



# Interactive workflows and data provenance with HELIPORT

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June 12, 2023

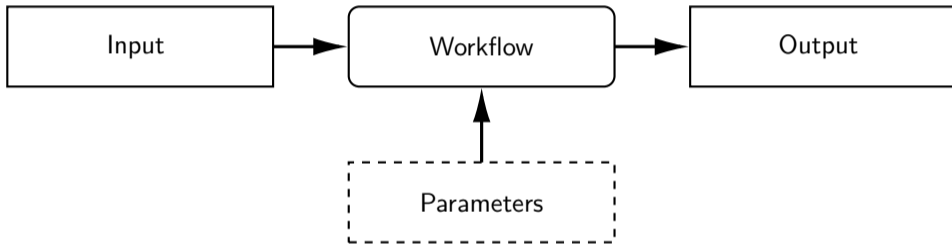
**1** Automated Workflows and Data Provenance

**2** Interactive Workflows

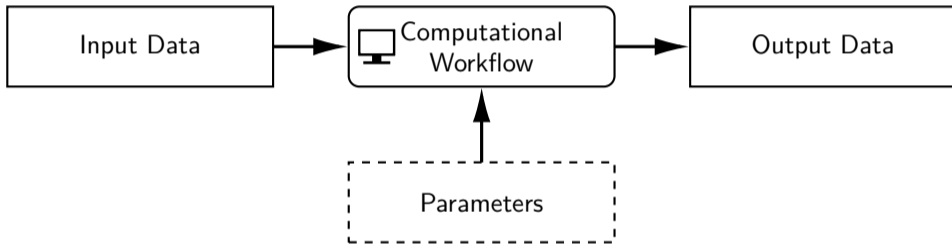
**3** Outlook: Interactive Workflows and Data Provenance

# Automated Workflows and Data Provenance

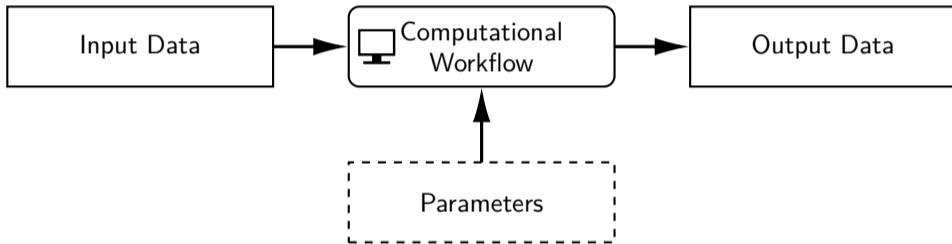
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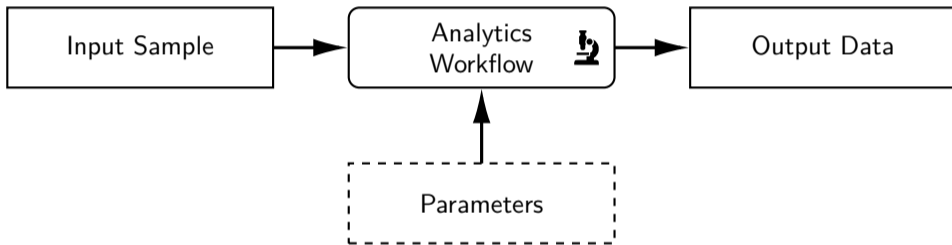
## Computational Workflows



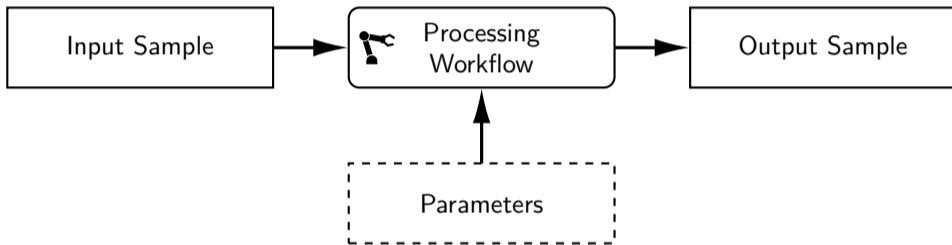
Computational Workflows  
CWL, Unicore, shell skript, ...



## Lab Workflows

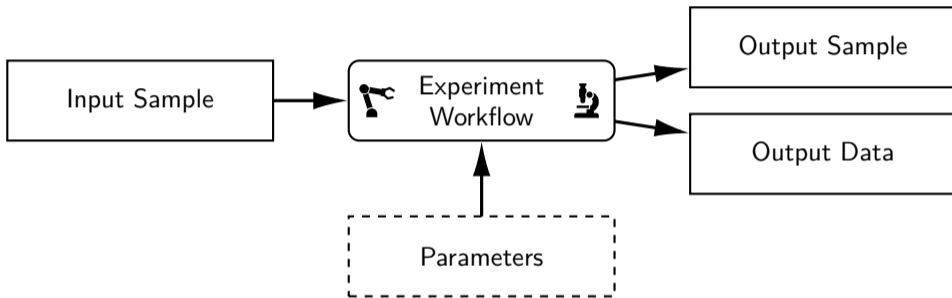


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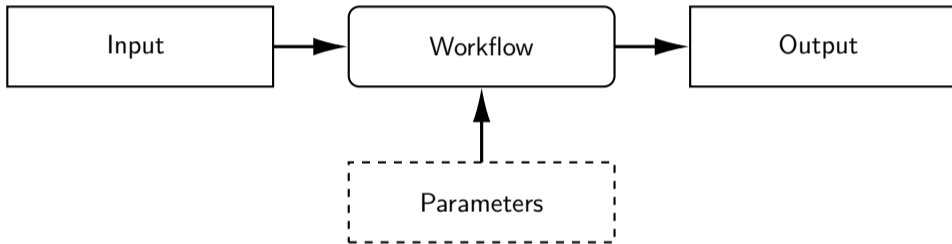




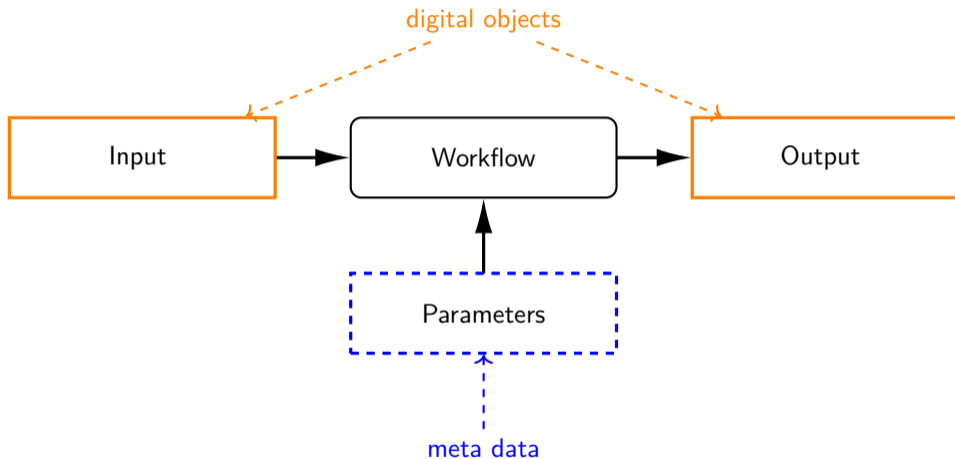
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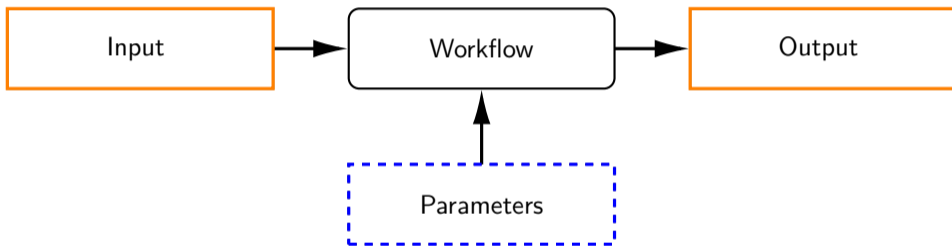
# Workflows and Data Provenance?



# Data Provenance

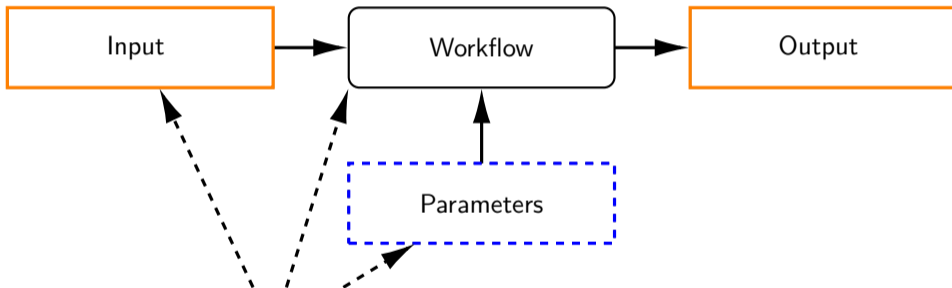


# Data Provenance



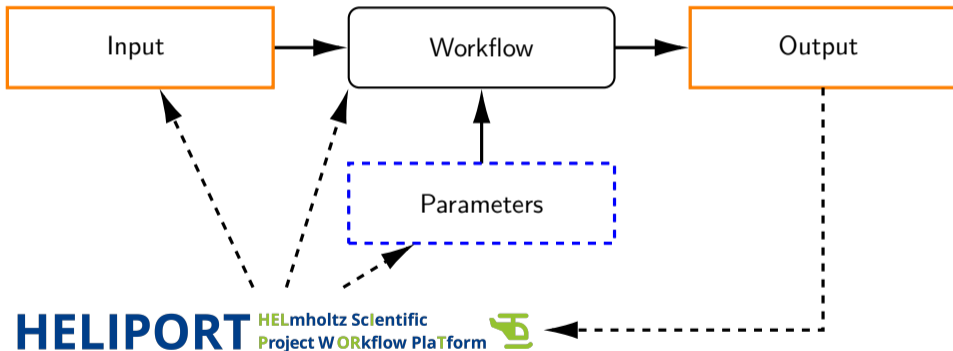
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Project WORKflow PlaTform 

# Data Provenance



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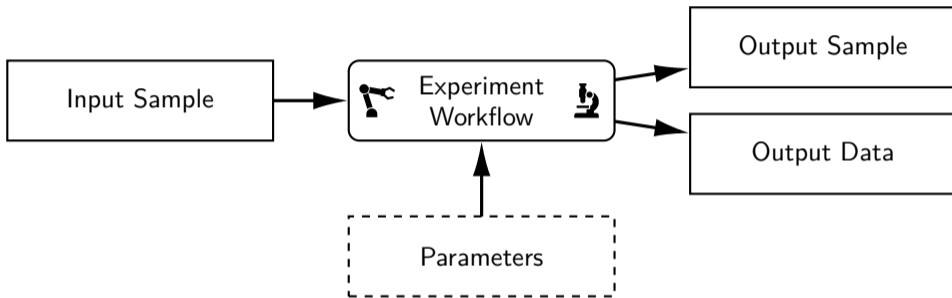


# Interactive Workflows

- 1 Automated Workflows and Data Provenance
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- 3 Outlook: Interactive Workflows and Data Provenance

# Interactive Workflows

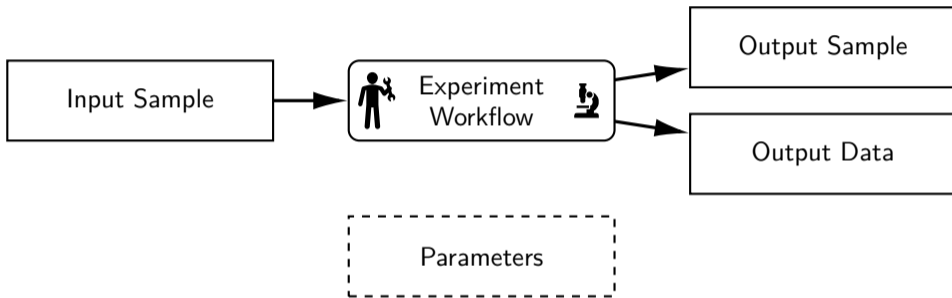
## Lab Workflows





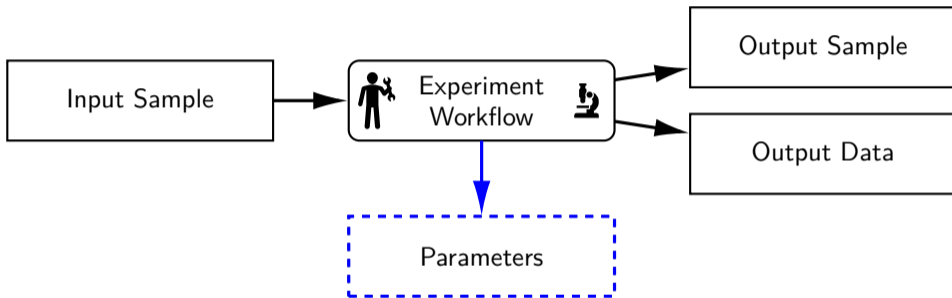
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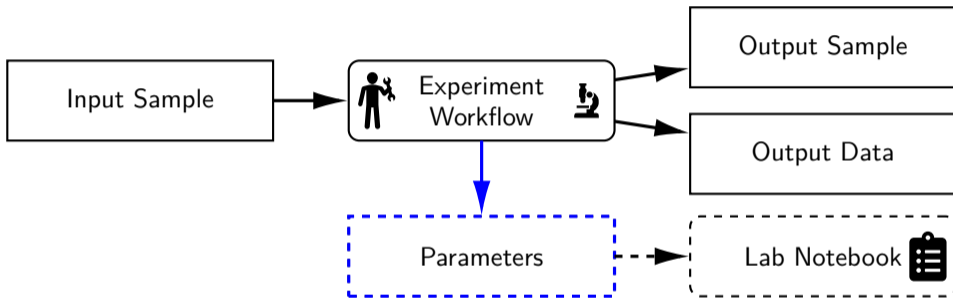
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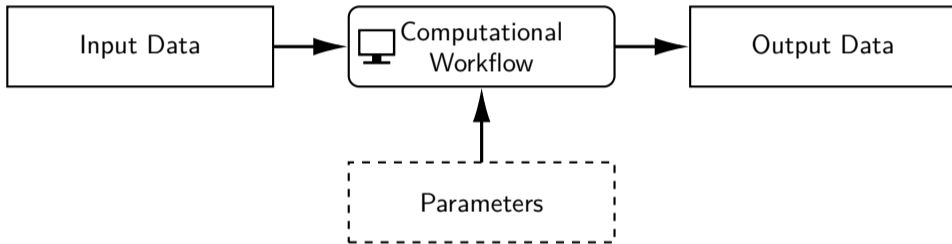
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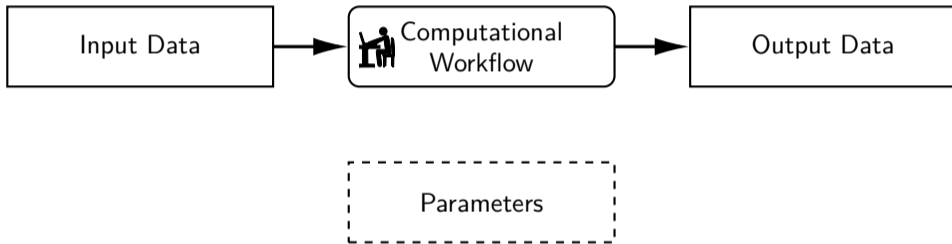
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# Interactive Workflows

Computational Workflows

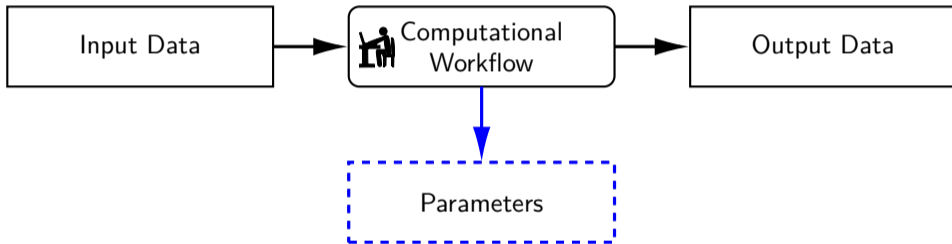
\*, ...



# Interactive Workflows

Computational Workflows

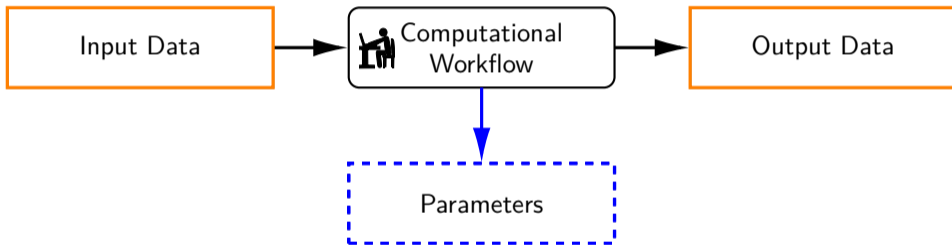
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# Interactive Workflows

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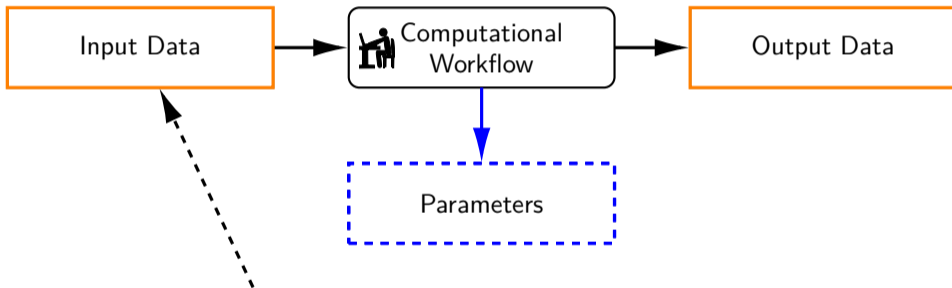


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# Interactive Workflows

Computational Workflows

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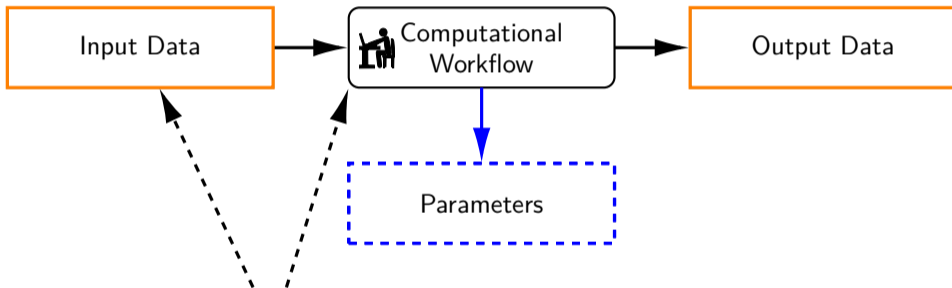
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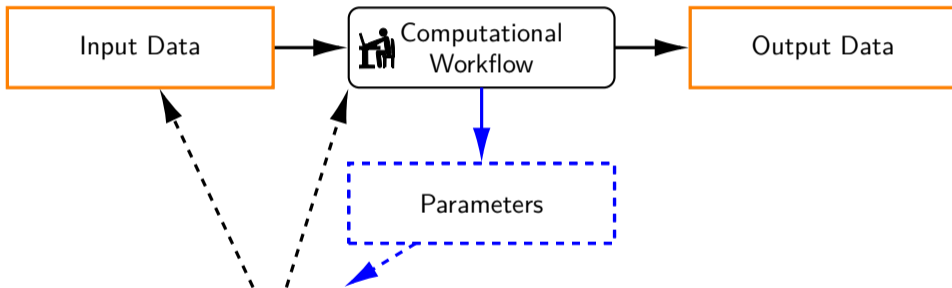


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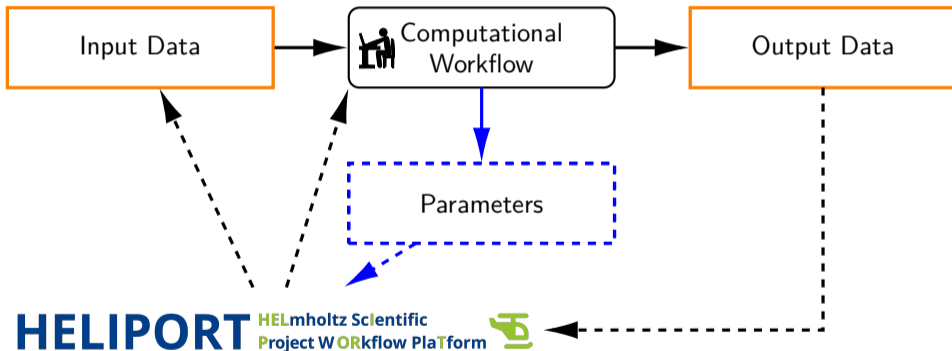


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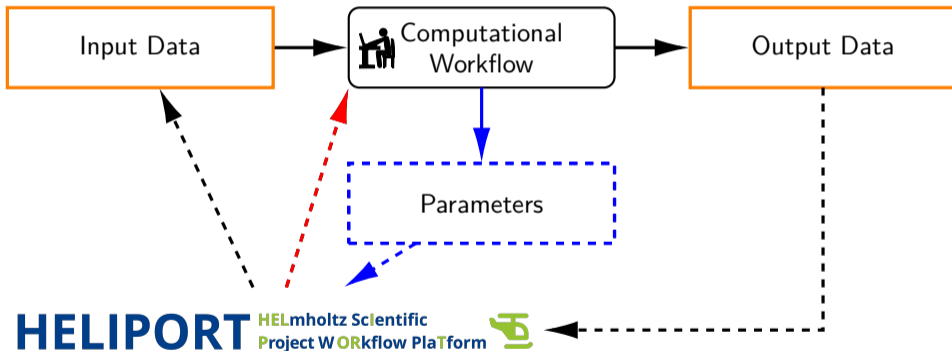
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# Interactive Workflows

Computational Workflows

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# Example Demo

<https://hemera5.fz-rossendorf.de/submit?service=SpekNG&>

# Interactive Workflow Examples

## Experimental Data Analysis

localhost:8080 50%

load operations file import operations dataset load data console

Remove No files selected

remove all files

Input Filter

Select source file format for import:

ascii, or

self-describing binary ADRIS container format.

import dataset

Preprocessing

number of rows values: 25  
number of items: 3  
number of measurements: 250

2. Fractional composition matrix

3. Fractional composition matrix

fractionator

Analysis Method

Select an analysis method:

PCA

Performs iterative target factor analysis by doing principal component analysis and various rotations on the spectra to compute abstract component spectra when target vectors are provided iterative target test is performed to improve the abstract solution.

Parameters for PCA

weighting coefficient: 0

number of components: 3

scale to unit variance scores

rotation Method

rotation Method

iterations

Performs target tests on vectors of fraction profiles of single components to see if they are in accordance with computed abstract fractions. If 0 vectors are given, a heuristic is used to construct incomplete target vectors from the maximum variance of the abstract fraction profile for each component.

Parameters for ICP rotation

rotate

Analysis Method results: PCA

Parameters for PCA

Analysis results

Import of PCA

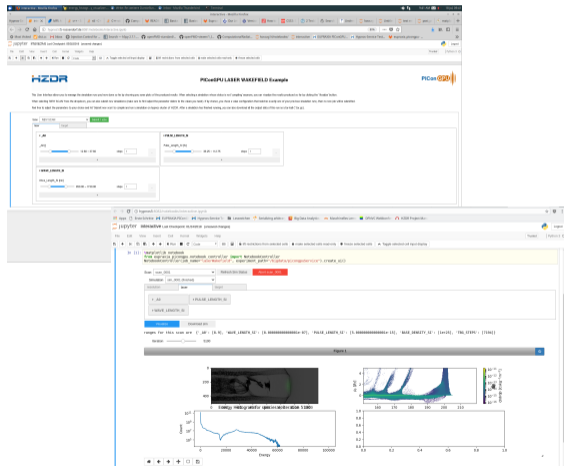
Rotation for PCA

# Interactive Workflow Examples

## Experimental Data Analysis



# Simulation Control and Visualization

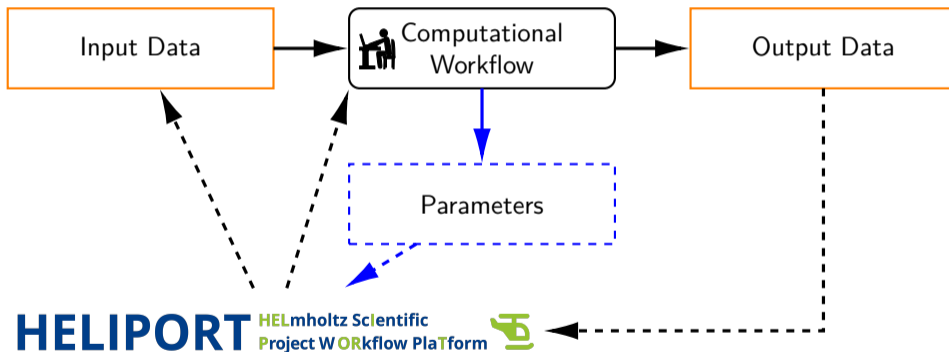


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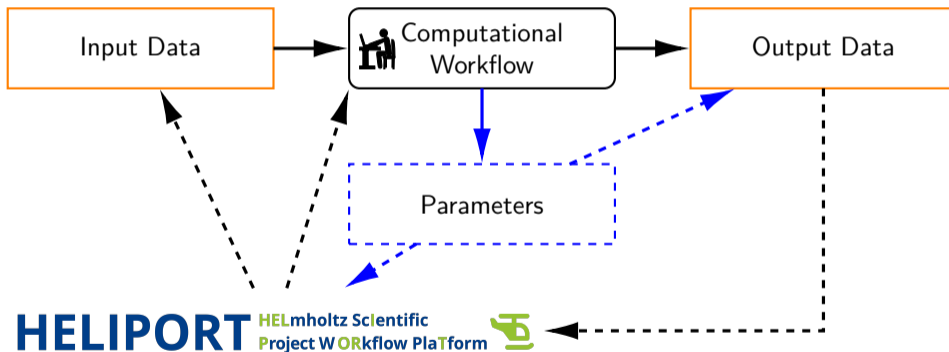
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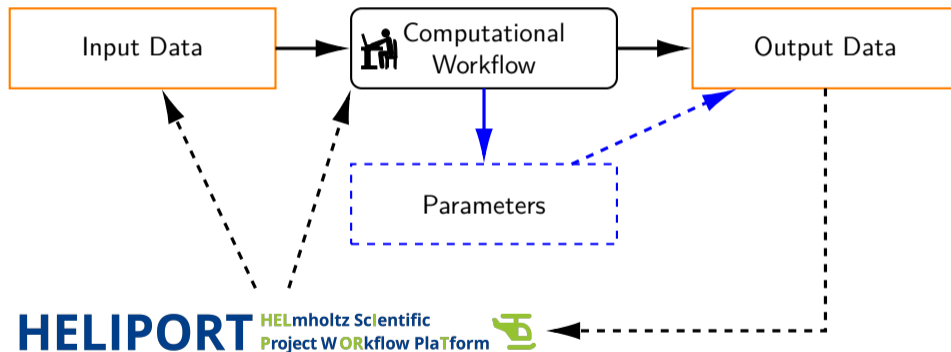
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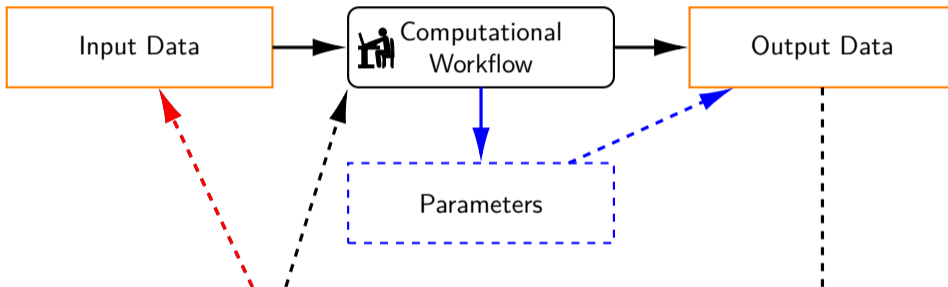


# Interactive Workflows and Data Provenance



# Interactive Workflows and Data Provenance

- User chooses managed dataset,
- system aware of which workflows may use it.

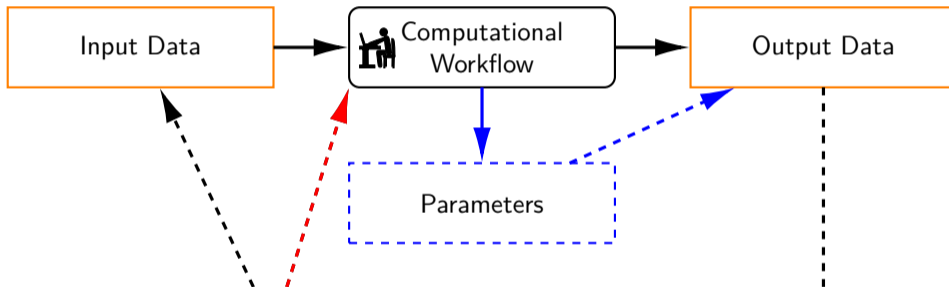


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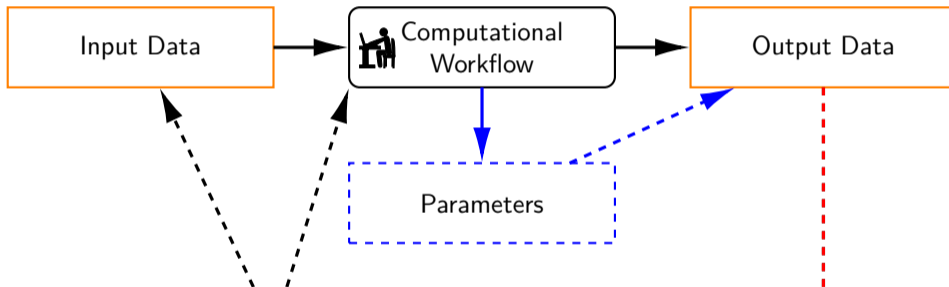
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- Pass handle to input data.



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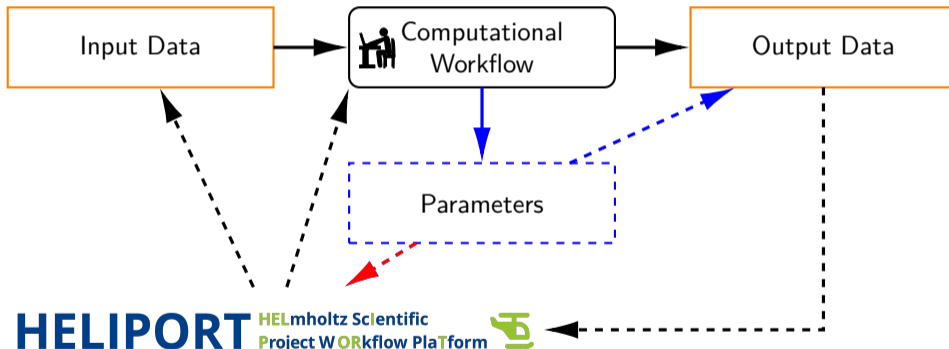
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- Ingest produced data, or
- workflow submits handle.



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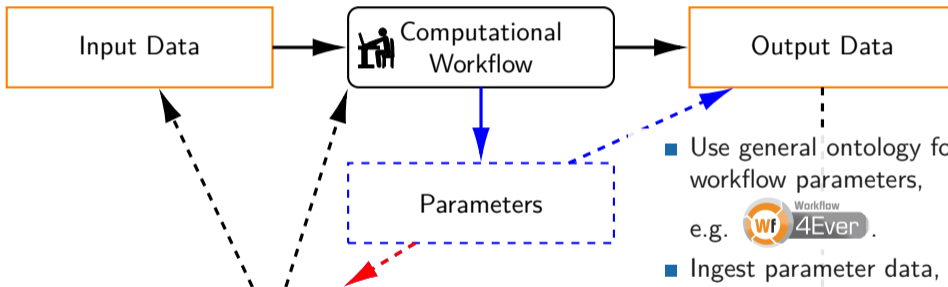



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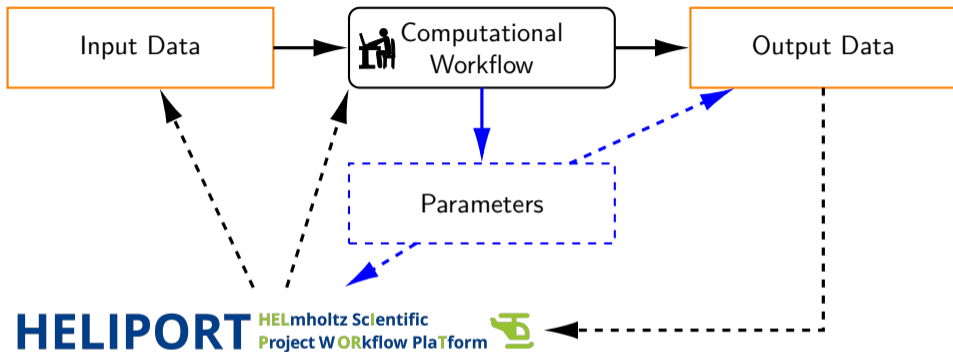


- Use general ontology for workflow parameters, e.g.  .
- Ingest parameter data, or
- workflow submits to manager.

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# Summary



- In interactive workflows meta data about the process is output not input.
- Interactive workflows require integration with digital-object management as client or slave.

# Acknowledgments

- Guido Juckeland
- Michael Bussmann
- Norbert Jordan
- Richard Pausch
- Melanie Rödel
- André Roßberg

**Thank You.**