Coupled Process Chain Modeling

IGF Project No. 21884 N

5th Project Advisory Committee Meeting

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28th Nov, 2023

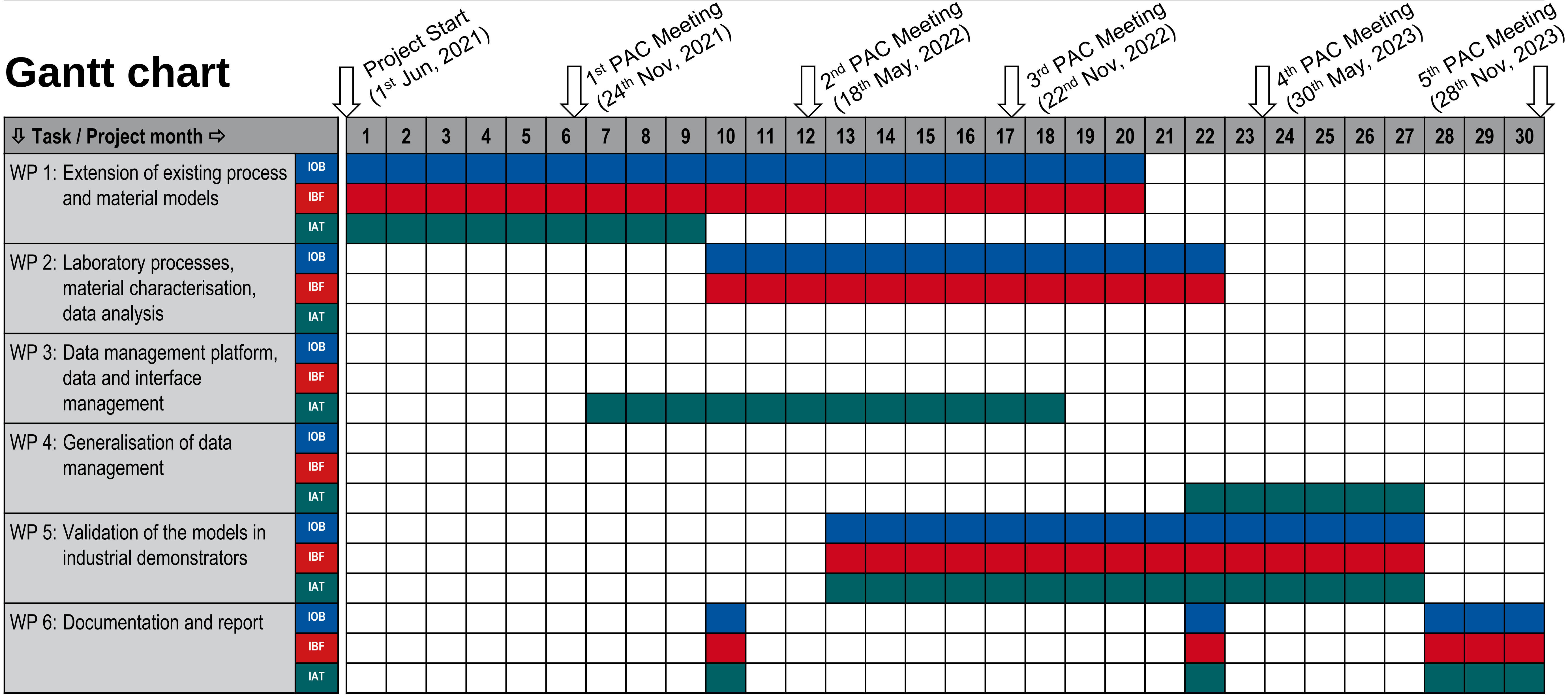
Project Framework

Project advisory committee (PAC)

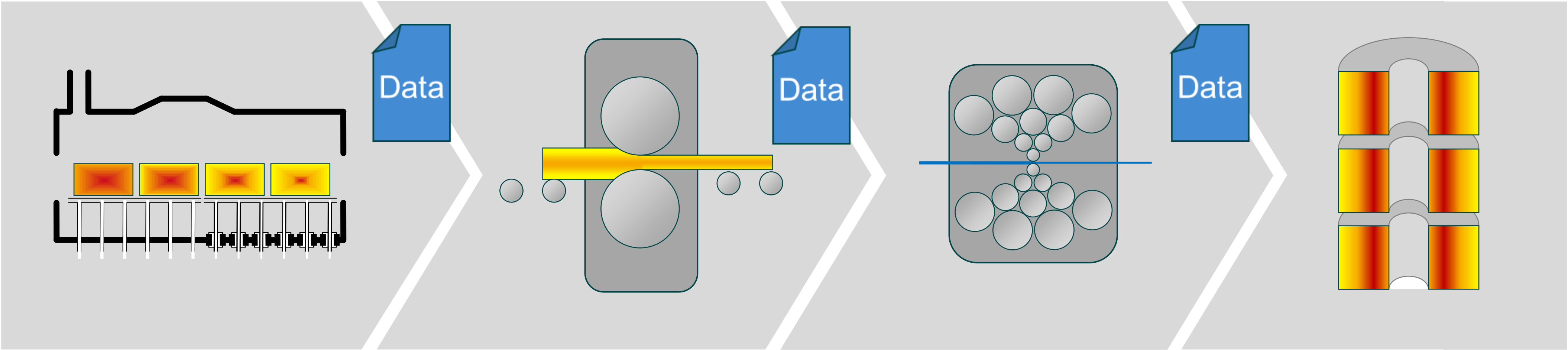
PAC chairperson: *Dr. Hansjochen Oertel, GIWEP GmbH*

Project Framework

Gantt chart



Coupled Process Chain Modelling



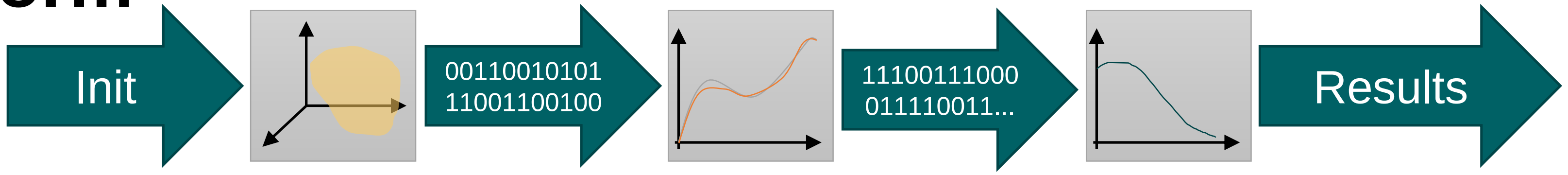
- Analysis of existing process models
  - Data basis
  - Considered physical quantities
- Define relevant input and output data for coupling
- Model adaptation / model extension
  - Providing output data
  - Use of new input data
- Data exchange with a „data platform“
  - Uniform data formats
  - Semantic annotation
  - Defined interfaces
- Unified execution environment for process models

Data management and simulation platform

Linking of data and models

Structure of the simulation platform

- Programmed with Python3 language on Linux operating system
- Communication with the user through a Flask based RESTful API
  - stateless
  - HTTP protocol
  - JSON message format
- Data storage in MongoDB, MinIO and Redis
- Components are running on their own Docker containers as services



Wrapper library

- Upload und download process and simulation data
- Generating the data structure
- Automatic unit conversion

Wrapper scripts

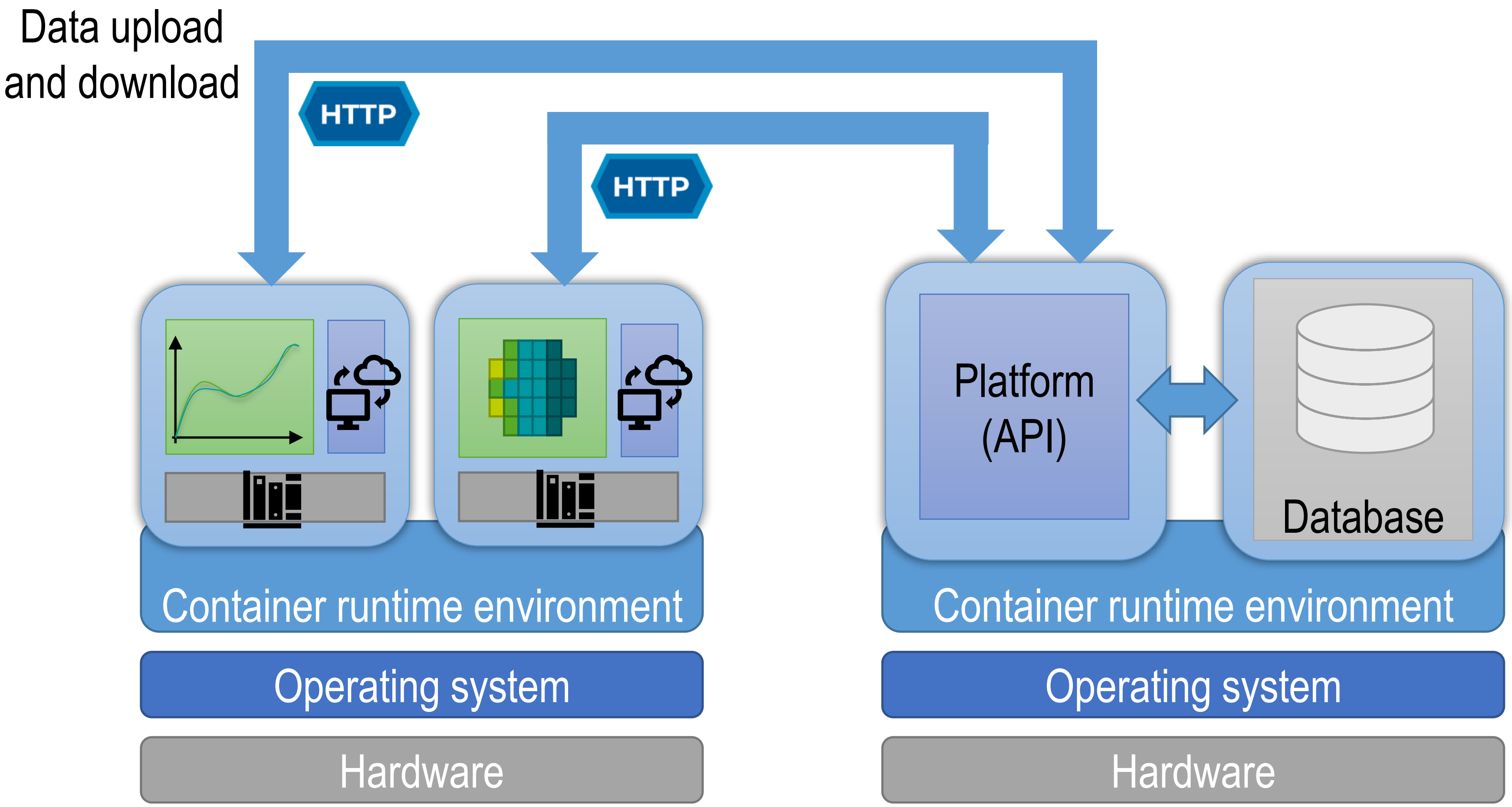
- Configure and start the simulations
- Communication with the platfrom’s API

Docker container

- Executable software package, which contains every element for running a simulation
- Several containers can run simultaneously
- Encapsulates its content

Data management and simulation platform

Structure of the simulation platform



Data storage

- API is stateless

→ Use of database storage technologies

MongoDB

- NoSQL
- Storage for metadata
- Speicherung einzelner Ergebnisse
- JSON-LD (JavaScript Object Notation for Linked Data)


```
"sosa:observedProperty": {
    "@type": ["qudt:Quantity", "sosa:ObservableProperty"],
    "qudt:hasQuantityKind": [{"@id": "cpmProcess:atmosphereTemperature"}],
    "rdfs:label": "Temperature in the oven 04",
    "ssn:isPropertyOf": {
        "@id": "http://acplt.org/individual/gpkm/factory/productionUnits#oven04",
        "@type": "cpm:ProductionUnit"
    }
},
"cpm:relativeAccuracy": 0.01,
"sosa:hasResult": {
    "@type": ["sosa:Result", "qudt:QuantityValue"],
    "qudt:numericValue": 25.5,
    "qudt:unit": {"@id": "unit:DEG_C"}
},
```


What kind of measurement?

What value?

MinIO

- Object storage
- Arbitrary data formats (e.g. zip)
- Multidimensional data (matrices)
- HDF5 (Hierarchical Data Format)

Redis

- RedisQueue stores its data in Redis

Data management and simulation platform

Database structure

mongoDB

Collection „datasets“

- ID
- observations
- metadata
  e.g. creator

Collection „simulators“

- ID
- Docker container registry URL
- metadata

Collection „input“

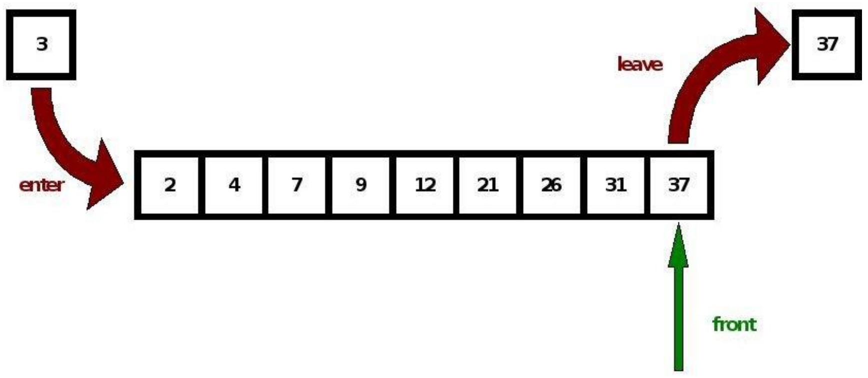
- ID
- simulator (ref)
- external_input (ref)
- data (overwrite referenced external_input)
  - priority level for every observation
- metadata

Collection „step“

- ID
- simulator (reference)
- external_input (ref)
- previous step (ref)
- dataset (output) (ref)
- metadata

Automatic simulation execution

- Technology: Redis queue and Redis worker
- Workflow:
  - Base worker runs on the host and waits for setting up a simulation queue
  - For a simulation queue a new worker will be generated
  - With the start of a simulation queue the assigned model worker starts the next simulation container
  - As the simulation finishes the container will be terminated
  - The model worker starts the next container in the queue until it finishes the whole queue
- Parallel simulations can be started
- The platform API sets up the queue, after that the states are only stored in the queue → The API stays stateless



Source: https://de.wikipedia.org/wiki/Warteschlange_(Datenstruktur)#/media/Datei:Queue_algorithmn.jpg

Data management and simulation platform

Worker

- Functions:
  - List containers
  - Run container
  - Pull image
  - Kill container
  - Start worker
  - Kill worker
  - Set workers
  - Get workers

Queue list

PID list

Redis

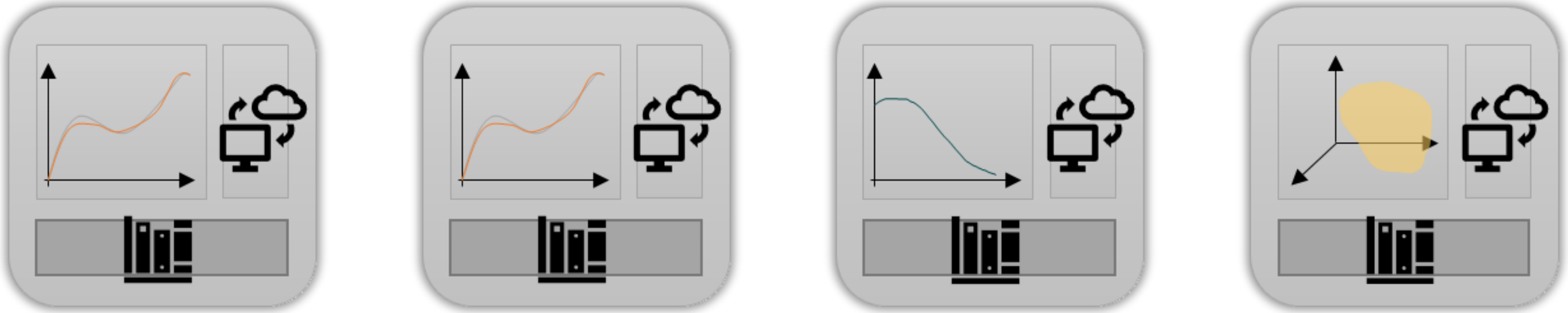
```
running_workers:burst = [burst:pid:simulation, …]
running_workers:noburst = [ ]
burst:pid:simulation = [4797, 5446, …]
```

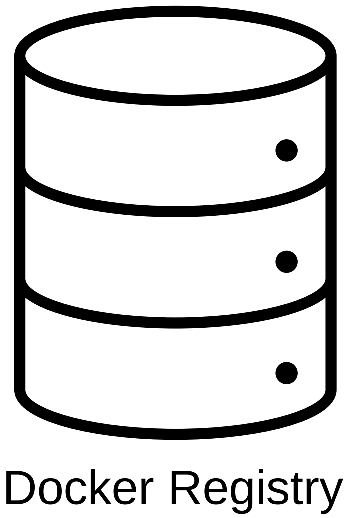
PIDs

- Storing actual process states
- Prevents processes to become orphan
- Uses the same Redis database as the RQ

Simulations

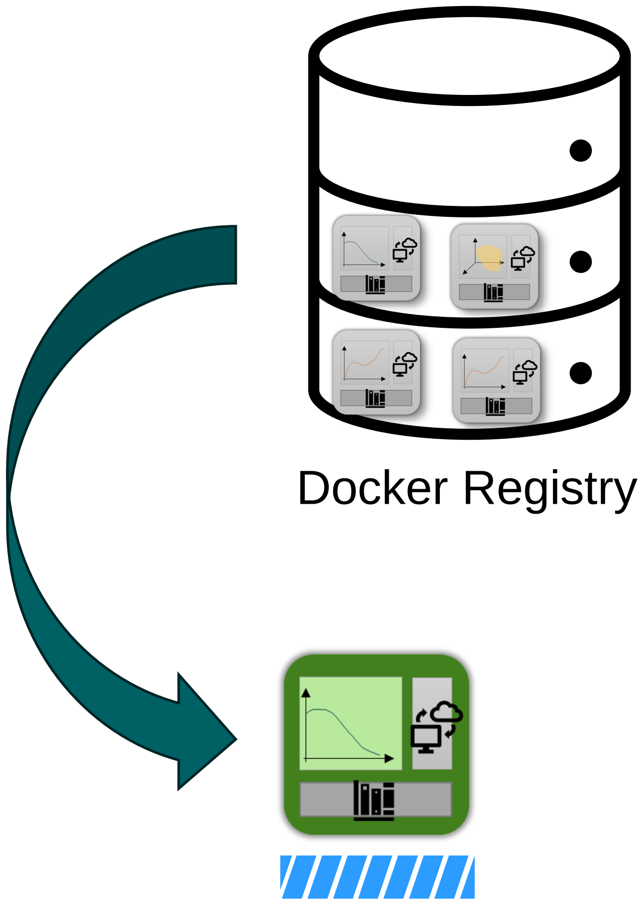
- Unified execution environment: Docker (if possible)





Simulations

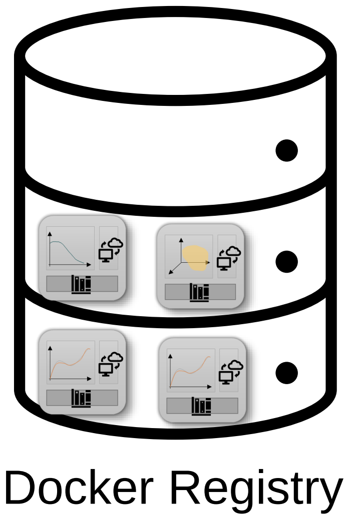
- Unified execution environment: Docker (if possible)
- Upload to local Docker Registry
- Contaioner execution by RQ-Workers[1]
  - Pull Container
  - Start next container in the Redis-Queue

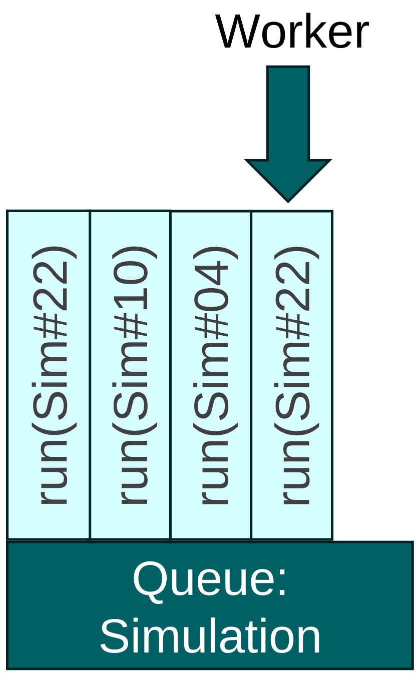


[1] https://python-rq.org/docs/workers/

Simulations

- Unified execution environment: Docker (if possible)
- Upload to local Docker Registry
- Contaioner execution by RQ-Workers[1]
  - Pull Container
  - Start next container in the Redis-Queue
  - If depends_on condition used, wait until previous job successfully executes





- Upload and download of the datasets inside of the container

[1] https://python-rq.org/docs/workers/

Remote simulation execution

Task-server

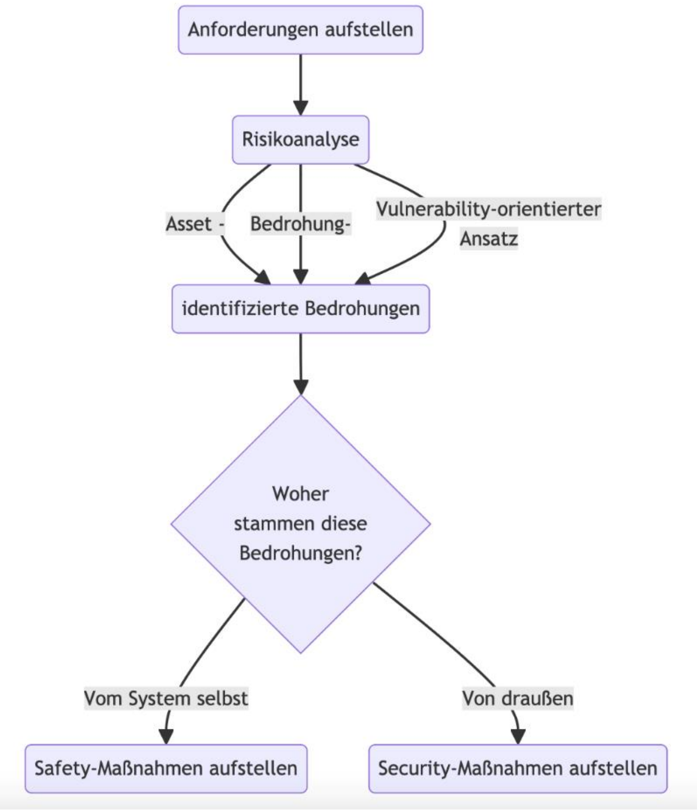
- If no dockerisation possible (e. g. no os compatibility, license bound to a certain computer)
- Flask server running on the remote machine
- Executes command
  - sent by the client (a docker container in the platform)
- Command configuration
  - Server checks, whether the requested command is permitted
  - Stores the path to the executable
- Sandbox environment
  - For every execution, new sandbox env generated
  - Inputs and the executable are than loaded
  - Results are sent back to the client

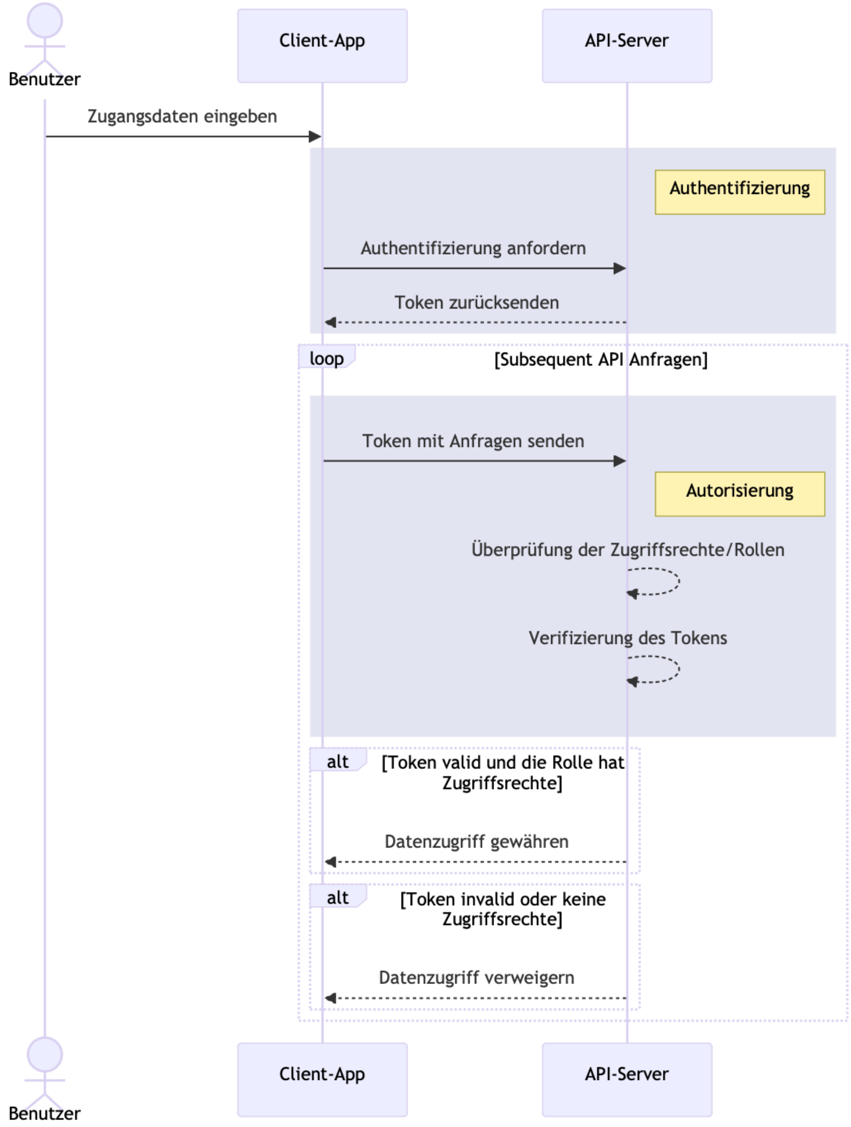

```
{
  "commands": [
    {
      "execute": "ls -l /some/directory"
    },
    {
      "execute": "grep -r 'some_pattern' /some/other/directory"
    },
    {
      "execute": "/path/to/your/customscript --option value"
    }
  ]
}
```

```
{
  "ls": "/bin/ls",
  "grep": "/bin/grep",
  "echo": "/bin/echo",
  "customscript": "/path/to/your/custom/script.sh",
  "main.sh": "/home/tamas/gPKM/test/server/main.sh"
}
```

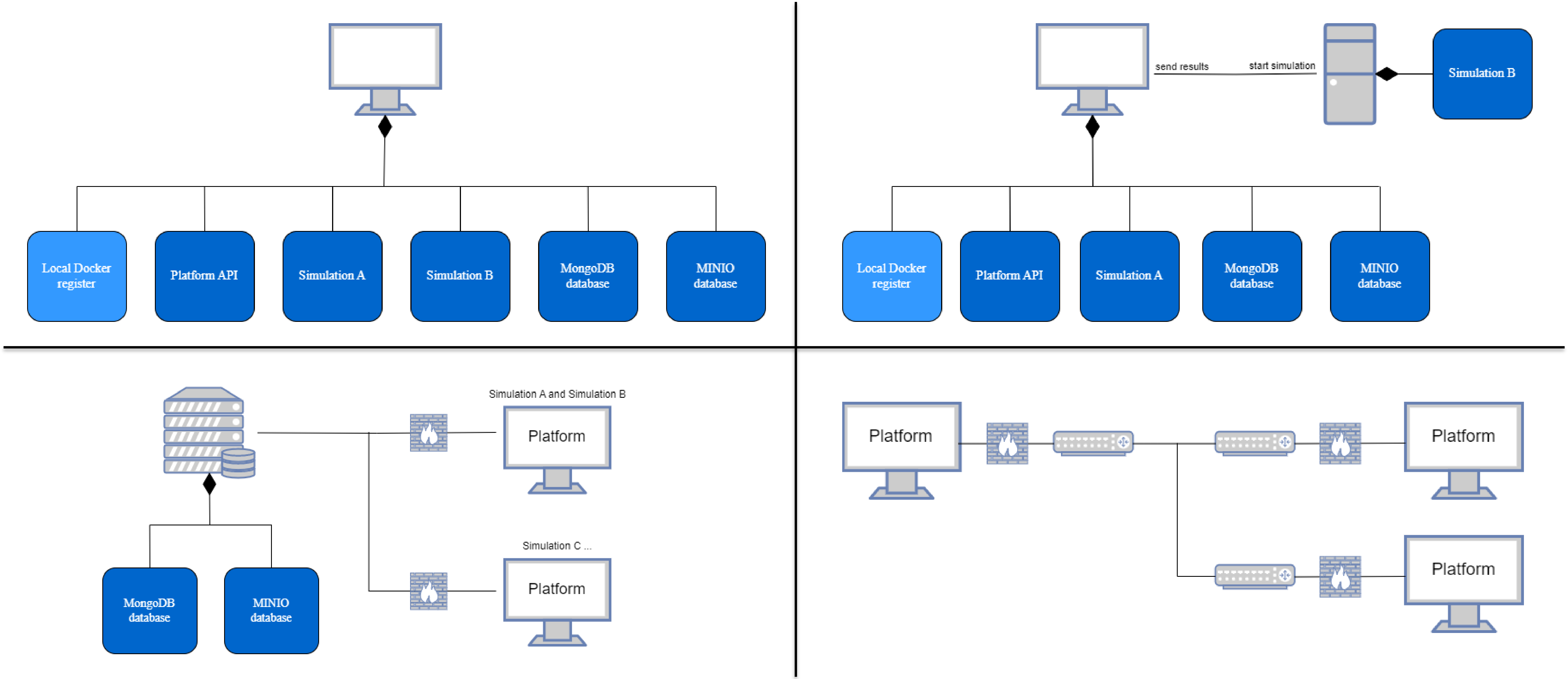
Security assessment

Inhaltsverzeichnis





Security assessment



Data management and simulation platform

Outlook

- TODO: Final report

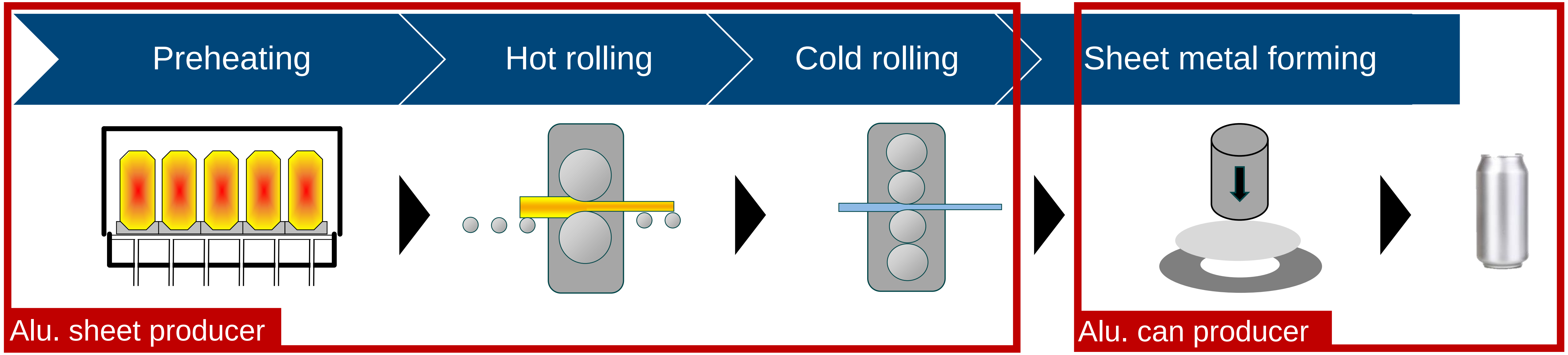
- Possible future project topics
  - Frontend, user interface
  - Failed job management
  - Process optimisation
  - Real-time simulations
  - Deployment in cloud environment
  - Access management, logging
  - Automatic reasoning based on ontologies
  - Distributed system
  - Test mode

If you are interested in the data platform, please feel free to contact us.

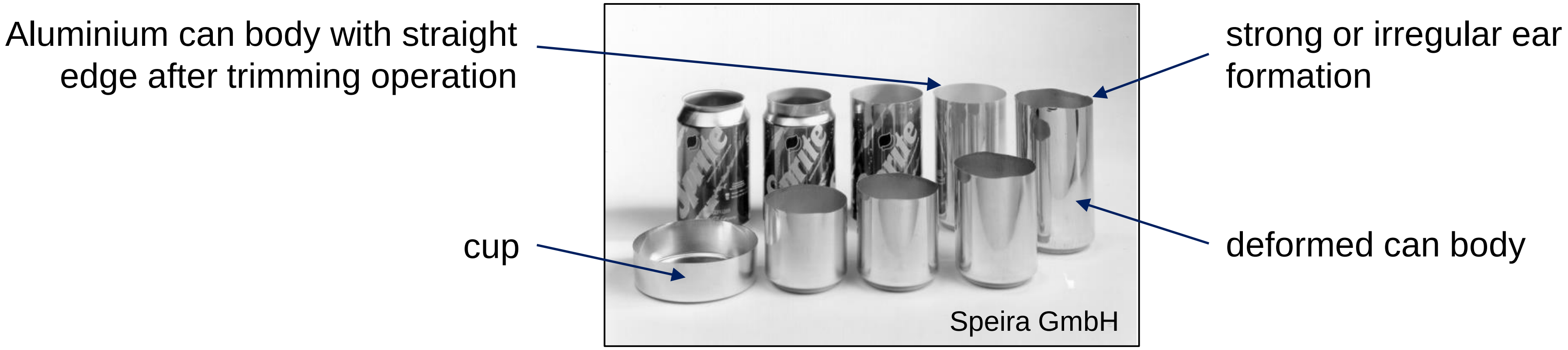
Demostrator – Speira & AluNorf

Quality improvement through reduction of ear formation in aluminium can production

Aluminium Demonstrator



Typical process chain of aluminium can production



Ear formation during aluminium can production

Aluminium Demonstrator

Motivation:

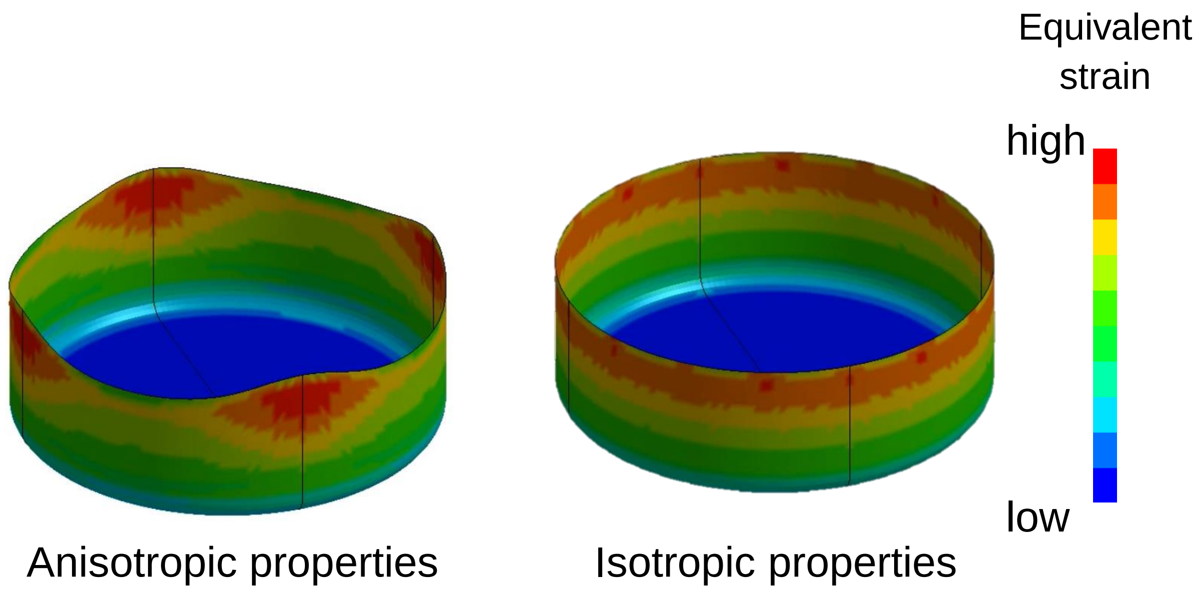
Ear formation due to anisotropic material behaviour

- Microstructure not correctly set
- Incomplete recrystallisation
- Rolling texture due to hot rolling process
- Precipitates

Uncoupled simulation models

- Different data formats
- Simulation of complete process chain - Time and cost expensive task

– Generation of material wastage through trimming of edges
– Shutdown of ultra fast can production process
– Economic efficiency of the process chain decreases



Influence of anisotropic material behaviour on ear formation

Aluminium Demonstrator

Goal:

- Minimization of ear formation by optimization of hot rolling process

Approach:

Coupling of process data and simulation models using a central data platform

- Extension/Modification of the hot rolling and earing model
- Validation of the simulation models
- Implementation of the concept for model coupling and generation of aggregated data

Analysis of the aggregated data to optimize the hot rolling parameters

- Provision of aggregated simulation and process data pia data platform
- Analyzing the correlation between ear formation and hot rolling parameters
- Determination of the optimum hot rolling parameters

Extension/Modification of the hot rolling and ear model

Analysis of existing models

- Procedure for process and model data management
- Management of input and output parameters
- Questionnaire study - area of application, existing interfaces, software technology, maintainability, archiving

Definition of transfer parameters and analysis of interfaces

- Identification of physical variables and their transfer
  - Spatial and temporal resolution
  - Number of dimensions
  - Data processing - data formats, data exchange technology
- Identification of coupling variables to achieve the goal
- Identification of model extension requirements

Implementation of the model extensions

- *Nein*
- *Clang mit Thermodynamik DB (intern aus verschiedenen DBs zusammengesucht)*

e) Anbindung/Integration

Dieser Abschnitt behandelt die (bereits umgesetzte) Integration bzw. Anbindung des Prozessmodells mit anderen Software-Komponenten.

- Werden von vorangegangenen Prozessschritten genutzt oder berechnete Daten an Simulationsmodelle bzw. Steuersysteme nachfolgender Prozessschritte weitergegeben?

Prozessmodelle sind gekoppelt

- wenn ja: *Versetzungsdichte, Temperatur*
- wenn ja: Wie starke Kopplung?
  - *manuelle Weitergabe von Daten (als Datei),*
- Werden Daten aus Produktionsdatenbanken, Stoffdatenbanken oder Prozessdaten-Erfassungssystemen genutzt oder die berechneten Daten an solche Systeme automatisch weitergegeben?

  Nein (outputs), parquet daten aus der Produktion (inputs)
- wenn ja, handelt es sich um „Cloud-basierte" Software (d.h. Software-as-a-Service-Angebot)?

  Nur Produktionsdaten werden archiviert, Prozessmodelldaten nicht

Requirements analysis conducted through questionnaire

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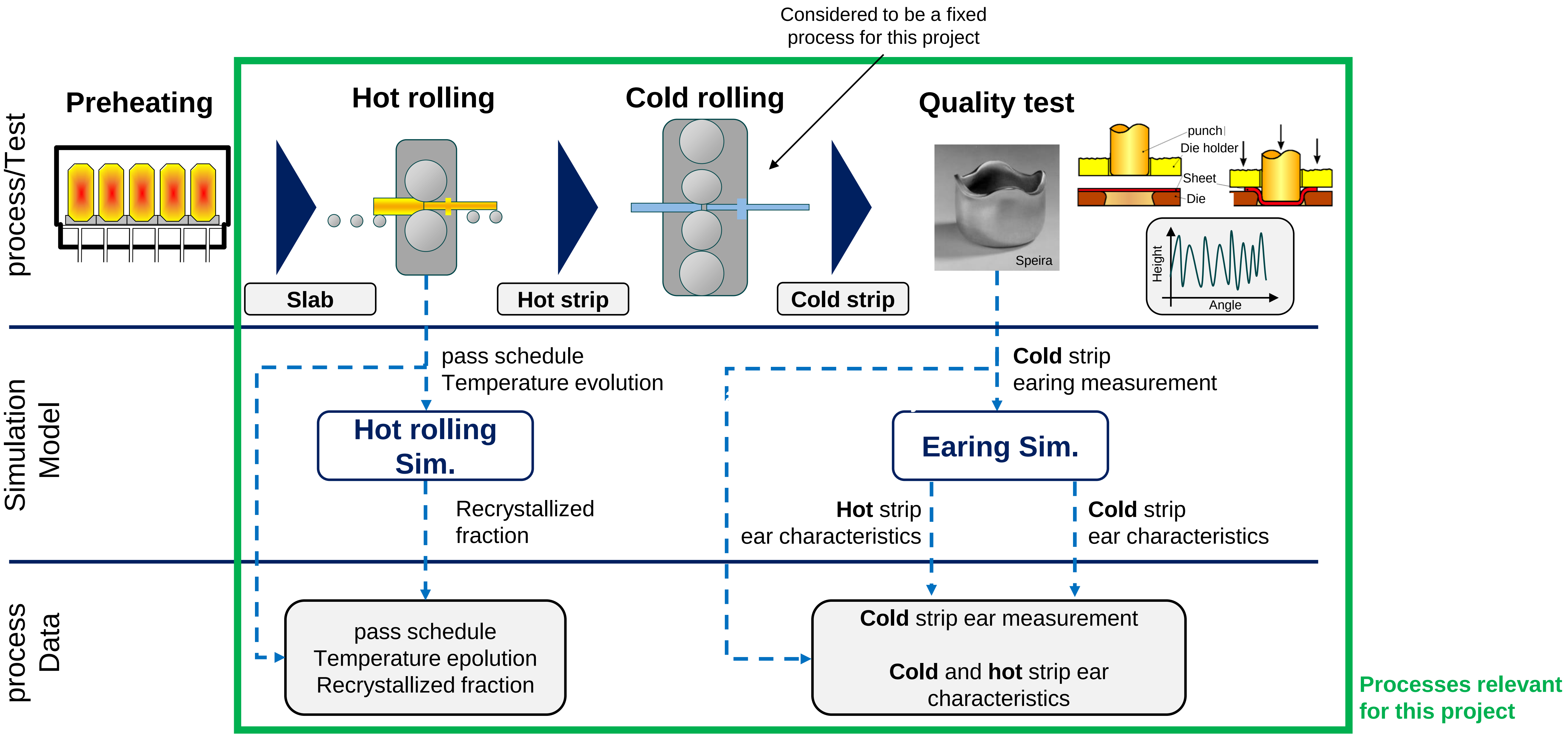

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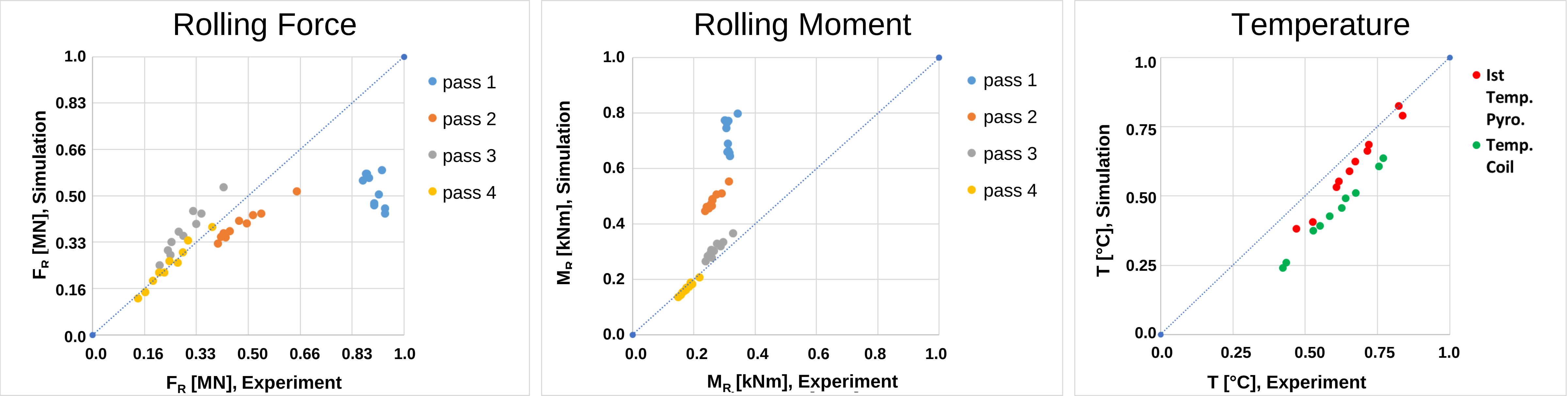
Validation of hot rolling model:

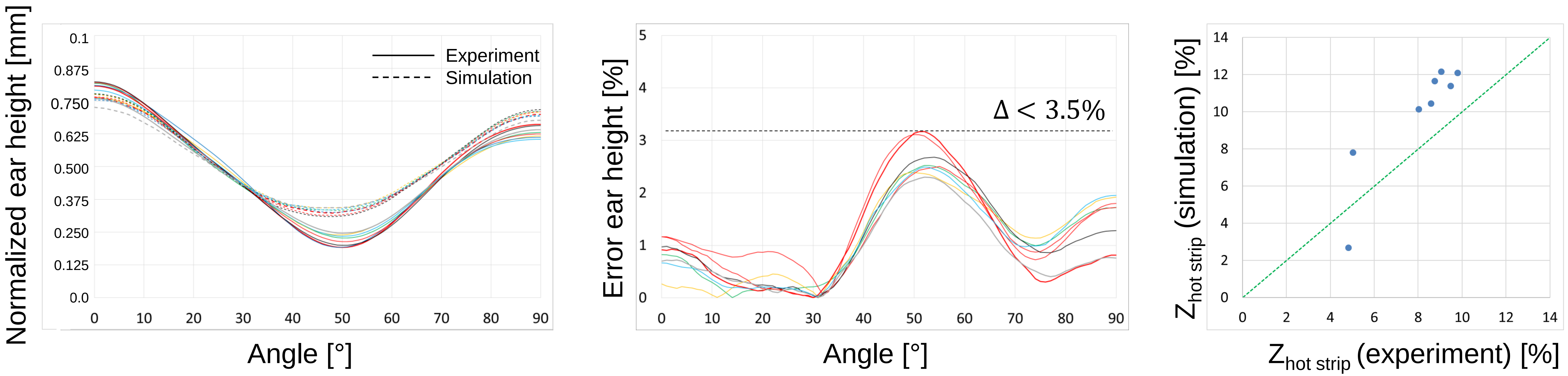
- Validation experiments conducted by Speira GmbH
- Comparison of simulation and experimental results show good accuracy for coil Temperature



Comparison of rolling force, rolling moment and coil temperature during hot rolling using experimental data and a simulation model

Validation of ear model:

- Validation experiments conducted by Speira GmbH
- Ear formation measured after both **hot** as well as **cold** rolling
- Comparison of experiment and simulation results show good agreement for hot strip ear formation

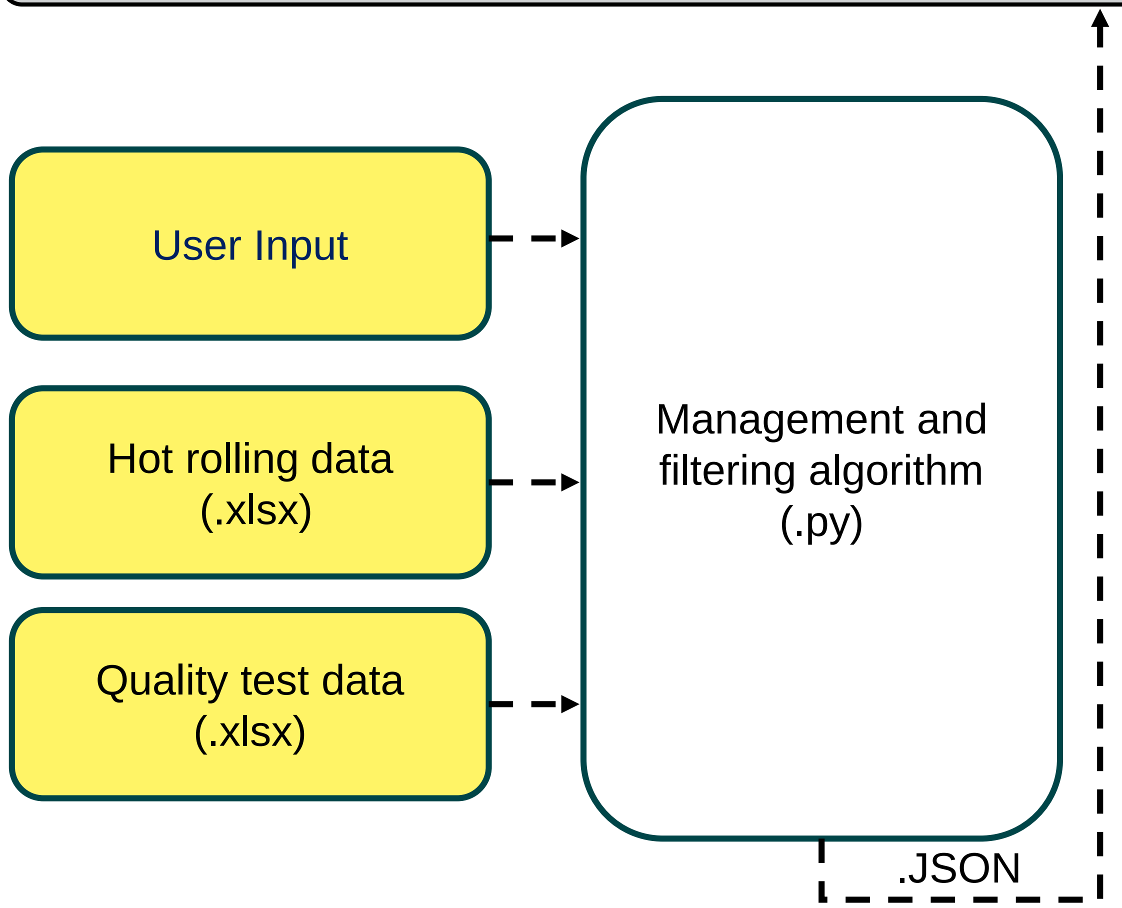


Comparison of hot strip ear characteristics calculated using the experiment and simulation model

Input / Output
Model / Calculation
Aggregate data

Concept for coupling of simulation models and process data

Data platform



User Input:

- Paths of production and quality files
- Number of ears

Management and filtering algorithm:

- Check cold strip earing measurements for errors
- Determination of material id
- Identification of hot rolling data with material id
- Production and quality data saved as .JSON
- Automated start of simulation, extraction and saving of simulation results as .JSON

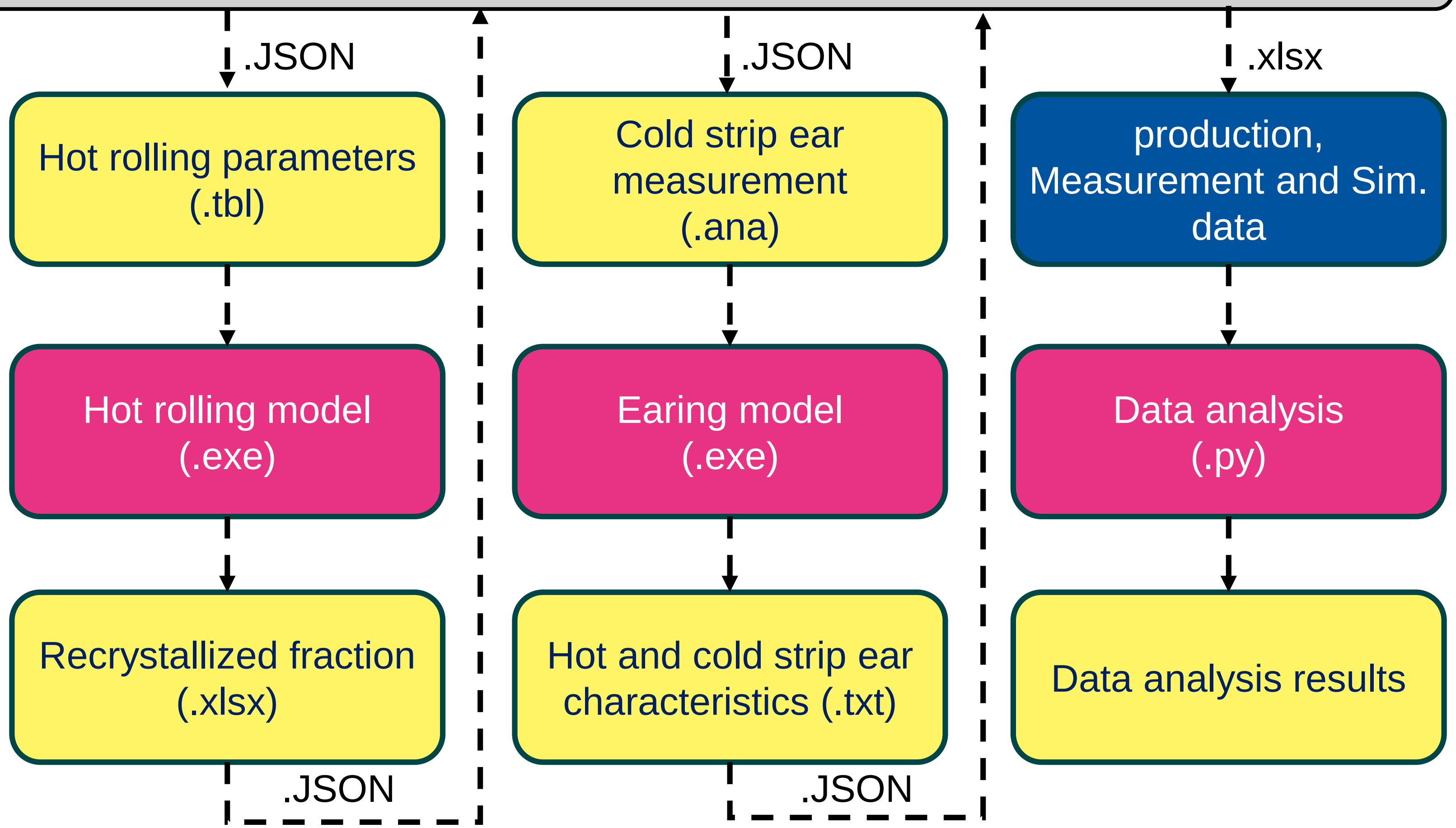
Input / Output
Model / Calculation
Aggregate data

Concept for coupling of simulation models and process data

Data platform

Simulation data:

- Preparation of model input file
  - .JSON to .tbl for hot rolling model
  - .JSON to .ana for earing model
- Execution of the simulations
- Extraction of simulation results
- Conversion of simulation results to .JSON
- Saving simulation data together with the production and quality data as .JSON



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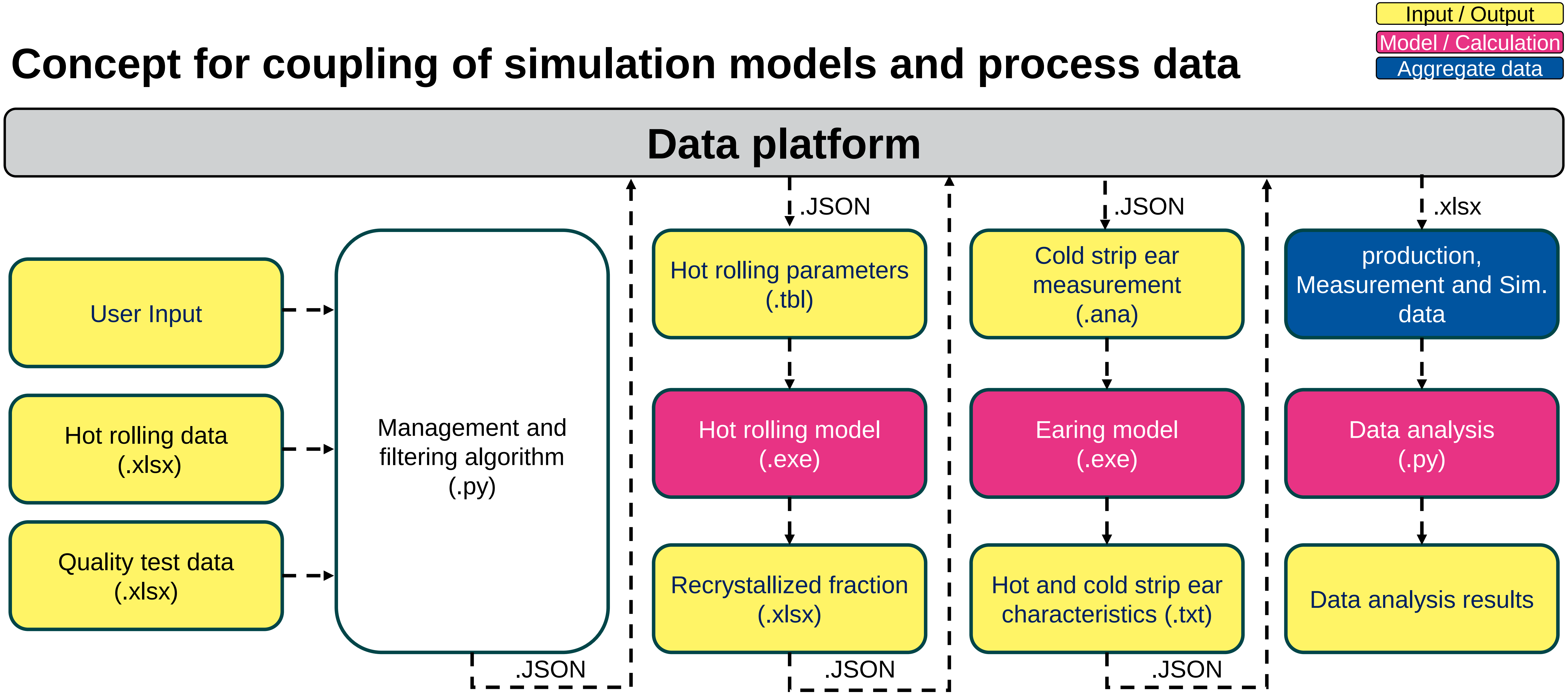
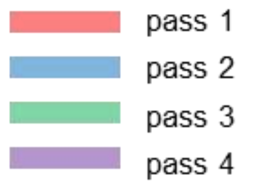
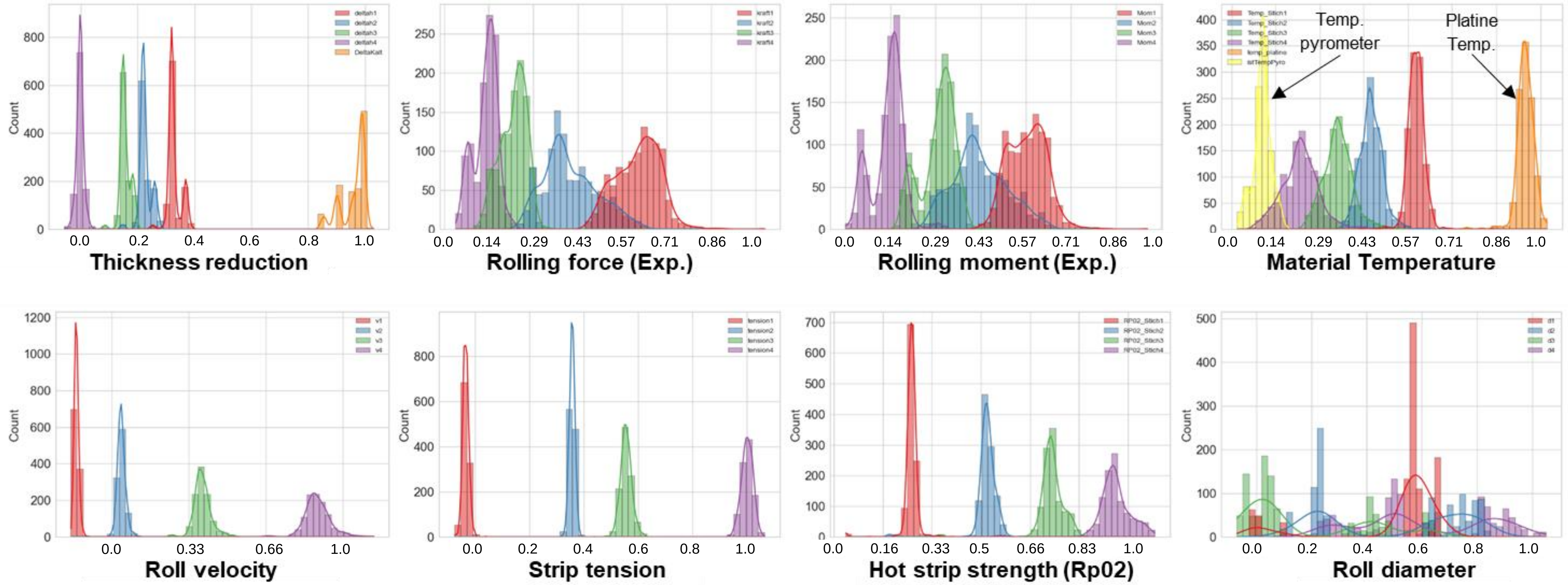
Concept for coupling of simulation models and process data



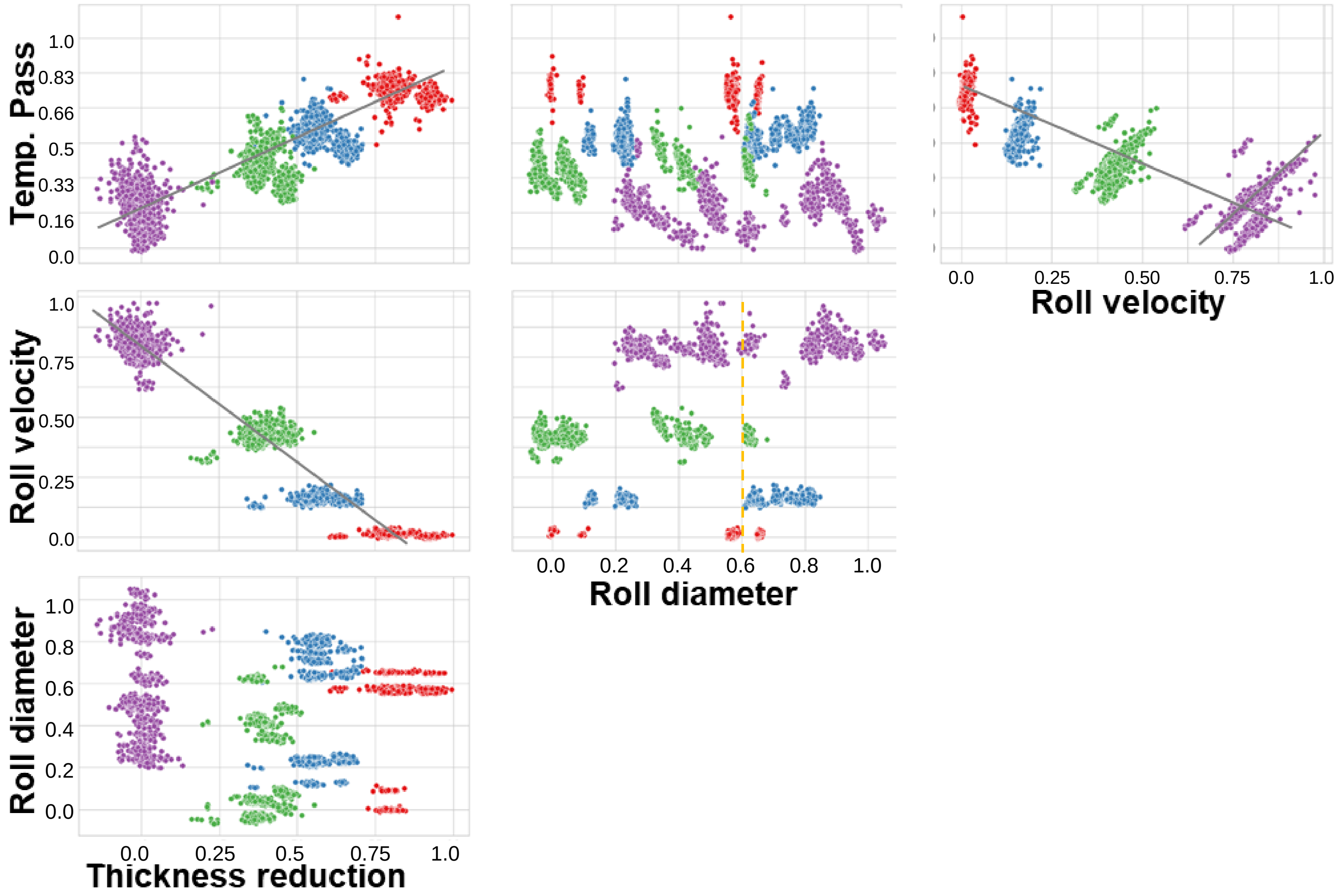
Aluminium Demonstrator

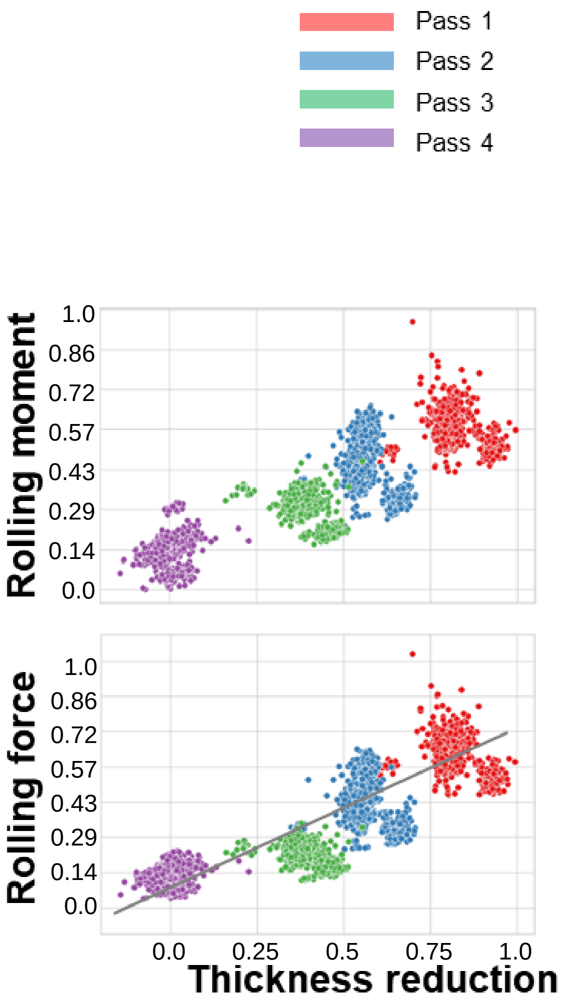
Data analysis - Process parameter





Data analysis - Process parameter





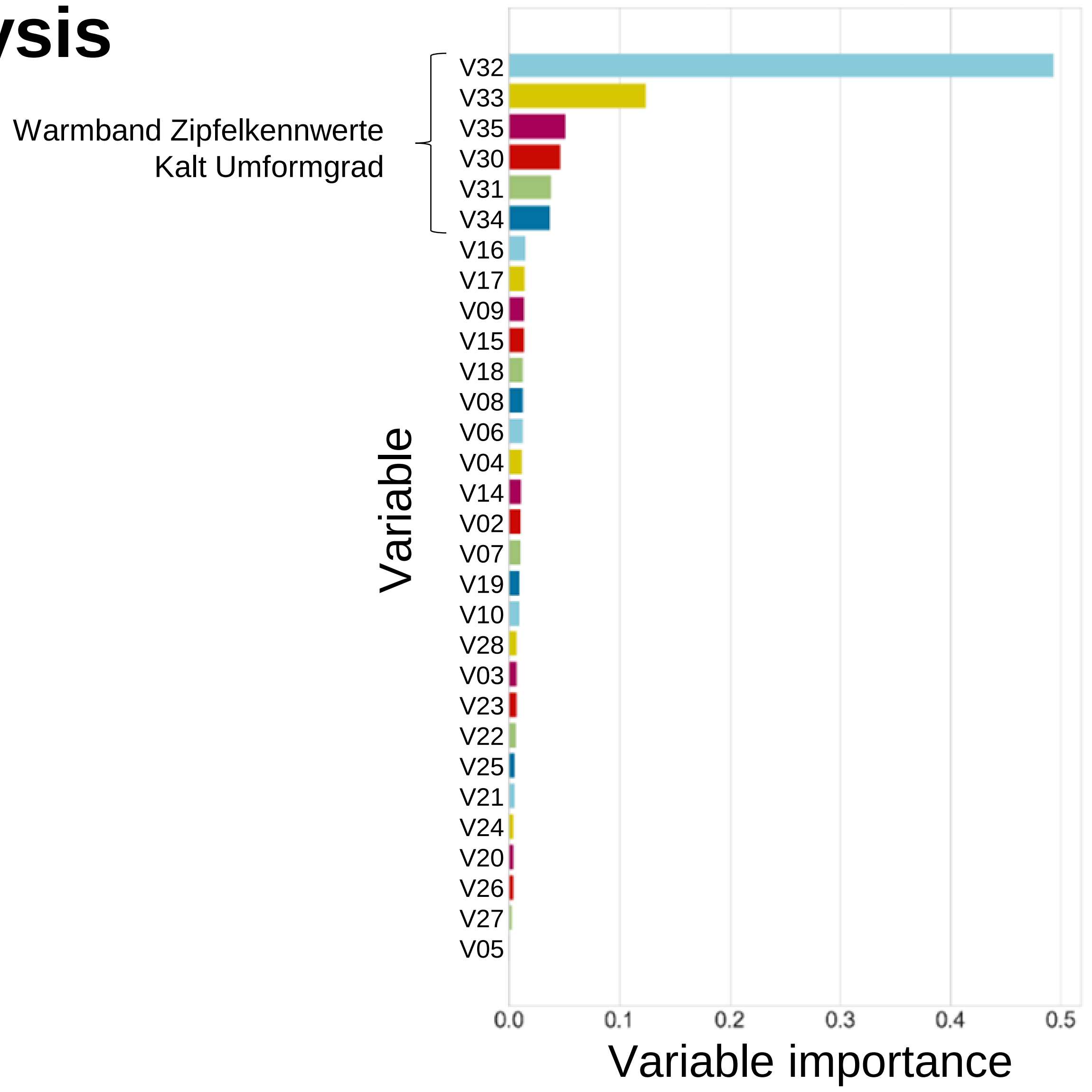
Aluminium Demonstrator

Data analysis - Parameter Importance Analysis

- ML Modell: Random Forrest Regression
  - **Input variables**: Material data, hot rolling parameters, hot strip ear characteristics
  - **Output variables**: Cold strip ear characteristics
- ML model learns the correlations between input- und output variables
- Explained variance as an indicator for input variable importance

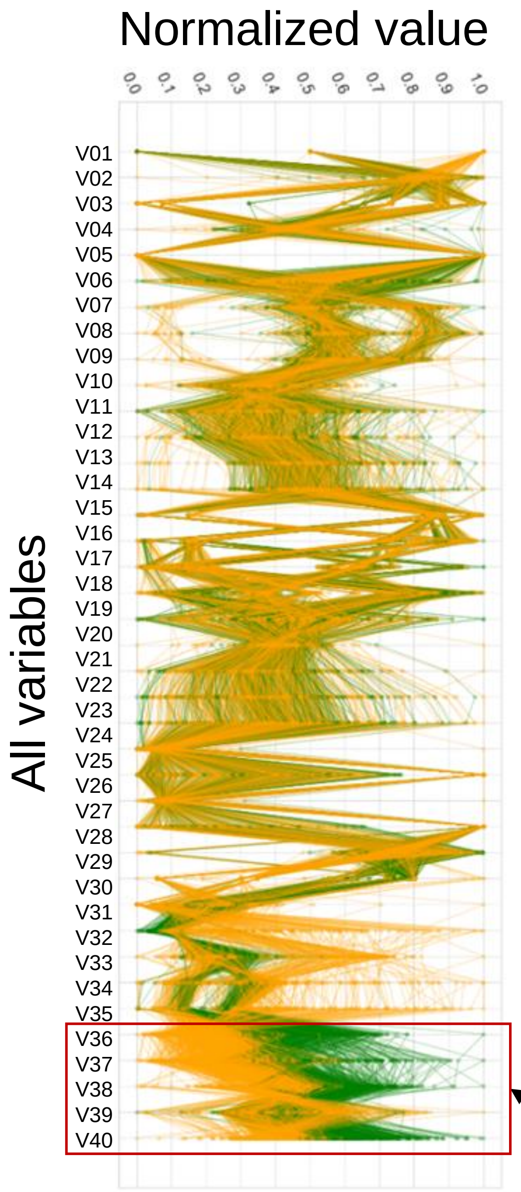
➢ Hot stip ear charateristics (V30-V34) have influence on cold strip ear characteristics

  – $dh_{\text{hot strip}}$ (V32) has most significant influence



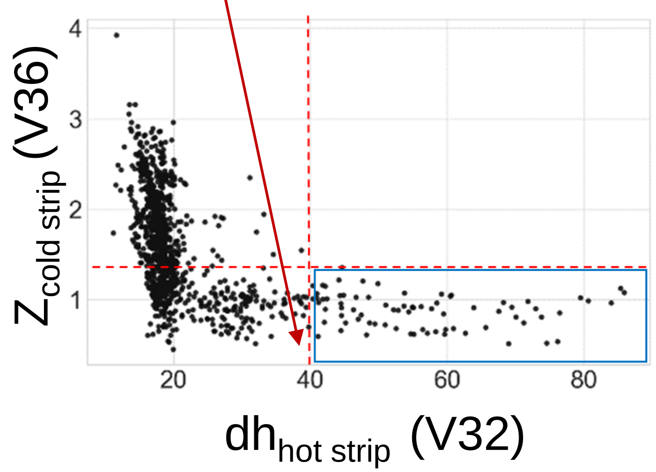
Data analysis - Cluster Analysis

- Clustering of processes into different groups having similar cold strip ear characteristics
- KMeans unsupervised ML method
  - **Input variables**: Cold strip ear characteristics
- Optimal clusters according to Silhouette Score: 2
  - Orange and green cluster
- Strong correlation between hot and cold strip ear characteristics
  - $dh_{hot\ strip}$ (V32) vs $Z_{cold\ strip}$ (V36)



Cold strip ear characteristics

For $dh_{hot\ strip}$ >= 40 % cold strip ear characteristics ($Z_{cold\ strip}$) is always less than 1.5 %



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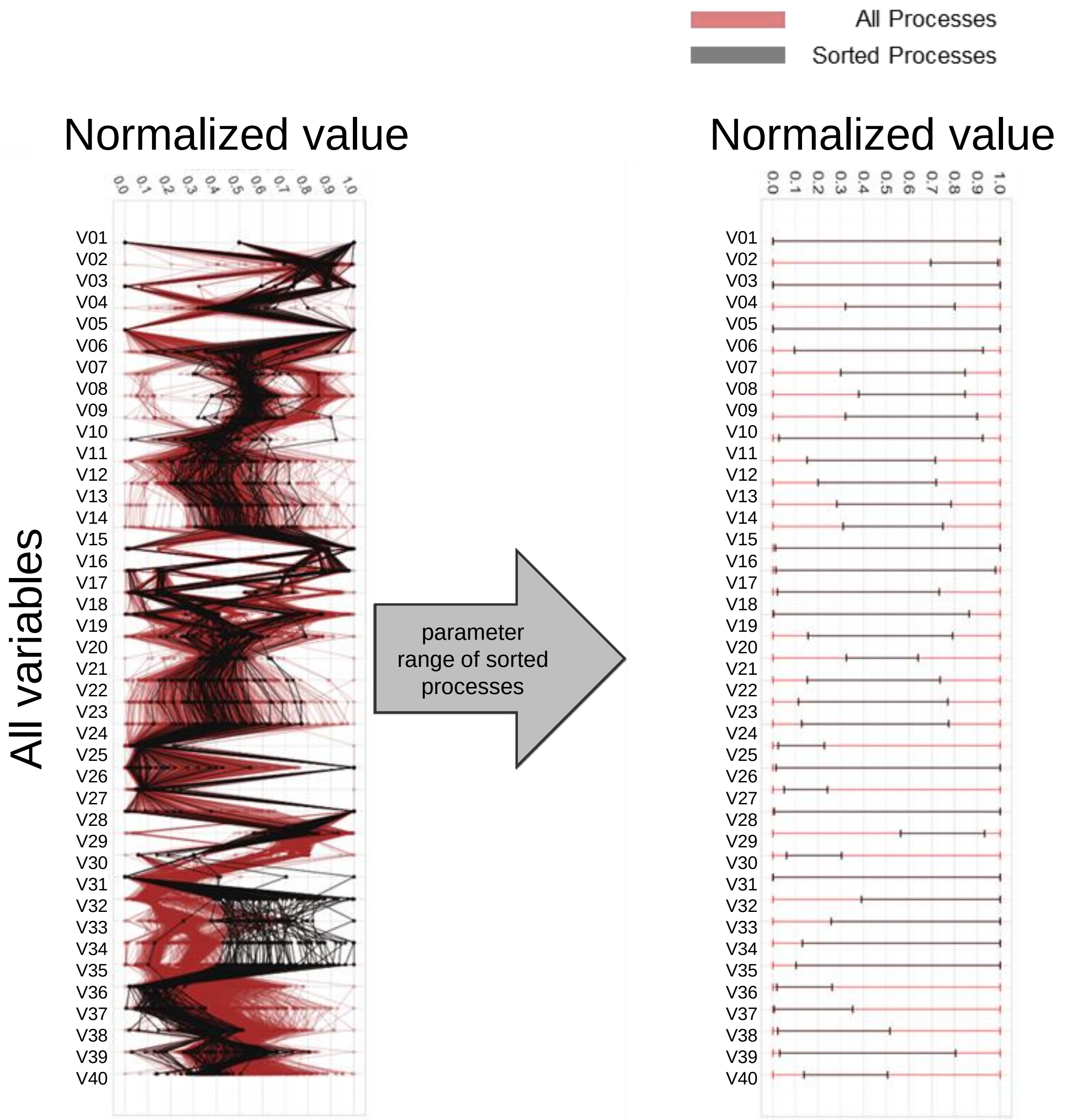
Data analysis - Cluster Analysis

Processes sorted using the criteria

- $dh_{hot\ strip}$ (V32) >= 40 %

Parameters of interest:

- Platine thickness (V04)
- Platine temp. (V02)
- Target temp. (V06)
- Roll diameter (V17 and V18)
- Fe/Si (V19)
- Degree of cold reduction (V30)



Data analysis - Optimal hot rolling parameter

Determination of optimal process to achieve the desired targets

- Evaluation function – Assign scalar value for each process
- User defined targets:
  - Minimize cold strip ear formation
  - Achieve customer desired cold strip strength and thickness
- Reference values required for the analysis

$$Evaluation\ function = \left(\frac{Z_0 - Z_{0,ref}}{Z_{0,ref}} \cdot 100\right)^2 \cdot w_1 + \left(\frac{Z_{45} - Z_{45,ref}}{Z_{45,ref}} \cdot 100\right)^2 \cdot w_2 + \left(\frac{Z_{90} - Z_{90,ref}}{Z_{90,ref}} \cdot 100\right)^2 \cdot w_3 +$$

← Earing characteristics

$$\left(\frac{R_{p02\ coldstrip} - R_{p02\ coldstrip,ref}}{R_{p02\ coldstrip,ref}} \cdot 100\right)^2 \cdot w_4 +$$

← Cold strip strength

$$\left(\frac{h_{fin} - h_{fin,ref}}{h_{fin,ref}} \cdot 100\right)^2 \cdot w_5$$

← Cold strip thickness

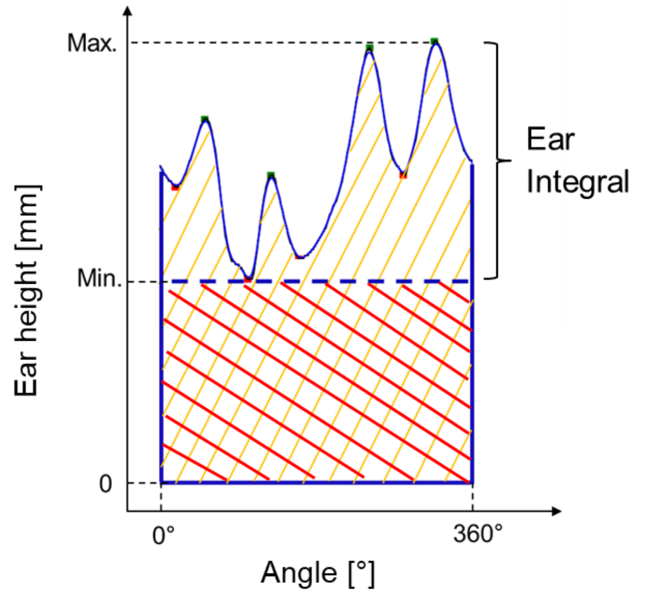
$w_{1,\ldots,5} = weights$

Aluminium Demonstrator

Data analysis - Optimal hot rolling parameter

- Ear integral: Material between max. and min. ear formation

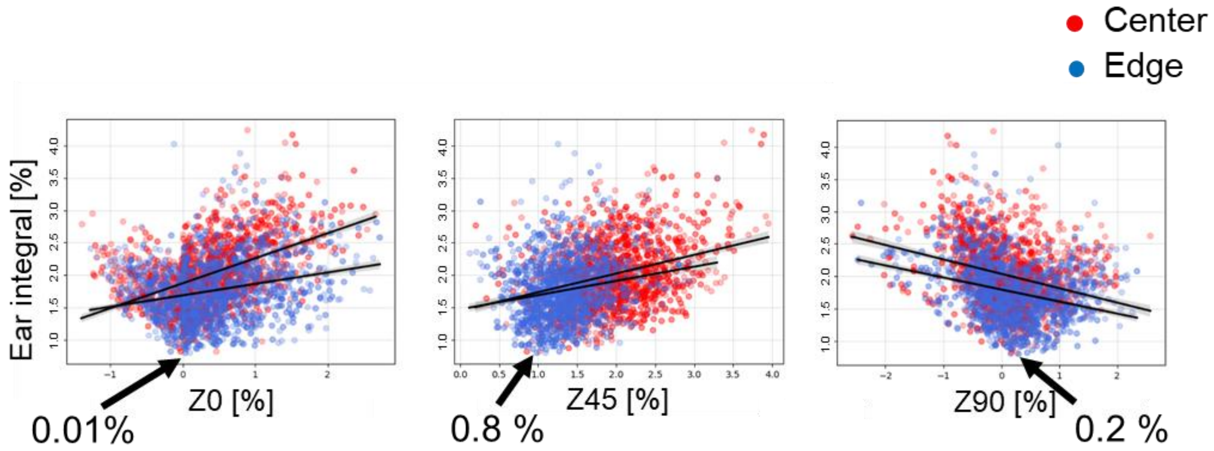
$$Ear\ integral = \left(\frac{A_{total} - A_{without\ ear}}{A_{total}}\right) \cdot 100\ [\%]$$



Calculation of ear integral

Reference values for evaluation function

- Cold strip ear characteristics:
  - Homogeneous ear formation at the edge and center of the coil
  - Z0 = 0.01 %
  - Z45 = 0.8 %
  - Z90 = 0.2 %
- Cold strip strength = 268 MPa
- Cold strip thickness = 0.24 mm



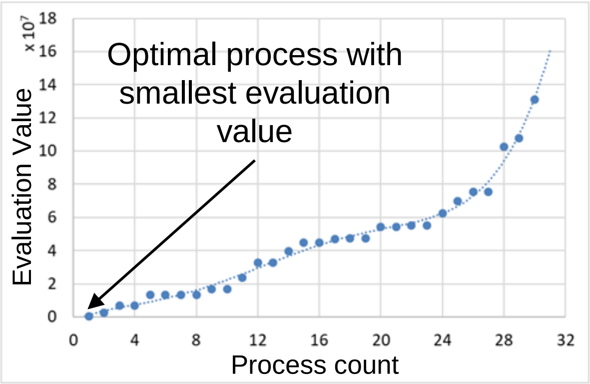
Determination of reference values using ear integral

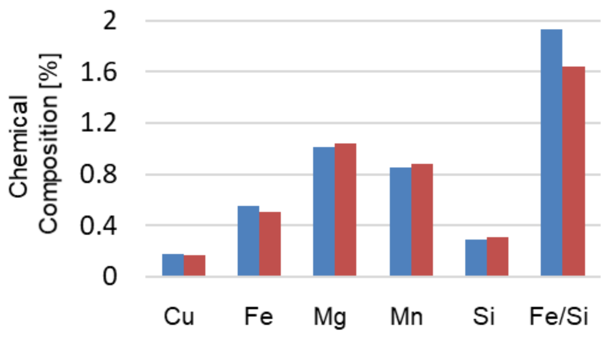
Determination of best and worst process

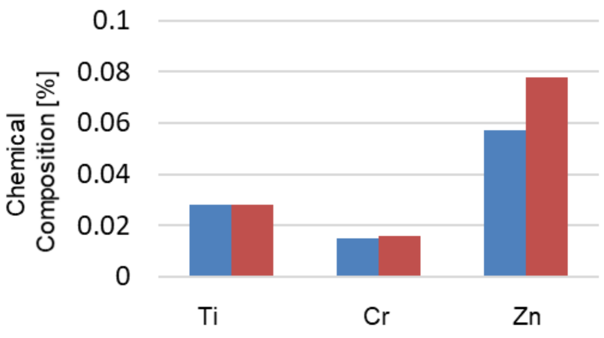
Aluminium Demonstrator

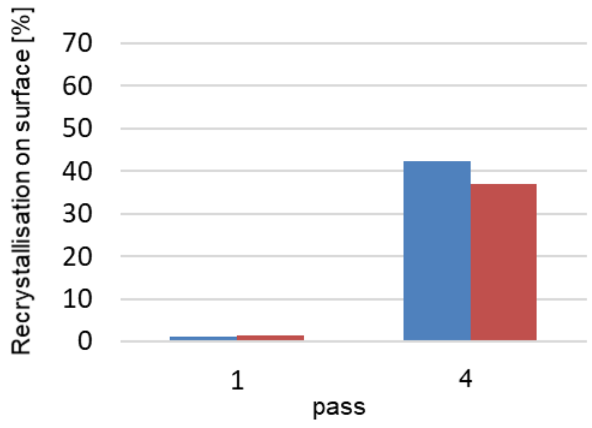
Data analysis - Optimal hot rolling parameter

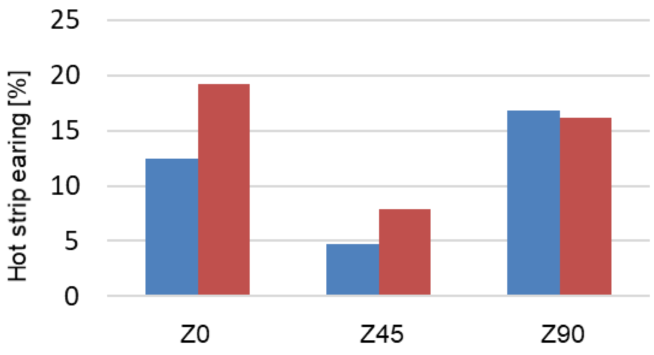
Best process
Worst process

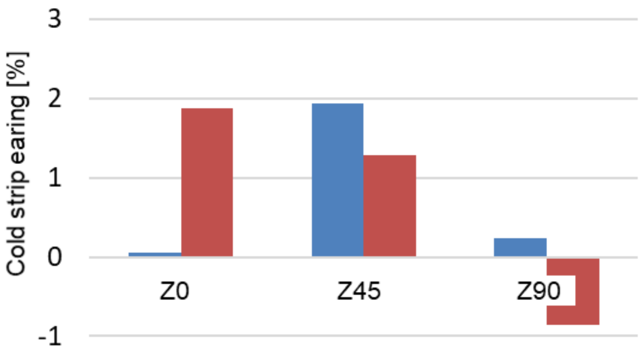












Summary

Coupling of process data and simulation models using a central data platform

- Extension/Modification of the hot rolling and ear model
- Validation of the simulation models
- Implementation of the concept for model coupling and generation of aggregated data

Analysis of the aggregated data to optimize the hot rolling parameters

- Provision of aggregated process and simulation data via data platform
- Analyzing the correlation between ear formation and hot rolling parameters
- Determination of the optimal hot rolling process

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Linking of Heating and Forming Processes

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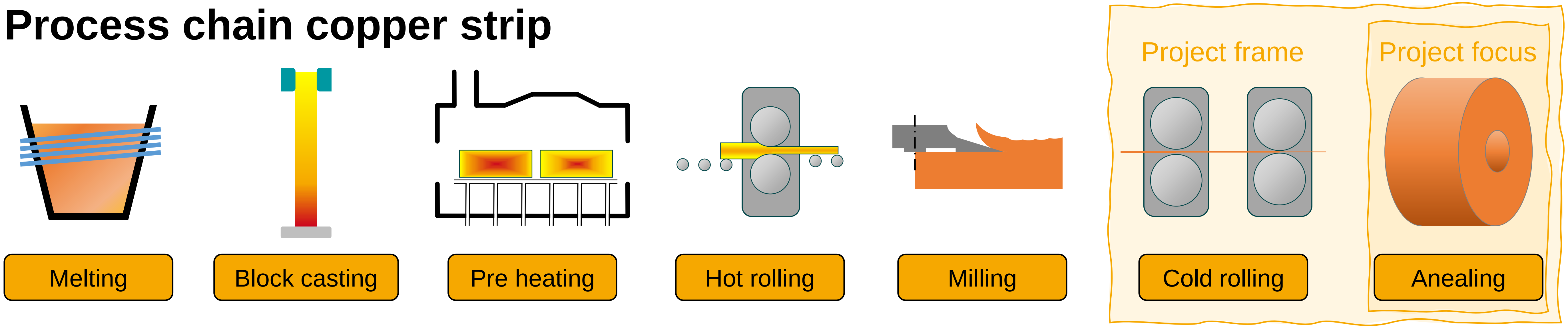
Process chain copper strip



- Main focus: Coil annealing
  - Temperature and stress state change in the coil
  - Change/homogenisation of material properties

  → High energy saving potential

  - Heat transfer in the coil dependent on previous process steps

- Secondary focus: coiling after cold rolling
  - Shaping of the coil
  - Stress distribution in the wound coil

- Tertiary focus: Further upstream steps
  - Shaping of the strip
  - Change in material properties (e.g. anisotropic structure)

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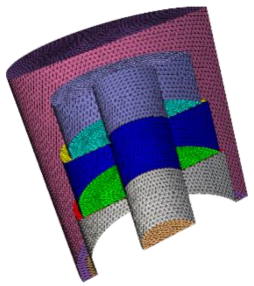
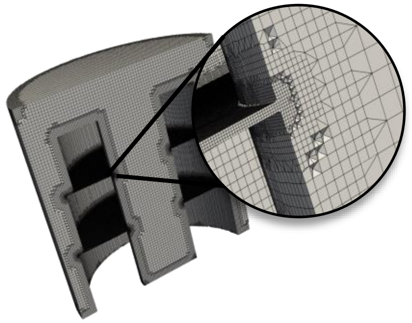
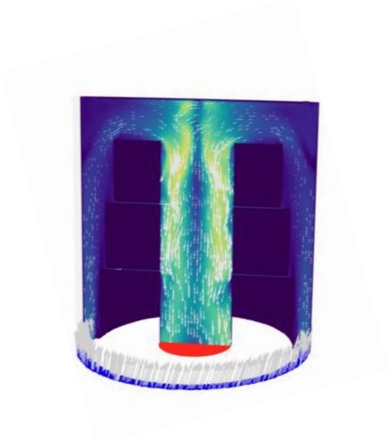
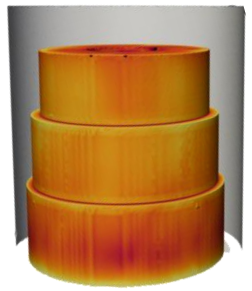
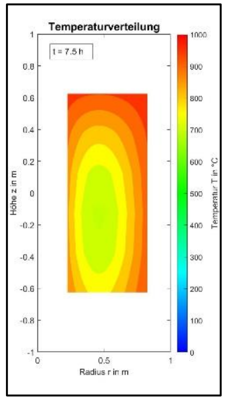
Modelling

- Step 1: Definition of parameters
  - Model parameters (user input)
    - Stacking in the bell type furnace
    - Furnace temperature curve
    - Alloy, surrounding gas
  - Strip geometry (e.g. from measurement data)
- Step 2: Material data
  - Input: Temperature range
  - Output: Material data (Good and gas)
- Step 3: Heat transfer coefficients
  - Input: Model parameters, geometry, material data
  - Creation of 3D CAD model bell type furnace with coils
  - Meshing, CFD simulation
  - Output: Heat transfer coefficients (HTCs)
- Step 4: Temperature distribution
  - Input: Model parameters, geometry, material data, HTCs
  - Stress distribution (coiling model)
  - Output: Time-dependent 2D temperature distribution

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Temperature-dependent Material Data

- Determination of material data
  - Simulations (e.g. JMatPro)
  - Measurements
  - Literature

- Interpolation
  - Curve fitting of the data
  - “Look up table”

- Tabular material data
  - Density
  - Thermal properties (heat capacity, thermal conductivity)
  - Mechanical properties (thermal expansion coefficient, Young’s modulus, Poisson’s ratio)
  - Emissivity

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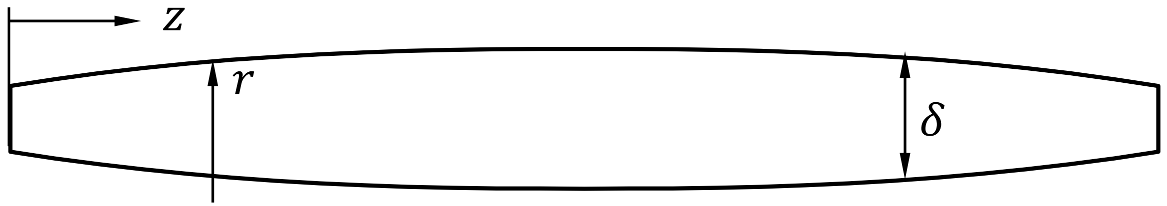
Process model: Coiling

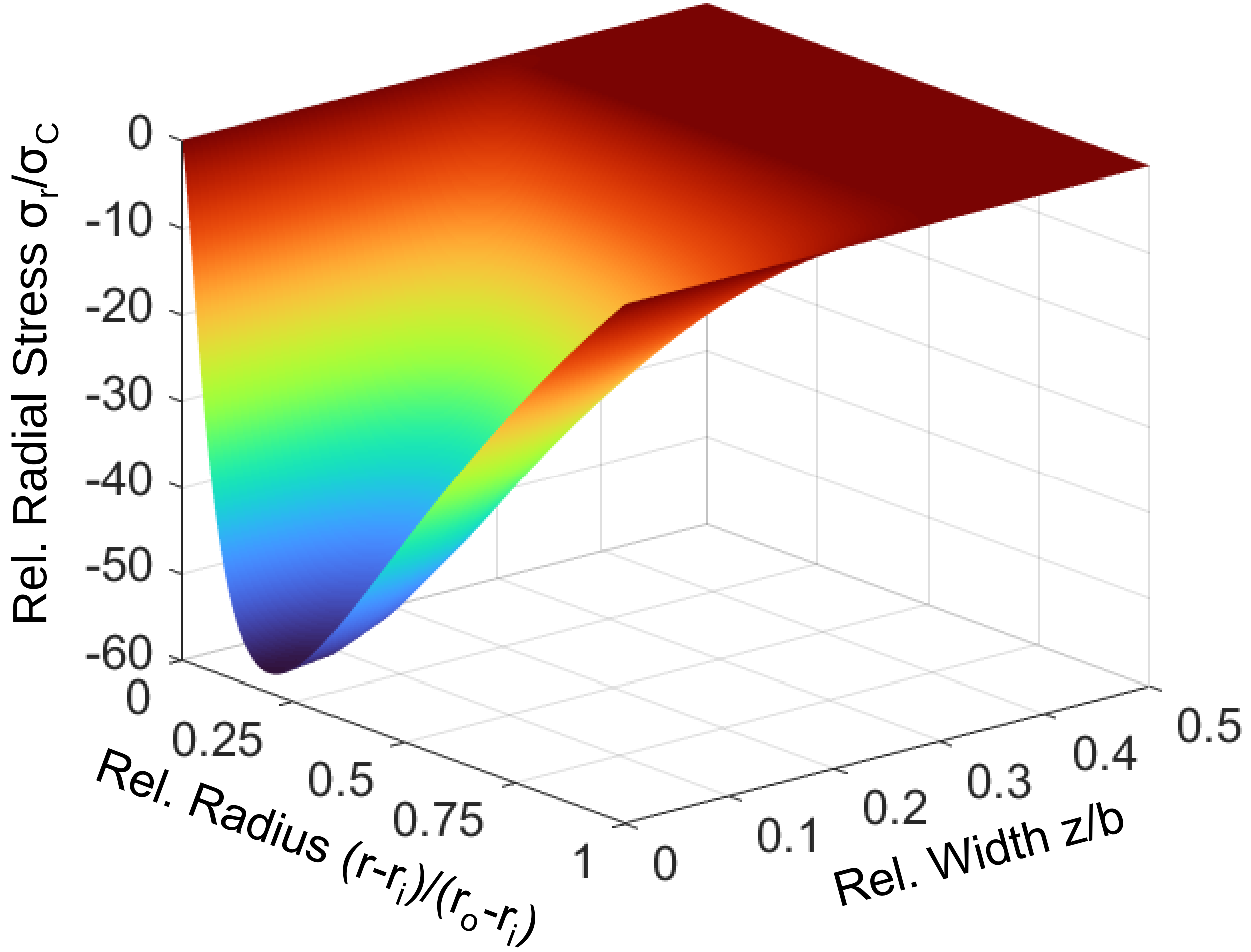


- Calculation of 2D radial stress distribution
- Coiling stress distribution over width

$$\sigma_C \int_{-b/2}^{b/2} \delta(z)dz = \int_{-b/2}^{b/2} \sigma_t(z)\,\delta(z)dz \quad , \qquad \sigma_t(z) \propto \ln(r(z))$$

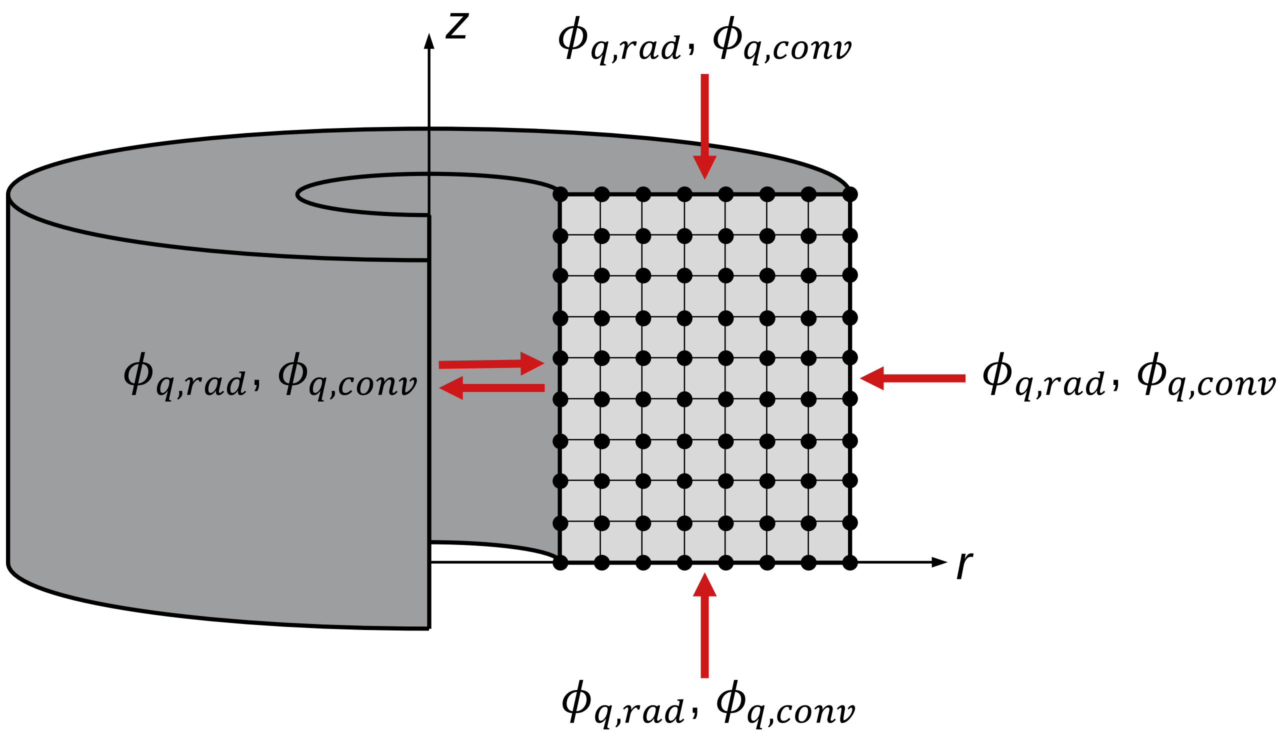
- Stress distribution over radius

$$\sigma_r(r,z) = \sigma_t(z)\left[\left(\frac{r_i}{r(z)}\right)^2 - 1\right]\frac{1}{2}\ln\left(\frac{r_o^2 - r_i^2}{r(z)^2 - r_i^2}\right)$$

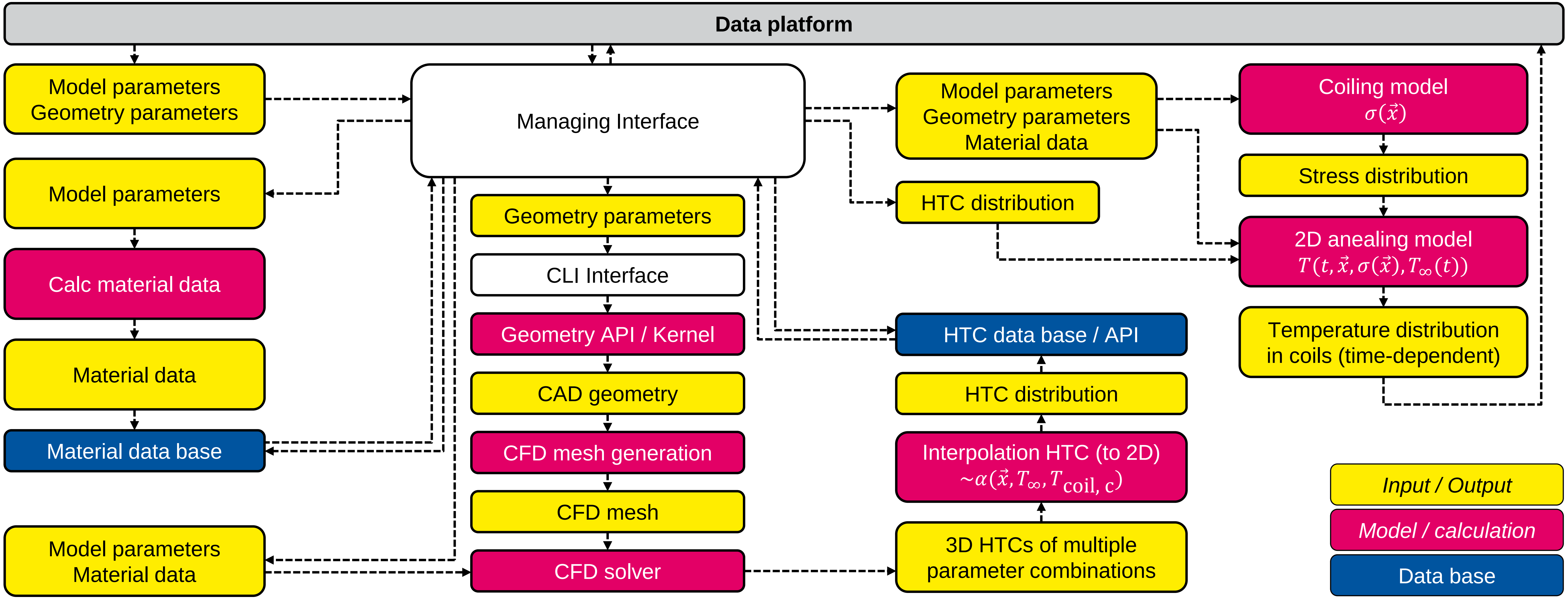


Process model: Coil annealing

- Optimisation of the process time
- Modelling
  - Numerical Solution of the Fourier equation with FDM
  - Rotation-symmetric 2D mesh
  - Anisotropic thermal conductivity (thermal contact resistance)
  - Boundary conditions from CFD simulation
- Results:
  - Time-dependent temperature distribution



Integration into the data platform



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Summary and outlook

- Completion of the individual models
  - Coiling model
  - CFD model
  - Annealing model
- Validation of the models by measurement data provided by Schwermetall
- Manual verification / optimisation of annealing times for typical occupancies
- Transfer of models to demonstrator platform
- Automatic verification of the annealing times through application of the demo platform

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Thinking the Future
Zukunft denken

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