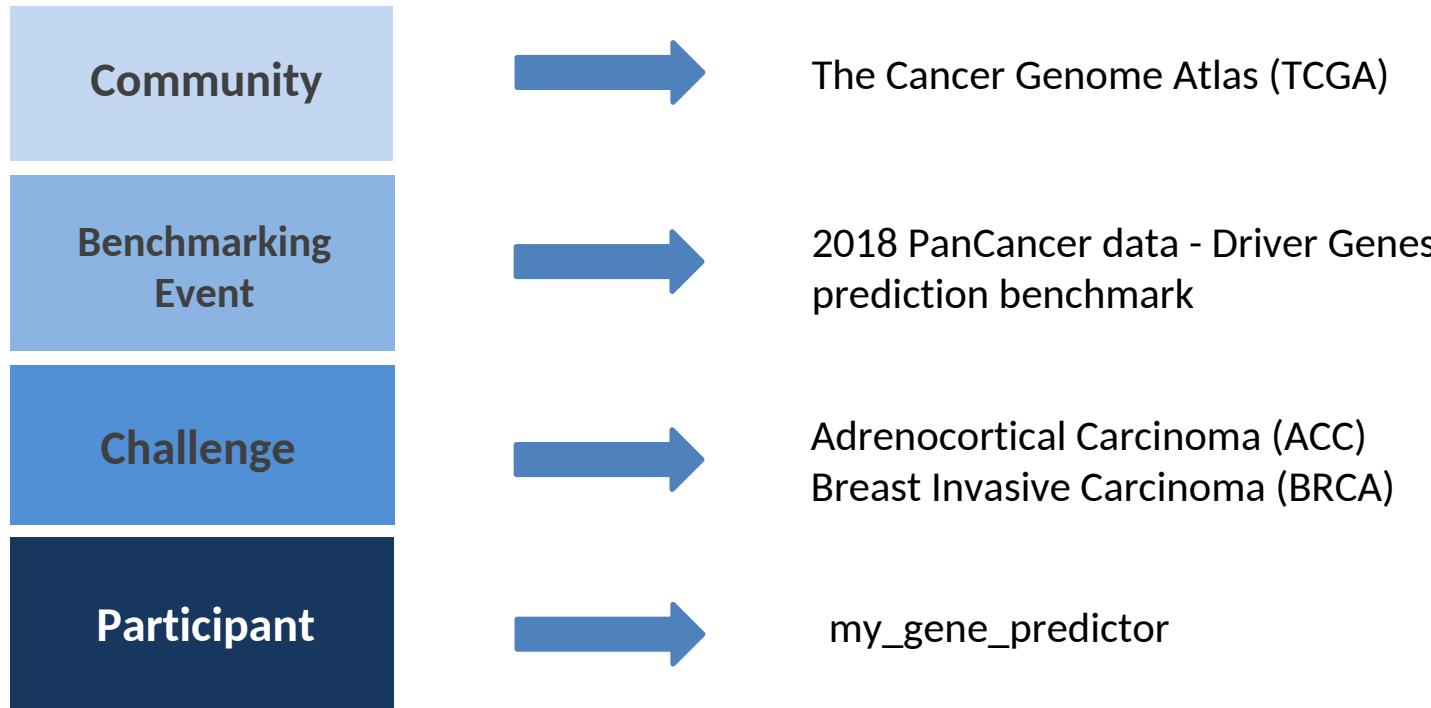
Running the TCGA benchmarking workflow

# 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:

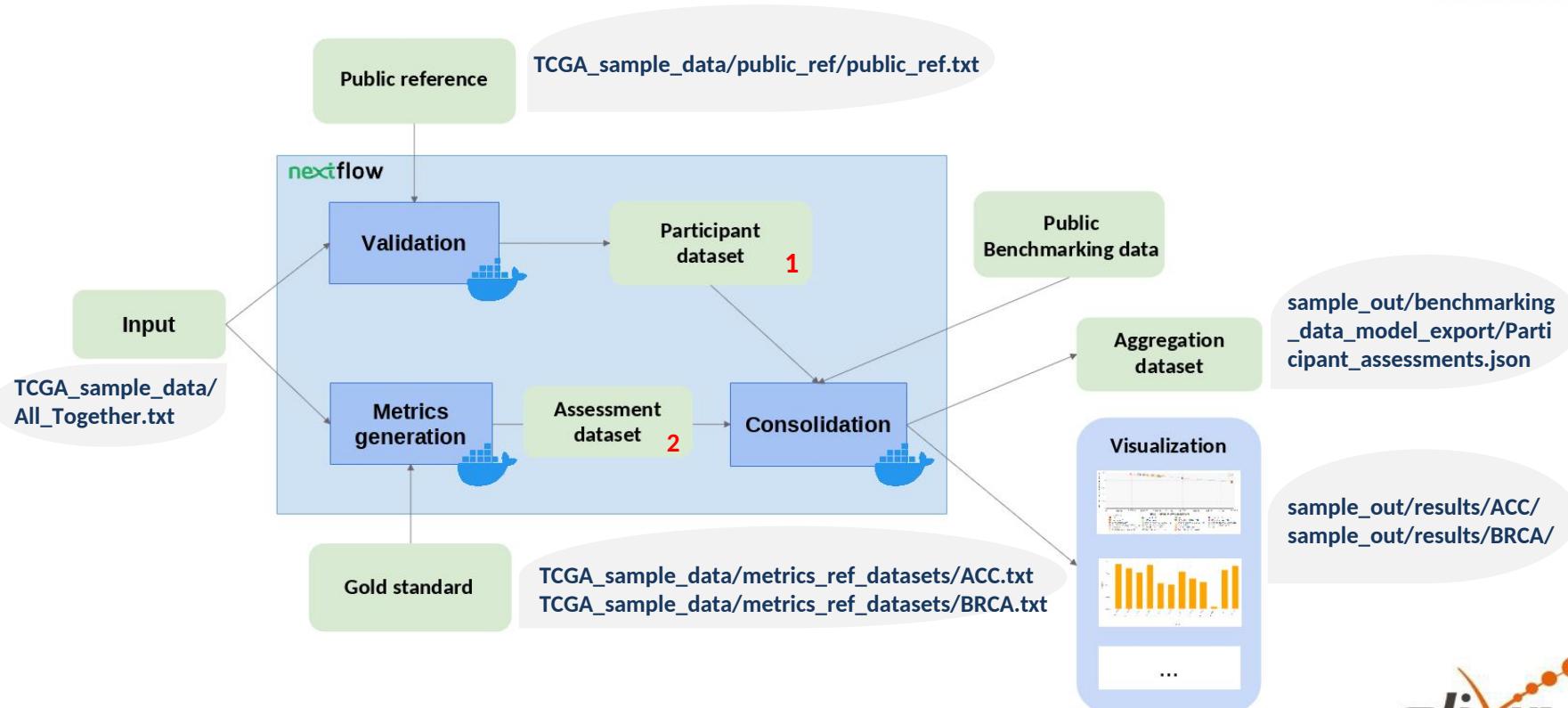
- Git
- Docker
- Nextflow ≥ 19.10.0 (it requires Bash ≥ 3.2 and Java ≥ 8 and ≤ 17 )

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)

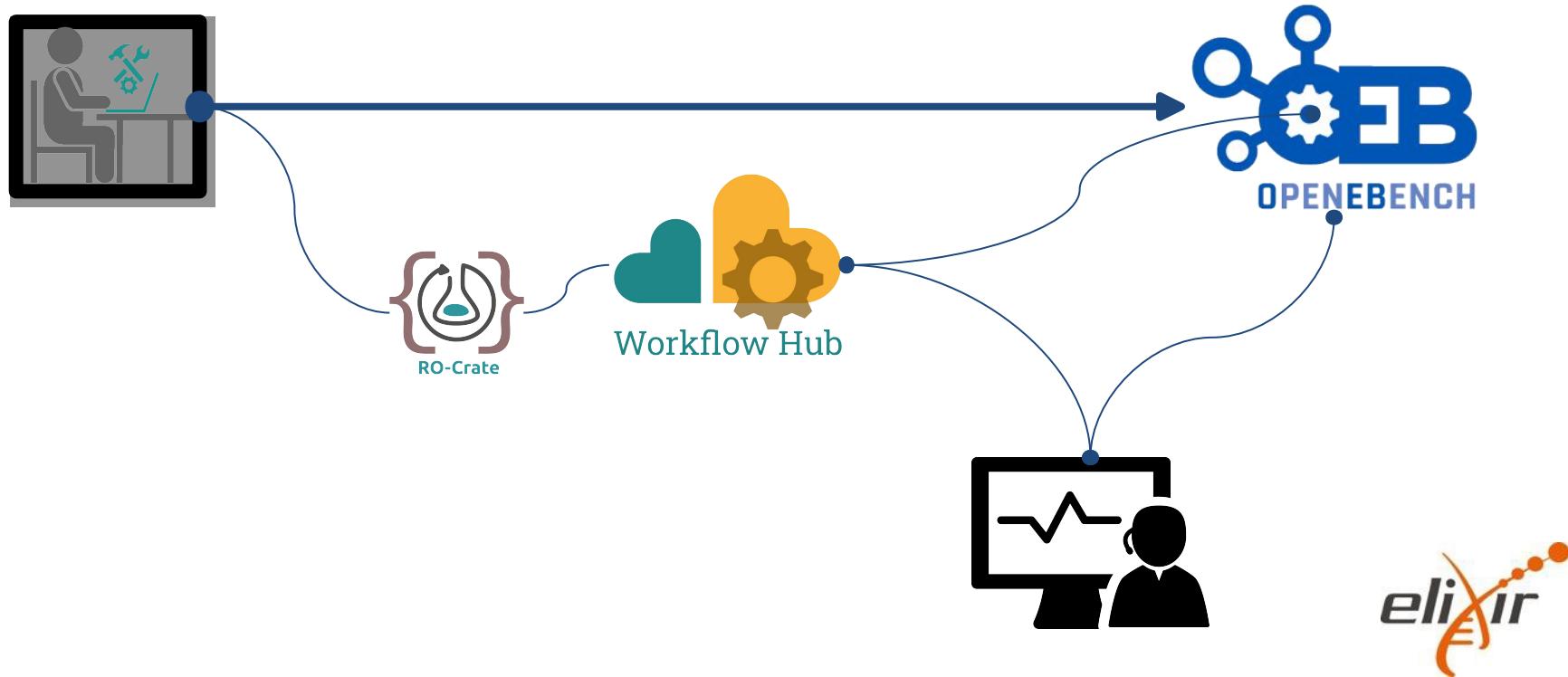
**Run same workflow in OpenEBench VRE**

<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 **Workflow Execution Service** 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 **Workflow Execution Service** 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):

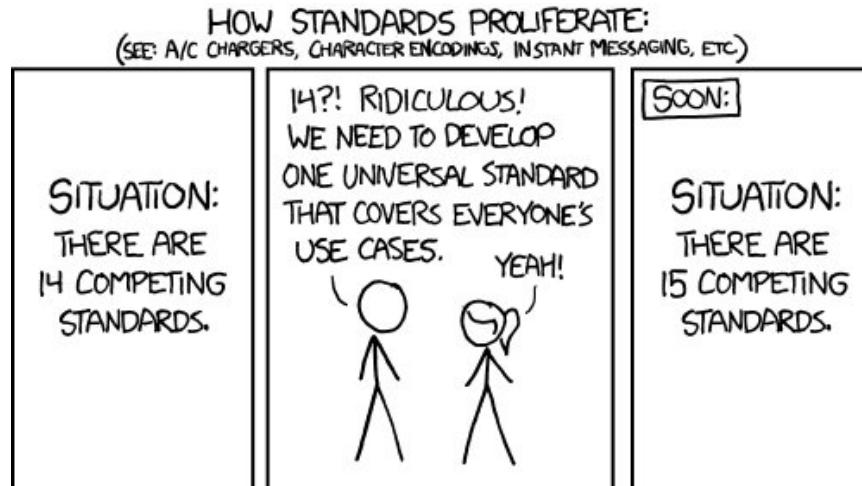
- Materialize **Nextflow** and **CWL** workflows from WorkflowHub.
- Materialize remote repositories that contain the materialized workflows.
- Materialize inputs and reference data to launch workflows.
- Setup **Nextflow** and **CWL** engines (currently working with [Nextflow](#) and [cwltool](#)).
- 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

Wf Ex S

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

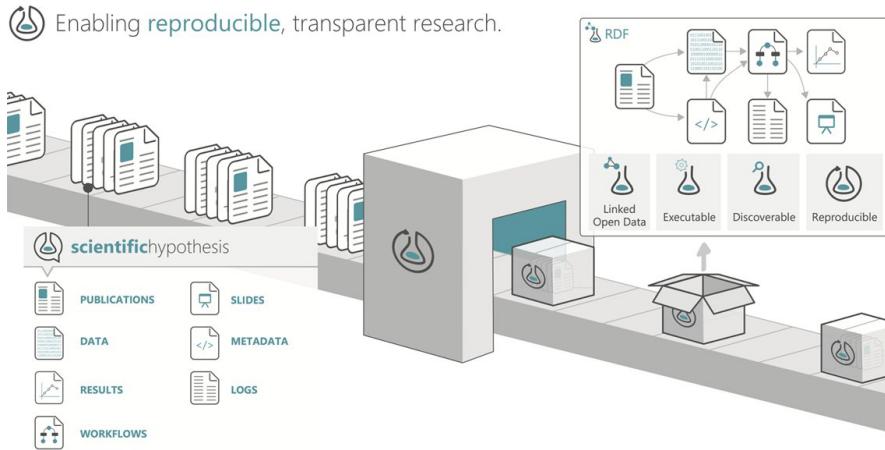


... we are not developing (or proposing to develop) the 300<sup>th</sup> workflow manager.

# Scientific benchmarking in OpenEBench

## Engagement level 3: Participants' tools execution

Wf Ex S

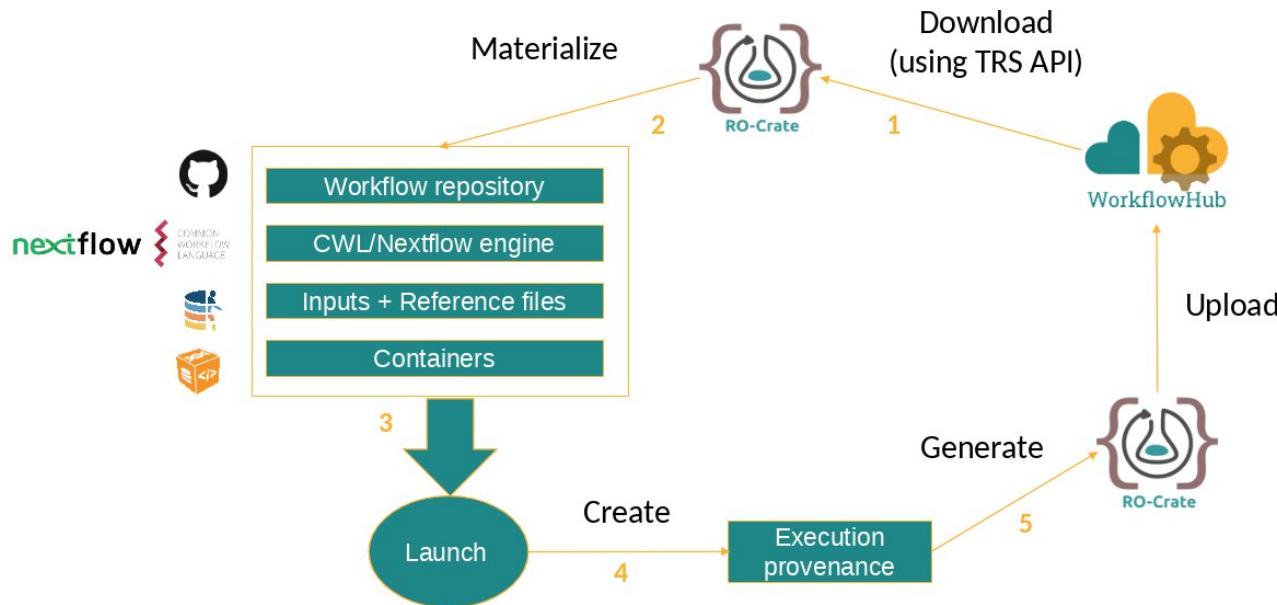


RO-Crate is a mechanism to bundle digital objects semantic metadata.

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...

# Scientific benchmarking in OpenEBench

## 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?

OpenEBench

Search docs

INTRODUCTION

- Overview
- Benchmarking Perspectives
- Background

OPENEBENCH GENERAL CONCEPTS

- Community-driven Scientific Benchmarking
- Assessment of Research Software Quality
- Platforms
- User Roles

TECHNICAL REFERENCES

- Scientific Benchmarking Data Model
- Scientific Benchmarking Datasets
- Software Metrics
- Benchmarking Workflows**

WEB COMPONENTS

- OpenEBench APIs
- Authentication and Authorization
- Source Code Repositories

HOWTO

- Explore Benchmarking Results
- Explore Tools Monitoring Data
- Participate in Benchmarking Events
- Organize Benchmarking Events
- Manage User Accounts and Roles

» Welcome to OpenEBench documentation!

[Edit on GitHub](#)

## Welcome to OpenEBench documentation!

OpenEBench, the ELIXIR platform for benchmarking, aims to address the main benchmarking challenges for life-sciences tools and workflows. It is based on three pillars:

BENCHMARKING EVENTS	ASSESSMENT OF RESEARCH SOFTWARE	
Support of <b>SCIENTIFIC BENCHMARKING</b>  protocols for assessing the scientific performance of bioinformatics methods in a qualitative and reproducible manner.	Systematic <b>SOFTWARE MONITORING</b>  of bioinformatics tools, server and workflows for assessing software-quality metrics at individual level.	Provision of a <b>SOFTWARE OBSERVATORY</b>  for assessing the technical efficiency of bioinformatics tools, servers and/or workflows.

Find more about the platform [here!](#)

### Introduction

- Overview
  - Community-driven Scientific Benchmarking efforts
  - Assessment of Research Software quality
  - Software Observatory of Quality Research Software
- Benchmarking Perspectives
- Background
  - Why benchmarking in bioinformatics?
  - OpenEBench in ELIXIR
    - Objectives of OpenEBench
    - Benefits to all stakeholders

Your feedback  
is welcome!

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





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INB/ELIXIR-ES Computational Team

Reach out to us at [openebench-support@bsc.es](mailto:openebench-support@bsc.es)



Thank you