TU WIEN Informatics

192.161 Management of Graph Data

(4.0 VU / 6.0 ECTS)

2025W

Advanced Topics

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Lecture Outline

- Advanced topics in graph data management
- Course feedback
- Exam information

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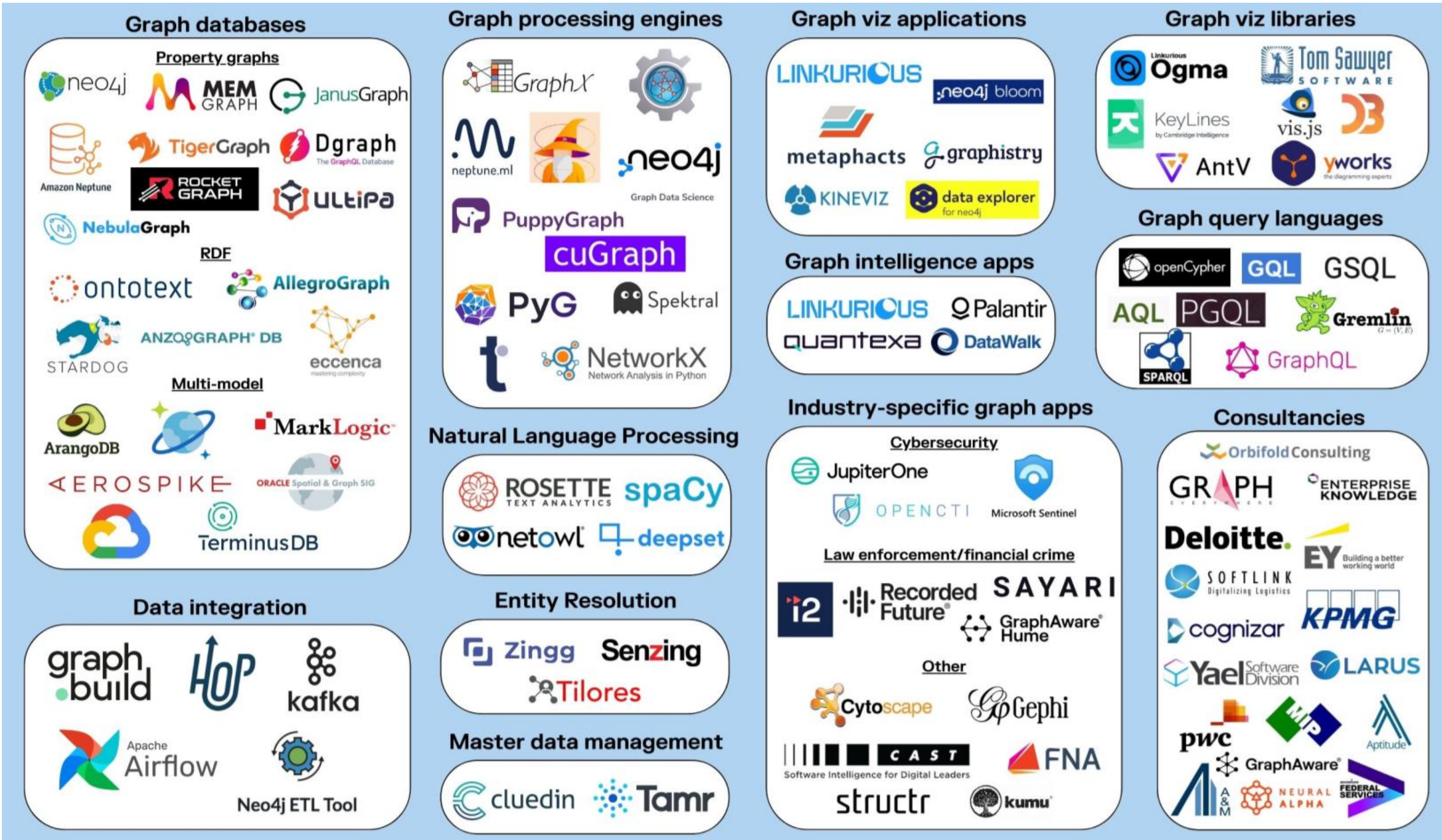
Graph technology landscape



https://linkurious.com/blog/introduction-graph-technology-landscape/

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Knowledge graph challenges for GDBMS and AI

Data Modeling and Interoperability

- alternative graph data models (RDF, property graphs) and query languages (SPARQL, Cypher, GQL)
- schema modeling (ontologies, PG-schema)
- multimodal data
- data integration (OBDA, entity resolution, virtual KGs, etc.)

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Scalability and Querying

- efficiently handling large-scale graphs
- indexing, statistics, query optimization
- centralized/cluster/federated
- example-driven analytics and exploration

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Quality, Provenance, and Dynamics

- ensuring accuracy, completeness, and consistency (SHACL, SHeX, PG-schema)
- Knowledge evolution, temporal knowledge graphs
- provenance, lineage

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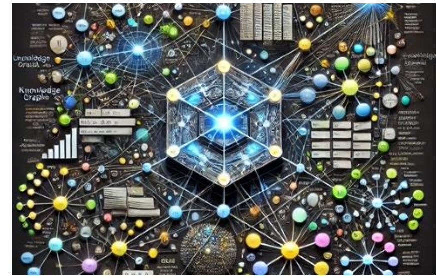
Reasoning and Neurosymbolic AI



- combining logical reasoning with machine learning
- embeddings, vector representations
- graph neural networks
- multi-modal ML

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- Semantic Data Lakes
- information retrieval
- AutoML
- data catalogs
- explainable AI
- digital twins

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KGs as Enabling Technology

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Generative AI

- LLMs and hallucinations
- Conversational agents
- Agentic AI
- GraphRAG

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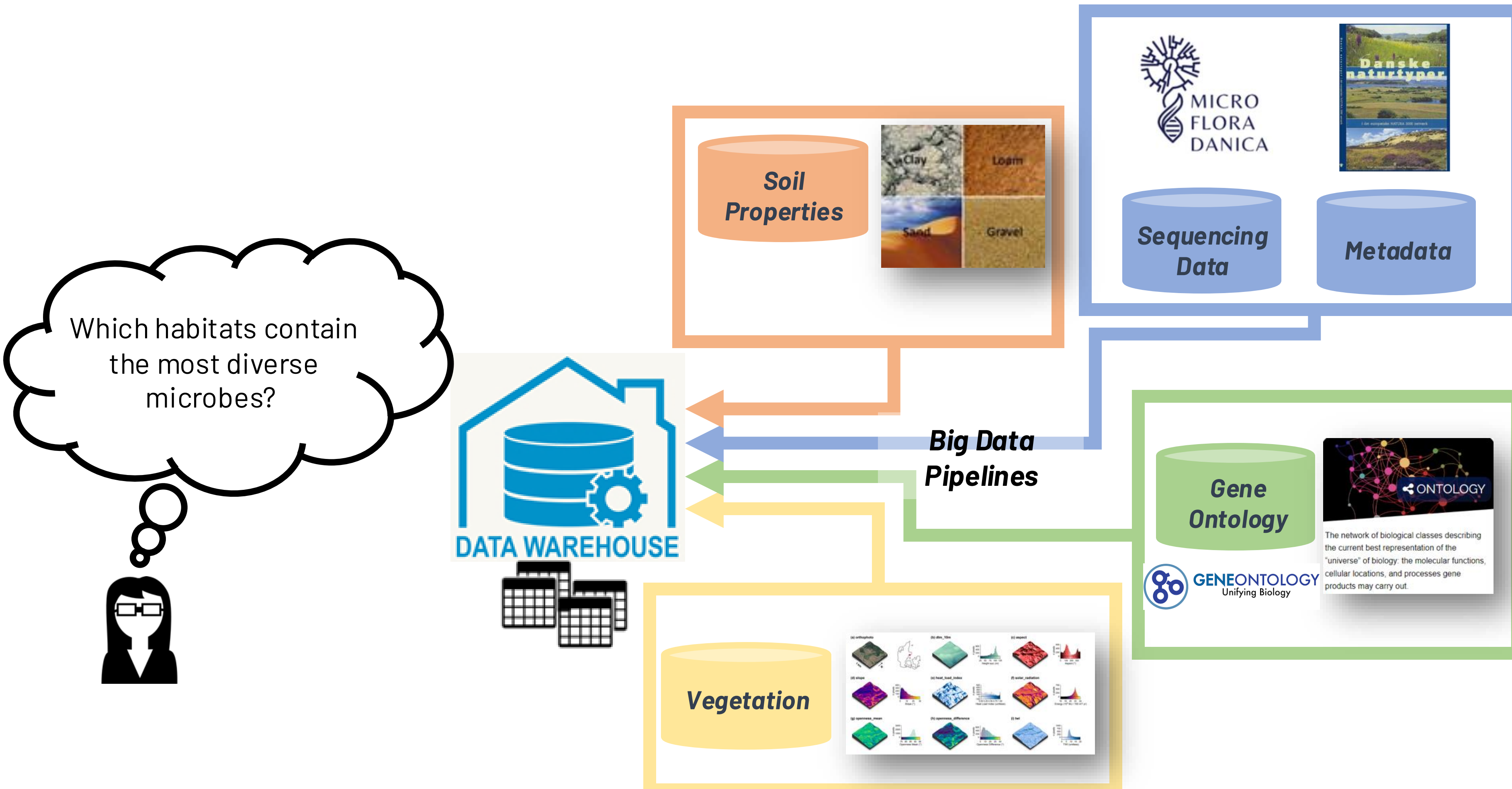
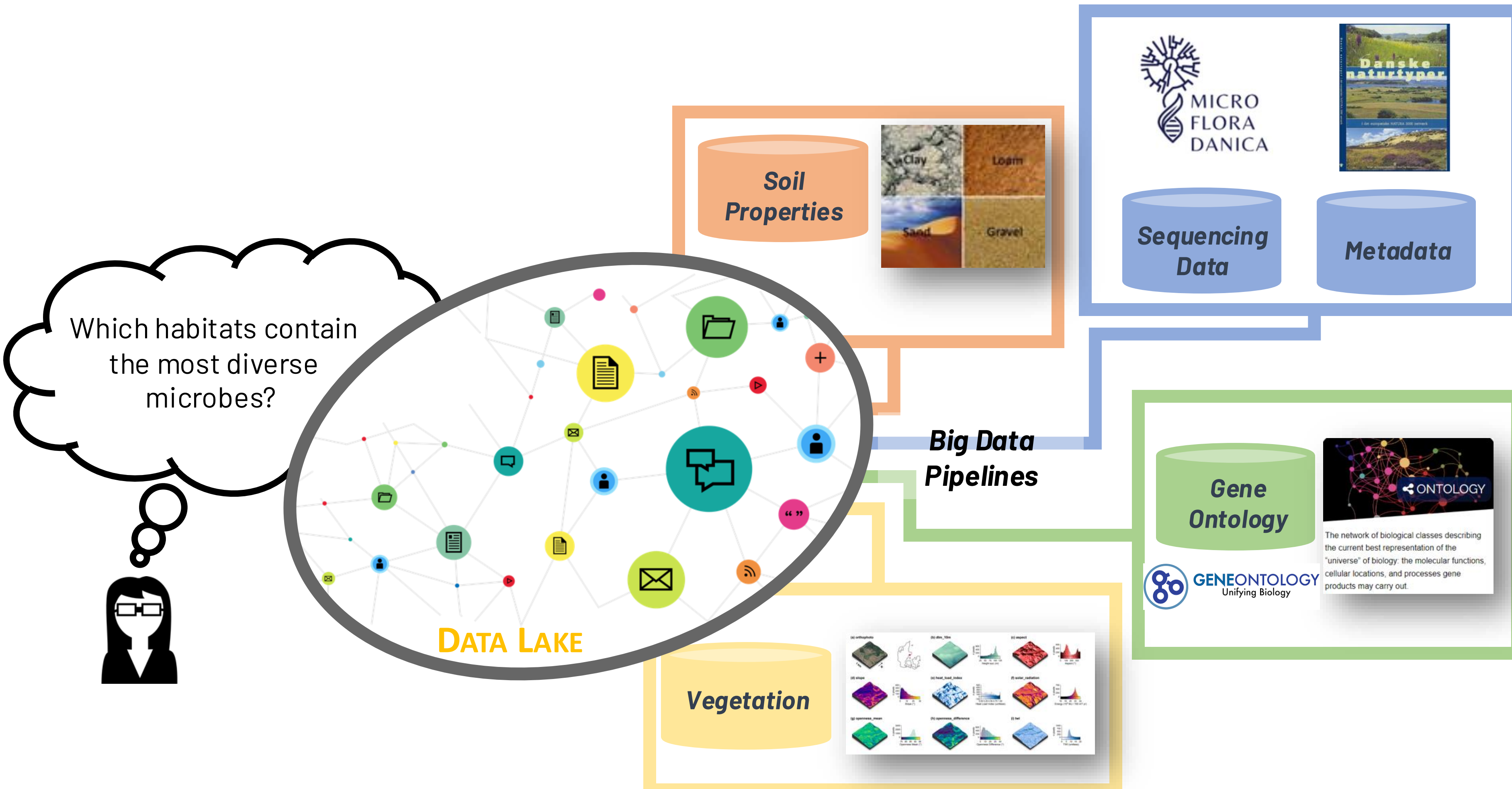
Data Warehouses



Knowledge-Graph based Integration, Data Lakes, Data Fabrics, Enterprise Knowledge Graphs



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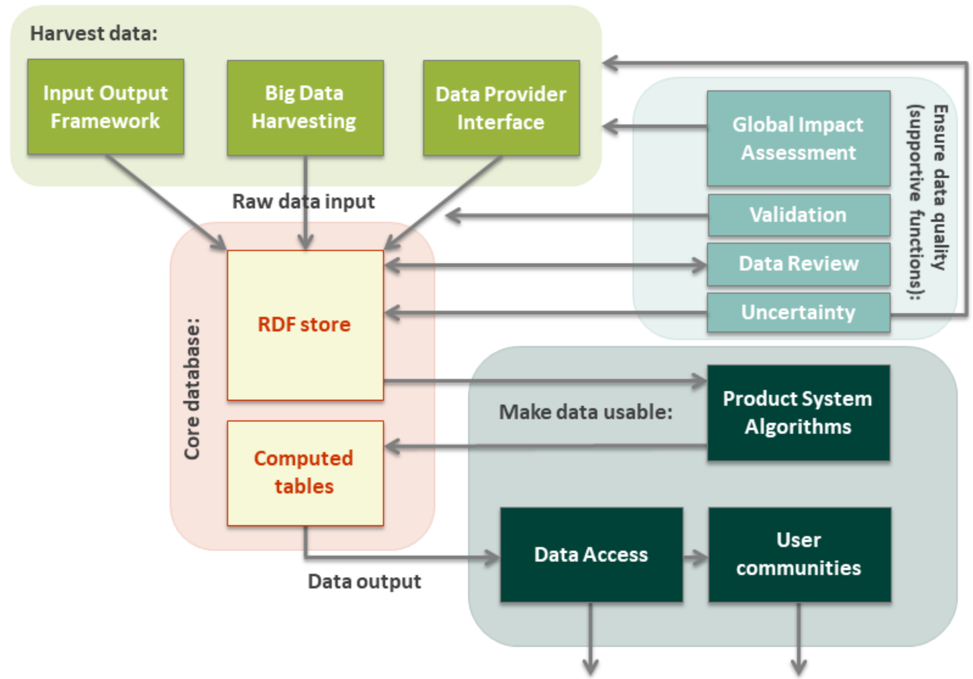
Data integration and sharing

Use case
Lifecycle sustainability assessment

Goal
Overcoming closed data silos

Framework
- Harvest data: data extraction
- Core database: pipeline for data integration, provenance for tracing data
- Ensuring data quality (LCA reasoning)
- Capturing provenance (PROV-O)
- Make data usable (user interfaces and APIs)

140M triples of instance-level data
2K triples of schema-level data



E. R. Hansen, M. Lissandrini, A. Ghose, S. Løkke, C. Thomsen, K. Hose: Transparent Integration and Sharing of Life Cycle Sustainability Data with Provenance. ISWC 2020

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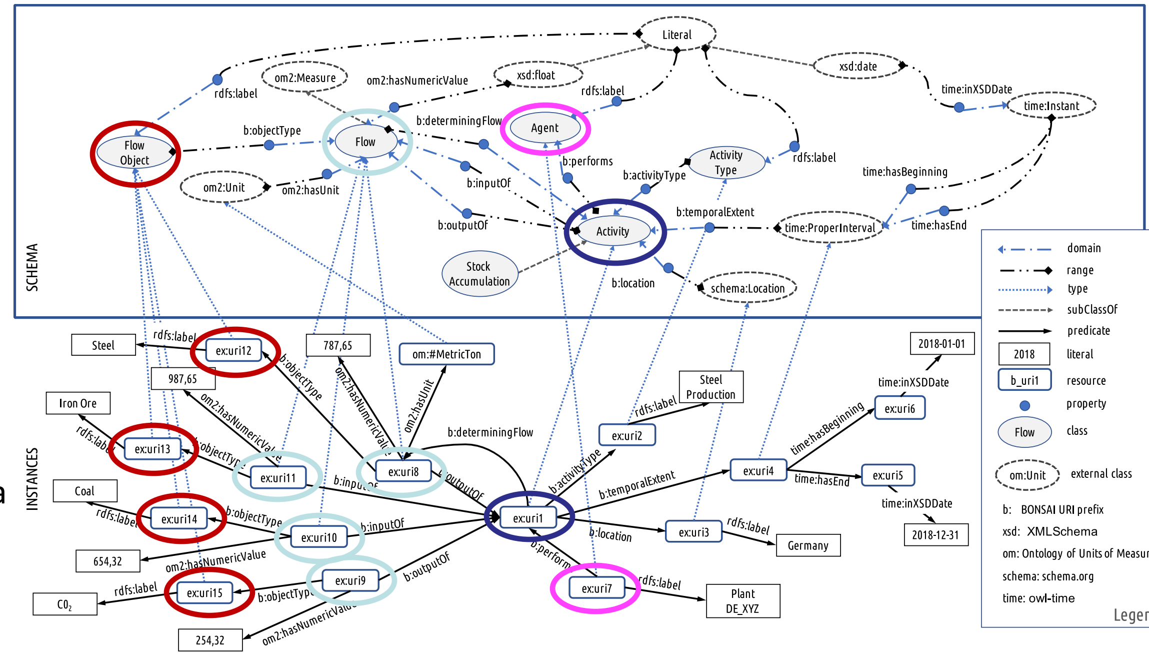
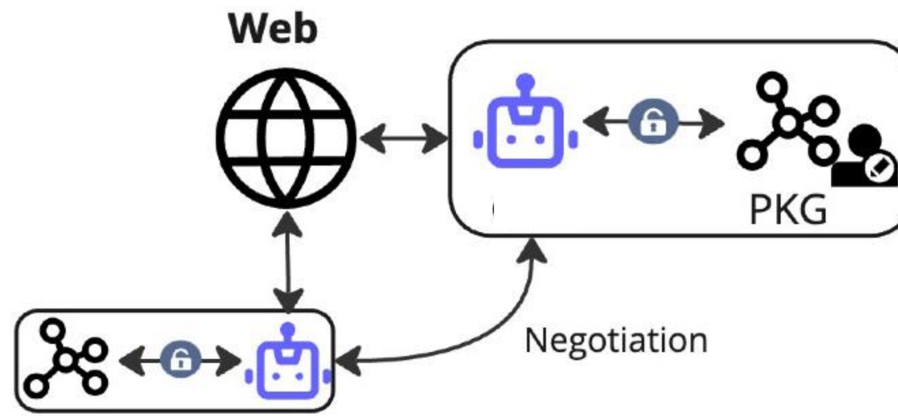


A. Ghose, K. Hose, M. Lissandrini, B. Weidema
An Open Source Dataset and Ontology
for Product Footprinting. In: ESWC 2019

Personalized agents

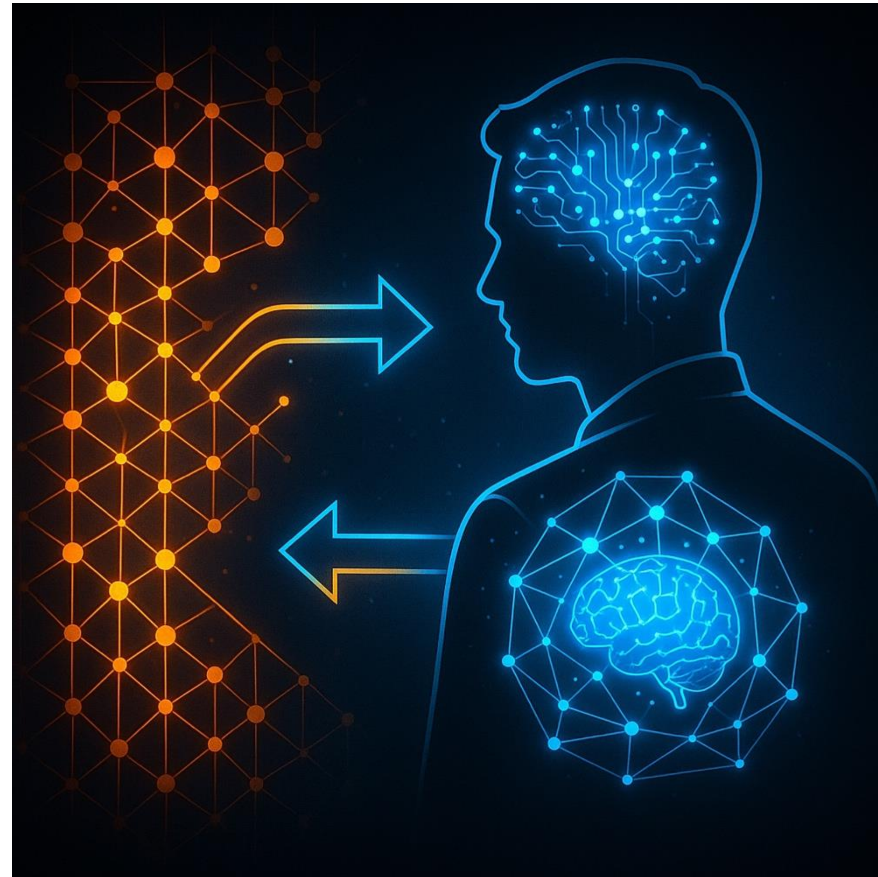
- Advancing Agentic AI
- Combine LLMs + Personal Knowledge Graphs (PKG)
- Goal
    - Personal automation with trust , structure, and control



Piero A. Bonatti, J. Domingue, A. L. Gentile, A. Harth, Olaf. Hartig, A. Hogan, K. Hose, E. Jimenez-Ruiz, D. L. McGuinness, I. Pickup, C. Sun, R. Verborgh, J. Wright: Towards Computer-Using Personal Agents, arxiv.org, 2025.

Use case: planning a dinner date

- Agent assists in meal choice and shopping
- Coordinates between users‘ agents (diet, allergies, schedule)
- Learns from outcomes (e.g., heartburn → avoid next time)
- Challenge: autonomy + privacy + policy-aware reasoning



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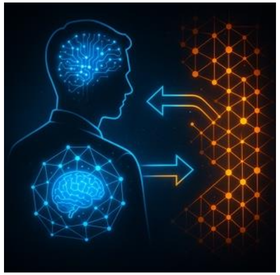
Sam: Jane is coming over for dinner, propose Thai food recipes.

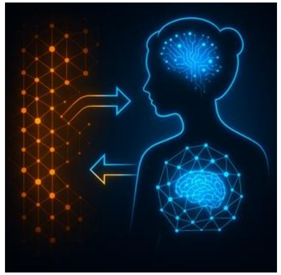
Sam + Agent



recipes →

← No coriander, no shellfish (allergy)

Jane + Agent



Use case: planning a dinner date

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→ agent proposes recipes (Sam is pre-diabetic)
→ find out which ones Jane probably likes

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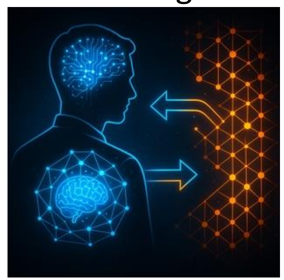

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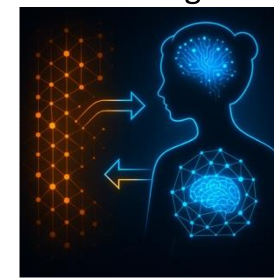

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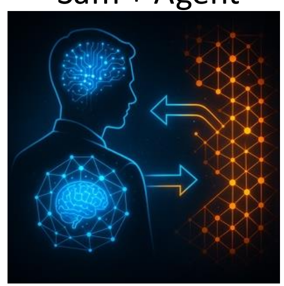
Sam: dinner at 7pm?

Sam + Agent



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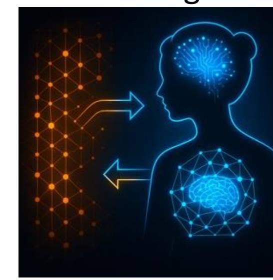

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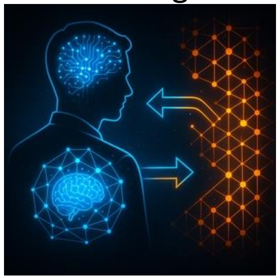

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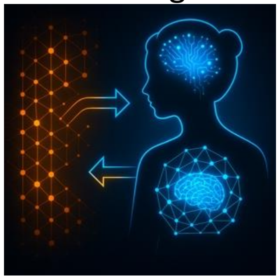
dinner at 7pm →

← 8pm, traffic jam because of an accident

Jane + Agent



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Sam: dinner at 7pm?

Sam: I have a heartburn
→ agent for the future

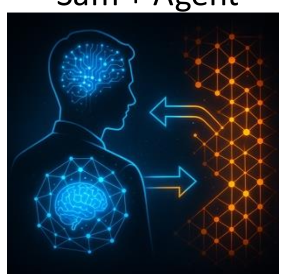
recipes

No coriander, no shellfish (allergy)

dinner at 7pm

8pm, traffic jam because of an accident

Sam + Agent



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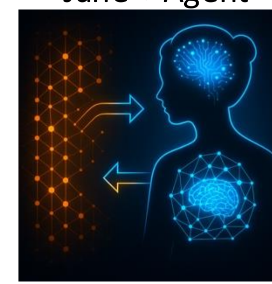

Some Topics Around SHACL

One of our research focus points

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Bridging Gaps in RDF Validation

A community survey on the use of schema languages for RDF

Data quality with SHACL

Language for validating RDF graphs against a set of conditions

W3C recommendation since July 2017: https://www.w3.org/TR/shacl/

SHACL allows validation of knowledge graphs in RDF by defining a shapes graph to validate a data graph.

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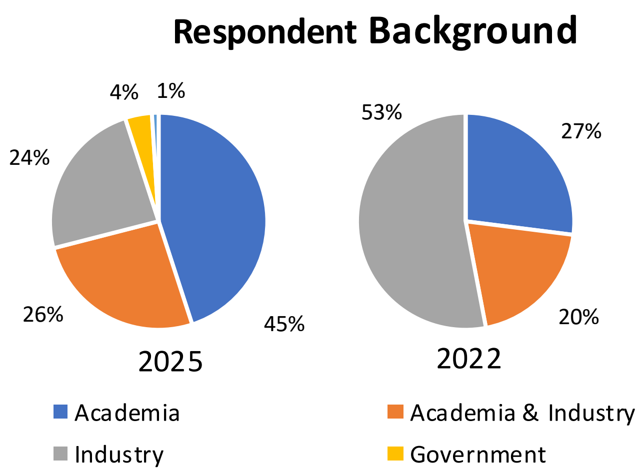
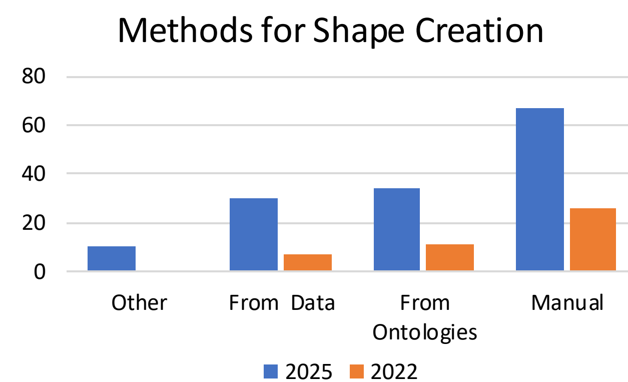
Validating RDF Data



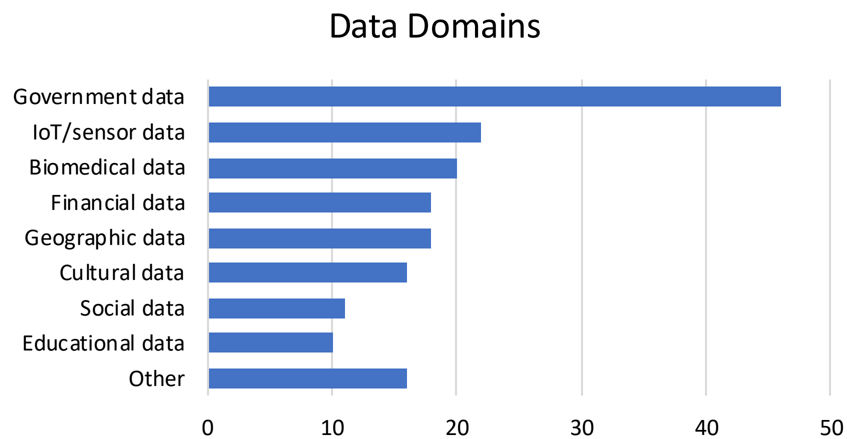
- Online survey from 2025
- Comparison to a survey from 2022

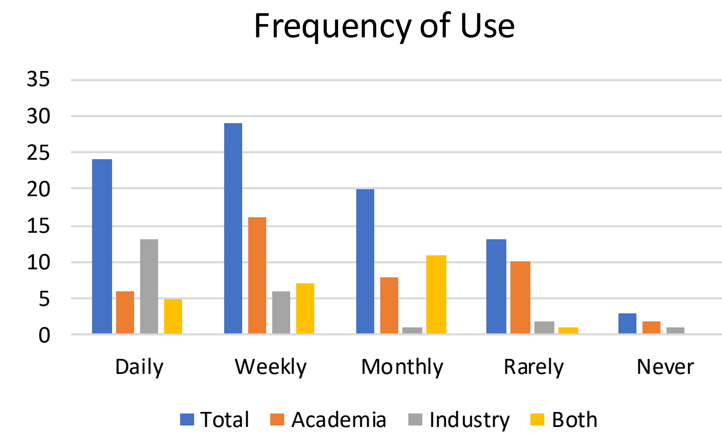


- Overwhelmingly manual
- Often created from other artifacts
- OWL Ontologies
- JSON Schema
- Conceptual Models

M. Jakubowski, D. Tomaszuk, K. Hose: Bridging Gaps in RDF Validation – Insights and Innovation Opportunities in RDF Validation Practices. SEMANTiCS 2025

Data Domains and Frequency of Use





Challenges

Issue / Limitation	Academia	Industry	Both
Documentation and tutorials	22	8	11
Community and tool support	20	11	8
Performance and scalability	17	9	11
Features or functionality	14	11	8
Missing constraint types	11	11	10

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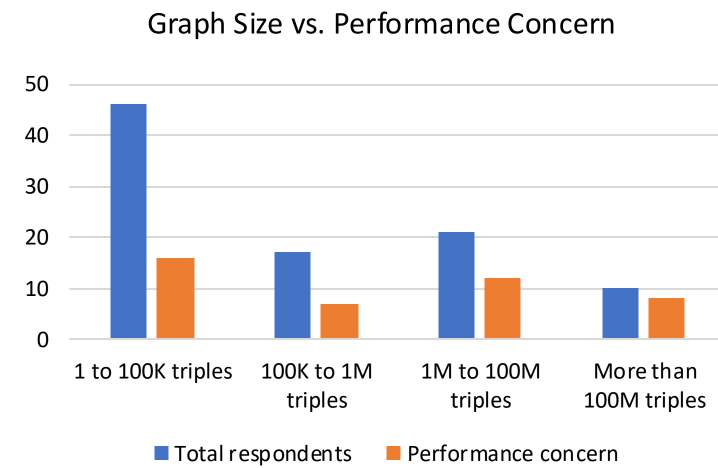

- Performance bottleneck for large datasets
- Few validators focus on performance
- Comparatively little academic literature
  - Idea: bring known techniques for query processing to SHACL/ShEx
  - Our work: [Compiling SHACL Into SQL] at ISWC 2024

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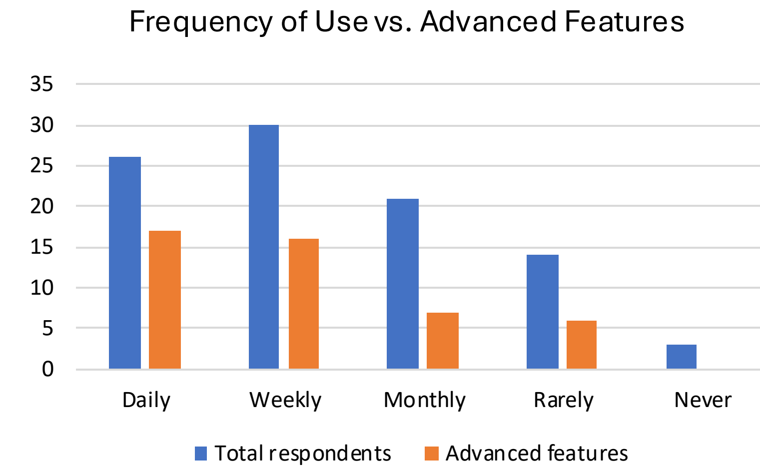
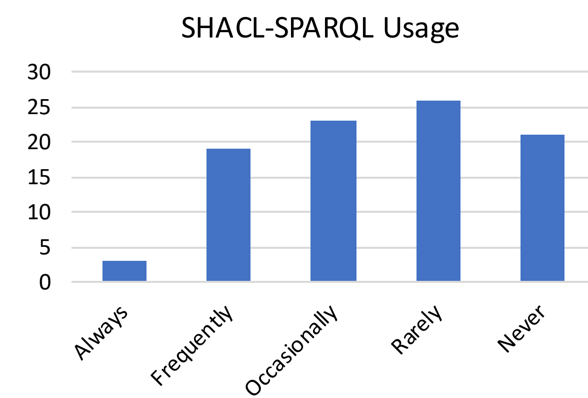
- Advanced Features extends SHACL
  - Expressive power
  - Widen the scope of SHACL
- Need for greater expressiveness
- Need for expansion of SHACL’s scope:
  - SHACL rules often cited





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Graph Subsetting and Neighborhoods

An alternative use for SHACL

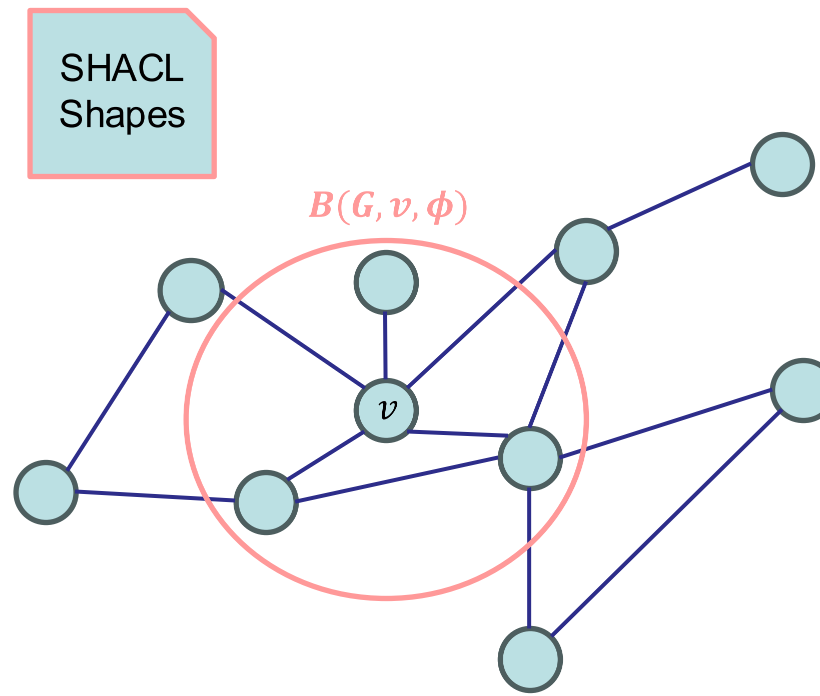
Neighborhoods

Goal:
Provide **a subgraph** that only contains triples that are "relevant"

We define the **neighborhood**: $B(G, v, \phi)$

- G a graph
- v a node
- ϕ a shape

What part of G is relevant to decide that v satisfies ϕ in G?



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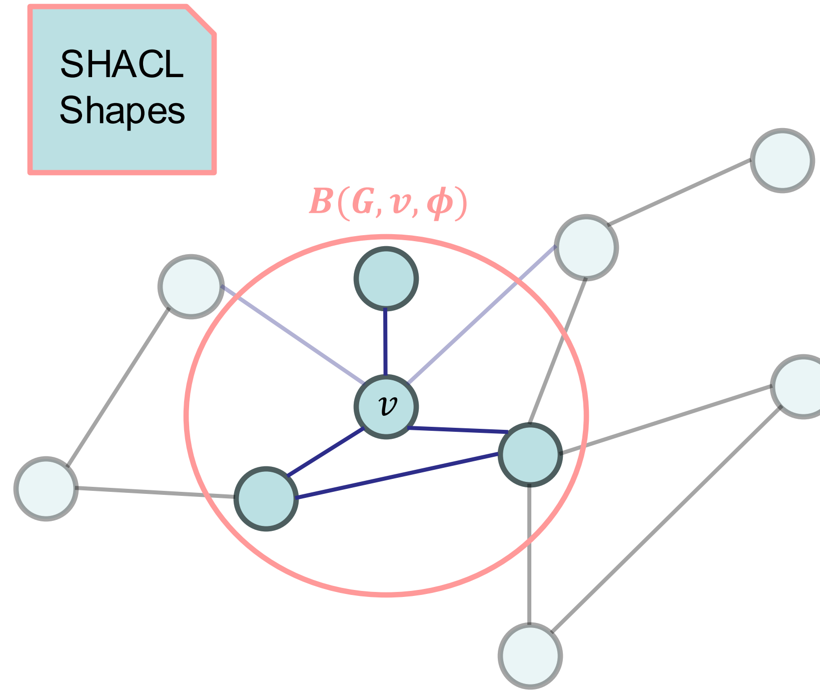


Sufficiency and design principles

Sufficiency Property	If a node v satisfies a shape ϕ in a graph G, then: v also satisfies ϕ in G' for any subgraph G' with $B(G, v, \phi) \subseteq G' \subseteq G$.

"Strong" sufficiency: it holds for all G' where $B(G, v, \phi) \subseteq G' \subseteq G$.

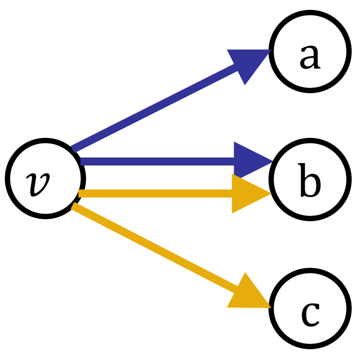
- Technical necessity
- Allows for leniency in implementations of neighborhoods

When defining neighborhoods we want to be both **deterministic** and **minimal**

Nonequality: $\neg eq(p, q)$

```
<myshape> sh:not [
  sh:path <p>;
  sh:equals <q>;
].
```

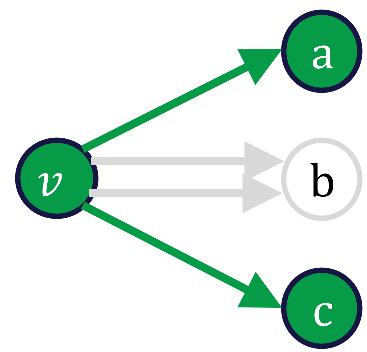
G



Options:
- Only edges to a and/or c
- All edges

$B(G, v, \mathrm{myshape})$

“symetric difference”

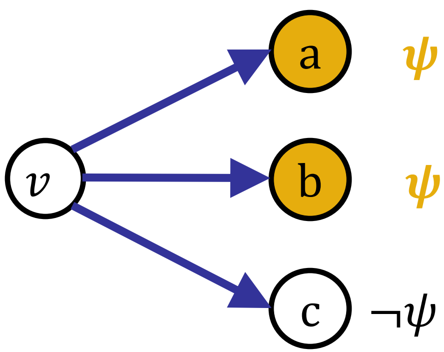


Reasons:
- Determinism
- Somehow minimal

Quantifiers: $\geq_1 p.\psi$

```
<myshape> sh:property [
  sh:path <p>;
  sh:qualifiedValueShape ψ ;
  sh:qualifiedMinCount 1 ;
].
```

G



Options:

- Only edges to a and/or b
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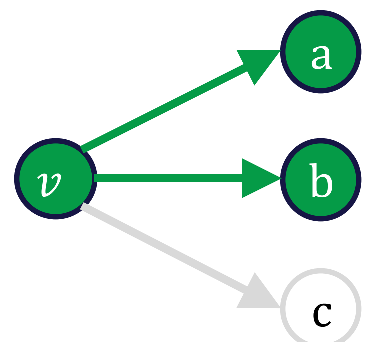
$B(G, v, \phi)$



Reasons:

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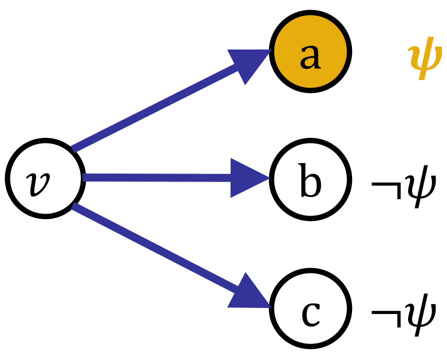
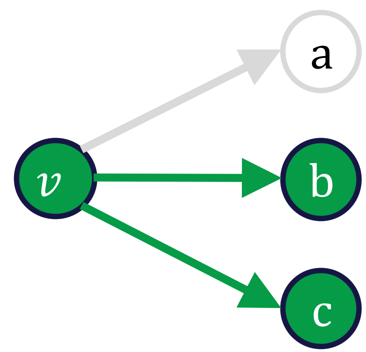


Options:
- No edges
- Edge to a
- All edges

$B(G, v, \phi)$



Reasons:
- Determinism
- Somehow minimal
- Adding edges to the neighborhood may not break sufficiency

Shape Fragments

We define $\mathbf{Frag}(\boldsymbol{G}, \boldsymbol{S})$ as the union of all neighborhoods of nodes satisfying the shapes from S in G.

Let H be a shape schema, we define:

$$\mathbf{Frag}(\boldsymbol{G}, \boldsymbol{H}) \coloneqq \text{Frag}(G, S)$$

where $S = \{\phi \wedge \tau \mid \tau \textit{ is the target of } \phi \textit{ in } H\}$

Conformance Property	If a graph G satisfies a schema H, then $\mathrm{Frag}(G, H)$ also conforms to H.

Shape Fragments can be used for…

- Explaining validation
- Graph subsetting
- A notion of "coverage"

Want to know more? https://openproceedings.org/2023/conf/edbt/paper-3.pdf
Want to know even more? https://dl.acm.org/doi/10.1007/978-3-031-72407-7_1

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Common Foundations of SHACL, ShEx and PG-Schema

They are very different in nature, but closer than it seems

Understand differences and commonalities between SHACL, ShEx and PG-Schema

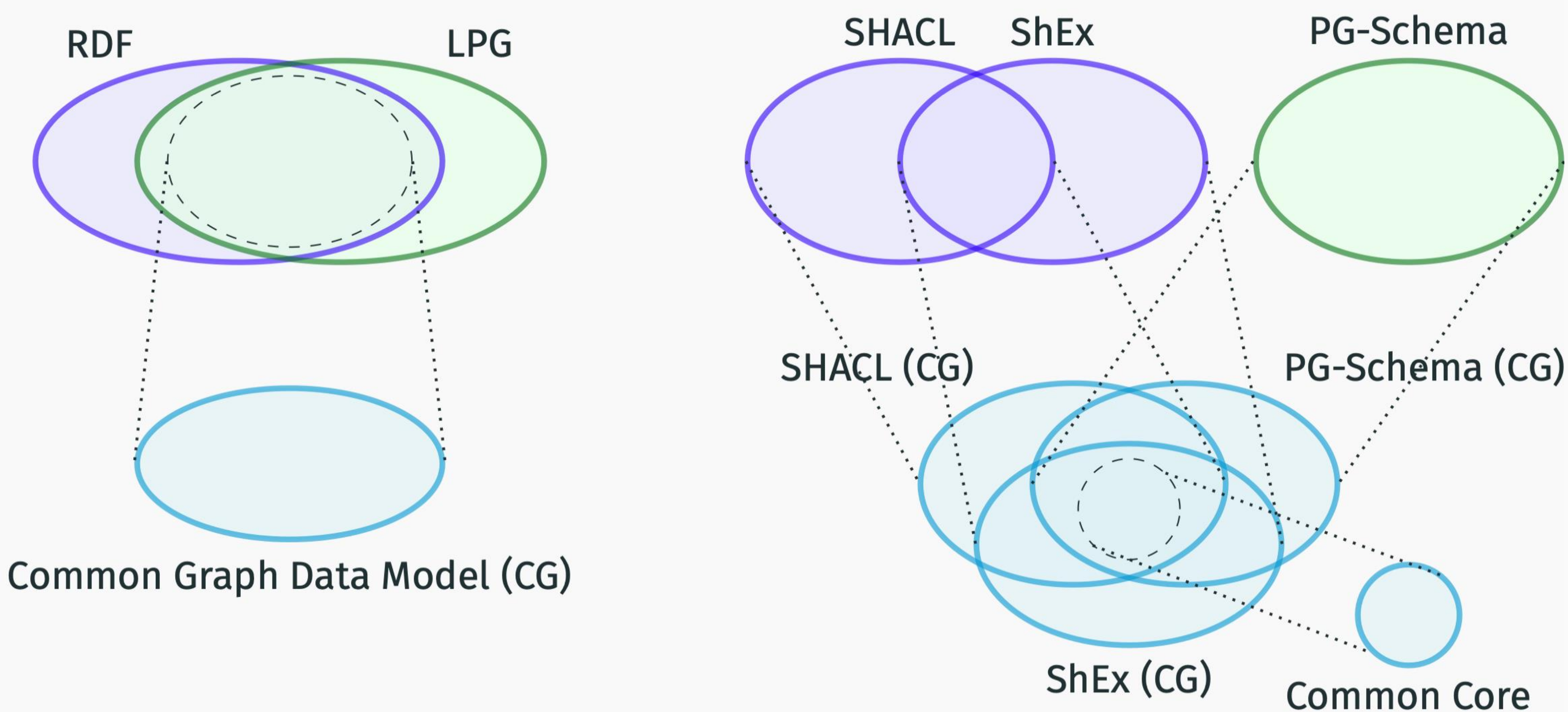
- **Users** are asking for this:
  - What are the fundamental differences? Is true interoperability possible?
- **Vendors** are asking for this:
  - What is actually used, and what is essential to support?
- **Designers** should be asking for this:
  - Why are there all these differences despite the similar objectives?
  - Do the superficial differences matter?

They certainly *look* different

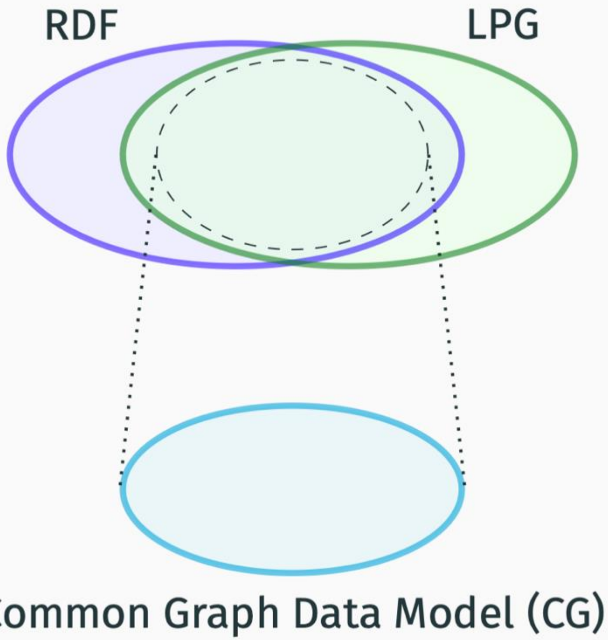
	SHACL	ShEx	PG-Schema
Data Model	RDF	RDF	LPG
Paradigm	Logical constraints	Regular expressions	Type-based + rich key constraints

- Their respective theoretical foundations seem only loosely related
- Defined for different data models
- Defined by different communities

Method


RDF
LPG
Common Graph Data Model (CG)
SHACL
ShEx
PG-Schema
SHACL (CG)
PG-Schema (CG)
ShEx (CG)
Common Core

Distilling the Common Graph Data Model



Features not present in both RDF and LPG are removed.

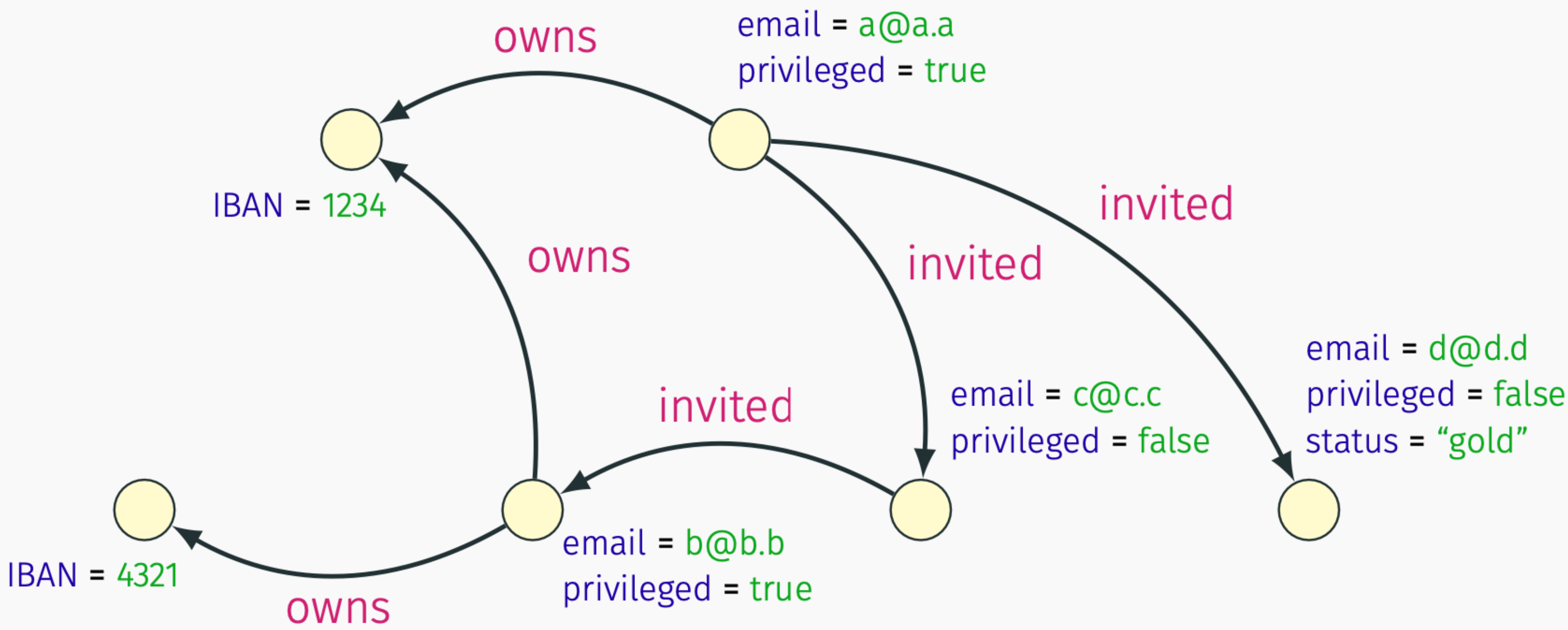
RDF Gives up:

- **Nodes** cannot be compared with an IRI
- **Predicates** …
  - associate at most one value with a node
  - cannot be compared with a node

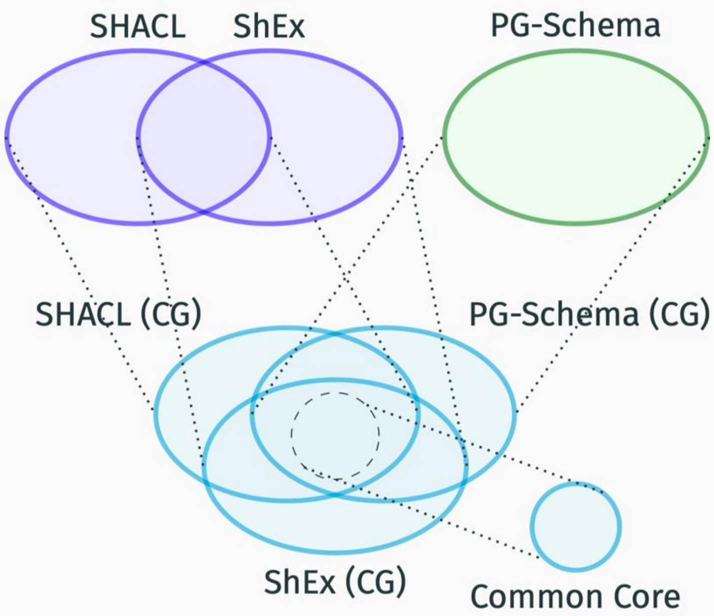
LPG Gives up:

- **Nodes** do not have labels
- **Edges** …
  - have exactly one label
  - have no properties
  - are identified by label and endpoints

Common Graph Example



Distilling the three schema languages

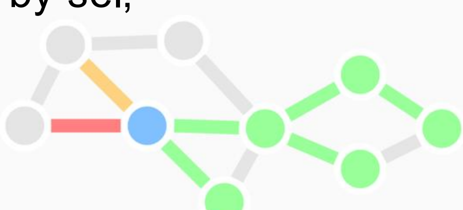


A **common shape** describes the graph's structure around a focus node or value.

A selector is a simple shape that indicates **focus** nodes or values.

A **schema** is a set of selector-shape pairs.

A graph G **conforms to** a schema S if,
for each selector-shape pair (sel, s) in S,
for every focus v indicated by sel,
v has shape s



Distilling the three schema languages

SHACL and ShEx give up

- disjunctions and negations,
- nesting of shapes.

```
<s> sh:or (
[ sh:path <invited>; sh:minCount 1 ]
[ sh:not [ sh:path <status> sh:hasValue “gold”]).
```

SHACL and PG-Schema give up

- unbounded path expressions.
- counting over multi-edge paths.

```
<s> sh:path [ sh:zeroOrMorePath <invited> ];
  sh:minCount 100 .
```

PG-Schema gives up

- closing properties and edges independently,
- testing properties under star.

ShEx gives up recursion.

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The Common Graph Schema Language (CoGSL)

Definition 12 (common shape). *A* common shape φ *is an expression given by the grammar*

$$\varphi ::= \exists\,\pi \mid \exists^{\leq n}\,\pi_1 \mid \exists^{\geq n}\,\pi_1 \mid \exists\,\mathbb{C} \land \nexists\,\neg P \mid \varphi \land \varphi\ .$$

$$\mathbb{C} ::= \{\} \mid \{k : \mathbb{V}\} \mid \mathbb{C}\ \&\ \mathbb{C} \mid \mathbb{C} \mid \mathbb{C}\ .$$

$$\pi_0 ::= [k = c] \mid \neg[k = c] \mid \mathbb{C}\ \&\ \top \mid \neg(\mathbb{C}\ \&\ \top) \mid \pi_0 \cdot \pi_0\ .$$

$$\pi_1 ::= \pi_0 \cdot p \cdot \pi_0 \mid \pi_0 \cdot p^- \cdot \pi_0 \mid \pi_0 \cdot k \mid k^- \cdot \pi_0\ .$$

$$\bar{\pi} ::= \pi_0 \mid p \mid \bar{\pi}^- \mid \bar{\pi} \cdot \bar{\pi} \mid \bar{\pi} \cup \bar{\pi}\ .$$

$$\pi ::= \bar{\pi} \mid \bar{\pi} \cdot k \mid k^- \cdot \bar{\pi} \mid k^- \cdot \bar{\pi} \cdot k'\ .$$

where $n \in \mathbb{N}$, $P \subseteq_{fin} \mathcal{P}$, $k, k' \in \mathcal{K}$, $c \in \mathcal{V}$, *and* $p \in \mathcal{P}$.

Want to know more? https://dl.acm.org/doi/10.1145/3696410.3714694

What have we gained?

- A common **framework** to talk about SHACL, ShEx, and PG-Schema, compare their core mechanisms and expressive power:
  - a high-level notion of a shape-based graph schema;
  - a uniform syntax for shapes and selectors.
- A **foundation** for automating interoperability:
  - a data model that can be supported by both RDF and LPG;
  - a schema language that can be compiled to SHACL, ShEx, and PG-Schema.

Master Thesis Topics

Master Thesis Topics

- Schema-related topics:
  - Creating a fast and scalable SHACL validator
  - Generating RDF data from SHACL shapes
  - Validating virtual graph data
  - Mining schemas from graph data
- Applied Data Management
  - Integrating biological datasets into graph data
  - Federated exploration of microbial and environmental data
- Evolving graph data
  - Visualizing evolving graph data
  - Benchmarking evolving property graphs
- Please contact us for more details, or to sit together and develop a topic!

Course Feedback

Please provide feedback to the course using the form on TUWEL (anonymous)

Exam Information

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Exam & Course Feedback

- Project hand-in: 18th of January 2026
- Written exam: 9th of January 2026
- Second chance: 2nd of March 2026
- Points: Project (60) + Exam (40)
  - You must pass both (at least 50%)
  - For the exam, the last attempt counts

- Exam structure
  - Theory: a set of yes/no questions
  - Understanding and interpreting queries/schemas
    - Either open questions;
    - Or complex multiple-choice questions