How the PO2/TransformON and FermentON domain ontologies can help us achieve interoperability and reuse of data on (bio)processes.

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How the PO2/TransformON and FermentON domain ontologies can help us achieve interoperability and reuse of data on (bio)processes

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Food, Bioproducts
& Waste

Mathematics & Digital
Technologies

Microbiology
& the Food Chain

Human Nutrition
& Food Safety

Plant biology
& Breeding

Agroecosystems

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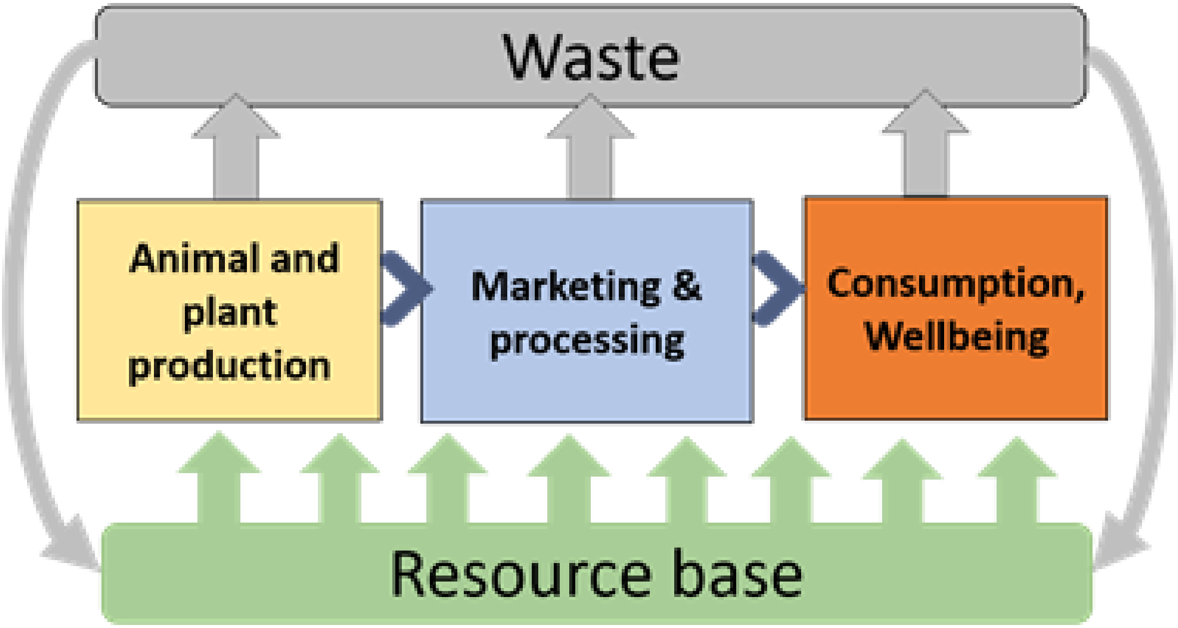
Numerous collaborators…

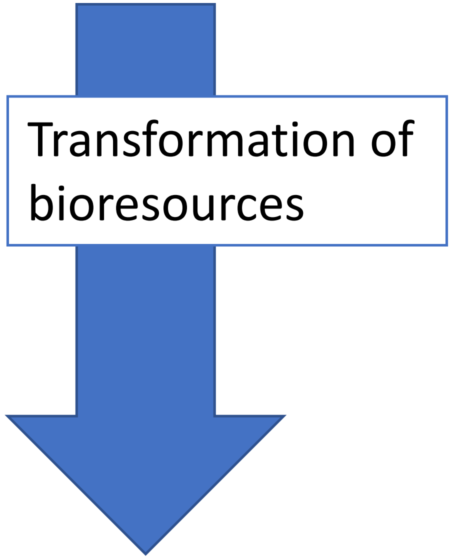
Challenges & solution

A tour on PO2/TransformON and FermentON

Food, Bioproducts and Waste engineering in the context of bioeconomy and global agri-food systems



Socio-economic drivers
Environmental drivers
Nutrition & Health



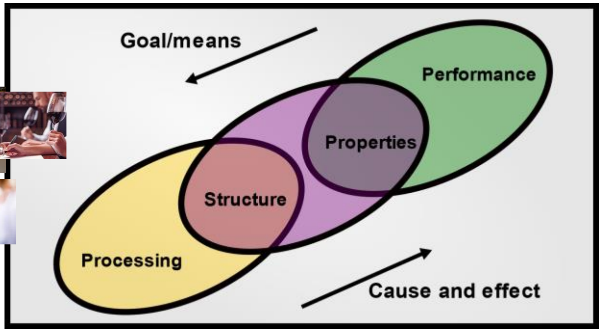
Towards a circular & sustainable agri-food system

Research challenges /ontology purposes:

- Designing food quality, from agricultural production to the impact of diets on health and the environment
- Designing biomass construction/deconstruction processes for the production of bioproducts and the use of waste (or residues) generated by human activities.

Knowledge discovery in Food and Bioproducts engineering is challenging

Complex research questions on both process performances & product usages...



Multidisciplinary fields & disciplines : Chemistry, Physics, Biology, Microbiology, Process engineering, Analytical chemistry, Sensometrics, ….

Heterogeneous experimental data,
multi-source, multi-format, multi-scale, sometimes incomplete, imprecise…

How to reason under uncertainty ??

Need for
STRUCTURING data

STANDARDISING metadata

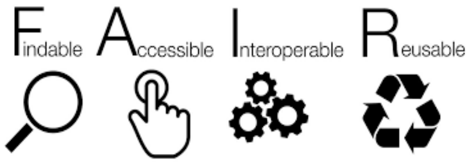
QUERYING &
LINKING data (W3C)

SHARE ------> **Re-USE**

STATISTICAL MODELLING & MACHINE LEARNING

Feedback with rules & constraints

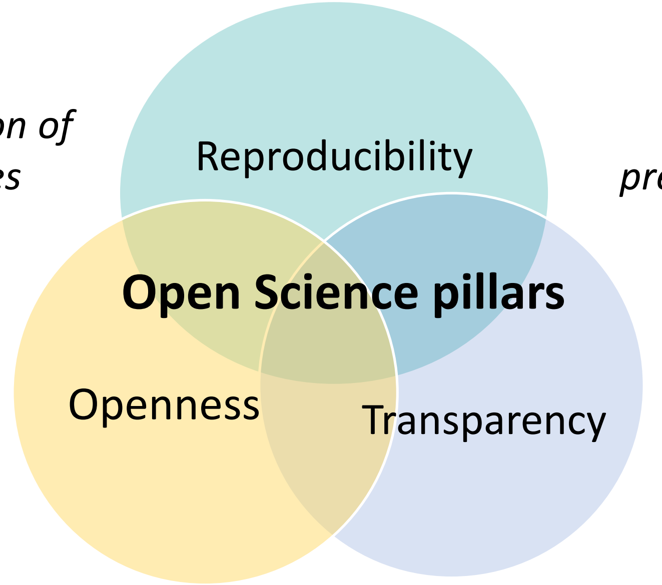
KNOWLEDGE DISCOVERY



W3C Semantic Web

How to collect, manage and provide FAIR data (by-design)

Effective collaboration of research communities



Long-term preservation of data

Build Machine-Learning models

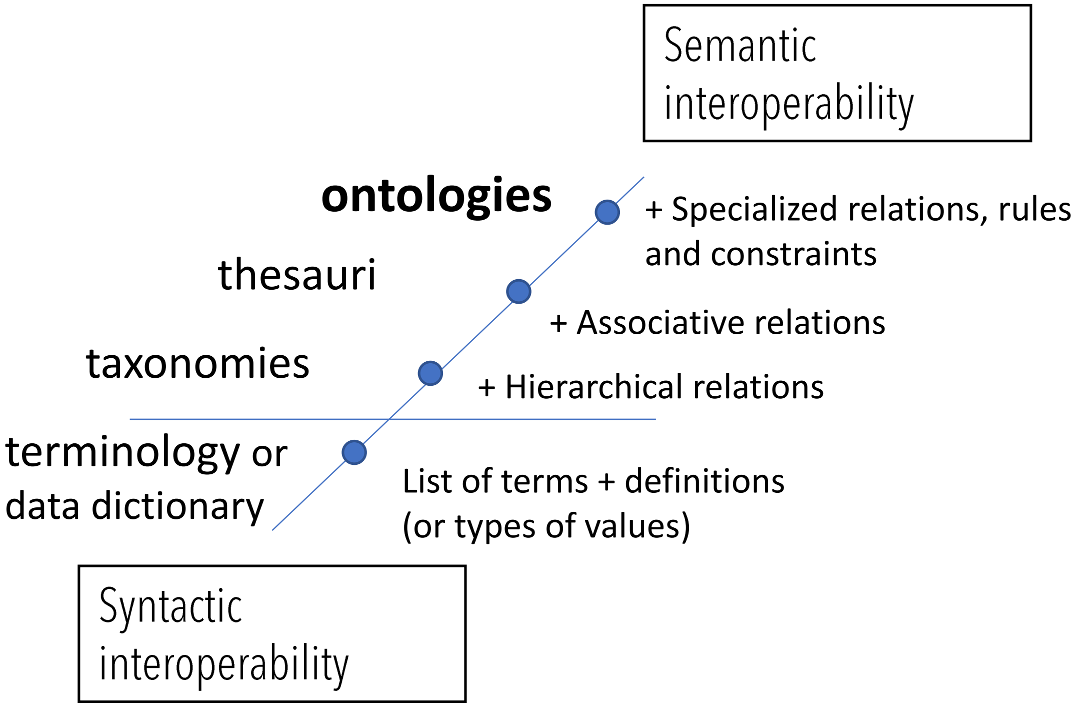
In the context of « Data-driven research » and Open Science, we need to formalize knowledge to make it "explicit" and "shareable": ***not** just data* but also **information about data (*metadata*)** to share the context and provenance of data

Ontologies are a key solution for interoperability & reusability (I & R)

Why are ontologies so useful?

Semantic interoperability is **unambiguous**, leaving few room for error or misinterpretation.

Semantically interoperable systems share the **same conceptual understanding of what the underlying data conveys,** thanks to ontologies.



There is a broad spectrum of ontologies :

- **Upper-level : foundational ontologies**
  - *BFO, DOLCE, …*
- **Mid-level : core ontologies, task ontologies**
  - *SOSA/SSN, PROV-O, Time ontology…*
- **Application level : domain ontologies , termino-ontologies**
  - *Vocabulary specific to the field (labels+ definitions)*

➢ *The domain ontologies, PO2/TransformON and FermentON are based on the PO2 core model*

Syntactic interoperability provides a **consistent data format** that can be interpreted by different systems.

Ontologies allow us to reach *Semantic interoperability*

The Process and Observation Ontology (PO2)

<u>A generic model in OWL</u>,

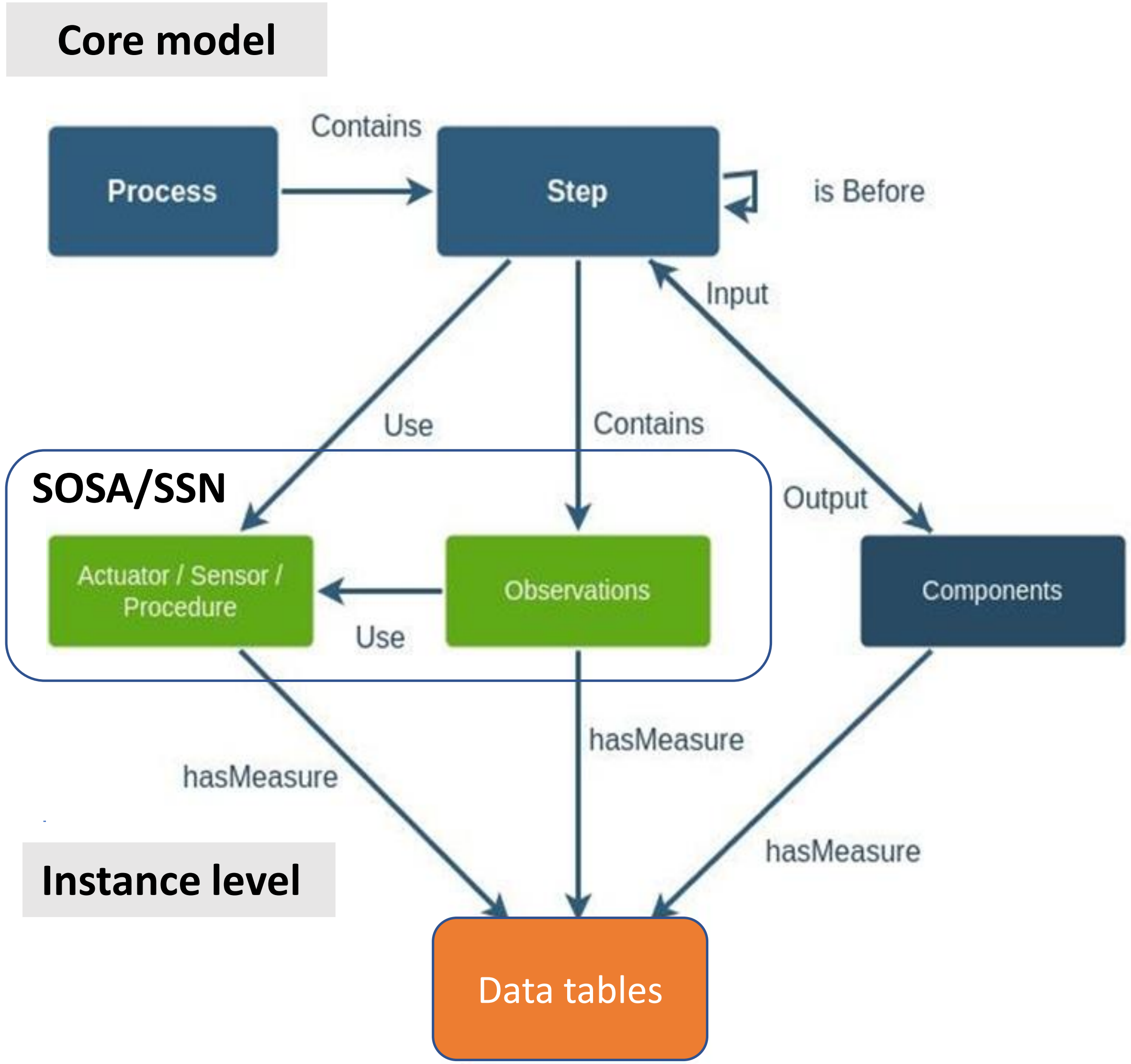
reusing SOSA/SSN concepts

together with other ontologies (BFO, IAO, Time ontology, QUDT), metadata schemas (DCAT, Schema.org), and the Unified Code for Units of Measure (UCUM)

<u>designed to describe :</u>

- Processes as a sequence of steps
- Input and output components
- Observations with materials and methods
- Results described in data tables at the instance level

- **Quantitative and qualitative values in the data tables conform to the I-ADOPT Variable Design Patterns** (https://catalogue.fair-impact.eu/resources/i-adopt)



Ibanescu et al. 2016

A unified vocabulary (TransformON) specializing the PO2 core concepts

Process Part

- PO2 / Component
  - living organism
    - algae (as living organism)
    - animal (as living organism)
    - bacteria (as living organism)
    - fungi (as living organism)
    - lichen (as living organism)
    - plant (as living organism)
  - substance
    - biochemical constituent
    - feed
    - food
    - non-food substance
    - water (generic)

- PO2 / Process
  - physiological process
    - human physiological process
    - microbial physiological process
    - plant physiological process
  - planned process
    - characterization process
    - transformation process

- PO2 / Step
  - characterization step
  - physiological process step
  - transformation step
    - cleaning
    - handling
    - harvesting
    - packaging
    - pre-processing
    - processing
    - slaughtering
    - storage
    - transport

Result Part

- PO2 / Attribute
  - calculation outcome
    - experimental data attribute
    - LCIA
    - nutritional score
  - inherent quality
    - identification attribute
    - label or labelling claim
    - physical state
    - status of food name
  - measurement attribute
    - biological attribute
    - mensuration
    - physico-chemical attribute
    - quantity
    - temporality

Observation Part

- PO2 / Material
  - measuring instrument
  - processing equipment

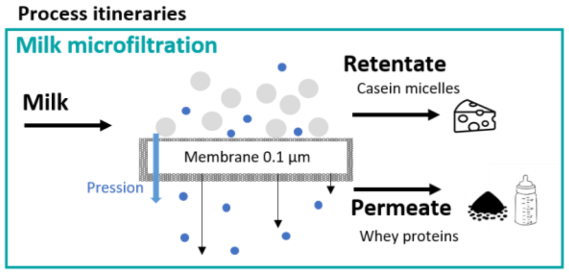
- PO2 / Method
  - analytical method
  - assessment method
  - computation and modelling
  - semi-empiric instrumental method
  - standard operating procedure

- PO2 / Scale
  - measurement scale
  - process scale

Weber et al. 2023

A variety of use cases and research objectives have been addressed

Objective: Predicting the performance of the milk microfiltration process

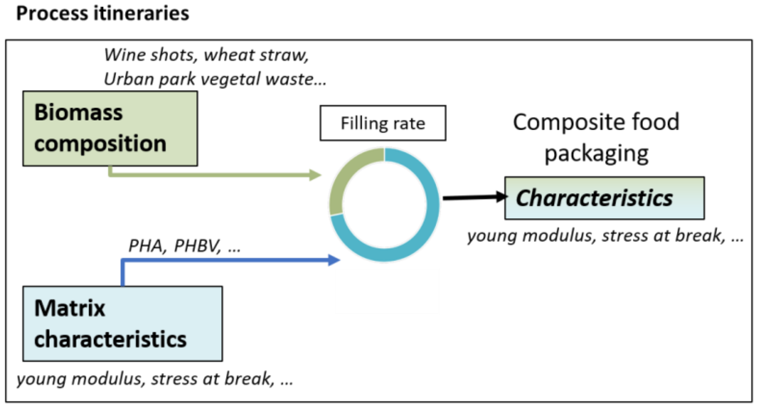


Baudrit et al. 2022

Problem to be solved:

- **Very heterogeneous and incomplete data**
- **Existing models limited to a specific range of operating conditions**

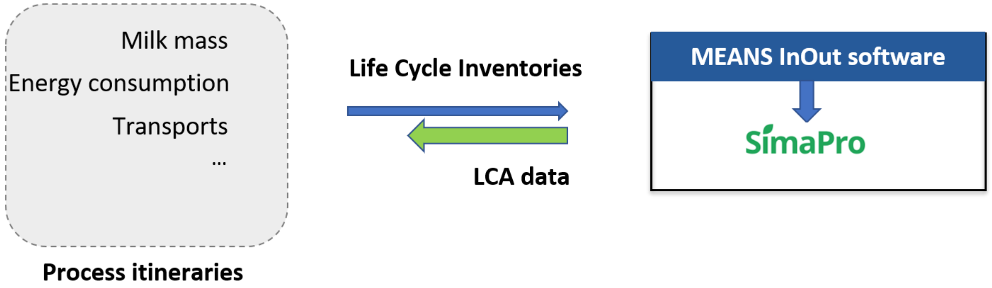
Objective: optimization of composite food packaging formulation



Münch et al. 2022

Problem to be solved : find what biomass and what loading rate to achieve the desired mechanical characteristics

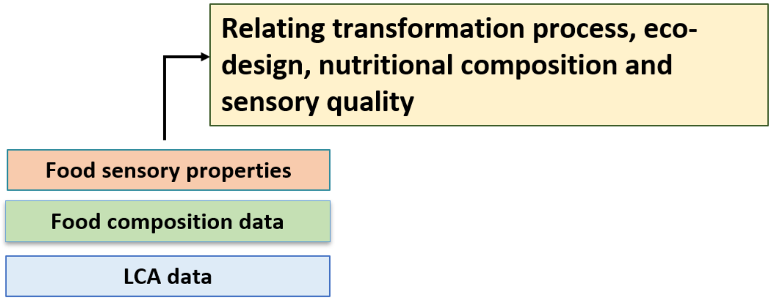
Objective: to study the environmental impacts of cheeses



Auberger et al. 2022

Problem to be solved : providing the process flowchart and inventory data needed for Life Cycle Impact Assessment

Objective: to design healthy, sustainable and acceptable food



Pénicaud et al. 2019

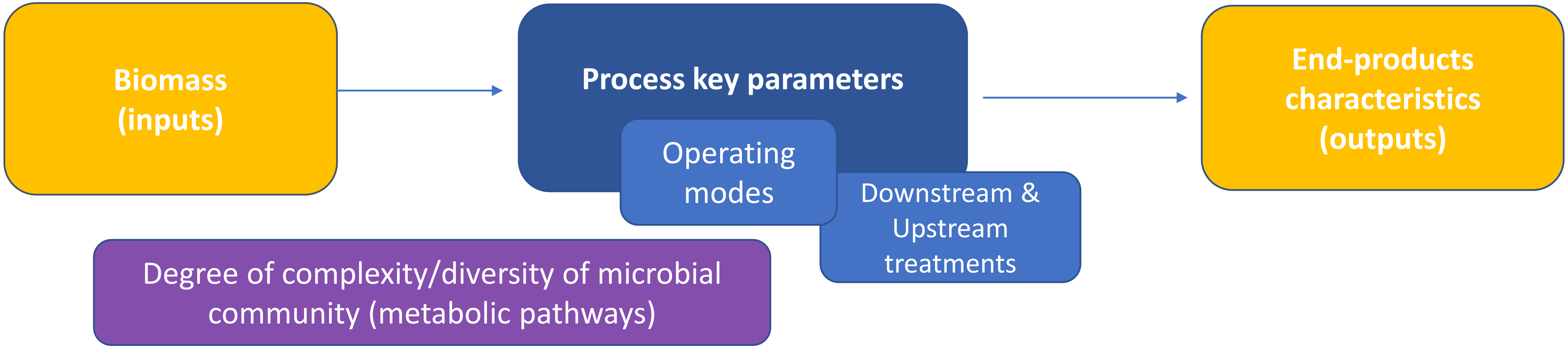
Problem to be solved: integration of heterogeneous data to provide a global quality score

What's next ?

Ongoing project FermentON

FermentON : extension of PO2/TransformON to bioprocesses

Scope: key concepts to describe **fermentation processes** (= using microbial agents) and, more broadly, **biological processes** (= using microbial agents and/or enzymes).



Examples of questions to be answered :

What combination of substrate/agent/target product and available equipment is needed to choose the cultivation method?

What products result from metabolic activity (intermediates and/or metabolites)? With which enzymes?

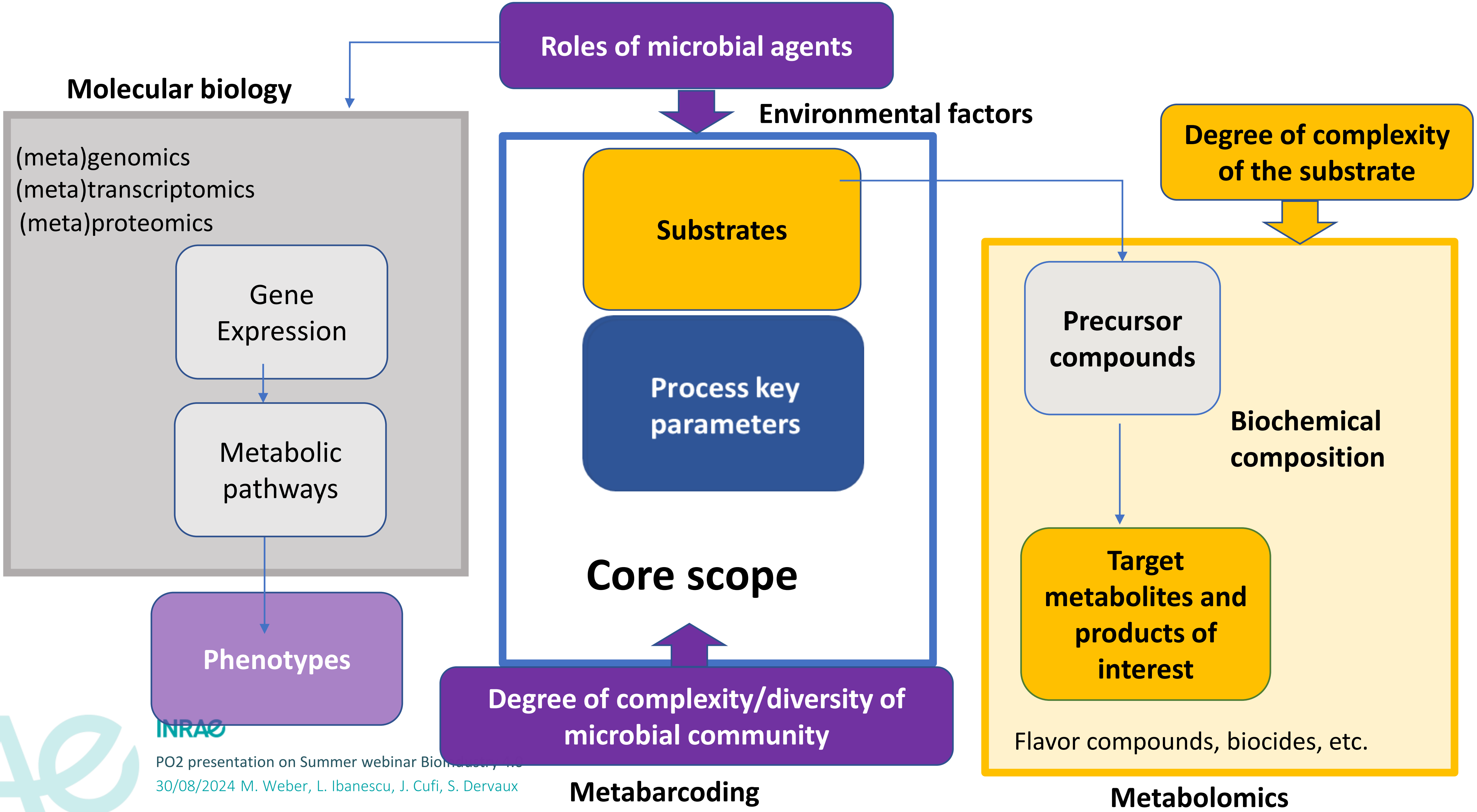
Use cases in FermentON

Food fermentation	Wine making	Composite making	Environmental biorefinery & biotech
(i) cheese, (ii) mixed dairy and plant-based yogurts, and (iii) fermented vegetables	A continuous line from vine to wine & a multiscale study of alcoholic fermentation	Production of PHA/PHBV for composite packaging materials	(i) Electrofermentation (ii) Design of soft sensors

Fermented food & Beverage

Bioproducts, matter & energy

Scope to be covered

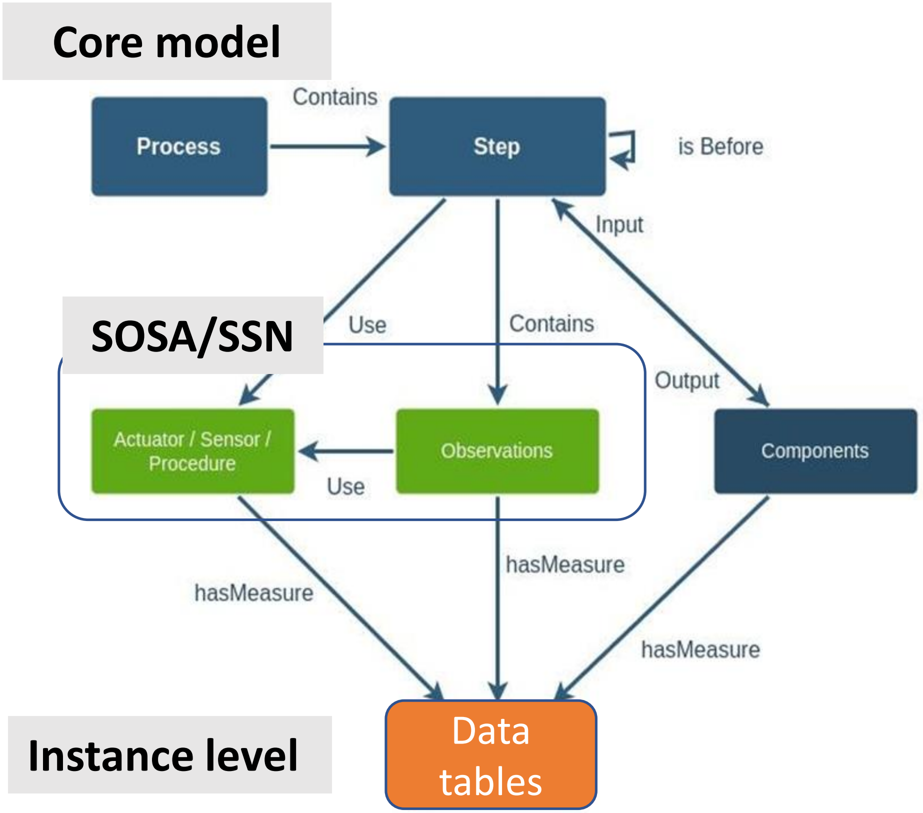


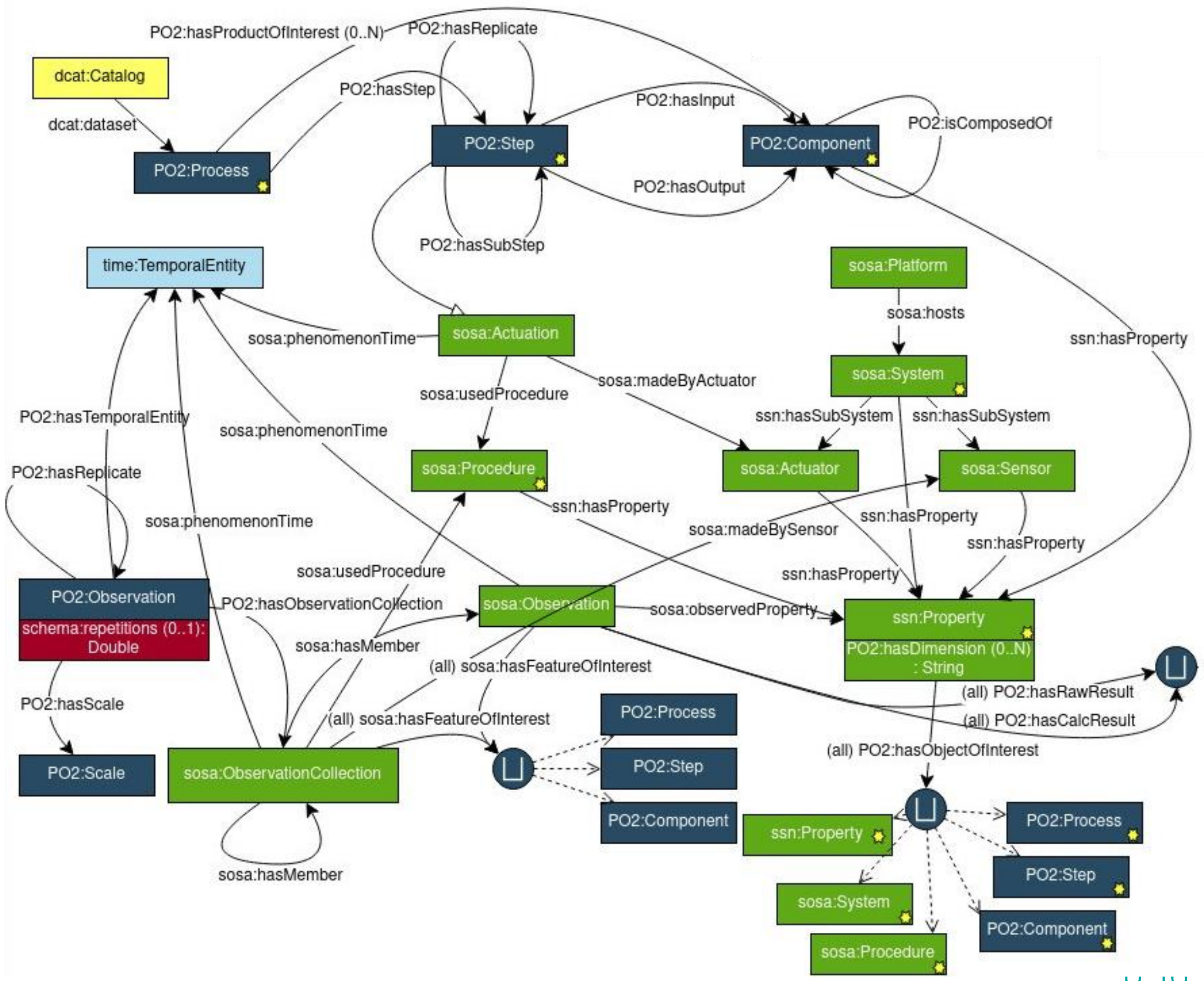
How to produce FAIR by-design and AI-ready data in practice ?

Deep dive into the ecosystem !

How to produce FAIR by-design and AI-ready data in practice ?

Simplified ontology representation VS reality …





How to produce FAIR by-design and AI-ready data in practice ?

Producing FAIR data requires Ontology driven Information System

These Information System address main needs like

- Data Entry
- Data Querying

… and relies on a Software Architecture who ensure

- Security and Access Management
- Interoperability

Data entry

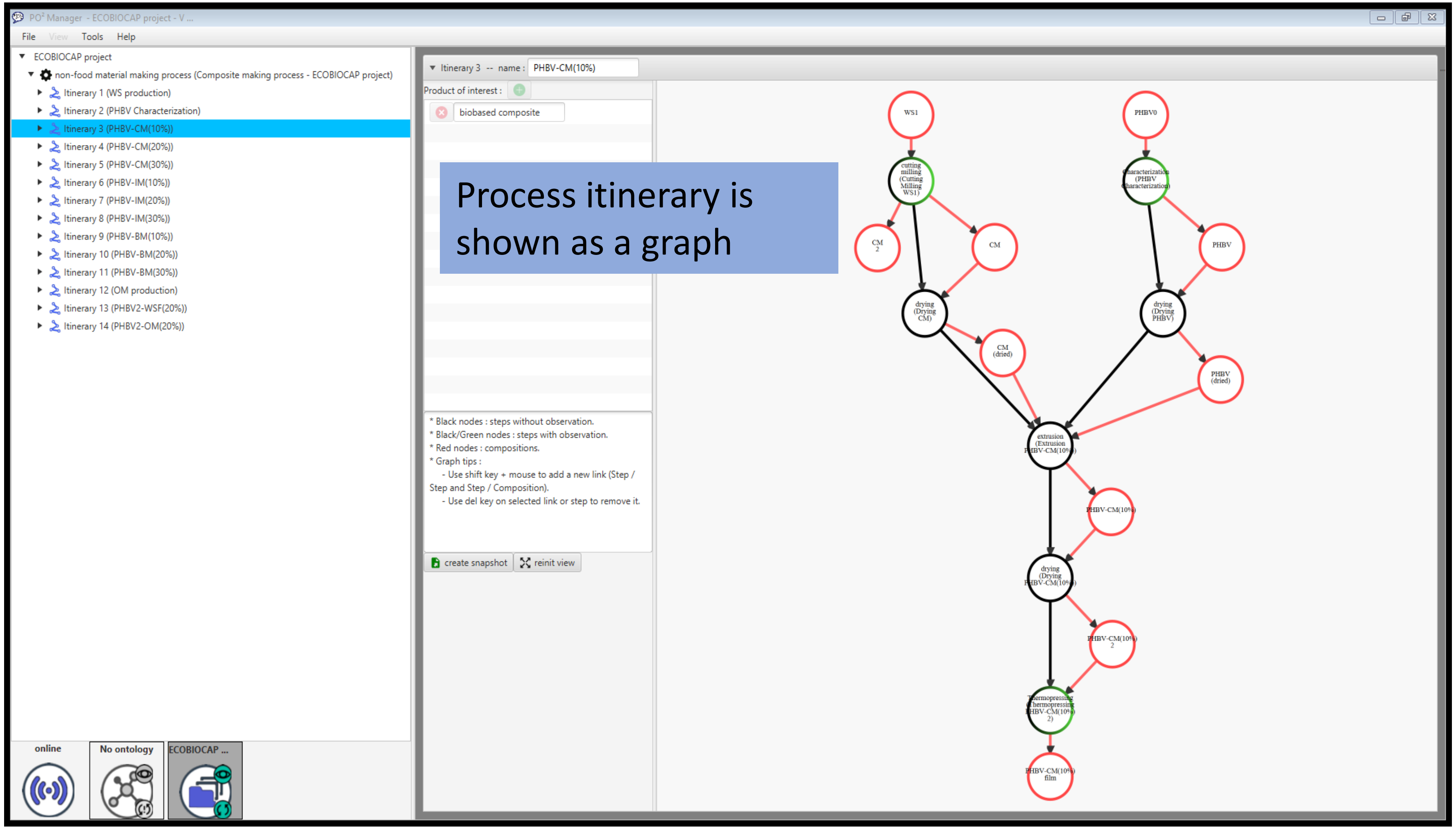
Desktop Application PO² Manager

- Main features
  - Data entry with visualization directly through the application
  - Import/Export of Excel template files
  - Data quality checks
    - Terminological consistency checks
    - Data checks on allowed value range (including dimensions for SI units)
  - Semantization process *i.e* remote publication to save and share data
- Benefits
  - Ontologies are stored on a centralized database

    → **One shared vision applied to ≠ context**
  - Data understanding through visualisation of the studied process
  - Standardized vocabulary used but no « Semantics prerequisites » required
  - Linked with international W3C standards
    - (e.g., Semantic Sensor Network Ontology, Time Ontology, ...)

Data entry

PO² Manager User Interface



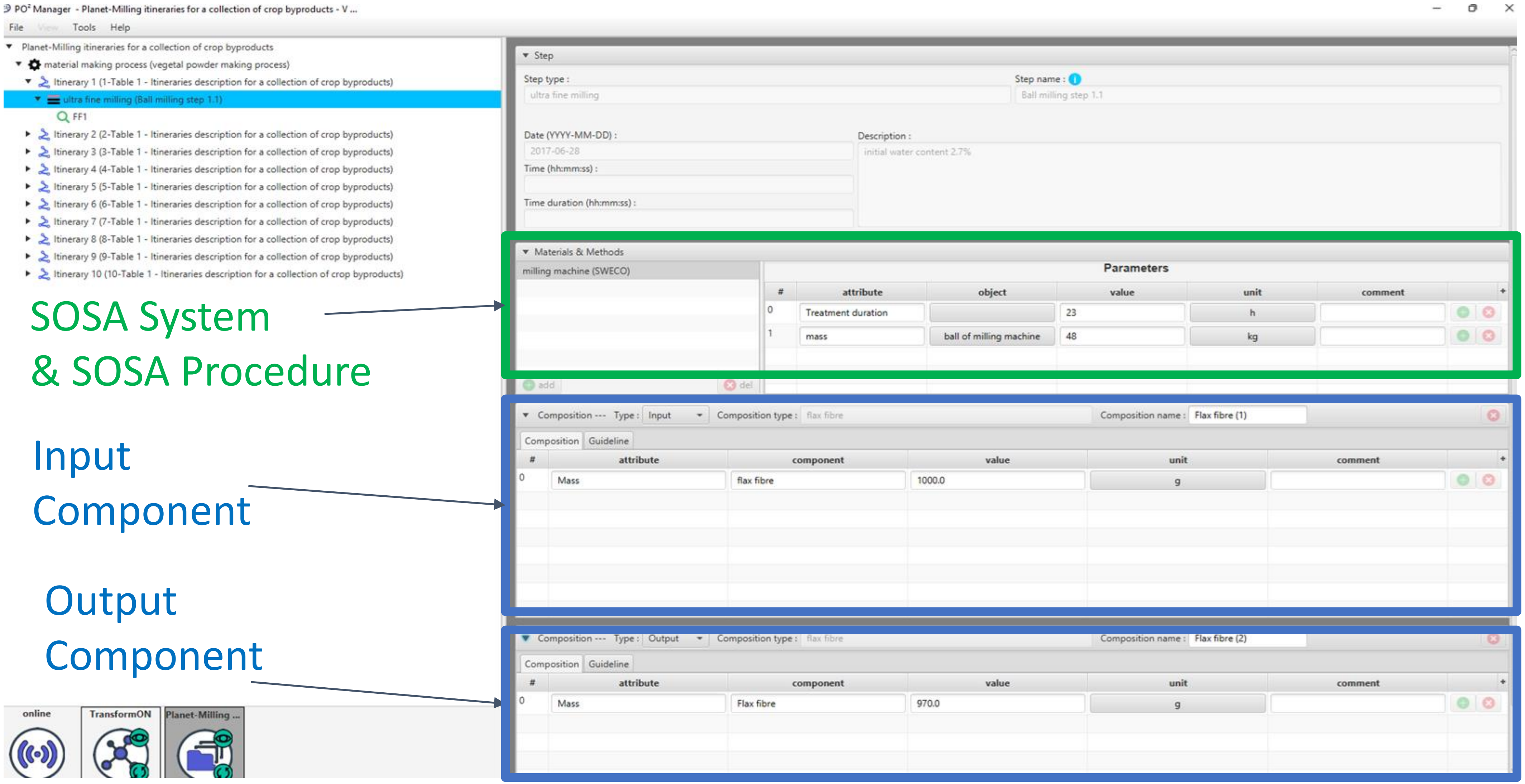
Red Circle : Component

Black Circle : Step

Black + Green: Observations

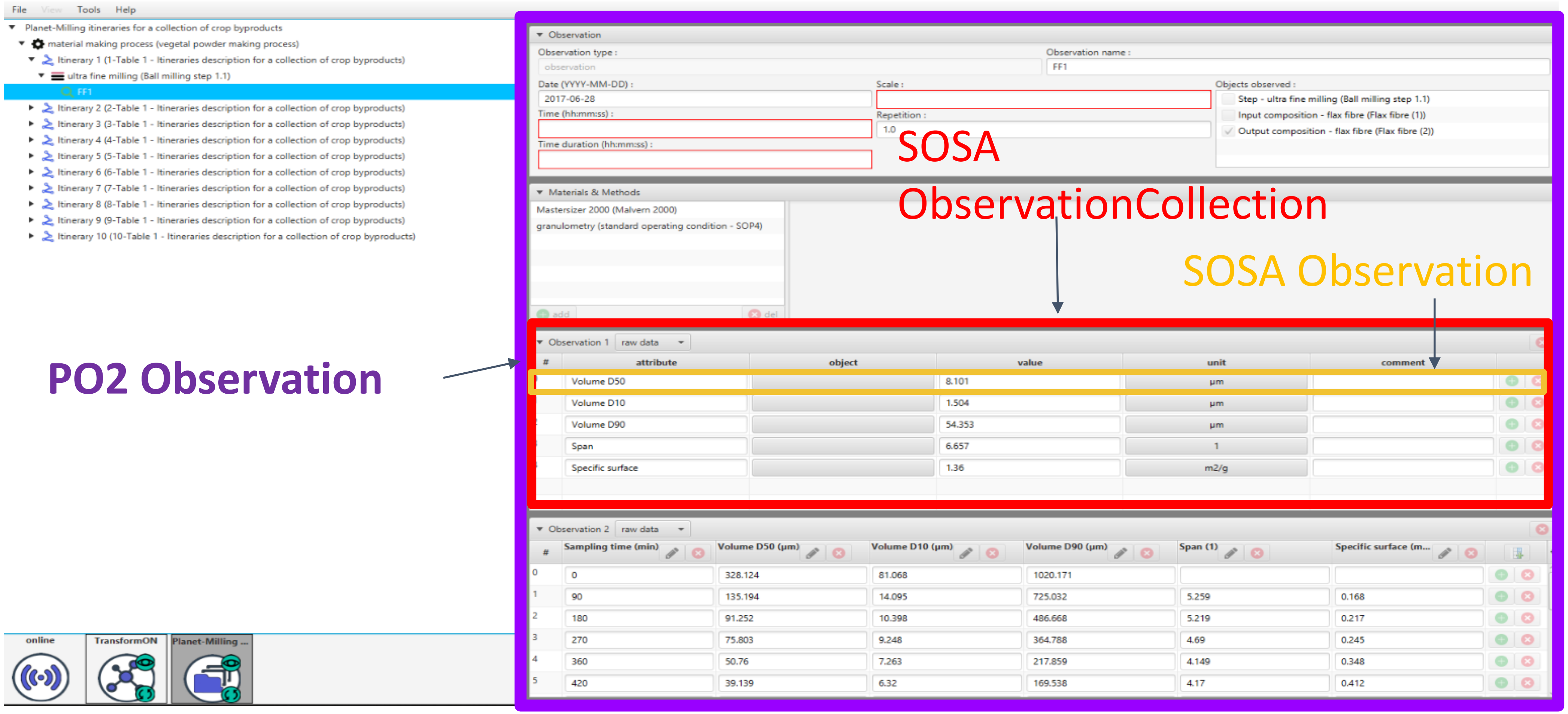
Data entry

PO² Manager User Interface : link with underlying ontologies



Data entry

PO² Manager User Interface : link with underlying ontologies



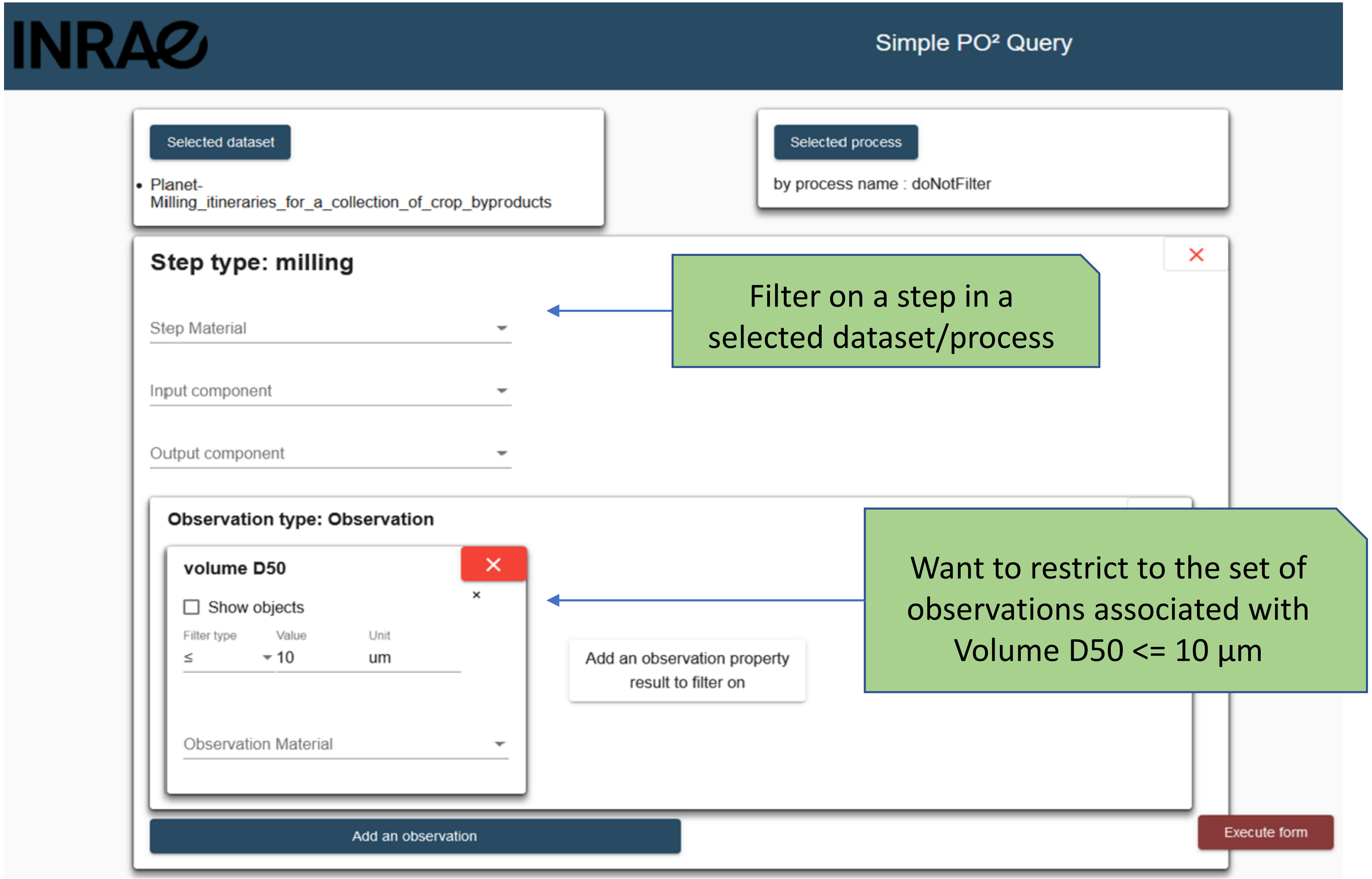
Data query

Web application SPO²Q

- Main Features
  - Search engine with two modes :
    - **Simplified** for standard data users via classic web forms
      - No « technical » knowledge required
    - **Advanced** for « power users »
      - Assisted complex query writing
      - Fine-tuning of the SPARQL query
  - Automatic conversion : querying data with ≠ units of measure
  - Save most frequent queries for re-execution
  - Query result export (CSV, JSON, …)
- Benefits
  - Controlled vocabularies used to query data
  - Query public and private project's data
  - Cross querying between opened data sources

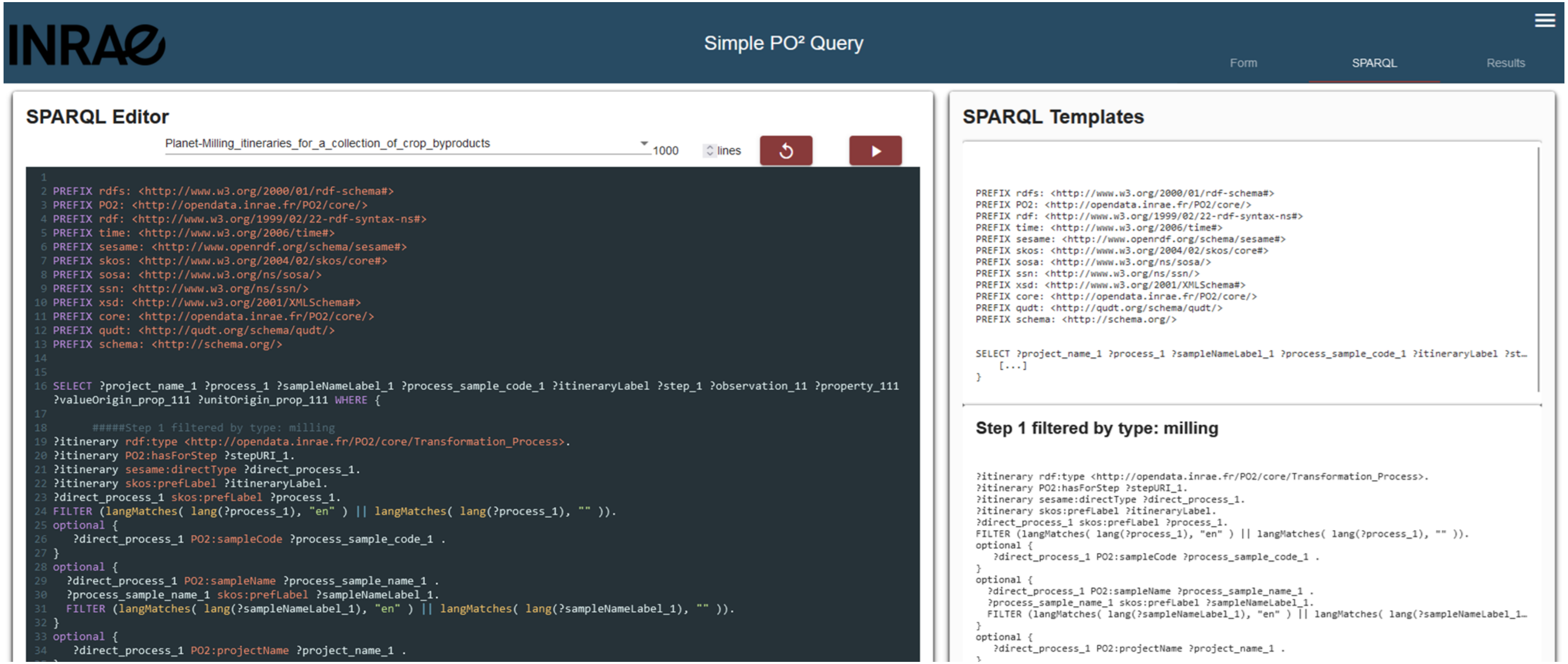
Data query

SPO²Q User interface : Simple mode



Data query

SPO²Q User interface : Advanced mode

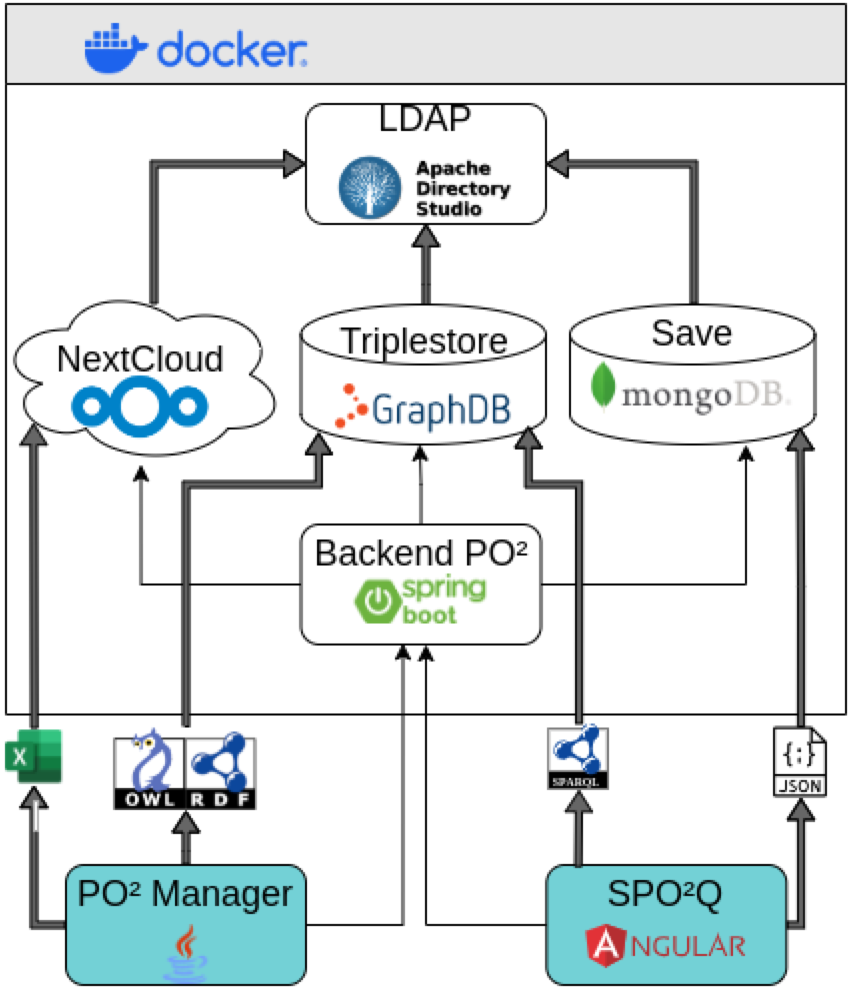


Security and Access Management

- **Data is FAIR but not necessarily immediately open**

→ Possibility of private project creation

- Account management internal LDAP shared with PO2 Manager and SPO²Q
    - One single account per user
    - Flexibility in account creation (not necessarily institutional)
- Management of read/write access by users
- Querying private and public data



What's next ?

- Collaborative ontology construction
  - → Share and improve domain ontology by integrating scientific point of views
  - → Workflow construction based on Git/Gitlab
- Develop and enforce AI applications
  - → Improve quality checks and user's feedback
- Large dataset management
  - → Be able to perform semantic queries on large dataset (Ex : Long times series)
    - Proof of Concept « Best of two worlds » in progress
      - BigData technology stack for performance
      - Semantic technology stack for knowledge representation

      → SANSA https://sansa-stack.net/
- Interface improvement (UX design)

In a nutshell

Summary

Data of interest

STRUCTURING data

STANDARDISING metadata

QUERYING &
LINKING data (W3C)

AI-READY Data

Re-USE

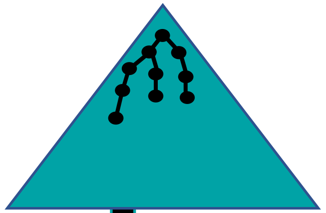
SHARE (PUBLISH)

Open data publication option

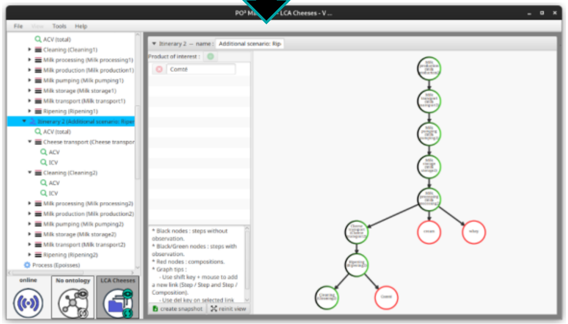
STATISTICAL MODELLING & MACHINE LEARNING

KNOWLEDGE DISCOVERY

PO2 core and domain ontologies



PO2 Manager



SPO2Q

Graph DB

FAIR by-design Data

PO2/TransformON : An ontology for modelling biomass transformation process and characterization of food, feed, bioproducts & biowaste

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PO2/TransformON, an ontology for data integration on food, feed, bioproducts and biowaste engineering

Magalie Weber, Patrice Buche, Liliana Ibanescu, Stéphane Dervaux, Hervé Guillemin, Julien Cufi, Michel Visalli, Elisabeth Guichard & Caroline Pénicaud

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Ouvrir la science !

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TRANSFORM

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Documentation and support:
https://quantum.mia-ps.inrae.fr/PO2/

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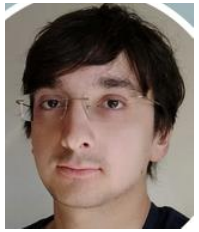

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Hervé Guillemin
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PAM Dijon/Poligny

& PLASTIC Platform

PAM
Food and wine sciences & Technology

Softwares

- Dervaux et al. 2023: PO2 Manager, an annotation tool to edit biomass transformation and characterization itineraries using the Process and Observation (PO2) Ontology. ⟨swh:1:dir:b9983f579ca087d946a9c3e4818e4507de395937⟩. ⟨hal-04313202⟩
- Dervaux et al. 2024: PO2 Engine, an application programming interface associated with the Process and Observation (PO2) software ecosystem. ⟨swh:1:dir:076aa8ecc70160ac3c9c333570c8d495d7e2ff19⟩. ⟨hal-04387669⟩
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Reused standards and ontologies

- SOSA/SSN https://www.w3.org/TR/vocab-ssn/
- BFO https://obofoundry.org/ontology/bfo.html
- IAO https://obofoundry.org/ontology/iao.html
- Time Ontology https://www.w3.org/TR/vocab-owl-time-rel/
- QUDT https://qudt.org/
- UCUM https://ucum.org/
- Schema.org https://schema.org/
- DCAT https://www.w3.org/TR/vocab-dcat/
- I-ADOPT https://i-adopt.github.io/ontology/

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