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Insights from an OTTR-centric Ontology Engineering Methodology

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GEFÖRDERT VOM
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SIRIUS
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Motivation: Ontology Engineering with OTTR

- development of large ontologies = multiple design decisions at the same time
- OTTR is a language for ontology modelling patterns → instances build ontology
  - hide complexity from the domain experts
  - separating what to model from how to model
- our approach
  - ⬆️ bottom-up: begin with existing data
  - ⬇️ top-down: OTTR template headers first, and bodies are developed iteratively

💬 enhanced communication with domain experts

⚙️ agile engineering process

Figure 1: Example Template Hierarchy

Reasonable Ontology Templates (OTTR)

a template library

a template definition

```
pz:Pizza[ ?name , ?label ] :: {
    ottr:Triple( ?name, rdf:type, owl:Class ),
    ax:SubClassOf( ?name, p:Pizza ),
    ottr:Triple( ?name, rdfs:label, ?label )
} .
```

Reasonable Ontology Templates (OTTR)

a template library

a template definition

```
ax:SubClassOf[ ?sub, ?super ] :: {
    ottr:Triple( ?sub, rdfs:subClassOf, ?super )
} .
```

a template definition

```
pz:Pizza[ ?name , ?label ] :: {
    ottr:Triple( ?name, rdf:type, owl:Class ),
    ax:SubClassOf( ?name, p:Pizza ),
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} .
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pz:Pizza[ ?name , ?label ] :: {
   ottr:Triple( ?name, rdf:type, owl:Class ),
   ax:SubClassOf( ?name, p:Pizza ),
   ottr:Triple( ?name, rdfs:label, ?label )
} .
```

a template instance

```
pz:Pizza( p:Margherita, "Margherita"@it )
```

result of instantiation

```
p:Margherita rdf:type owl:Class .
p:Margherita rdfs:subClassOf p:Pizza .
p:Margherita rdfs:label "Margherita"@it .
```


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Domain: Material Science 

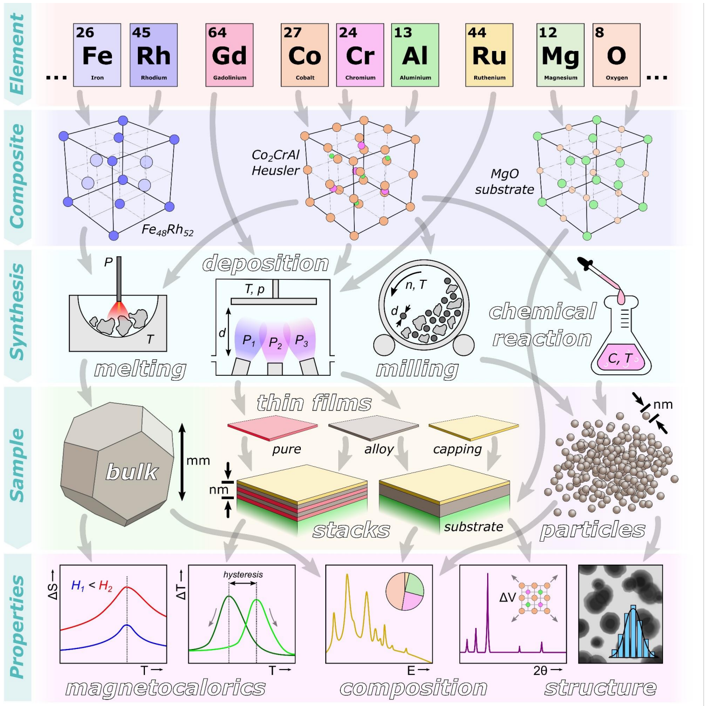

Figure 2: Material science workflow

- project DiProMag: model experiments related to magnetocaloric alloys from the production, over the characterization to the prototypical application in an application ontology
- close collaboration between ontology engineers and domain experts
- favors a bottom-up ontology engineering approach

Project Website: https://www.dipromag.de/

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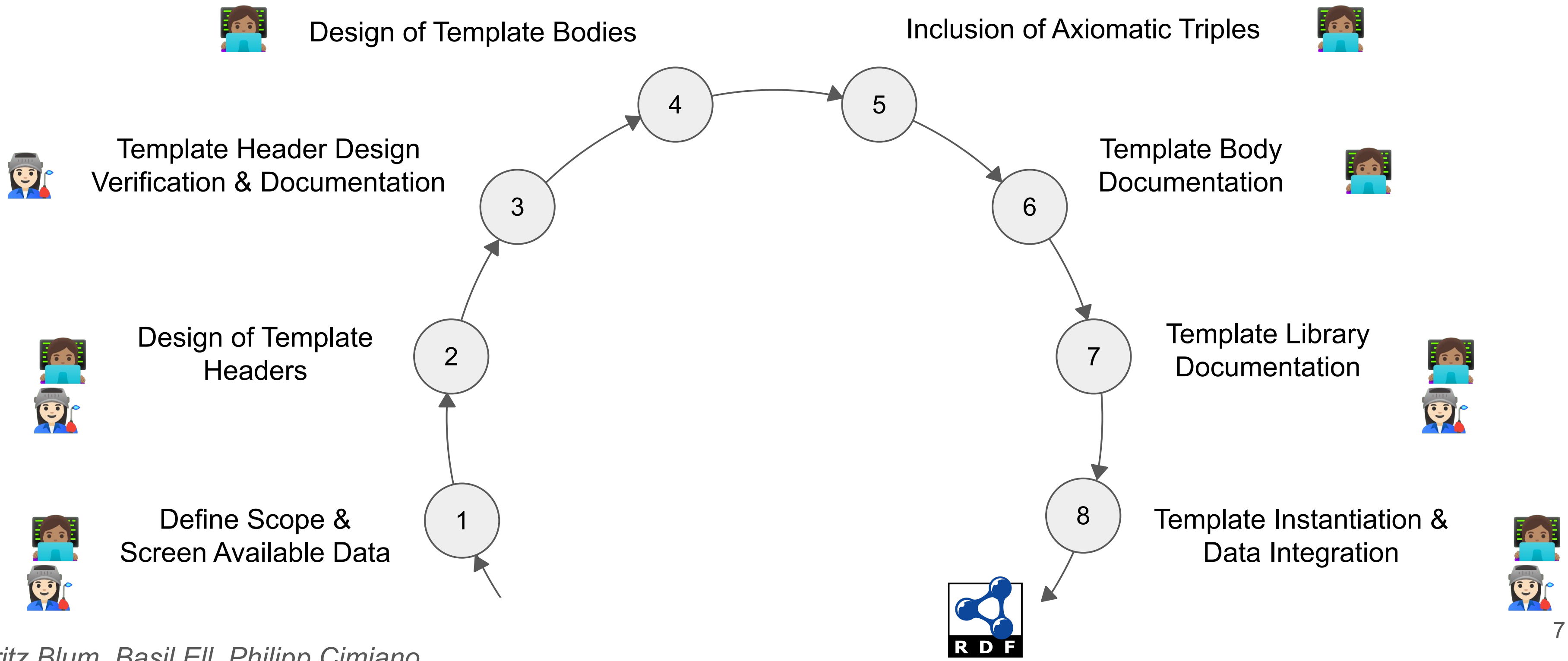
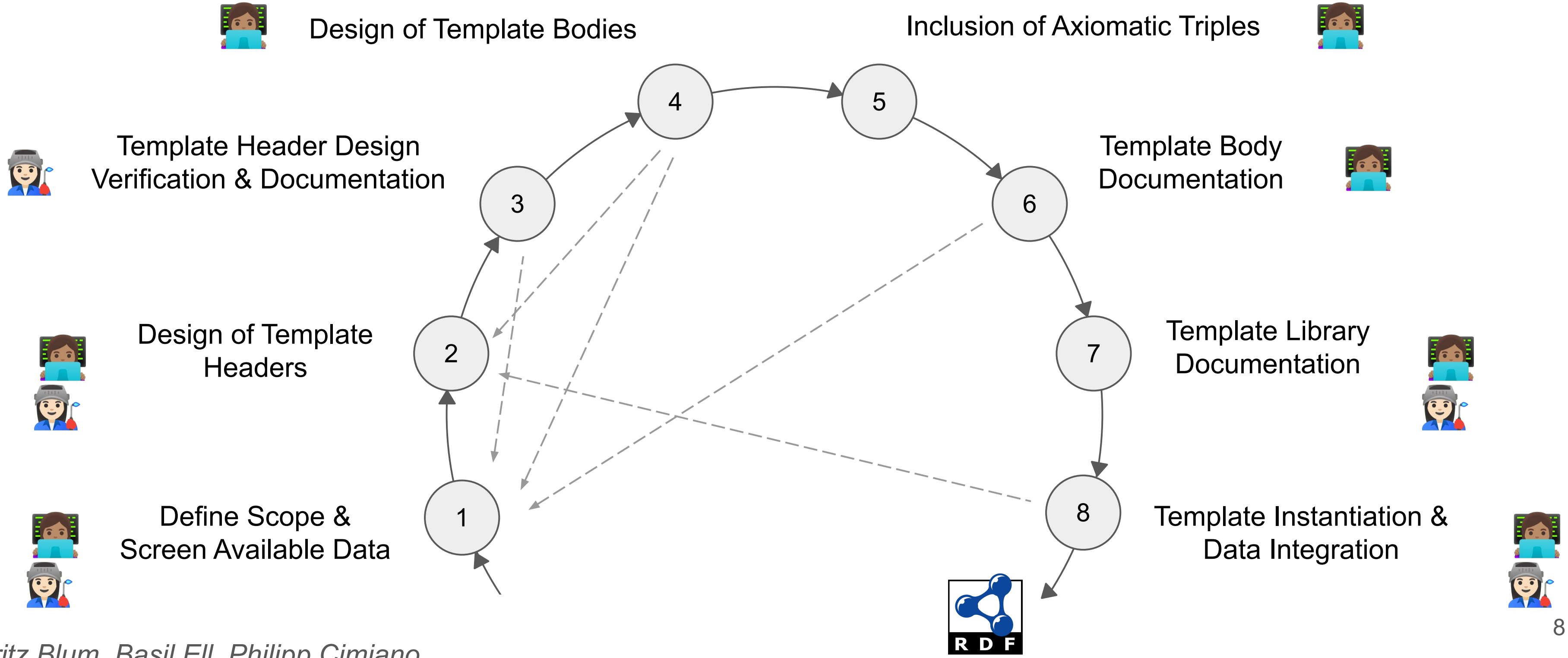
Methodology



Methodology



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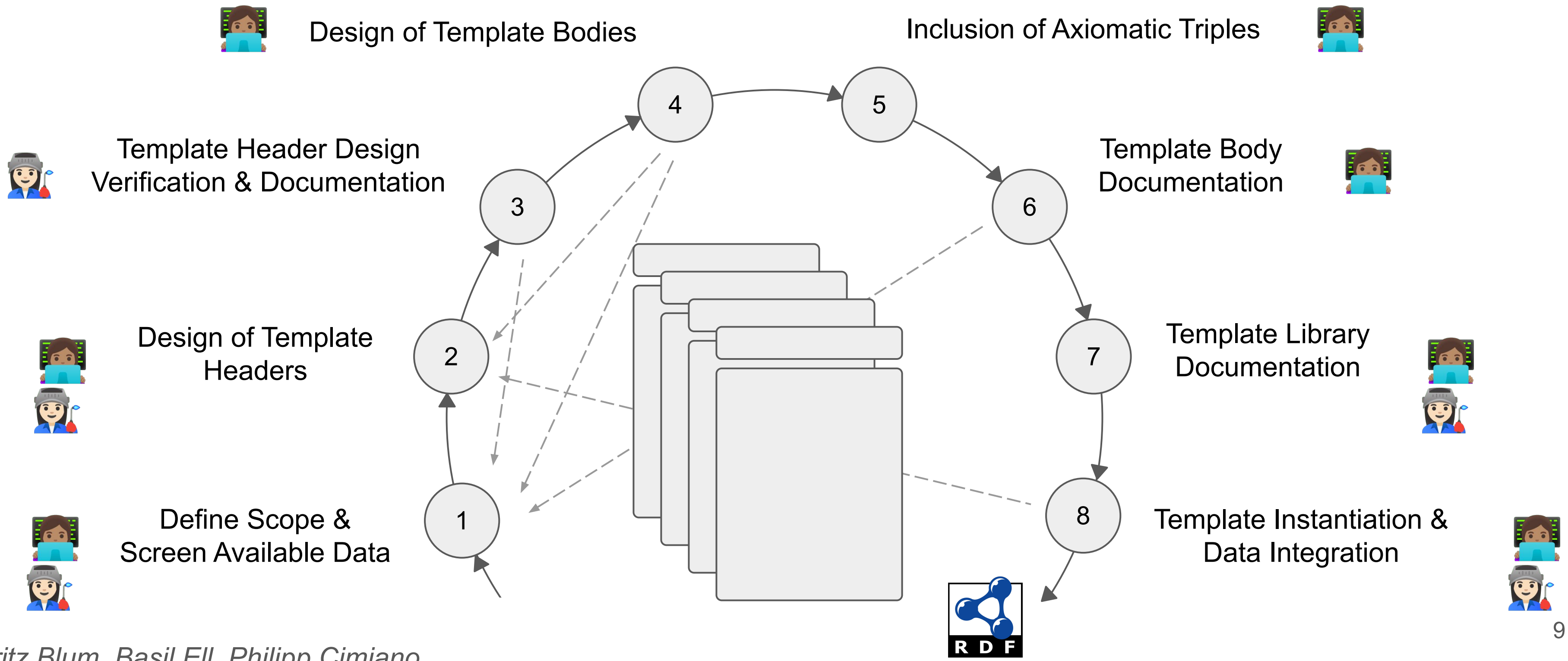
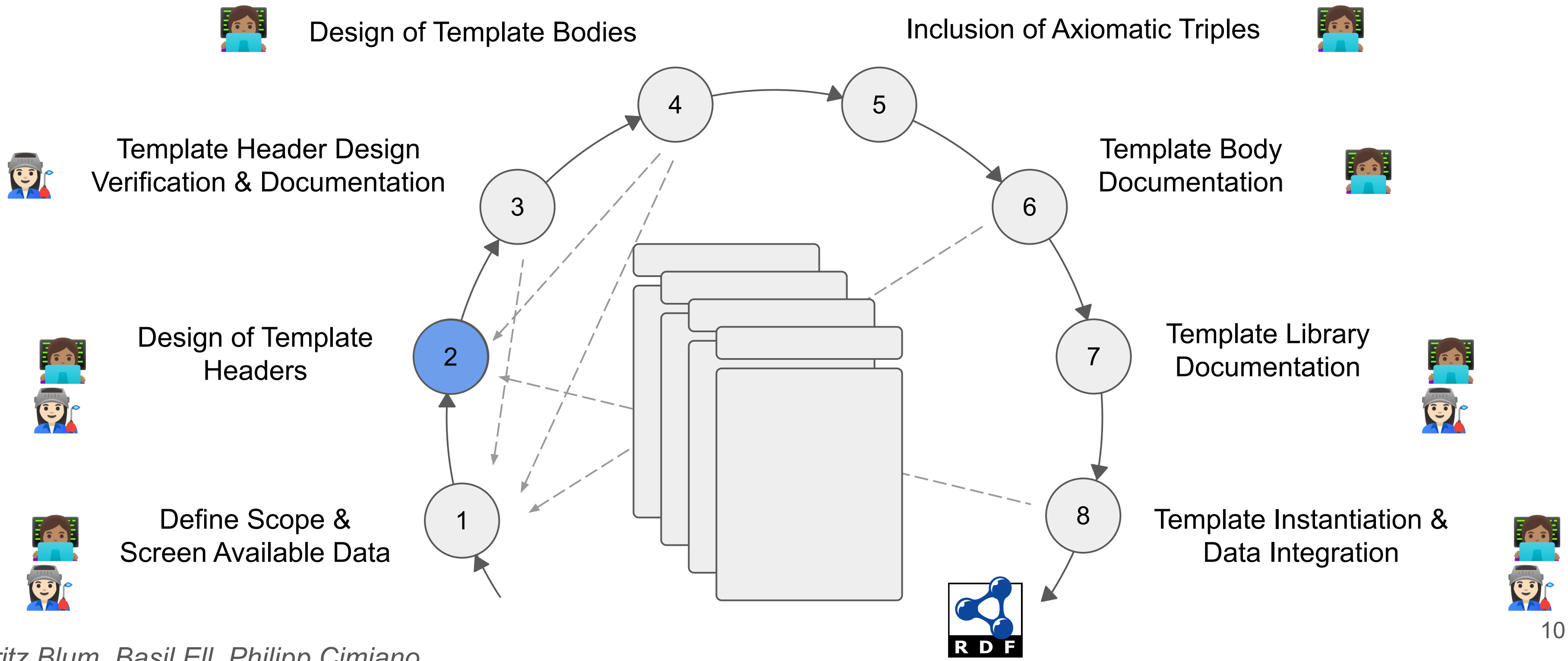
Methodology



Methodology



Step 2 – Design of Template Headers

Template header: **ex:Pizza[ottr:IRI ?name, xsd:string ?label]**

- abstraction simplifies the communication with domain experts
- design trade-offs like
  - complexity of templates vs. complexity of template relations
    `ex:Pizza[ottr:IRI ?name, xsd:string ?label, ottr:IRI ?cheese, ottr:IRI ?cheese_age]`
    vs.
    `ex:Pizza[ottr:IRI ?name, xsd:string ?label, ottr:IRI ?cheese] &`
    `ex:Cheese[ottr:IRI ?cheese, ottr:IRI ?cheese_age]`

  - multiple similar but specific templates vs. few general templates
    `ex:PizzaLarge` & `ex:PizzaMedium` & `ex:PizzaSmall`
    vs.
    `ex:PizzaOfDiffSize`
- result = initial collection of template headers (improve iteratively)

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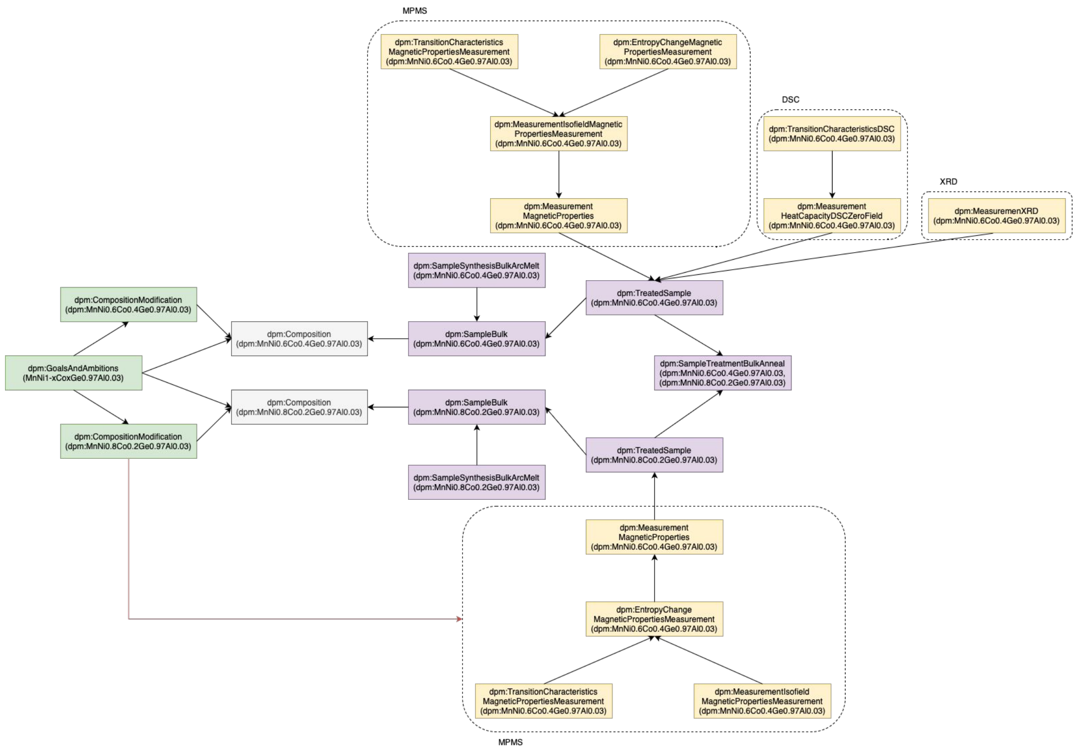
Step 2 – Design of Template Headers

Experiences:

- derived template parameters directly from the available data
- one template per process step, i.e., one template per material type, one template per synthesis method, and one template per measurement method
- encountered trade-offs: splitting data across multiple templates concerns the correlations and dependencies between data points



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Methodology

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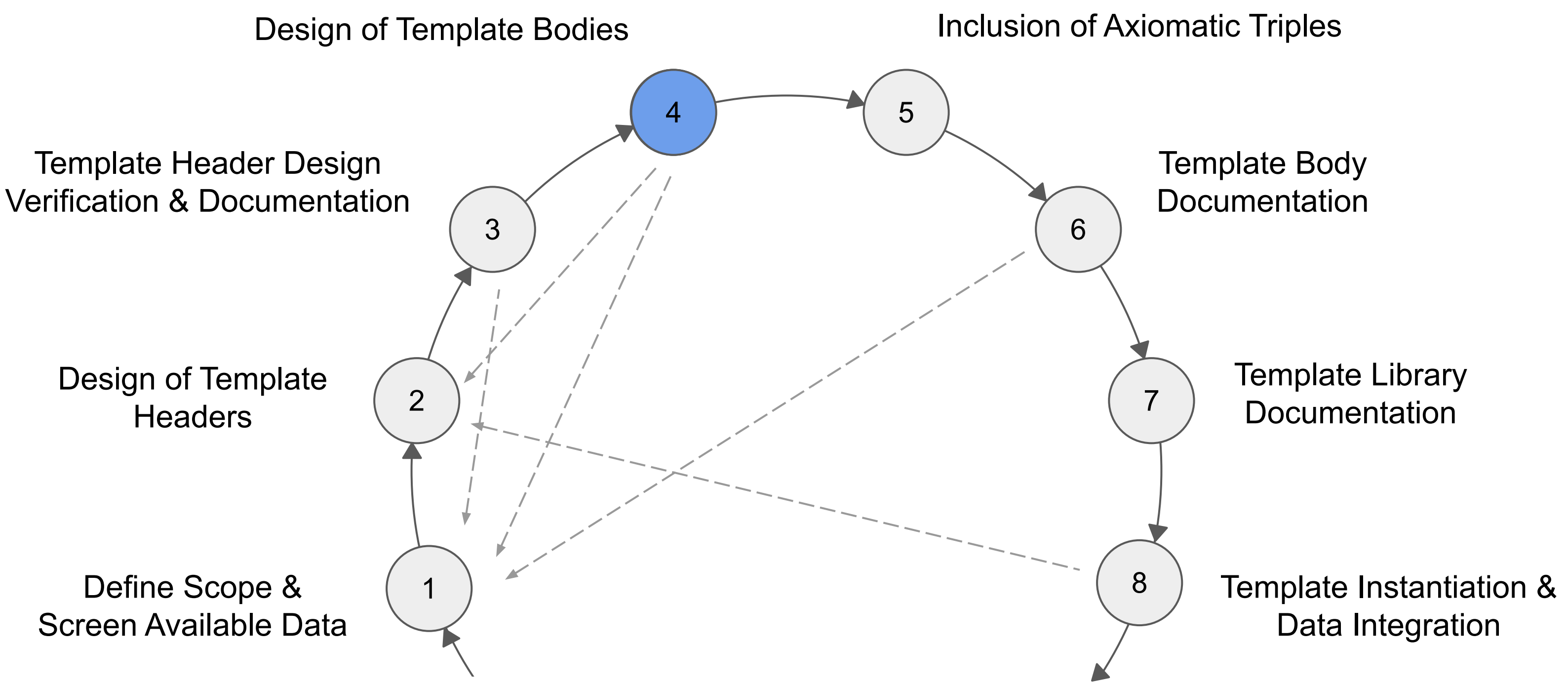

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Step 4 – Design of Template Bodies

- straightforward, as a pre-structuring is already done
- use template header documentation
  - benefit from collected domain knowledge about, e.g., domain-specific terms
  - to identify sub-templates (🔄 iterative development – step back to template header design)
  - to identify and reuse existing ontologies
- possible difficulties
  - incompatibility to the ontologies selected for reuse
  - modeling redundancy → potential inconsistency: avoid by introducing appropriate sub-templates

Experiences:

- modelling processes according to existing ontologies like EMMO required to revisit *"Design of Template Headers"* to introduce additional template parameters
- a collection of similar physical experiments shares the same parameters (e.g., about the environment) → sub-templates were introduced

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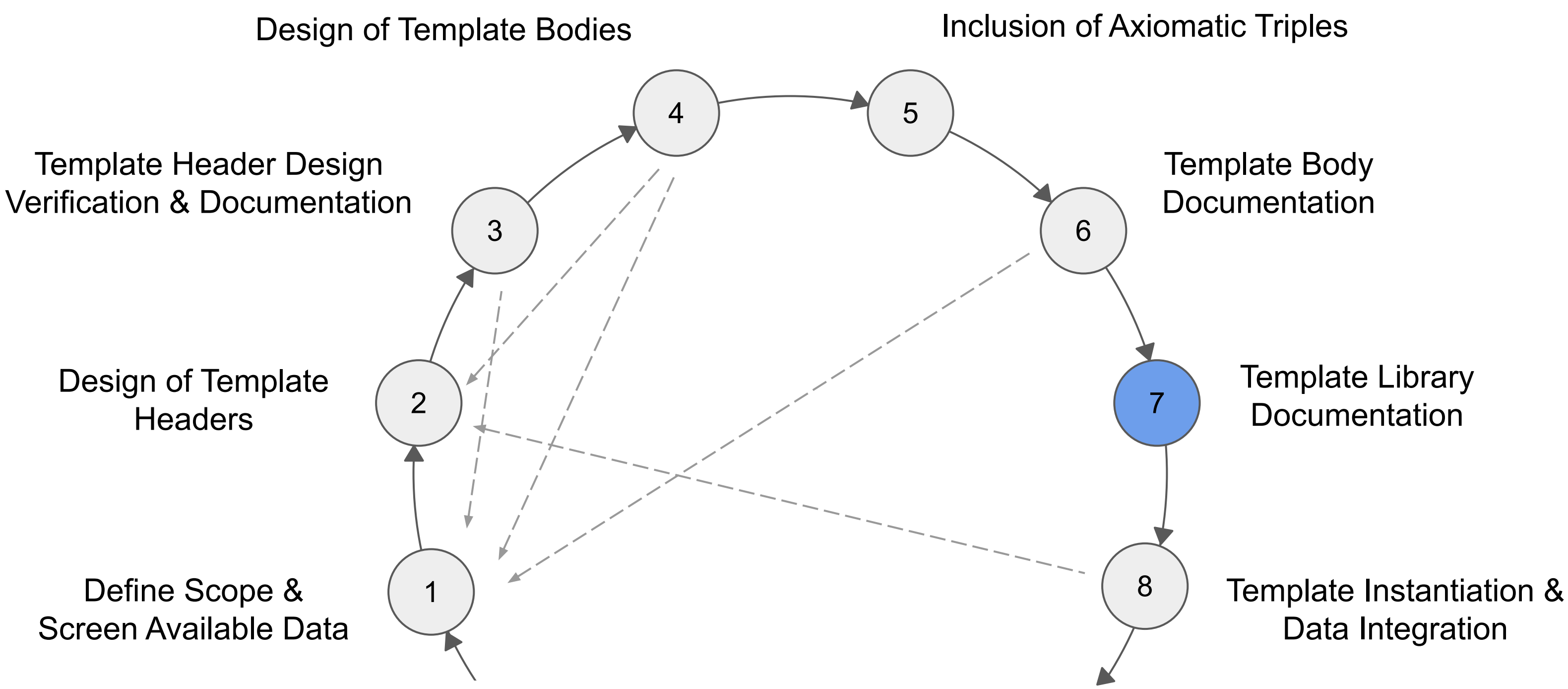
Methodology



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Step 7 – Template Library Documentation

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Template: dpm:CreateComposition

URI: http://dipromag.de/ottr-templates/0.1/CreateComposition

Parameters

The parameters defined by the signature are listed here. Unfortunately parameter names are not informative; fixing it is a planned future feature. An optional parameter will accept the value ottr:none as an argument. A parameter which allows blanks will accept a blank node as argument value.

Index	Name	Type	Optional	Blanks allowed	Default value
1	material	ottr:IRI	no	yes	no
2	elements	NEList<ottr:IRI>	no	yes	no
3	stoichiometry_portion_unit_at_percent	NEList<xsd:float>	no	yes	no
4	user	ottr:IRI	no	yes	no
5	date	xsd:date	no	yes	no
6	comment	xsd:string	no	yes	""^^http://www.w3.org/2001/XMLSchema#string
7	verified	xsd:boolean	no	yes	"true"^^http://www.w3.org/2001/XMLSchema#boolean

Pattern

stOTTR

stOTTR serialisation of the template without annotation instances.

```
dpm:CreateComposition[
    ottr:IRI ?material,
    NEList<ottr:IRI> ?elements,
    NEList<xsd:float> ?stoichiometry_portion_unit_at_percent,
    ottr:IRI ?user,
    xsd:date ?date,
    xsd:string ?comment="",
    xsd:boolean ?verified="true"^^xsd:boolean
] :: {
    zipMin | dpm:CompositionElement(?material, ++?elements, ++?stoichiometry_portion_unit_at_percent),
    dpm:HasMetaData(?material, ?user, ?date, ?comment, ?verified),
    o-rdf:Type(?material, pmd:ChemicalComposition)
} .
```

The pattern of the template is illustrated by expanding a generated instance. Below the generated instance is shown in different serialisations, and its expansion is presented in different formats.

Generated instance

stOTTR

```
dpm:CreateComposition(x:argument1, (x:argument2-1, x:argument2-2), (_:argument3-1, _:argument3-2), x:argument4,
```

RDF/wOTTR

```
[ ottr:of      dpm:CreateComposition ;
  ottr:values  ( x:argument1 ( x:argument2-1 x:argument2-2 ) ( []
                                                              []
                                                            ) x:argument4
                 []
                 []
                 []
               )
] .
```

Visualisation of expanded RDF graph

Each resource node is linked to its IRI. Type relationships are not visualised, rather each node contains its type.

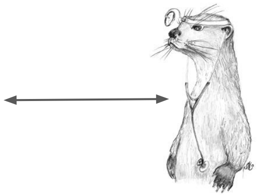
▼ Hierarchical horizontal layout (dot)

▶ Hierarchical vertical layout (dot)
▶ Spring model layout (neato)
▶ Spring model layout (fdp)
▶ Radial layout (twopi)
▶ Circular layout (circo)

Expanded RDF graph

```
x:argument1  rdf:type     pmd:ChemicalComposition ;
        dpm:comment       []  ;
        dpm:isVerified    []  ;
        dcterms:created   []  ;
        dcterms:creator   x:argument4 ;
        pmd:composedOf    [ rdf:type            dpm:Element , pmd:Object ;
                            dpm:hasStoichiometry  [ rdf:type   pmd:Measurement , pmd:Metadata ;
                                                    pmd:unit   dpm:at_percent ;
                                                    pmd:value  []
                                                  ] ;
                            pmd:relatesToElement  x:argument2-2
                          ] ;
```

Figure 3: OTTR documentation



- list of all templates
- template inclusion/call hierarchy
- individual template documentation

- instantiation order and naming guidelines, e.g., *“BulkSample”* + *\w{2} initials of the creator* + *YYMMDD* + *[0-9]{2} enumerator*

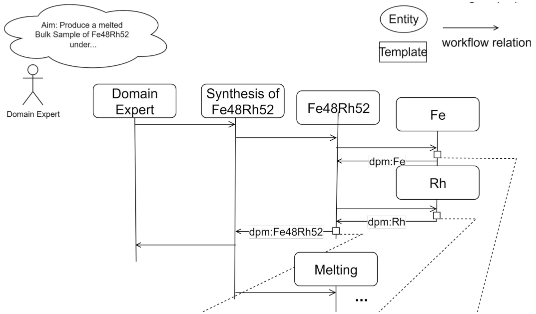


Figure 4: Template instantiation workflow

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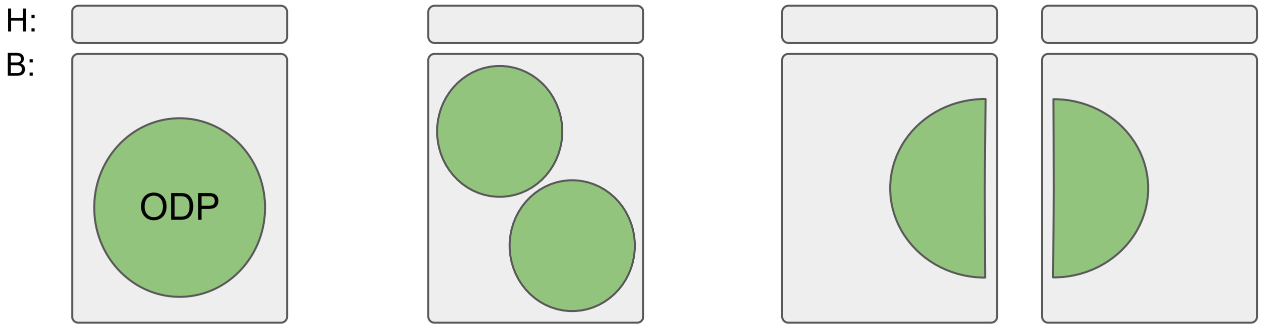
ODPs are compatible with OTTR



a template can instantiate <u>one</u> ODP

a template can instantiate <u>multiple</u> ODP

multiple templates can instantiate one or more ODPs

\+ benefit of OTTR features, e.g., dealing with optional/default parameters or checking data type constraints

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Conclusion

- ontology engineering methodology that relies on OTTR templates
  - key steps: defining the ontology's scope, …, instantiating templates and integrating data
  - our OTTR-based method should be combined with existing ontology engineering practices
  - compatible with ODPs
- experience from a project (~90 templates)
  - low efforts when we had to revisit design decisions
  - greatly helped for communicating with domain experts

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Thank you for your attention!

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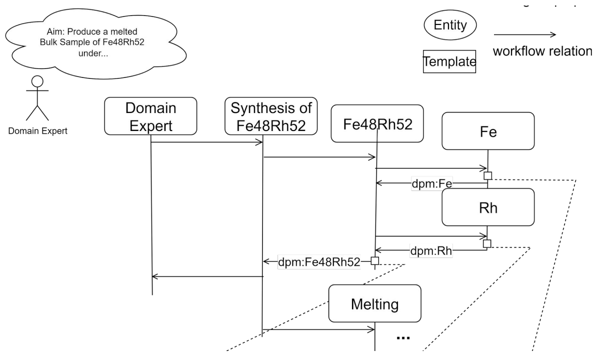

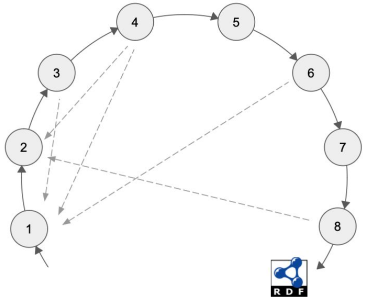

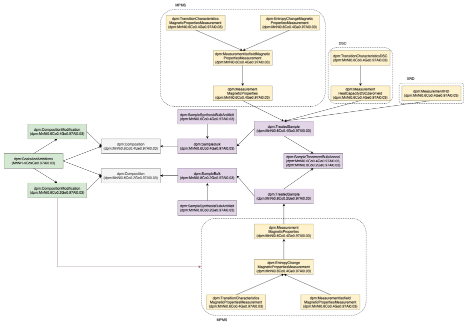

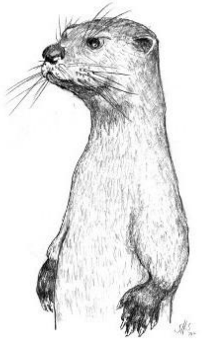

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