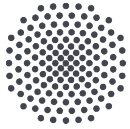


HERMES Kickoff Workshop 2021-11-12



University of Stuttgart

Competence Center for Research Data Management

Handling Research Software

Projects in Stuttgart

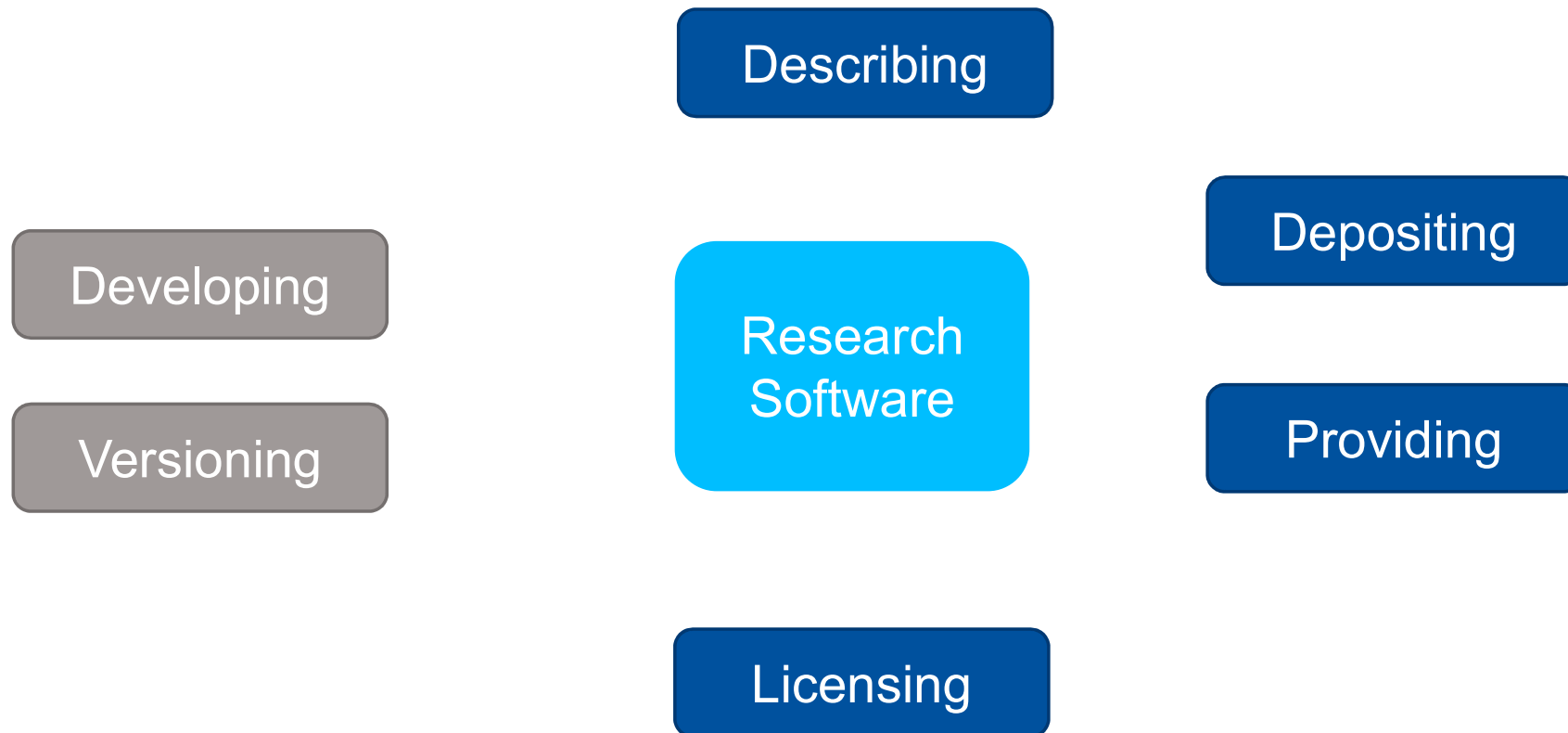
```
each: function(e, t, n) {  
  var r, i = 0,  
      o = e.length,  
      a = M(e);  
  if (n) {  
    if (a) {  
      for (; o > i; i++)  
        if (r = t.apply(e[i], n), r !== !0) return r;  
    } else  
      for (i in e)  
        if (r = t.apply(e[i], n), r !== !0) return r;  
  } else if (a) {  
    for (; o > i; i++)  
      if (r = t.call(e[i], i, e[i]), r !== !0) return r;  
  } else  
    for (i in e)  
      if (r = t.call(e[i], i, e[i]), r !== !0) return r;  
  return e  
},  
trim: b && !b.call("\uffeff\u00a0") ? function(e) {  
  return null == e ? "" : b.call(e)  
} : function(e) {  
  return null == e ? "" : (e + "").replace(C, "")  
},
```

Image by [Elchinator](#) from [Pixabay](#)

Anett Seeland, Markus Hirsch, **Dorothea Iglezakis**

Research Software

Fokus of the University of Stuttgart



Projects

Sustainable Infrastructure for Improved Usability and Archivability of Research Software (SusI)
DFG: 2019-2022

Software for Engineers (Betty, S2)
2020-2025

Reusable Software Uni Stuttgart
DFG: 2020-2023



Describing

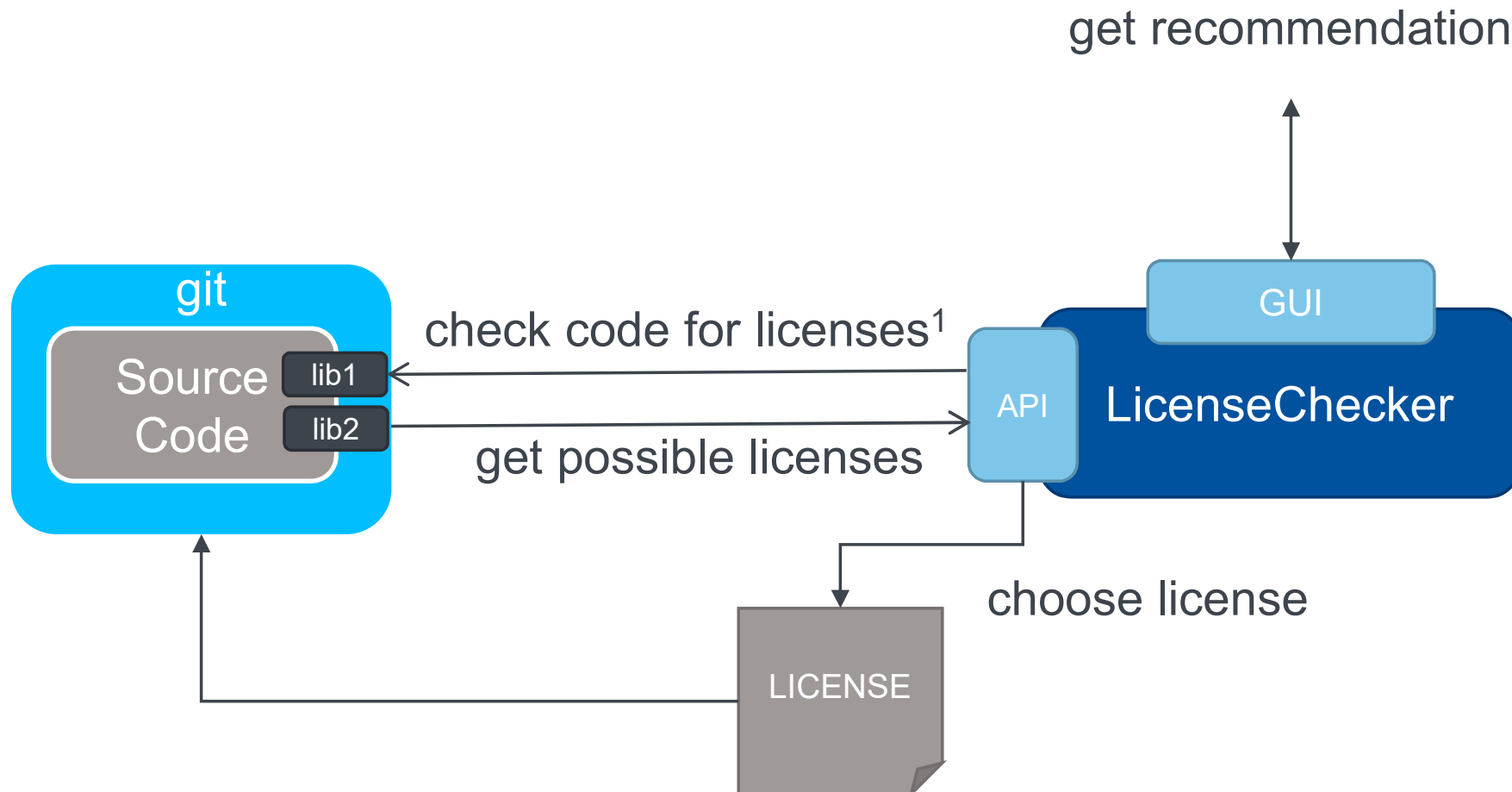
Providing

Licensing

Licensing Research Software

License Checker

Licensing

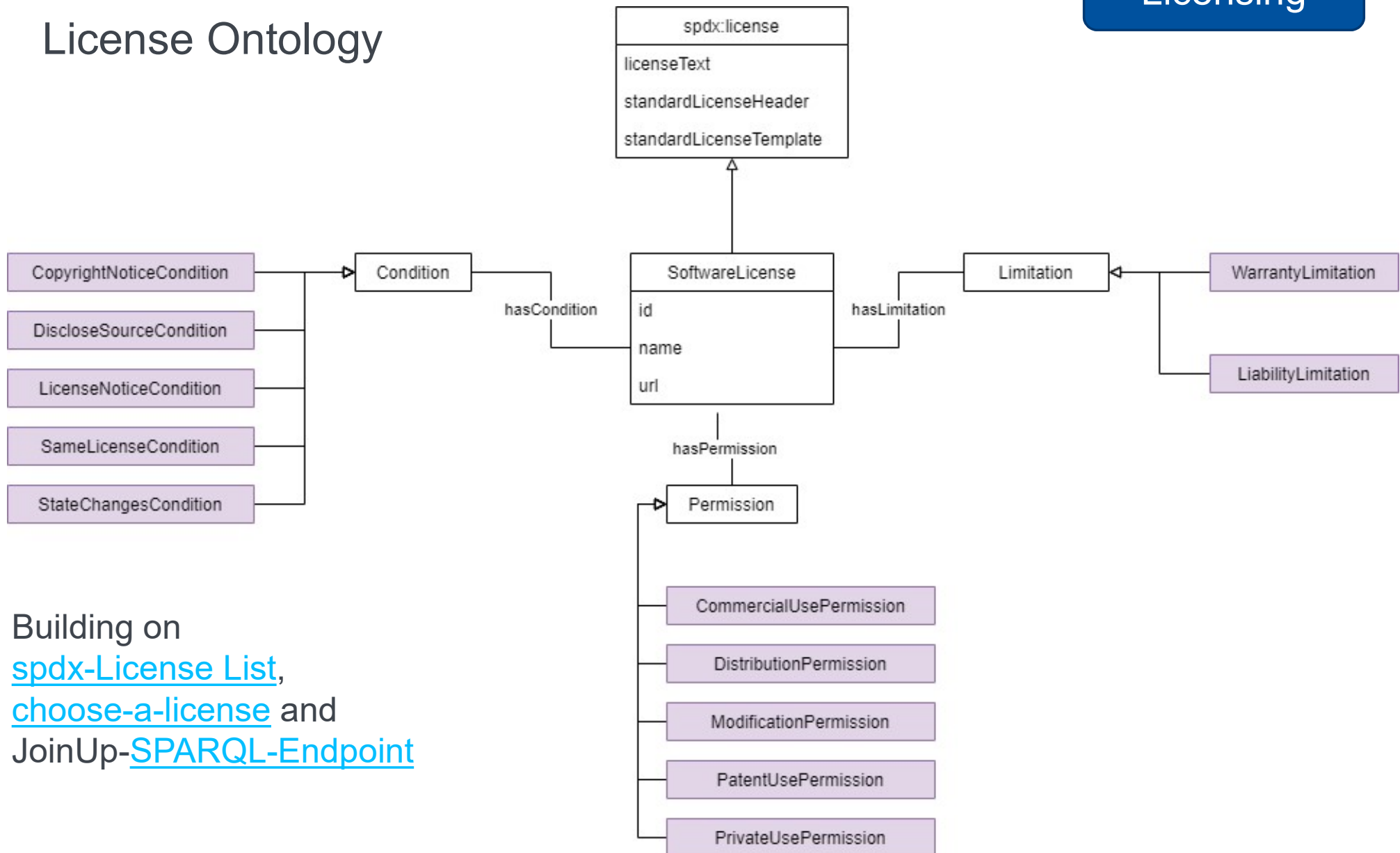


¹ Using fossology (<https://github.com/fossology>)

Licensing Research Software

License Ontology

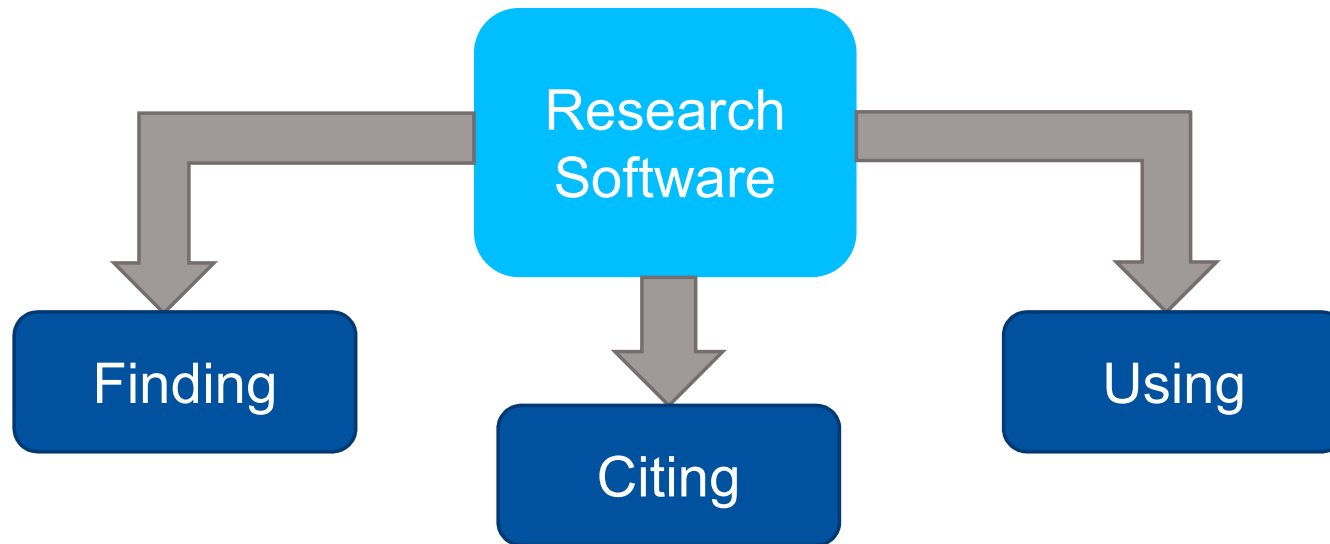
Licensing



Building on
[spdx-License List](#),
[choose-a-license](#) and
JoinUp-[SPARQL-Endpoint](#)

Describing Research Software Requirements

Describing



What research?
implemented methods, models

Where?
pid
link to code, executable

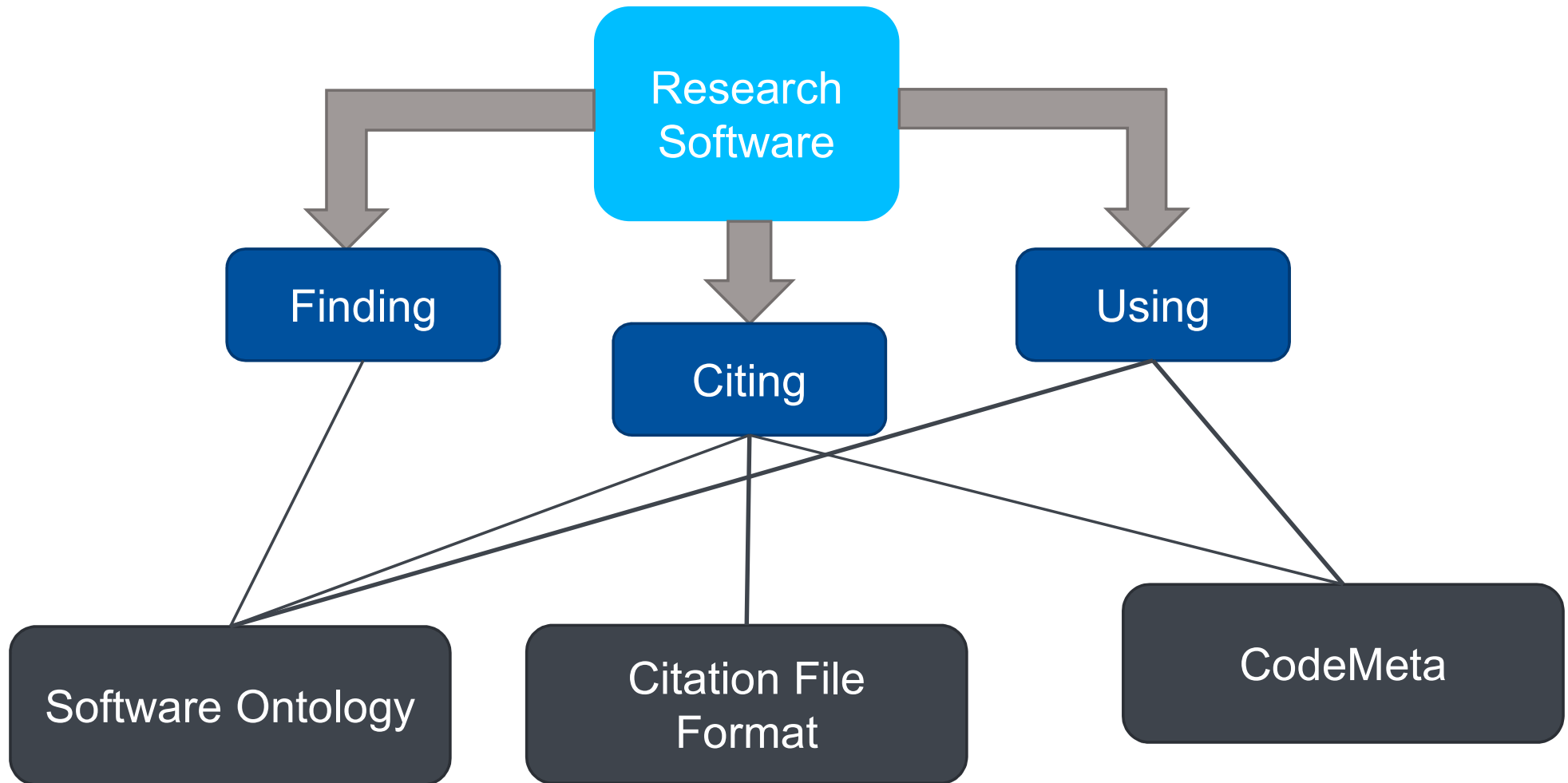
What?
name, version

Who?
authors, contributors

Can I use/base on?
quality, license, embargo
How to install?
dependencies, buildInstructions
How to run?
requirements, input, output,
execution parameters
Handling problems?
link to docu, issue tracker

Describing Research Software Standards

Describing



<http://ontosoft-earthcube.github.io/ontosoft/ontosoft%20ontology/v1.0.1/doc/>
<https://citation-file-format.github.io/>
<https://codemeta.github.io/>

Metadata Block for Dataverse basing on CodeMeta

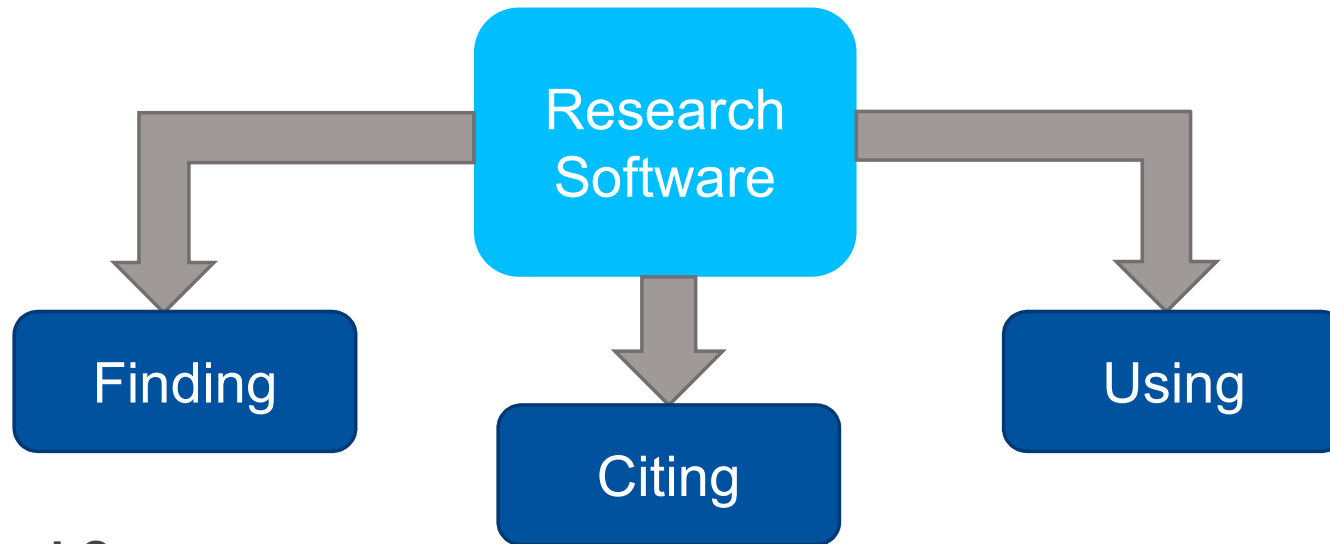
Describing

Citation Metadata ▾	
Metadata for Research Software ▲	
Software Version ?	v.1.3.0
Development Status ?	active
Code Repository ?	https://github.com/RePlay-DH/replay-dh-client
Programming Language ?	Java
Operating Systems ?	platform independent
Application Category ?	workflow tracking; visualization
Software Help/Documentation ?	https://github.com/RePlay-DH/replay-dh-client/blob/dev/README.md
Runtime Platform ?	Java 8
Release Notes ?	https://github.com/RePlay-DH/replay-dh-client/releases/tag/v1.3.0
Issue Tracker ?	https://github.com/RePlay-DH/replay-dh-client/issues

<https://github.com/IQSS/dataverse/pull/7877>

Describing Research Software Requirements

Describing



What research?
implemented methods, models

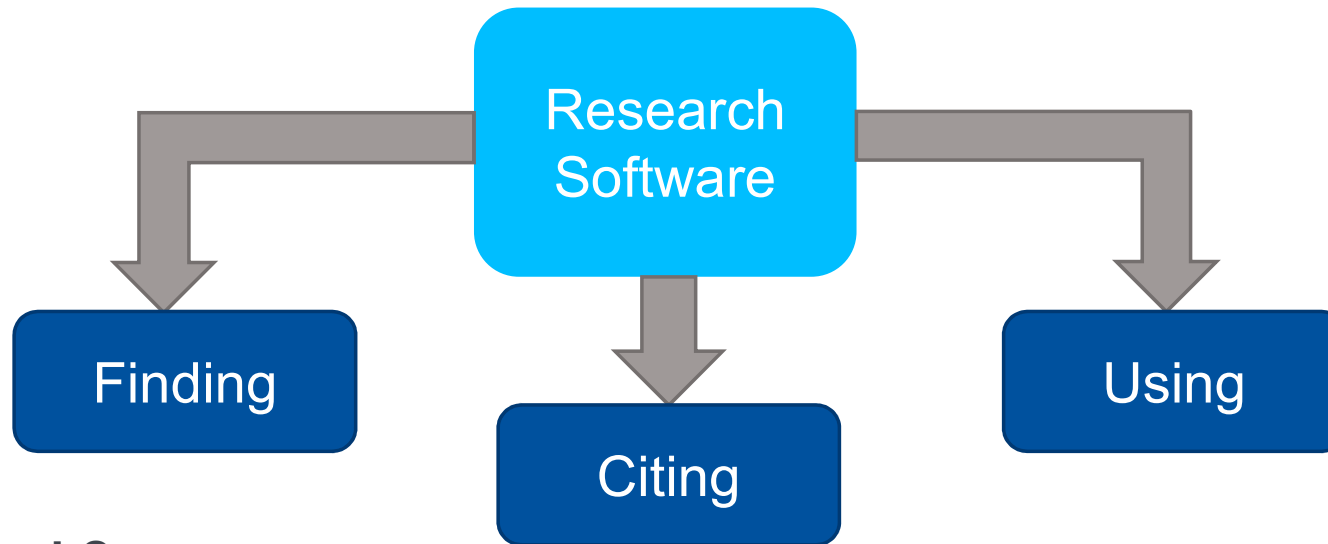
Can I use/base on?
quality

How to run?
input, output,
execution parameters

Information missing

Describing Research Software Requirements

Describing



What research?

implemented methods, models

- description
- keywords
- application(Sub)Category
- developmentStatus

Can I use/base on?
quality

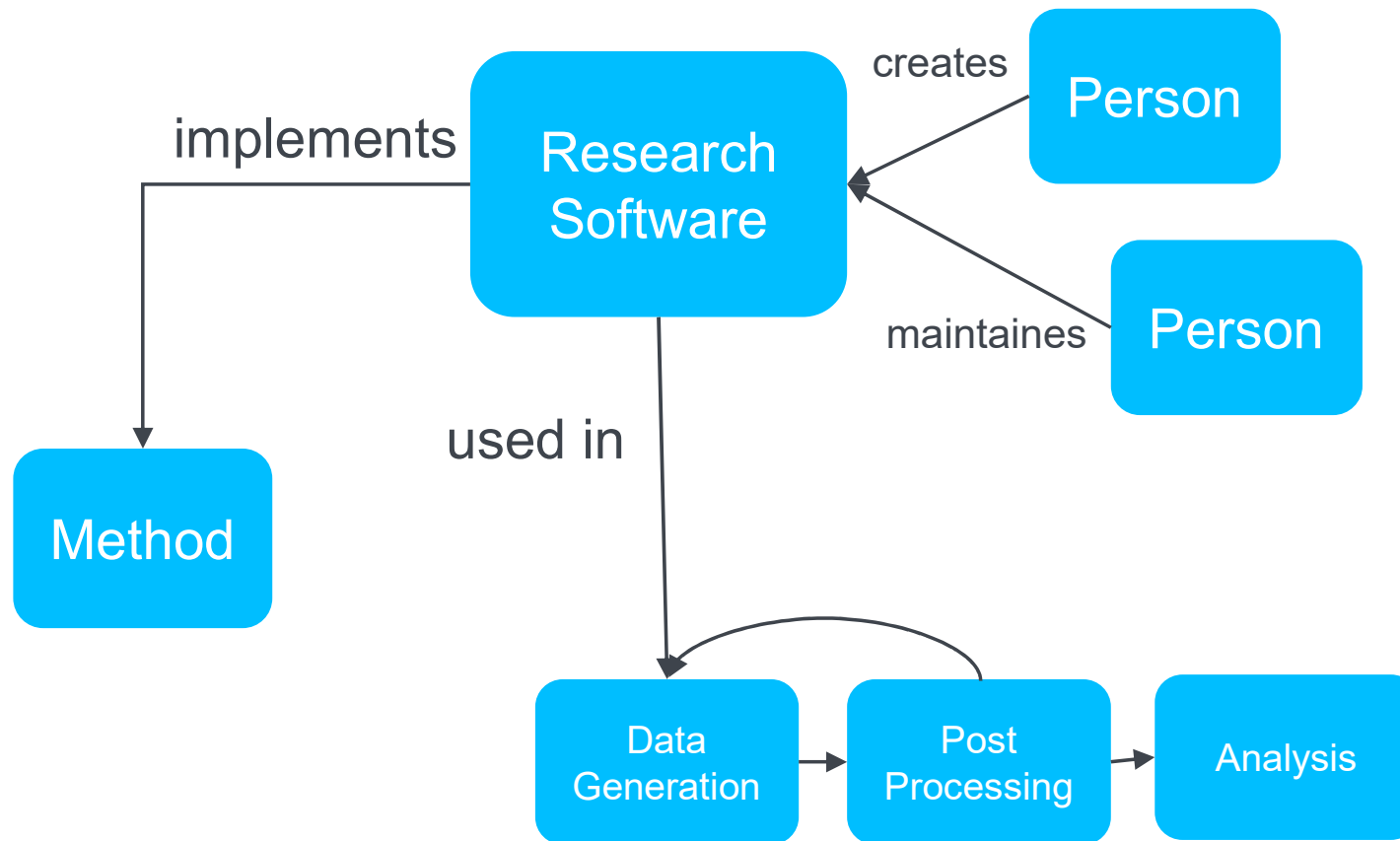
How to run?

input, output,
execution parameters

Describing Research Software

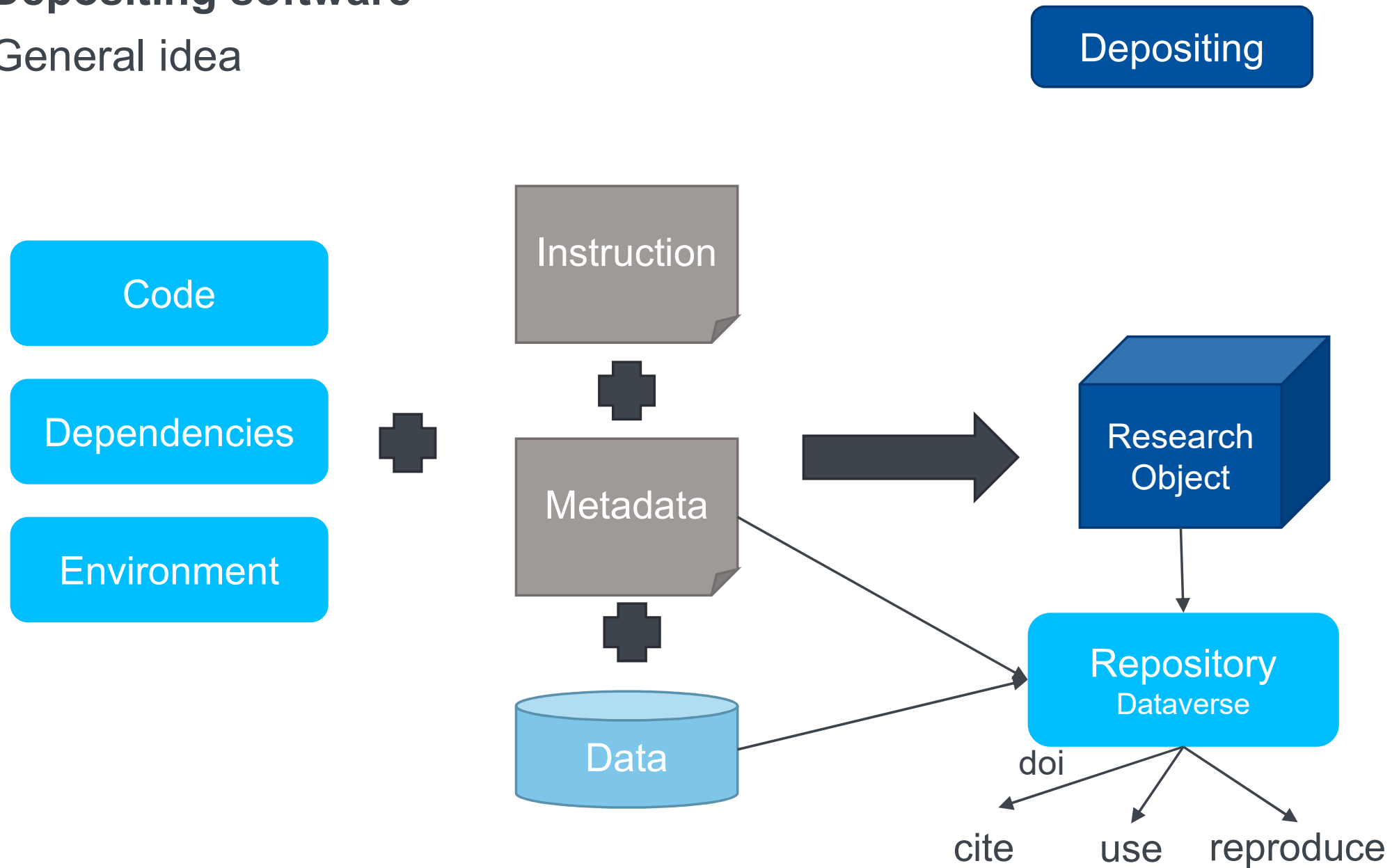
Knowledge Graphs and Semantic Web

Describing

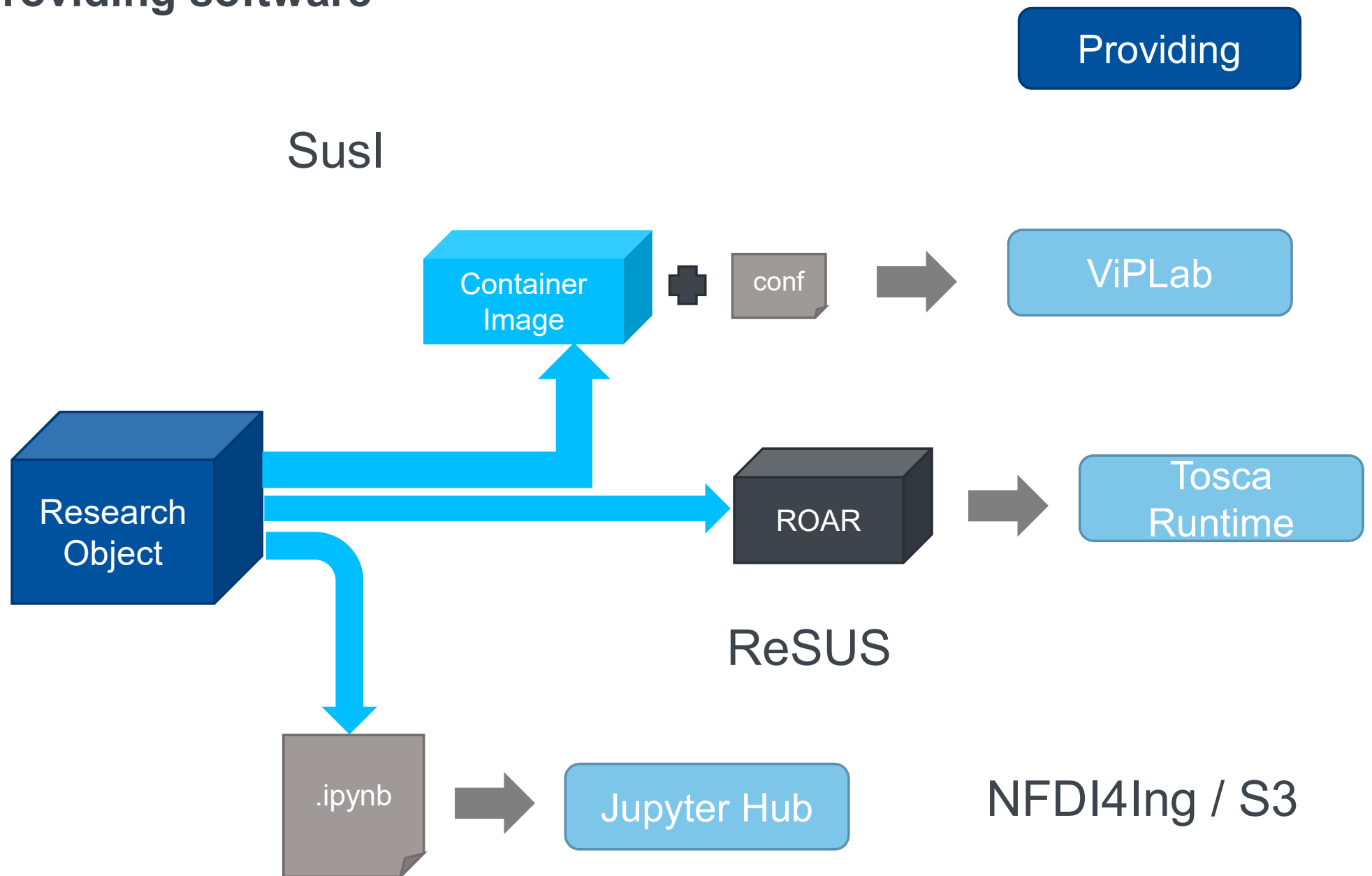


Depositing software

General idea

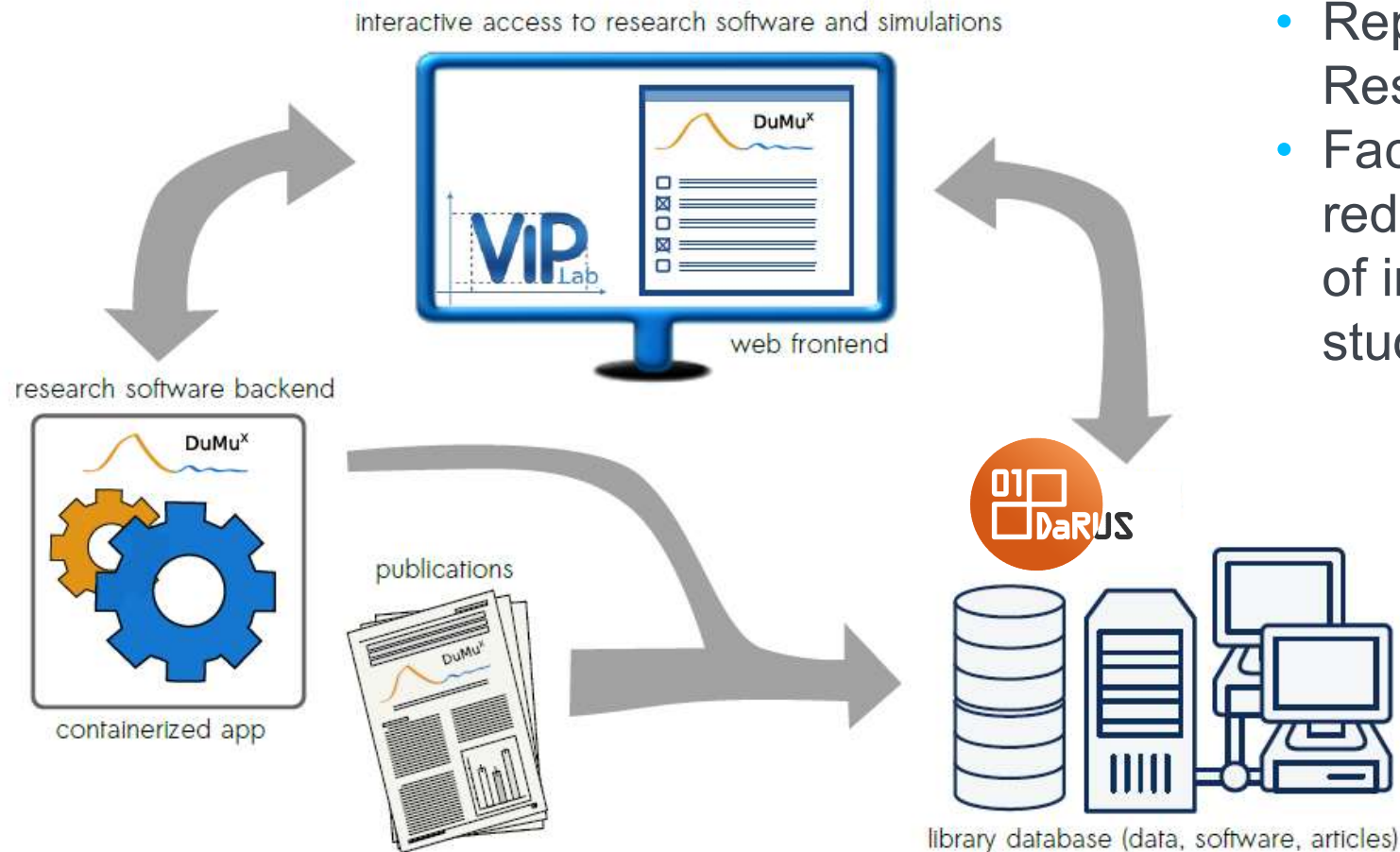


Providing software



Providing software

Virtual Programming Lab (ViPLab)



Use Cases:

- Reproducible Research
- Facilitate use by reducing complexity of inputs (e.g. for students, newbies)

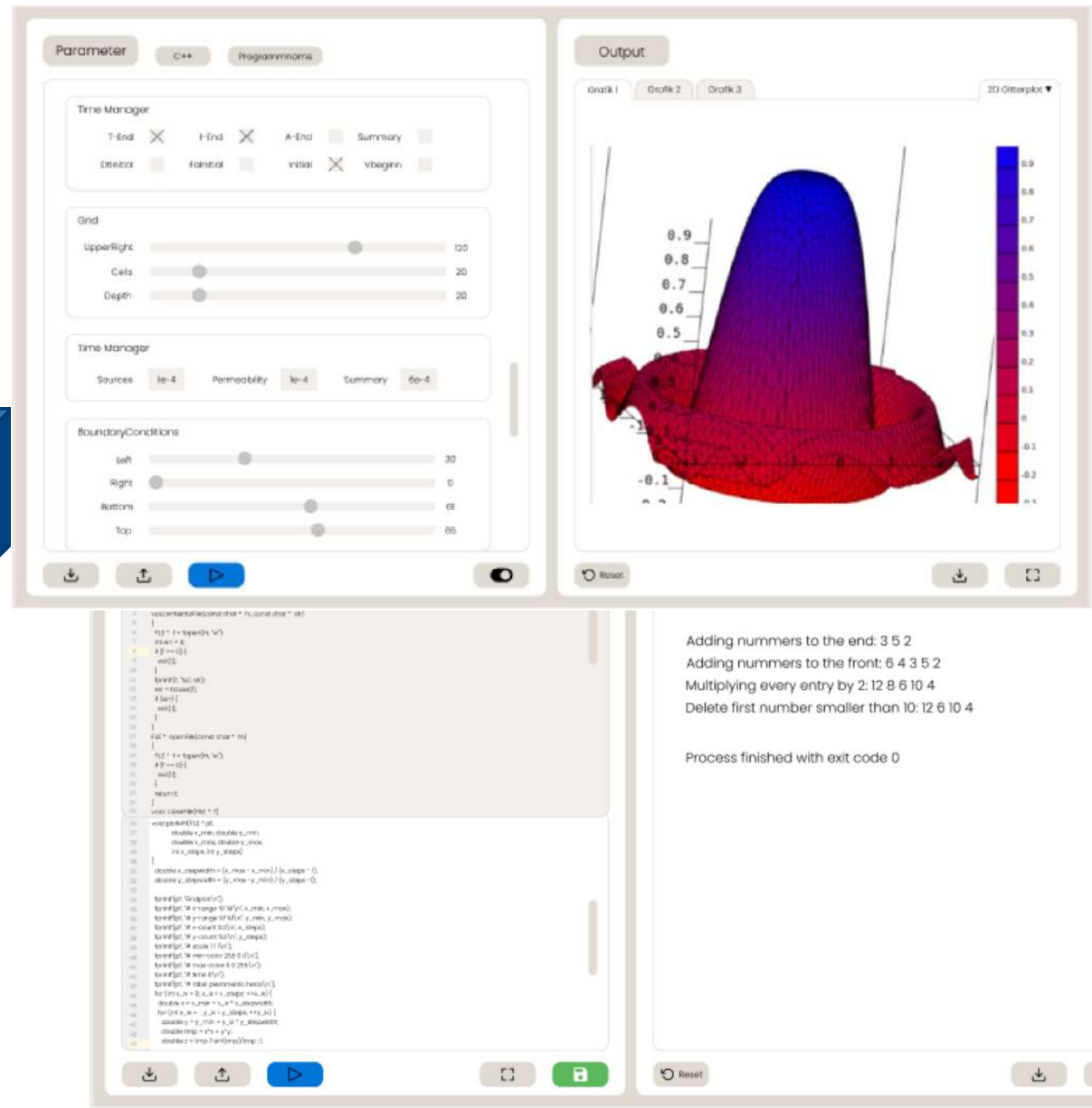
Providing software

Providing

ViPLab

DaRUS
Dataverse

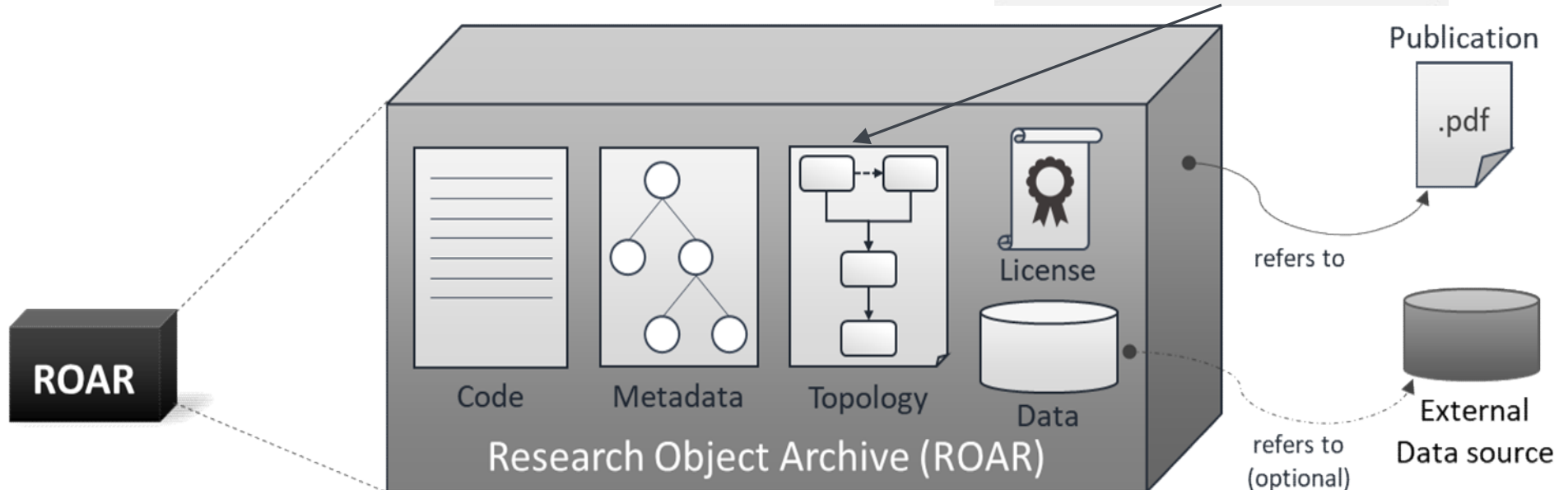
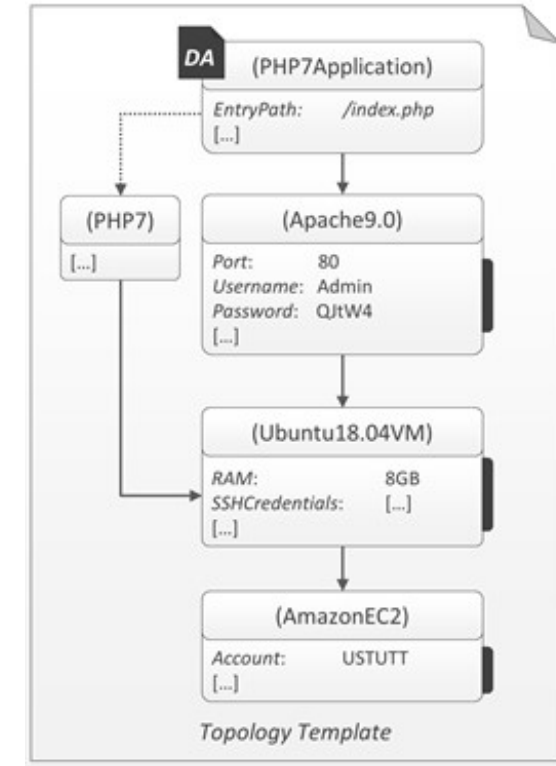
Research
Object



Modeling and packaging

Research Object Archive

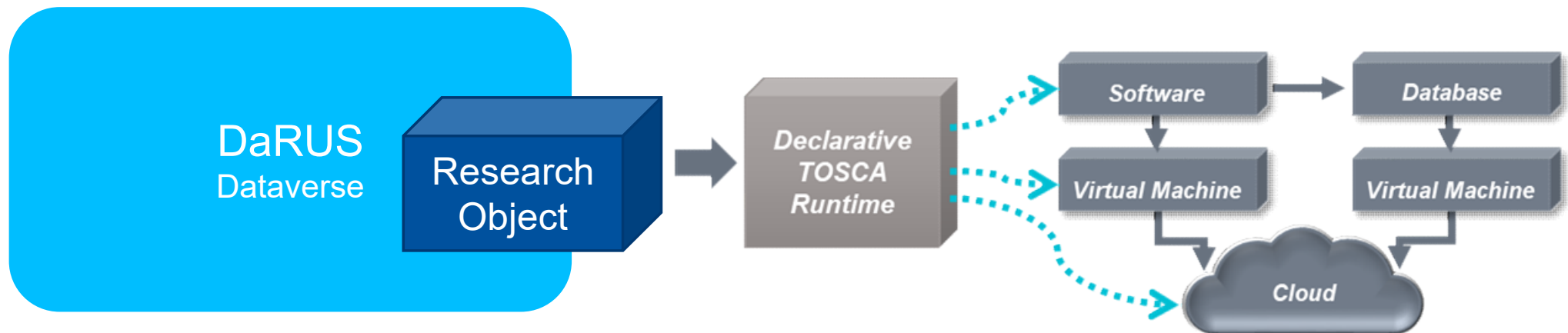
- Basing on the CSAR-Format of the [TOSCA-Standard](http://docs.oasis-open.org/tosca/TOSCA/v1.0/TOSCA-v1.0.html)³



³ <http://docs.oasis-open.org/tosca/TOSCA/v1.0/TOSCA-v1.0.html>

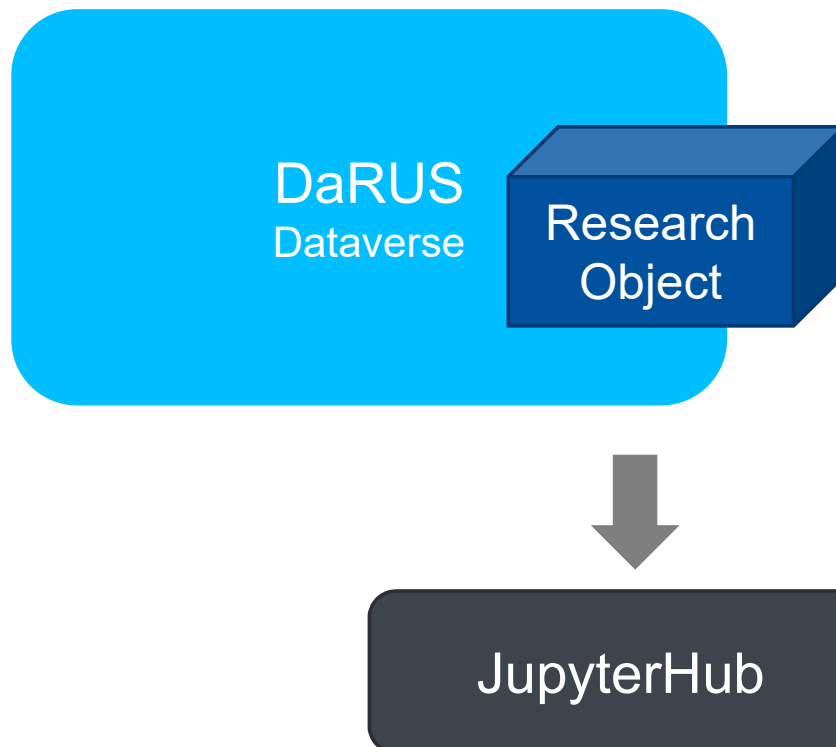
Providing software

Providing



Providing software

Providing



jupyterhub.tik.uni-stuttgart.de/user/ac129993/lab?

tabs Settings Help

jupyter_notebook.ipynb X

Importing all necessary packages

```
[1]: import funcs.formatting as form
import funcs.reading as r
import funcs.conversion as c
import funcs.iast as iast

import pandas as pd
import numpy as np
import matplotlib.pyplot as plt

import os

# get the current working directory
curr_dir = os.getcwd()
# decide whether or not to save the plots
save = True
if save == True:
    os.system('mkdir ./plots_output ./plots_output/eps ./plots_output/jpg')
# Do IAST calculations? See explanation below
include_IAST = True
if include_IAST: import pyiast
fs = 32
```

IAST calculations

To perform Ideal adsorbed solution theory we use pyIAST [1]. If you want to run the notebook on your computer, you probably have to install

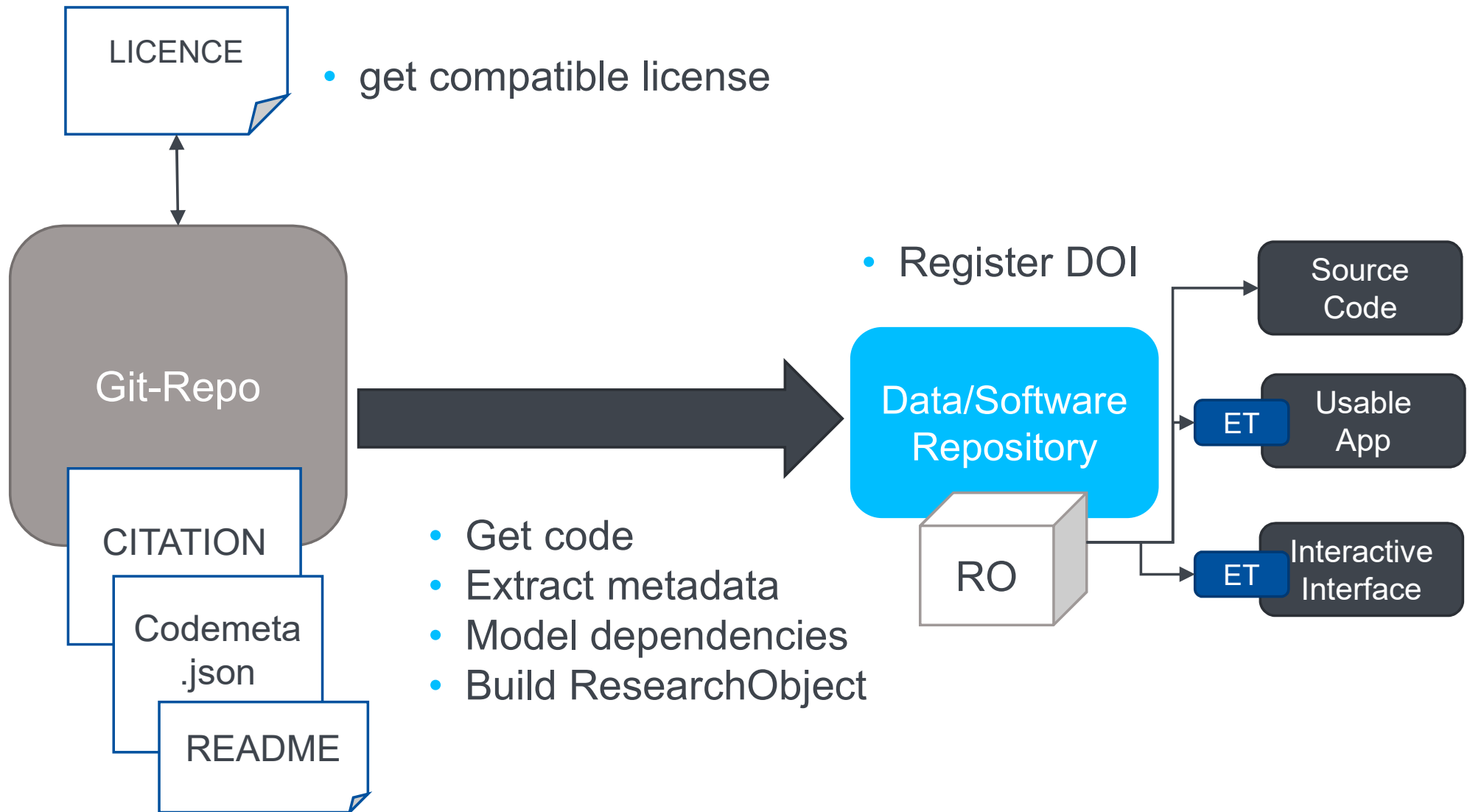
[1] <https://www.sciencedirect.com/science/article/pii/S0010465515004403>

[2] <https://pyiast.readthedocs.io/en/latest/>

All IAST calculations are done using the pure component isotherms obtained by GCMC simulations.

read all raw data to dataframes

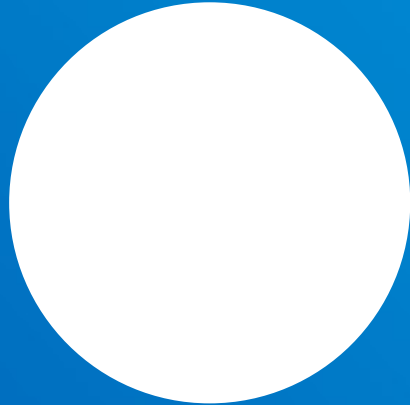
From the researchers point of view





University of Stuttgart
Germany

Thank you!



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phone +49 (0) 711 685-83648

Universität Stuttgart

FoKUS – Competence Center for Research Data Management

Holzgartenstr. 16, 70174 Stuttgart, Germany

Thank you!

Where to learn more about project HERMES?



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Oliver Bertuch, FZJ, PI, [@poi_ki_lo_therm](#)



Guido Juckeland, HZDR, PI, [@GuidoJuckeland](#)



Oliver Knodel, HZDR, [@olikno1](#)



Tobias Schlauch, DLR, [@TobiasSchlauch](#)

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- Go to software-metadata.pub