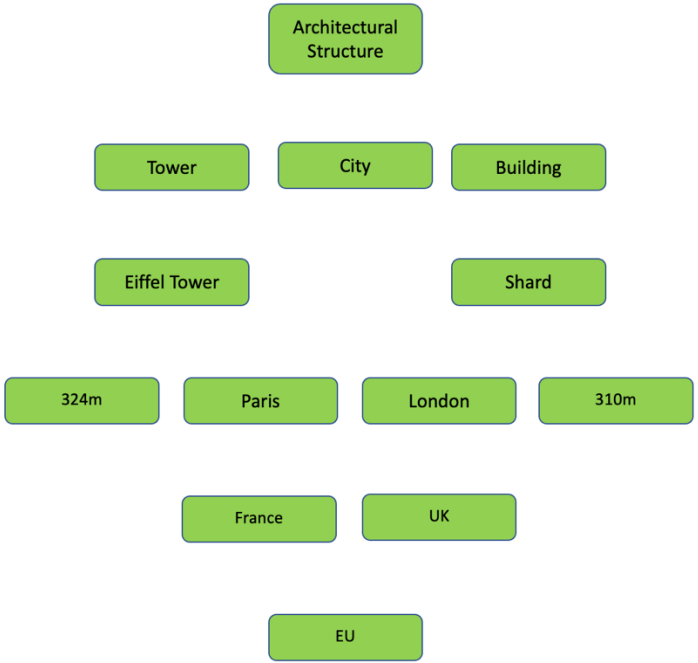
Knowledge Graphs: Theory, Applications & Challenges

Ian Horrocks
University of Oxford & Oxford Semantic Technologies

Introduction to Knowledge Graphs

Anatomy of a Knowledge Graph



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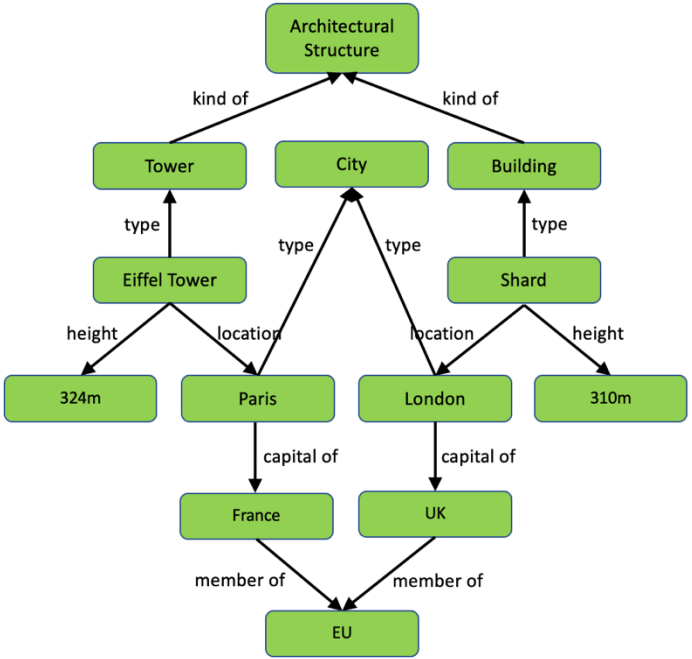

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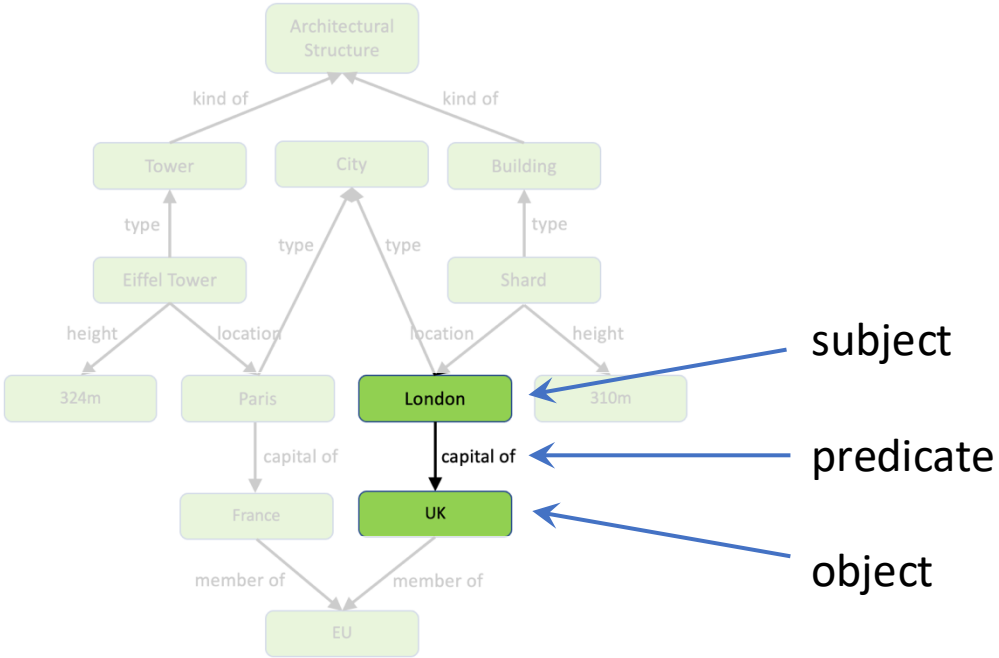

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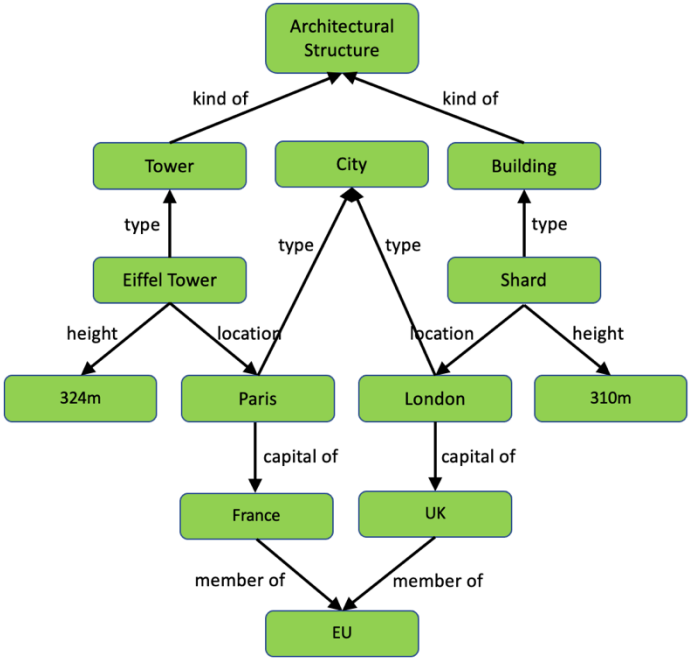

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Architectural Structure		
Name	Height	Location
Eiffel Tower	324	Paris
Shard	310	London

Tower
Name
Eiffel Tower

Building
Name
Shard

City	
Name	Capital Of
Paris	France
London	UK

Member	
Country	Union
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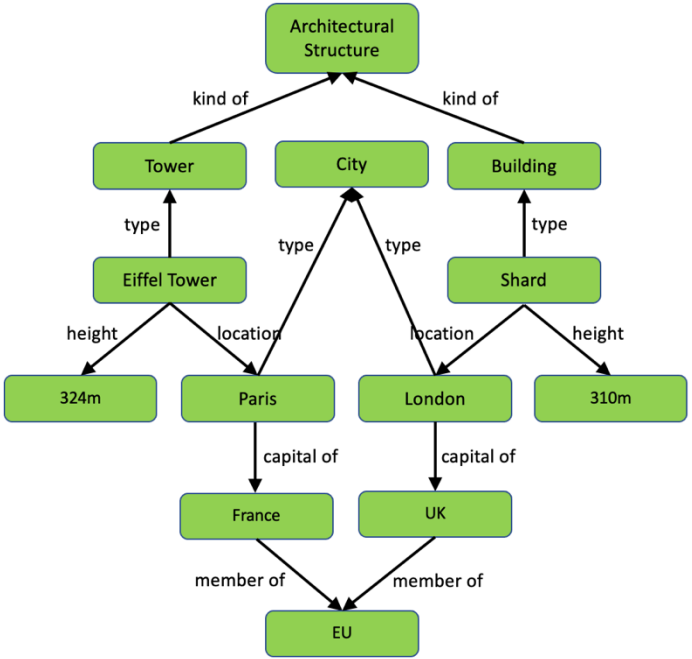

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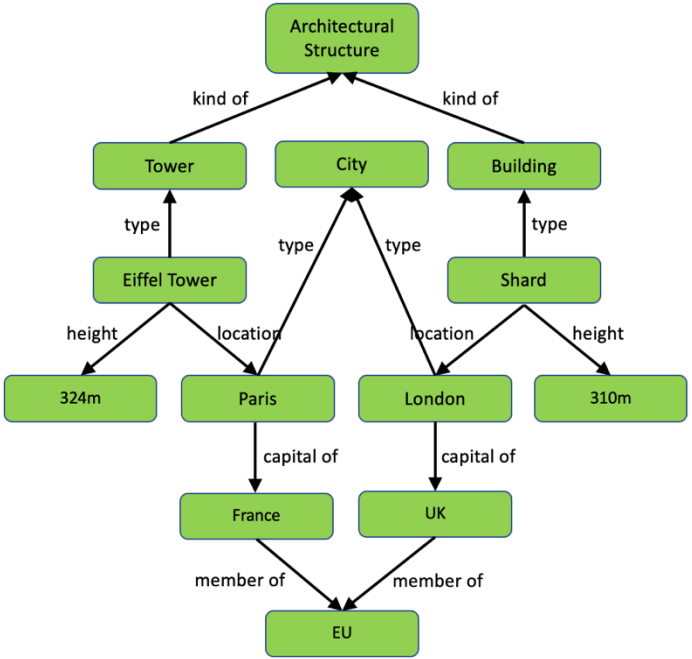

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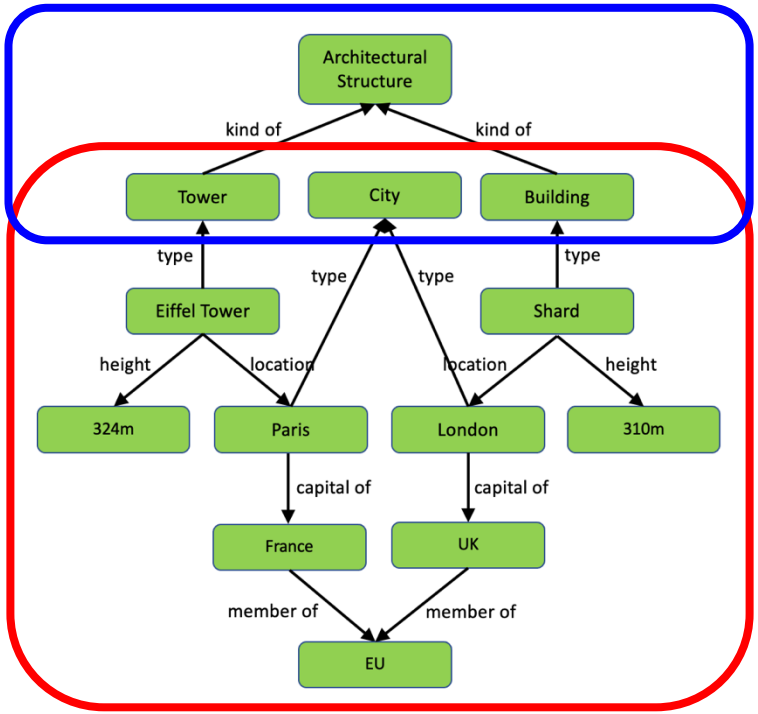

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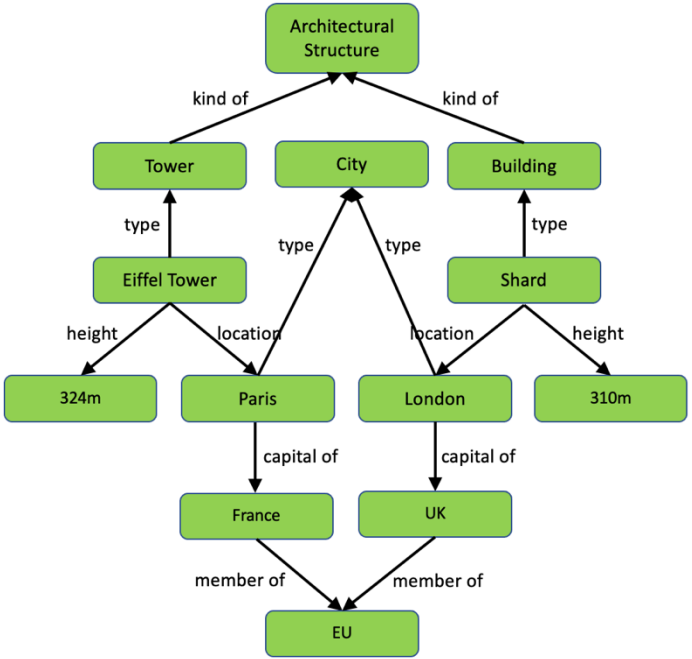

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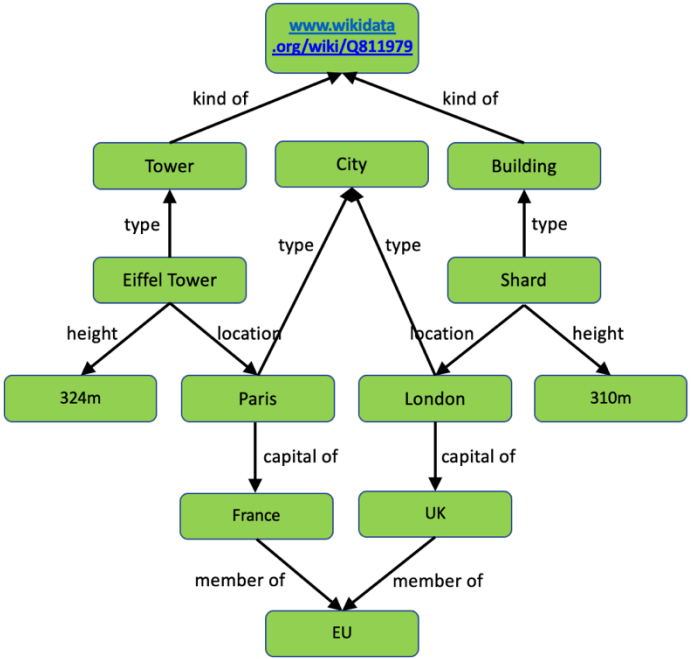

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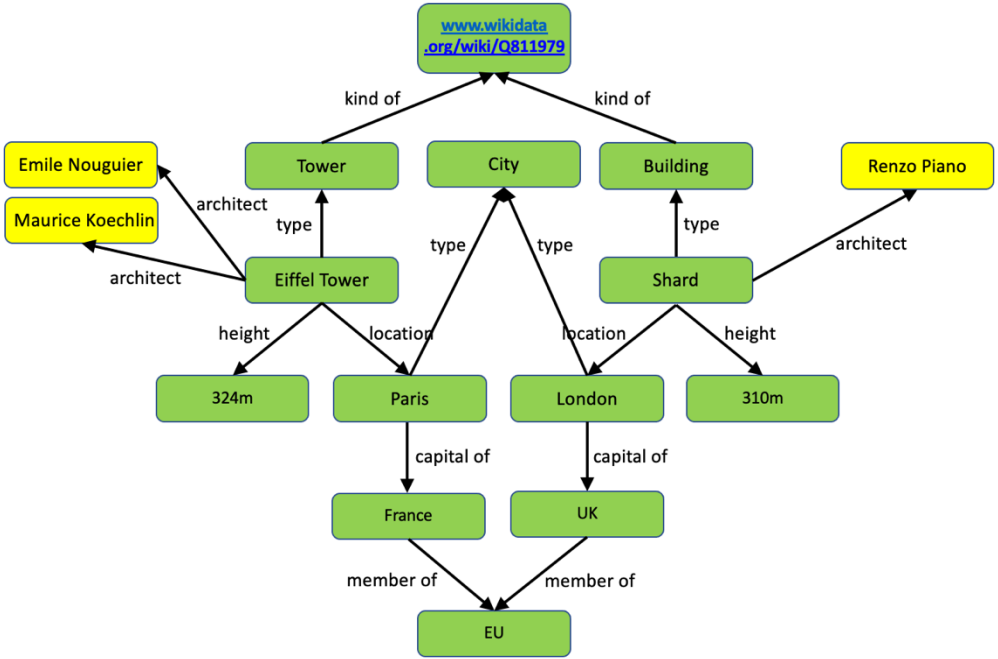

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- ✓ Flexible & extensible

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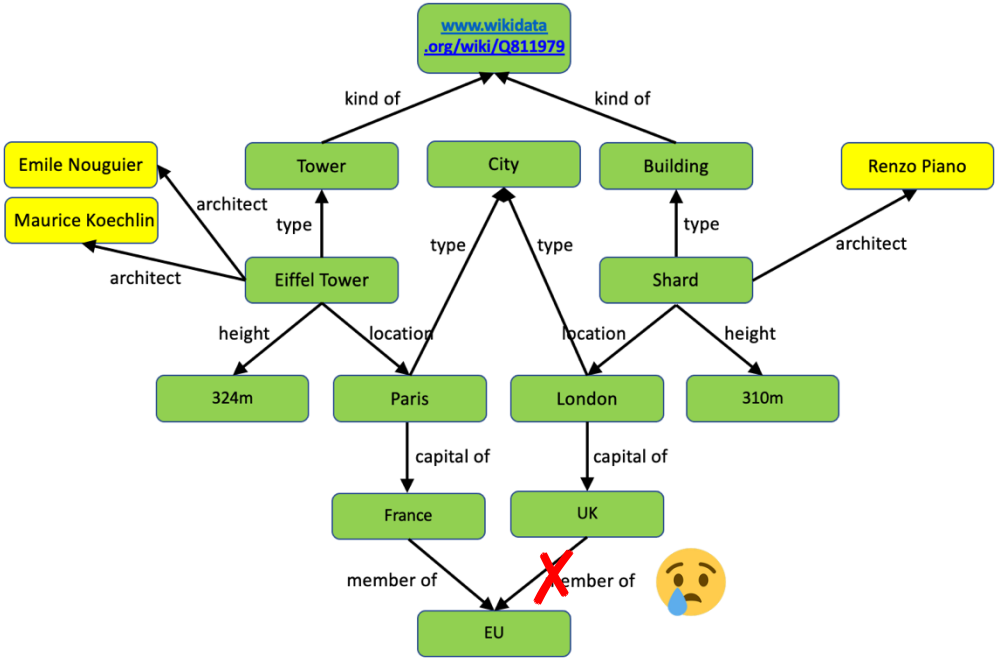

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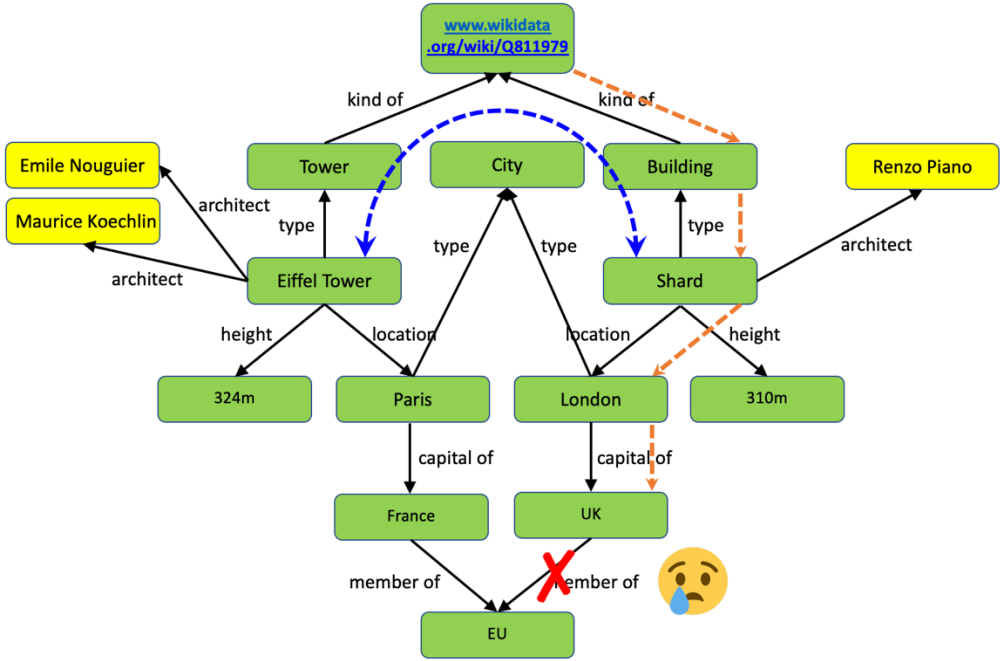

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- ✓ Other kinds of query
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  - similarity & locality

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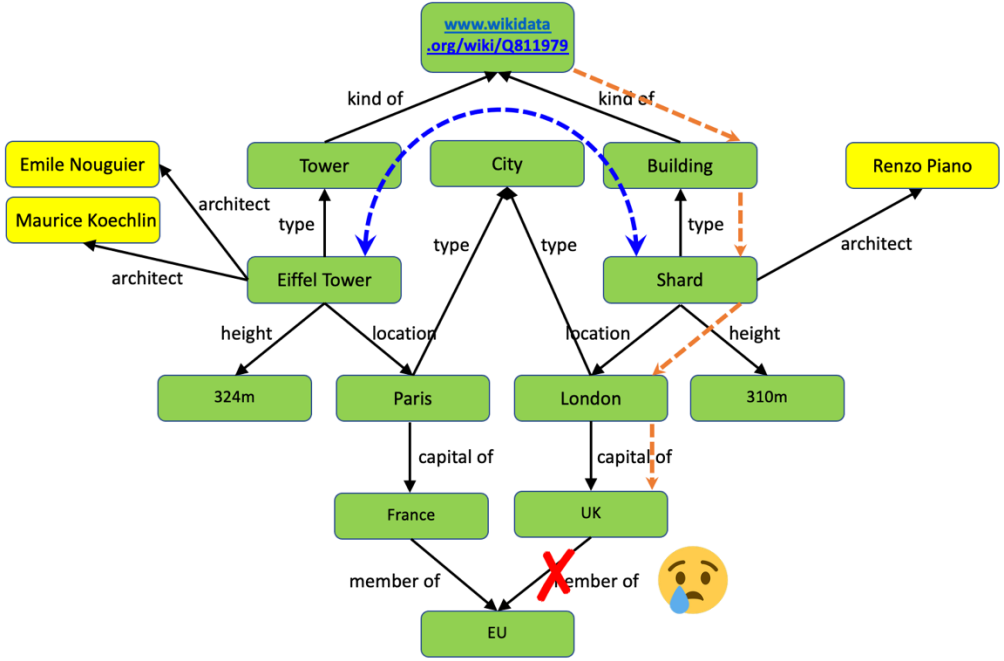

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- ✓ **Data** + **schema (ontology)**
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- ✓ Other kinds of query
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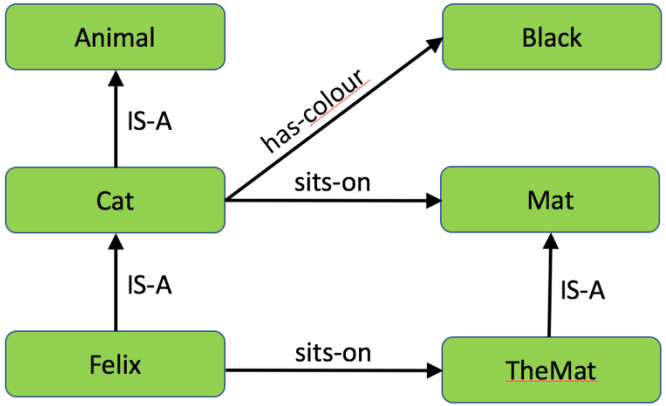
- ✗ Views
  - Data integration & restructuring
  - Security
  - Query simplification & optimization
  - …

Challenges and Solutions (1)

Vague Semantics



[Quillian, 1967]

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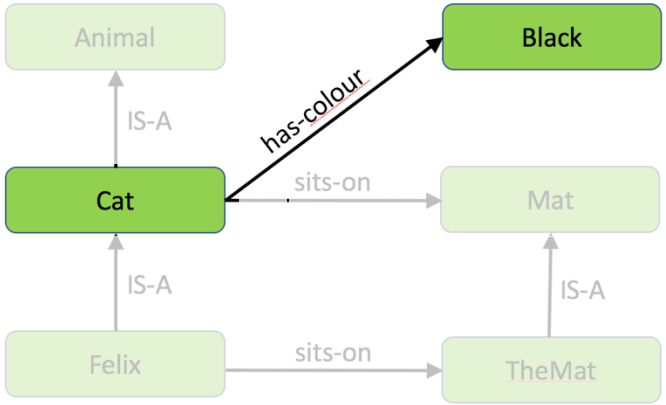

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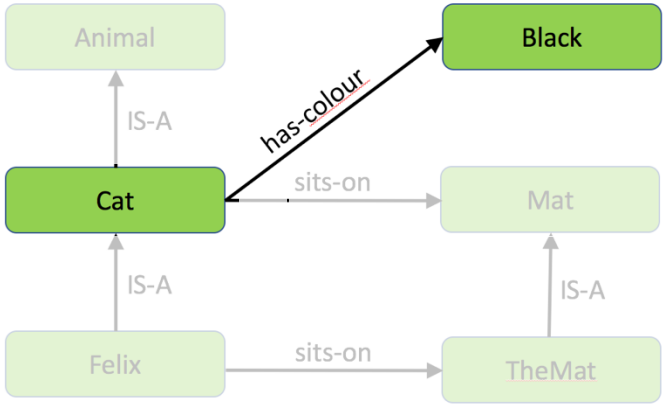

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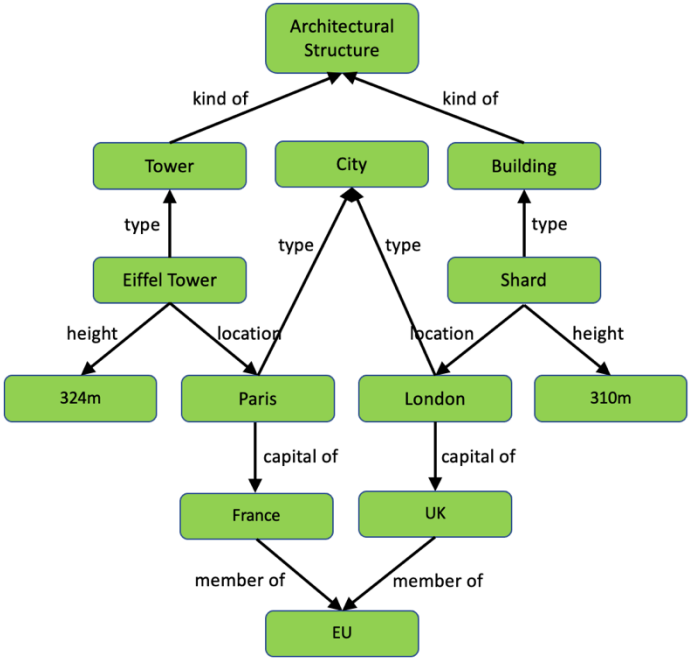

- Architectural Structure with location in the EU?

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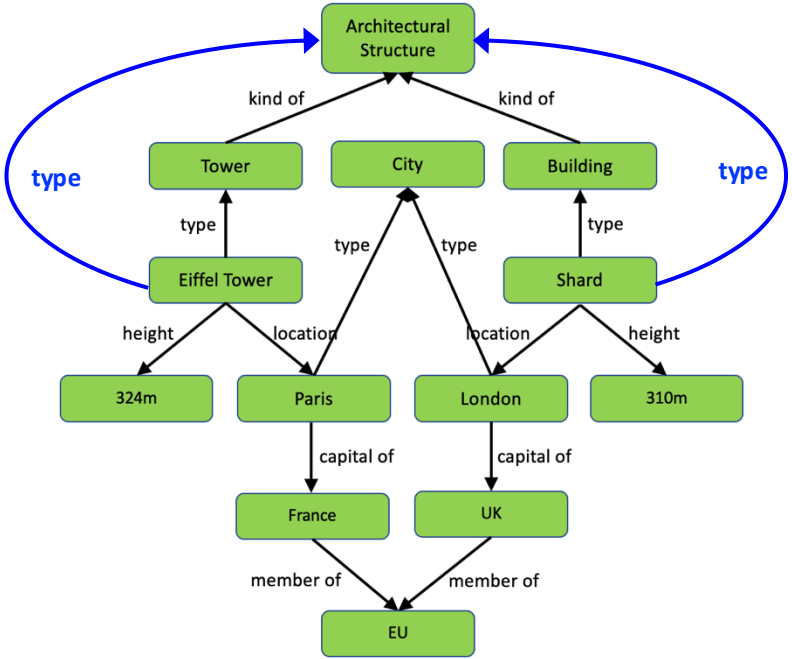

- Architectural Structure with location in the EU?
- Semantics of type and kind of edges?

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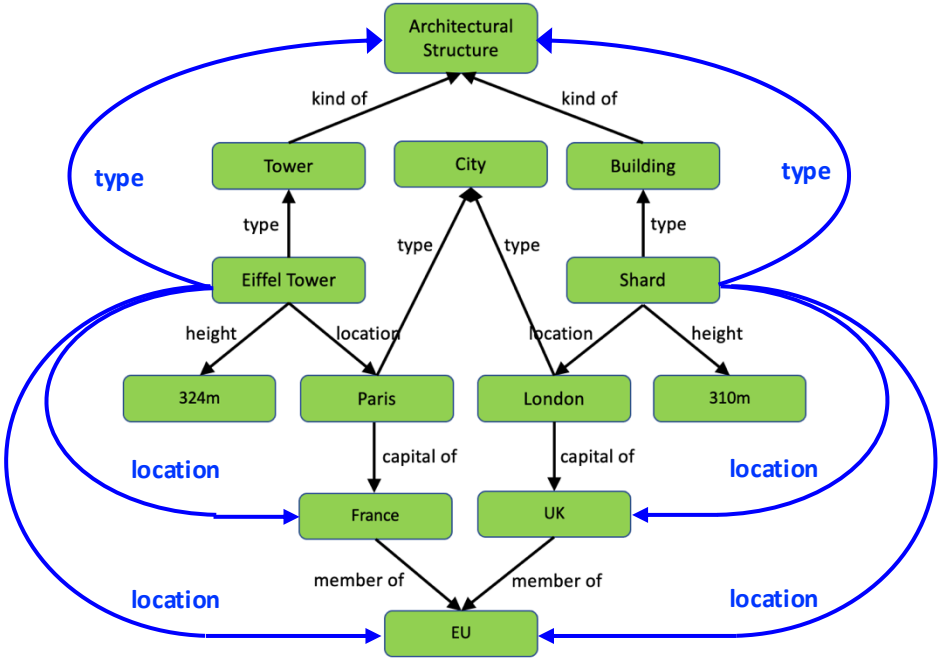
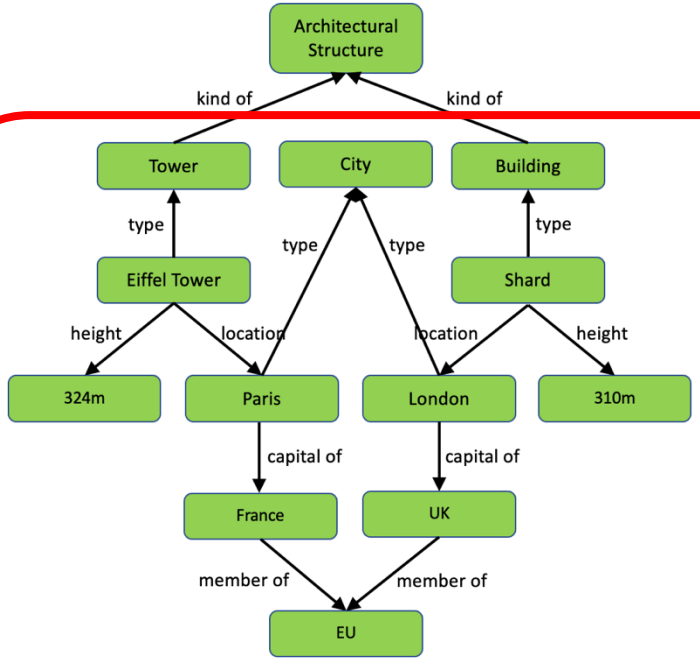


- Architectural Structure with location in the EU?
- Semantics of type and kind of edges?
- Semantics of location + capital of + member of edges?

Solution: Logic!



Tower(EiffelTower)
City(Paris)
location(EiffelTower, Paris)
location(Shard, London)
capital_of(Paris, France)
member_of(France, EU)

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height(EiffelTower, 324m)
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(RDF) graph / facts / data

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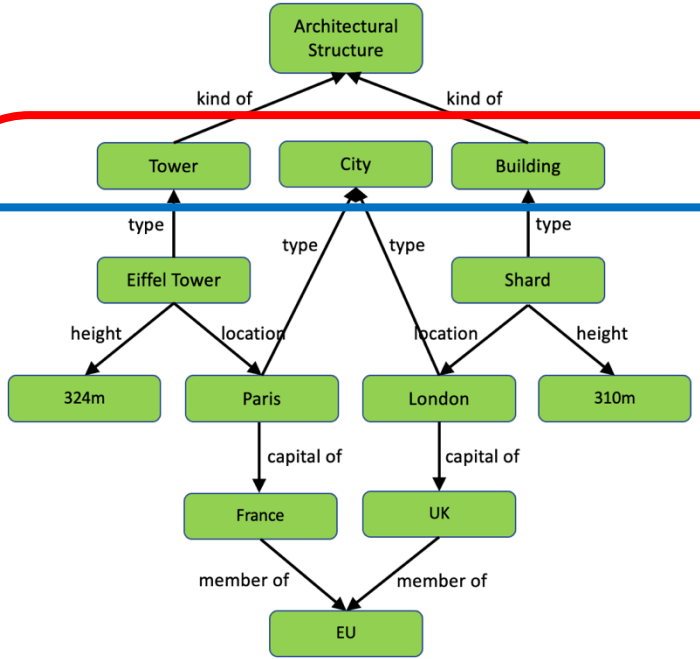

(OWL) ontology / conceptual schema

$\forall x$ Tower$(x) \rightarrow$ ArchitecturalStructure(x)
$\forall x$ Building$(x) \rightarrow$ ArchitecturalStructure(x)

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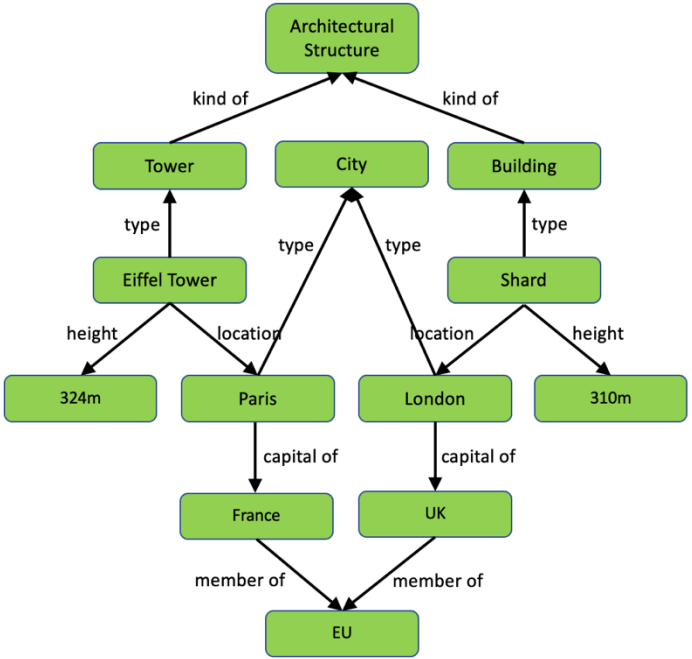
Knowledge base/graph



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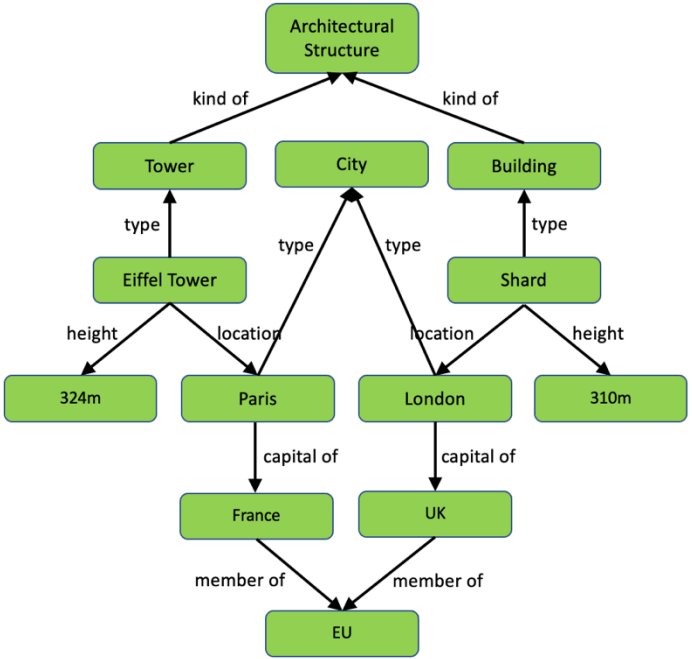

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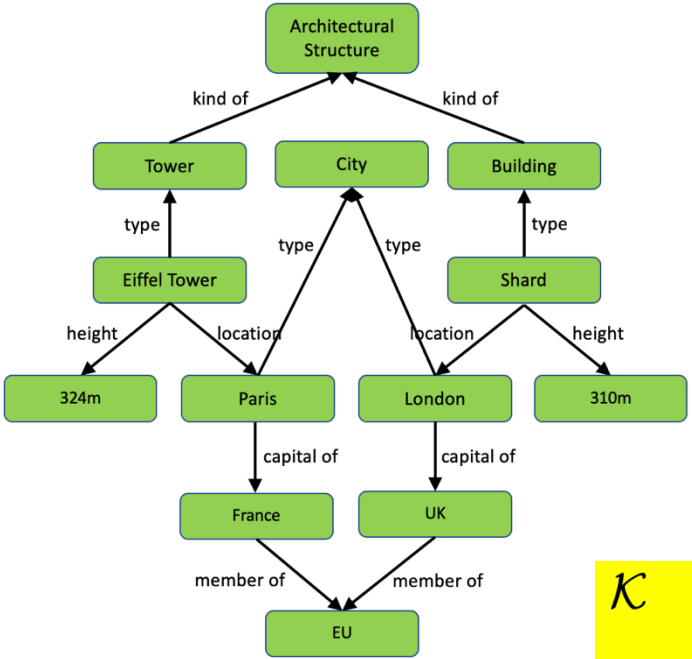

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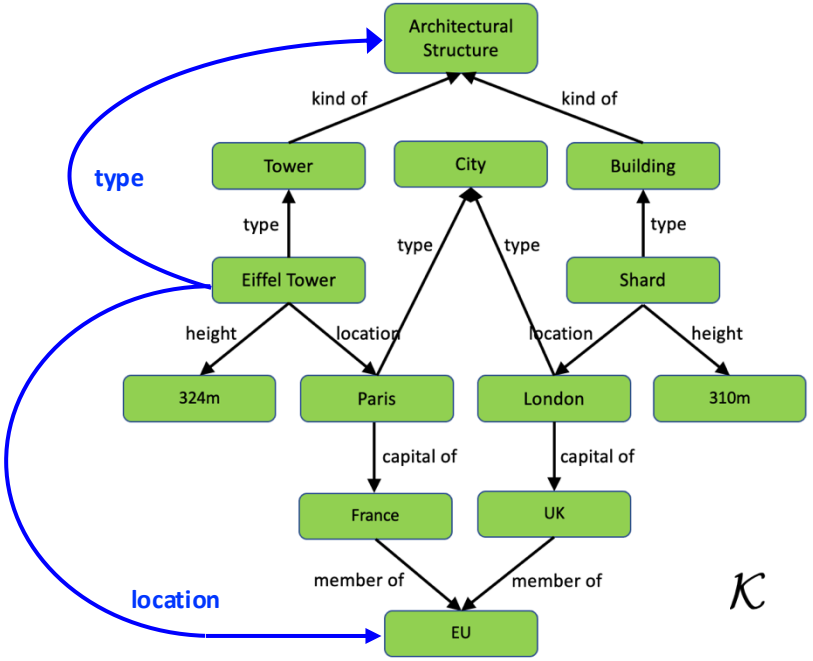
$\mathcal{K} \models$ ArchitecturalStructure(EiffelTower) $\wedge$ location(EiffelTower, EU)

Solution: Logic!

Knowledge base/graph



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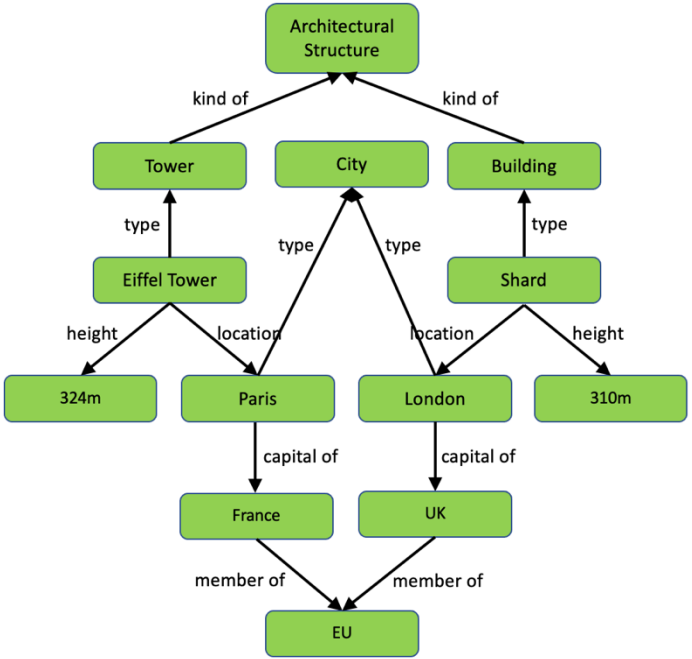
Rules and Views



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$\text{ArchitecturalStructure}(x) \wedge \text{location}(x, EU) \rightarrow \text{EUStruc}(x)$

Views & Rules

- Integration & restructuring (e.g., introduce EUStruc)
- Security (e.g., only allow access to EUStruc)
- Simplification (e.g., use EUSruc in other queries/rules)
- Optimisation (e.g., materialize EUStruc)

Rules

- Recursive definitions (e.g., location)
- Critical for, e.g., part-whole, connectivity, causation, …

Solution: Logic!

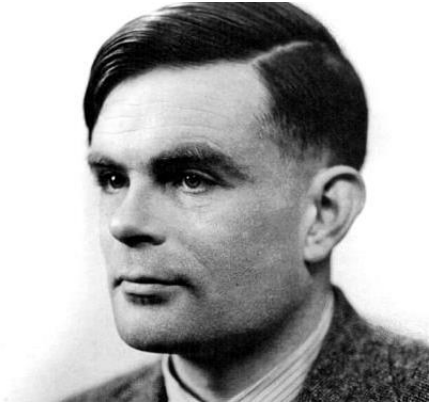
- Identify/devise algorithms that compute query answers
- E.g., using natural deduction rules:

$$\frac{Q(a)}{\forall x P(x) \rightarrow Q(x) \quad P(a)} \qquad \frac{\mathsf{ArchitecturalStructure}(\mathsf{EiffelTower})}{\forall x\, \mathsf{Building}(x) \rightarrow \mathsf{ArchitecturalStructure}(x) \quad \mathsf{Building}(\mathsf{EiffelTower})}$$

- Can check/prove algorithms are sound and complete w.r.t. semantics

Problem Solved?

- Some problems cannot be completely solved using standard computational model
  - halting problem
  - **FOL entailment problem**



- Even if decidable, reasoning might be of inherently high complexity and so take an infeasibly long time

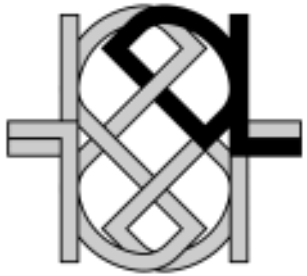
So what to do?

- These are worst case results
  - Even if *logic* is undecidable, some *problems* may still be decidable
  - Even if *logic* is intractable, some *problems* may still be tractable

- **Study** KR languages to find suitable balance of expressive power and computability
- **Design** reasoning algorithms that work well in typical cases
- **Develop** highly optimised implementations

Description Logic

- Family of logic-based KR languages
- Most are decidable subsets of FOPC (usually in C2)
- Provide a range of different constructors
  - Booleans (and, or, not)
  - Restricted forms of quantification (exists, forall)
  - Counting (atmost, atleast)
  - …
- Decidability/complexity and (efficient) algorithms known for many combinations of constructors
- Effective reasoners available for several “sweet-spot” DLs



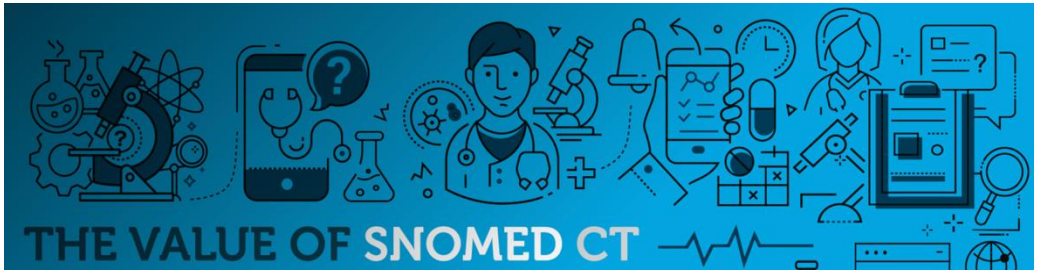
W3C and the Semantic Web

- Goal: to make web data machine-readable
  - KRR on the web
- Standardized **RDF**
  - Graphical data model for representing facts
- Extended RDF with **OWL**
  - Ontology language based on expressive DL (**SROIQ)**
- Developed **SPARQL** query language
  - Similar to SQL
  - Tailored to graphical data model

Challenges and Solutions (2)

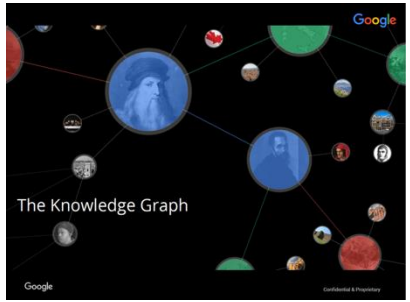
Ontology-centric Applications

- Development of large/complex ontologies
  - Class axioms (usually $<10^6$ classes) with few or no facts
  - Main reasoning task is consistency/subsumption
- OWL/DL reasoners such as **HermiT** and **ELK** used
  - to identify errors and inconsistencies
  - to compute class hierarchy (classification)
- Widely used in medicine and life sciences
  - Bioportal (900+ ontologies)
  - **SNOMED CT**
  - …



Data-centric Applications

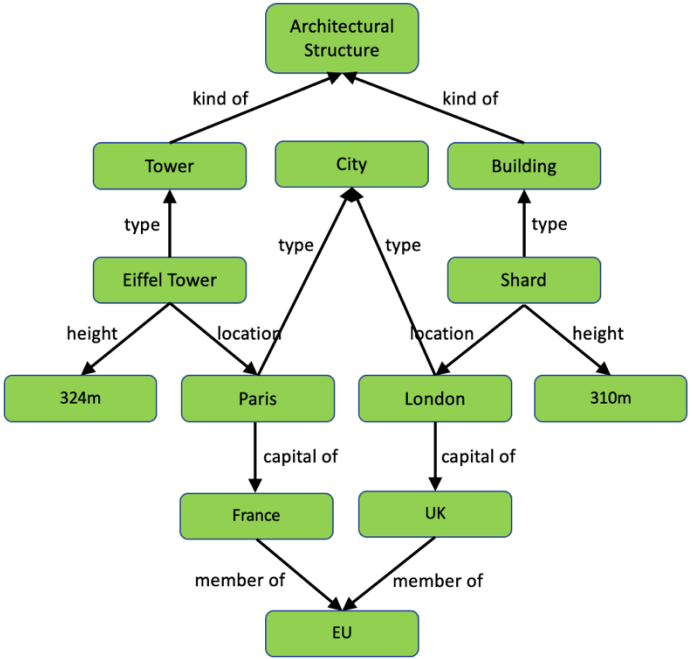
- Development and deployment of large knowledge graphs
  - Ontology/rules plus large number of facts (can be >10^9 edges)
  - Main reasoning task is (SPARQL) query answering
- OWL/DL reasoners don't scale well to this task
  - Query answering reduces to multiple entailment checks
  - Number of checks is polynomial in size of graph
  - Each such check can be costly



OWL 2 Profiles

- OWL 2 is based on powerful but still decidable DL (SROIQ)
- OWL 2 also introduced three “profiles” based on tractable subsets
  - **QL**: based on the DL-Lite description logic
  - **EL**: based on the EL description logic
  - **RL**: based on the DL fragment of Datalog (aka DLP)
- Profiles allow for algorithmic techniques suited to query answering
  - **Query rewriting** for QL
  - **Materialisation** for RL
  - **Combined approach** for EL

Query Rewriting for OWL QL



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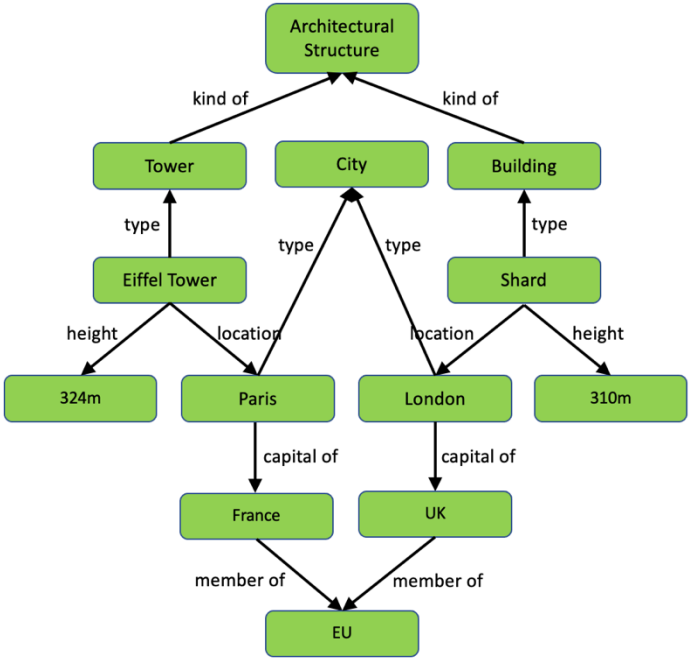

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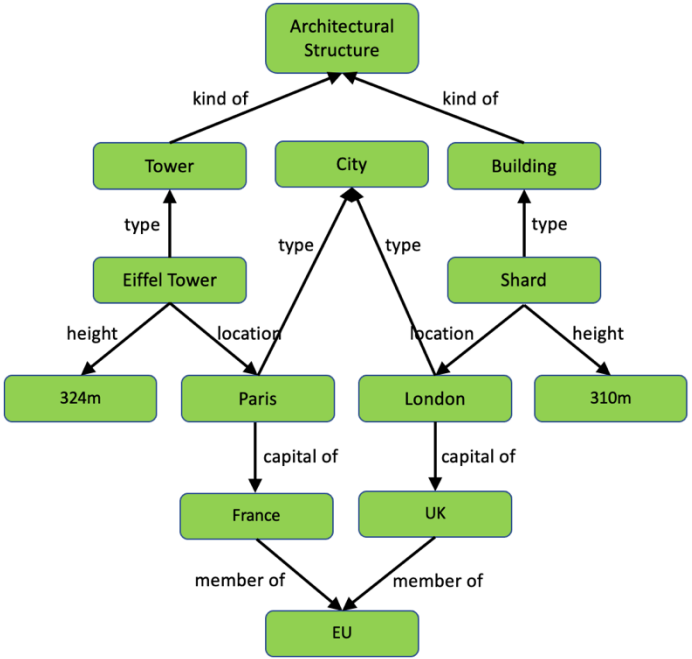

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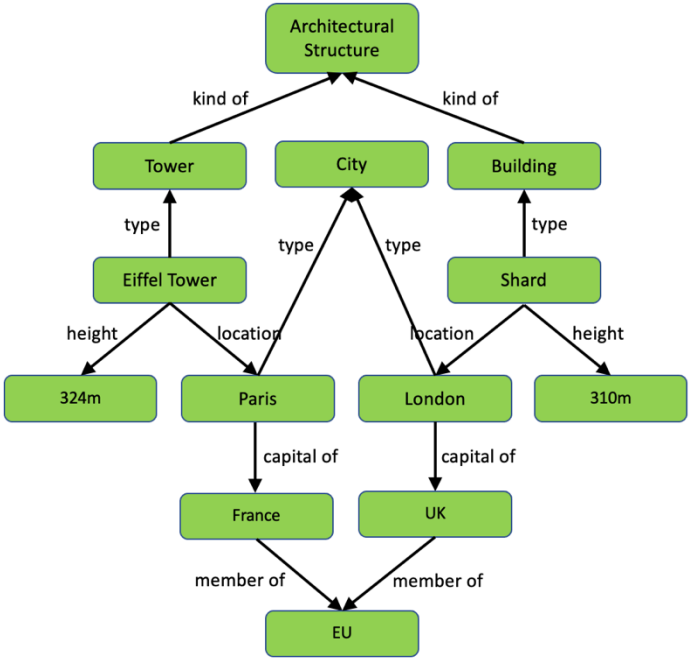
```
SELECT Name FROM Architectural_Structure
UNION SELECT Name FROM Tower
UNION SELECT Name FROM Building
```

Query Rewriting for OWL QL



$$Q(x) \leftarrow \text{Architectural\_Structure}(x)$$

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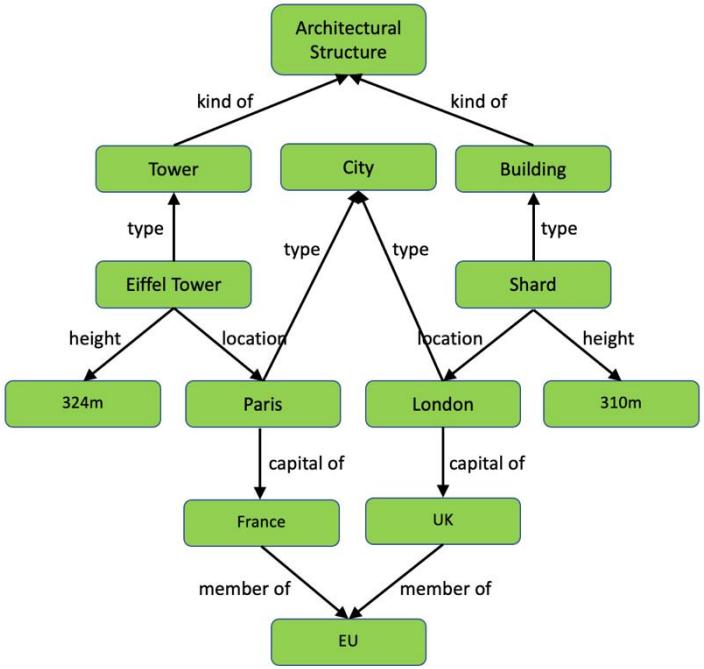
$$\begin{aligned} Q(x) \leftarrow\ & \text{Architectural\_Structure}(x) \vee \\ & \text{Tower}(x) \vee \\ & \text{Building}(x) \end{aligned}$$

```
SELECT Name FROM Architectural_Structure
UNION SELECT Name FROM Tower
UNION SELECT Name FROM Building
```

$$\text{location}(x, y) \wedge \text{capital\_of}(y, z) \rightarrow \text{location}(x, z)$$

Materialisation for OWL RL



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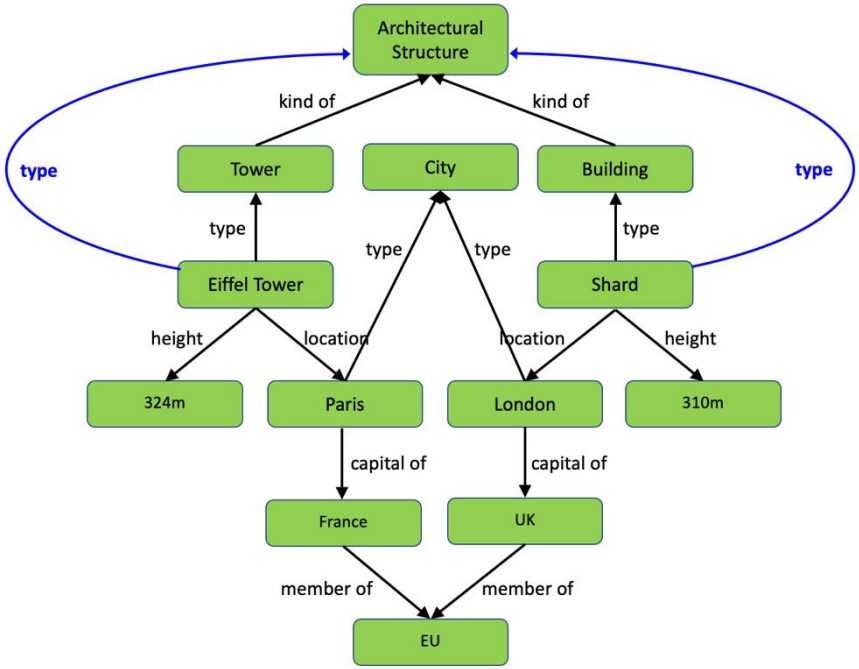

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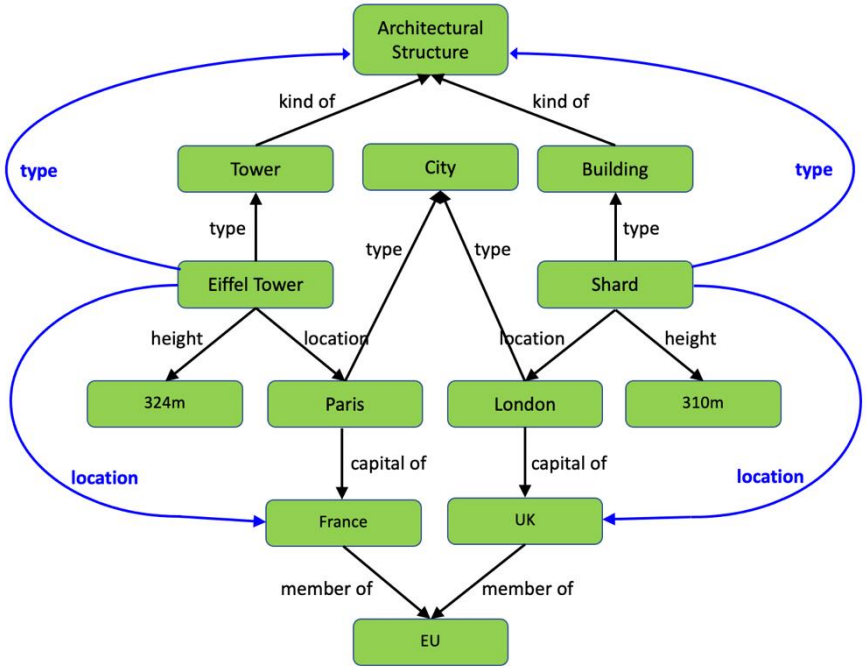

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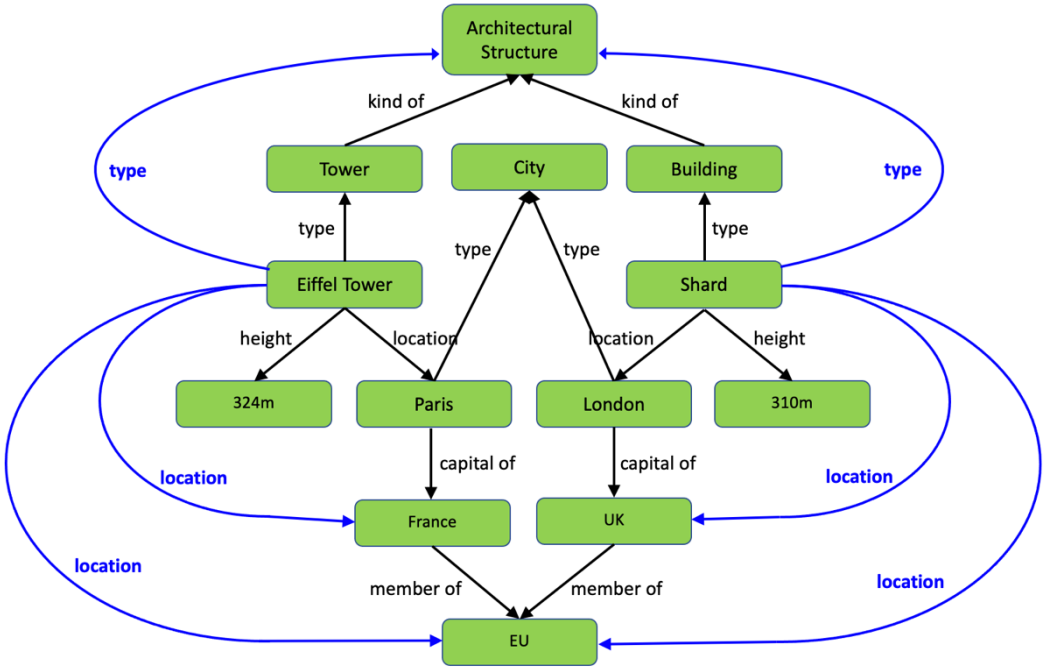

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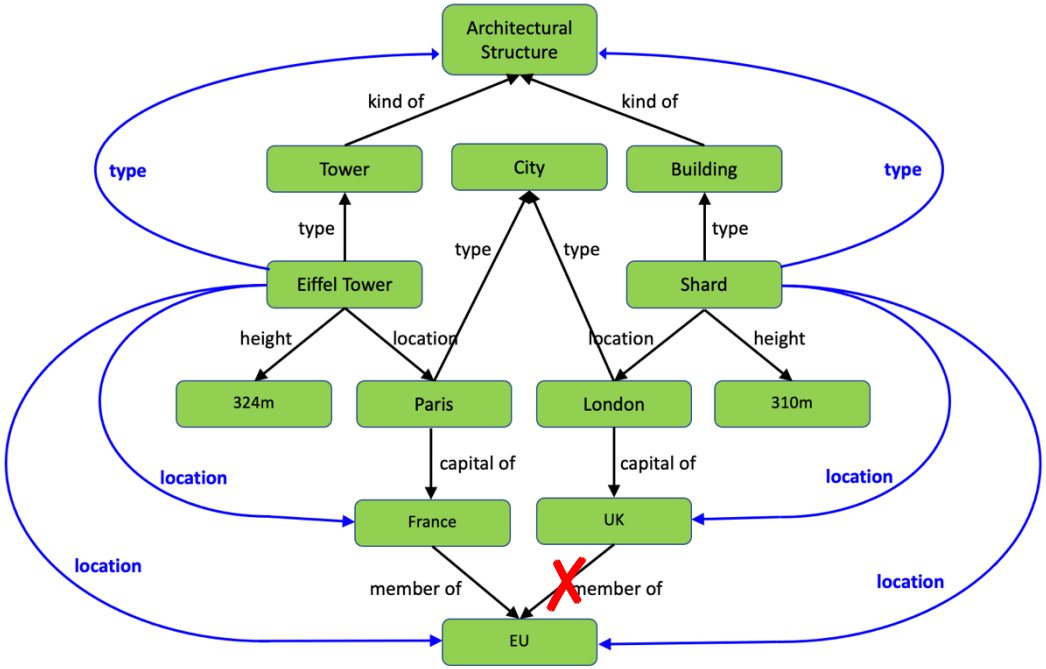
Materialisation for OWL RL



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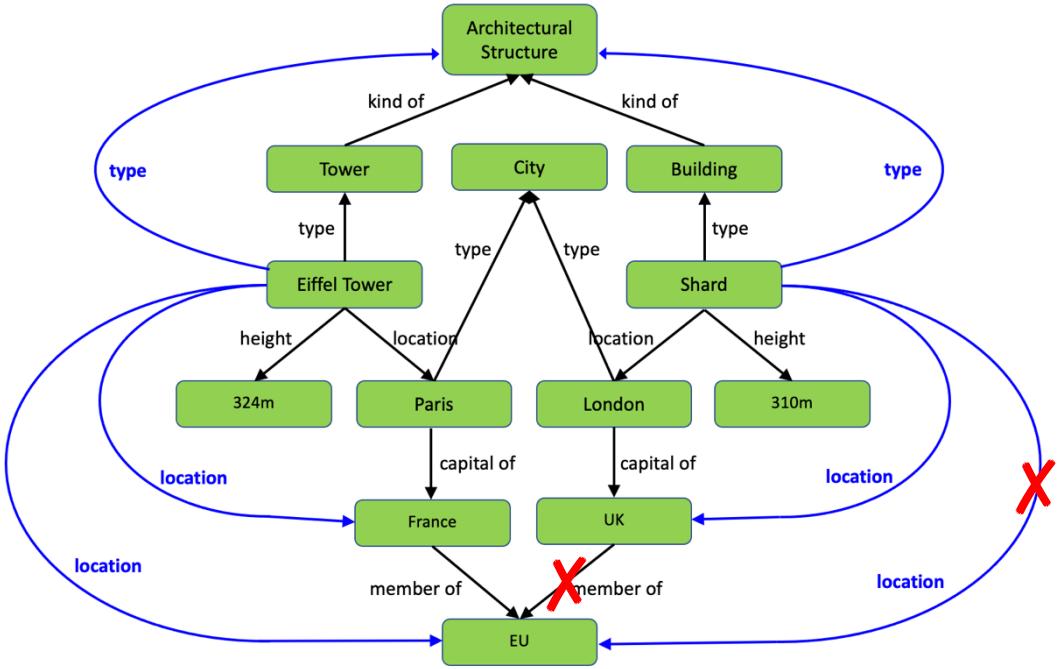
Materialisation for OWL RL



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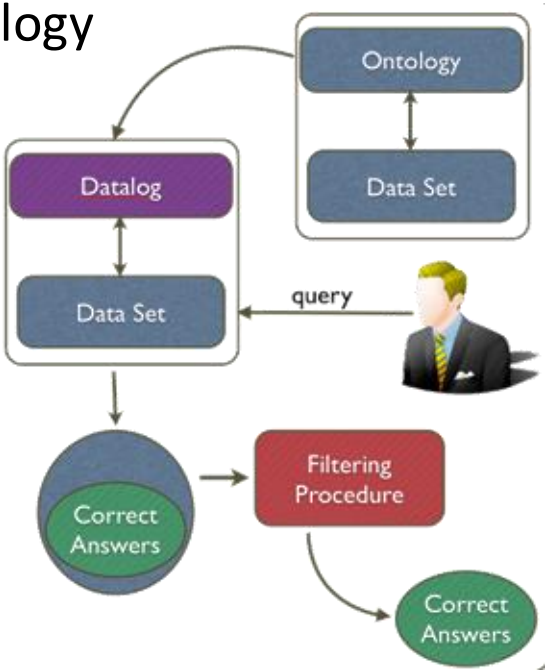
Combined Approach for OWL EL

Given (RDF) graph G and EL ontology O:

- **Overapproximate** O → O’ s.t. O’ is an OWL RL ontology
  - In particular, Skolemise existentials
- **Evaluate** queries against G and O’
  - E.g., using materialization-based reasoner
  - Answers will be complete, but may be unsound
- **Filter** results to remove any spurious answers
  - Filtration process is also polynomial



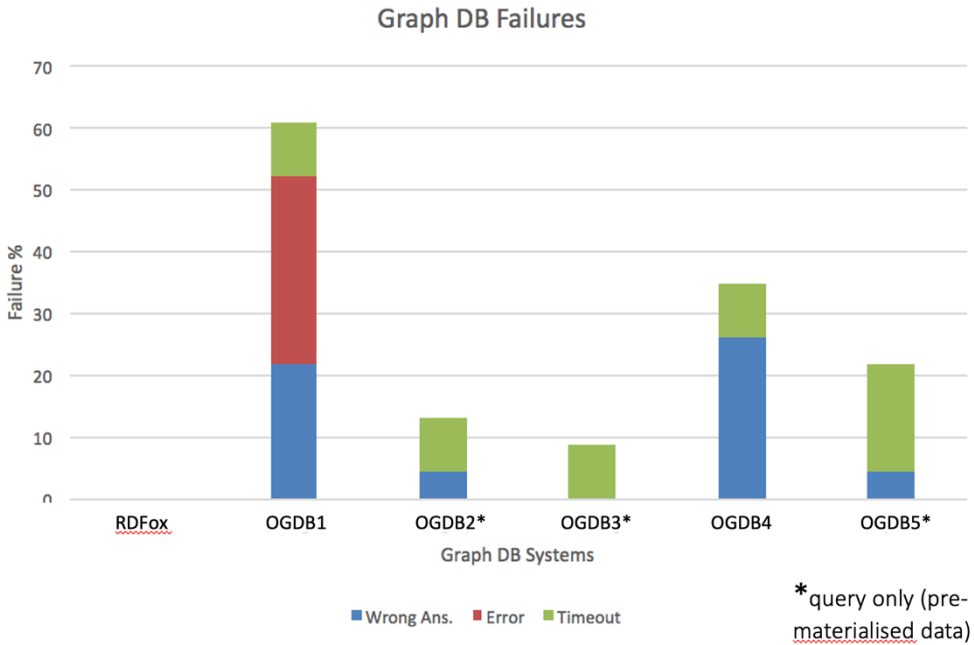
- Materialization reasoning seems ideal for data-centric applications
  - Can support expressive ontology languages
  - Fast query answering over very large graphs

- Challenges
  - Materialisation can be costly in time and memory
  - Materialisation may need to be repeated if data changes

- Solution: RDFox
  - Optimised materialization exploiting modern multi-core architectures
  - Incremental maintenance as data changes

RDFOX

- **Novel algorithms developed at Oxford**
  - Proven correctness



*query only (pre-materialised data)

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- **Novel algorithms developed at Oxford**
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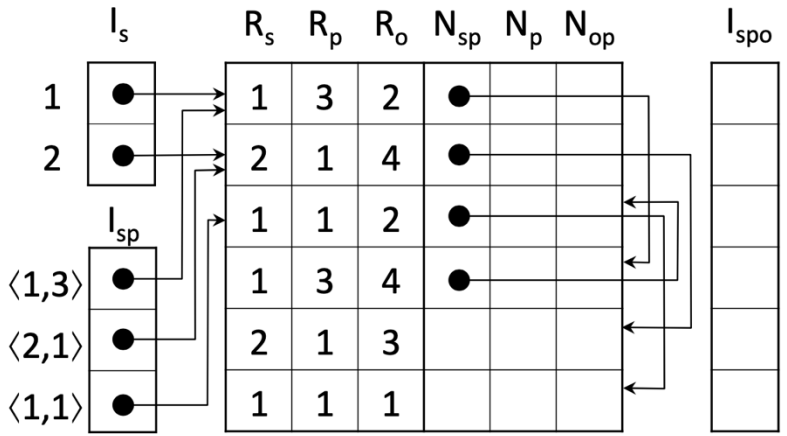
  - >10^9 triples on 128 Gb entry level server
  - >10^{10} triples on 1 Tb server



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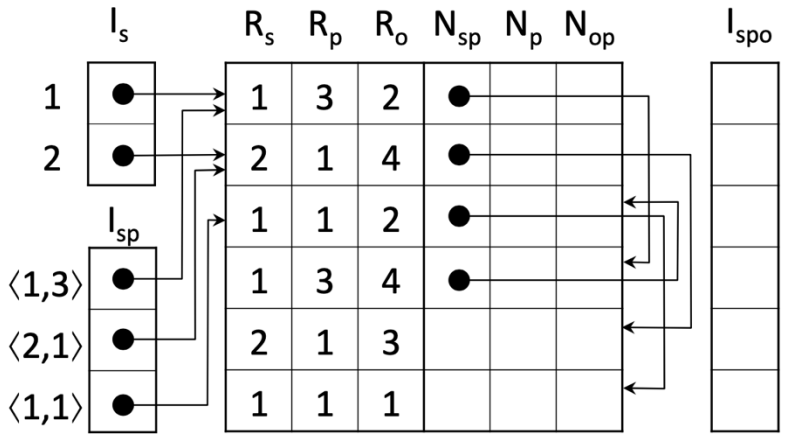

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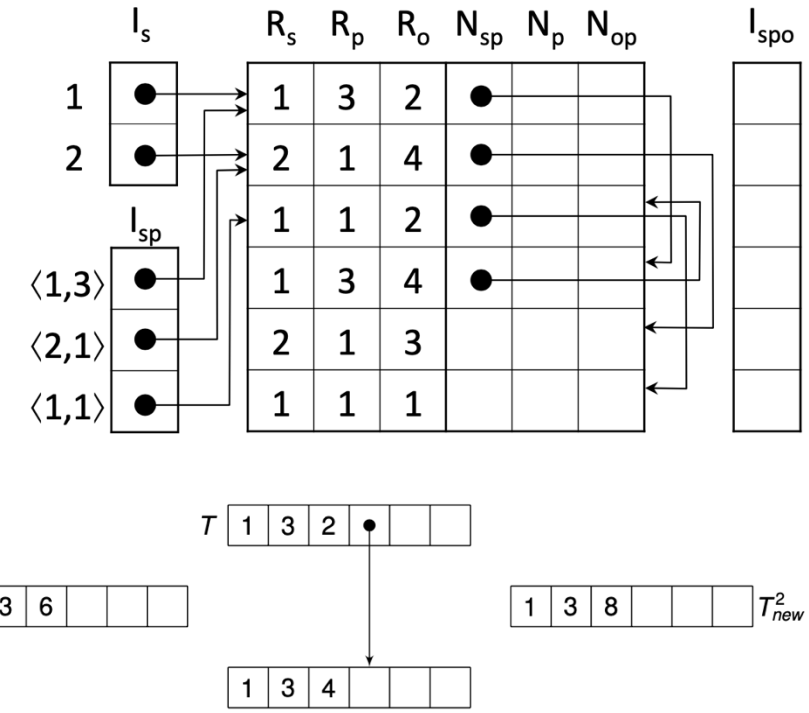

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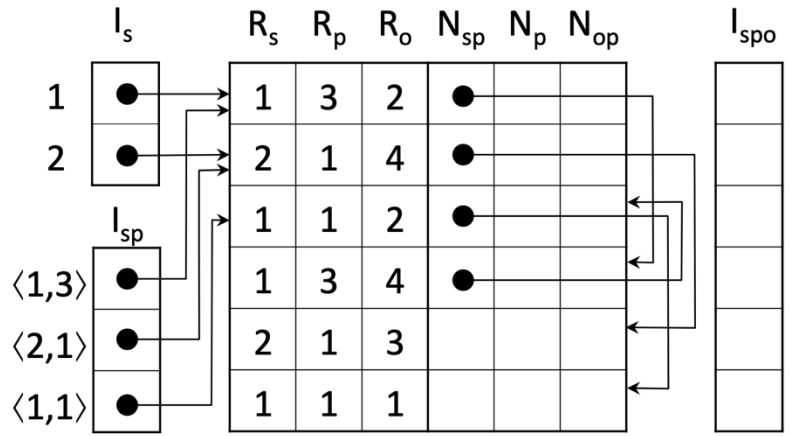

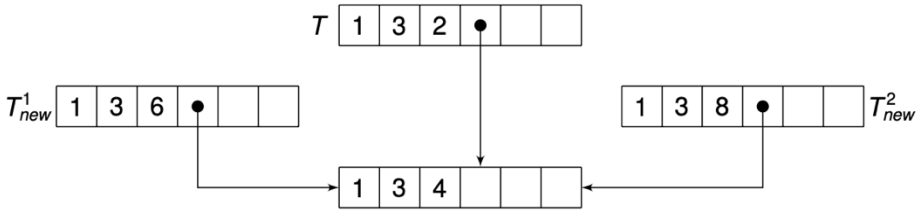

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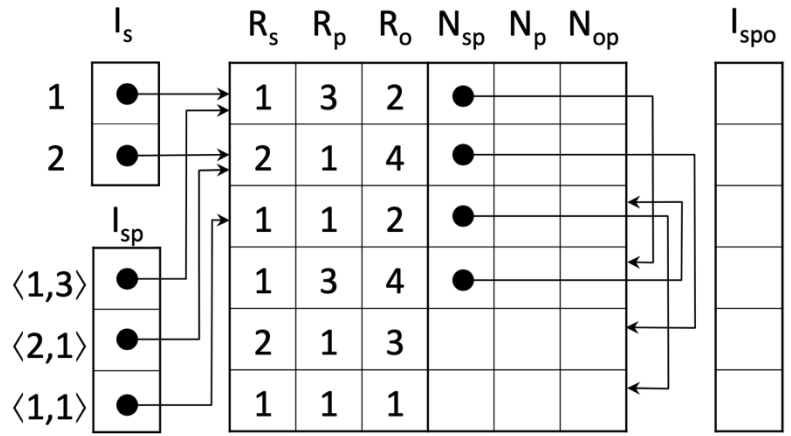

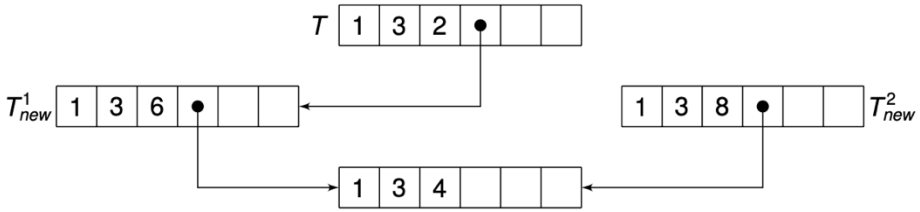

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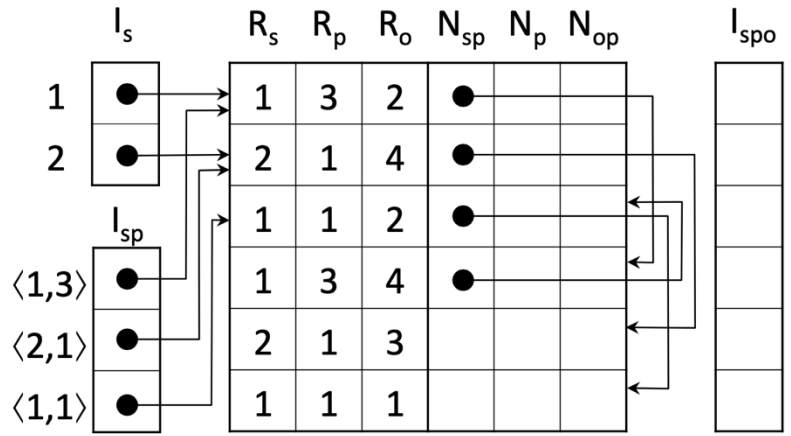

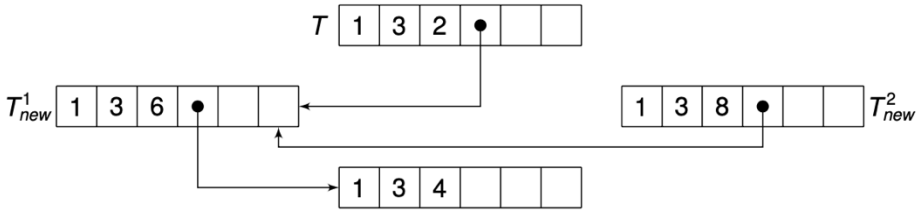

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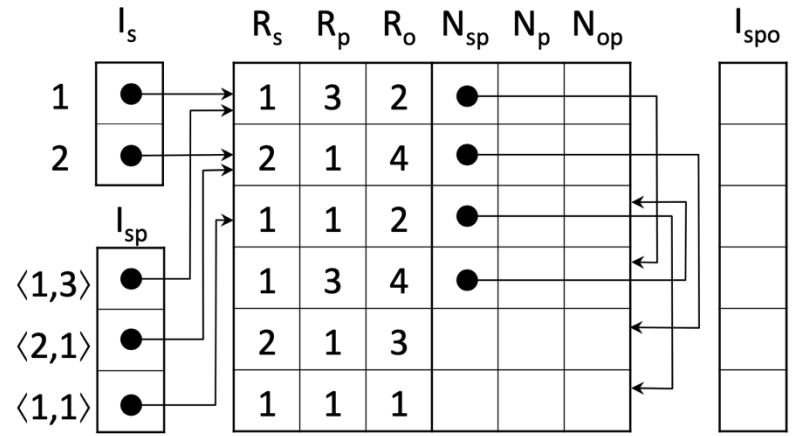

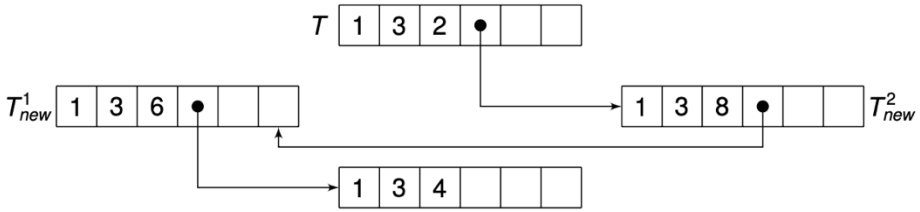

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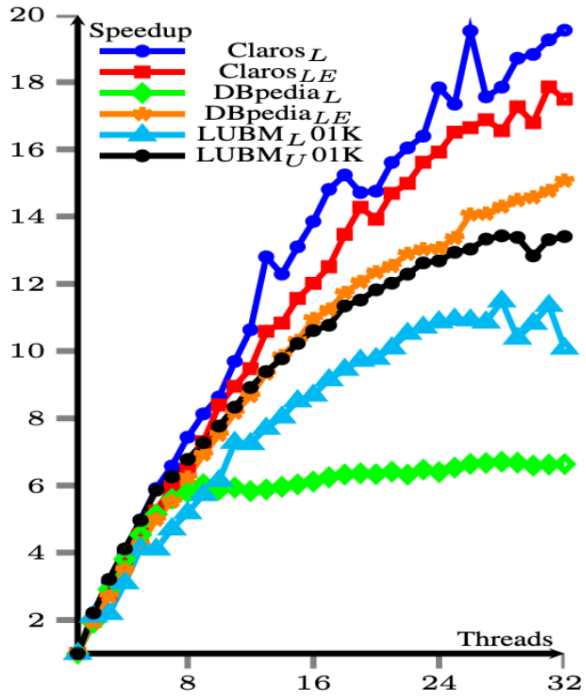

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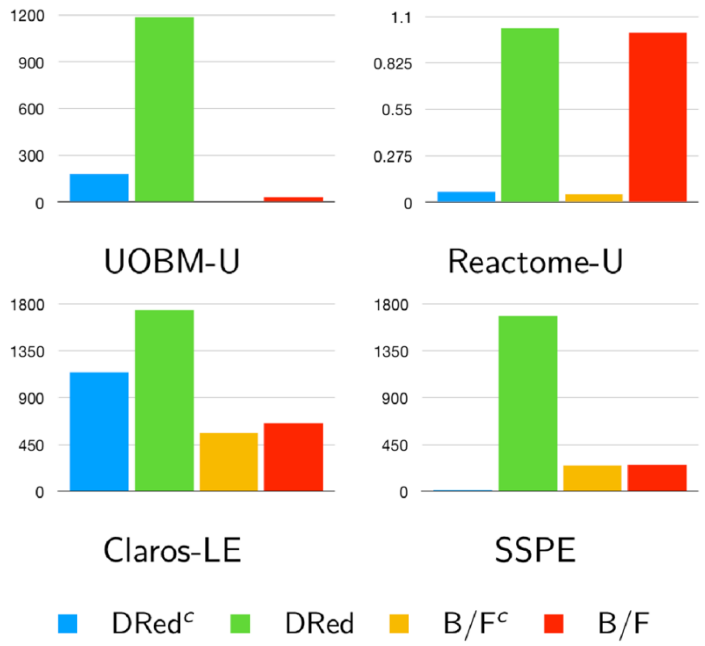
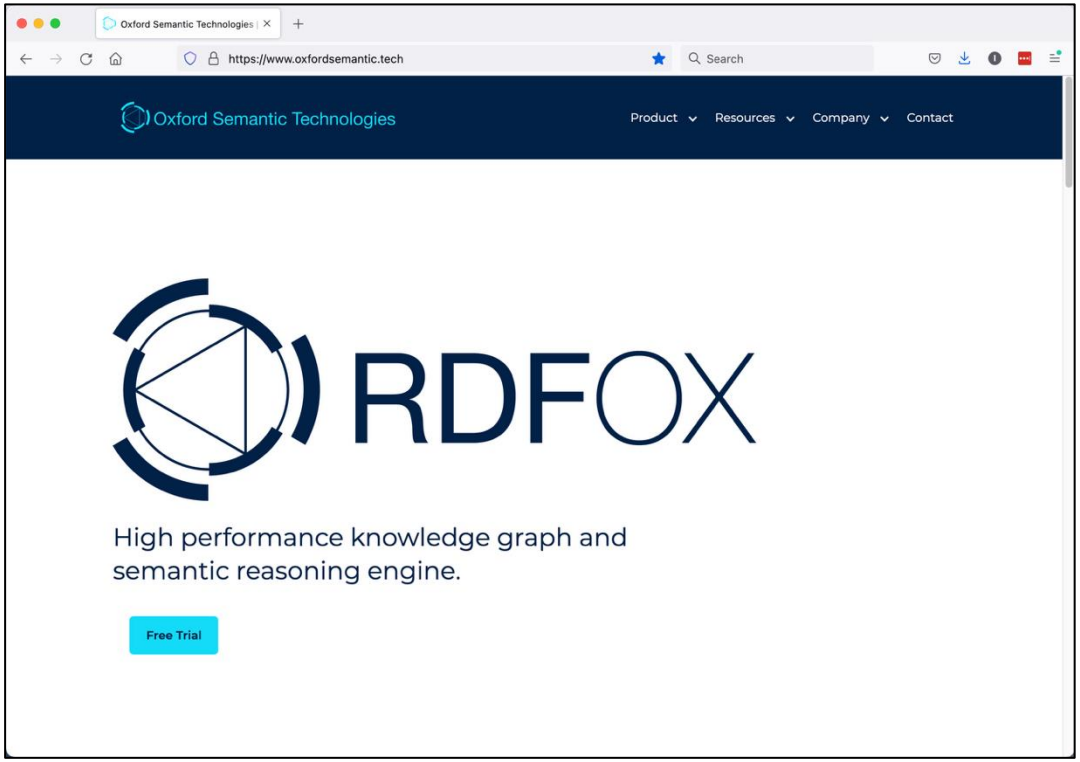
- **Incremental addition and retraction**
  - Novel B/F materialisation maintenance algorithm



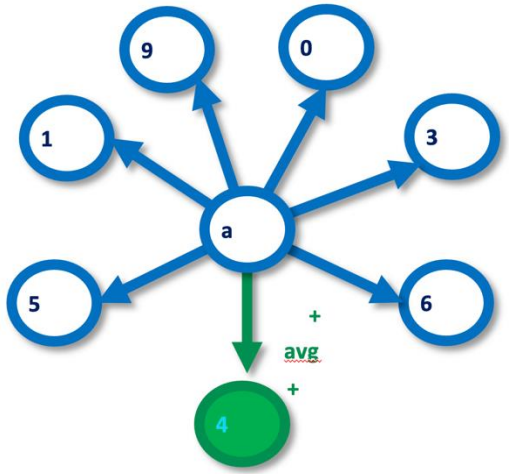
Challenges and Solutions (3)

Oxford Semantic Technologies

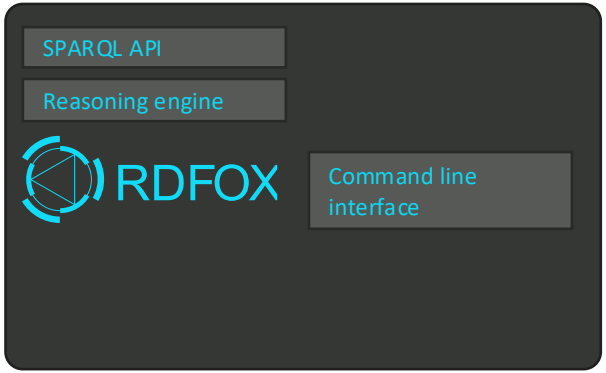


Extensions

- Arbitrary rules
  - No restriction to OWL RL (tree-shaped) rules
- Data types and values
  - Numbers, strings, dates, …
  - Built in functions and aggregation
- Value invention
  - Add new (possibly computed) values to graph
  - Add new URI nodes to graph
- Constraints and negation as failure
  - SHACL+



System Architecture



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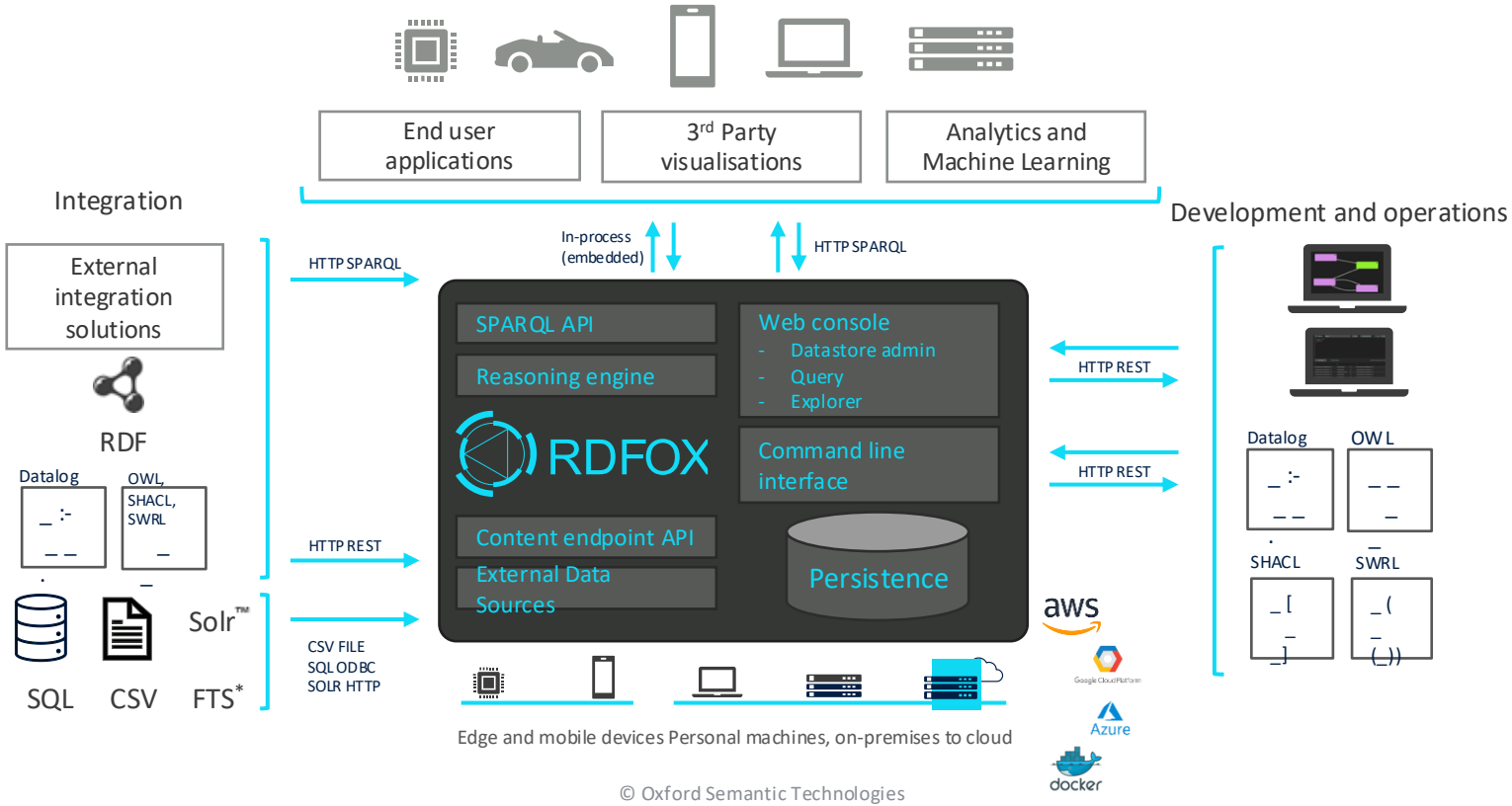
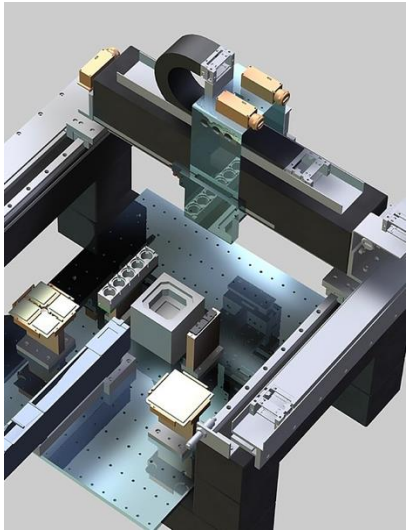


Knowledge Graph Use Cases

Configuration management

FESTO



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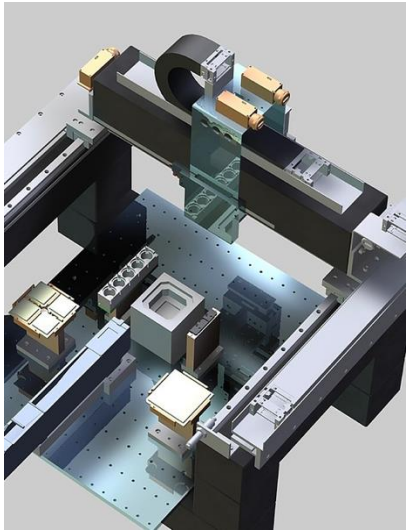
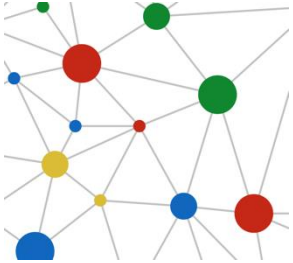




- Components
- Their attributes & constraints

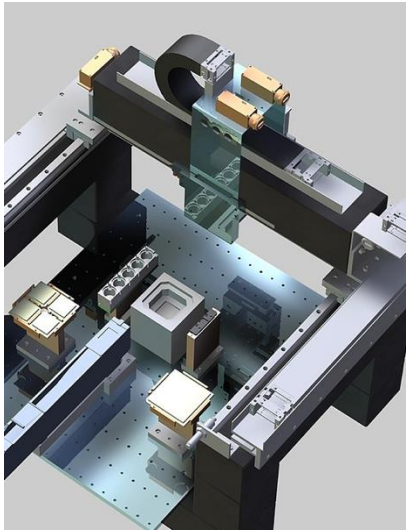
DATA _

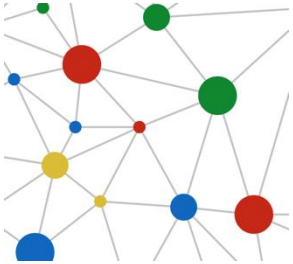
- Definitions of compatibility &
- Valid configurations

RULES

Configuration management

FESTO





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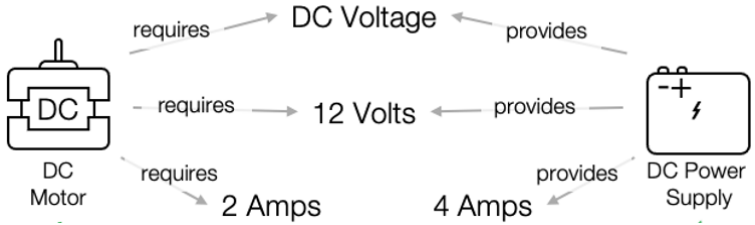

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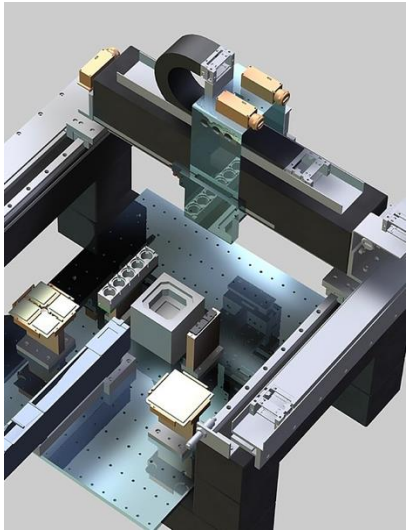

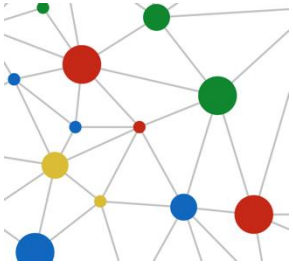

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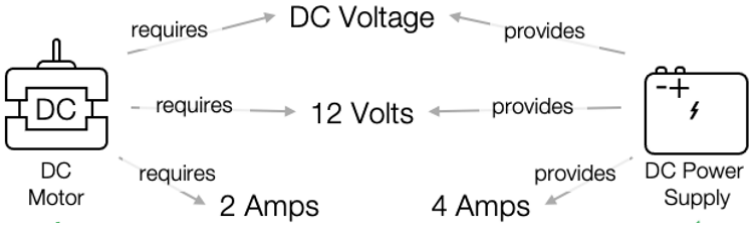


```
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   :DCPowerSupply[?PS] ,
   [?PS, :provides, :DCVoltage] ,
   [?PS, :providedVoltage, ?pv] ,
   [?PS, :providedCurrent, ?pc] ,
   [?M,  :requires, :DCVoltage] ,
   [?M,  :requiredVoltage, ?rv] ,
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   FILTER (?pv = ?rv && ?pc >= ?rc) .
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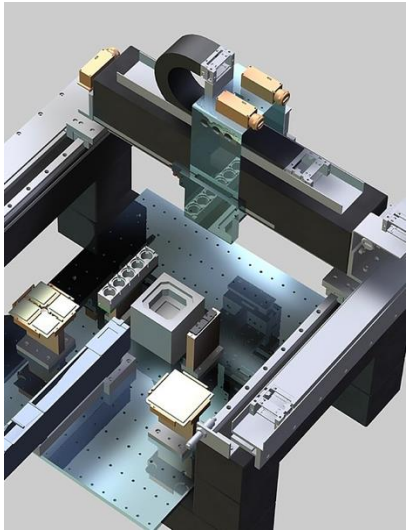
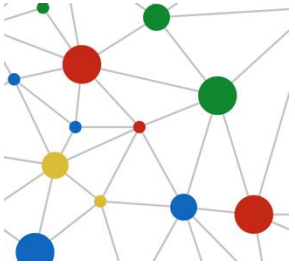
Configuration management

FESTO





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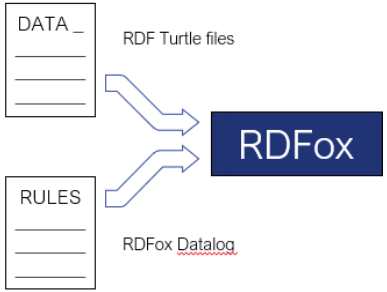

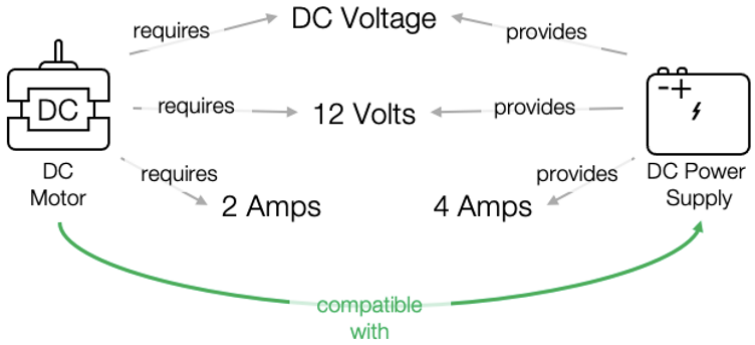


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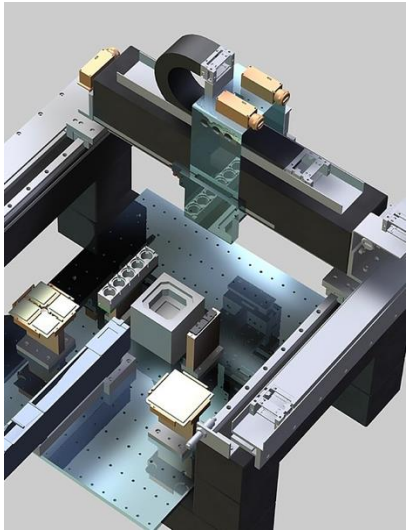

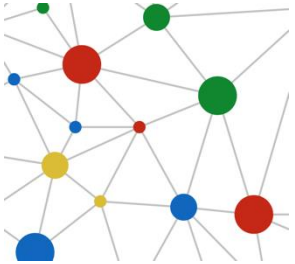

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DATA _

RDF Turtle files

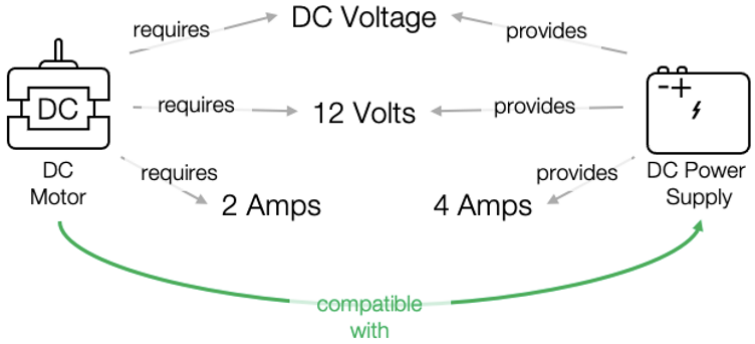
RULES

RDFox Datalog

RDFox

Rotation Solutions

Query via SPARQL over REST

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   :DCMotor[?M] ,
   :DCPowerSupply[?PS] ,
   [?PS, :provides, :DCVoltage] ,
   [?PS, :providedVoltage, ?pv] ,
   [?PS, :providedCurrent, ?pc] ,
   [?M,  :requires, :DCVoltage] ,
   [?M,  :requiredVoltage, ?rv] ,
   [?M,  :requiredCurrent, ?rc] ,
   FILTER (?pv = ?rv && ?pc >= ?rc) .
```
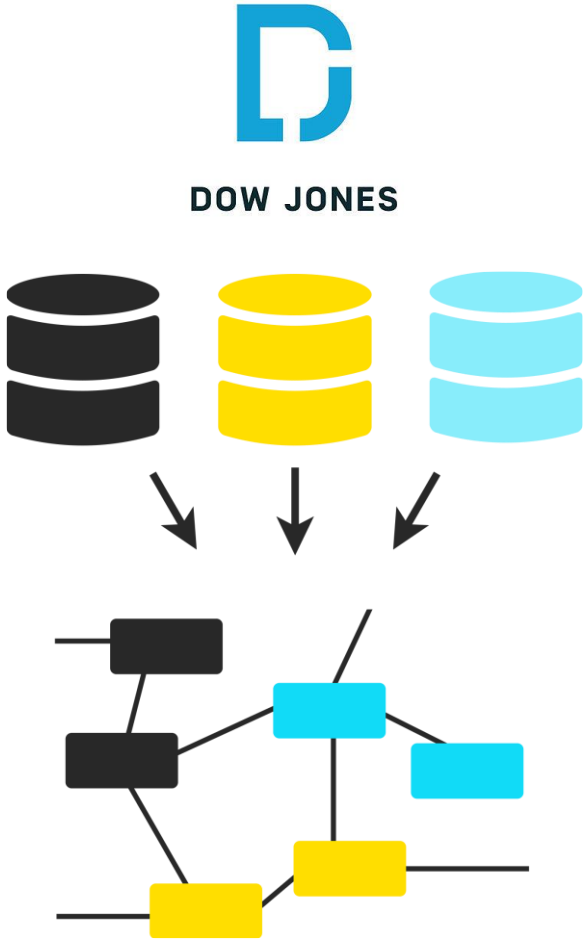
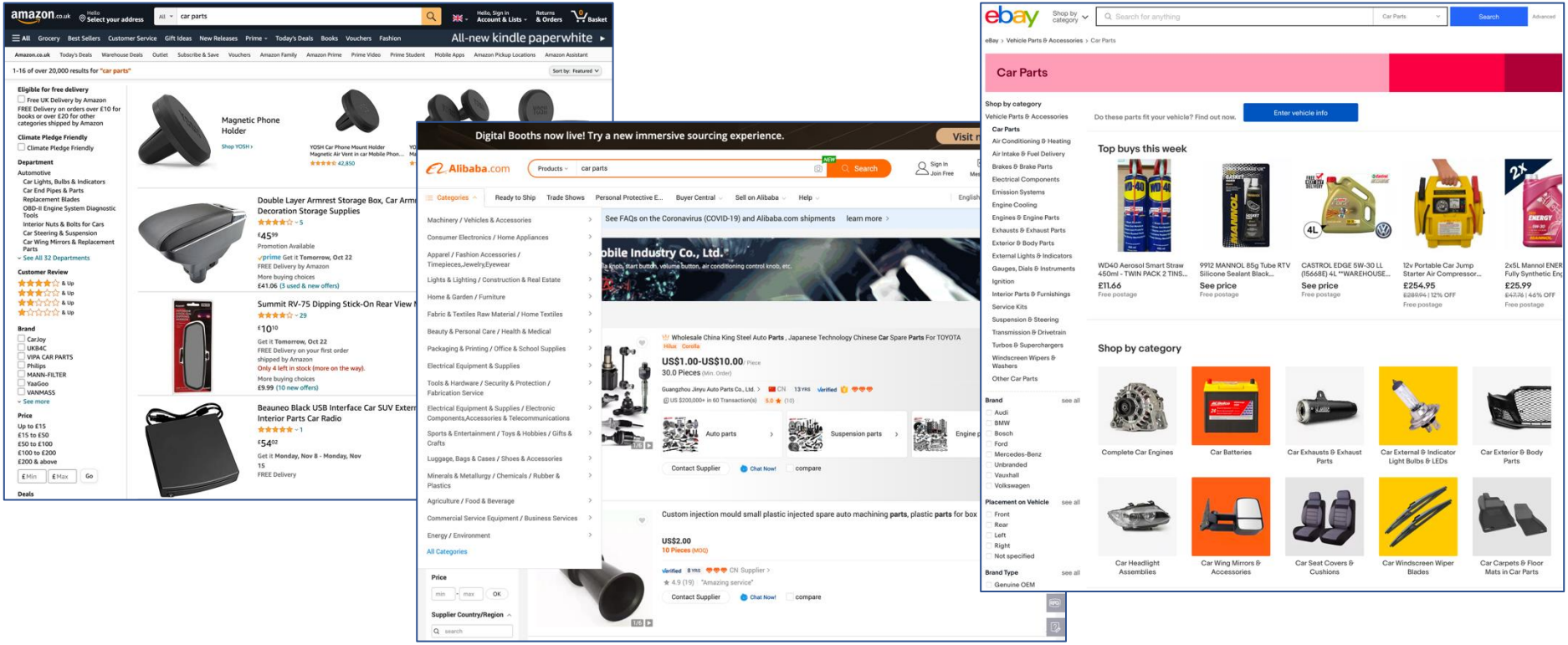

Data Integration

- Integrate data from multiple sources
  - Companies
  - Executives
  - Stock markets
  - Geonames
  - Articles from WSJ, Factiva, …
- Query integrated data
  - Competitor companies that are NASDAQ listed and have subsidiaries in same or related sector
  - Article published between 2020-05-24 and 2020-05-26 that talk about company C and mention an African country

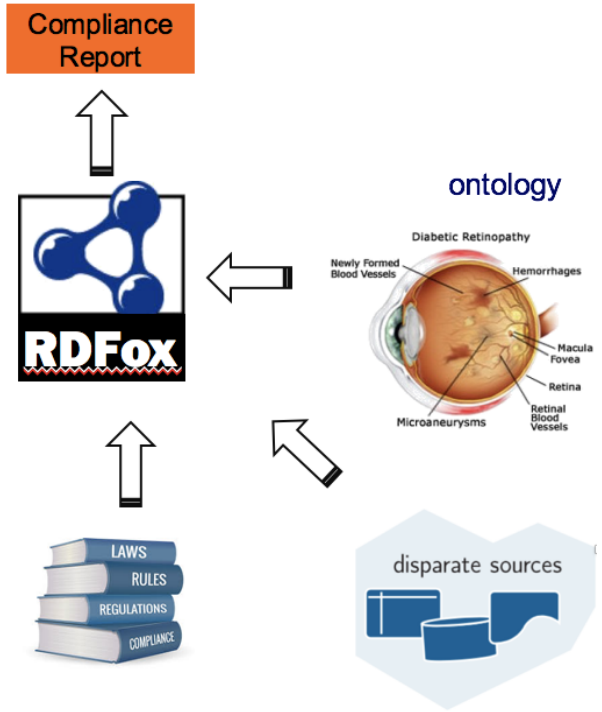


Semantic Search & Browse



Regulatory Compliance / Fraud Detection

- Domain knowledge captured in ontology/rules
- Regulations captured as rules
- Data describes real-life situation
- RDFox generates compliance report highlighting any non-compliance



Wrap-up

Summary

- **KGs are powerful tool** for representing & reasoning about knowledge
- **Many applications**: configuration, data integration, compliance, …
- **Technical challenges**: complexity, scalability, extensions, systems, …
- **Solutions** based on foundational research + systems engineering

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SAMSUNG

SIEMENS

ebay

EDF

ORACLE

Thanks for Listening
Any Questions?

: **www.oxfordsemantic.tech**

Background reading:

- **Description Logic:** Baader, Horrocks, Lutz, and Sattler. *An Introduction to Description Logic*. Cambridge University Press, 2017.
- **OWL:** Horrocks, Patel-Schneider, and van Harmelen. *From SHIQ and RDF to OWL: The Making of a Web Ontology Language*. J. of Web Semantics, 1(1):7-26, 2003.
- **RDFox algorithms & data structures:** Motik, Nenov, Piro, Horrocks, and Olteanu. *Parallel Materialisation of Datalog Programs in Centralised, Main-Memory RDF Systems*. AAAI 2014.
- **Incremental maintenance:** Motik, Nenov, Robert Piro, and Horrocks. *Maintenance of datalog materialisations revisited*. Artificial Intelligence, 269:76-136, 2019.