Combining file-based with RDMS-based scientific workflows using the LinkAhead-crawler

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2024-03-06

Article

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Mapping Hierarchical File Structures to Semantic Data Models for Efficient Data Integration into Research Data Management Systems

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Data **2024**, *9*(2), 24; **https://doi.org/10.3390/data9020024**

Submission received: 15 August 2023 / Revised: 8 December 2023 / Accepted: 18 December 2023 / Published: 26 January 2024

(This article belongs to the Section **Information Systems and Data Management**)

tom Wörden et. al., *Data* 2024, 9, 24.
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Research Question

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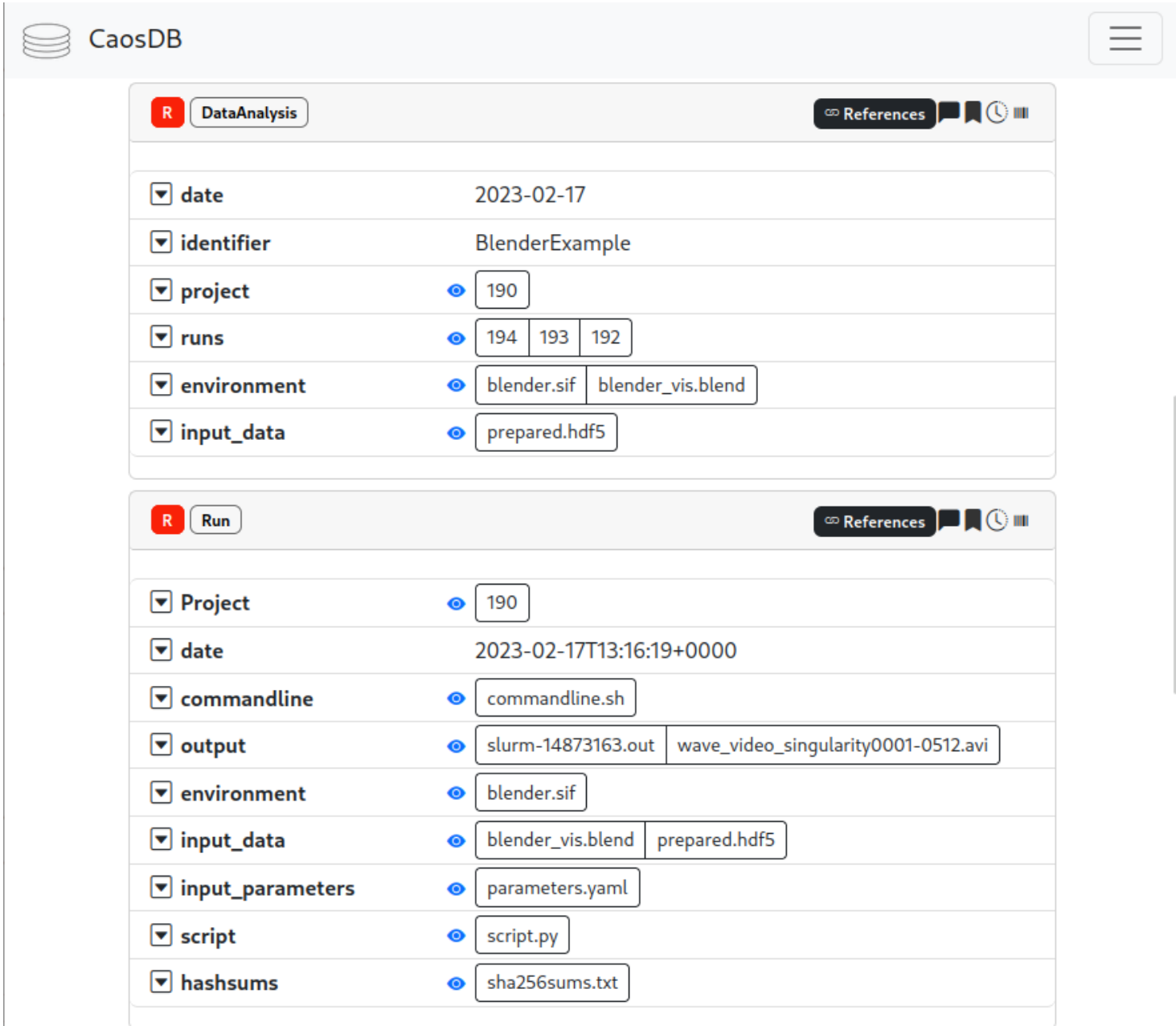
- How can we use the RDMS simultaneously to traditional file systems (for interoperability)?

LinkAhead (formerly: CaosDB)



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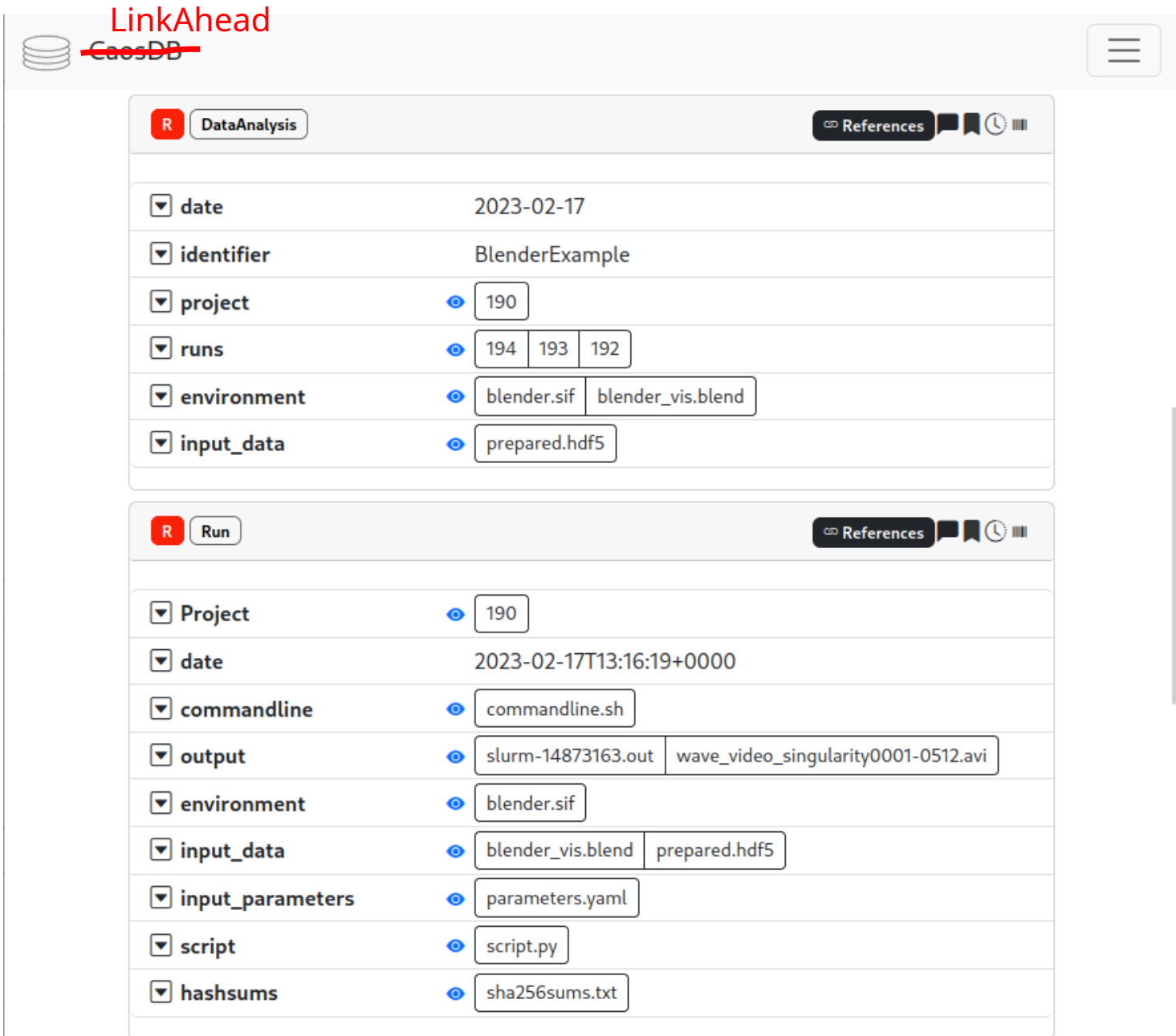

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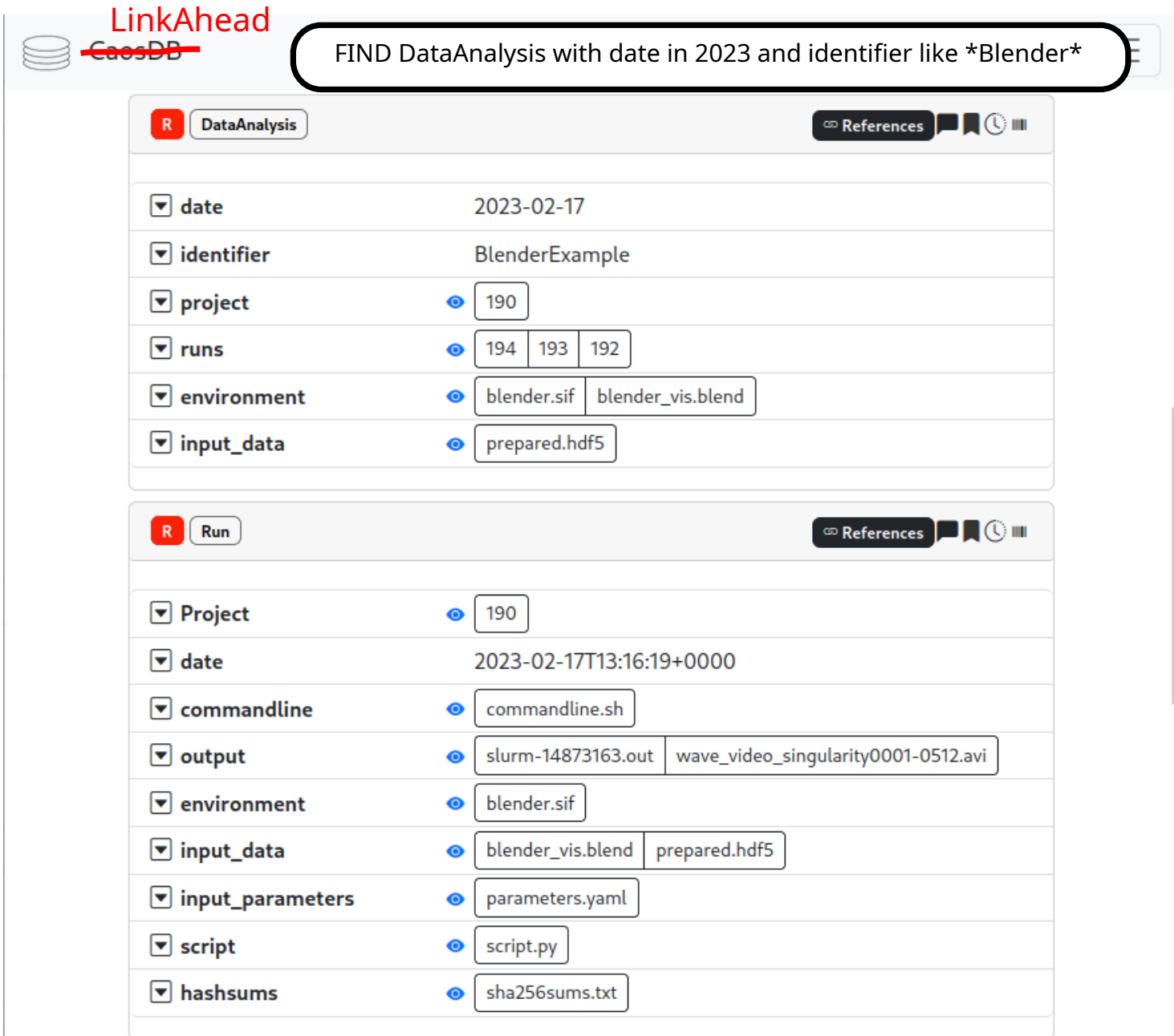

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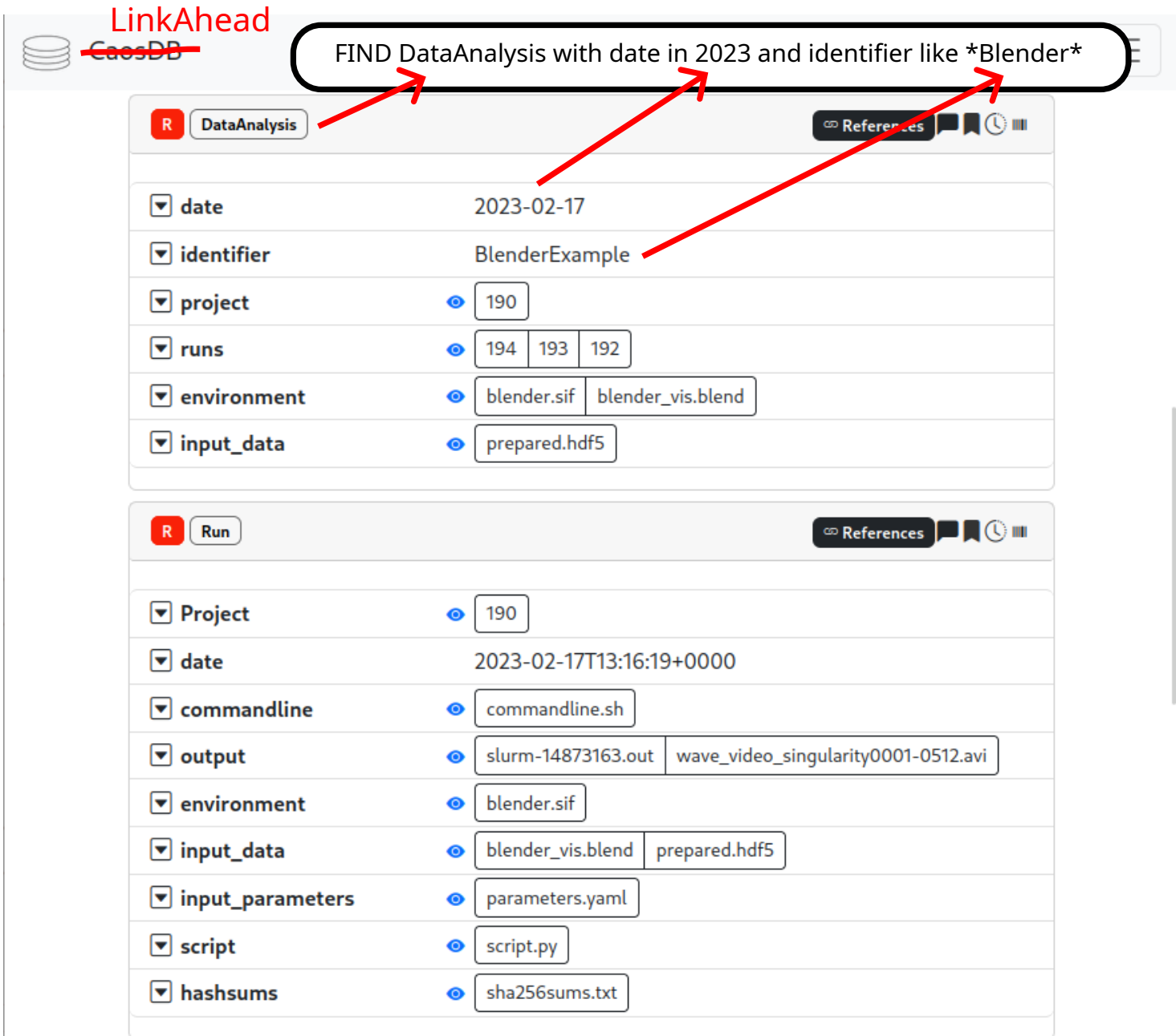

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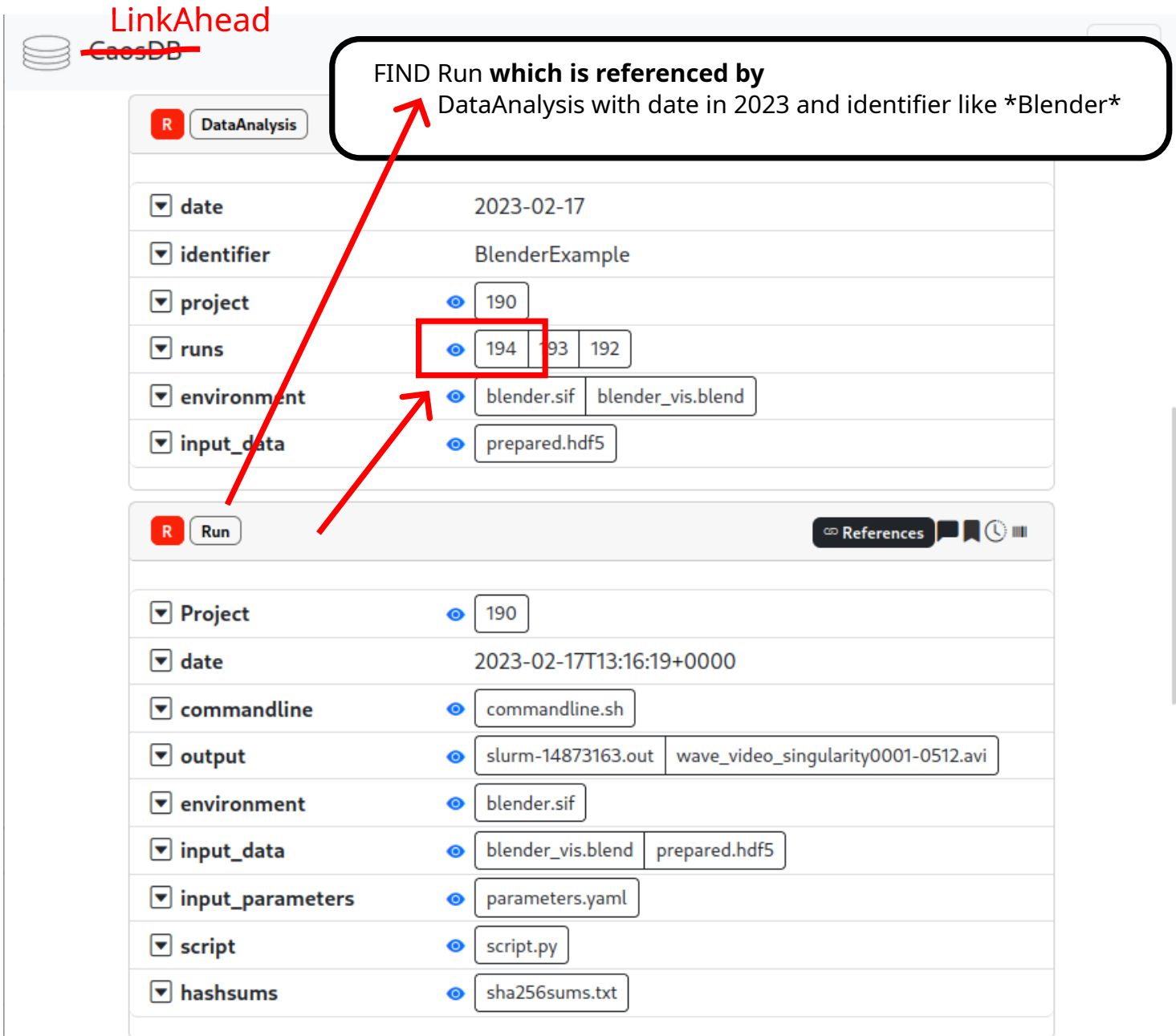

LinkAhead (formerly: CaosDB)

- Semantic Research Data Management System (RDMS)
  Fitschen et.al., *Data* 2019, 10.3390/data4020083
- Developed at the Max Planck Institute for Dynamics and Self-Organization (Göttingen) since 2010
- Open Source project since 2018: gitlab.com/linkahead
- Commercial support available by IndiScale GmbH[1] (since 2019)
- Currently approximately 20-30 instances in very different scientific disciplines
- Main features (very briefly): Flexible semantic data model, highly modular data crawler, semantic search

[1] A.S. is a co-founder of IndiScale.

Data Integration

```
example/
├ runs/
│   └ 2023-02-17T13_16/
│       ├ prepared.hdf5
│       ├ sha256sums.txt
│       ├ parameters.yaml
│       ├ commandline.sh
│       └ slurm-14873163.out
├ script.py
└ blender.sif
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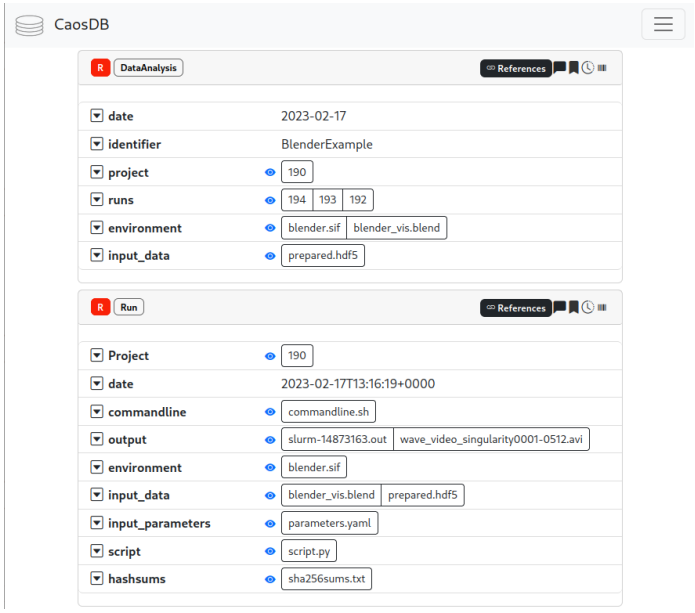

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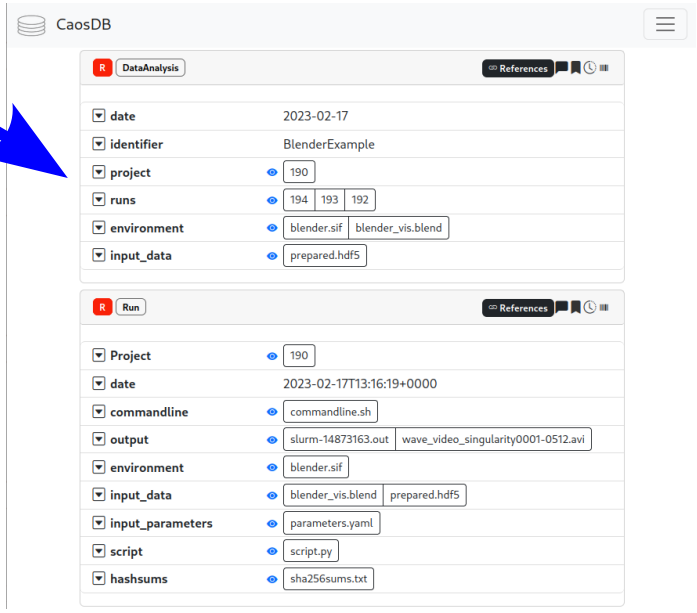

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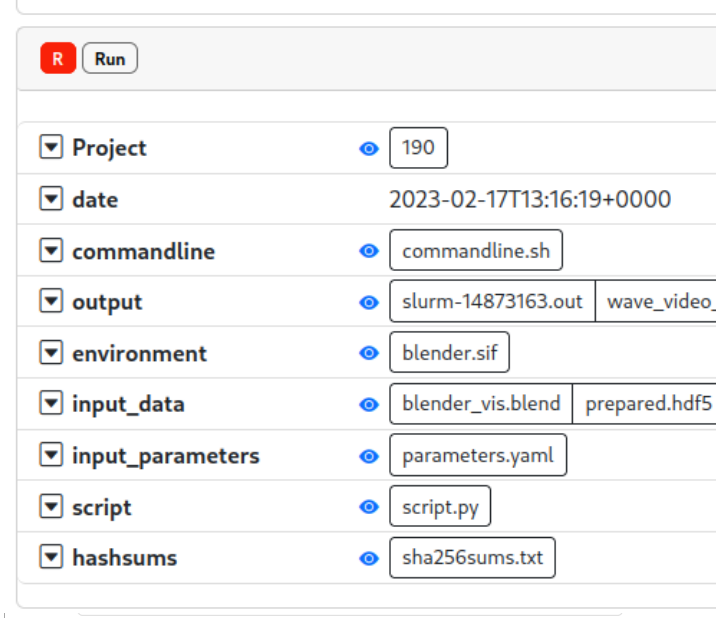

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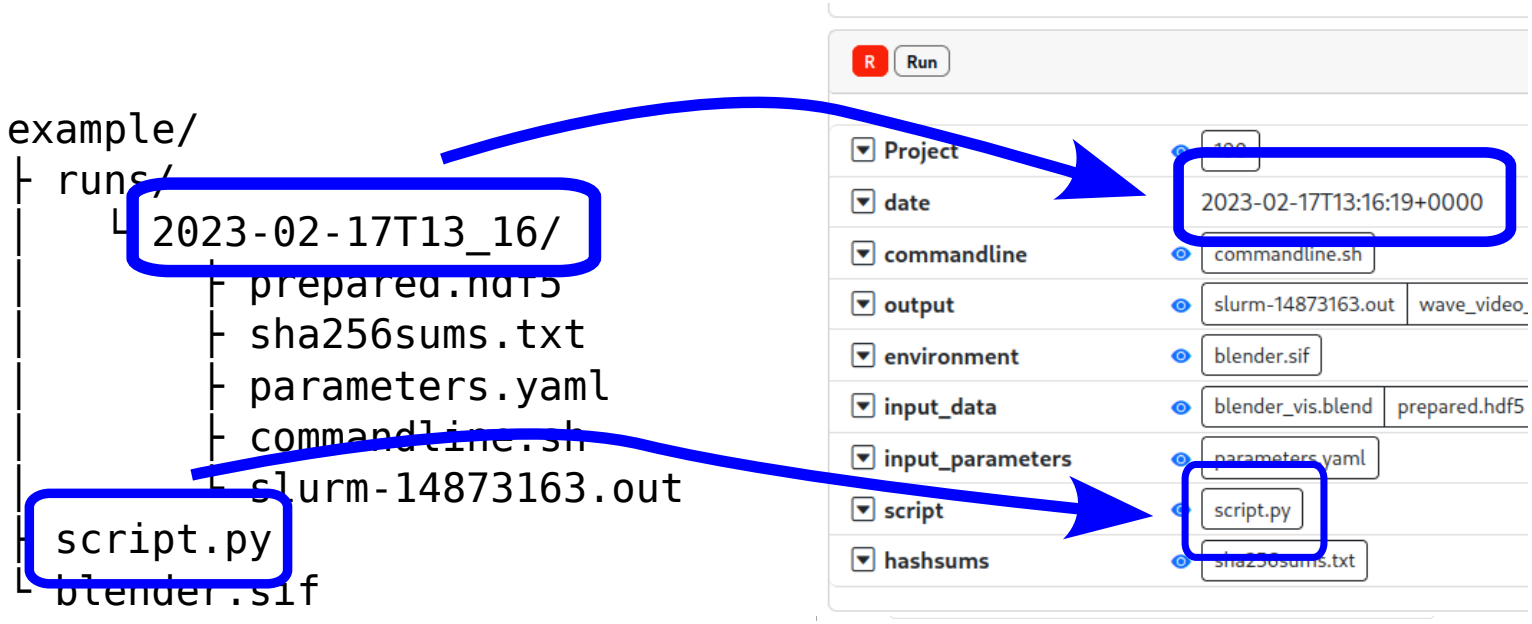

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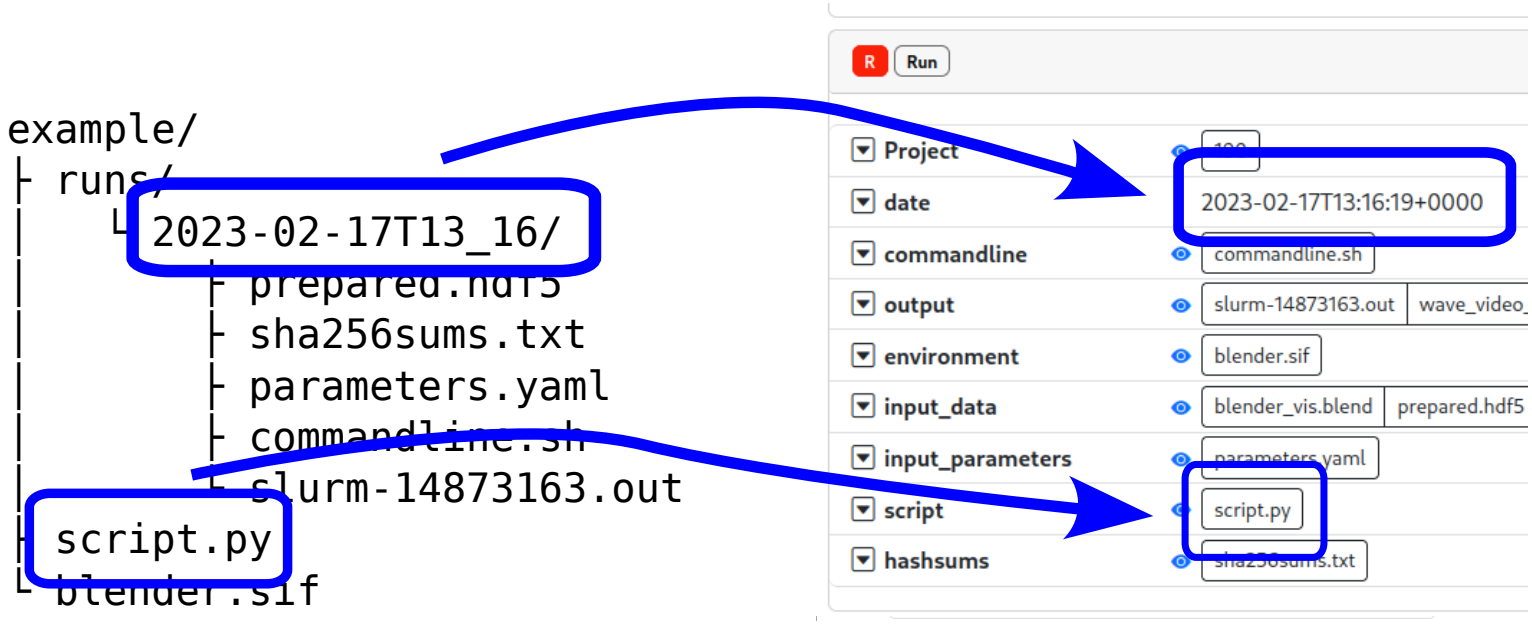

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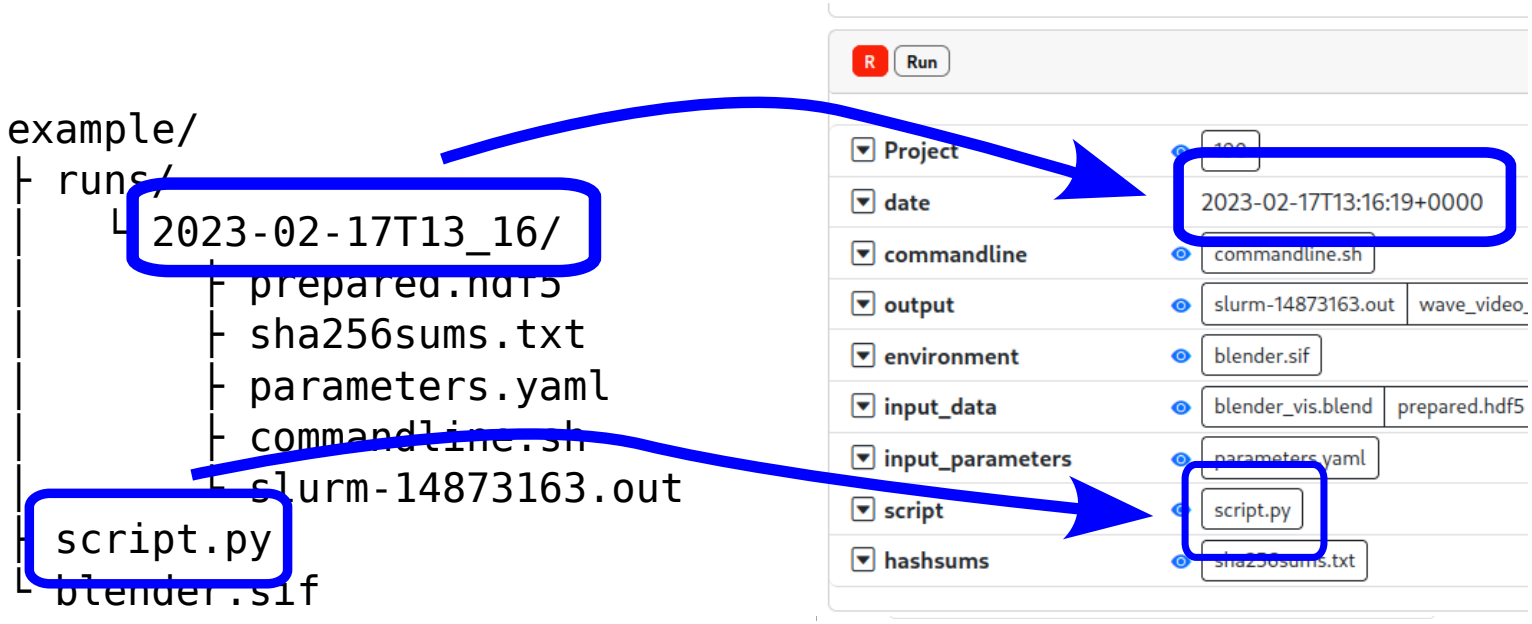
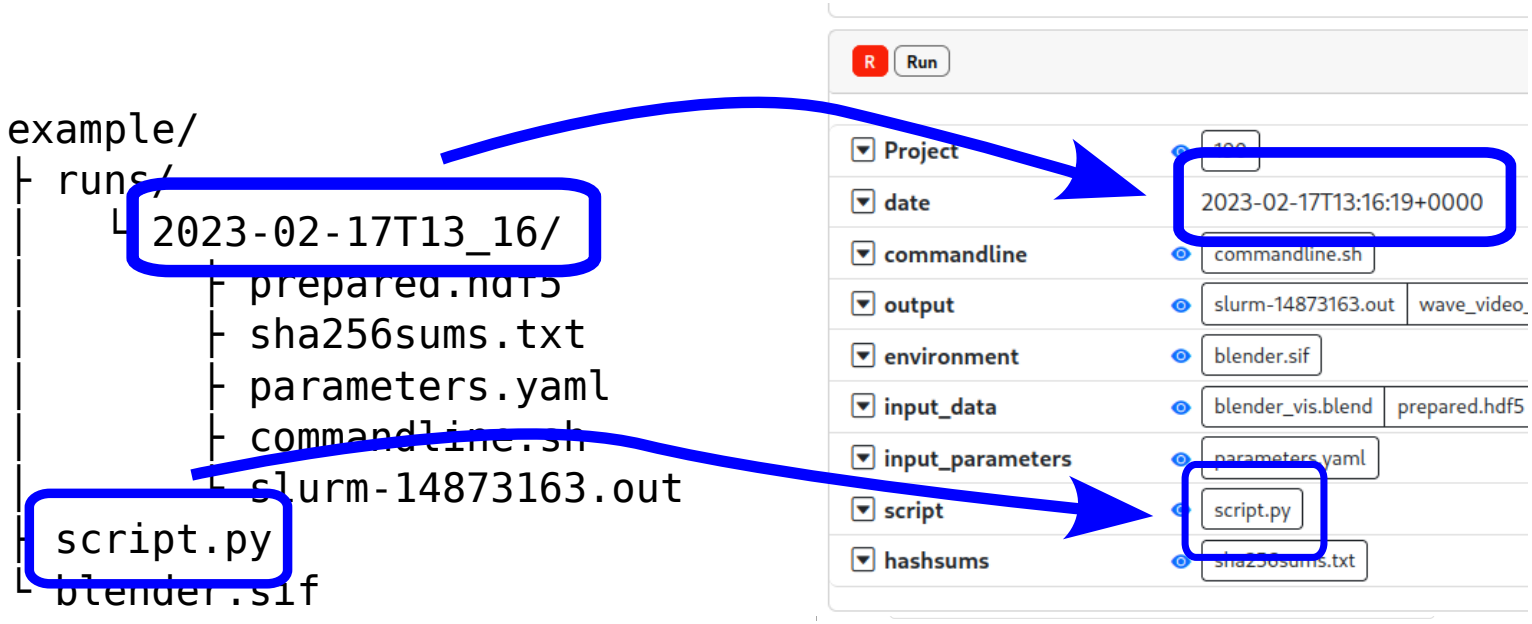


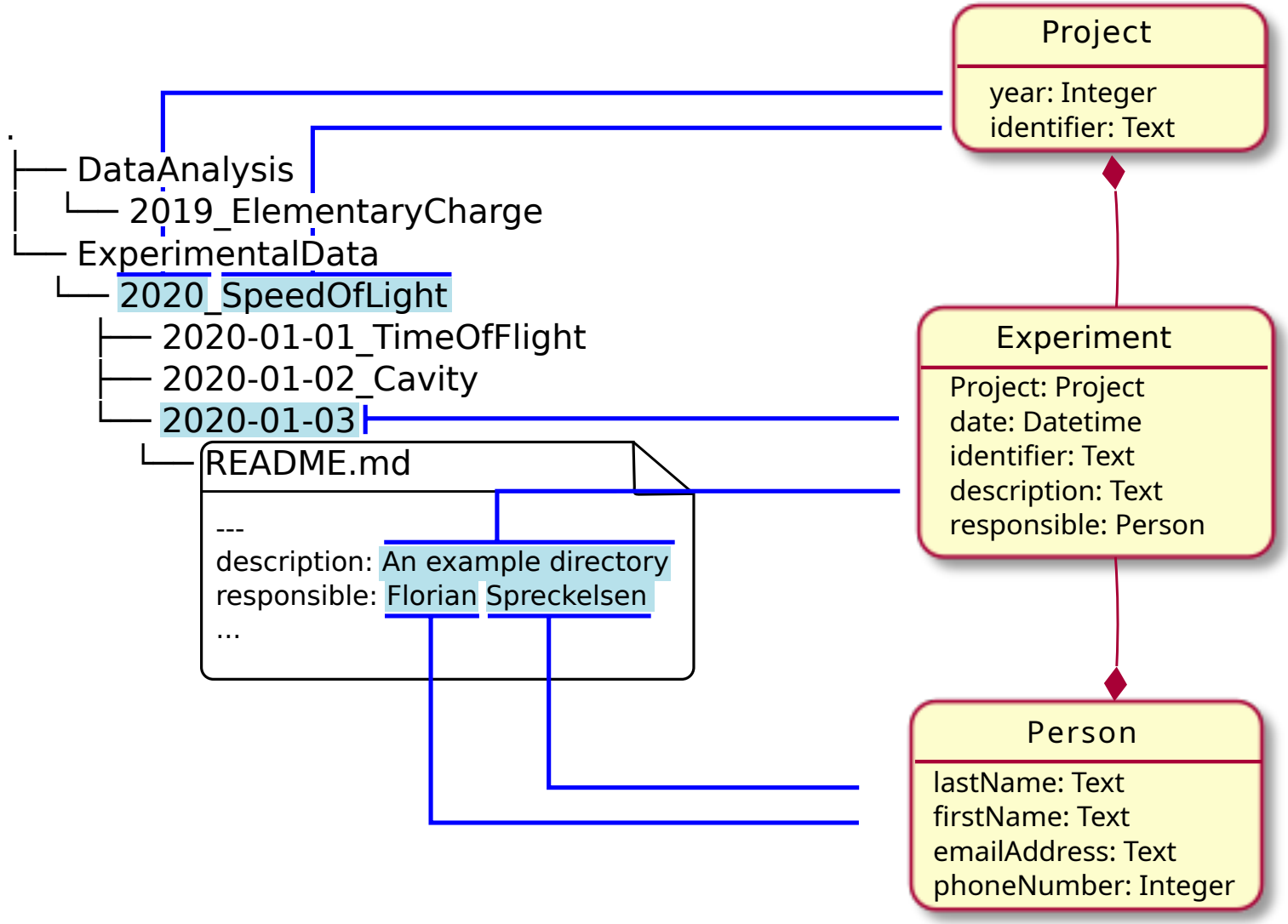
- Extract (meta) data from file names, directory names, and file contents

Data Integration



- Extract (meta) data from file names, directory names, and file contents
- Map these data onto a semantic data model (and store it in CaosDB/LinkAhead)

Example 2



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Crawler Design

- Modular file crawler (Python, AGPLv3)

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- Modular file crawler (Python, AGPLv3)
- Adaptable to file structure using YAML specification
- Extendable with Python modules (custom data formats, . . .)
- Synchronization into RDMS (instead of data ingest): Files and RDMS can be used simultaneously!

YAML specification

```yaml
ExperimentalData_Dir:
  type: Directory
  match: "ExperimentalData"
  subtree:
    Project_Dir:
    type: Directory
    match: (?P<year>[0-9]{4,4})_(?P<name>.*)
    records:
      Project:
        year: $year
        name: $name
# (...)
```

YAML specification

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# (...)
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Converter matching folders with name
ExperimentalData

YAML specification

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    records:
      Project:
        year: $year
        name: $name
# (...)
```

Converter matching folders with name containing numbers

Converter for subfolders
using a regexp, e.g.: **2024_deRSE**

YAML specification

```yaml
ExperimentalData_Dir:
  type: Directory
  match: "ExperimentalData"
  subtree:
    Project_Dir:
    type: Directory
    match: (?P<year>[0-9]{4,4})_(?P<name>.*)
    records:
      Project:
        year: $year
        name: $name
# (...)
```

For each subfolder, a record of type **Project** is created, setting 2 properties **year** and **name** from the regexp.

Extract contents from files

```
# (...)
DataFile:
  type: JSONFile
  match: results\.json
  subtree:
    frequency:
      type: DictTextElement
      match_name: frequency
      match_value: (?P<frequency>[0-9]+)
      records:
        DataAnalysis:
          frequency: $frequency
# (...)
```

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  type: JSONFile
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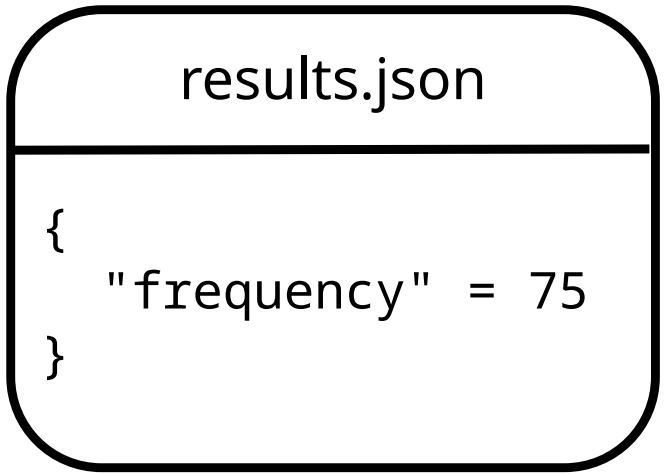

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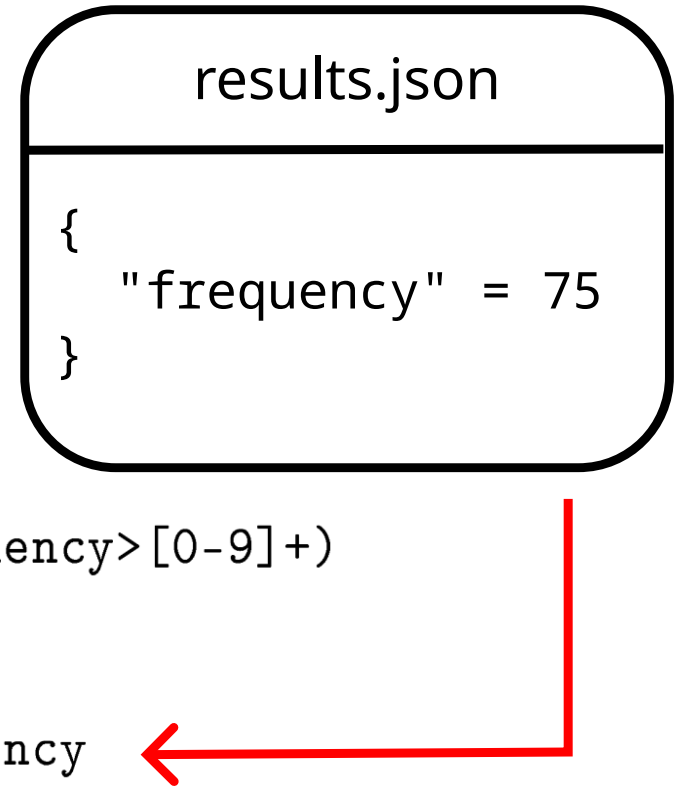

Create a record of type **DataAnalysis**
with property **frequency** = 75

Thank You! - Summary

- Crawler that continuously synchronizes (currently one-way) information from file system to semantic RDMS
- YAML based, extendable specification for adapting crawler to different file system layouts and data formats
- tom Wörden et. al., *Data* 2024, 9, 24. `https://doi.org/10.3390/data9020024`
- gitlab.com/linkahead AND gitlab.com/linkahead/linkahead-crawler