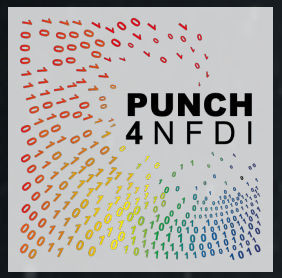

Funded by
DFG Deutsche Forschungsgemeinschaft
German Research Foundation

TA3-WP2

C4P integration into DESTINY using REANA: A first attempt

PUNCH4NFDI Annual Meeting 2025

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Jülich Supercomputing Centre, Forschungszentrum Jülich (FZJ), Jülich, Germany

MOTIVATION

> Reminder of funding period

Jülich DATA

A Centralised Repository for Research Data and Software Publications

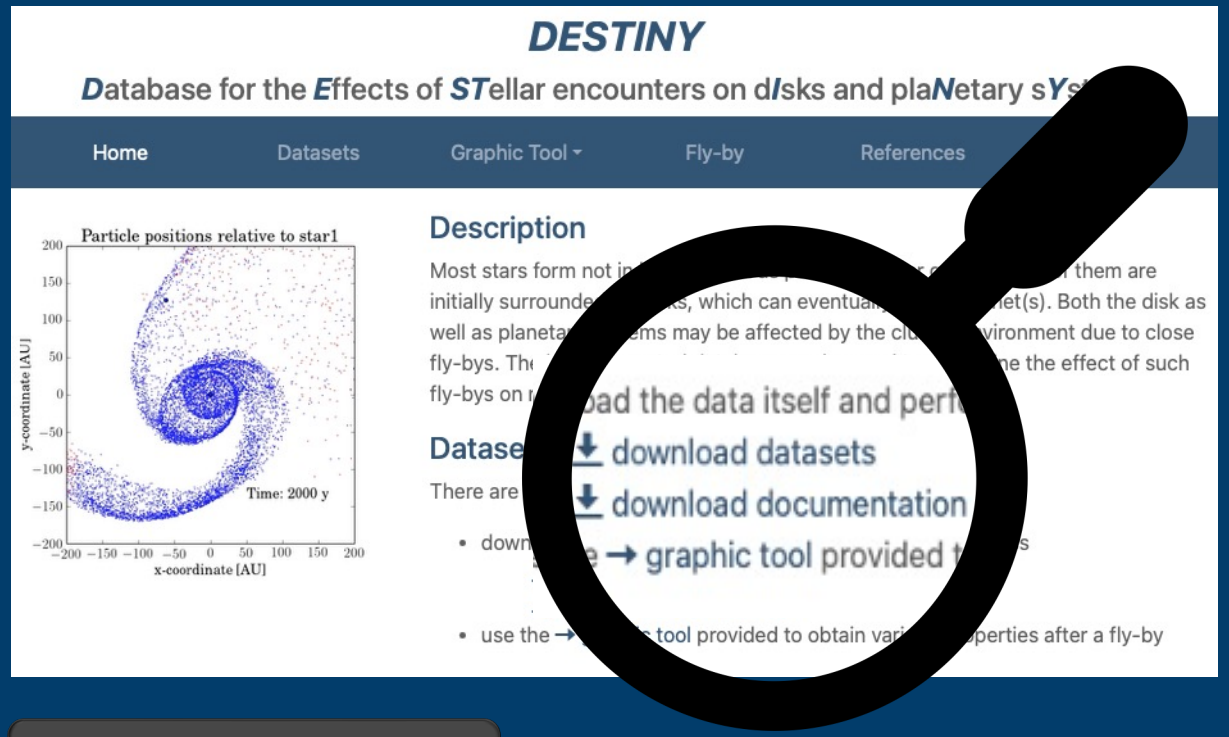
- Jülich DATA is the **institutional research data registry** for Forschungszentrum Jülich
- It is built on **Dataverse**, an **open-source web application**
- The registry indexes and provides access to all **research data** created at or related to FZJ
- It supports data and software publication with **DOI assignment** for citation
- Jülich DATA enables **global search** and **reuse** of research data from Jülich

https://data.fz-juelich.de

DESTINY

Database for the effects of stellar encounters on disks and planetary systems

- **Open-data initiative** for astrophysical *N*-body simulations of stellar flybys
- **4 datasets** from over **6000 simulations** and growing
- **Wide parameter space** covered in simulations
- **Flask-based web application** for easy maintenance
- Utilises **Pandas** for data processing and **Matplotlib** for visualisation



https://destiny.fz-juelich.de

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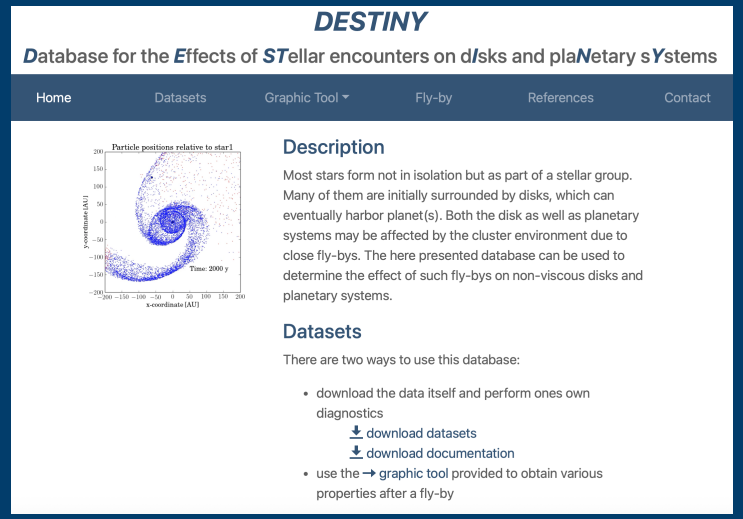
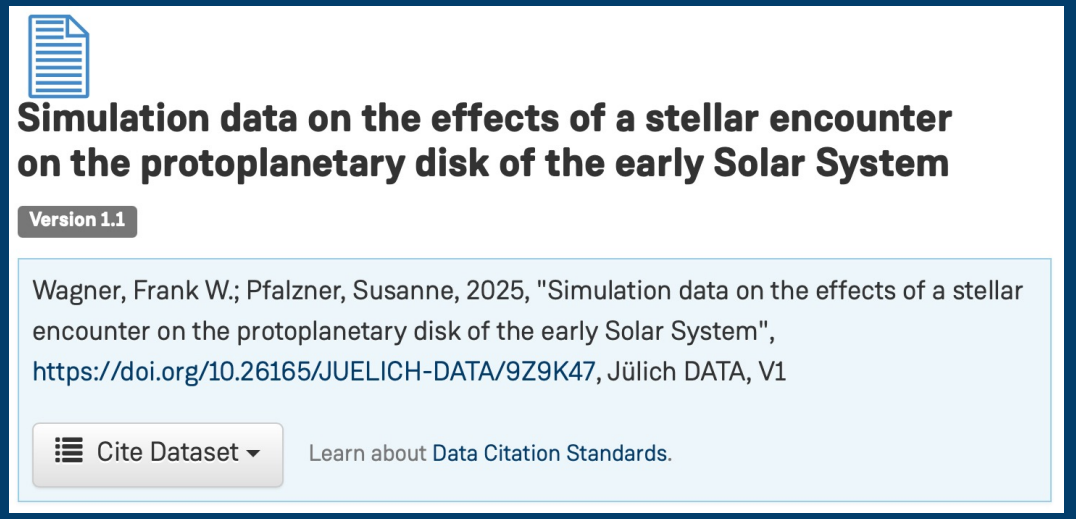
Making data FAIRer

DESTINY platform



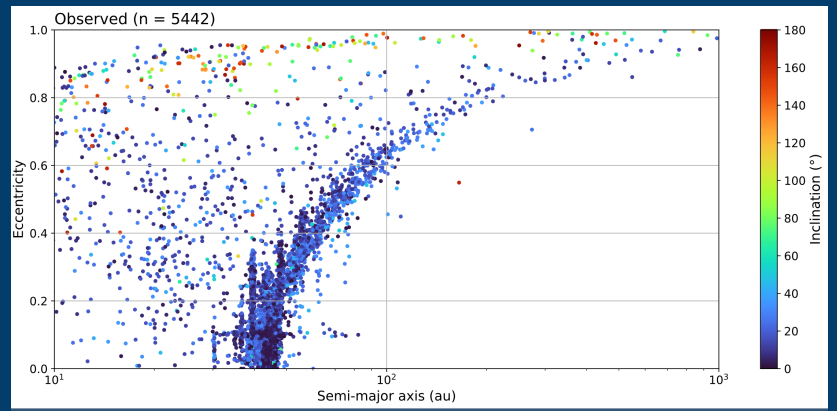
Dataverse API

Jülich DATA, digital repository



- Reuses data and provides tools for analysis and visualisation
- Preserves data and issues DOI

Leveraging PUNCH resources with REANA



Home | Datasets | Graphic Tool | Fly-by | References | Contact

Properties after a fly-by — Info

Model Parameters

Mass ratio (perturber mass / host mass)	0.8
Angle of periastron (degrees)	70
Orbital inclination (degrees)	70
Periastron distance (au)	110
Disk size (au)	150

Plot Settings

Property X-Axis	semimajor_axis	Logarithmic
Property Y-Axis	eccentricity	Logarithmic
Property Color-Axis	inclination	Logarithmic
Limits X-Axis (leave empty for auto)	min - max	
Limits Y-Axis (leave empty for auto)	min - max	
Limits Color-Axis (leave empty for auto)	min - max	

Submit | Reset | Download Data/Plots

reana

Compute4PUNCH, computing resources

- Provides scalable compute resources for data analysis workflows

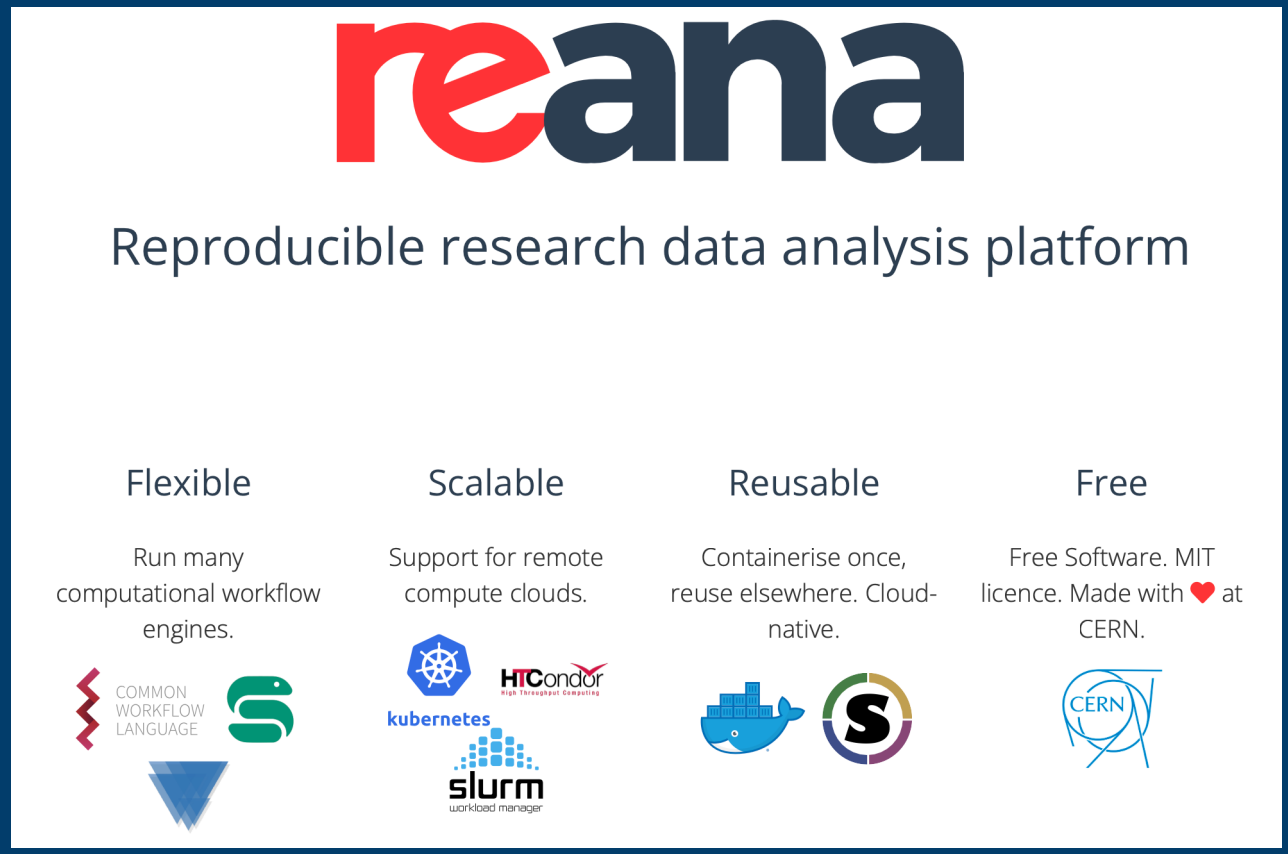
REANA

An Open-Source Workflow Engine for Reproducible Data Analysis

- REANA is an **open-source platform** developed by CERN for reproducible data analysis
- It is enhanced by AIP through integration with the **PUNCH infrastructure**

https://reana-p4n.aip.de

- REANA functions as a **workflow engine** that manages authentication, verification, and execution
- It provides direct access to federated compute (**Compute4PUNCH**) and storage (**Storage4PUNCH**) resources
- The platform is designed to be **scalable** and **flexible** for diverse analytical tasks



https://reanahub.io

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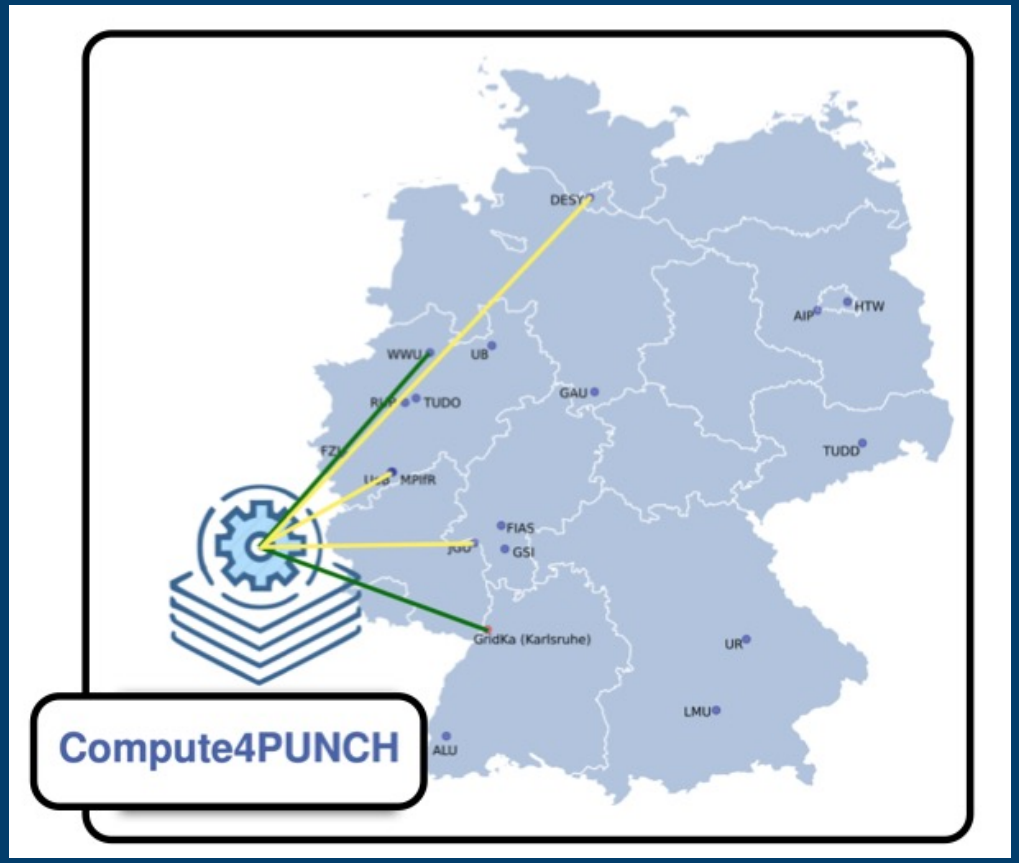
Compute4PUNCH

A Federated Network of Compute Resources for Efficient Data Processing

- **Federated compute resource network** across multiple institutions in **PUNCH4NFDI**
- Managed by an **HTCondor overlay batch system** for efficient resource allocation
- **Dynamic integration** of diverse computing systems via the **TARDIS resource manager**
- Serves as the **compute backend** for the **REANA workflow engine**
- **Single entry point with automated token-based authentication** for seamless, secure job submission
- **Containers for data analysis workflows** are stored and maintained in **PUNCH4NFDI's Docker Registry** with a **CI/CD pipeline**



TA2, https://punch4nfdi.de

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Higgs Boson Analysis Workflow

REANA-CERN Open Data Tutorial by Manuel Giffels

https://home.web.cern.ch

Higgs Boson Analysis Workflow

Description

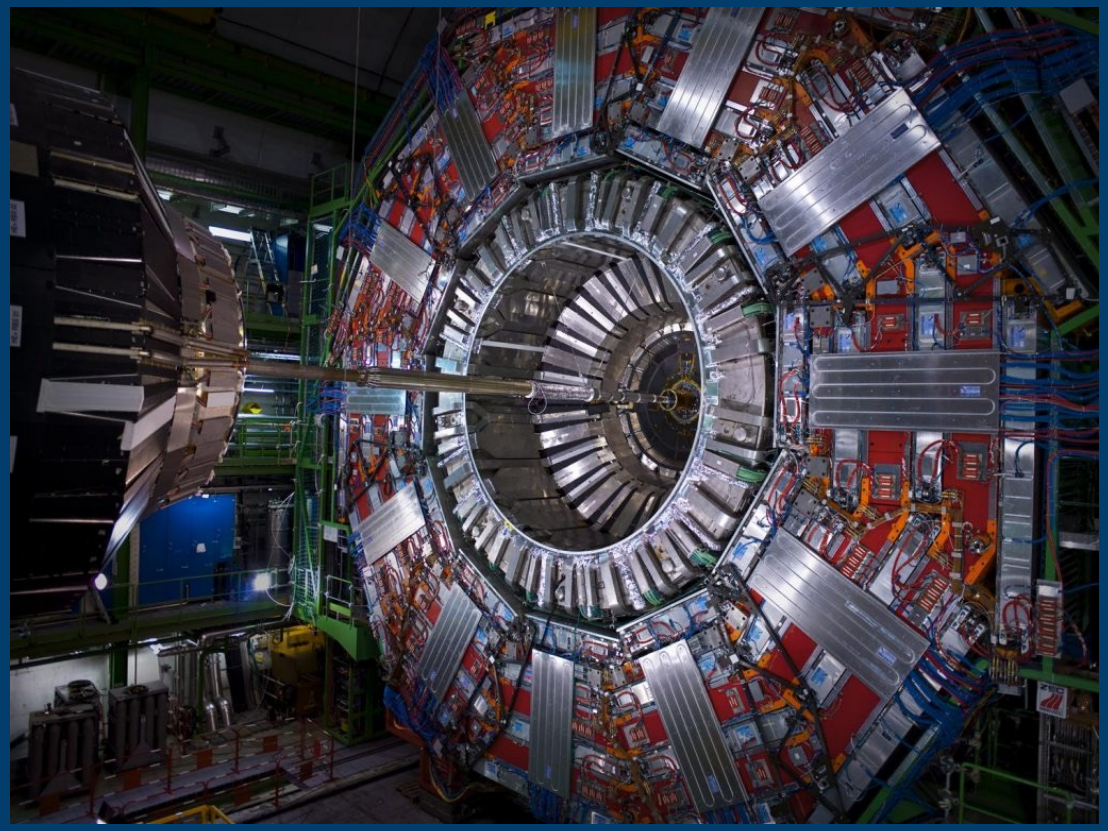
This workflow analyzes real CMS detector data from 2012 to reconstruct the Higgs boson decaying to two Z bosons from events with four leptons. The analysis processes collision events and produces plots showing the invariant mass distribution with evidence of the Higgs boson at approximately 125 GeV.

Workflow Details

- **Input Files:** ROOT analysis code (C++)
- **Environment:** ROOT 6.30.02 on AlmaLinux 9
- **Steps:**
  1. Run Higgs analysis on CMS Open Data
  2. Generate PDF plots from results
- **Outputs:** 4 PDF plots (4μ, 4e, 2e2μ, combined)
- **Execution Time:** ~5-15 minutes (fast mode)

Configuration File

The workflow is defined in `reana.yaml`. View configuration



https://gitlab-p4n.aip.de/compute4punch/tutorials/reana-cern-open-data-tutorial

DESTINY

*D*atabase for the *E*ffects of *ST*ellar encounters on d*I*sks and pla*N*etary s*Y*stems

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REANA Workflow Jobs

Submit and monitor REANA workflows.

✓ **REANA Client Configured**
Connected to: https://reana-p4n.aip.de

Submit Workflow

Workflow Name

higgs-analysis

🚀 Submit Workflow

✓ Workflow 'higgs-analysis' submitted successfully!

```
==> Creating a workflow...
==> Verifying REANA specification file... /Users/frawa/PycharmProjects/desti
  -> SUCCESS: Valid REANA specification file.
==> Verifying REANA specification parameters...
  -> SUCCESS: REANA specification parameters appear valid.
==> Verifying workflow parameters and commands...
  -> SUCCESS: Workflow parameters and commands appear valid.
==> Verifying dangerous workflow operations...
  -> SUCCESS: Workflow operations appear valid.
==> Verifying compute backends in REANA specification file...
  -> SUCCESS: Workflow compute backends appear to be valid.
higgs-analysis.9
==> SUCCESS: File /reana.yaml was successfully uploaded.
==> Uploading files...
==> Detected .gitignore file. Some files might get ignored.
==> SUCCESS: File /code/df103_NanoAODHiggsAnalysis.C was successfully upload
==> SUCCESS: File /code/PrintHistos.C was successfully uploaded.
==> Starting workflow...
==> SUCCESS: higgs-analysis.9 has been queued
```

Visit your REANA dashboard to monitor the workflow progress.

Your Workflow Runs

Workflow Name	Run #	Started	Ended	Status
compute4punch	1	2025-11-18T15:44:05	2025-11-18T15:45:07	failed
kubernetes	1	2025-11-18T15:32:52	2025-11-18T16:19:03	finished
higgs-analysis	1	2025-11-17T18:01:21	2025-11-17T18:40:10	finished

Visit your REANA dashboard to view detailed workflow information and download results.

Workflow Result Files

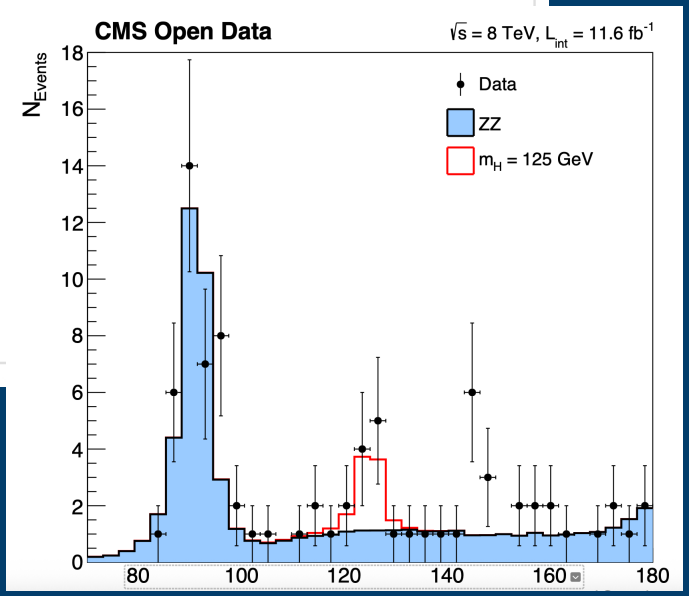
compute4punch.1

higgs-analysis.1

- results/higgs_2el2mu.pdf (available)
- results/higgs_4el.pdf (available)
- results/higgs_4l.pdf (available)
- results/higgs_4mu.pdf (available)

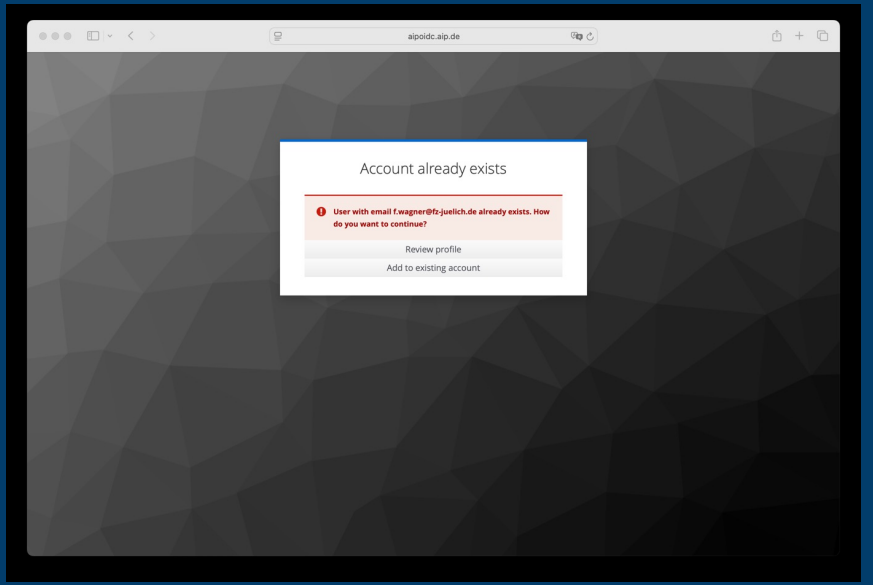
kubernetes.1

- results/higgs_2el2mu.pdf (available)
- results/higgs_4el.pdf (available)
- results/higgs_4l.pdf (available)
- results/higgs_4mu.pdf (available)



CHALLENGES AND LIMITATIONS

- **DESTINY:** Some web technologies outdated, modernisation with React needed
- **Jülich DATA:** DOI assigned instantly, but data curation takes 2-3 days
- **REANA:** No automated access token generation; obtaining a working token takes 2-3 days via support
- **REANA:** Initially, very limited CPU time for workflows — only 1 hour allowed
- **REANA:** FZJ members cannot access the REANA dashboard
- **C4P:** An additional time-limited access token is required for C4P resources
- **C4P:** Kubernetes backend worked, but C4P example failed




```
$ reana-client run -w higgs-analysis -f reana-c4p.yaml
==> ERROR: Cannot create workflow higgs-analysis:
User quota exceeded.
Resource: cpu, usage: 6h 3m 58s out of 1h used (607%)
Please see: https://docs.reana.io/advanced-usage/user-quotas
```

SUMMARY AND OUTLOOK

- **DESTINY:** A FAIR data platform for stellar flyby simulations. We used Jülich DATA for data archiving and to issue DOIs for DESTINY data. We demonstrated a prototype implementation of an example workflow to integrate C4P resources using the REANA workflow manager.
- **Next Steps:** Replace the example workflow with a real astrophysical use case, such as TNO classification using a ML pipeline.
- **Announcement:** See you at Astroinformatics 2026!

https://ai2026.astro.uni-koeln.de

THANK YOU FOR LISTENING!

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