

Project Kupfer*Digital*2

Enhancing Efficiency and Sustainability of the Copper Life Cycle with Semantic Technology

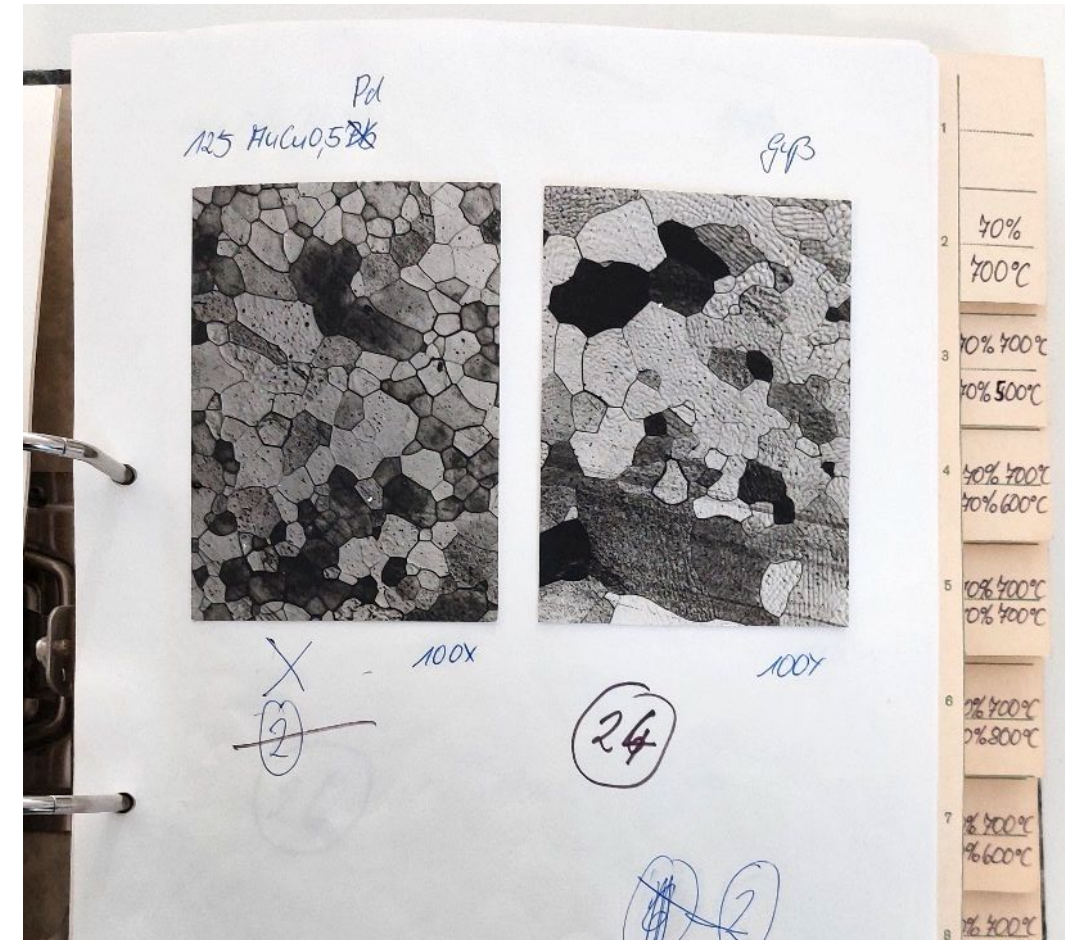
Konstantin Gubaev, Felix Bauer, Miriam Eisenbart
fem Forschungsinstitut

Data Week Leipzig, 03.06.2026

Alloy development data from the past

Analoguous data

- Example of not-FAIR data
- Such experiments have to be repeated if
 - Important information is missing (e.g. metadata)
 - Data is not known to exist / not findable



Historical data
from our archive

Project coordination: Wieland Electric



Consortium



Duration

1.2.2025 – 31.1.2028

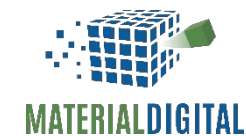
Acknowledgement

The project 13XP5230 is funded by the Federal Ministry of Education and Research as part of the **MaterialDigital** innovation platform.

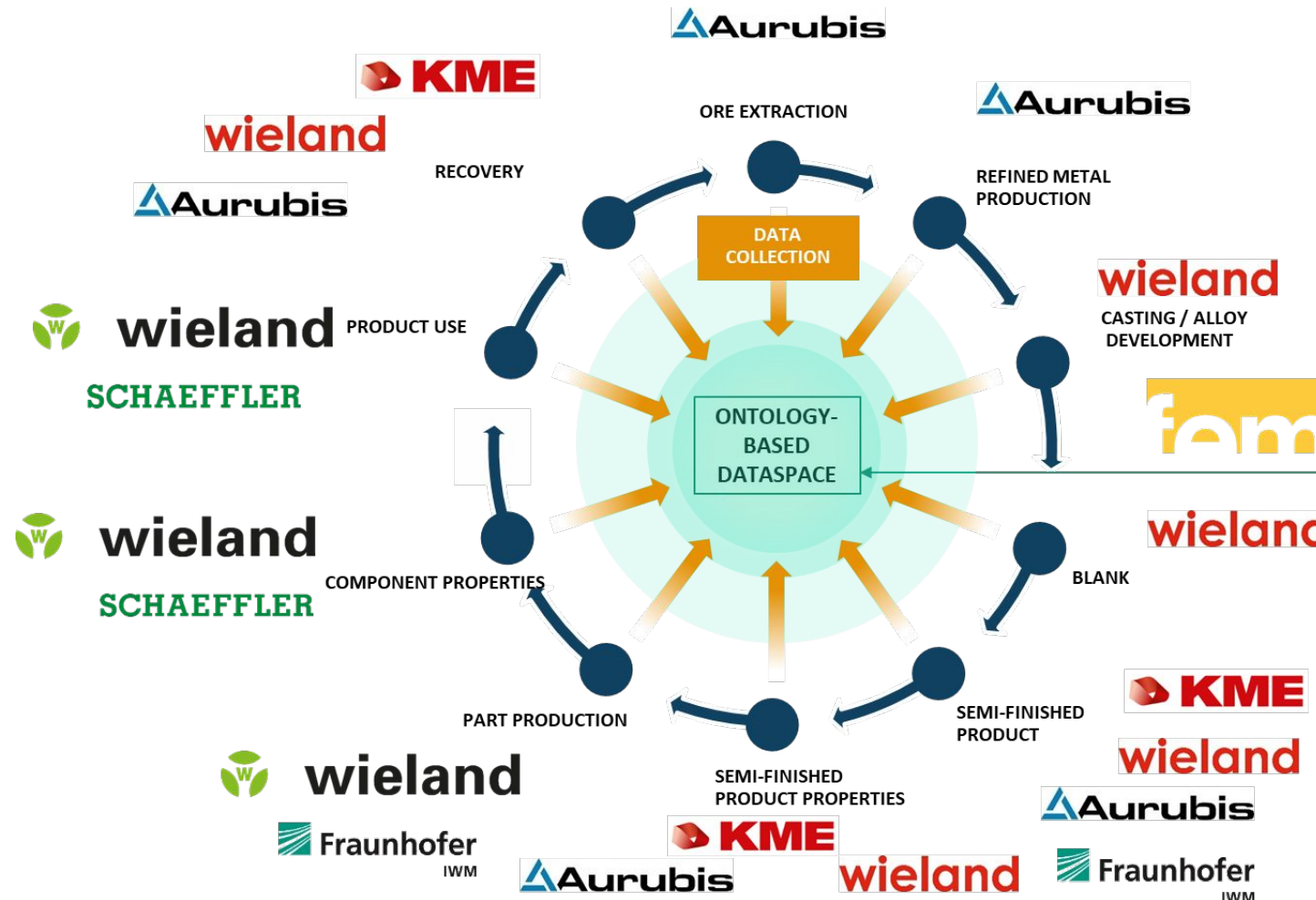
With funding from the:



Platform Material Digital Project



Material data space to increase the efficiency and sustainability of the copper lifecycle



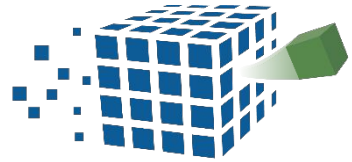
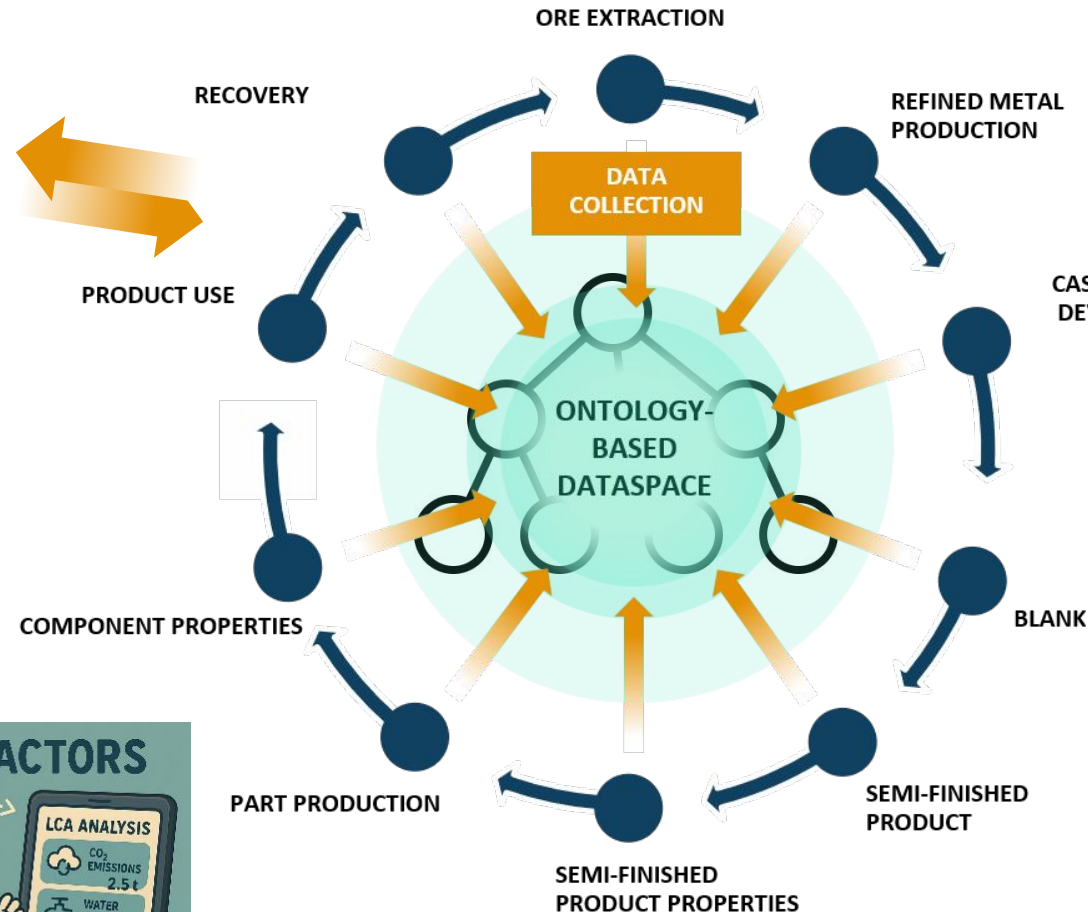
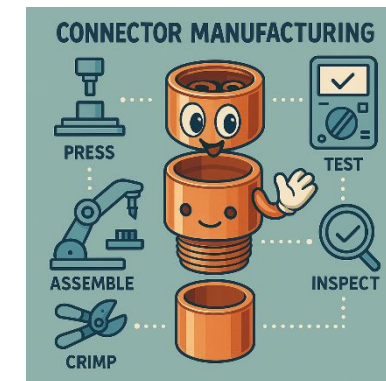
Topics in KupferDigital2



Digital Product Passport



Demonstrator Process Chain



MATERIALDIGITAL

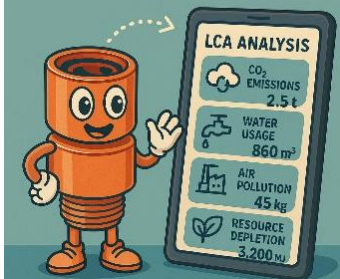


Catena-X
Your Automotive Network

STANDARDIZATION



LCA FACTORS



Background and Experience

Education:

- Master ☐ **theoretical physics**, analytics, simulation
- Doctorate ☐ **atomistic simulations** / machine learning

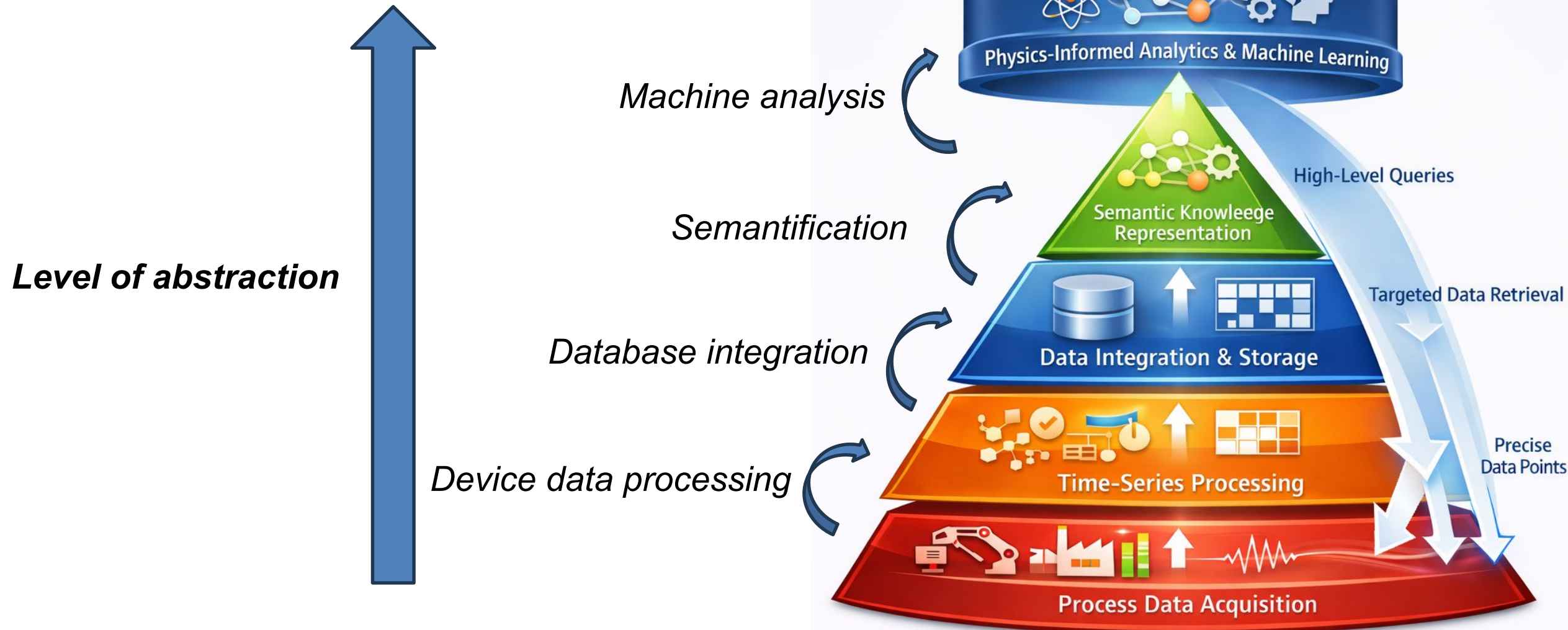
Work:

- TU Delft
 - Uni Stuttgart
 - FIZ Karlsruhe
 - fem Forschungsinstitut
- ☐ **Machine Learning**
- ☐ **Semantics/Ontologies**
- ☐ **AI & Digitalization**
- for **Mat. Sci.**



*Konstantin Gubaev
(Abt. Digitalisierung & KI,
fem Forschungsinstitut)*

Knowledge transformation



Presentation plan: alloy casting ontology



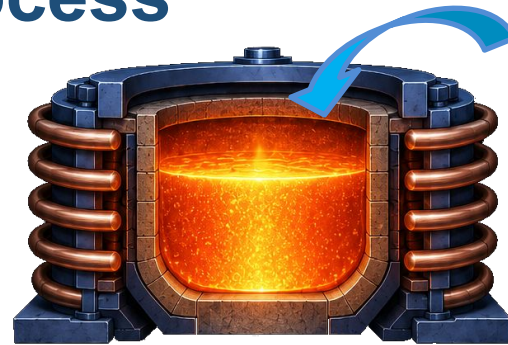
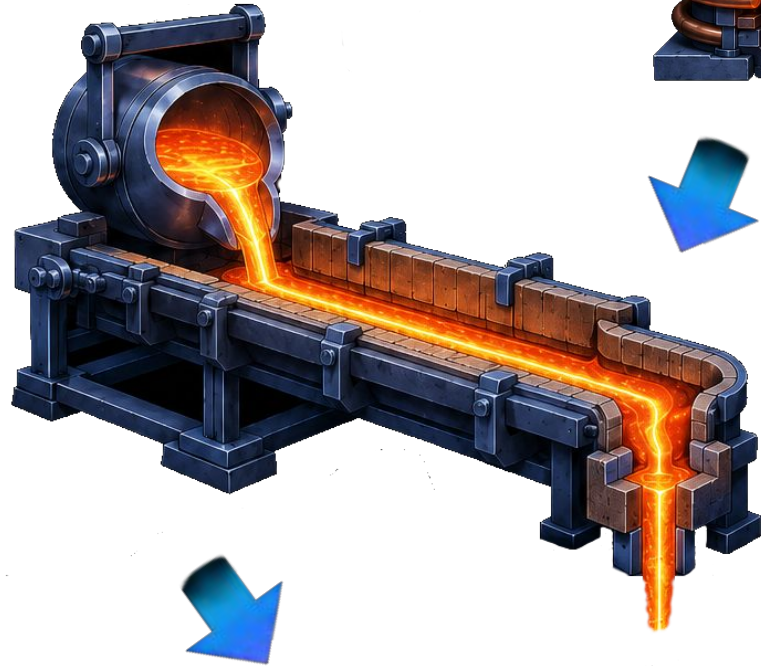
- Casting process overview
- The semantic approach
- LCA integration

BFO
&
PMDco3

alignment

Generic Casting Process

Transporting



Heating + Melting

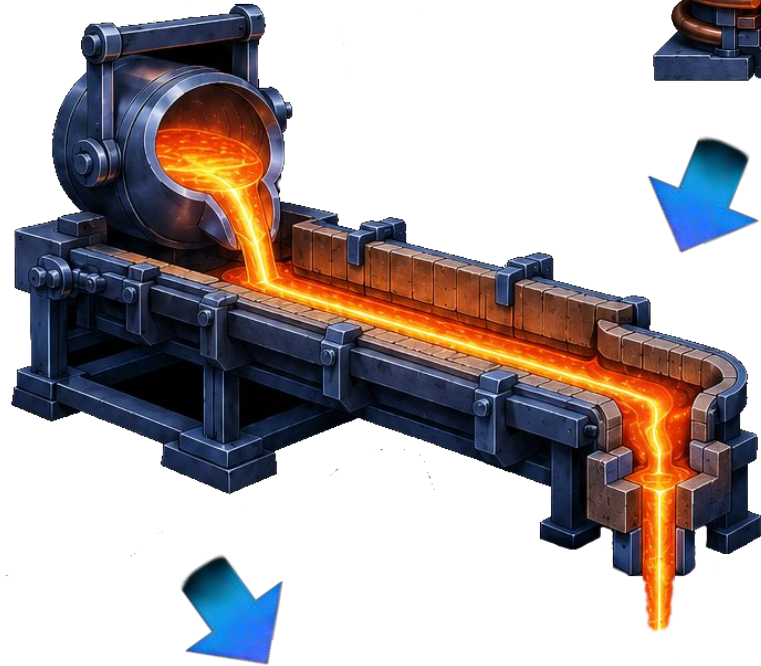
Solidifying

Mold
Filling

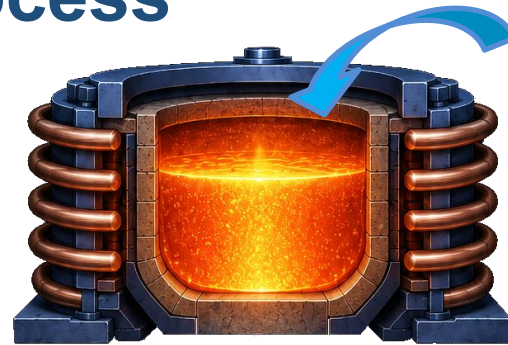


Generic Casting Process

Transporting



Mold
Filling



Heating + Melting

T_{melt} , $Power$

$V_{per\ minute}$

Planned values
&
Actual values

Solidifying

$T_{coolant}$



Alloy Casting Application Ontology

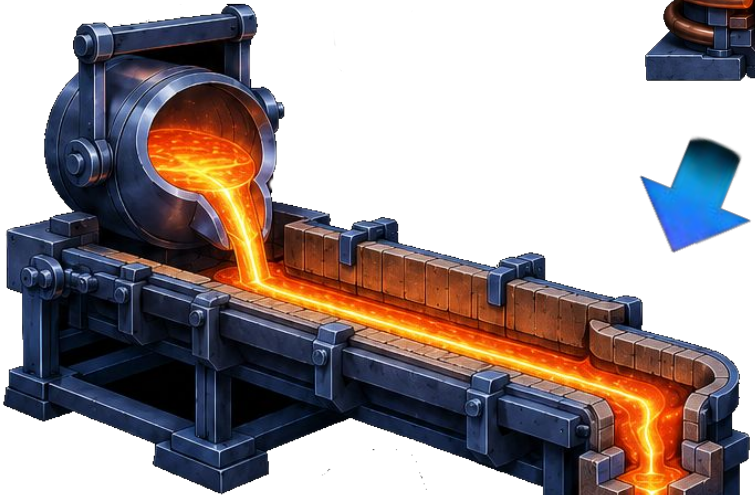
- Generic module — *Physical grounding*
- Casting module — *Equipment and processes*
- Operational module — *Parameters/ Time series*
- LCA module — *Environmental impact*



ACAO
GitHub repository

Generic Casting Process

Transporting



Heating + Melting

Batch regime

Driving force

Discrete
Continuous

Gravity
Pressure
Centrifugal F.

Mold Filling

Reusable
Expendable
Architecture, Reusability



Solidifying

Casting Module: definition of casting type

*Classification
dimensions*

Formalizing
the
domain
knowledge

Annotations +

label [language: en]

investment casting production process

skos:definition

Casting process where waxes are embedded into investment and destroyed during dewaxing and burnout to produce near net shaped metal components.

definition source

ISO 19376-1:2025(en)

Investment casting production process

Equivalent To +

SubClass Of +

'discrete casting production process'

'has part' some
(('casting mold filling process'
and ('has participant' some
(('shell mold'
and 'expendable casting mold'))))

'has part' some
(('casting mold filling process'
and ('stimulated by' some
(('physical stimulus'
and ('has basis in' some 'gravity field condition'))))

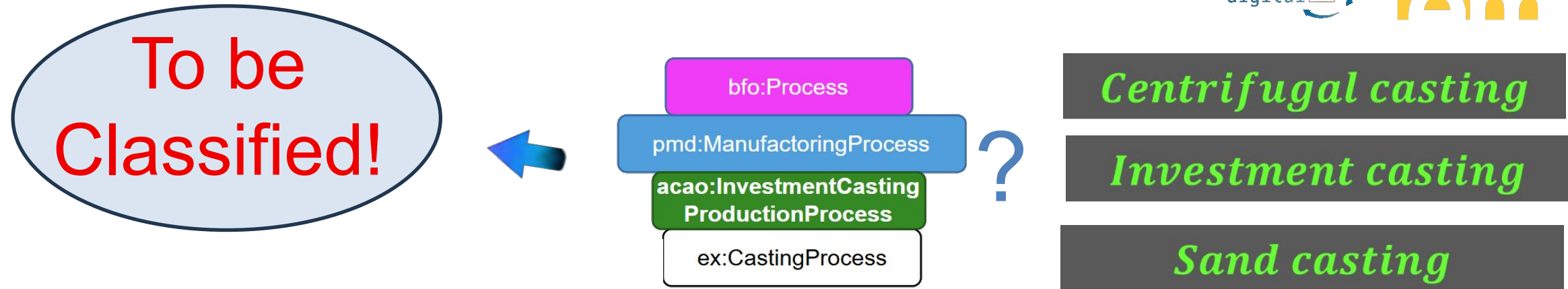
Batch regime

Architecture of mold

Reusability of mold

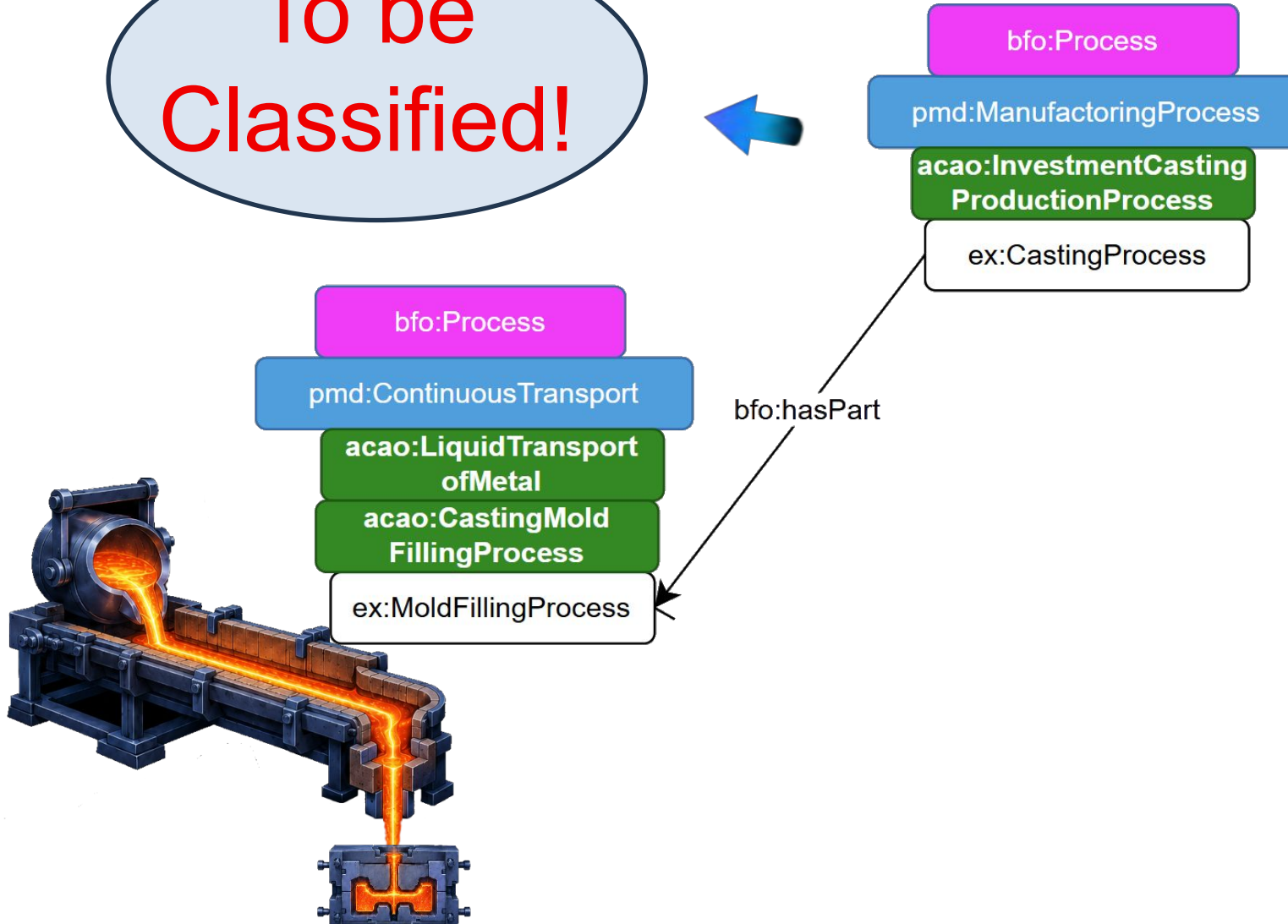
Driving force for liq. metal

Generic Module: physical basis for domain semantics

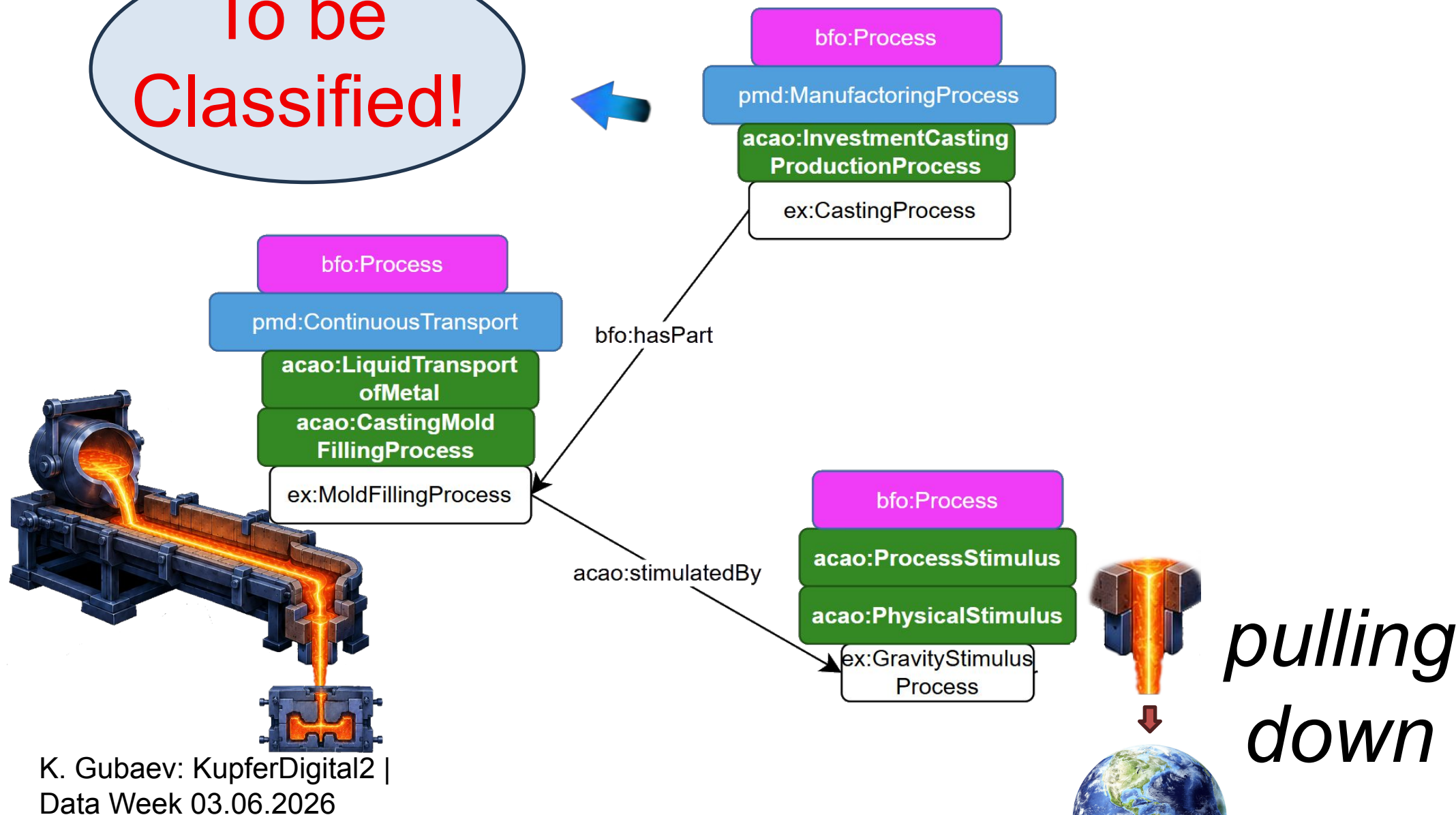


Generic Module: physical basis for domain semantics

To be
Classified!

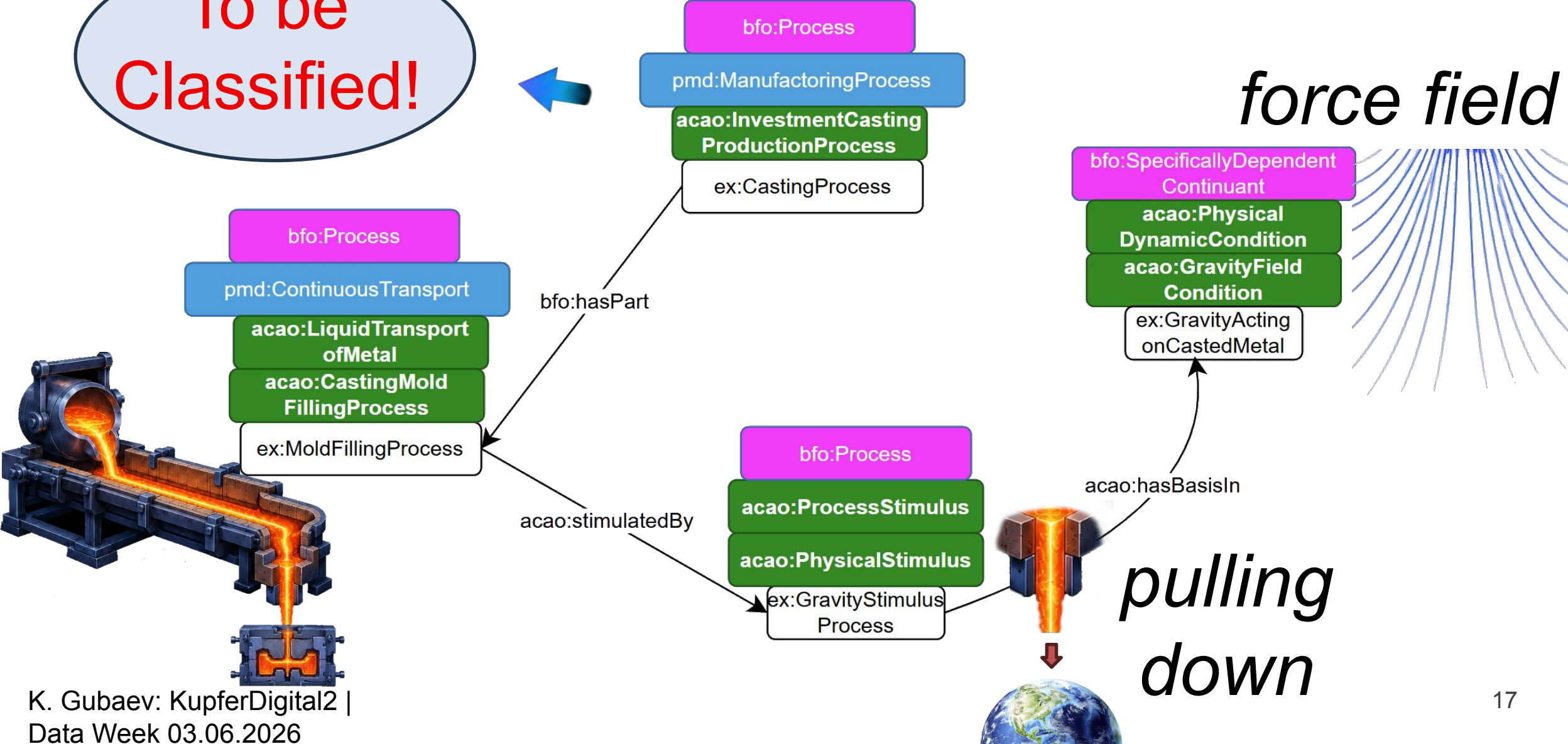


To be
Classified!



Generic Module: physical basis for domain semantics

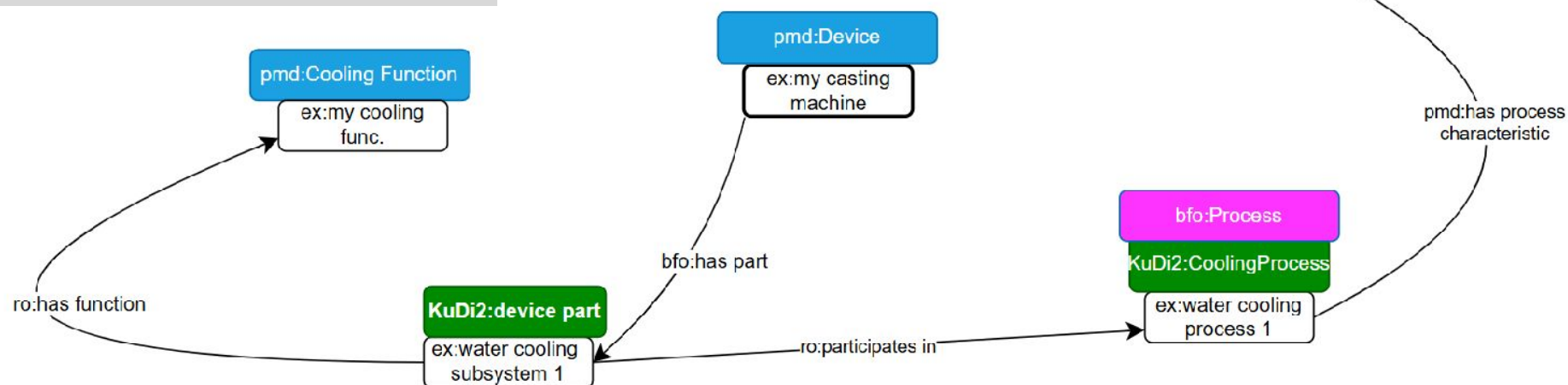
To be
Classified!



*PMDco pattern***Planned value
(device setting)***PMDco pattern***Actual value
(measurement datum)**

Connecting:

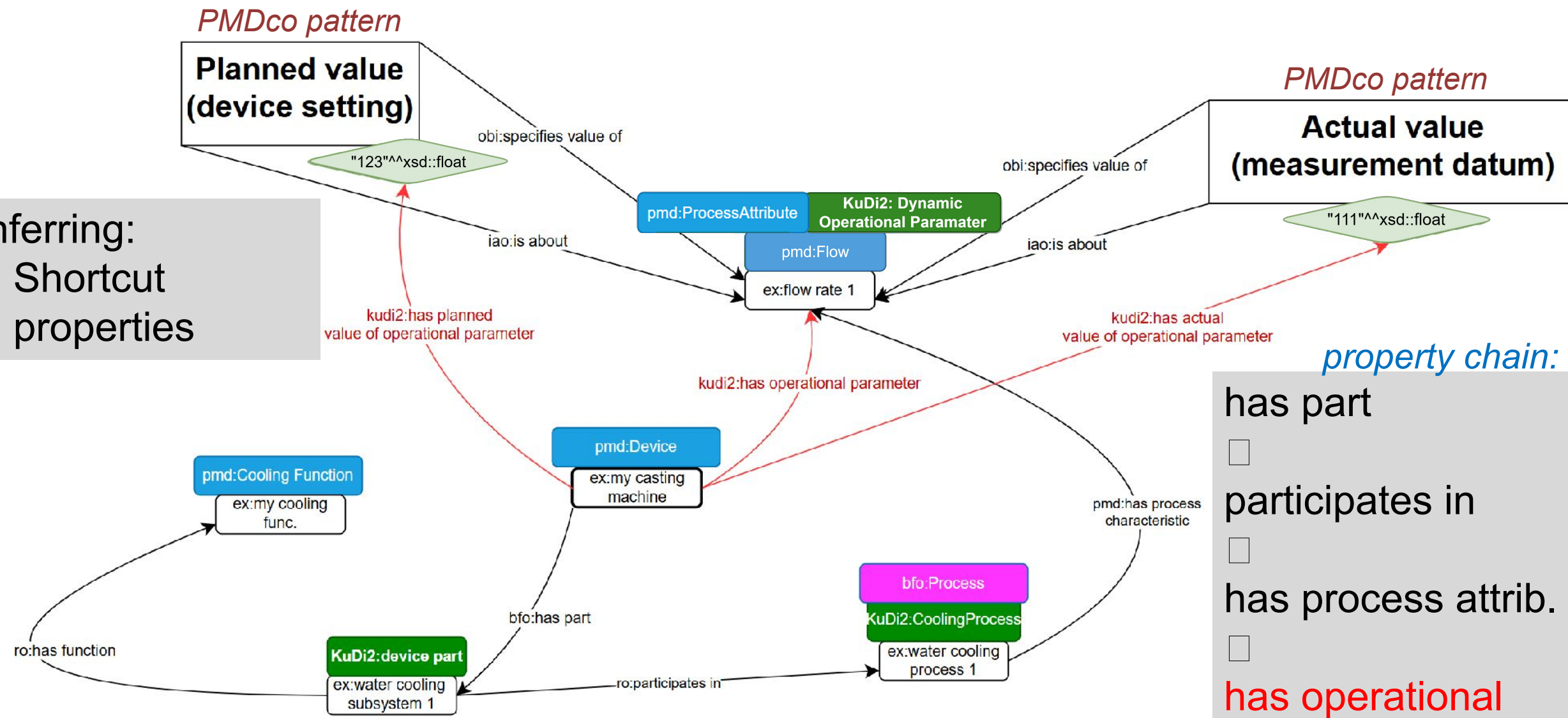
- Big Device
- Executing system
- Executed process
- Process parameter



Operational Module: semantic data organization

Inferring:

- Shortcut properties



property chain:

has part

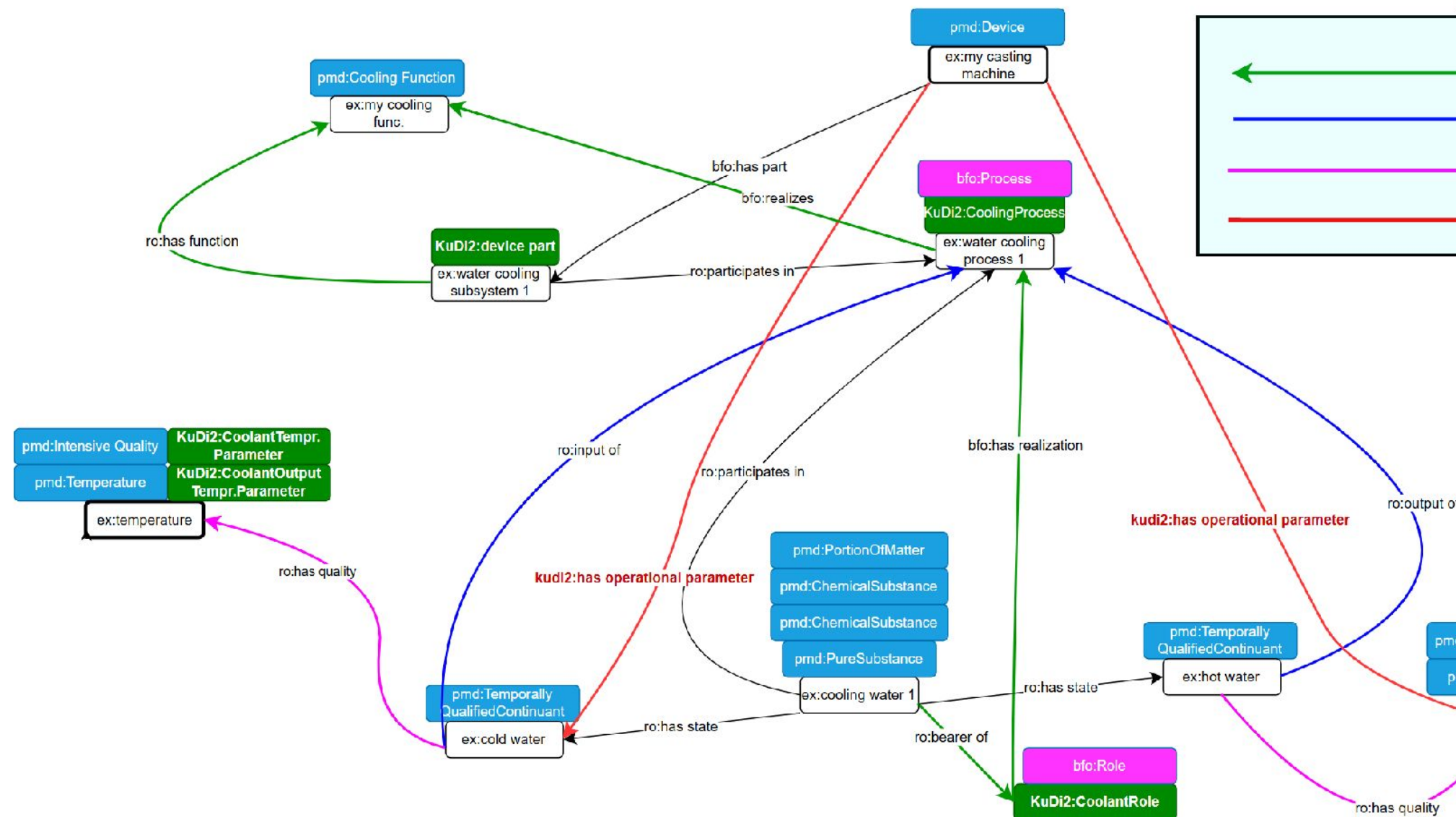
participates in

has process attrib.

has operational parameter

- ← - role/function bearing
- - process input/output
- - quality bearing
- - operational parameter

property chain:



has part

--	--

participates in

f

has input/output

--	--

has quality

- has operational parameter

Querying (inferred) operational parameters:

- Single property for dynamic & static
- Easy to wrap-up in complex queries

Snap SPARQL Query:

```
#has operational parameter: obo:KD2_d4c01cd7_acdc_4784_9b31_06b44c46d2ba

SELECT DISTINCT ?host_device ?parameter
WHERE{
  ?cls rdfs:label ?clsLabel .
  FILTER( LCASE(STR(?clsLabel)) = "device" )

  ?host_dev rdf:type ?cls .
  ?host_dev obo:KD2_d4c01cd7_acdc_4784_9b31_06b44c46d2ba ?par .
  OPTIONAL { ?par rdfs:label ?parameter }
  OPTIONAL { ?host_dev rdfs:label ?host_device }
}
ORDER BY ?label|
```

Execute

?host_device	JSON fields
ContinuousCastingMachine@en	H2O_out_Zone2_quality
ContinuousCastingMachine@en	H2O_out_Zone1_quality
ContinuousCastingMachine@en	L1_quality_exp2
ContinuousCastingMachine@en	t_Pause_Anfahren_quality
ContinuousCastingMachine@en	t_Pause_quality
ContinuousCastingMachine@en	T_Kok_quality
ContinuousCastingMachine@en	t_Anfahren_quality
ContinuousCastingMachine@en	H20_in_quality
ContinuousCastingMachine@en	v_gieß_quality
ContinuousCastingMachine@en	H20_out_Sek_quality
ContinuousCastingMachine@en	Vol_Zone3_quality
ContinuousCastingMachine@en	Vol_Sek_quality
ContinuousCastingMachine@en	P_Heiz_Kok_quality
ContinuousCastingMachine@en	T_Tiegel_quality
ContinuousCastingMachine@en	Vol_Zone2_quality
ContinuousCastingMachine@en	m0_quality_exp2
ContinuousCastingMachine@en	Abschnitt_quality
ContinuousCastingMachine@en	Vol_Zone1_quality
ContinuousCastingMachine@en	B1_quality_exp2
ContinuousCastingMachine@en	T_Kühler_quality
ContinuousCastingMachine@en	H1_quality_exp2

25 results

Querying values of operational parameters:

- Where difference planned vs actual is > 5 ?
- At which time step?

?host_device	?quality_label	?actual_val	?planned_val	?diff	?unit	?timestep_seconds
ContinuousCastingMachine@en	T_Tiegel_quality	1240	1230	10.0	degree Celsius@en	190
ContinuousCastingMachine@en	T_Tiegel_quality	1238	1230	8.0	degree Celsius@en	180
ContinuousCastingMachine@en	T_Tiegel_quality	1238	1230	8.0	degree Celsius@en	170
ContinuousCastingMachine@en	T_Tiegel_quality	1236	1230	6.0	degree Celsius@en	160
ContinuousCastingMachine@en	T_Tiegel_quality	1236	1230	6.0	degree Celsius@en	150
ContinuousCastingMachine@en	T_Tiegel_quality	1236	1230	6.0	degree Celsius@en	140
ContinuousCastingMachine@en	Vol_Zone1_quality	307	300	7.0	litre per hour@en	10
ContinuousCastingMachine@en	Vol_Zone1_quality	306	300	6.0	litre per hour@en	0
ContinuousCastingMachine@en	Vol_Zone1_quality	407	400	7.0	litre per hour@en	60
ContinuousCastingMachine@en	Vol_Zone1_quality	257	300	43.0	litre per hour@en	20
ContinuousCastingMachine@en	Vol_Zone1_quality	480	500	20.0	litre per hour@en	170
ContinuousCastingMachine@en	Vol_Zone1_quality	500	500	0.0	litre per hour@en	180

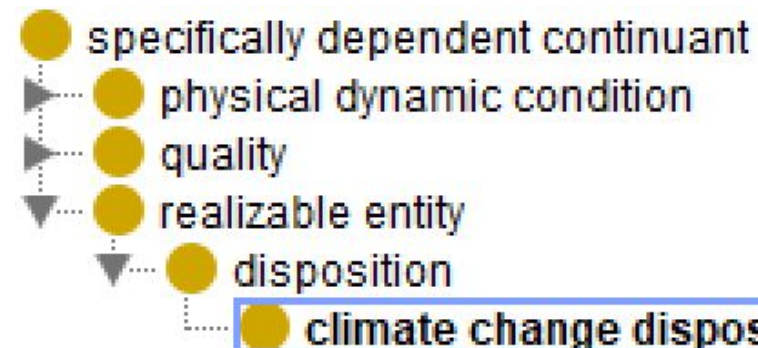
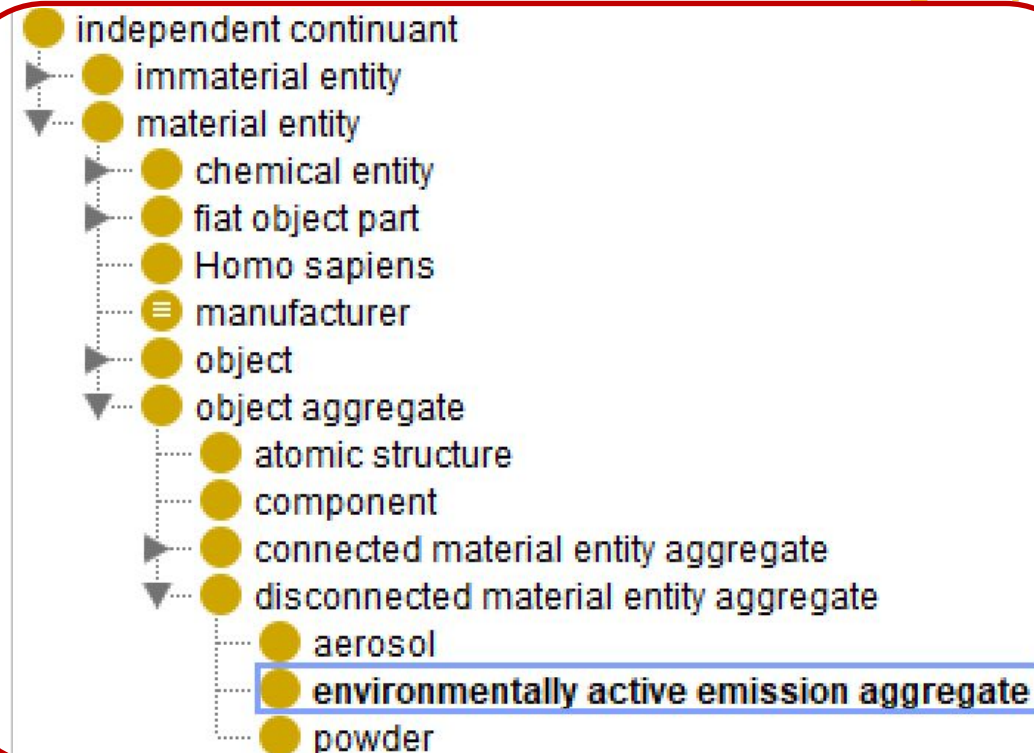
87 results

State of the art:

- **ORIONT***: ontology for product LCSA
- **No BFO-conformant LCA ontology found**

Minimal semantic effort for LCA:

- Material entity – emissions (acids, ions, H₂)
- Realizable entity – CO₂-equivalent
- PMDco patterns for calculations & method



*<https://ecoinvent.org/projects/orienting/>

Takeaway message

- **WHAT:**
 - Alloy Casting Ontology / Knowledge Graph for aggregation / querying / analysis
- **WHY:**
 - Make data **meaningful + auditable**: embedding **domain semantics** and **LCA**
- **HOW:**
 - *Now*: Reusing PMD patterns + dedicated extensions
 - *Next*: **Thermodynamics** for **Machine-Learning** analysis
- **SO WHAT:**
 - *From raw process data to explainable environmental impact.*



ACAO

GitHub repository ²⁴

Our project partners in KupferDigital



Projektkoordination: **Wieland Electric**



Konsortialpartner



Laufzeit

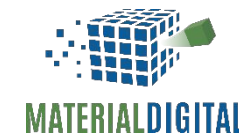
1.2.2025 – 31.1.2028

Danksagung

Das Vorhaben 13XP5230 wird im Rahmen der Innovationsplattform **MaterialDigital** vom Bundesministerium für Bildung und Forschung gefördert.



Platform Material Digital Project



Thermodynamic ontology: semantic data integration



Mat. Sci. Article

IDE for Mat. Sci.

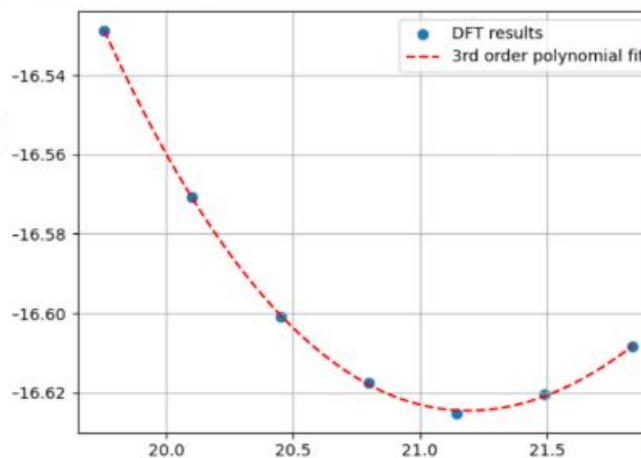
Calculations Database

OPEN ACCESS

Compare 2nd
derivative (bulk
modulus)

Constant	MTP*	SNAP ^c	GAP ^d	DFT*	Exp.
Lattice Parameter a_0 (Å) Bulk Modulus B (GPa)	3.322(1) 175.0(7)	3.327 183	3.308 172	3.322 171	3.303 ^g 174

Potential Energy, eV

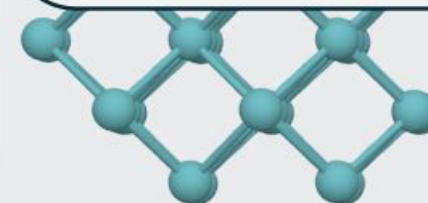


Volume, Å³

$$\frac{d^2}{dV^2}$$

$$\frac{d}{dV} = 0$$

Compare
equilibrium
volume



Nb

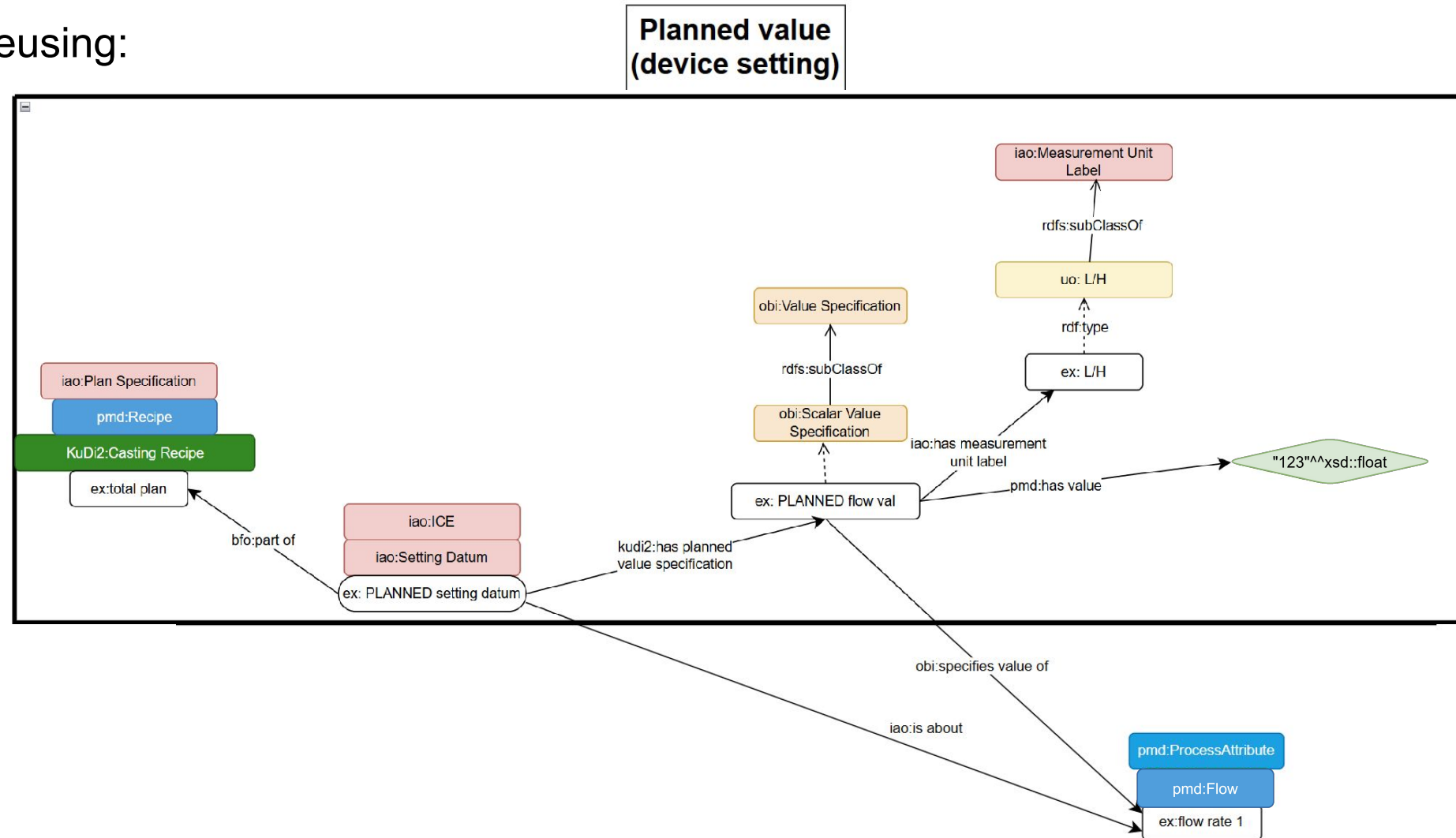
a b c
0 0 0

Volume **18.306 Å³**

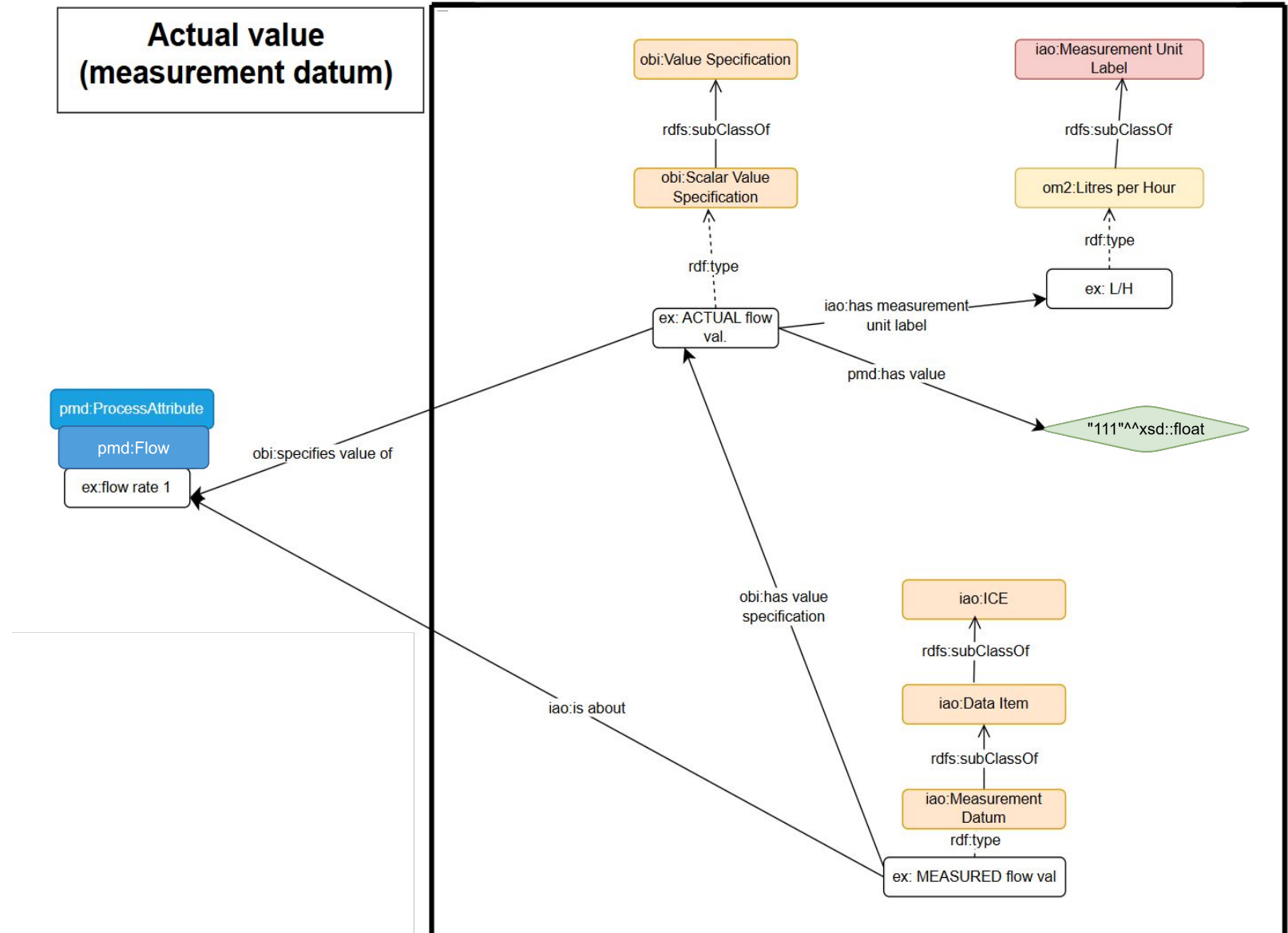
- BFO/PMDco3 patterns reusing:

- Planned settings are part of the plan
- Value specification with unit and value

- OM2 ontology for units



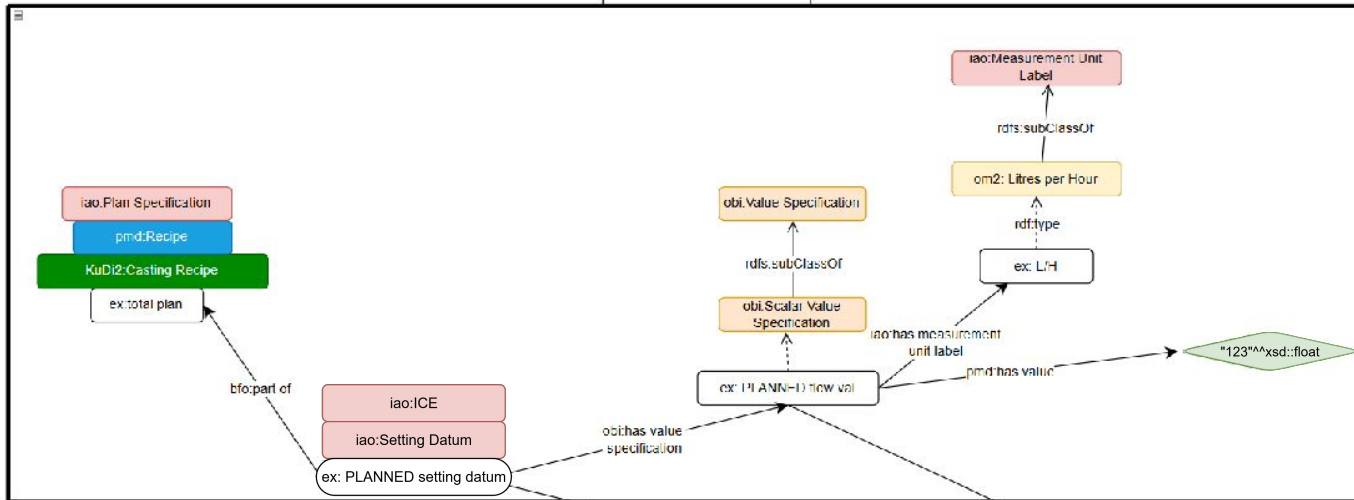
- BFO/PMDco3 patterns reusing:
 - Actual values come from measurements
 - Value specification with unit and value
- OM2 ontology for units



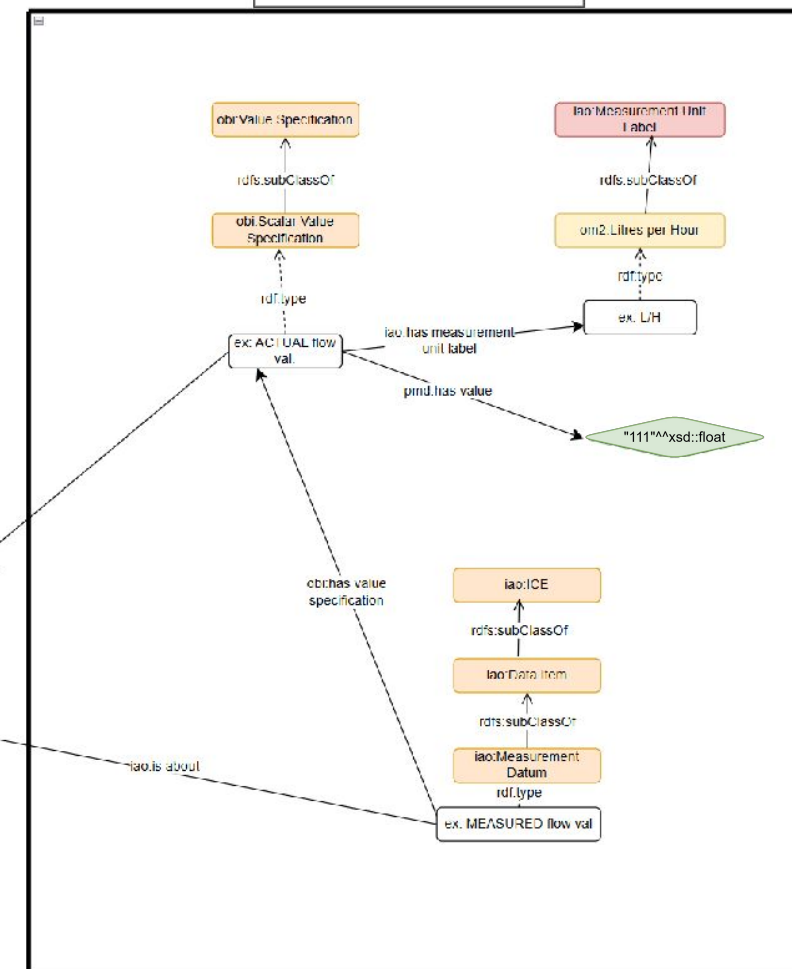
KUPFERDIGITAL 2

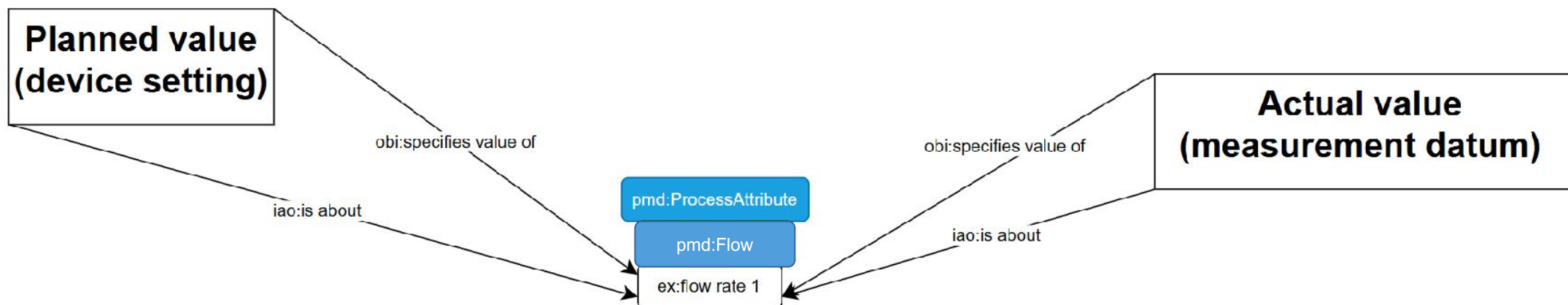
PMDco style: flow rate

Planned value
(device setting)



Actual value
(measurement datum)



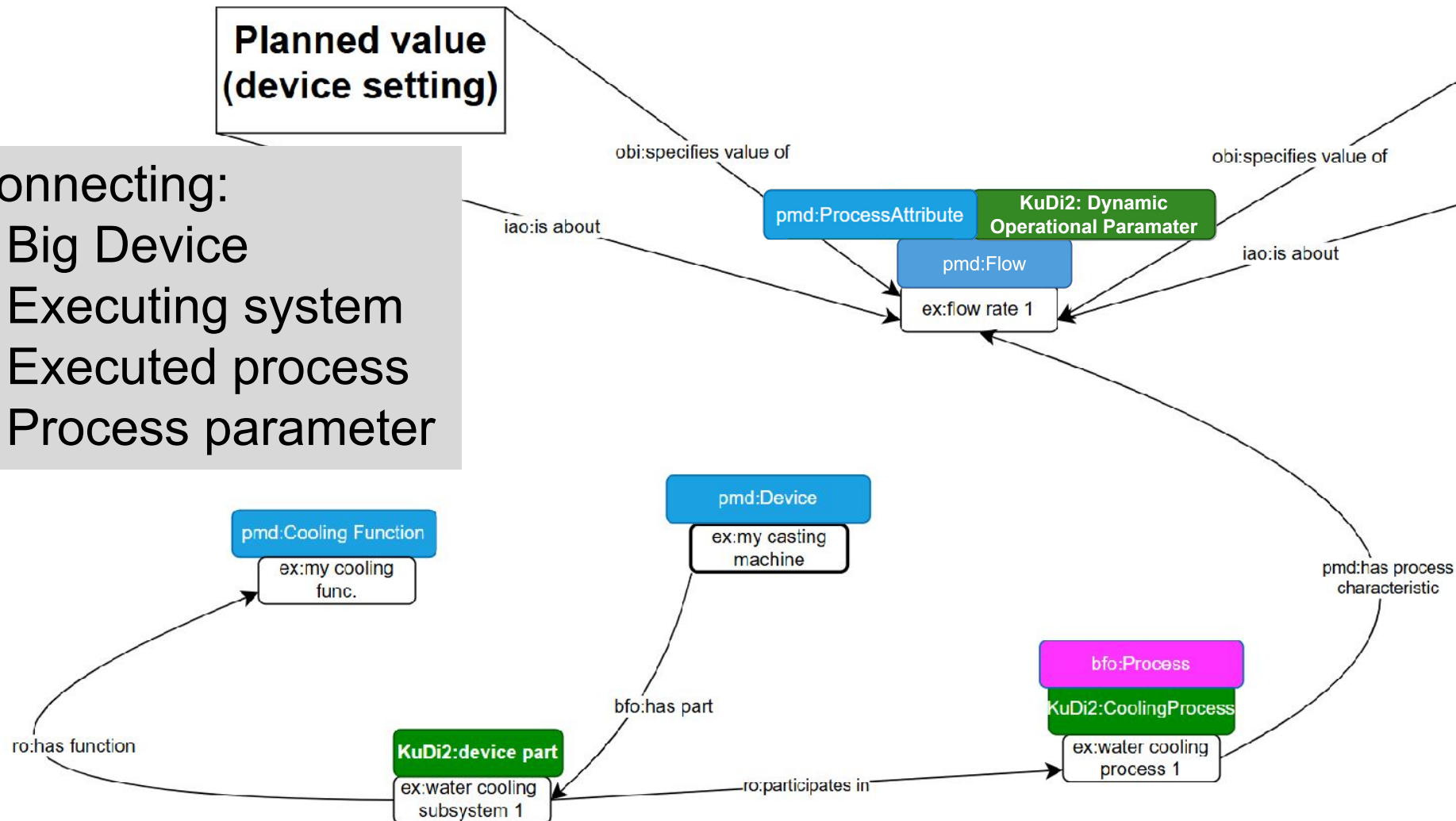


**Planned value
(device setting)**

**Actual value
(measurement datum)**

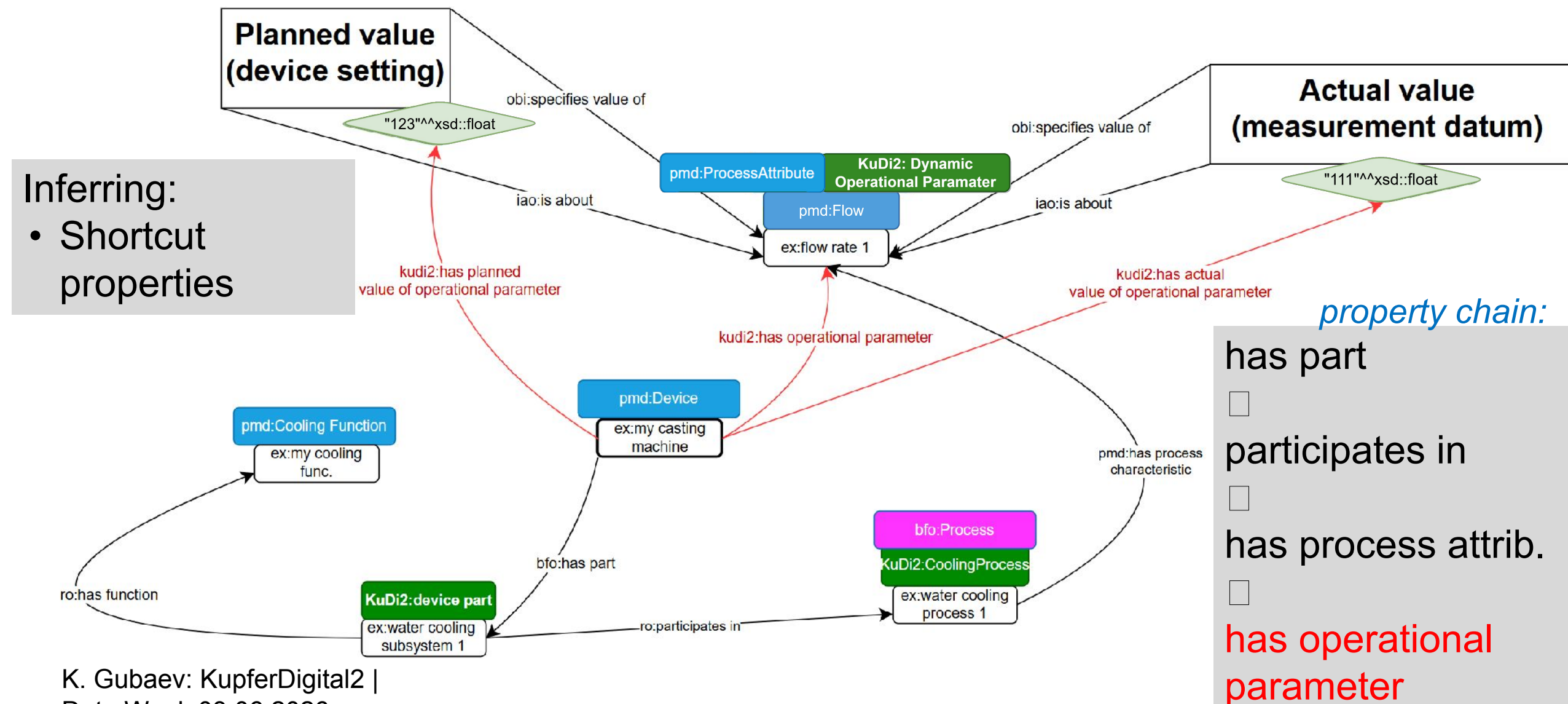
Connecting:

- Big Device
- Executing system
- Executed process
- Process parameter



KUPFERDIGITAL 2

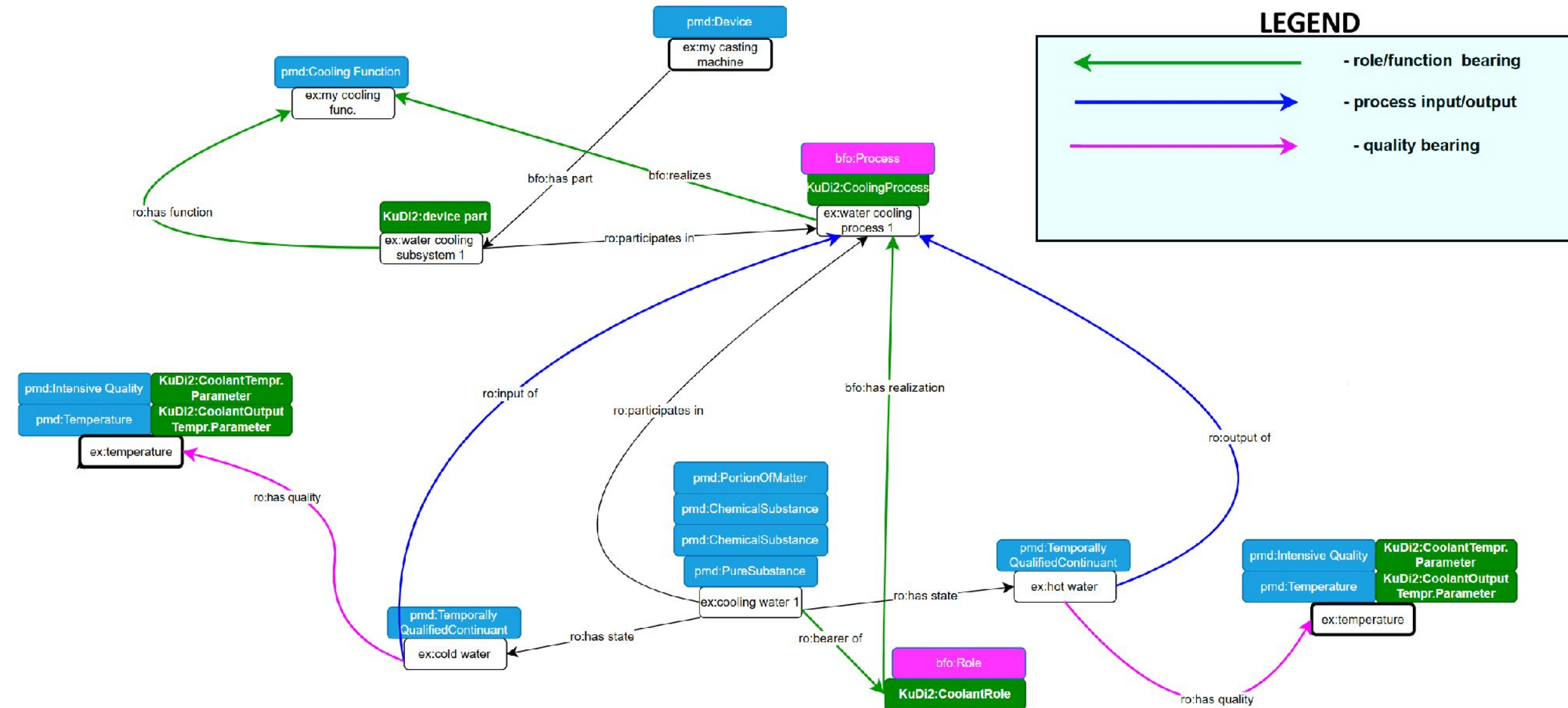
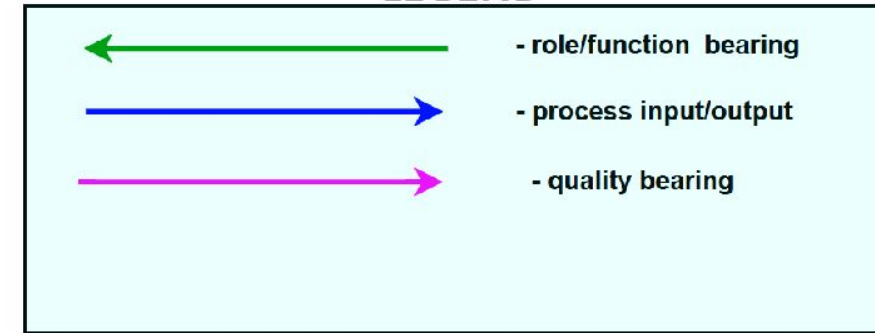
Casting ontology: operational module



KUPFERDIGITAL 2

Casting ontology: operational module

LEGEND



The background of the slide is a photograph of a modern, angular building with a facade made of many small, square windows in various colors (yellow, orange, blue, grey). The building is situated on a hill overlooking a river. In the foreground, there are stone steps leading down to the river, and several people are walking and sitting on the steps. The sky is blue with some clouds.

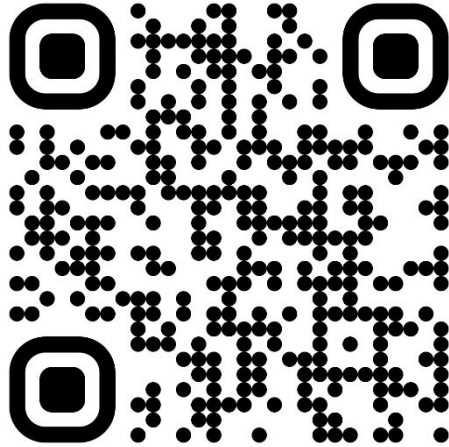
Kupfersymposium 2025

We look forward to welcoming you
to Schwäbisch Gmünd! Home of the
fem Research Institute since 1922.

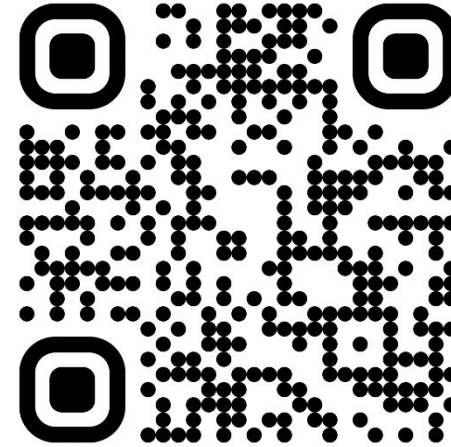
With a Digitalization Workshop tailored for Engineers and Material Experts

Some Links:

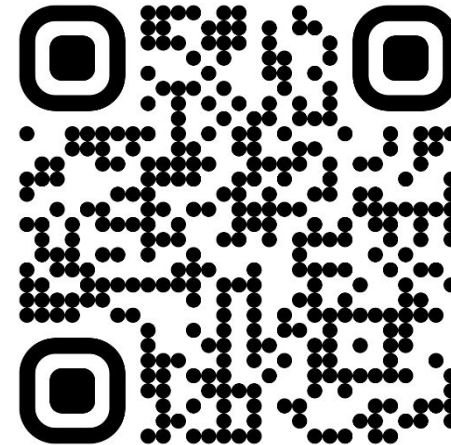
The PMD Data Portal can be found here:



Publications can be found here:



Showcases to explore can be found here:



Thank you very much for your attention.

Miriam Eisenbart, fem Forschungsinstitut

