

EMMC International Workshop 2019  
Feb. 25 – 27, 2019  
Vienna, Austria

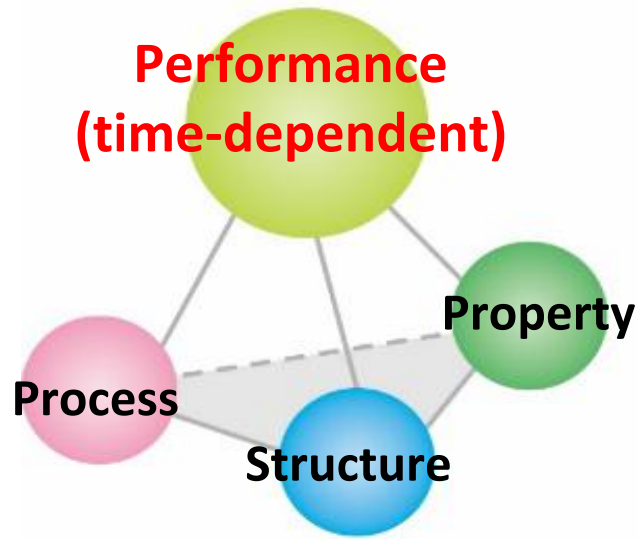
# Materials integration

National Institute for Materials Science (NIMS)  
Research service division of  
Materials Data and Integrated System (MaDIS)

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# Materials integration (SIP-MI)

Under the program Strategic Innovation Promotion Program (SIP)  
Structural Materials for Innovation (SM4i) project



Key elements in  
Materials S&E

**Goal:**  
Predict performance from  
process, linking among the four  
elements with a fusion of  
experiments, computation,  
database, and data science.

Long life time of structure materials > Long-time & high-cost R&D



10~15 yr.



15~20 yr.



20~25 yr.



30~40 yr.



100 yr.

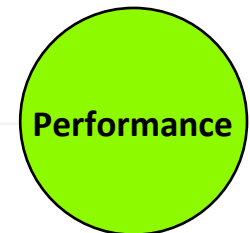
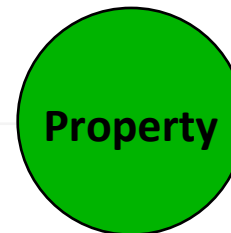
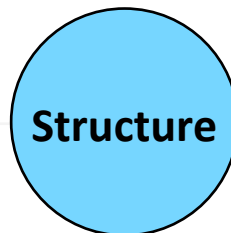
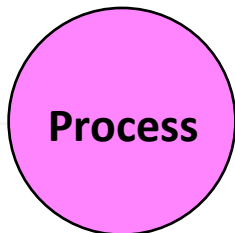
# PSPP design space

## Huge design space under PSPP linkage

- Variation of Processing
- Variation of Structure (esp. in meso-scale)
- Variation of Targeted Properties
- Trade-off among targeted properties
- Dependencies of Performances under usage environment

**Computers and computational methods could help us to explore the design space.**

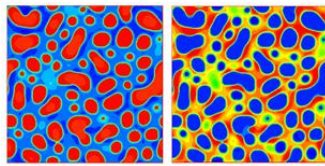
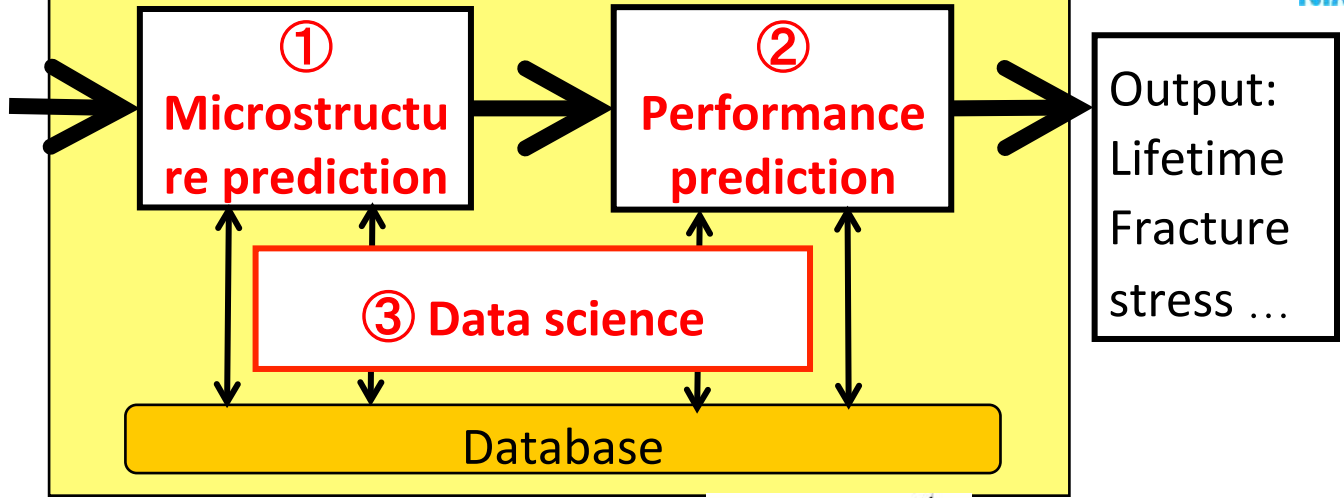
Design ←



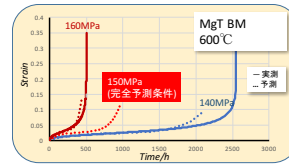
→ Prediction 3

Input:  
Composition,  
Process, Use  
conditions

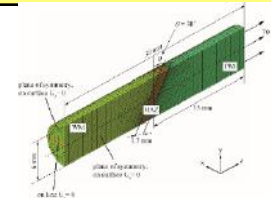
### ④ Integrated system



Phase field

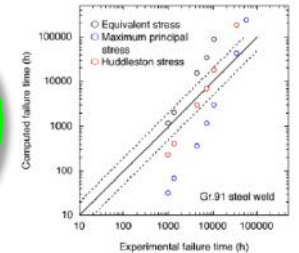
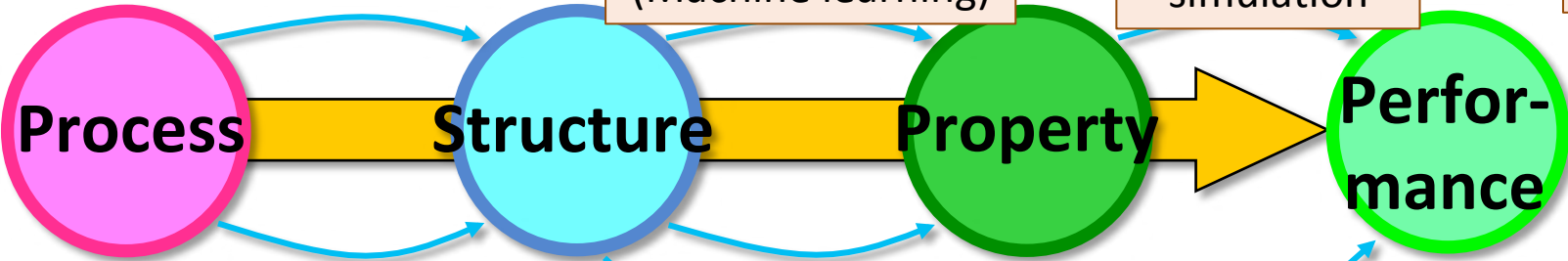


Constitutive law (Machine learning)

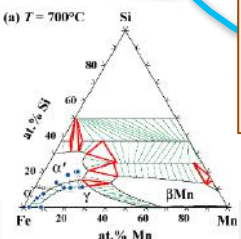


FEM Life time simulation

Life time prediction of a heat-resistant part



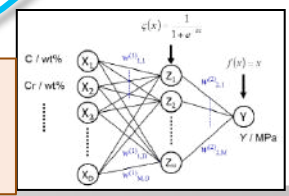
Calphad phase diagram



Empirical rule

$$\sigma_y = f(\sigma_0, k, d)$$

Creep life time (Machine learning)



# Resources of the MI system

Executed Results

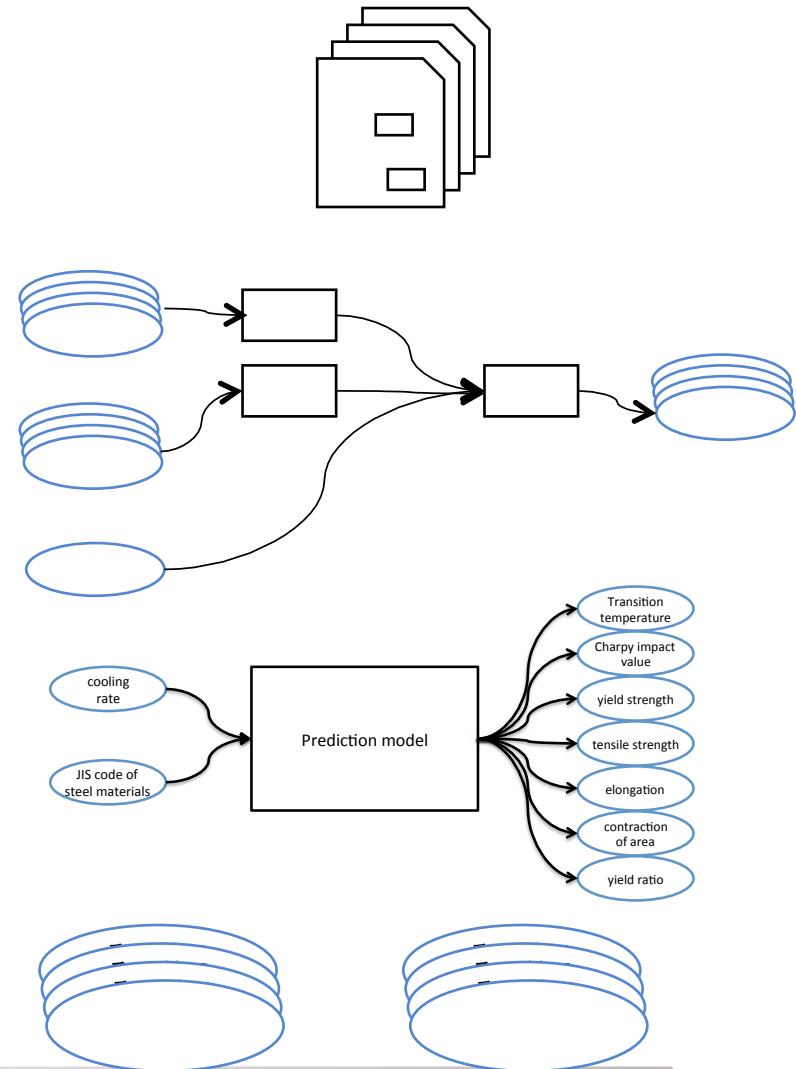
Workflows

Prediction Models / Modules

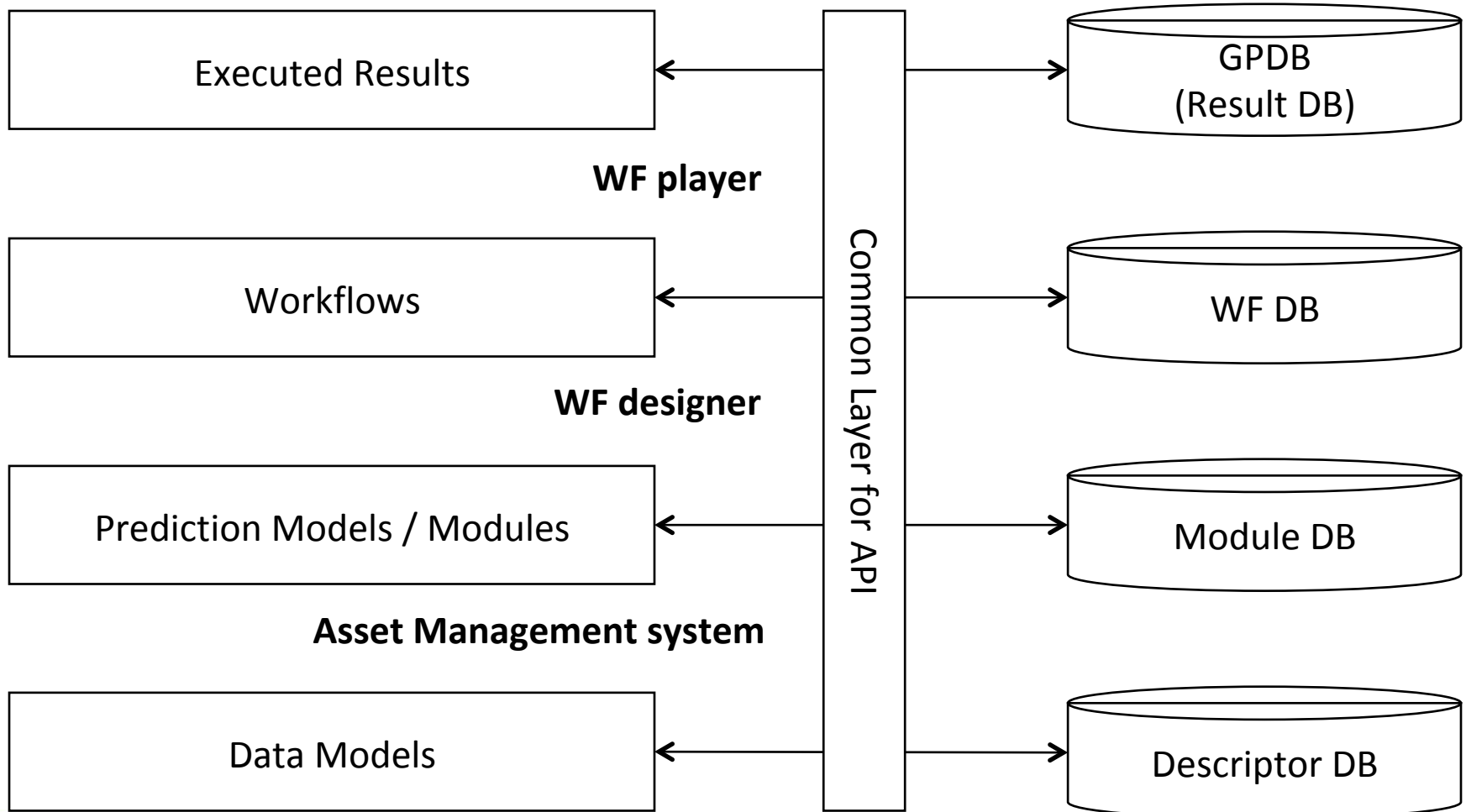
Measurement/Testing/Simulation/Database/etc.

Data Models / Data Instances

Parameters / Physical Quantities/etc.



# Systems for management of resources



# Use cases of the MI system

- **For Researchers**

- Collaboration / Sharing tool
- Design of data, model, module and workflows
- Optimization tool

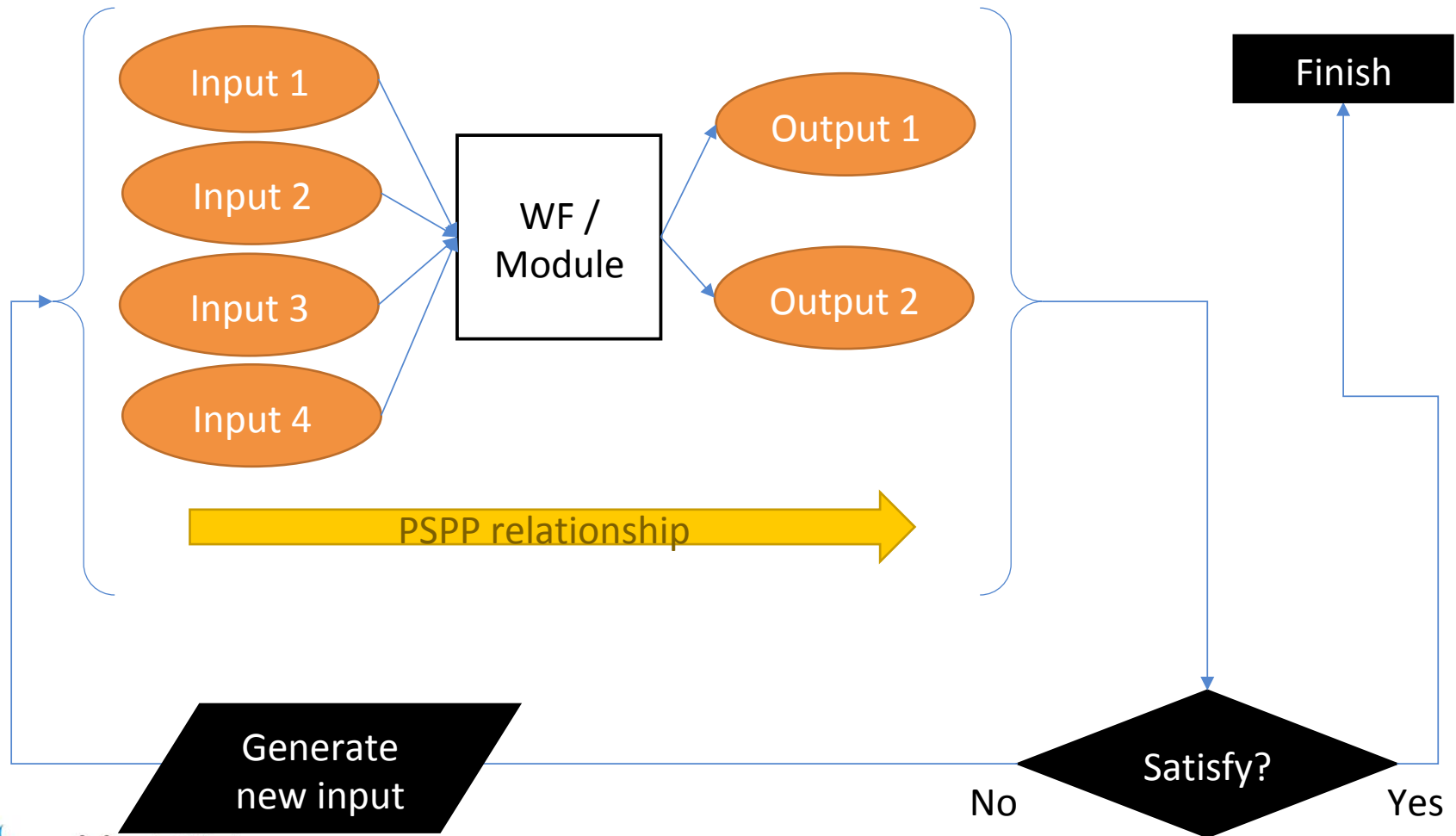
- **For Material suppliers / users**

- Standards for data exchange between different sectors (like “mill sheet”)
- Optimization tool

- **For Teachers / students**

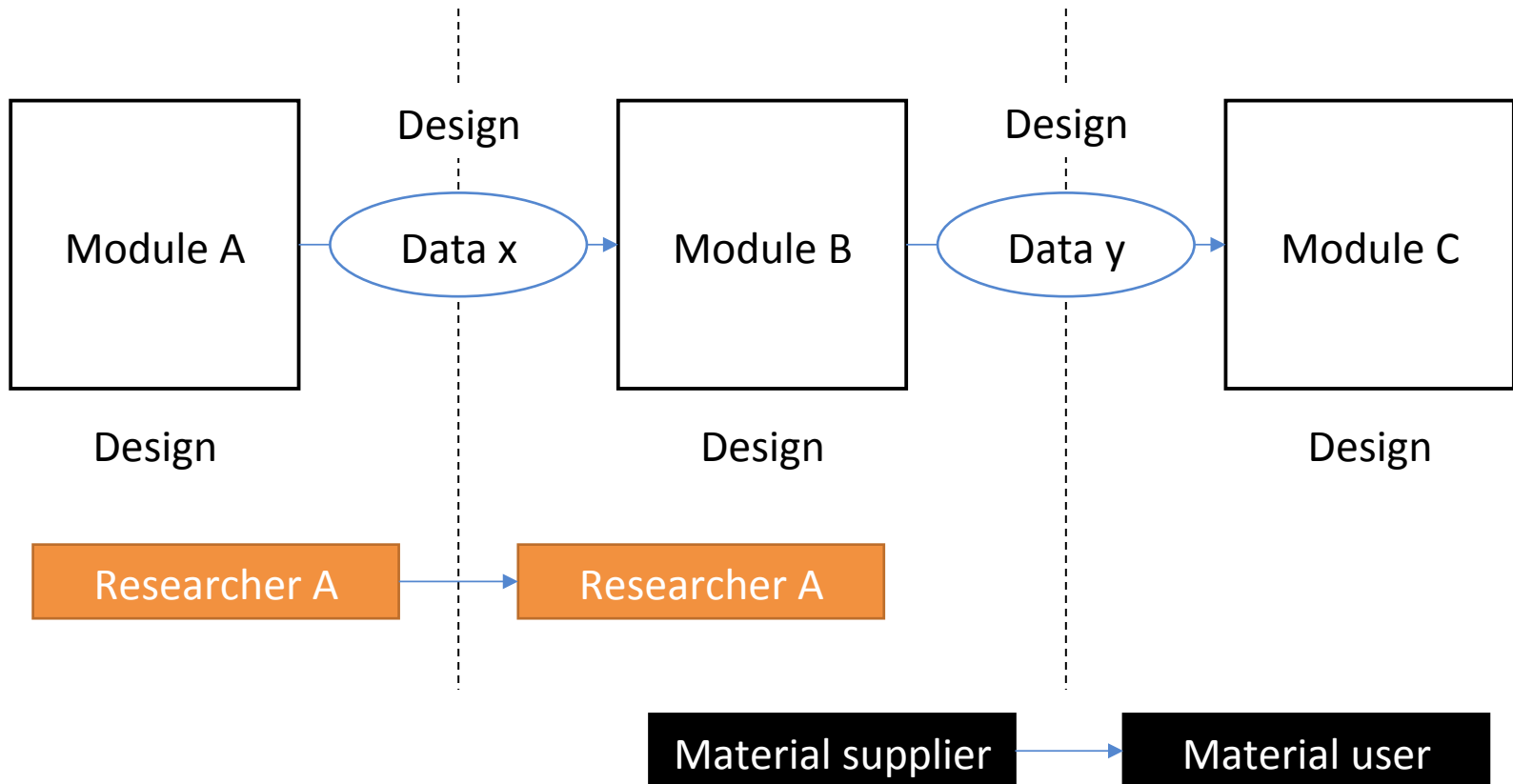
- e-learning resources
- Training tool for design of materials

# Use case example 1: Tool for PSPP optimization





# Use case example 2: Collaboration and sharing



Standards for data exchange between different sectors (like mill sheet)

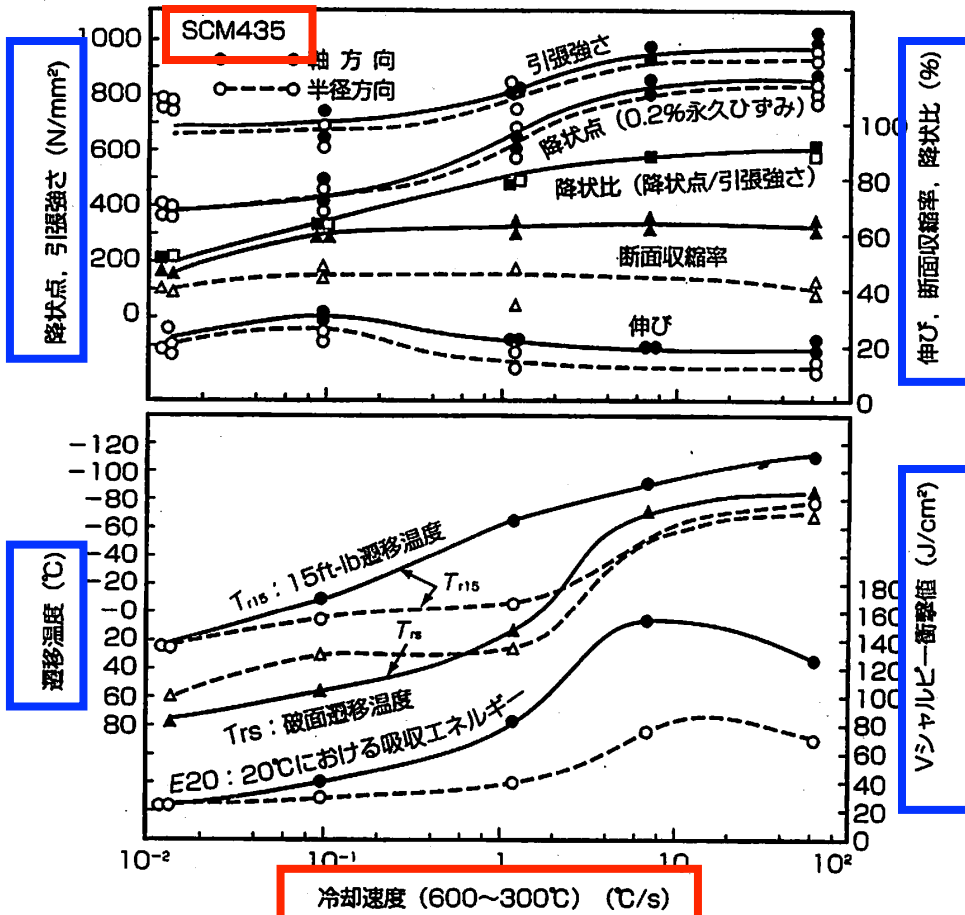
# Use case example 3: Design opportunities

- **Data models**
  - Metadata concerning MSE
  - Data schema toward interoperability among models/modules
- **Prediction models**
  - Relationships between I/O descriptors including their selections
- **Executable modules**
  - Calculation algorithms based on materials theories and/or calculation tools such as *ab initio* calculation
  - Queries for DBs of materials properties
  - Correlation models generated by Machine Learning techniques
  - Quantitative empirical rules
- **Workflows**
  - Solvers for direct problems along PSPP relationships

# Design opportunities

Resources	Design opportunities	Who in charge
Data models	<ul style="list-style-type: none"> <li>● Metadata concerning MSE</li> <li>● Data schema</li> </ul>	<ul style="list-style-type: none"> <li>● Dictionary editors</li> <li>● Data curators</li> <li>● Software owners</li> <li>● MSE professionals</li> </ul>
Prediction models	<ul style="list-style-type: none"> <li>● I/O relationships</li> </ul>	<ul style="list-style-type: none"> <li>● MSE professionals</li> <li>● Teachers / students</li> </ul>
Executable modules	<ul style="list-style-type: none"> <li>● Calculation algorithms</li> <li>● Queries for DBs</li> <li>● Correlation models generated by ML</li> <li>● Empirical rules</li> </ul>	<ul style="list-style-type: none"> <li>● Statisticians</li> <li>● Physicists</li> <li>● Data collectors</li> <li>● Software owners</li> <li>● MSE professionals</li> </ul>
Workflows	<ul style="list-style-type: none"> <li>● Solvers for direct problem along with PSPP</li> </ul>	<ul style="list-style-type: none"> <li>● MSE professionals</li> <li>● Innovators</li> <li>● Teachers / students</li> </ul>

# Use case example 4: e-learning resources



- i: cooling rate
- i: material code
- o: transition temp.
- o: Charpy impact value
- o: yield strength
- o: tensile strength
- o: elongation
- o: contraction of area
- o: yield ratio

図 3.9 焼入冷却速度と 620°C 焼戻後の機械的性質、靱性値\*

# Knowledge in the MI system translated from textbooks

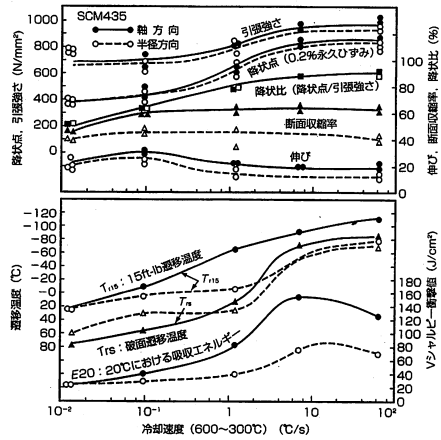
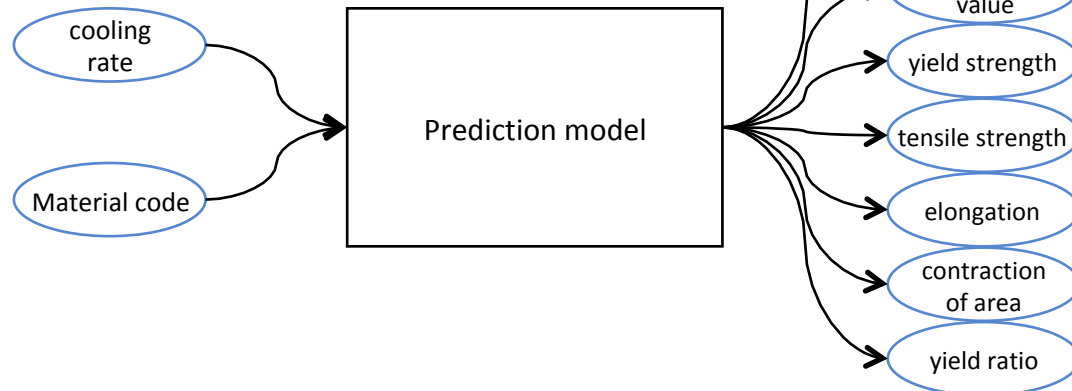
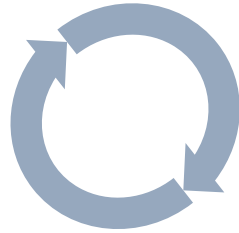


図 3.9 焼入冷却速度と 620℃ 焼戻後の機械的性質、靱性値\*

cooling rate	transition temperature	Charpy impact value	yield strength	tensile strength	elongation	contraction of area	yield ratio
°C/s	°C	J/cm2	N/mm2	N/mm2	%	%	%



# Toward sustainable operation of the MI system

- **Developer team (= Translators)**
  - Is very important for prompt translation between stakeholders from different sectors
- **Documentation**
  - Is very important for succession of rules, knowhow, concepts and philosophies
- **Public funding**
  - Is very important for accumulation of examples and contents, particularly in startup phase
- **Intellectual property management**
  - Is very important for smooth collaborations and strengthen the system
- **Consortium / Center of Excellence**
  - Is very important for maintenance of communities of users, designers and tool providers
- **(Usage fee)**
  - will be very important for maintenance of systems

... and we want to know your ideas and experiences about sustainable operation.

# Resources chain for sustainability

=> : can generate

- Data model
  - => Data instance in a common manner
- Series of inputs (Data instances)
  - => Series of outputs (data instances)
- Accumulation of data instances
  - => Correlative modules using machine learning techniques
- Series of modules
  - => workflows
- Accumulation of relationships between descriptors
  - => Suggestion on workflows

# Summary

- Focusing on design of performances of structural materials, we have developed the MI system which has a potential to describe knowledge on materials widely.
- The system works as a collaboration tool between different sectors.
- Sustainable operation is the most important issue for the MI system. Some focusing points based on our experiences have been presented and still be necessary to discuss.