QPTDat
Quality | Plasma Technology | Data

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Ontologies and Knowledge Graphs for FAIR Research Data Management

Prof. Dr. Harald Sack
FAIR Research Data in Plasma Medicine
28 October 2020

650

650 cm

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650 cm

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650 cm
http://oberwesel.spatialhumanities.de/

650

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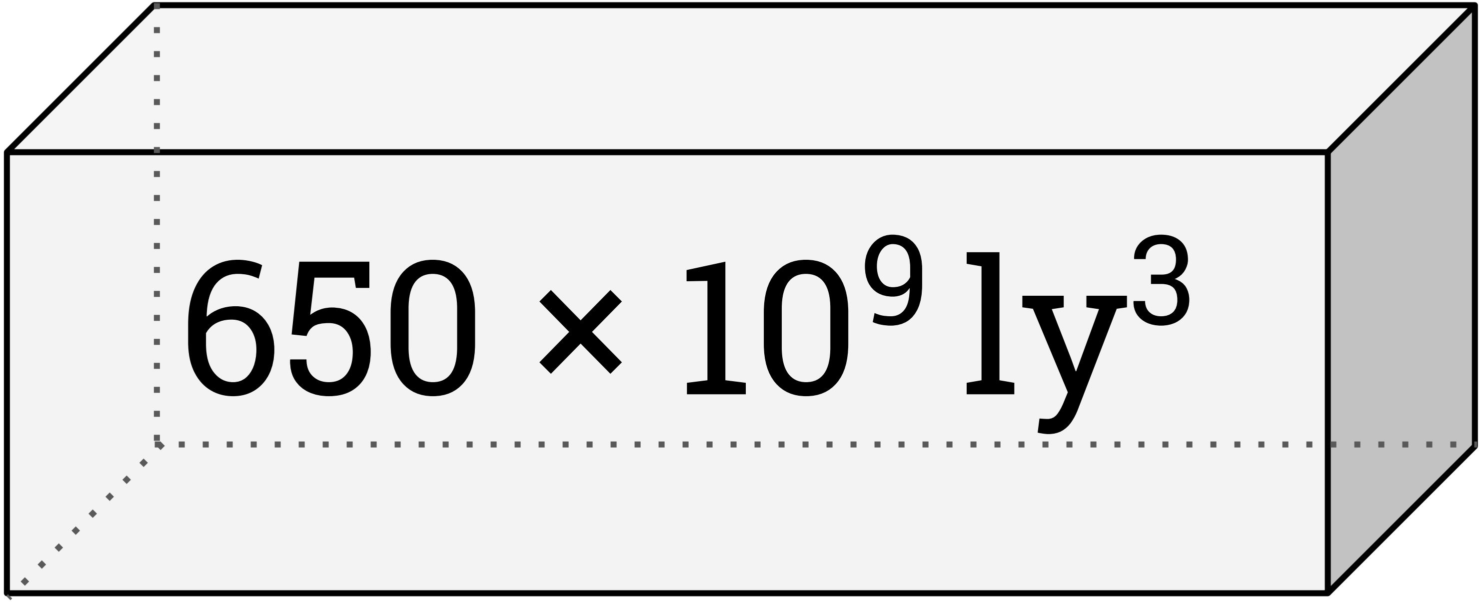
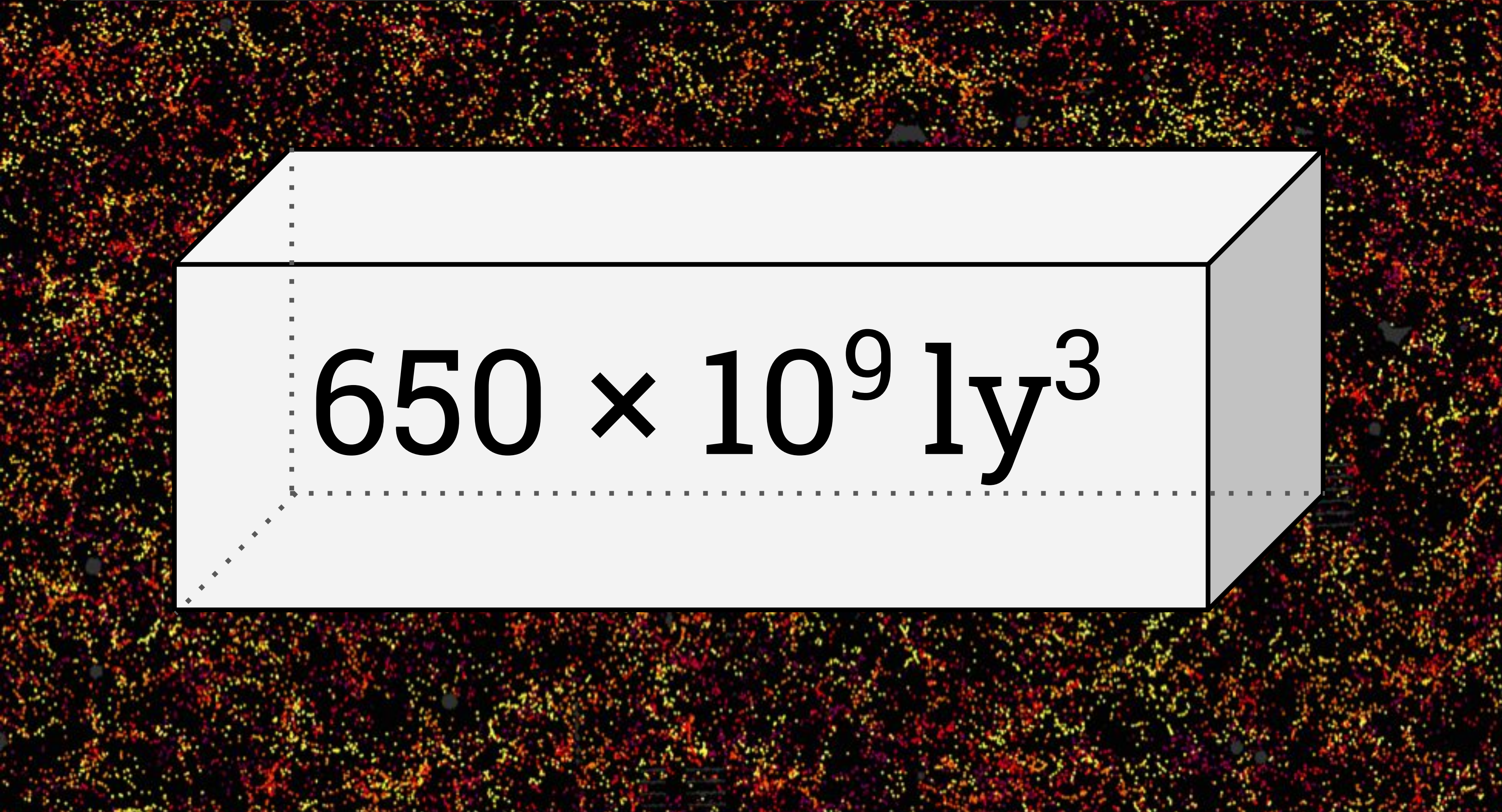
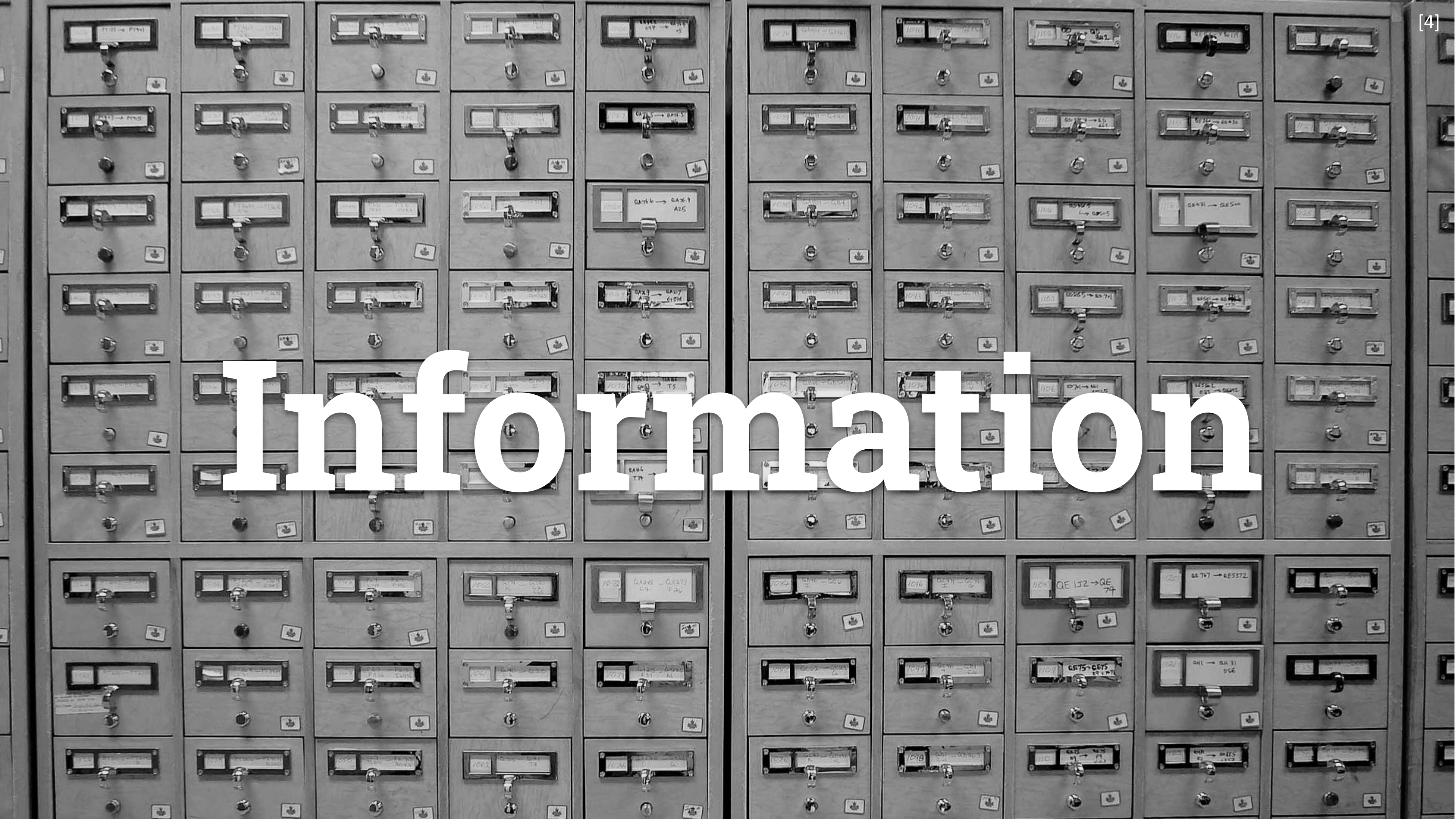
$$650 \times 10^9 \, \mathrm{ly}^3$$

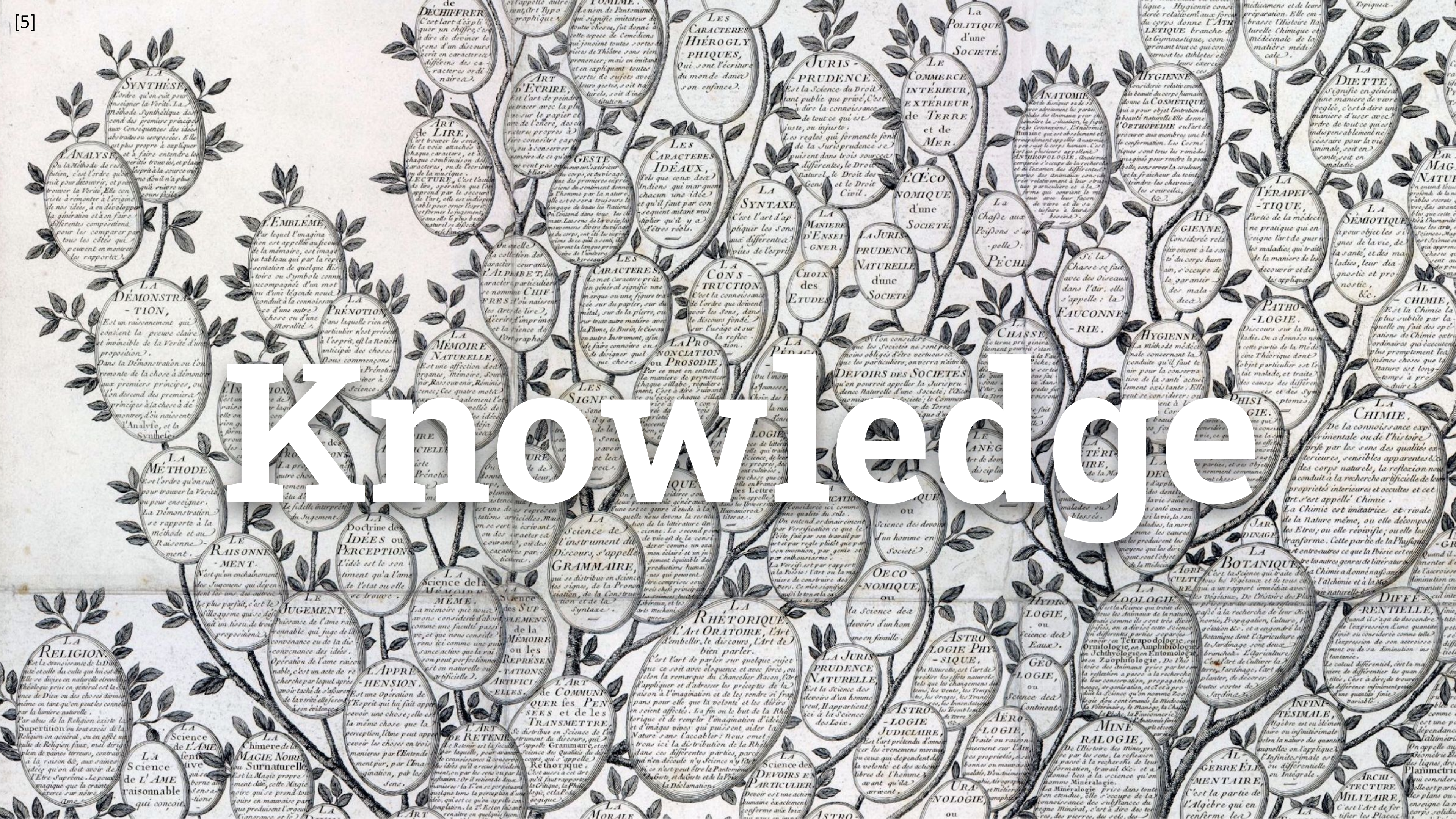

$650 \times 10^9\,\mathrm{ly}^3$


$650 \times 10^9\ \mathrm{ly}^3$

Data

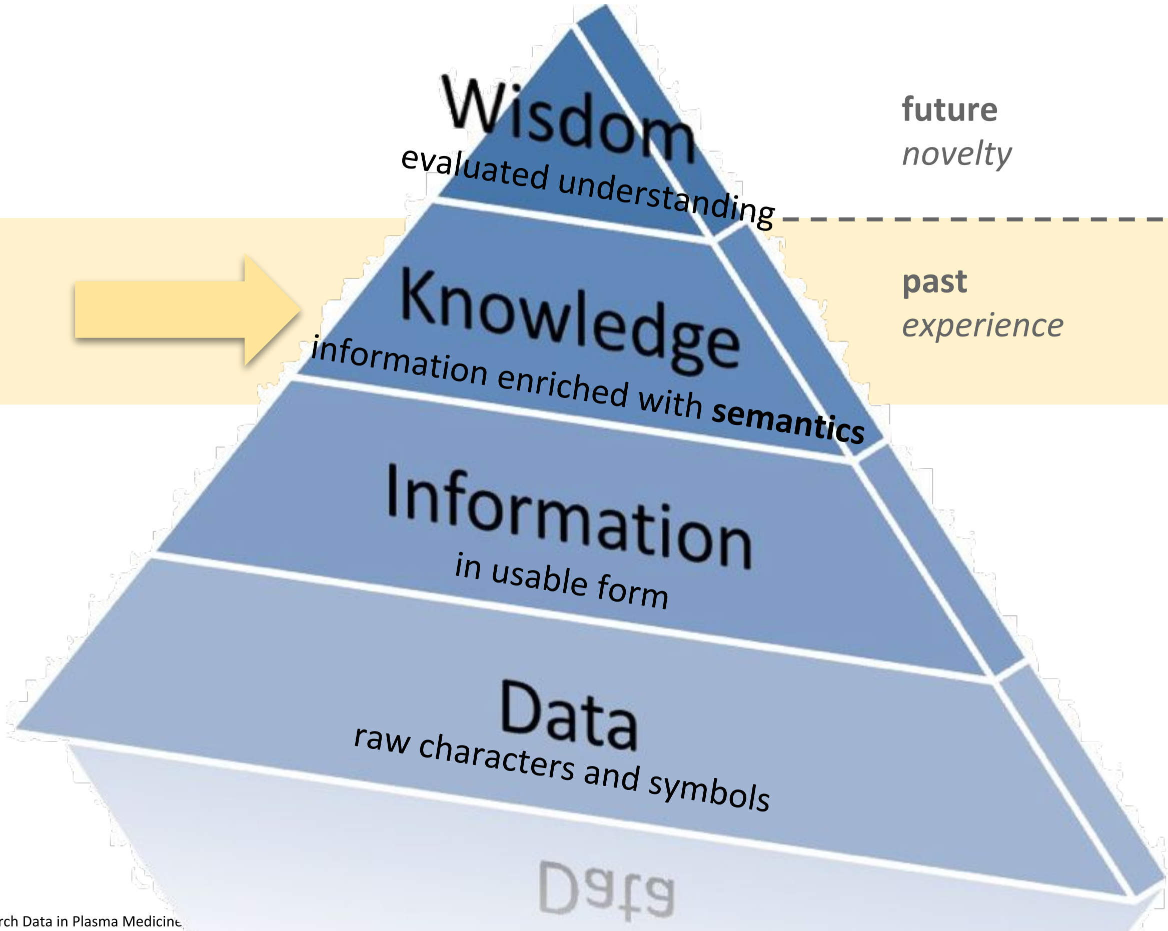

[4]
Information

[5]



Knowledge

From Data to Knowledge



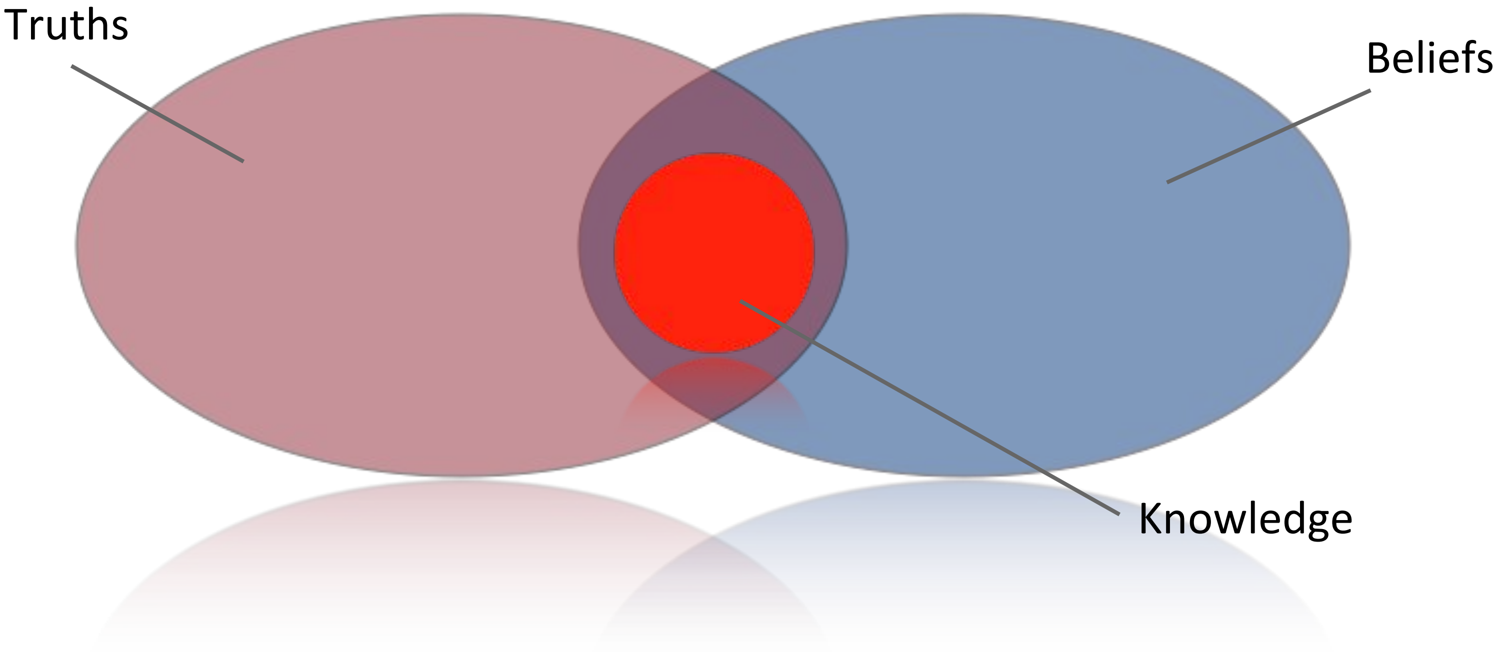
DIKW Pyramid, *Ackoff 1989*

[6]

„People can‘t share knowledge if they don‘t speak a common language“

Thomas Davenport (1997)

What is Knowledge?

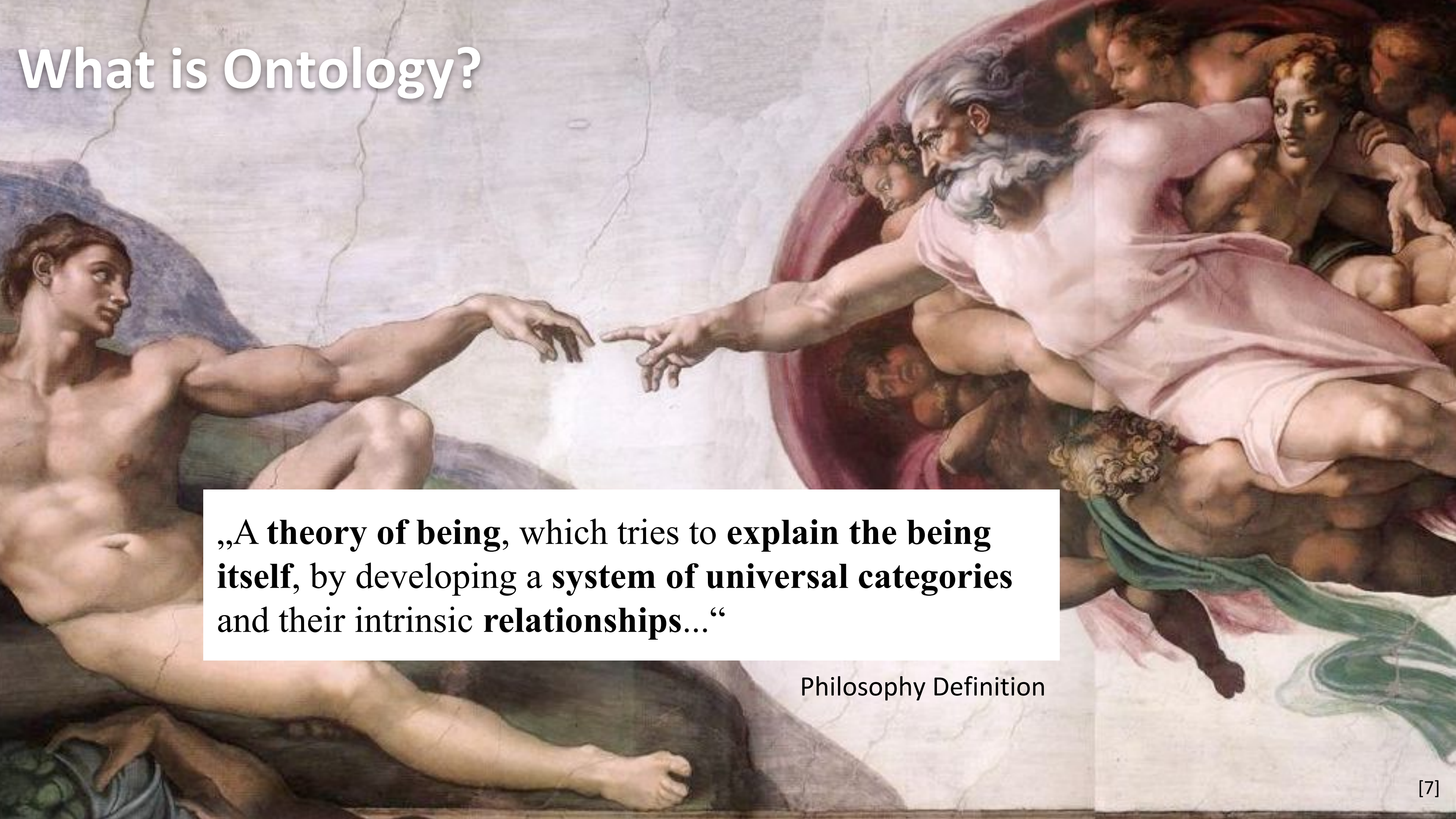


Traditional Definition: „Knowledge is a subset of all true beliefs“

...to speak a common Language:

- common symbols and concepts **(Syntax)**
- agreement about their meaning **(Semantics)**
- classification of concepts **(Taxonomy)**
- associations and relations of concepts **(Thesauri)**
- rules and knowledge about which relations are allowed and make sense **(Ontologies)**

But what exactly are Ontologies?



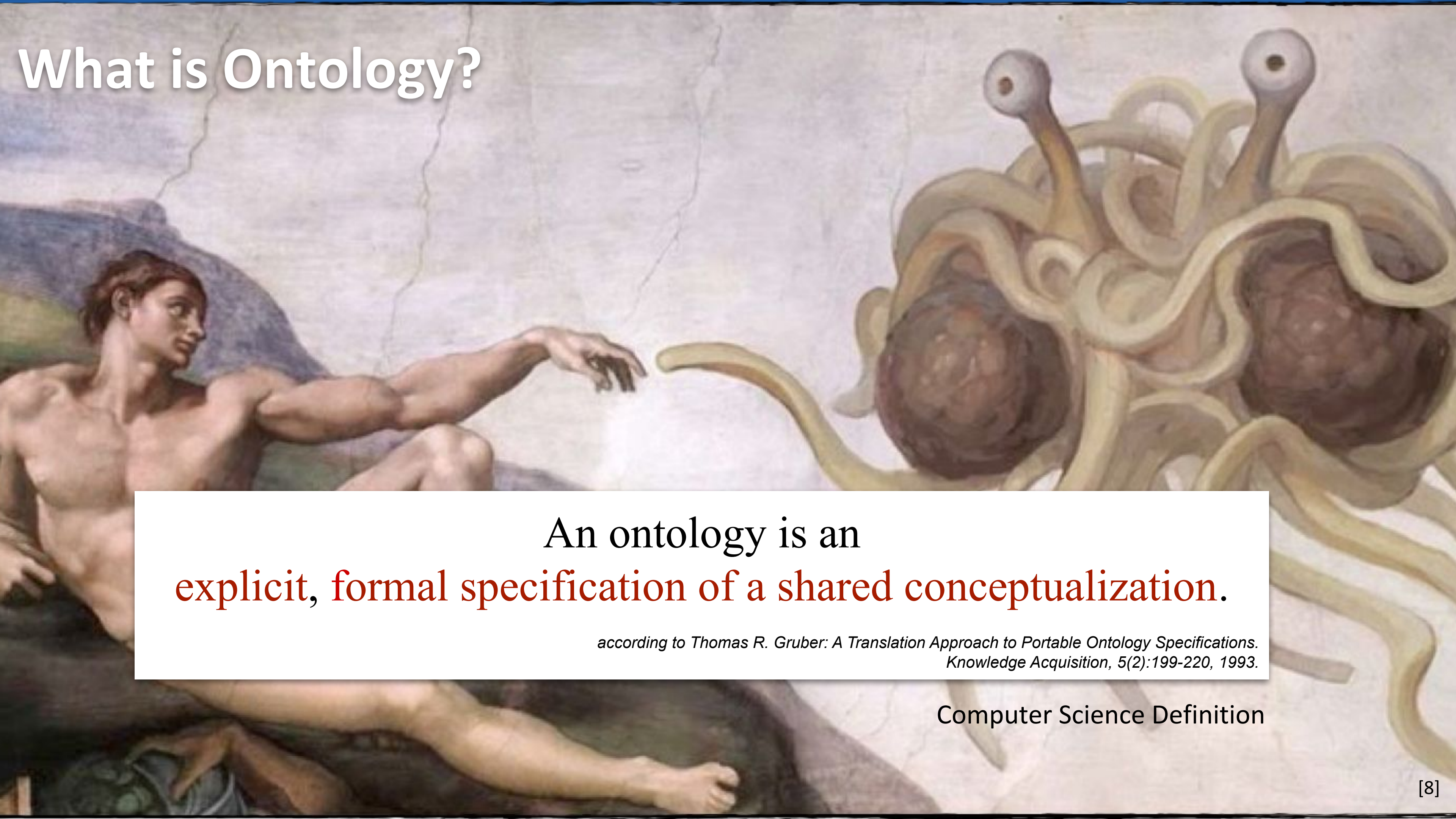
What is Ontology?

„A **theory of being**, which tries to **explain the being itself**, by developing a **system of universal categories** and their intrinsic **relationships**...“

Philosophy Definition

[7]

What is Ontology?



An ontology is an
explicit, formal specification of a shared conceptualization.

according to Thomas R. Gruber: A Translation Approach to Portable Ontology Specifications. Knowledge Acquisition, 5(2):199-220, 1993.

Computer Science Definition

[8]

What is Ontology?

An ontology is an
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according to Thomas R. Gruber: A Translation Approach to Portable Ontology Specifications.
Knowledge Acquisition, 5(2):199-220, 1993.

conceptualization: abstract model
(domain, identified relevant concepts, relations)

explicit: meaning of all concepts must be defined

formal: machine understandable

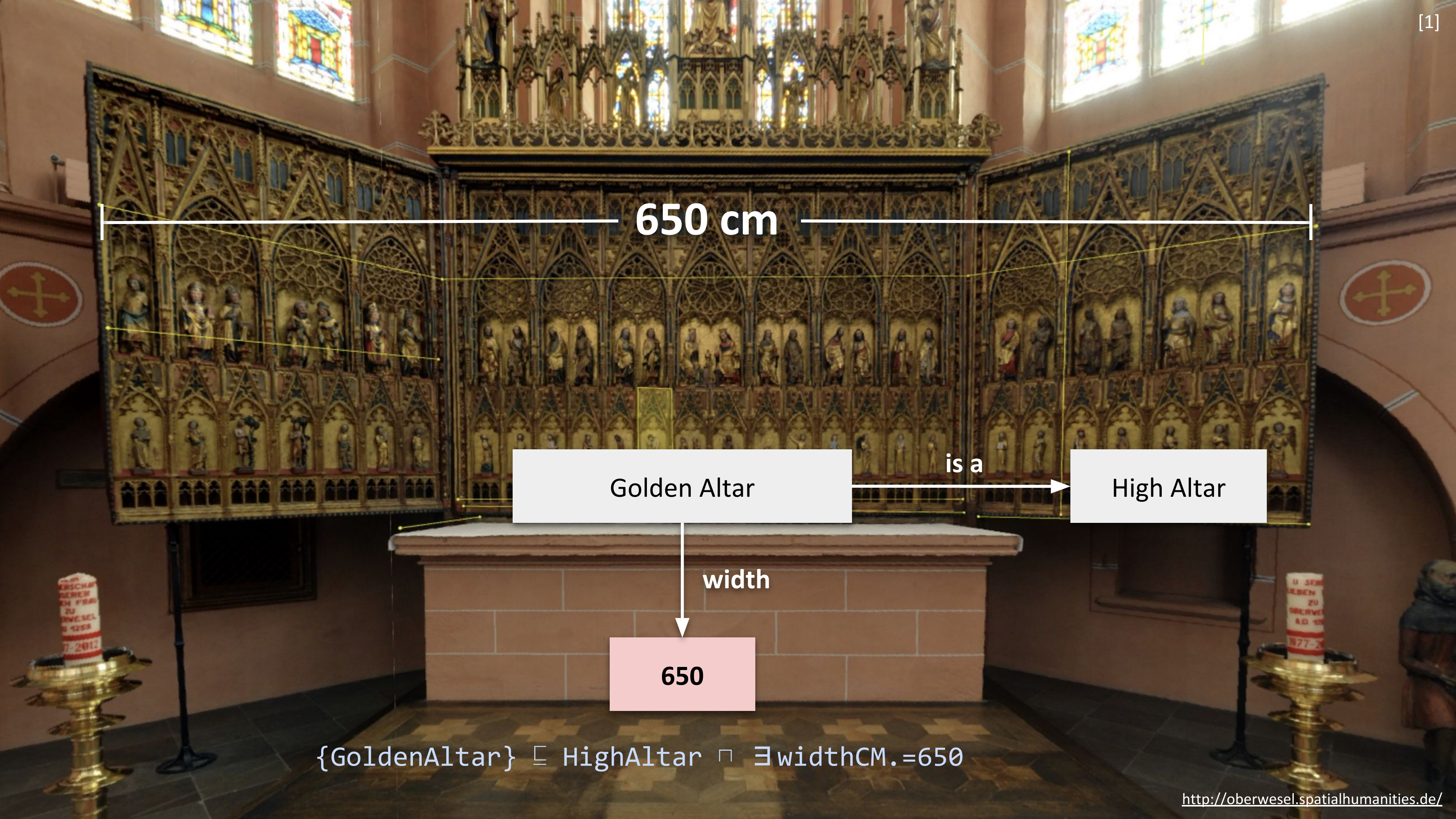
shared: consensus about ontology

[8]

PARENTAL

ADVISORY

EXPLICIT SEMANTICS


[1]
650 cm
Golden Altar
is a
High Altar
width
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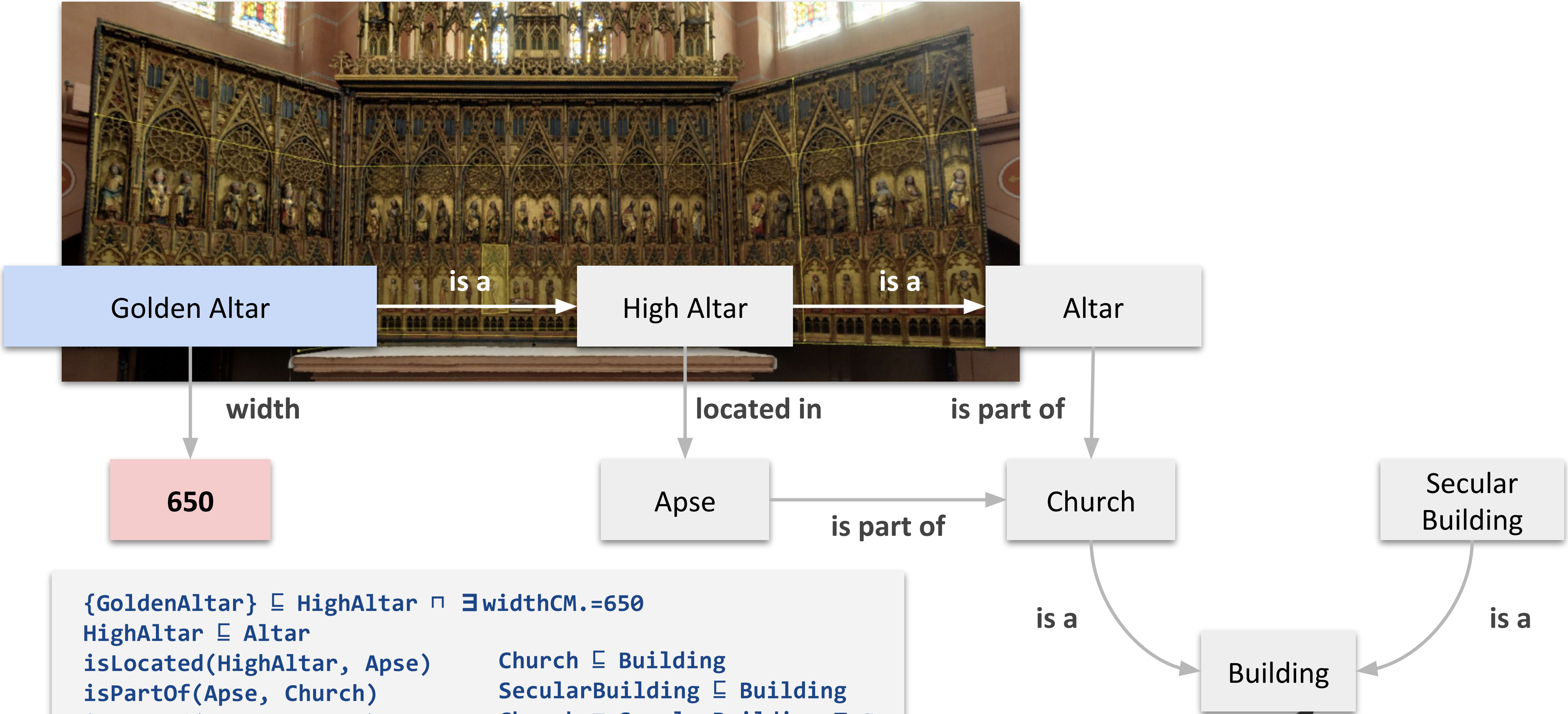
{GoldenAltar} ⊑ HighAltar ⊓ ∃widthCM.=650
http://oberwesel.spatialhumanities.de/

From Ontology to Knowledge Graphs



$\{GoldenAltar\} \sqsubseteq HighAltar \sqcap \exists widthCM.{=}650$
$HighAltar \sqsubseteq Altar$
$isLocated(HighAltar, Apse)$
$isPartOf(Apse, Church)$
$isPartOf(Apse, Church)$

$Church \sqsubseteq Building$
$SecularBuilding \sqsubseteq Building$
$Church \sqcap SecularBuilding \equiv \varnothing$

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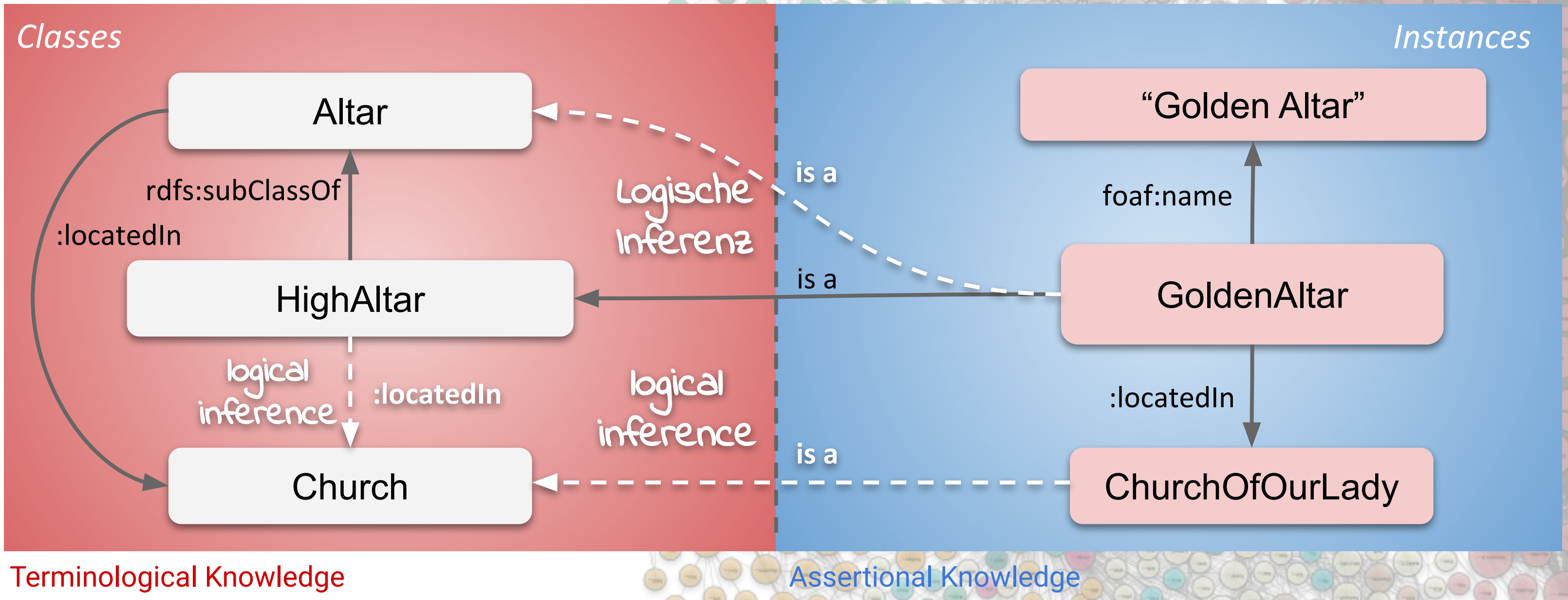
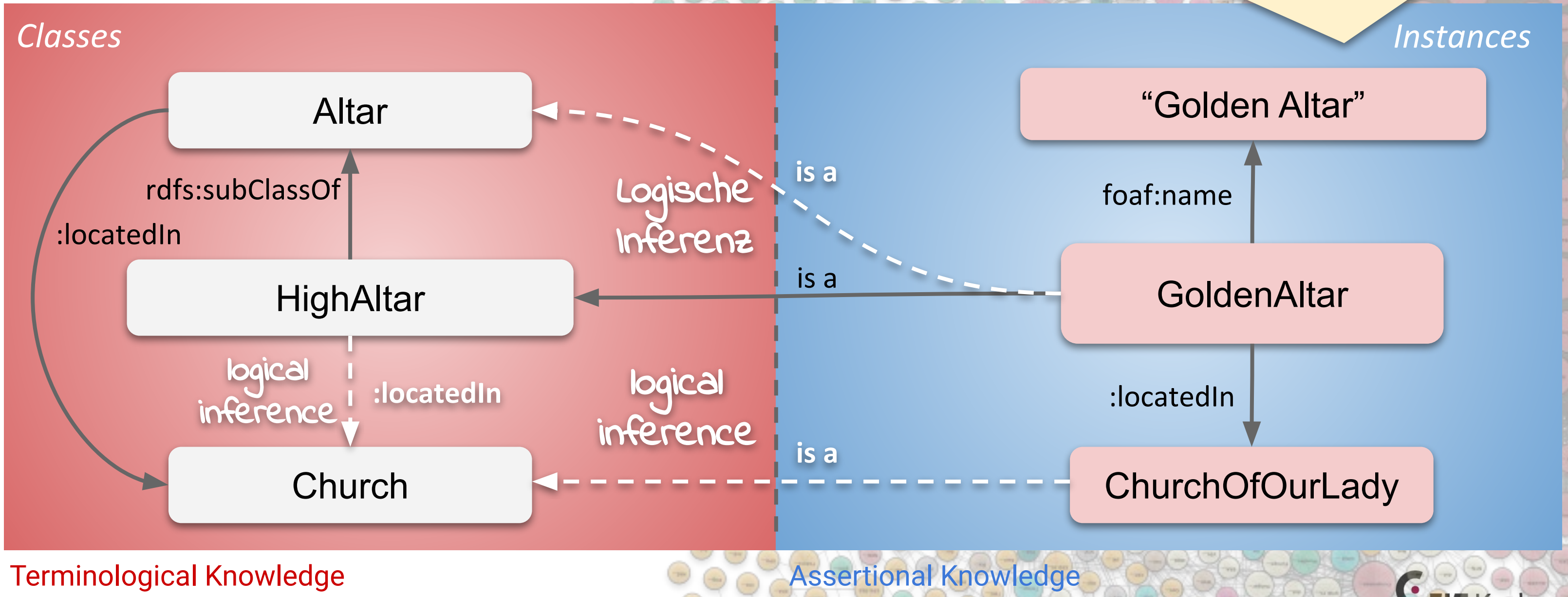
From Ontology to Knowledge Graphs



From Ontology to Knowledge Graphs

Encoded via **RDF**:

```
:GoldenAltar foaf:name   "Golden Altar" .
:GoldenAltar :locatedIn dbr:ChurchOfOurLady .
:GoldenAltar rdf:type    :HighAltar .
```



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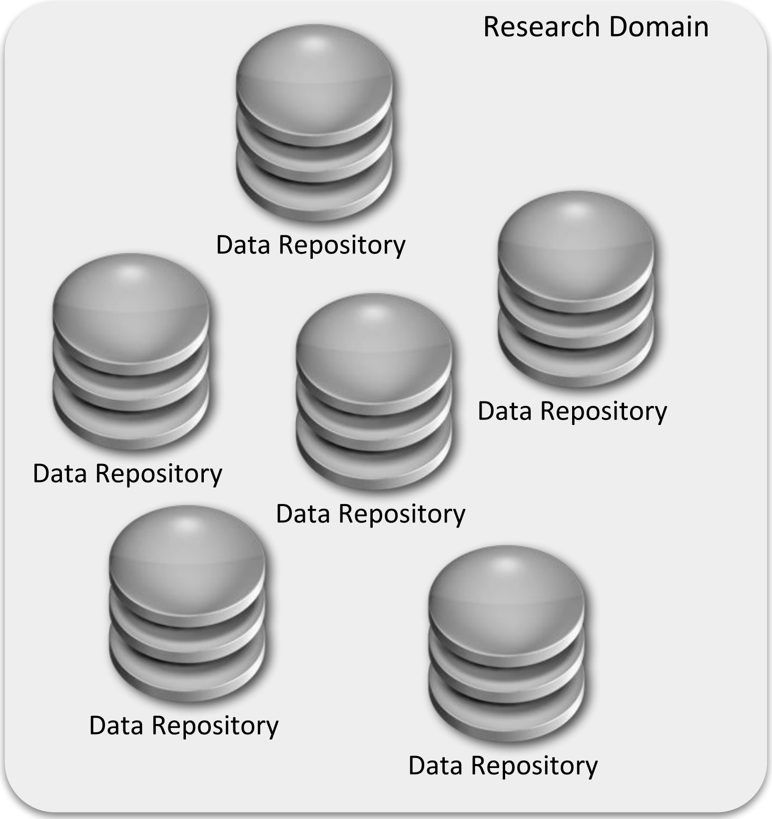
Research Data Management

without Ontologies and Knowledge Graphs



- Research Data is locked up in s**mall data islands**
- Access only via **proprietary APIs**
- Without prior knowledge specific **Research Data is difficult to find**
- **Cross connections** between Data Repositories are **next to impossible**
- **FAIR principles** are only **hard to implement**

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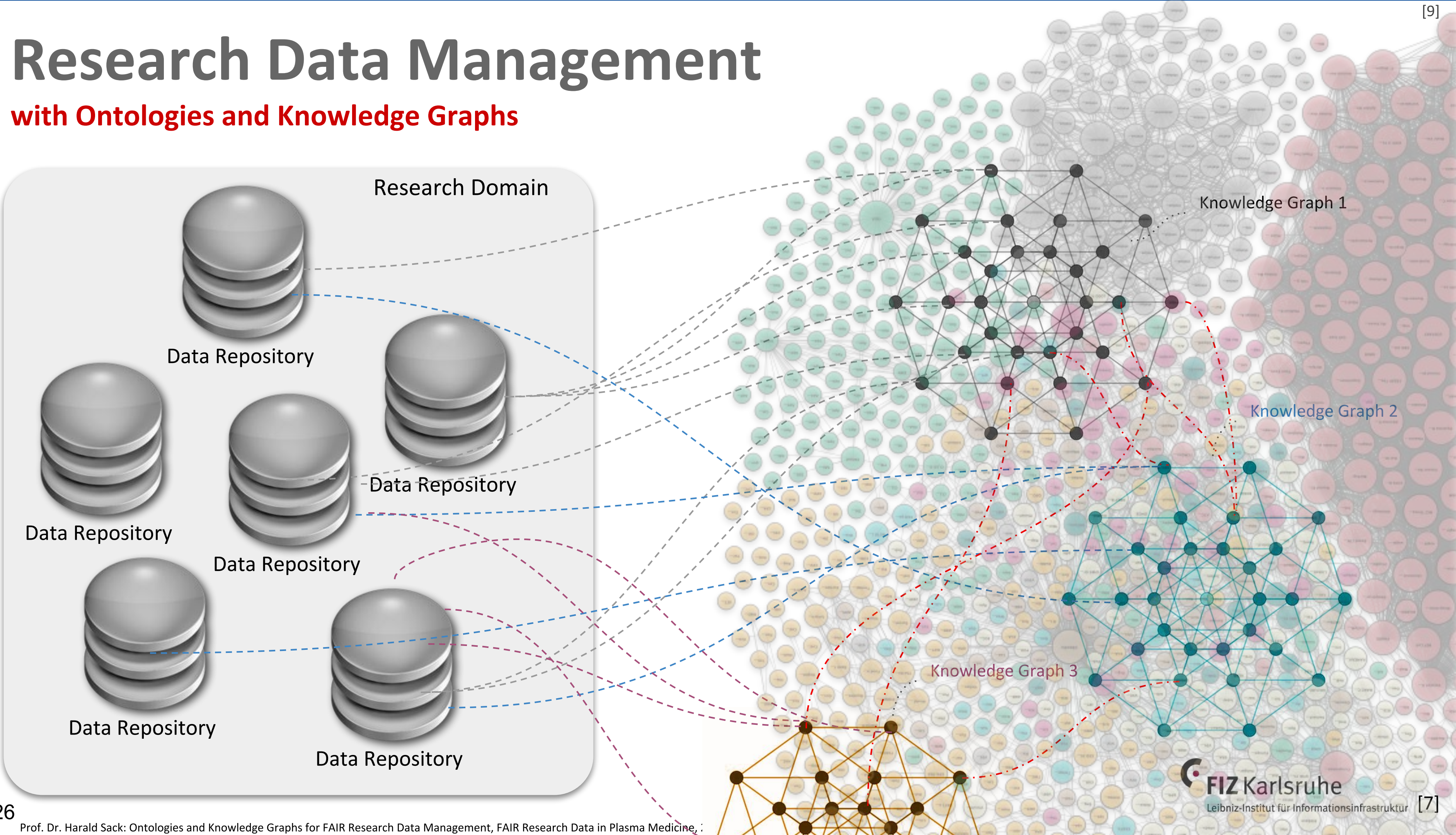
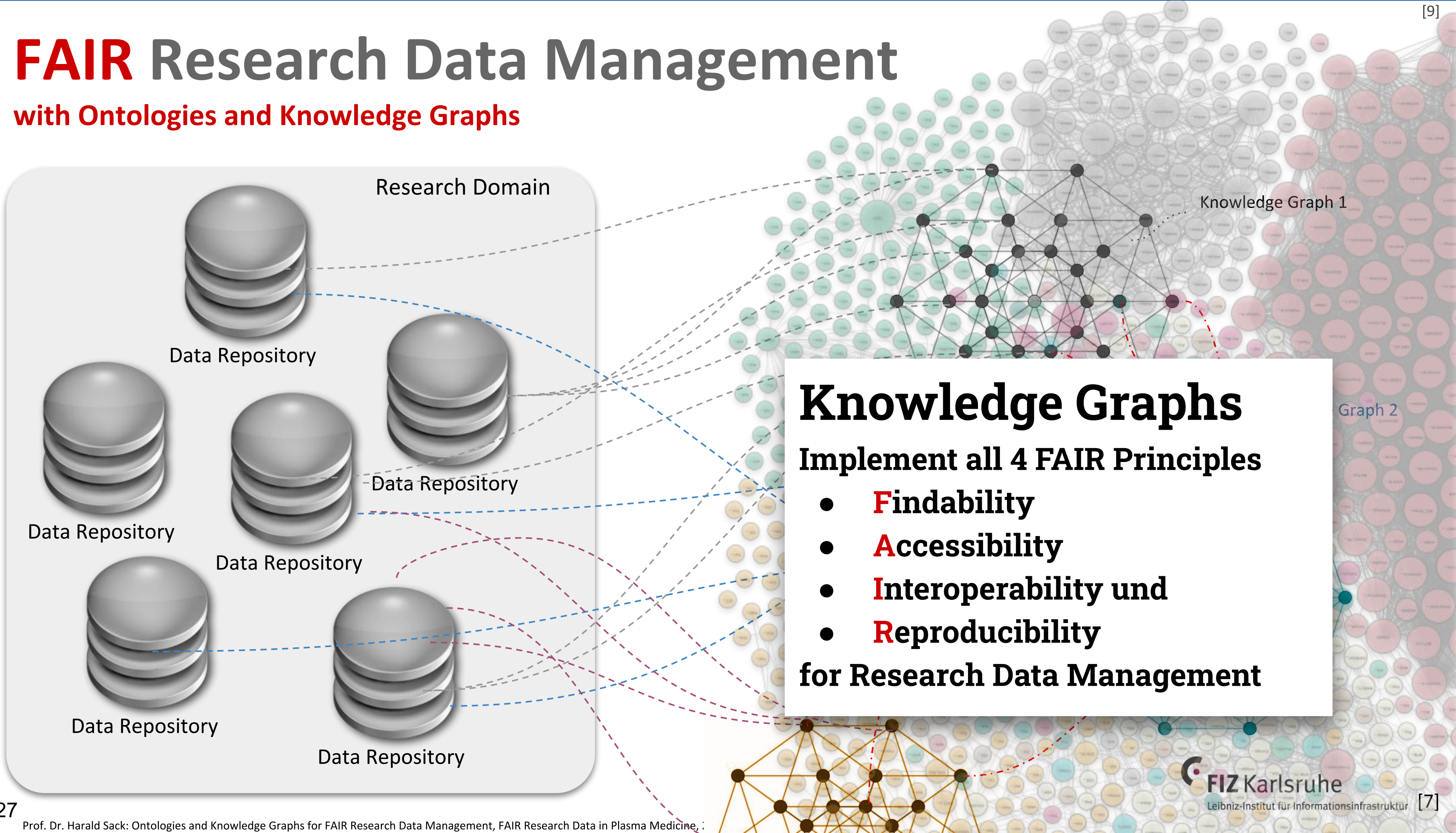
Research Data Management

with Ontologies and Knowledge Graphs



FAIR Research Data Management

with Ontologies and Knowledge Graphs



Knowledge Graphs

Implement all 4 FAIR Principles

- **Findability**
- **Accessibility**
- **Interoperability und**
- **Reproducibility**

for Research Data Management

But how to Begin...?

Caspar David Friedrich, Wanderer über dem Nebelmeer, 1818 [10]

[7]

Ontology Types and Categories

according to their level of Generality

general, cross domain ontologies; represent very general concepts as e.g., Time, Space, Event; independent of a specific domain or problem

Top-Level Ontology (Upper Ontology, Foundation Ontology)

Domain Ontology

fundamental concepts according to a generic domain; specializes terms introduced in top-level ontology

Task Ontology

fundamental concepts according to a general activity or task; specializes terms introduced in top-level ontology

Application Ontology

specialized ontology focussed on a specific task and domain; often a specialization of both task and domain ontology; often specify roles played by domain entities for specific activity

(according to Guarino: Formal Ontology in Information Systems, 1998)

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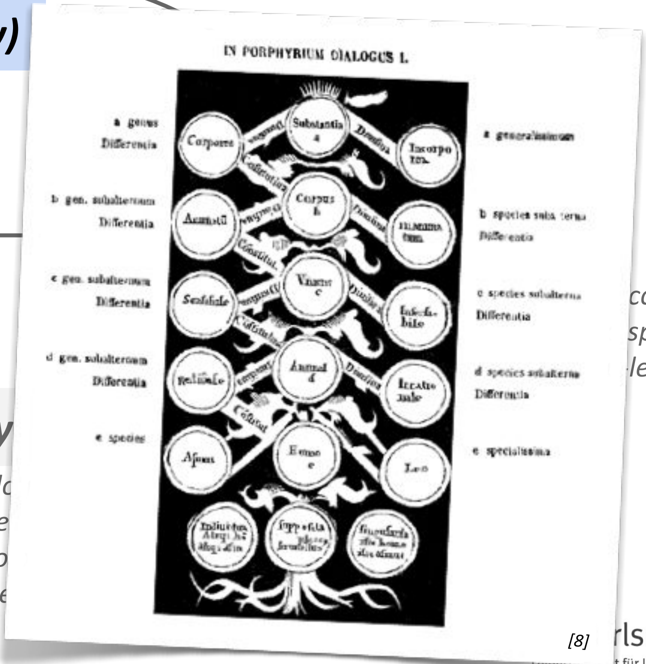

[8]

(according to Guarino: Formal Ontology in Information Systems, 1998)

[11]

Ontology Types and Categories

according to their level of Generality

Top-
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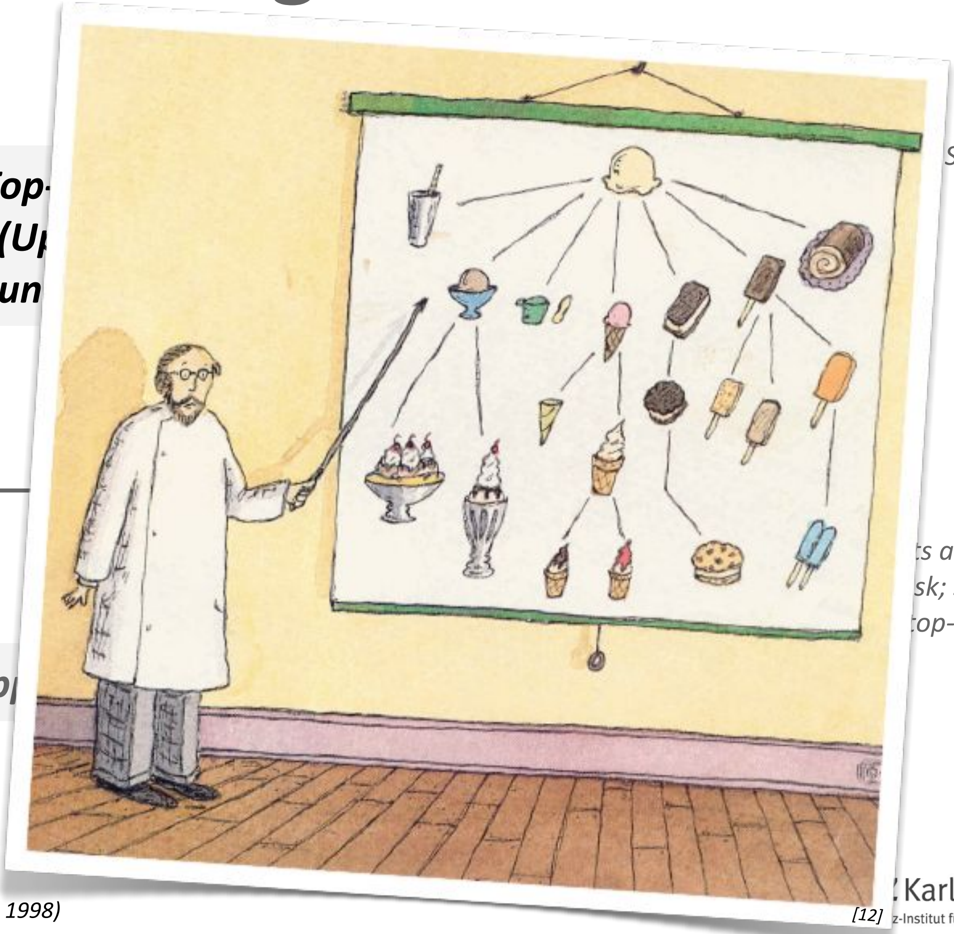
Space, Event;



Domain Ontology

*fundamental concepts according to a **generic domain**; specializes terms introduced in top-level ontology*

ts according to a
sk; specializes
top-level ontology

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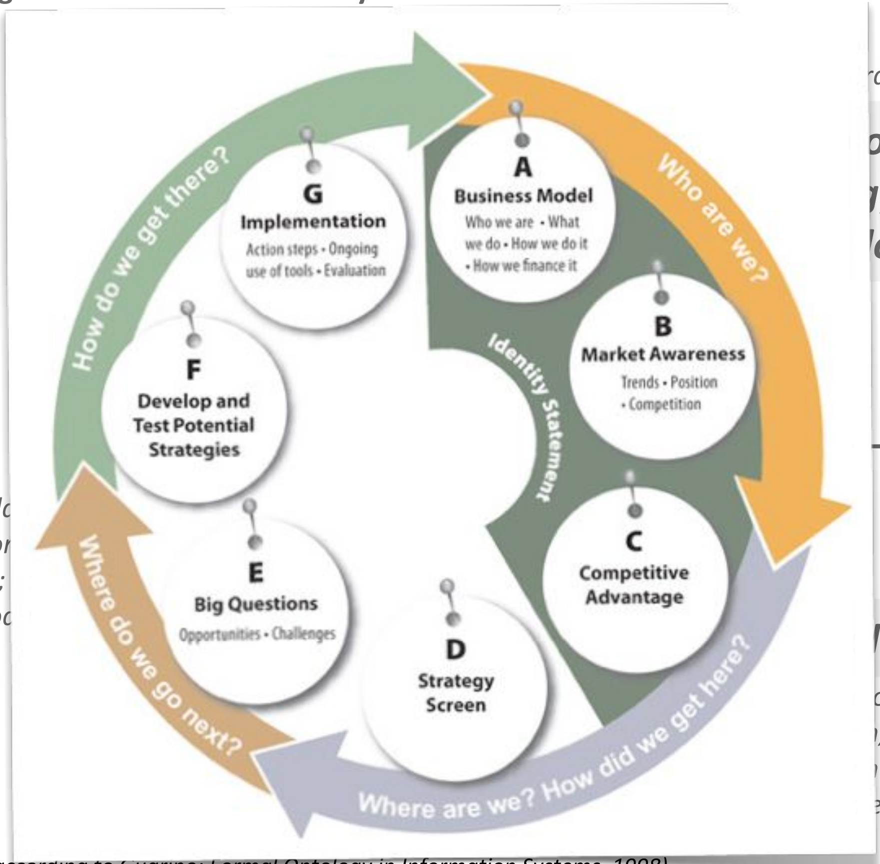
[12]

(according to Guarino: Formal Ontology in Information Systems, 1998)

Ontology Types and Categories

according to their level of Generality



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Ontology Types and Categor

according to their level of Generality

general, cross

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a

logy

[13]

(according to Guarino: Formal Ontology in Information Systems, 1998)

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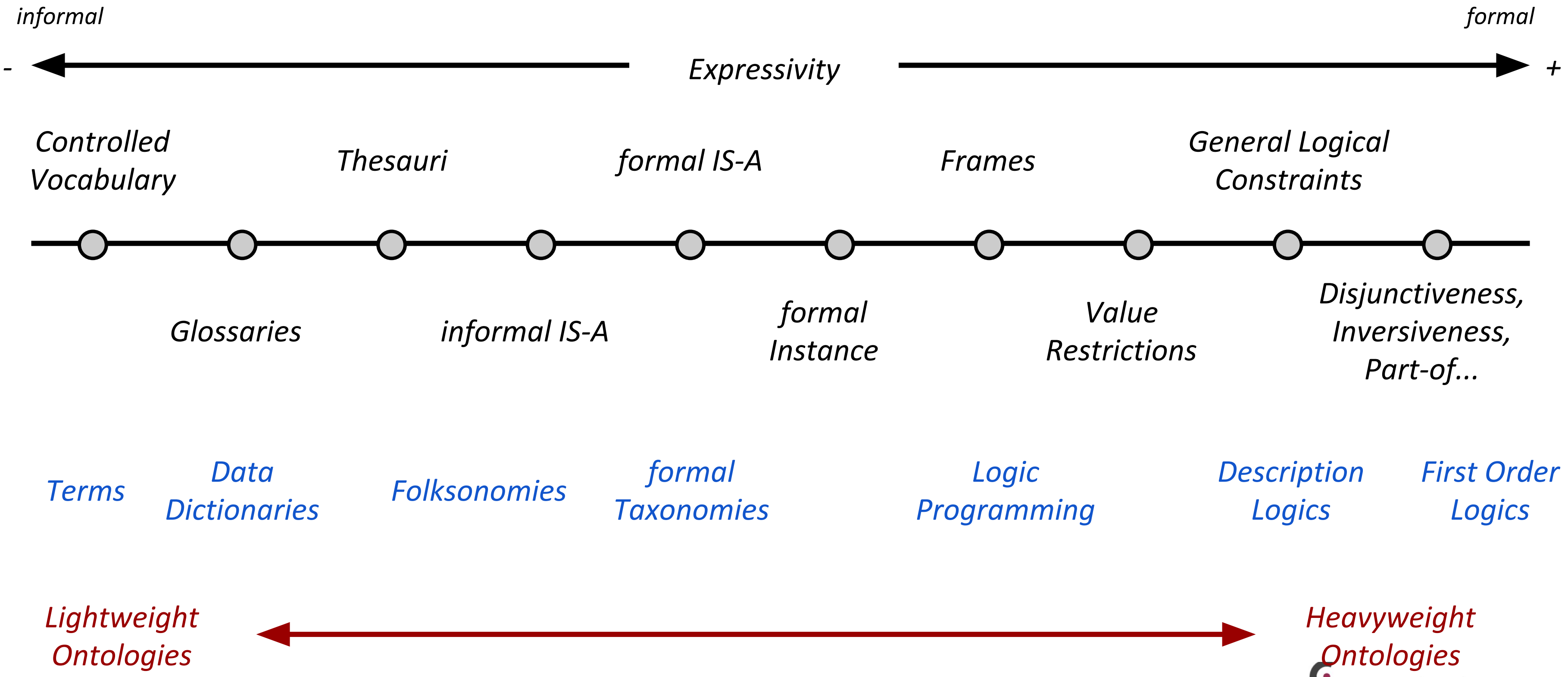
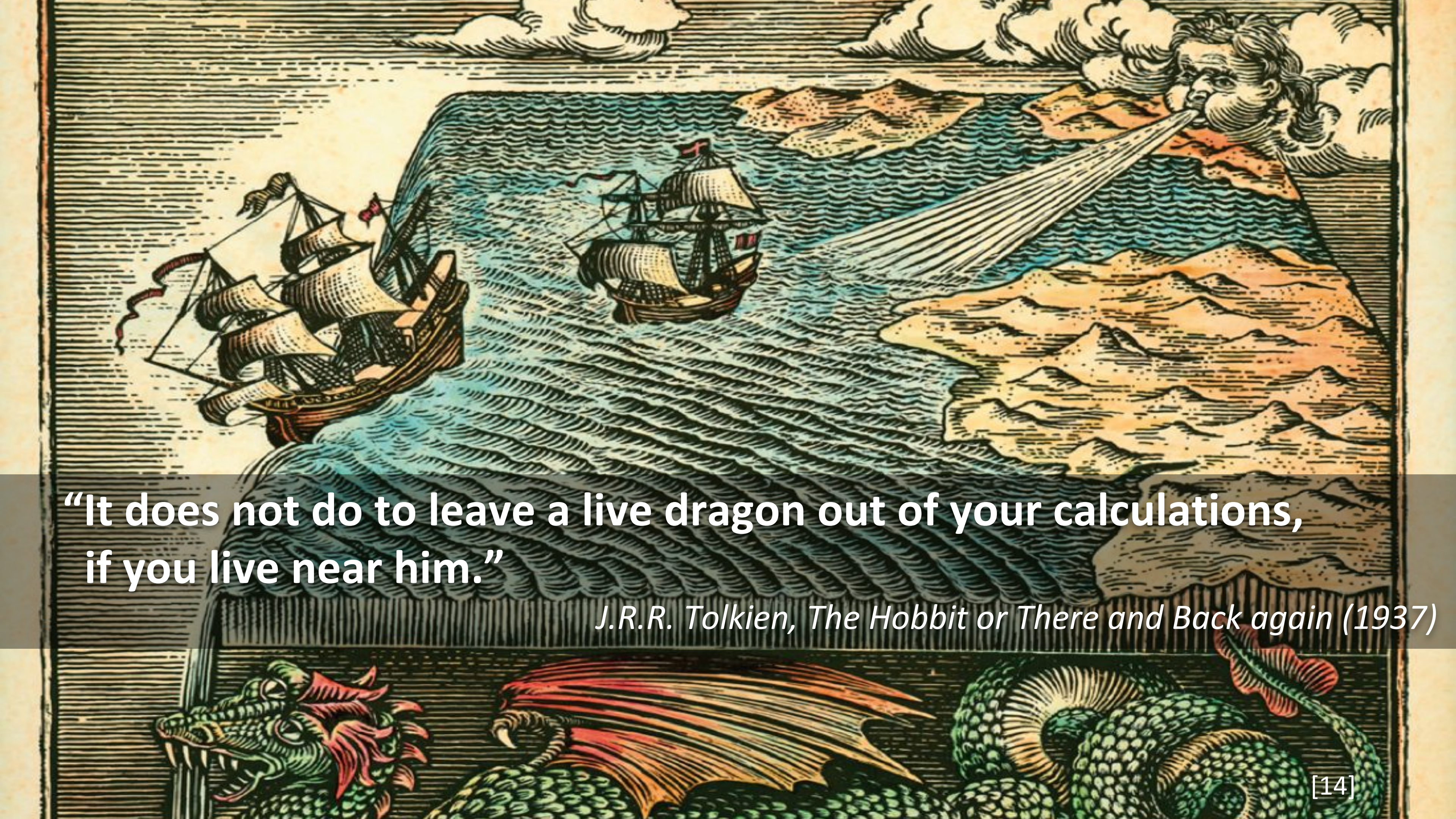
Ontology Types and Categories

according to their level of Semantic Expressivity



(according to Guarino: Formal Ontology in Information Systems, 1998)

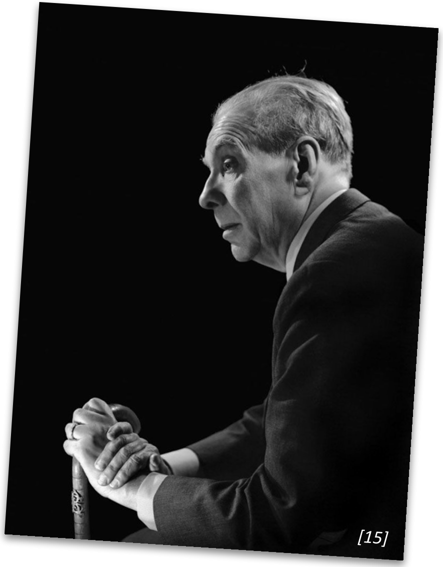
(according to Lassila and McGuiness:The Role of Frame-Based Representation on the Semantic Web, 2001


"It does not do to leave a live dragon out of your calculations,
if you live near him."
J.R.R. Tolkien, The Hobbit or There and Back again (1937)
[14]

Ontologies as Interpretations of Reality

*Various **categories of animals** from "a certain Chinese encyclopedia"* according to Jorge Luis Borges:

- Those that belong to the emperor
- Embalmed ones
- Those that are trained
- Suckling pigs
- Mermaids (or Sirens)
- Fabulous ones
- Stray dogs
- Those that are included in this classification
- Those that tremble as if they were mad
- Innumerable ones
- Those drawn with a very fine camel hair brush
- Et cetera
- Those that have just broken the flower vase
- Those that, at a distance, resemble flies



Jorge Luis Borges
(1899-1986)

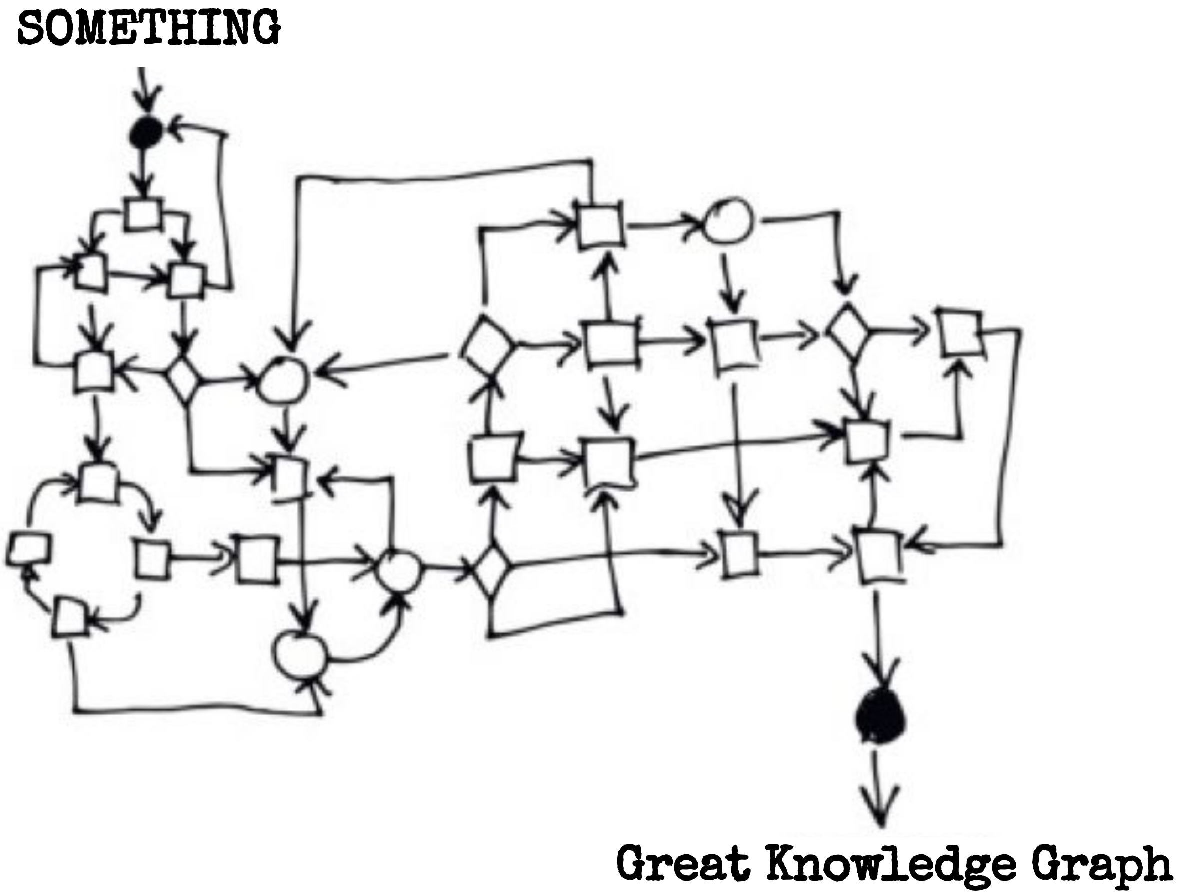
Jorge Luis Borges: The Analytical Language of John Wilkins (1942)

Follow an Approved Methodology

Niles, John Jacob, An Early Flying Machine, c. 1908, University of Kentucky

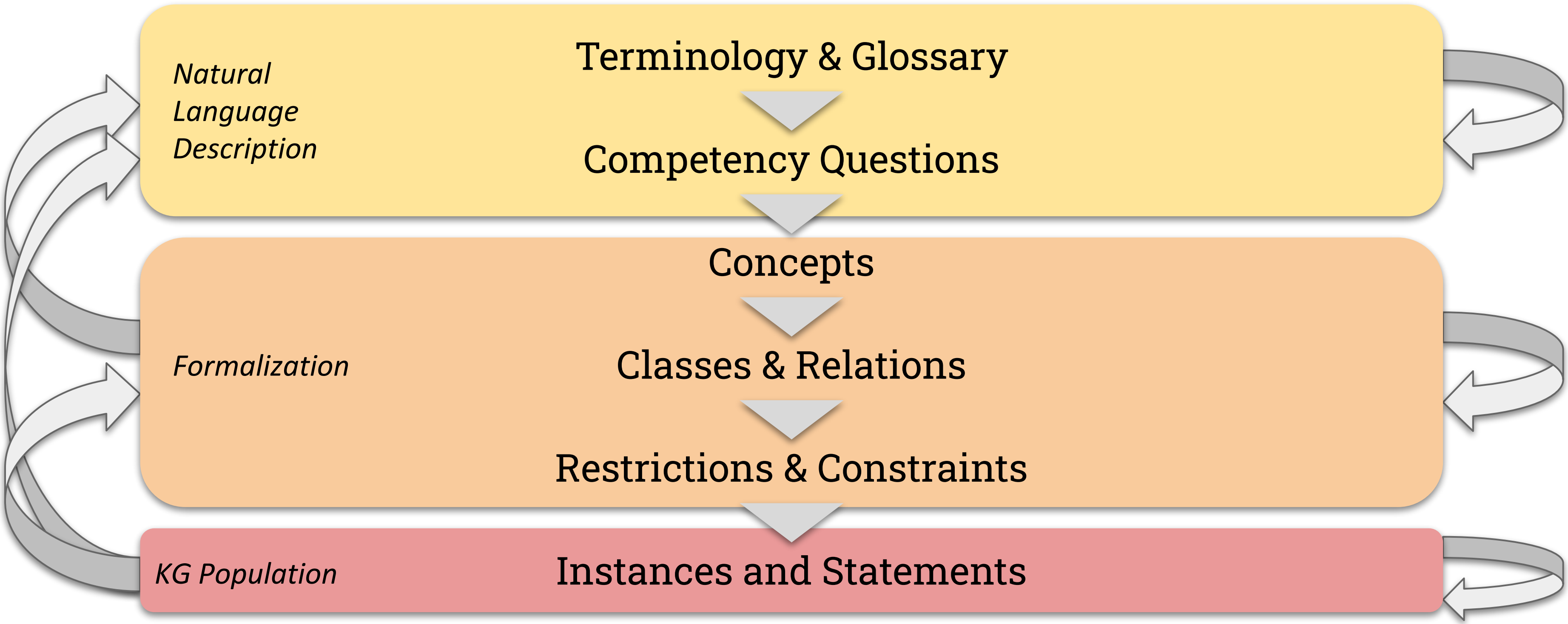
[16]

Follow an Approved Methodology



[17]

Follow an Approved Methodology



Ontologies and Knowledge Graphs for Research Data Management

(1) (Raw) Research Data

z/d [1]	Ion density (PIC-ITAP) [10^15 m^(-3)]	Ion density (PIC-INP) [10^15 m^(-3)]
0.0000000e+00	2.1538249e-01	2.2127591e-01
1.0000000e-02	2.2320410e-01	2.2851489e-01
2.0000000e-02	2.3078706e-01	2.3700471e-01
3.0000000e-02	2.3957809e-01	2.4612475e-01
4.0000000e-02	2.4898703e-01	2.5569295e-01
5.0000000e-02	2.5889461e-01	2.6656408e-01
6.0000000e-02	2.7120663e-01	2.7901766e-01
7.0000000e-02	2.8447237e-01	2.9209201e-01
8.0000000e-02	2.9853002e-01	3.0861118e-01
9.0000000e-02	3.1697947e-01	3.2641678e-01
1.0000000e-01	3.3656863e-01	3.4837557e-01
1.1000000e-01	3.6049250e-01	3.7427430e-01
1.2000000e-01	3.8862354e-01	4.0343478e-01
1.3000000e-01	4.2297845e-01	4.3891770e-01
1.4000000e-01	4.6555629e-01	4.8310615e-01
1.5000000e-01	5.1581989e-01	5.3864561e-01
1.6000000e-01	5.7837521e-01	6.0616555e-01
1.7000000e-01	6.4984874e-01	6.8350098e-01
1.8000000e-01	7.3012722e-01	7.6446633e-01
1.9000000e-01	8.1671138e-01	8.5748202e-01
2.0000000e-01	9.0375181e-01	9.4726775e-01

Ontologies and Knowledge Graphs for Research Data Management

(1) (Raw) Research Data

(2) Schema Information

Fields +

- z/d [1] string »
- Ion density (PIC-ITAP) [10^15 m^(-3)] string »
- Ion density (PIC-INP) [10^15 m^(-3)] string »
- Ion density (Fluid-DDAn) [10^15 m^(-3)] string »
- Ion density (Fluid-DDA53) [10^15 m^(-3)] string »

Benchmark data for fluid modelling of low-pressure CCRF discharge plasmas

Plasma Chemical Processes

The dataset contains data from comparative studies of capacitively coupled radio-frequency (CCRF) discharges in helium and argon at pressures between 10 and 80 Pa applying two different fluid modeling approaches as well as two independently developed particle-in-cell Monte Carlo collision (PIC-MCC) codes. The dataset provides a test bed for future studies of simple ccrf discharge configurations in helium and argon at pressures ranging from 10 to 80 Pa.

plasma modelling/simulation | benchmark data

structured information | **unstructured information**

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Ontologies and Knowledge Graphs for Research Data Management

(1) (Raw) Research Data
(2) Schema Information
(3) Metadata

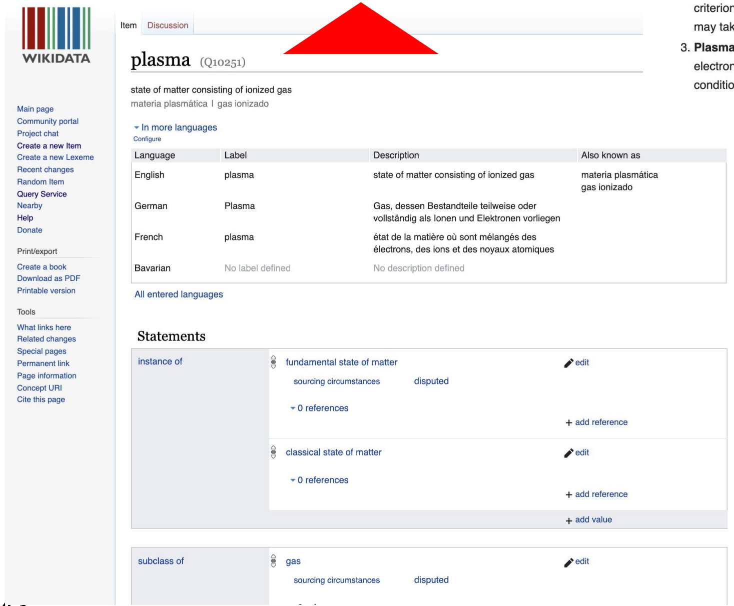
structured
+
unstructured
information

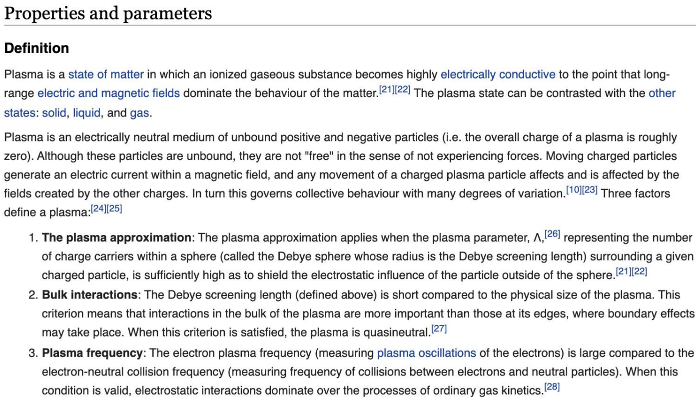
Field	Value
Group	Plasma Modelling
Authors	Becker, Markus M. Kählert, Hanno Sun, Anbang Loffhagen, Detlef
Release Date	2019-06-14
Resources	Benchmark data for CCRF discharge plasmas - time averaged ion density (argon, 20 Pa) Benchmark data for CCRF discharge plasmas - time averaged ion density (argon, 40 Pa) Benchmark data for CCRF discharge plasmas - time averaged ion density (argon, 80 Pa) Benchmark data for CCRF discharge plasmas - time averaged ion density (helium, 10 Pa) Benchmark data for CCRF discharge plasmas - time averaged ion density (helium, 20 Pa) Benchmark data for CCRF discharge plasmas - time averaged ion density (helium, 40 Pa) Show more Benchmark data for CCRF discharge plasmas - time averaged ion density (helium, 80 Pa)
Identifier	60dbcdd4-8be4-4f41-896c-e725bdb37fe2
Permanent Identifier (DOI)	doi:10.34711/inptdat.72
Permanent Identifier (URI)	https://www.inptdat.de/node/72
Is supplementing	M. M. Becker et al., Plasma Sources Sci. Technol. 26 (2017) 044001
Plasma Source Name	CCP
Plasma Source Specification	AC high frequency low pressure non-thermal
Plasma Source Properties	Low-pressure RF plasma between plane electrodes separated by the distance d, driven by a sinusoidal voltage with amplitude V0 and frequency f; d = 2.5 cm (argon) resp. 6.7 cm (helium); V0 = 50-250 V; f = 13.56 MHz; Current density: 10 A/m^2

Ontologies and Knowledge Graphs for Research Data Management

(1) (Raw) Research Data
(2) Schema Information
(3) Metadata
(4) External Resources

semantic information





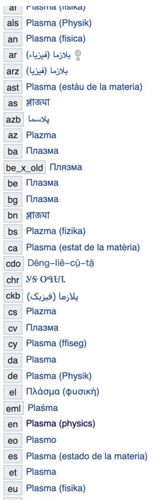
Properties and parameters

Definition

Plasma is a state of matter in which an ionized gaseous substance becomes highly electrically conductive to the point that long-range electric and magnetic fields dominate the behaviour of the matter.[21][22] The plasma state can be contrasted with the other states: solid, liquid, and gas.

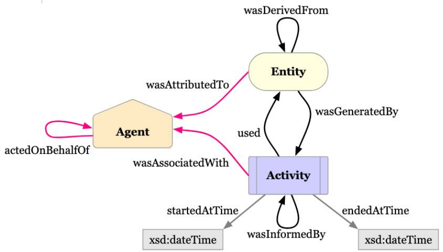
Plasma is an electrically neutral medium of unbound positive and negative particles (i.e. the overall charge of a plasma is roughly zero). Although these particles are unbound, they are not "free" in the sense of not experiencing forces. Moving charged particles generate an electric current within a magnetic field, and any movement of a charged plasma particle affects and is affected by the fields created by the other charges. In turn this governs collective behaviour with many degrees of variation.[10][23] Three factors define a plasma:[24][25]

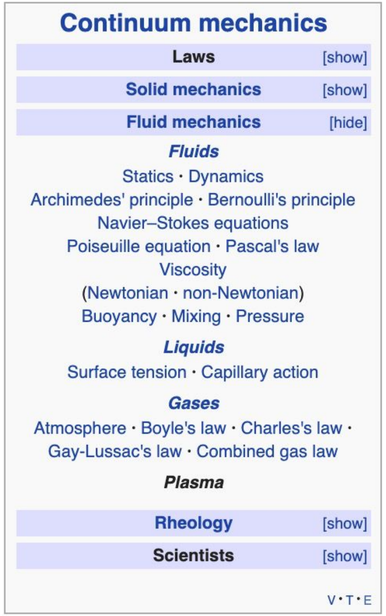
1. **The plasma approximation**: The plasma approximation applies when the plasma parameter, Λ,[26] representing the number of charge carriers within a sphere (called the Debye sphere whose radius is the Debye screening length) surrounding a given charged particle, is sufficiently high as to shield the electrostatic influence of the particle outside of the sphere.[21][22]
2. **Bulk interactions**: The Debye screening length (defined above) is short compared to the physical size of the plasma. This criterion means that interactions in the bulk of the plasma are more important than those at its edges, where boundary effects may take place. When this criterion is satisfied, the plasma is quasineutral.[27]
3. **Plasma frequency**: The electron plasma frequency (measuring plasma oscillations of the electrons) is large compared to the electron-neutral collision frequency (measuring frequency of collisions between electrons and neutral particles). When this condition is valid, electrostatic interactions dominate over the processes of ordinary gas kinetics.[28]



unstructured information

semantic information





structured information

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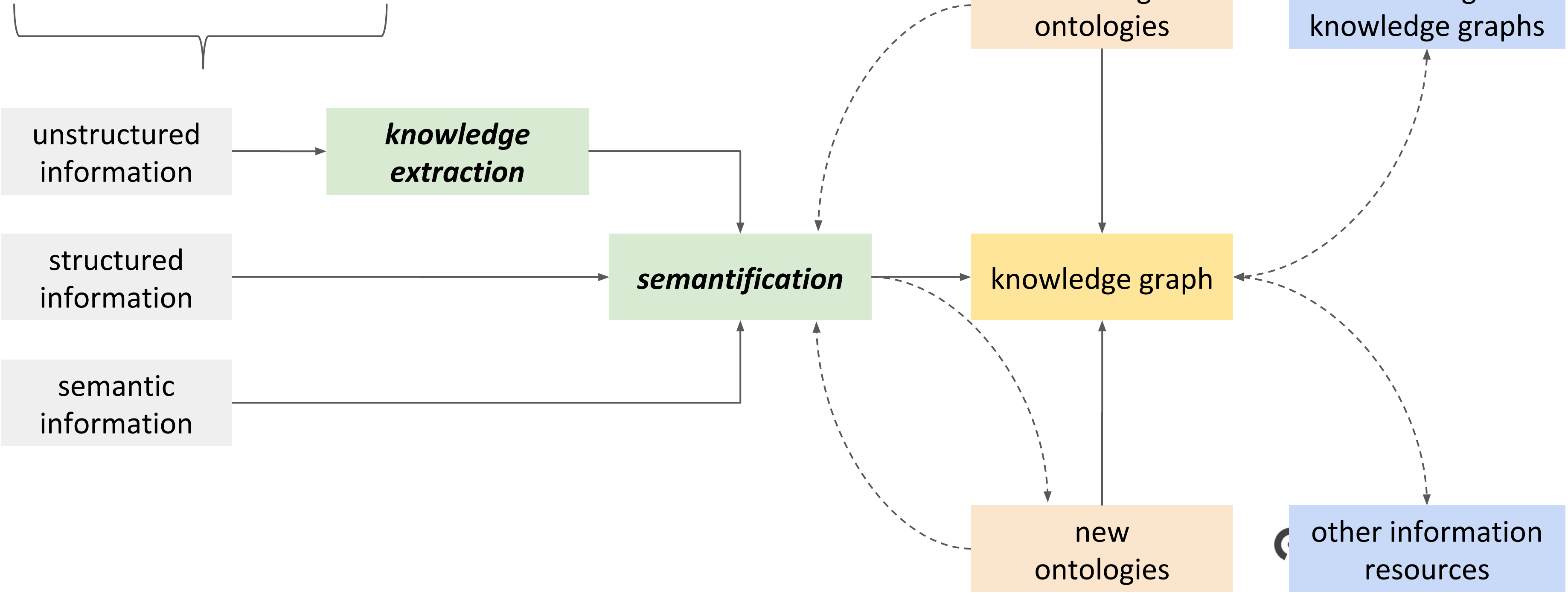
Ontologies and Knowledge Graphs for Research Data Management

(1) (Raw) Research Data
(2) Schema Information
(3) Metadata
(4) External Ressources

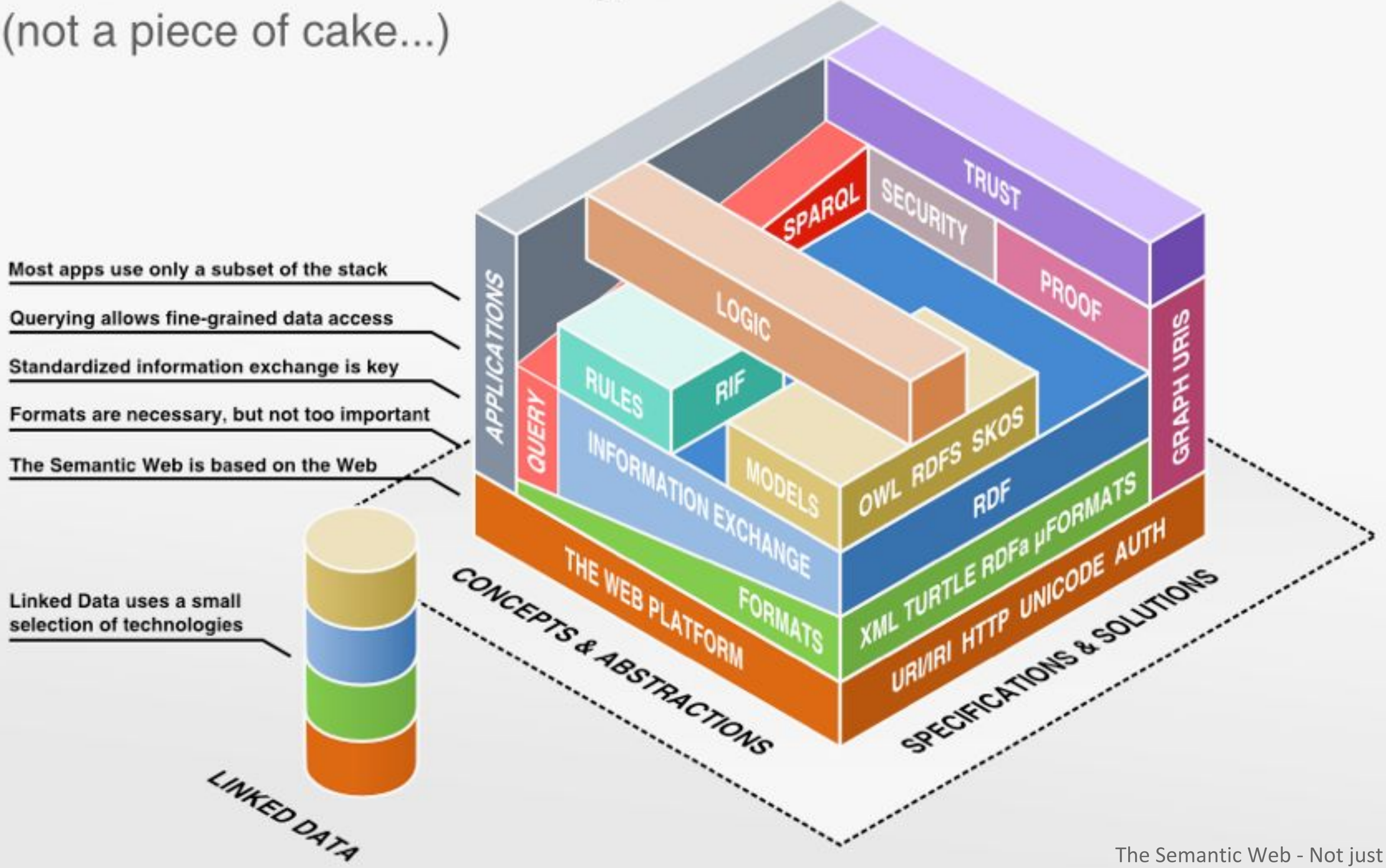


The Liberty Statue, work in progress, 1884 [18]

“Though this be madness, yet there is method in it”

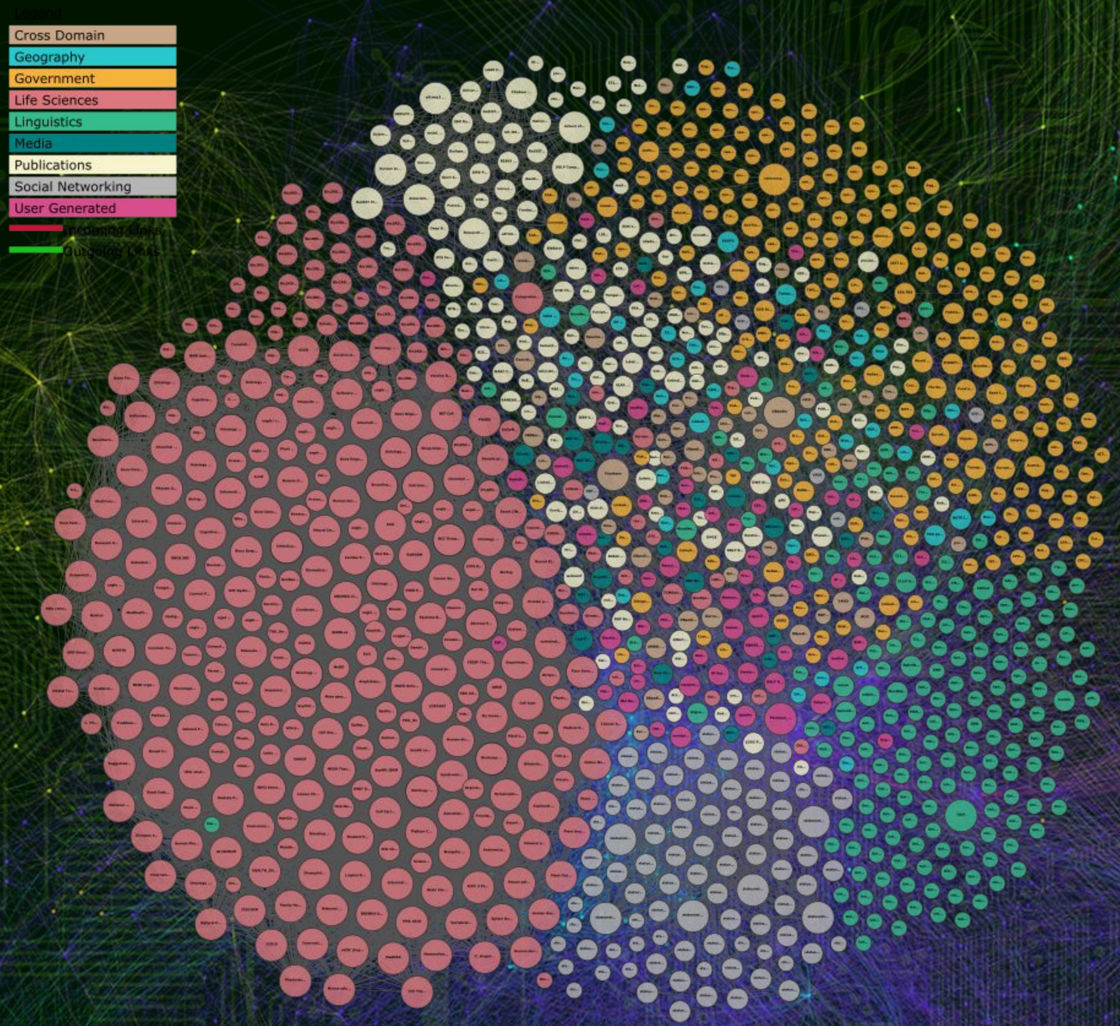
William Shakespeare, Hamlet (1602)

The Semantic Web Technology Stack
(not a piece of cake...)



The Semantic Web - Not just a piece of cake, [16]

Linked Data and Knowledge Graphs



The Linked Data Cloud, 2019 [9]

Semantic Search & Retrieval

Ontology & Knowledge Graph Applications

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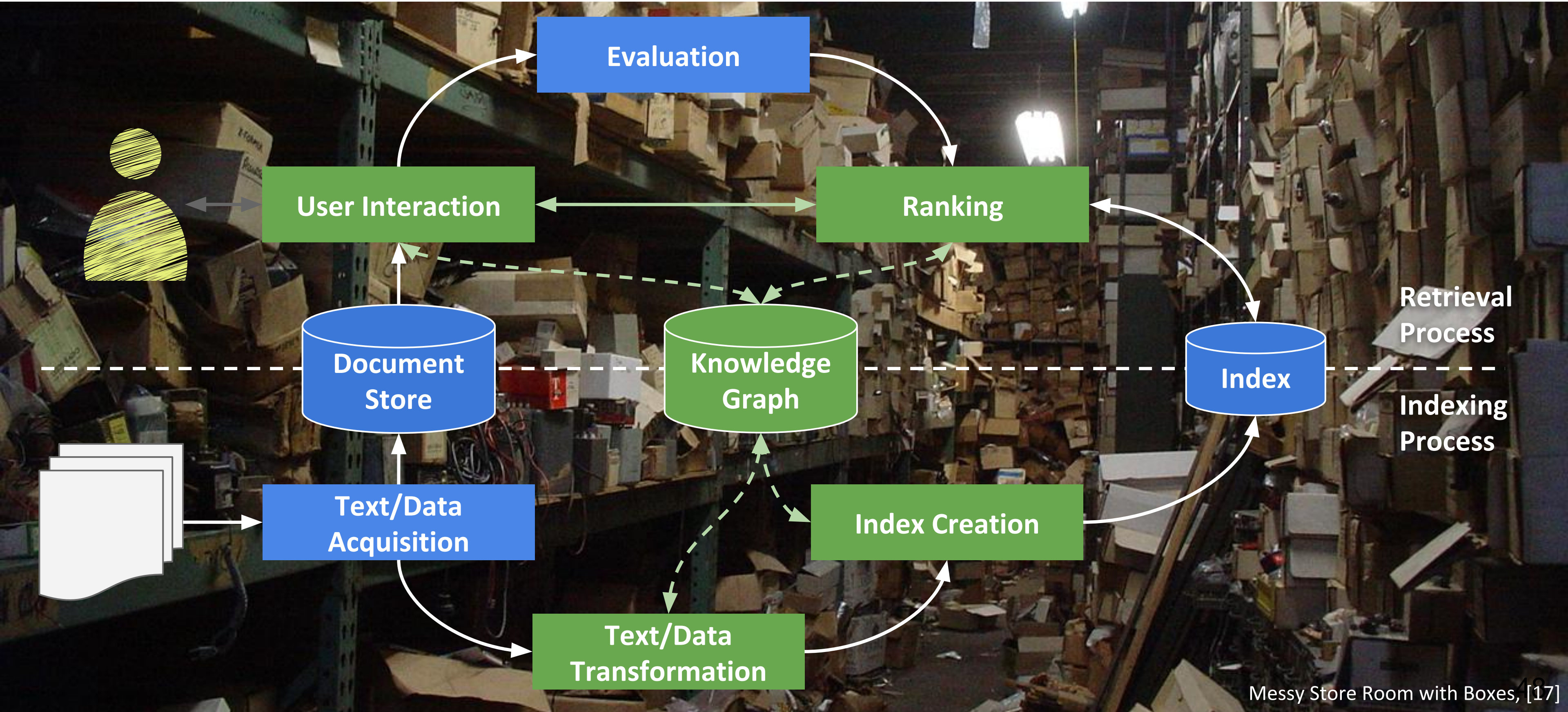
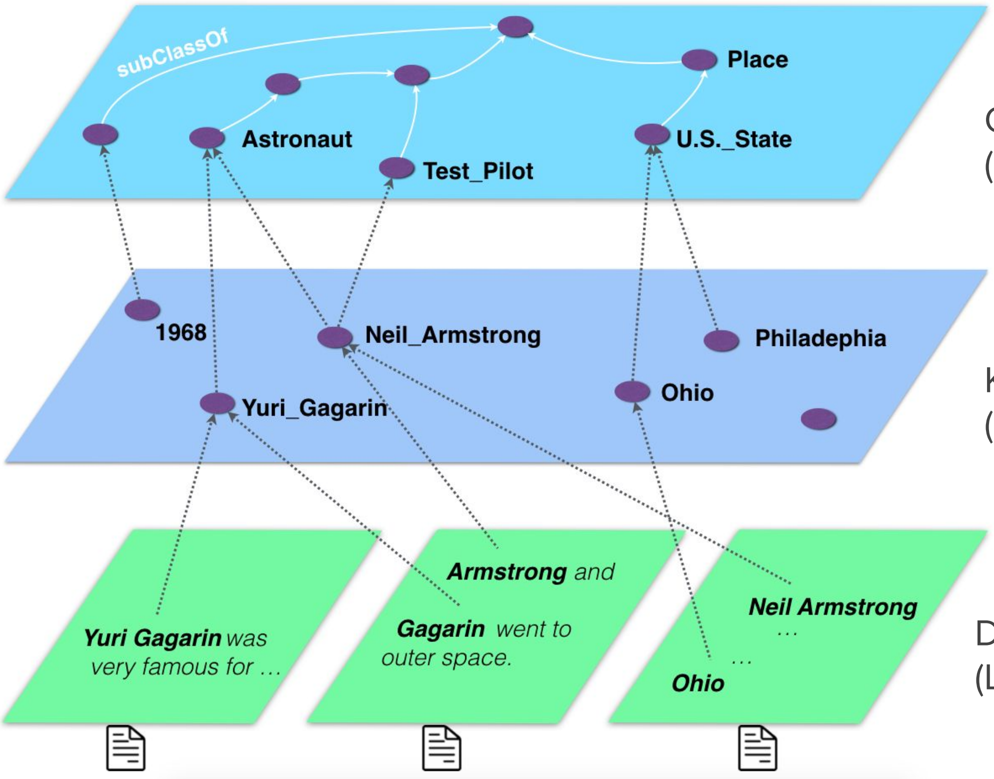


Messy Store Room with Boxes, [17]

Semantic Search & Retrieval

Ontology & Knowledge Graph Applications



Ontology
(Classes & Relations)

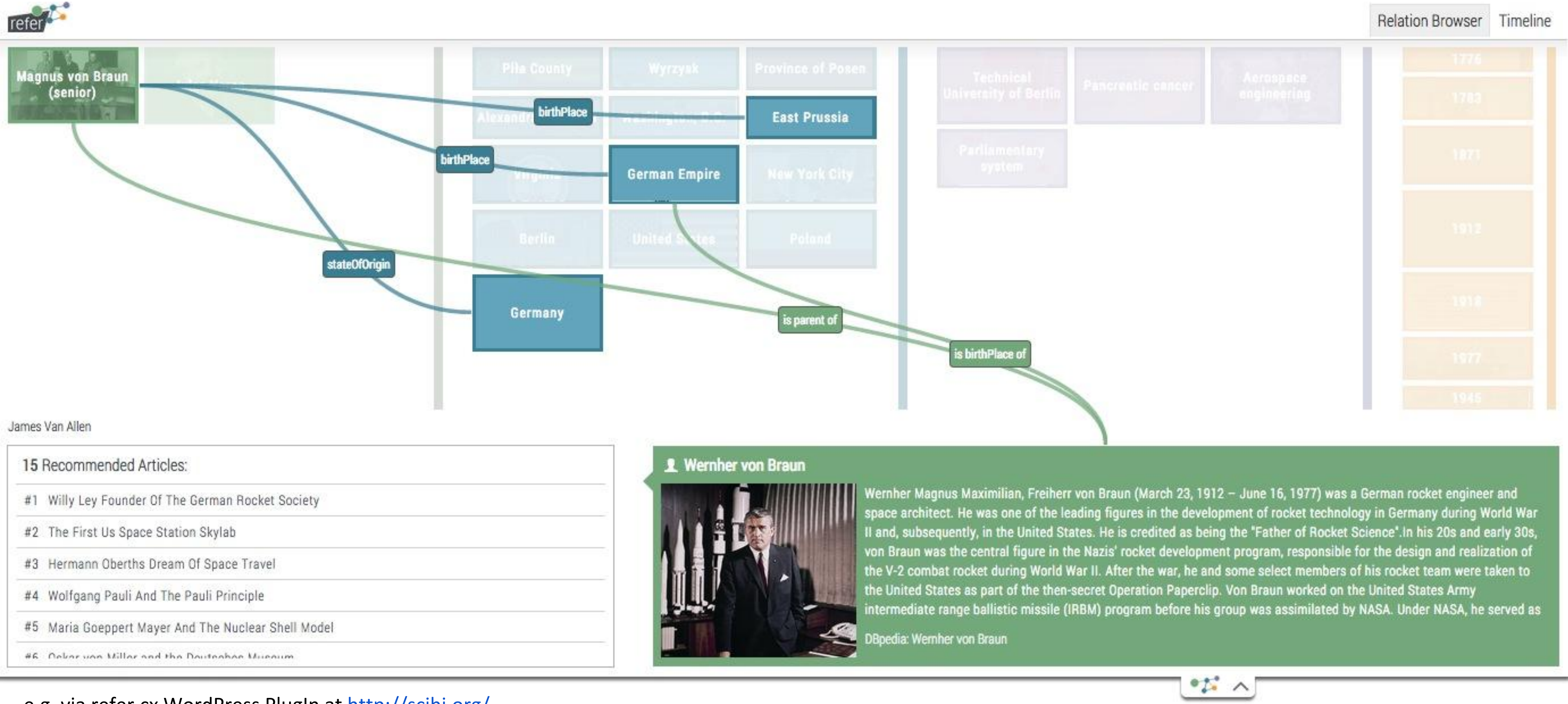
Knowledge Graph
(Instances)

Document Text
(Labels)

Jörg Waitelonis, Claudia Exeler, and Harald Sack. **Linked Data enabled Generalized Vector Space Model to improve document retrieval.** In Proc. of NLP & DBpedia 2015 workshop in conjunction with 14th International Semantic Web Conference (ISWC2015), CEUR Workshop Proceedings, Vol1581, pp 33-44, 2015.

Exploration & Recommendation

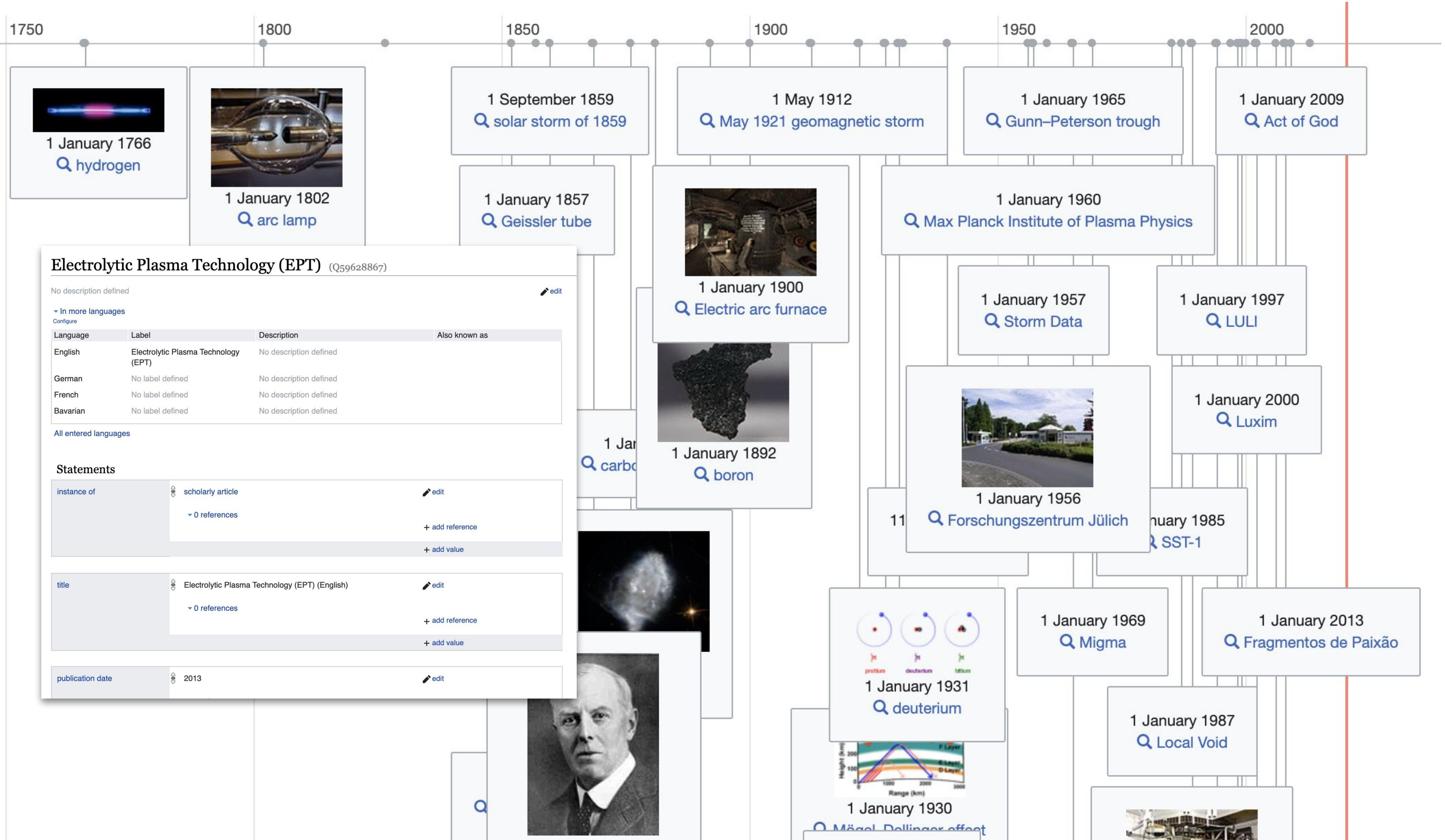
Ontology & Knowledge Graph Applications



e.g. via refer.cx WordPress PlugIn at http://scihi.org/

An Evolving Knowledge Graph

For Plasma Technology



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Ontologies and Knowledge Graphs for
FAIR Research Data Management

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FAIR Research Data in Plasma Medicine
28 October 2020

QPTDat
Quality | Plasma Technology | Data

FIZ Karlsruhe
Leibniz-Institut für Informationsinfrastruktur

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