

# Reproducibility of workflows and containers at OpenEBench

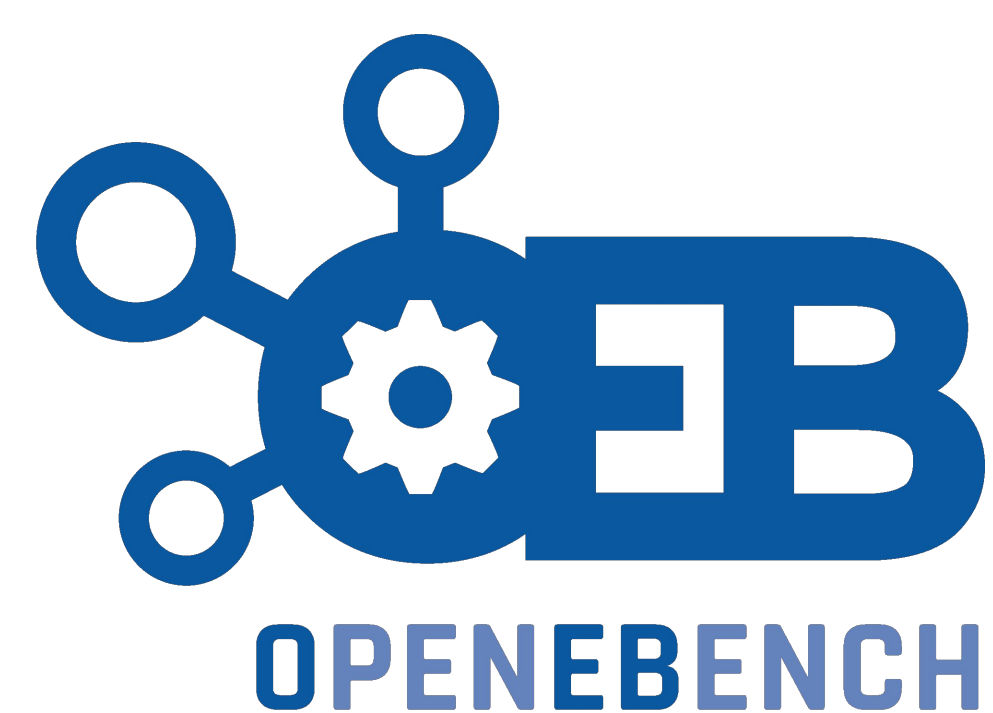


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## <https://openebench.bsc.es>

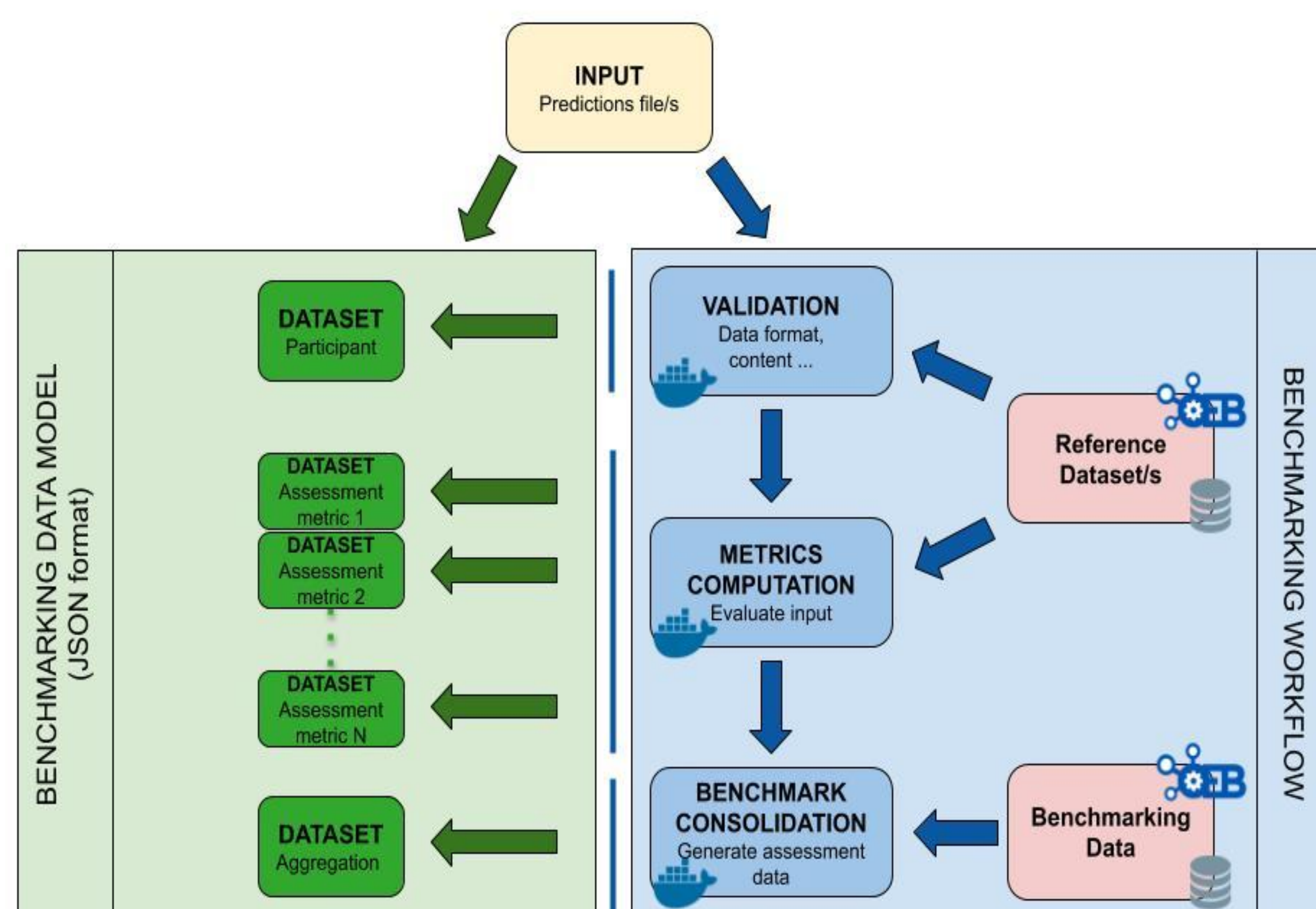
OpenEBench is designed to establish an automated benchmarking system for bioinformatics tools, web servers and workflows. Gathered results help users to choose the most suitable software for the problem at hand, and they provide a reference to developers when they want to improve their methods.

One of the main issues in benchmarking nowadays is the low reusability of its workflows and components, mainly due to lack of standardization, ambiguity in tools and parameters, as well as problems in sharing and maintenance. Also, the proposed workflows are usually not well specified, making it complicated to understand the flow and utilization of data.

## Benchmarking workflows standardization:

We are addressing those limitations in our infrastructure by defining **reproducible, reusable and interoperable** benchmarking workflows in order to make those challenges available to the scientific community. This can be achieved by standardizing the required steps any benchmark challenge needs (Figure 1). On the other hand, we also recommend the usage of workflow managers such as Nextflow for its implementation, as well as software container technologies such as Docker or Singularity (with stable base images that enable reproducibility of those workflows across time).

The usage of those technologies together with the specification of expected input and output parameters, allows to easily deploy any benchmarking workflow in the **OpenEBench' Virtual Research Environment** (<https://openebench.bsc.es/vre>), where end-users can automatically test their methods and compare themselves against the rest of members in the community. What is more, if the workflow outputs are also standardized (Figure 1), the results can be automatically exported to our benchmarking data model, thus, enabling their long-term storage and sharing.



**Figure 1. OpenEBench Workflows architecture.** Based in three conceptual blocks (blue boxes): 1 - **Validation and preprocessing**: the input file format is checked and, if required, the content of the file is validated. 2 - **Metrics Computation**: the predictions are compared with the 'Gold Standards' provided by the community, which results in one or more performance metrics (e.g. Precision & Recall). 3 - **Results Consolidation**: the benchmark itself is performed by merging the tool metrics with the rest of the community' reference data. Standard output formats are also specified (green boxes) for compatibility with Benchmarking Data Model (<https://github.com/inab/benchmarking-data-model>).

Regarding the creation and use of a **benchmarking ontology** (<https://github.com/inab/OEB-ontologies>), this effort will allow to provide additional metadata to the data model used in OpenEBench. Such additional metadata will facilitate the data exchange across challenges within the same community and across communities as well as it will provide a formal description of datasets and workflows.

OpenEBench benchmarking workflows system has already been successfully used to run benchmarking experiments in very diverse areas such as on orthology and paralogy predictions e.g. Quest for Orthologs Consortium; and in the identification of cancer driver genes e.g. The Cancer Genome Atlas' Benchmarking group. Moreover, those workflows are supporting ongoing efforts, like some of the DREAM challenges, or the ones by the Spanish Network of Biomedical Research Center on Rare Diseases (CIBERER).

## Workflows submission system:

Once the workflow' steps have been encapsulated in containers, and the parameters have been standardized, those containerized blocks can be reused across different events. Thus OpenEBench is developing a modularized workflow submission system, which allows community managers to specify their benchmarking metrics, containers, parameters through a user-friendly form (Figure 2) which results in an automatically deployed workflow in the Virtual Research Environment.

**Figure 2. VRE workflow submission form.** Community managers can upload their workflows with an easy four-step formulary. First, complete the general information for the workflow (description, workflow engine...), then add generic or custom keywords to make it findable; provide the workflow files contained within a Github Repository, and, finally, specify the parameters and arguments.

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