

Adamant: A JSON-Based Metadata Editor for Researchers

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Gemeinschaf

FROM IDEA TO PROTOTYPE



Outline

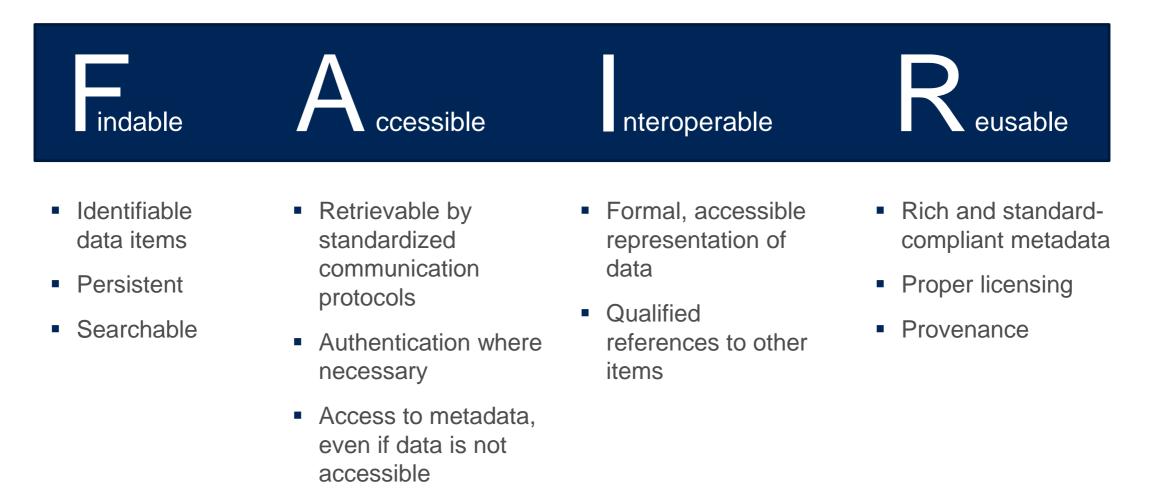
- Basics
 - FAIR data principles
 - Metadata
 - JSON Schema
 - Electronic lab. notebook (eLabFTW)
- Adamant
 - Architecture
 - Main features
- Live Demo
 - Setting up Adamant
 - RDM workflows with Adamant
 - Other workflows
- Outlook





Basics FAIR data principles

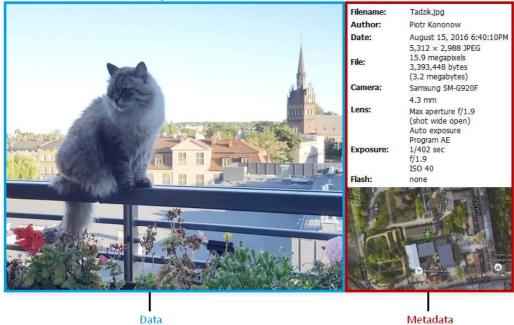
Seminal paper of M. Wilkinson *et al.* 2016 *Sci Data* **3**, 160018, https://doi.org/10.1038/sdata.2016.18 **The FAIR Guiding Principles for scientific data management and stewardship**



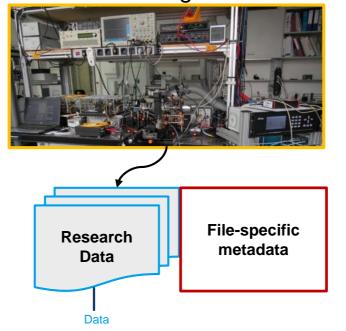


Basics What is metadata?

General setting



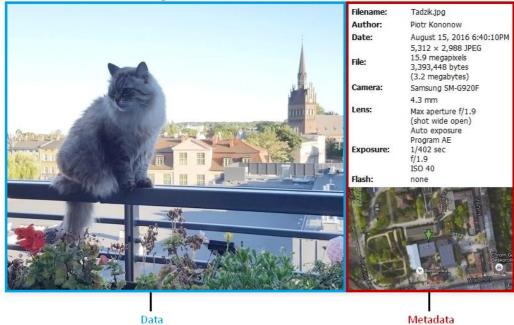
Research setting



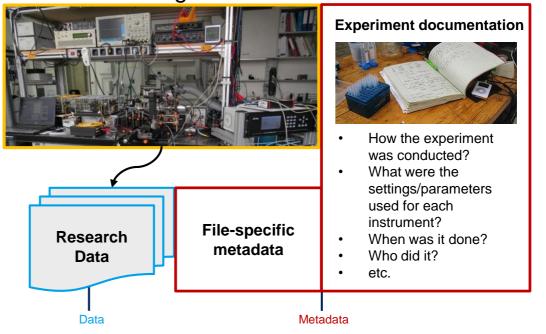


Basics What is metadata?

General setting



Research setting

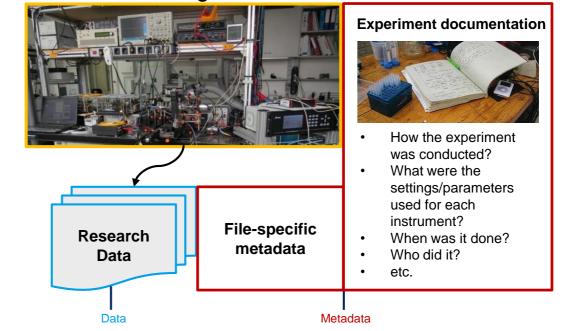




Basics What is metadata?

General setting Filename: Tadzik.jpg Author: Piotr Kononow August 15, 2016 6:40:10PM Date: 5.312 × 2.988 JPEG 15.9 megapixels File: 3,393,448 bytes (3.2 megabytes) Camera: Samsung SM-G920F 4.3 mm Lens: Max aperture f/1.9 (shot wide open) Auto exposure Program AE Exposure: 1/402 sec f/1.9 **ISO 40** none Data Metadata

Research setting



Metadata is simply data about data!





• From the main site:

"JSON Schema is a declarative language that allows you to annotate and validate JSON documents." – <u>https://json-schema.org/</u>



Basics JSON Schema – examples and validation

type": "string", ninLength": 2, naxLength": 3	<pre>{ "type": "object", "properties": { "number": { "type": "number" }, "street_name": { "type": "string" }, "street_name": { "type: "street_name": { "type: "street_name": { "type: "street_name": { "type: "street_name": { "type: "street_name": { "type: "street_name": { "type: "street_name": { "type: "street_name": { "type: "street_name": { "type: "street_name": { "type: "street_name": { "type: "street_name": { "type: "street_name": { "type: "street_name": { "type: "street_name": { "type: "street_name": { "type: "street_name": { "type: "street_name": { "type: "street_name": { "type: "street_name": { "type: "street_name": { "type</pre>
"A"	<pre>"street_type": { "enum": ["Street", "Avenue", "Boulevard"] } }</pre>
"AB"	<pre>{ "number": 1600, "street_name": "Pennsylvania", "street_type": "Avenue" }</pre>
"ABC"	If we provide the number in the wrong type, it is invalid:
"ABCD"	<pre>{ "number": "1600", "street_name": "Pennsylvania", "street_type": "Avenue" }</pre>
	By default, leaving out properties is valid. See Required Properties.
/pe": "number" }	<pre>{ "number": 1600, "street_name": "Pennsylvania" }</pre>
42	By extension, even an empty object is valid:
	{ }
-1 Simple floating point number:	By default, providing additional properties is valid:
	<pre>{ "number": 1600, "street_name": "Pennsylvania", "street_type": "Avenue", "direction": "NW" }</pre>
Exponential notation also works:	
2.99792458e8	JS package implementing JSON Schema validation:
Numbers as strings are rejected:	
"42"	🖌 🛛 🗛 🗸 Ajv JSON schema validator

nue", "Boulevard"] } nsylvania", "street_type": "Avenue" } pe, it is invalid: ennsylvania", "street_type": "Avenue" } See Required Properties. nsylvania" } lid: s is valid: nsylvania", "street_type": "Avenue", "direction": "NW" }



https://json-schema.org, https://ajv.js.org/



Basics Electronic lab. notebook – ElabFTW: an open-source general purpose ELN

- It's free and open source
- You can self-host it
- Flexible and generic, not only for notebook purposes
 - Experiment templates, easy to create and to tailor
 - Item database
 - Scheduler
 - And many other features

Experiments Back to listing < View mode	< Create
Started on 12.06.2022 Status Running Title Untitled Tass Add a tag	eLabFTW
File Edit View Insert Format Tools Table	
Procedure : Resulta : H1 - SMN	 Attached file JSON-metadatajson JSON-metadatajson Click to add a comment Load into JSON Editor
Linked items Add a step	Strip: Son Editor Corr
	 Save s Draw something ∑ Molecule drawer
	V 〇 恒 査 USER PANEL Powered by cLubTW 4.5.3 Page generated in 5.10572 seconds





Adamant

Technical paper (open peer review)



GitHub repository: https://github.com/plasma-mds/adamant

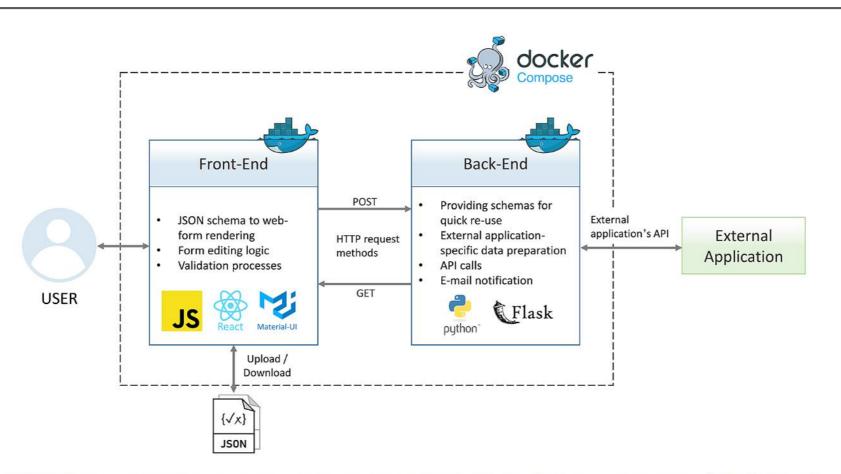
Live playground: https://plasma-mds.github.io/adamant/

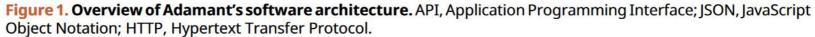
Chaerony Siffa I, Schäfer J and Becker MM. Adamant: a JSON schema-based metadata editor for research data management workflows [version 2; peer review: 3 approved]. *F1000Research* 2022, **11**:475





Adamant Architecture







Adamant Main features – rendering of editable user-friendly web-form

Input: JSON Schema file

```
{
   "$schema": "http://json-schema.org/draft-04/schema#",
   "id": "http://scanning-electron-microscopy",
   "title": "Scanning Electron Microscopy (SEM)",
   "description": "A schema to describe a Scanning Electron Microscopy used in an
       experiment (demo schema)",
   "type": "object",
   "required":["DeviceModel","SEMParameters"],
    "properties": {
        "DeviceModel": {
           "title": "Model of SEM Device",
            "description": "SEM device model used in the experiment",
            "type":"string"
       },
        "SEMParameters":{
            "title": "SEM Parameters",
            "description": "SEM parameters used in the experiment",
            "type":"object",
            "properties": {
                "AccelerationVoltage": {
                   "title": "Acceleration Voltage [kV]",
                    "description": "Voltage applied to accelerate the electrons",
                    "type": "number"
               },
                "WorkingDistance":{
                   "title": "Working Distance [mm]",
                    "description": "Distance from the lens to the sample/specimen",
                    "type": "number"
               },
                "ProbeCurrent":{
                   "title": "Probe Current [nA]",
                    "description": "Electrical current or electron beam focused on the
                       sample/specimen",
                    "type": "number"
               }
           }
      }
   }
```

Listing 1. Example of a draft-4 JSON schema containing typical schema-specific keywords presented in blue with their values presented in black, and field element keywords presented in red. JSON, JavaScript Object Notation.

Output: rendered editable web-form

Ad <u>amant</u> { 王 }		Edit "Working Distance [mm]"	×
BROWSE SCHEMA OR Gemo-schema json • OR CREATE FROM SCRATCH		Basic Descriptors: Field Keyword* WorkingDistance	
demo-schema,ison is a valid schema. You can now render the form. RENDER CLEAR	_ 1	A unique jaon keyword for this field. Usually short and has no Spaces are replaced automatically with "_" upon saving.	spaces (use "_" instead).
	B 🖌 🕓	Field ID/URI	
A schema to describe a Scanning Electron Microscopy used in an experiment (demo schema)	2	ID or URI for this field if available.	
Model of SEM Device *	 (1) 	Field Title Working Distance [mm]	
SEM device model used in the experiment		Label or title of the field. For a field that requires a unit, the u	mit can be placed within a
BEM Parameters* SEM parameters used in the experiment	 (a) 	square bracket, e.g., "Chamber Pressure [Pa]". Field Description Distance from the lens to the sample/specimen	
	5-22°		
	kV 🖌 📕	A detailed description of the field, how the input should be for Validation Related	maled, elc.
4)	kV 🖌 📕	A detailed description of the field, how the input should be for Validation Related: - Field Onto Type	maled, etc.
4) II Acceleration Voltage [kV]	kV × •	Validation Related: Field Data Type number	mated, etc.
Acceleration Voltage (kV) Voltage applied to accelerate the electrons		Validation Related:	-
A A A Acceleration Voltage [kV] Voltage applied to accelerate the electrons. Working Distance [mm]		Validation Related: Field Data Type number Data type of the field input. Minimum Value None None	-
Acceleration Voltage [kV] Voltage applied to accelerate the electrons. Working Distance [mm] Distance from the lens to the sampletpectmen	mm (5).	Validation Related: Field Data Type number Data type of the field input. Minimum Value None Set the minimum and macmum values of this field.	¥ 10
4) II Acceleration Voltage [kV] Voltage applied to accelerate the electrons. II Working Distance [mm] Distance from the ions to the sample/specimen II Probe Current [nA]	mm (5).	Validation Related: Field Data Type number Data type of the field input. Minimum Value None None	re
4) II Acceleration Voltage [kV] Voltage applied to accelerate the electrons. II Working Distance [mm] Distance from the ions to the sample/specimen II Probe Current [nA]	mm (55)	Validation Related: Field Data Type number Data type of the field input. Minimum Value None Set the minimum and maximum values of the field. Enumerated. Provide a list of possible inputs fi	re

Figure 3. Overview of the Adamant UI with a rendered web-form based on the schema in Listing 1 as an example. (A) Main corpus of the UI; (1) from left to right: JSON schema viewer, auto-populate form, edit schema description, revert all changes; (2) remove form field; (3) collapse or expand the field container; (4) field drag handle; (5) edit field description and (B) field editing panel (as a pop-up on top of the main UI) triggered by clicking (5) the edit button. UI, user interface; JSON, JavaScript Object Notation.

Adamant Main features – rendering of editable user-friendly web-form

Input: JSON Schema file

Fo	rm field specification in the schema
"Dev	<pre>riceModel":{ "title": "Model of SEM Device", "description": "SEM device model used in the experiment", "type":"string"</pre>
- ,	

Listing 1. Example of a draft-4 JSON schema containing typical schema-specific keywords presented in blue with their values presented in black, and field element keywords presented in red. JSON, JavaScript Object Notation.

o schema, joon is a valid schema. You can now render the form. RENDER CL

Rendered field

Model of SEM Device *

SEM device model used in the experiment

Figure 3. Overview of the Adamant UI with a rendered web-form based on the schema in Listing 1 as an example. (A) Main corpus of the UI; (1) from left to right: JSON schema viewer, auto-populate form, edit schema description, revert all changes; (2) remove form field; (3) collapse or expand the field container; (4) field drag handle; (5) edit field description and (B) field editing panel (as a pop-up on top of the main UI) triggered by clicking (5) the edit button. UI, user interface; JSON, JavaScript Object Notation.



Adamant Main features – validation of input data

Type checking and visual feedback

Scanning Electron Microscopy (SEM) schema to describe a Scanning Electron Microscopy used in an experiment (demo s	schema)
Model of SEM Device *	
SEM device model used in the experiment	
SEM Parameters* SEM parameters used in the experiment	^
Acceleration Voltage [kV] 15	kV
Voltage applied to accelerate the electrons	
Working Distance [mm] 6.7	mm
Distance from the lens to the sample/specimen	
Probe Current [nA]	nA
Electrical current or electron beam focused on the sample/specimen	

canning Electron Microscopy (SEM) schema to describe a Scanning Electron Microscopy used in an experiment (de	نیا mo schema)]
Nodel of SEM Device *		
Nodel of SEM Device' field must be filled (required)		
SEM Parameters* SEM parameters used in the experiment - Acceleration Voltage [kV]- 15		kV
Voltage applied to accelerate the electrons		κv
Working Distance [mm]		mm
Distance from the lens to the sample/specimen Probe Current [nA] 850		nA
Electrical current or electron beam focused on the sample/specimen		



Adamant Main features – downloadable schema and JSON data

Type checking and visual feedback

Scanning Electron Microscopy (SEM) A schema to describe a Scanning Electron Microscopy used in an experiment	(demo schema)
Model of SEM Device *	
SEM device model used in the experiment	
SEM Parameters* SEM parameters used in the experiment	^
Acceleration Voltage [kV] 15	kV
Voltage applied to accelerate the electrons	
Working Distance [mm]6.7	mm
Distance from the lens to the sample/specimen	
Probe Current [nA] 850	nA
Electrical current or electron beam focused on the sample/specimen	

canning Electron Microscopy (SEM) schema to describe a Scanning Electron Microscopy used in an experim	u u	
Model of SEM Device *		
Model of SEM Device' field must be filled (required)		
SEM Parameters* SEM parameters used in the experiment Acceleration Voltage [kV]		
15		kV
Voltage applied to accelerate the electrons Working Distance [mm]		
6.7		mm
Distance from the lens to the sample/specimen		
- Probe Current [nA]		nA
Electrical current or electron beam focused on the sample/specimen		
Electrical current or electron beam focused on the sample/specimen		





Adamant Main features – downloadable schema and JSON data

Downloaded JSON data collected / metadata

JSON	Ra	w Data H	eader	S	
Save	Сору	Collapse All	Expar	nd All	🗑 Filter JSON
Dev	iceMod	el:		"JEOL	JSM-7500F"
▼ SEMI	Parame	ters:			
A	ccele	rationVolta	ge:	15	
h	WorkingDistance:			6.7	
F	ProbeCurrent:			850	

JSON	Raw Data	Headers
Save C	opy Pretty P	Print
"SEMP "Ac "Wo	arameters":	/oltage": 15, nce": 6.7,





Live Demo Setting up Adamant for development and deployment

GitHub repository: https://github.com/plasma-mds/adamant

Development

Setting up Adamant on a local machine for development:

- \$ git clone https://github.com/csihda/adamant.git —clone the repository
- \$ cd adamant —go to adamant project directory
- adamant\$ npm install —install the dependencies for the client-side
- adamant\$ cd backend —go to backend directory
- adamant/backend\$ python -m venv venv —create a python virtual environment
- adamant/backend\$./venv/Scripts/activate —activate the virtual environment
- adamant/backend\$ pip install -r requirements.txt —install the dependencies for the back-end
- adamant/backend\$ cd .. —go back to adamant project directory
- adamant\$ yarn start-api —start the back-end
- adamant\$ yarn start —on a new terminal, in the adamant project directory, start the front-end

By default, Adamant is accessible at http://localhost:3000 .

Deployment

We recommend deploying Adamant with docker-compose, which can be done with ease:

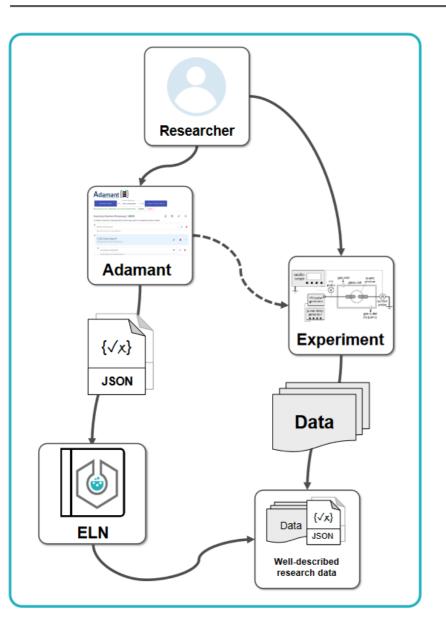
- \$ git clone https://github.com/csihda/adamant.git —clone the repository
- \$ cd adamant —go to adamant project directory
- adamant\$ docker-compose build —build the docker images for both back-end and front-end
- adamant\$ docker-compose up -d —start both client and server containers, i.e., the whole system

By default, the deployed system can be accessed at http://localhost:3000.



Live Demo

Generic schema-based metadata collection

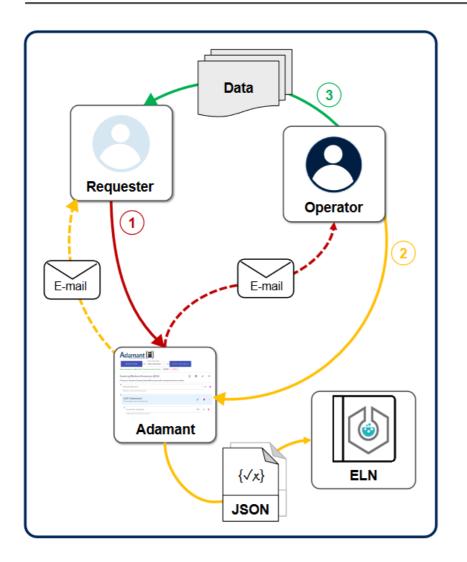


- Browse, select, or create experiment schema and render the web-form
- Fill in relevant information regarding the experiment
- Submit to store experiment metadata and the used schema in the ELN system
- Experiment metadata can be re-used for dataset publication and other automated processes



Live Demo

Job request of scientific instrument operation



□ Motivation:

Only a handful of researchers can operate a certain advanced scientific instrument. The instrument has to be more accessible to researchers with different skillsets to improve research outputs. A more automated workflow to request an instrument operation is required to make life easier.

Workflow:

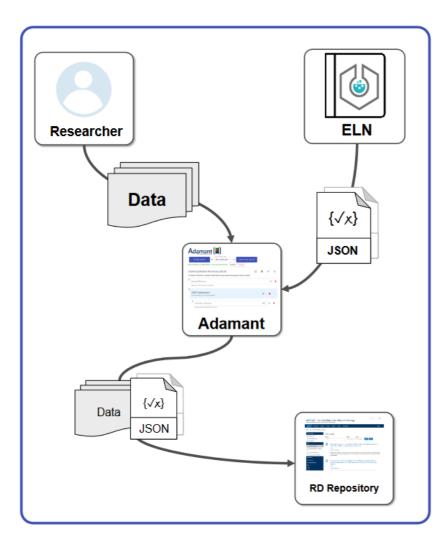
- (1) Job request initiation by the requester (researcher who is not an expert on the instrument);
- (2) Processing of the request by the operator (expert on the instrument), experiment metadata is stored in ELN;
- (3) Handing of research data (results) from operator to requester





Other workflows

Dataset preparation and publication (under preparation)



- Gather and load the data into Adamant
- Re-use experiment metadata stored in the ELN system

to describe the dataset

- Adjust or extend the metadata as needed
- Submit the prepared dataset to a research data repository system (e.g., <u>https://www.inptdat.de</u> for datasets related to plasma science and technology)



Other workflows

Compilation of input configurations for plasma simulations (under preparation)

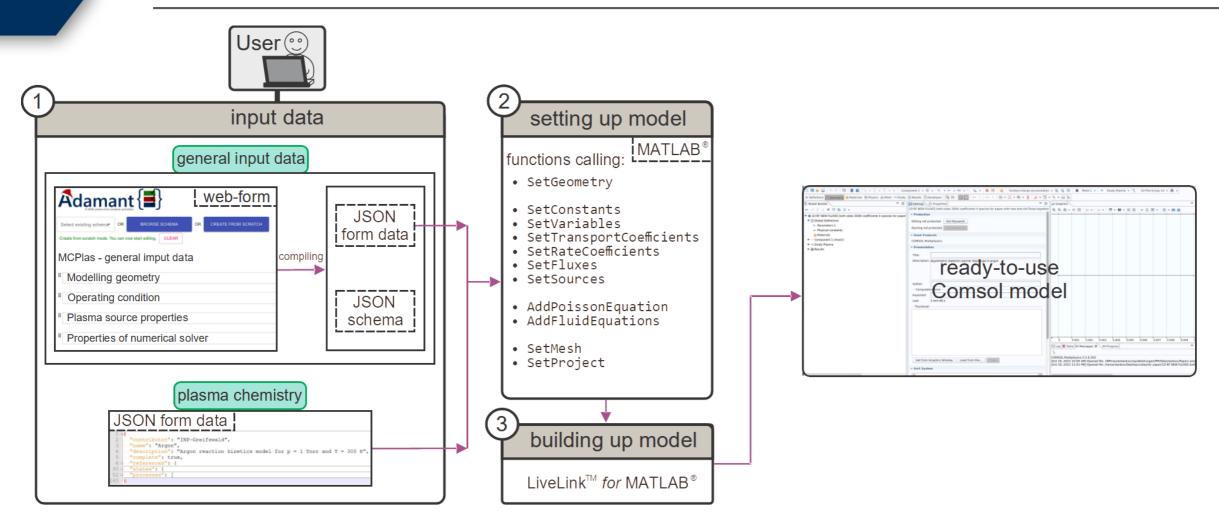


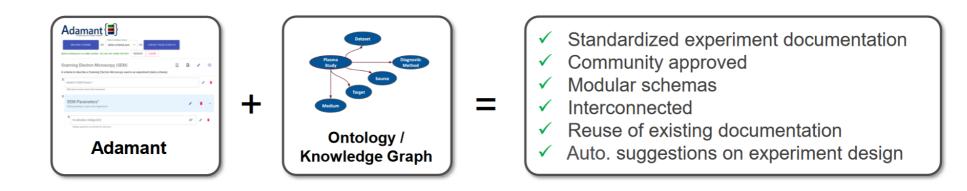
Figure credit: Marjan Stankov





Outlook Further feature developments

- More JSON Schema keyword implementations
- Better UI and UX
- Ontology / Knowledge graph integration



Many more!





Acknowledgement

RDM@INP

From left to right:

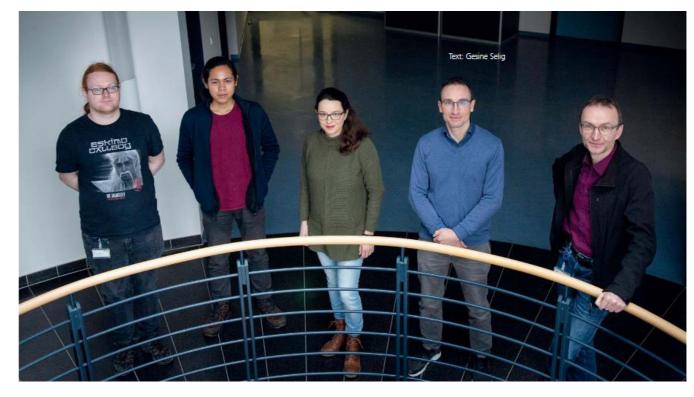
Nick Plathe

Ihda Chaerony Siffa

Laura Vilardell Scholten

Markus M. Becker

Steffen Franke (Alumnus)



BMBF Project:

SPONSORED BY THE

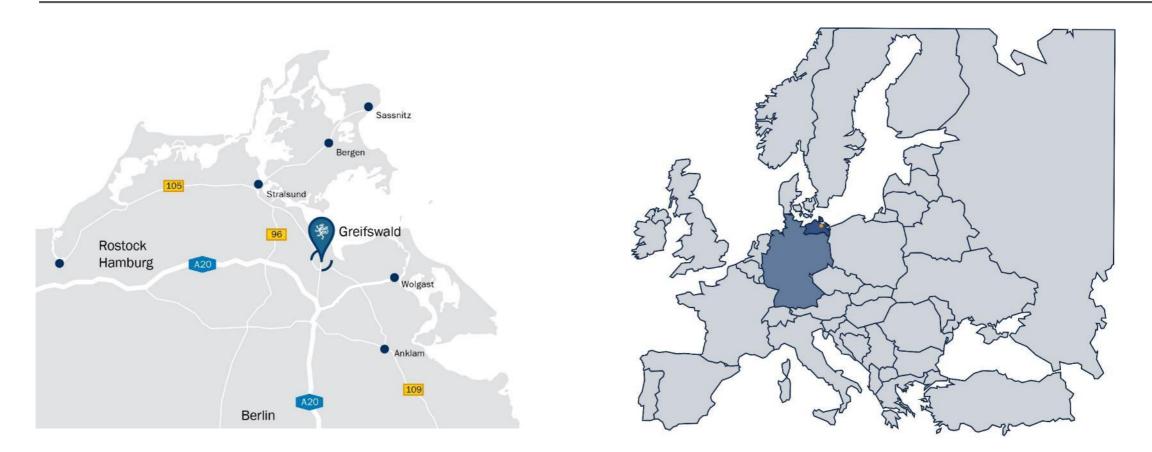


Federal Ministry of Education and Research The German Federal Ministry of Education and Research (BMBF) funded this work under the grant mark 16QK03A





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