Project DiMoGraph

Experiments → Data
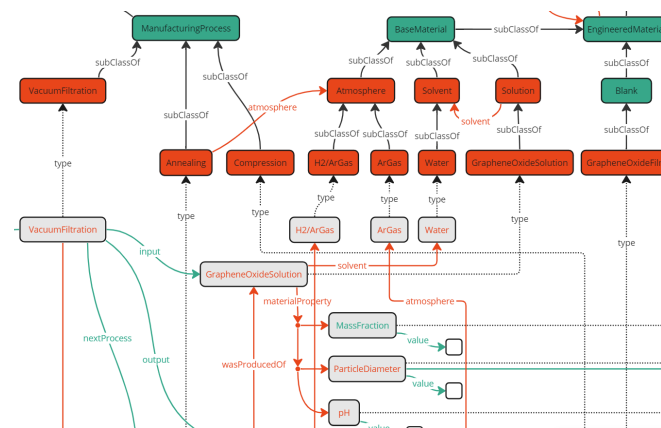
Production and characterization processes

Simulation → Data

Calculation of conductivity using a network model

Data-based surrogate model → Data

Fast, efficient model for data generation

Ontology & knowledge graph

- Semantic description
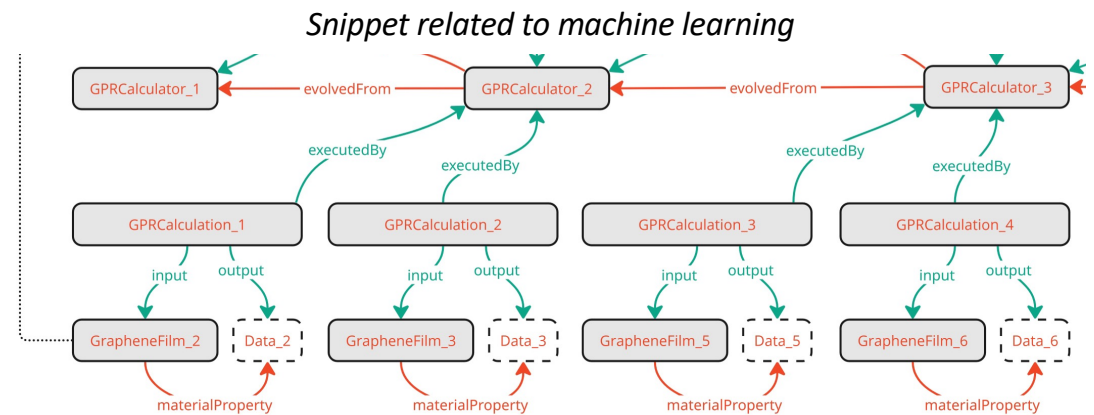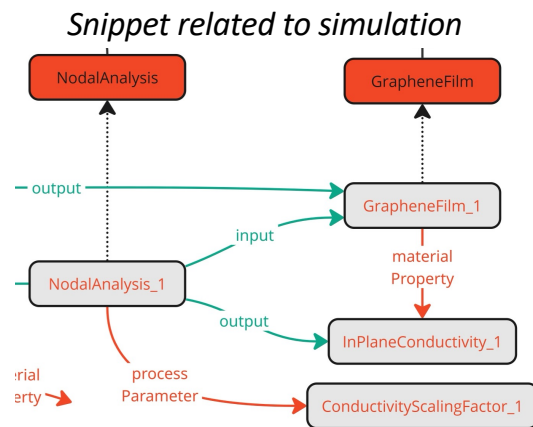- Uniform, standardized format

4 development stages

- Ontology concept
- Ontology implementation
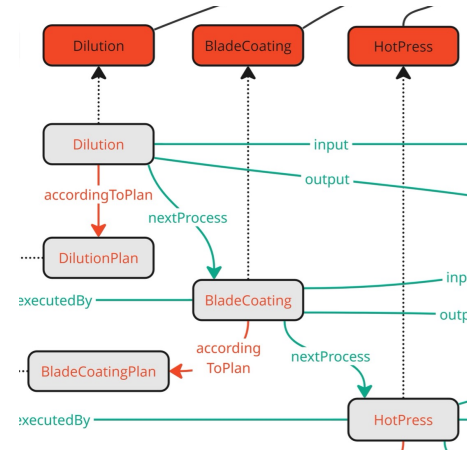- Database implementation
- Database creation
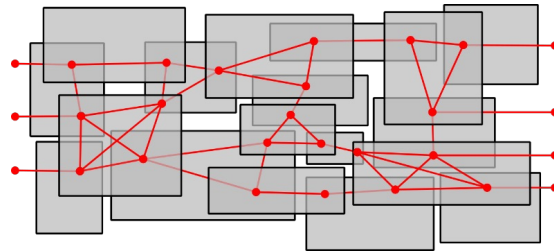
OntoGraph

OntoGraph

- An ontology for describing graphene based macromaterials
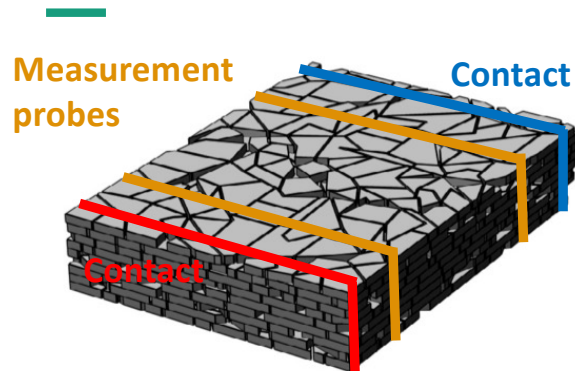- Based on PMD Core Ontology 2.0
- Can describe experimental data, simulation data, and machine learning data / training

Snippet related to experiment

Snippet related to simulation

Snippet related to machine learning

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Network model (GraConSi)

Measurement probes

Contact

Contact

σ_{in}^{micro}

σ_{out}^{micro}

$$\begin{pmatrix} G_{11} & G_{12} & \dots & G_{1N} \\ G_{21} & G_{22} & \dots & G_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ G_{N1} & G_{N1} & \dots & G_{NN} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_N \end{pmatrix} = \begin{pmatrix} i_1 \\ i_2 \\ \vdots \\ i_N \end{pmatrix}$$

1. Construction of the model

- Multiple layers of random flakes

Rizzi et al., *Comput. Mater. Sci.* **161**, 364 (2019)
Rizzi et al., *ACS Appl. Mater. Interfaces* **10**, 43088 (2018)

2. Calculation of flake overlaps between adjacent layers

- Finding all relevant connections
- Calculation of overlap areas

3. Computation using nodal analysis

- Conductance matrix creation
- Calculation of potentials
- Conductivity based on voltage drop between probes
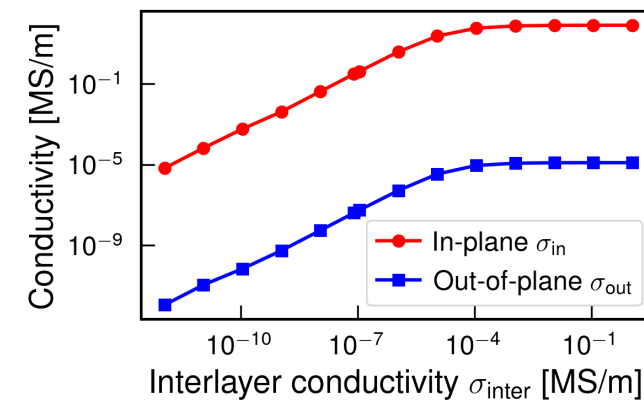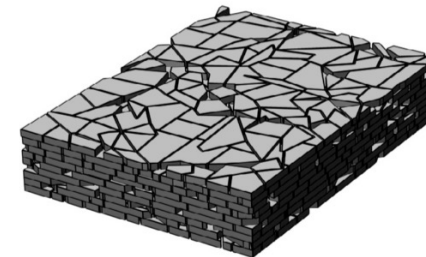
Project DiMoGraph

Use case 1: network simulation

GraConSi
- Own network simulation tool
- Nodal analysis to calculate the conductivity (in-plane, out-of-plane)

Digital description
- Semantic data description
- Store all input / output data in ontology / knowledge graph
- Workflow automatized with pyron

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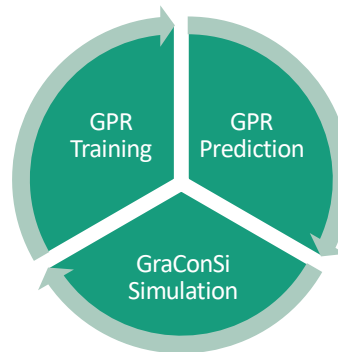
Use case 2: data model and training

Surrogate model

- Gaussian process regression (GPR)
- Fast, sufficient accuracy
- Uncertainty quantification
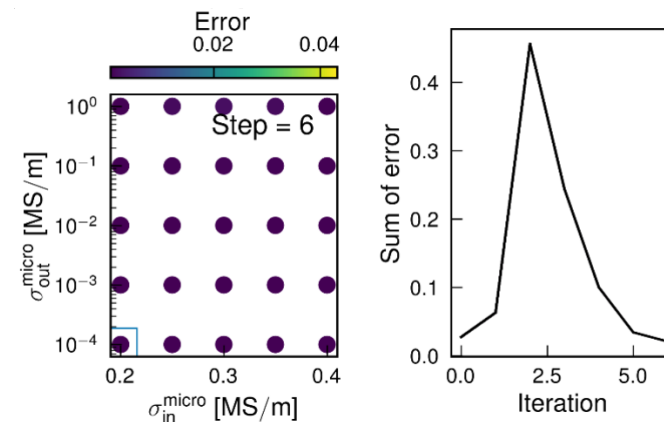
GPR training

Iteratively add new data points

(1) Predict properties with GPR
(2) Perform GraConSi simulation
    for data with highest uncertainty
(3) GPR training with new data

Digital description

- Semantic data description
- Store all input / output data in ontology / knowledge graph
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Project DiMoGraph

Use case 3: digital lab book

Production of graphene-based materials
- Dilution processes
- Vacuum filtration or blade coating
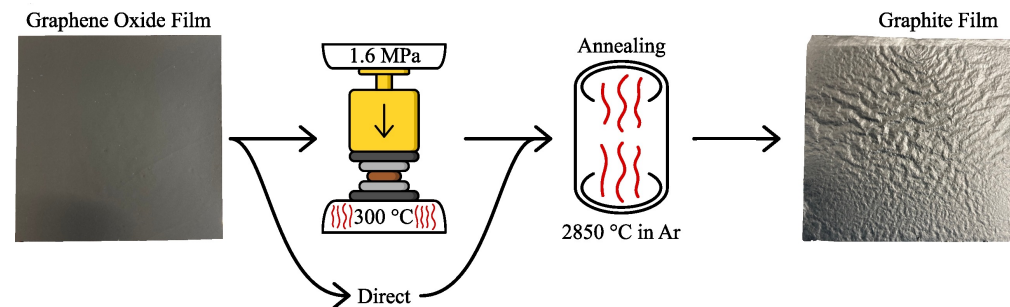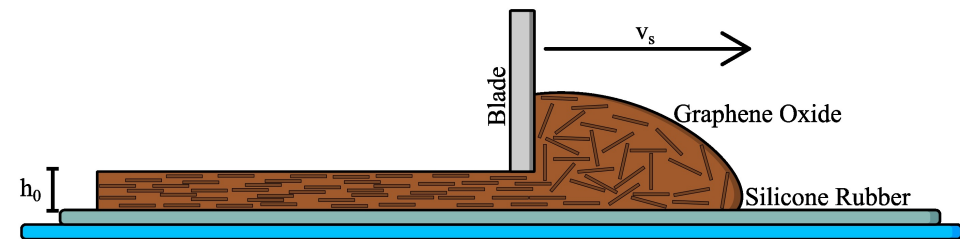- Post treatment with hot press and annealing

Various measurements
- Eddy current, viscosity, shear stress, thickness, mass

Digital description
- Standardized formats: Excel --> json --> rdf
- Interactive app to enter, change and store data
- Scripts for automatic data visualization

L. Niemann et al., *Diamond and Related Materials* **147**, 111310 (2024)

Project DiMoGraph

Graphene conductor database

Blade coating   Hot press   Annealing   **Samples**   Analyze data   SPARQL query

🛢 **Samples**	
91	

Select sample

GIC-022-1   ▼

Add new sample

Delete selected sample

Production   graphene oxide film   **graphene film**

Add property	Delete selected property ⓘ	Add dependend property	Delete selected dependent property ⓘ

property	value
diameter	35.0 mm
mass	(0.011 ± 0.0001) g
sheet resistance	(488.2924 ± 1.5065103) mOhm/sq

pressure	thickness	conductivity
2.0 kPa	(29.4 ± 2.4) μm	(70.0901 ± 1.14432812) kS/m
500.0 kPa	(5.5 ± 0.4) μm	(374.663 ± 27.24821818) kS/m

Eddy current measurement: Suragus output

Delete	Exchange

Eddy current measurement: Sheet resistance map

Project DiMoGraph

Graphene conductor database

Blade coating   Hot press   Annealing   Samples   **Analyze data**   SPARQL query
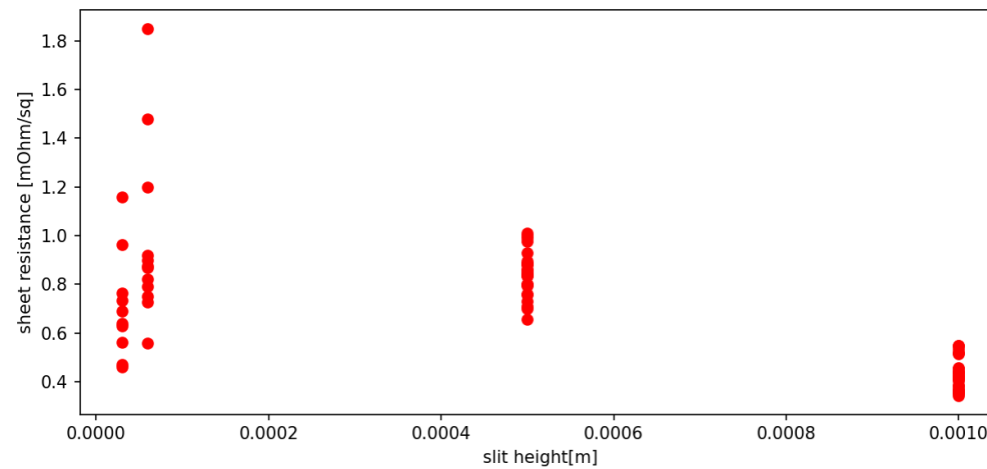
x axis property

blade coating: slit height ▾

y axis property

sheet resistance ▾

Correlation coefficient

-0.661

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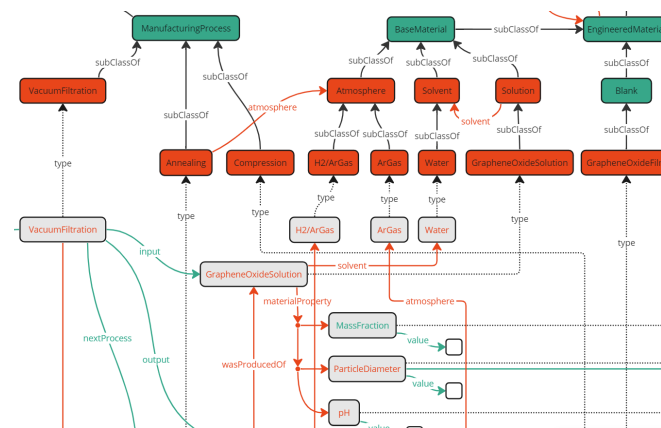- Uniform, standardized format

Simulation

Calculation of conductivity
using a network model

Data →

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- Database creation

**Data-based
surrogate model**

Fast, efficient model for
data generation

Data →