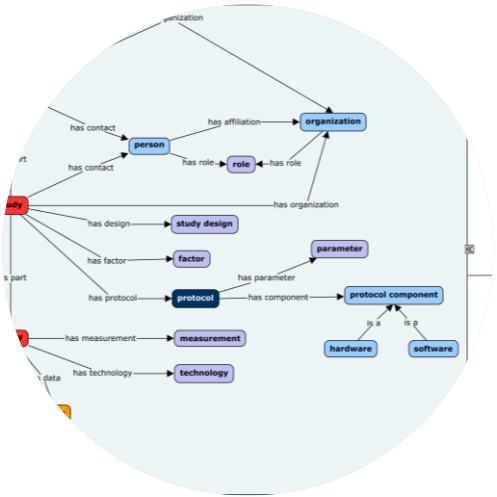
FAIR Data & ISA standard

Using the ISA standard for collecting and sharing data

2024, Sven Warris & Rick van de Zedde



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Data challenges in genomics & phenomics

- Collecting and pre-processing terabytes of data
  - Single and combined experiments
  - Many different sensors, technology platforms
  - Many different pre-processing steps
- Sharing and publishing data
- Metadata is as important as the data itself
  - Organisms, treatment, samples, etc
  - Sensor type, settings, etc

Project partners

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- Bioscience
- Biointeractions
- Biometrics

PHENET
PHENOTYPING & ENVIROTYPING
SOLUTIONS FOR AGROECOLOGY

NPEC

UNLOCK
MICROBIAL POTENTIAL

NARO
National Agriculture and Food Research Organization

vlpb
Virtual
Laboratory
Plant Breeding

RootEd
DOCTORAL NETWORK

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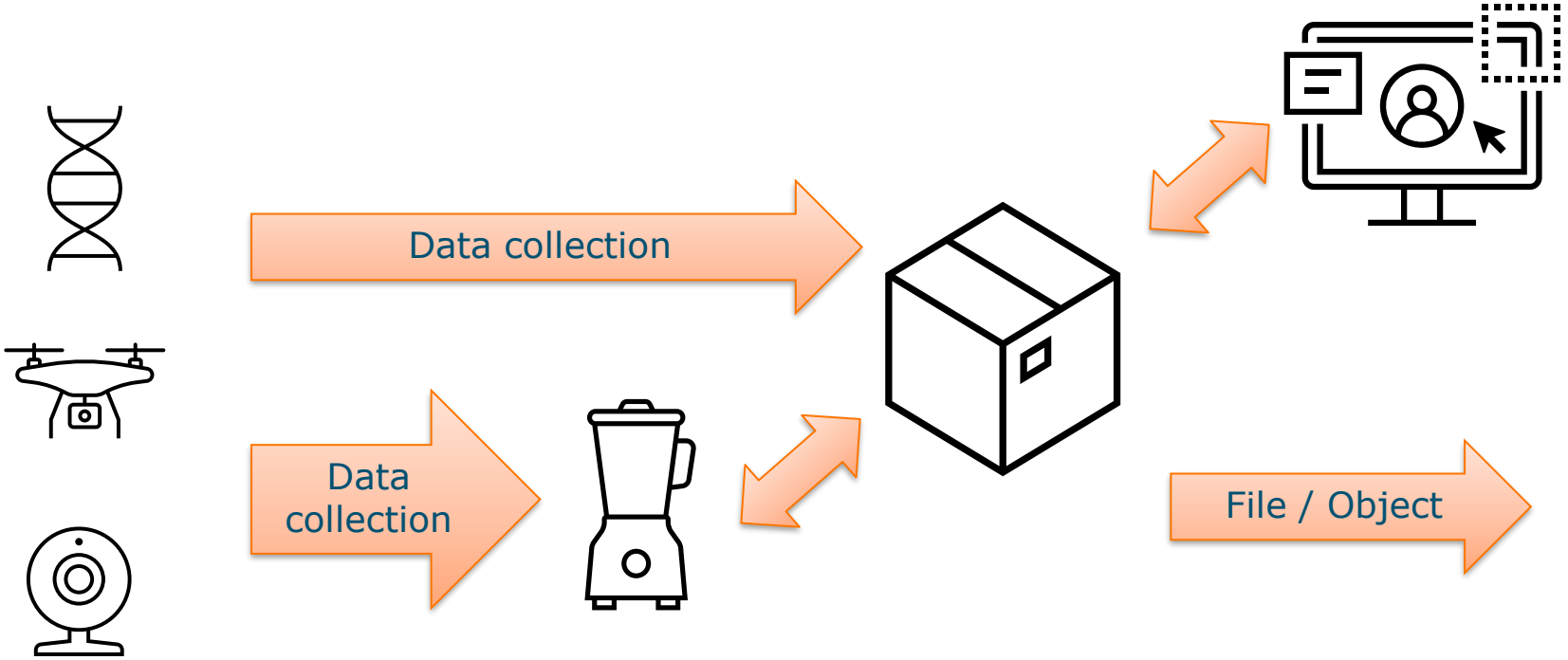
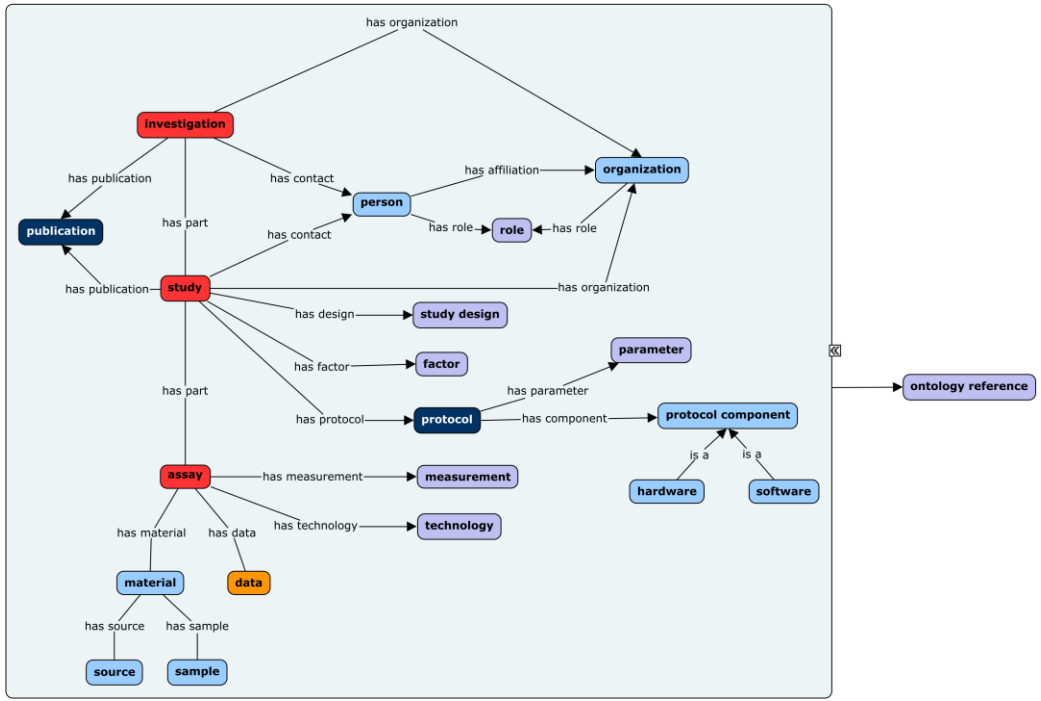
Data flow


Data collection
Data collection
File / Object
Source
Processing
Storage
Sharing

Investigation / study / assay

- Standardized way of structuring project metadata
- Data files, documents, etc
- Ontology-based
- Important entities:
    - Person, Assay, Data



- https://isa-specs.readthedocs.io/en/latest/isamodel.html

Investigation / study / assay

- Structure is the same in, for example:
  - eLabJournal
  - FAIRDOM-seek
- Python support through isatools:
  - ISAJSON / ISATAB
- R support:
  - ISATAB
  - ISAJSON currently being developed

FAIRDOM-seek

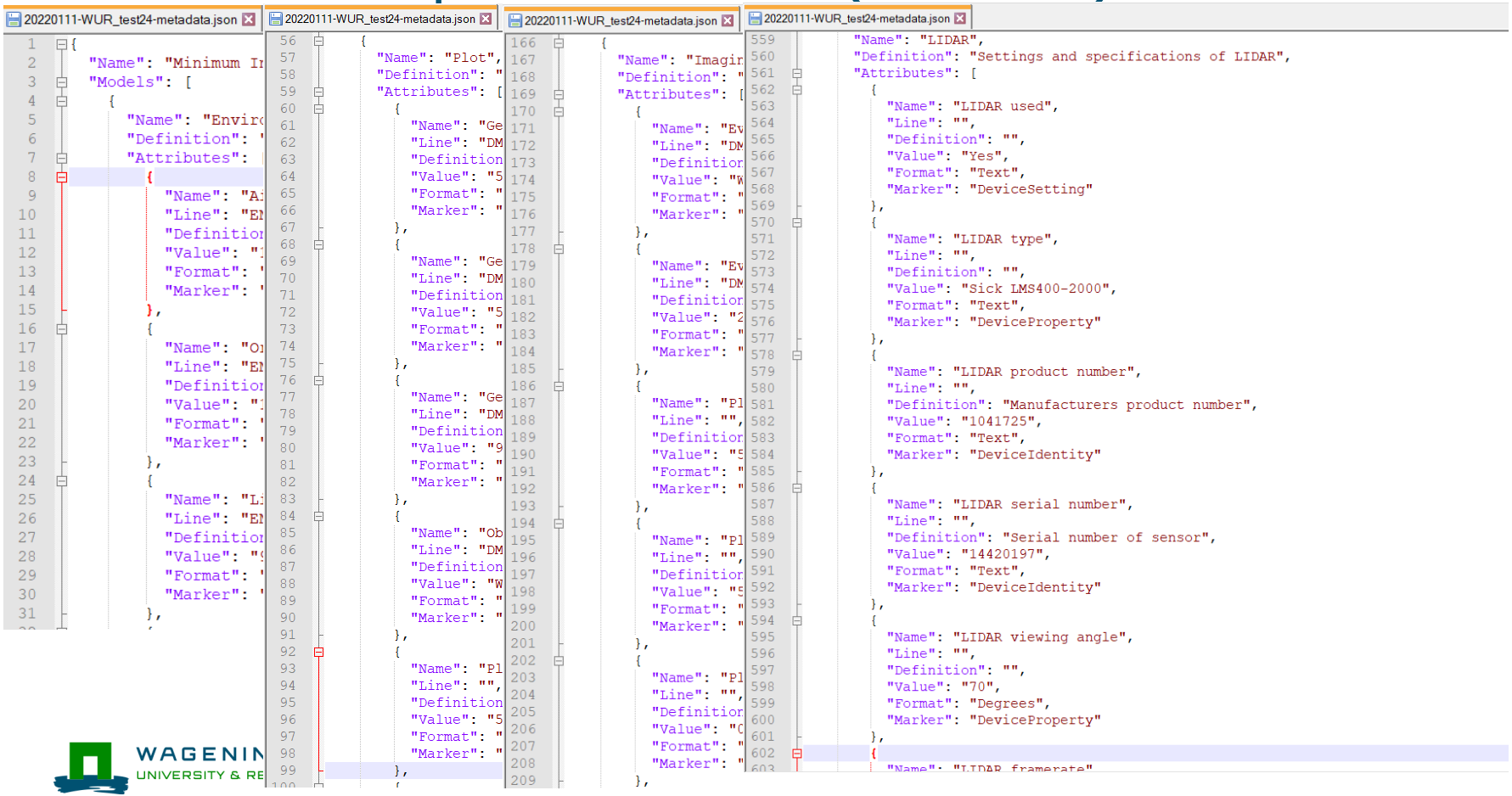
Open-source platform designed for the cataloguing and sharing of diverse scientific research data, including datasets, models, simulations, processes, and outcomes.

- **Preserves Associations**: It maintains relationships between various research components along with information about the involved people and organizations
- **ISA Infrastructure**: FAIRDOM-SEEK structures how experiments are part of broader studies and investigations
- **Configurable Structure:** structure is adaptable, making it suitable for various scientific fields

FAIRDOM-seek

- **Sharing Permissions:** flexible and detailed sharing permissions, supporting collaboration at different research stages, from initial collaboration to publishing final results
- **DOI Generation**: Digital Object Identifiers for individual items or entire collections packaged as Research Objects
- **Semantic Technology**: Advanced queries over its content
- **Metadata Collection:** standard Excel tools and processes (RightField)
- **MIAPPE** support: metadata from *Minimum Information About Plant Phenotyping Experiments*

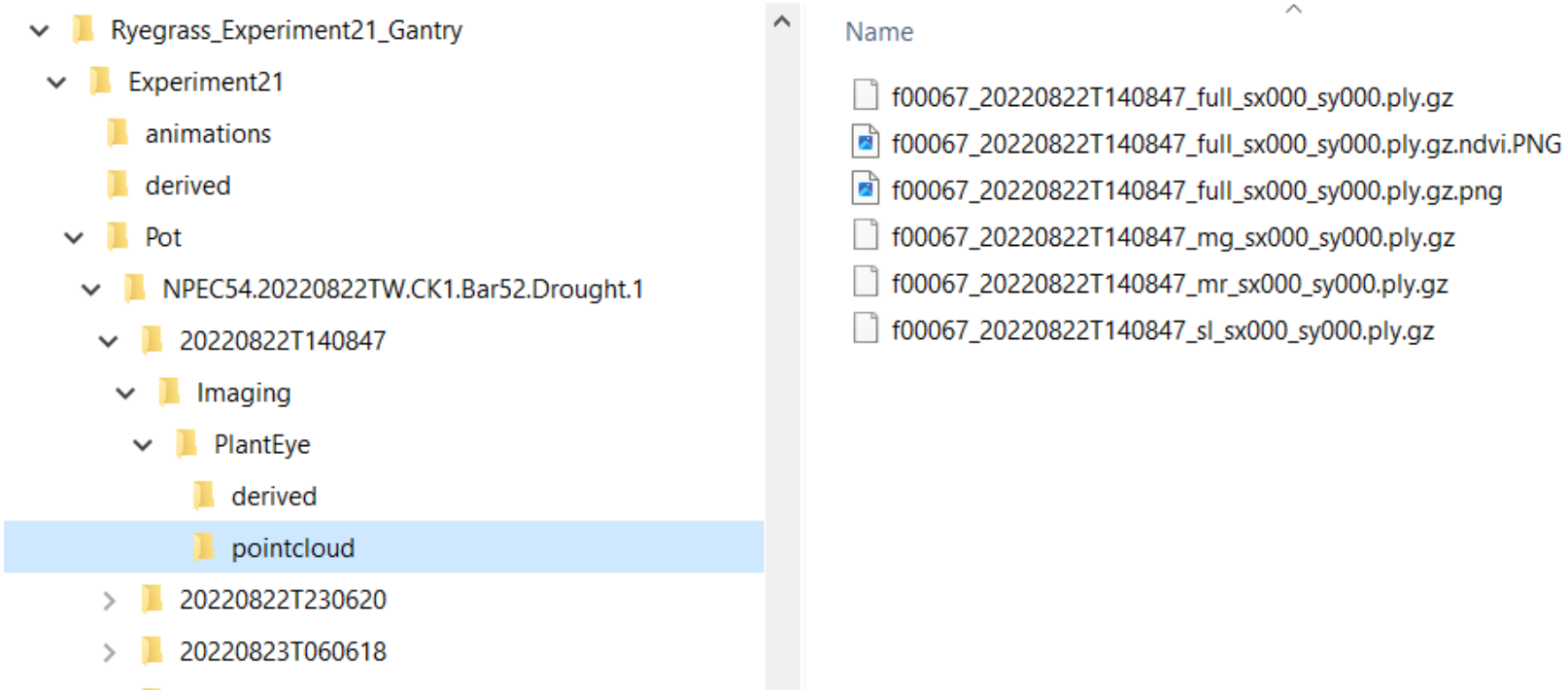
Metadata implementation (MIAPPE)



Extended ISA directory structure

- With thousands of measurements per experiment, the ISA structure is not suited for file storage
    - Operating / File systems and file browsers cannot deal with that many files in a single directory
- Extended ISA structure:
  Experiment / exp[id] / [Sample type] / [Pot ID] / [Assay timestamp] / Imaging / PlantEye / [data type]
- Makes data browsable (aka Findable) again

Extended ISA directory structure



ISA-JSON

- JSON file containing:
    - Project metadata
    - Samples & organisms
    - Sensor technologies
    - Location of the data files
    - And the type for each file (raw, derived)
- Computer (and little bit human) readable format
- Readily in and out Python & R isatools

```
{
    "@id": "#sample/a721c29a-5f86-4921-a5ce-024c39833d04",
    "characteristics": [
        {
            "category": {
                "@id": "#characteristic_category/040b5fbf-5d50-4631-ad8f-8d509ddcb0a5"
            },
            "comments": [],
            "value": {
                "@id": "#ontology_annotation/cb10d77d-dac2-4d6f-a218-e571e730208d",
                "annotationValue": "Plant",
                "comments": [],
                "termAccession": "http://purl.bioontology.org/ontology/NCBITAXON/33090",
                "termSource": "NCBITaxon"
            }
        }
    ],
    "comments": [],
    "derivesFrom": [
        {
            "@id": "#source/1cf2584b-e509-46ff
        }
    ],
    "factorValues": [],
    "name": "F1_6"
},
```


Sample

Assay (part)


```
        {
            "@id": "#data_file/0f65eadf-f045-4c0c-af40-bf91970627a9",
            "comments": [
                {
                    "name": "fullPath",
                    "value": "running_exp28_Gantry4/exp28/Pot/F2_5/20230725T111409/Imaging/PlantEye/derived/20230725T111409_psri.csv"
                }
            ],
            "name": "20230725T111409_psri.csv",
            "type": "Derived Data File"
        }
    ],
    "filename": "20230725T111409",
    "materials": {
        "otherMaterials": [],
        "samples": [
            {
                "@id": "#sample/a575a1be-6b2b-4b41-af26-c82fcabb6aa8"
            }
        ]
    },
    "measurementType": {
        "@id": "#ontology_annotation/2279abf0-7b79-478d-a11f-7da48bf11403",
        "annotationValue": "",
        "comments": [],
        "termAccession": "",
        "termSource": ""
    },
    "processSequence": [],
    "technologyPlatform": "PlantEye",
    "technologyType": {
        "@id": "#ontology_annotation/4dbb5726-90f0-4df2-bb43-eb16af6a3b6a",
        "annotationValue": "Imaging",
        "comments": [],
        "termAccession": "http://jermontology.org/ontology/JERMOntology#Imaging",
        "termSource": ""
    },
```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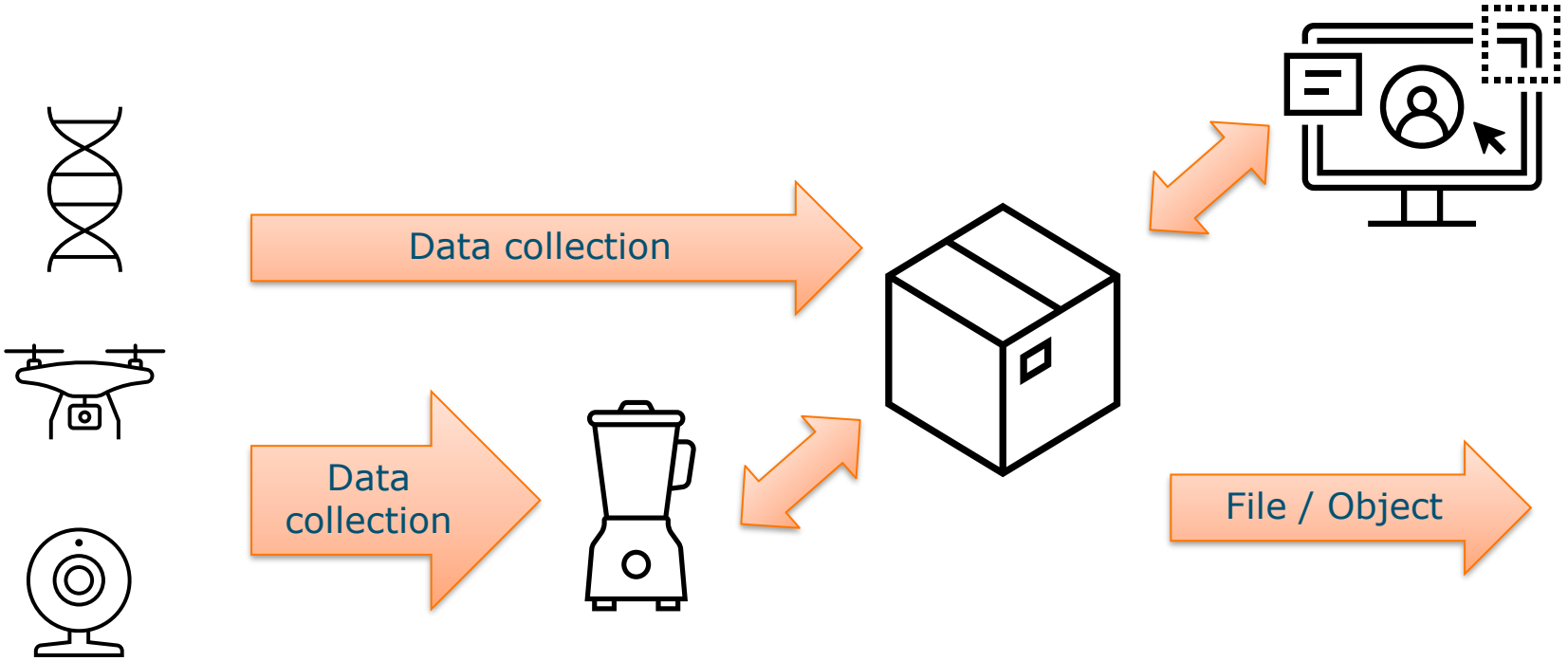
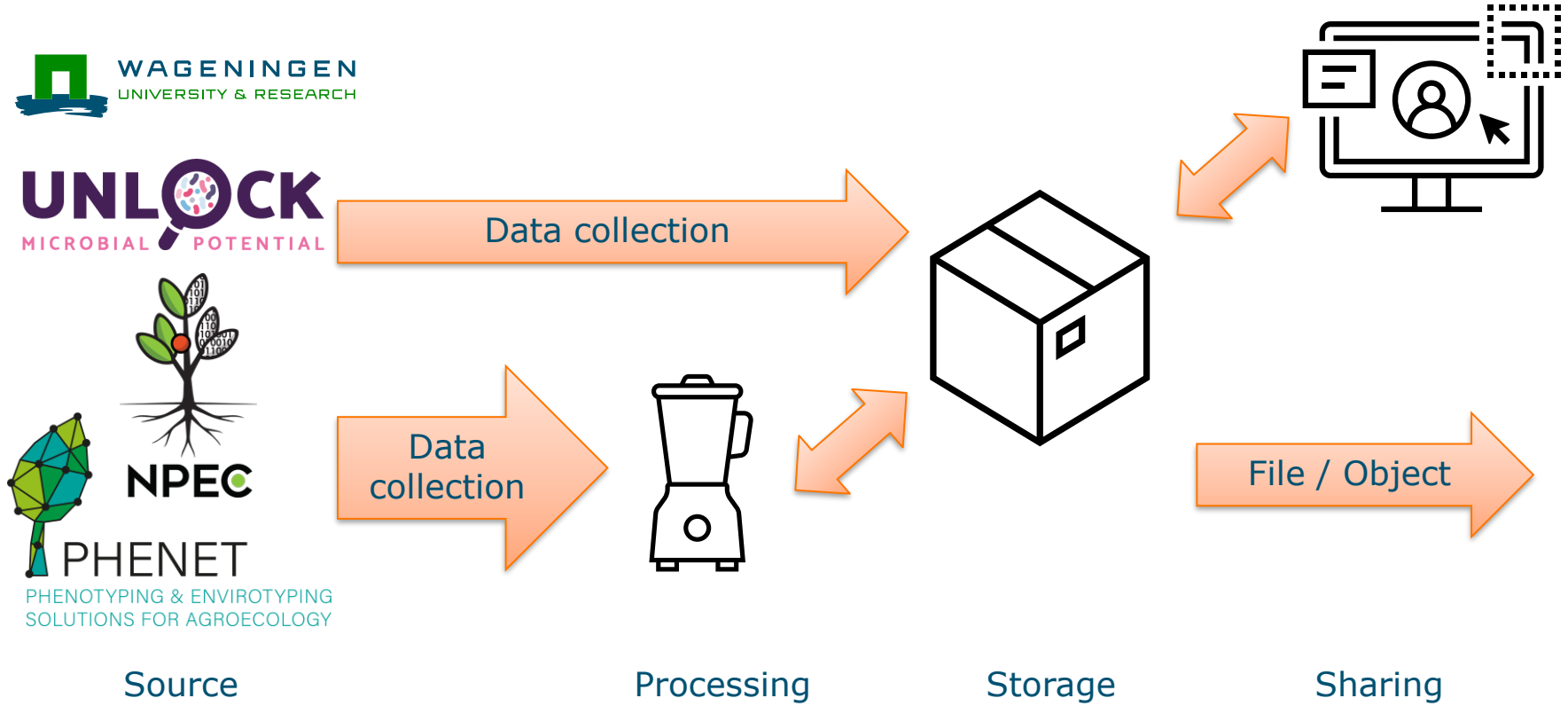
Use of ISA and ISA-JSON

- Adding pre-processing steps:
  - Get the relevant files
  - Process and store the location also in JSON
- For researchers:
  - Direct access to the relevant data files
  - Sharing makes the data more FAIR
- IT:
  - Use the metadata to store, archive or provide access to data

Data flow implementation



Data flow implementation



Data flow implementation

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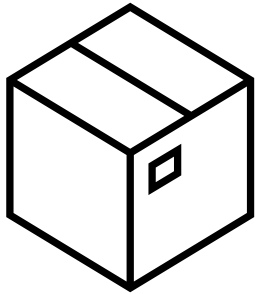
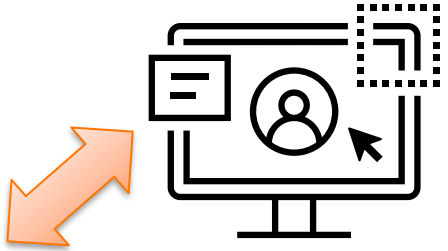
Data collection





File / Object

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Data flow implementation

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Data collection

Data collection

lustre

iRODS

File / Object

Source

Processing

Storage

Sharing

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Data flow implementation

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FAIRDOM SEEK

jupyter

ISA-JSON

Source | Processing | Storage | Sharing

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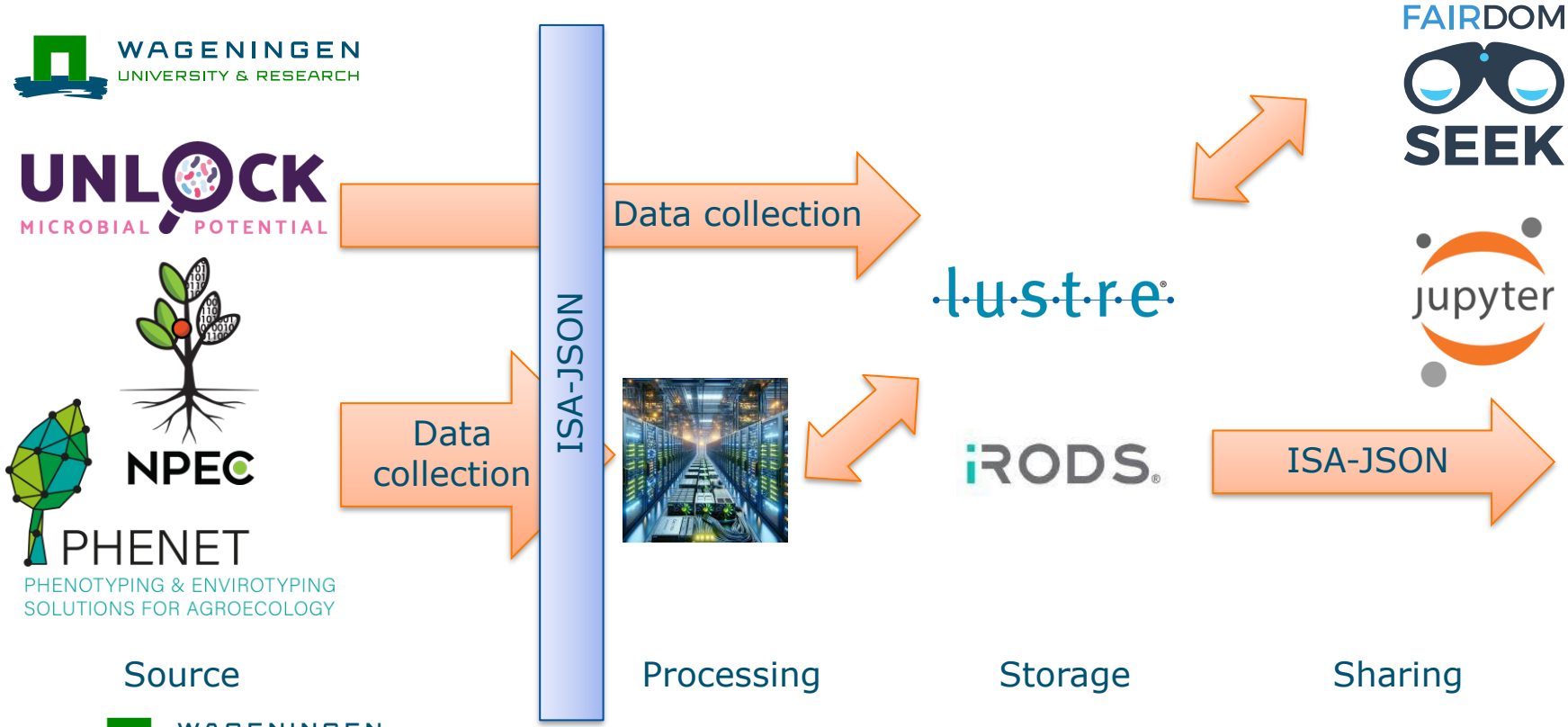
Data flow implementation



Ongoing implementations

- Data in iRODS
    - URL of file location in iRODS
- extISA structure for many projects
    - Automatic archiving on tape
- Create experiment related ISA-JSON files
- Processing ISA-JSON & data in iRODS using Python notebooks
    - Configurable upload to FAIRDOM-seek
- Upload datasets for data publications incl DOI

Question?

Balazs Brankovics

Bart-Jan van Rossum

Rick van de Zedde

Tim van Daalen

Sven Warris

Many others