Integrating data repositories with HPC resources for execution of VHT models

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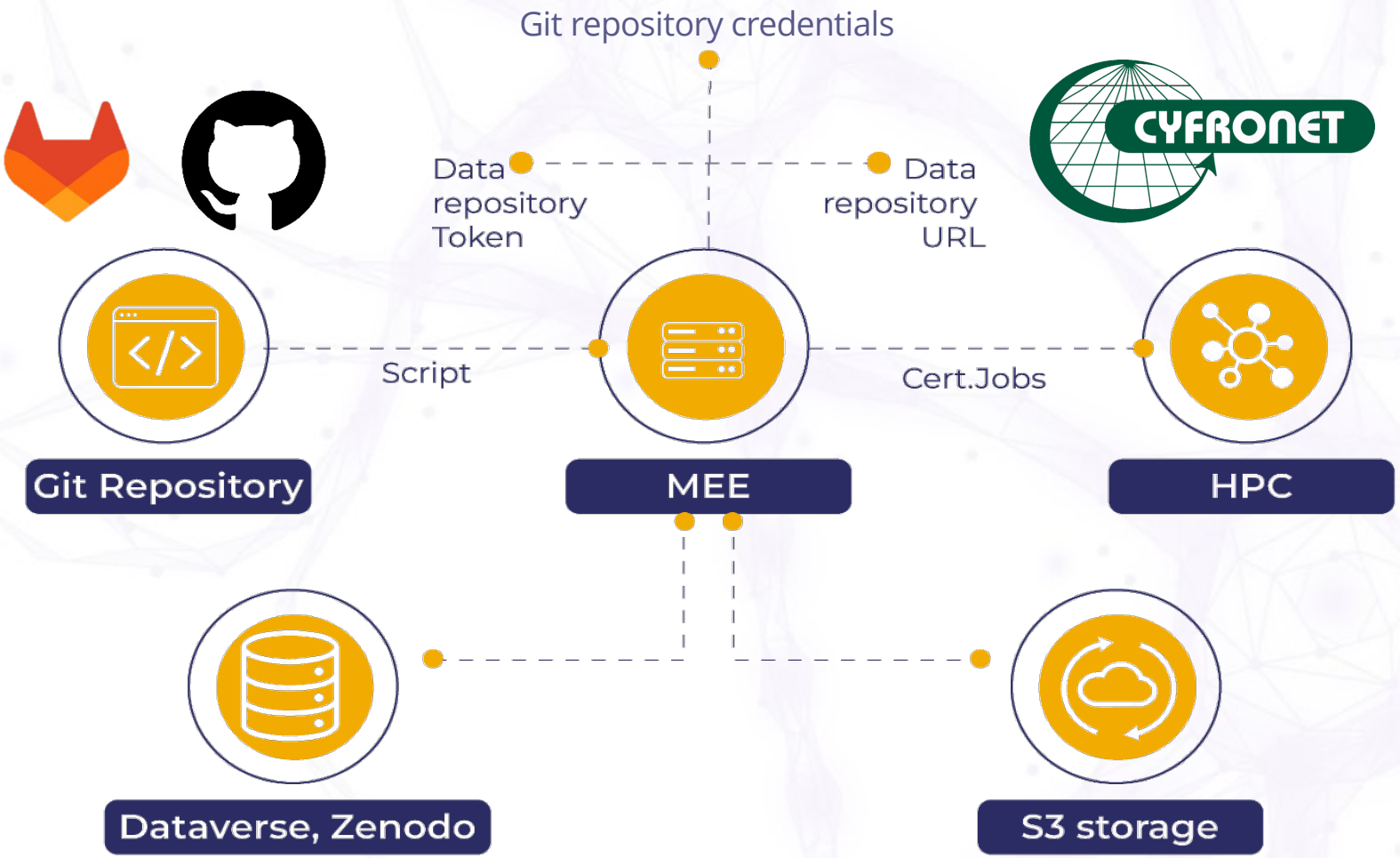
Technical Problems in Research

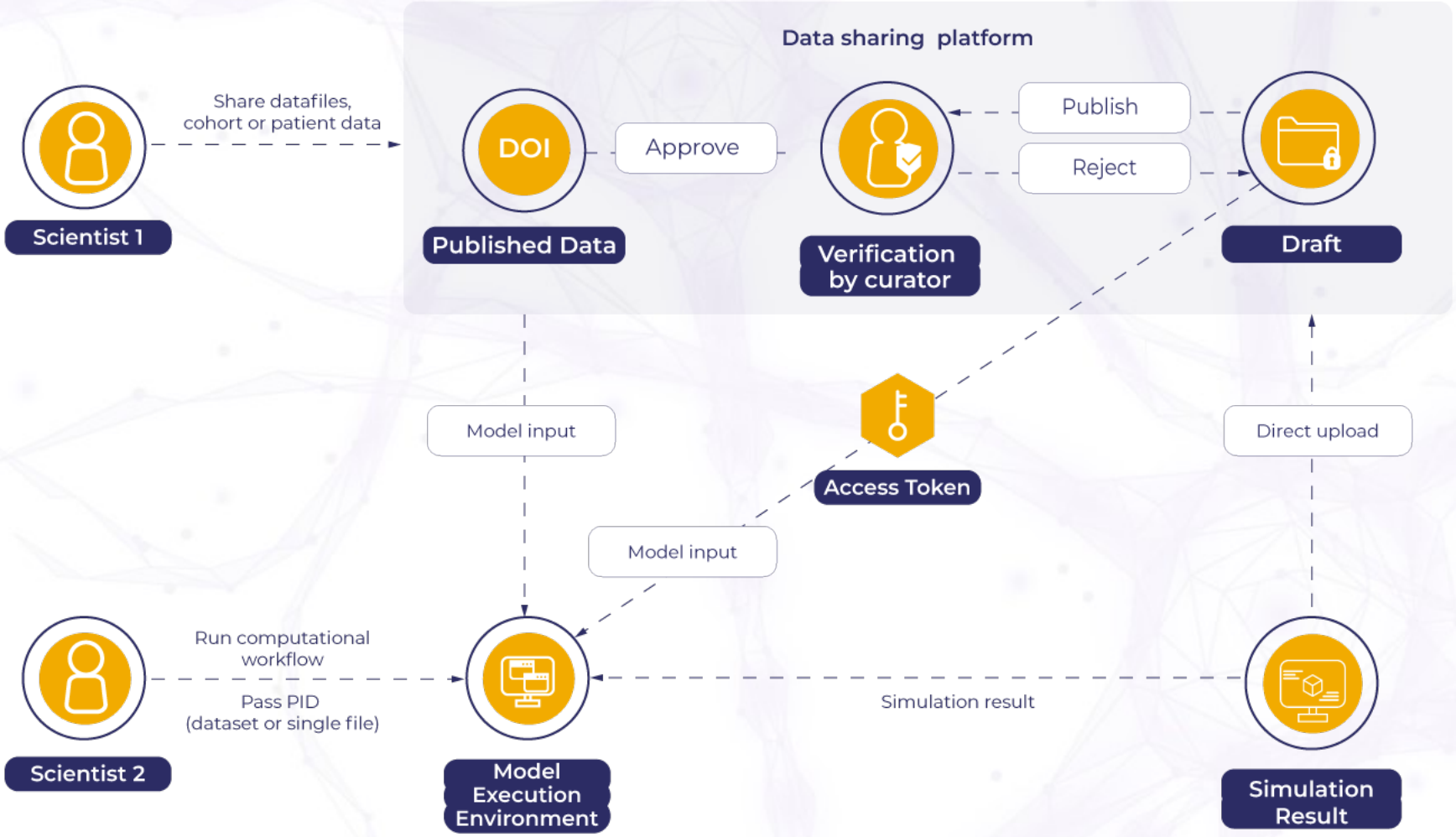
- **Virtual Human Twin** – safe and accurate experiments
- Models require computational power – HPC can help
- HPC is not easy to use for scientists
- Research data has to be **shared** between scientists
- **Publishing** results – supporting open science

Model Execution Environment – the connecting link



- MEE is developed in collaboration with the Academic Computer Centre Cyfronet
- Job execution on HPC using SSH certificates
- User-friendly interface for simulation execution
- Model versioning mechanism with GitHub and GitLab integrations
- Seamless two-way data sharing with Zenodo and Dataverse integrations

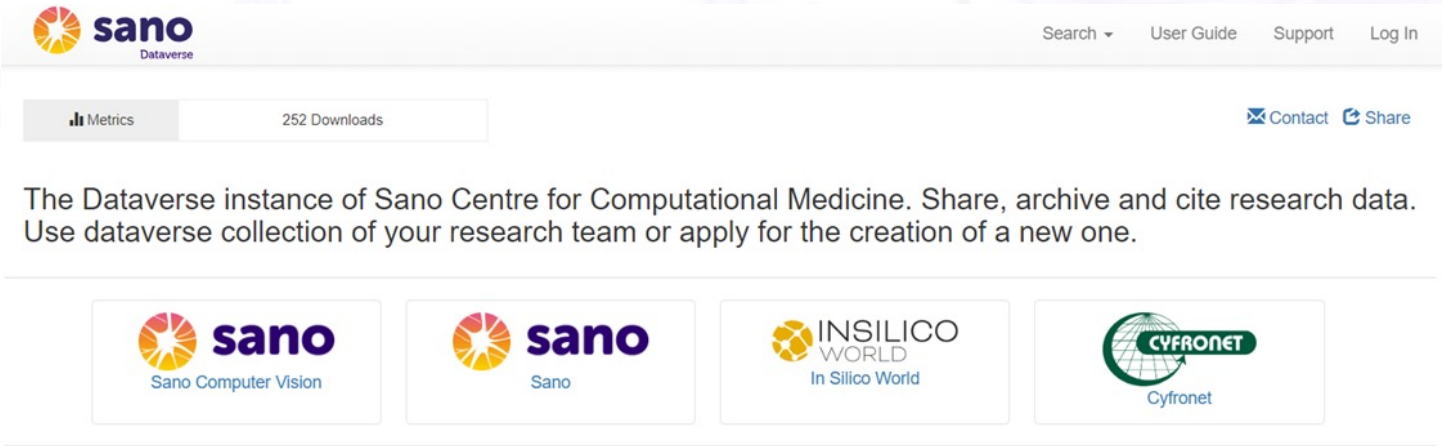
Data repositories and MEE – Example workflow



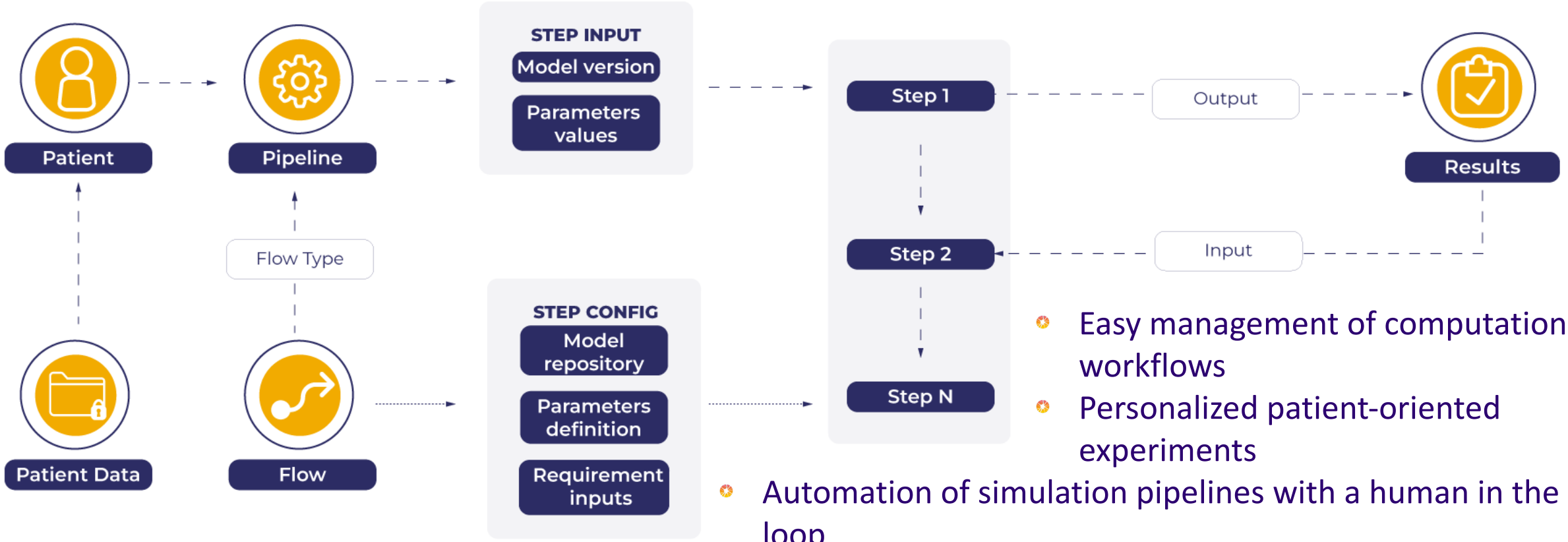
- Allows direct upload to the data-sharing platform
- Allows direct download of datasets and files as model inputs
- Datasets are verified before publication, but unpublished versions can still be used
- If a dataset is in draft form, an access token is required

Sano's Dataverse Instance

- Hosted for Sano research teams and project partners
- DataCite Fabrica account connected to register DOIs
- Joining RODBUK to disseminate datasets and ensure their reliability



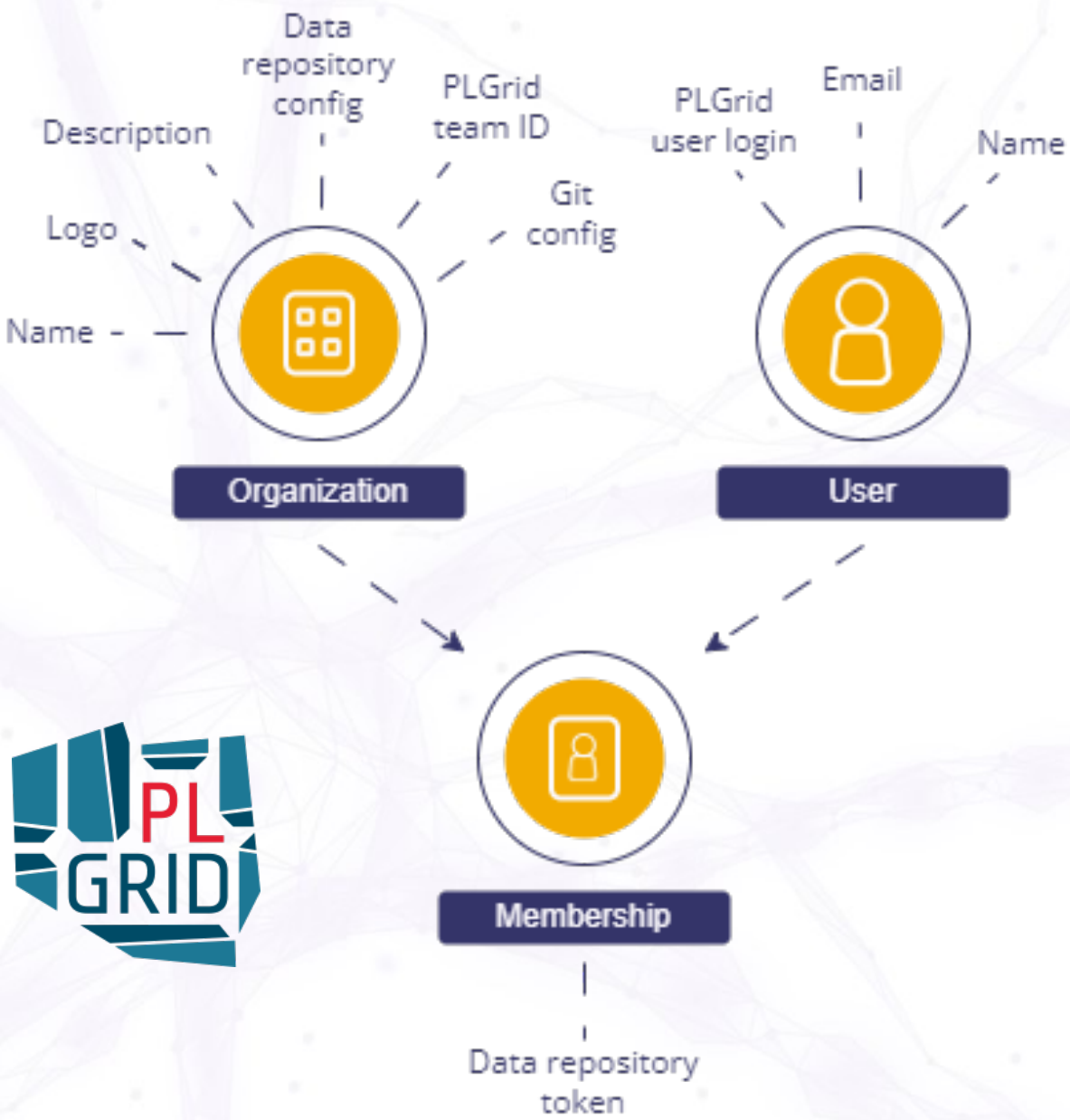
Model Execution Environment



- Easy management of computation workflows
- Personalized patient-oriented experiments
- Automation of simulation pipelines with a human in the loop
- Model versioning and pipeline history revision
- Monitoring execution status and logs of each workflow step
- Text and graphical viewers for visual comparison of results

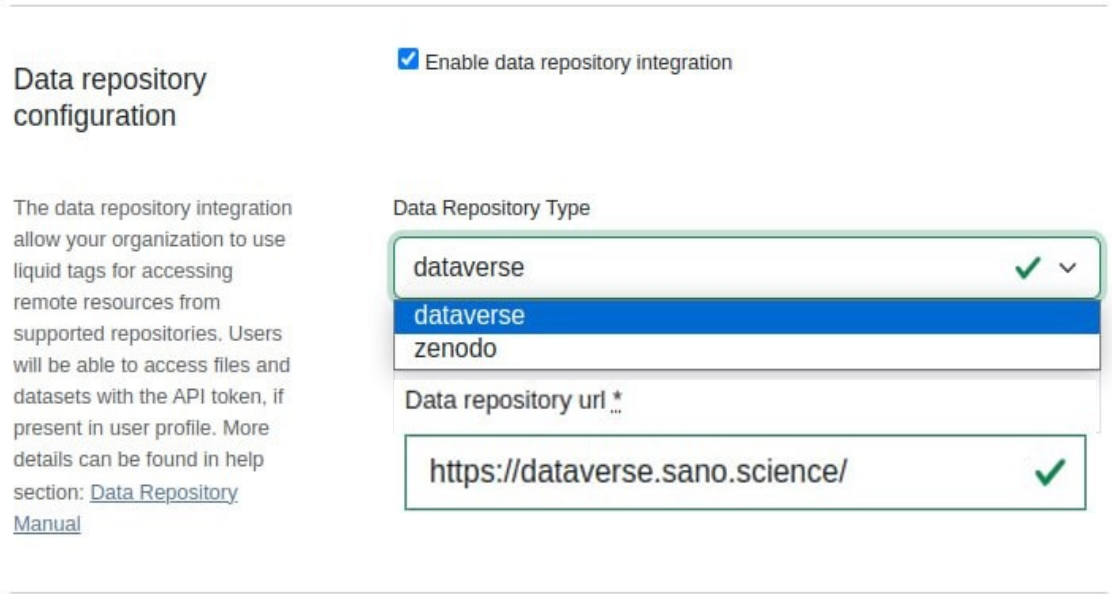
Model Execution Environment

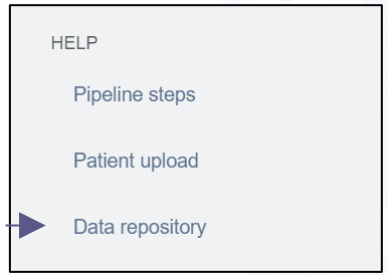
- Access delineation for HPC resources and integrated services
- PLGrid – Polish HPC managing infrastructure
- Membership – connection of a pair of a user with an organization
- Data repository token – API token from a data repository



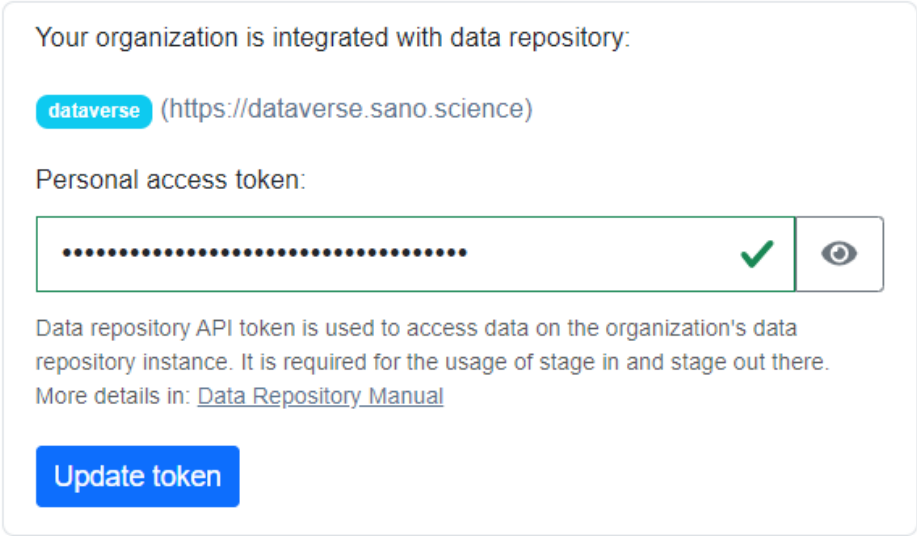
MEE and Data Repository Integration

- Data Repository Instance Configuration
  - In „Organization Details”
  - Configured by admin
- Data repository token
  - Configured only if Data Repository integration in current organization is turned on
  - Unique for every instance
  - Configured by user in each organization





User guide for the integration



MEE and Data Repository Integration

- Script features – liquid tags

```
{% dataverse_file_stage_out filePath persistentID metadata %}

{% dataverse_file_stage_in persistentID target %}

{% dataverse_dataset_stage_in persistentID target %}
```

- **filePath**: The path to the file that you want to upload to Dataverse.
- **persistentID**: The identifier for the target file or dataset in Dataverse, provided in a specific format, for example DOI (e.g., *"doi:10.12326/shoulder/23GF4H"*).
- **metadata**: An optional parameter that can be included in JSON format to provide additional file metadata. **(OPTIONAL)**
  For example:
  {"directoryLabel":"dir1/subdir","categories":["Data"], "restrict":"false"}
- **target**: The name of the file where downloaded content should be saved.(zip archive in case of dataset downloading) **(OPTIONAL)**

MEE and Data Repository Integration

- Script features – liquid tags

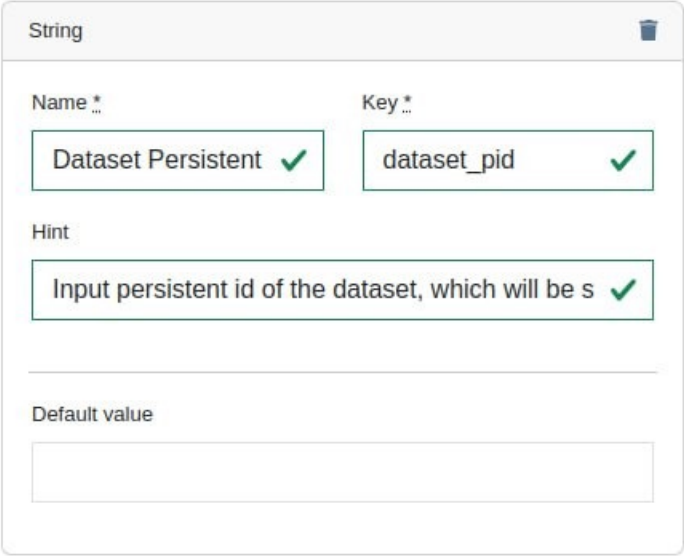
```
{% zenodo_file_stage_out filePath depositID %}

{% zenodo_file_stage_in recordID  filename  target %}

{% zenodo_dataset_stage_in recordID target %}
```

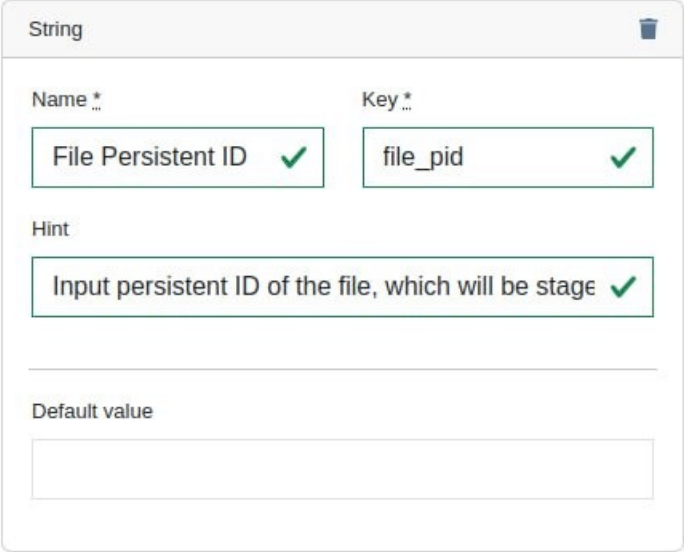
- **filePath**: The path to the file that you want to upload to Zenodo.
- **depositID**: The identifier for the upload deposition in Zenodo (may be unpublished).
- **recordID**: The identifier of the record (dataset) containing the file or a target to upload to in Zenodo .
- **filename**: The filename of the file that you want to download.
- **target**: The name of the file where downloaded content should be saved.(zip archive in case of dataset downloading) **(OPTIONAL)**

Integrated Simulation Workflow

- Example basic script and step configuration

```
echo Download dataset from dataverse
echo --------------------START----------------------------
dataset_pid={% value_of dataset_pid %}
file_pid={% value_of file_pid %}
{% dataverse_dataset_stage_in $dataset_pid %}
echo "Downloaded dataset"
{% dataverse_file_stage_in $file_pid %}
echo "Downloaded file"
echo --------------------END------------------------------

find . -type f -name "*.txt" -exec cat {} + > merged.out


echo Uploading results
echo --------------------START----------------------------
{% dataverse_file_stage_out merged.out $dataset_pid %}

{% dataverse_file_stage_out merged.out $dataset_pid {"description":"My description.",
"directoryLabel":"dataverse/subdir1","categories":["Data", "Dummy File"],
"restrict":"false", "tabIngest":"false", "jshfdbv":"sjhfd"} %}

echo --------------------END------------------------------
echo Finish
```





Integrated Simulation Workflow

- Example input and simulation result

Citation Metadata

Persistent Identifier	doi:10.82726/sano/GE7NAW
Publication Date	2023-07-26
Title	UISS-COVID19 Datafiles
Author	Zajac, Karol (Sano) - ORCID: 0000-0003-1393-8236
Point of Contact	
Description	
Subject	
Keyword	
Depositor	
Deposit Date	

dataverse_step

dataverse_step finished successfully, results stored in the outputs directory.

Computation details

Start time	27 Feb 15:45
Site	Ares
Revision	3f95751e3c0f937566fca9cfa62d9f0cc9354a2d
Execution time	00h 00m 19s
Outputs	stdout, stderr
Status	Finished

Saved parameter values

Model version	main
Dataset Persistent ID	doi:10.82726/sano/GE7NAW
File Persistent ID	doi:10.82726/sano/WOGMAR/8F9V3H
Grant	plgsano4-cpu

File Metadata

Preview

doi:10.82726/sano/WOGMAR/8F9V3H

Use the Download URL in a Wget command or a download manager to avoid interrupted downloads, time outs or other failures. User Guide - Downloading via URL

`https://dataverse.sano.science/api/access/datafile/:persistentId?persistentId=doi:10.82726/sano/WOGMAR/8F9V3H`

b8fe52d04d06845f2af9107f0b15b44d

2023-11-13

ate 2023-11-13

2023-11-13

1.0 KB

XML

Integrated Simulation Workflow

- Outcome on the repository

1 to 3 of 3 Files | Edit Files | Download

datafile_test_mild_moderate
Plain Text - 4.5 KB
Published Jul 26, 2023
42 Downloads
MD5: 569...273
Simply mild moderate

datafile_test_mild_moderate+47D11_therapeutic
Plain Text - 4.5 KB
Published Jul 26, 2023
13 Downloads
MD5: 826...34c
47D11 Treatment

datafile_vaccine+challenge
Plain Text - 4.7 KB
Published Jul 26, 2023
10 Downloads
MD5: 85a...749
Vaccine and challange

1 to 5 of 5 Files | Edit Files | Download

datafile_test_mild_moderate
Plain Text - 4.5 KB
Published Jul 26, 2023
42 Downloads
MD5: 569...273
Simply mild moderate

datafile_test_mild_moderate+47D11_therapeutic
Plain Text - 4.5 KB
Published Jul 26, 2023
13 Downloads
MD5: 826...34c
47D11 Treatment

datafile_vaccine+challenge
Plain Text - 4.7 KB
Published Jul 26, 2023
10 Downloads
MD5: 85a...749
Vaccine and challange

merged.out
Unknown - 0 B
Deposited Feb 27, 2024
MD5: d41...27e

merged.out
dataverse/subdir1/
Unknown - 0 B
Deposited Feb 27, 2024
MD5: d41...27e
My description.
Data | Dummy File

Current and Future Goals

- Large amounts of simulation data can be managed through external data repository integration
- Extreme-scale simulations are performed on MEE within the InSilicoWorld project
- Planning to make Sano's Dataverse one of the institution's primary storages
- Aiming to provide long-term storage services for both internal and partner datasets

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