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Vienna, Austria

Materials integration

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

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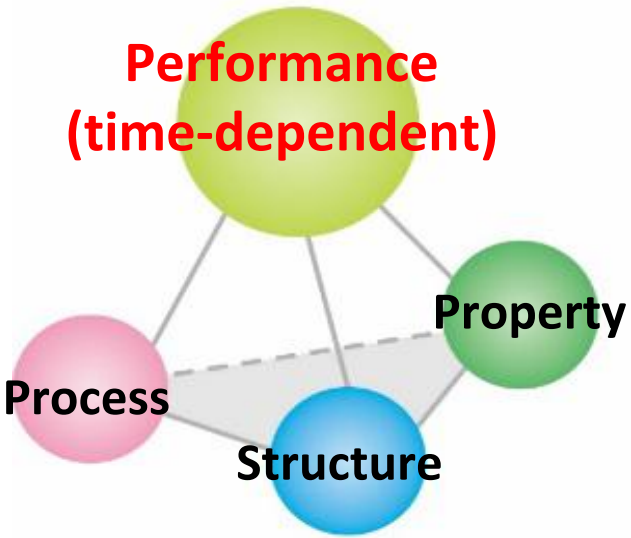
MaDIS
NIMS MATERIALS DATA and INTEGRATED SYSTEM

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.

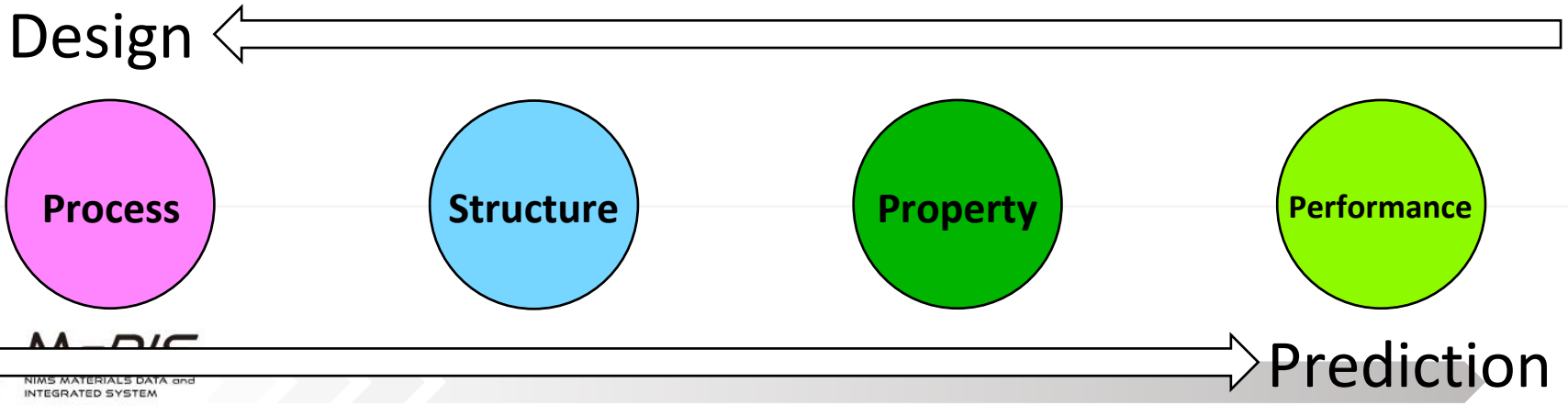

100 yr.

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.



④ Integrated system

Input: Composition, Process, Use conditions

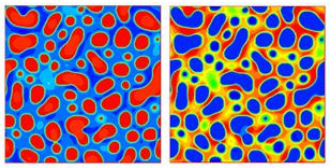
① Microstructure prediction

② Performance prediction

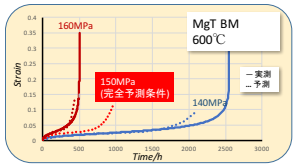
③ Data science

Database

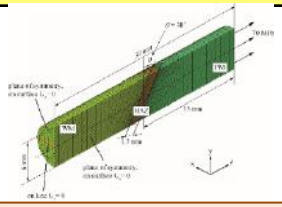
Output: Lifetime Fracture stress …



Phase field

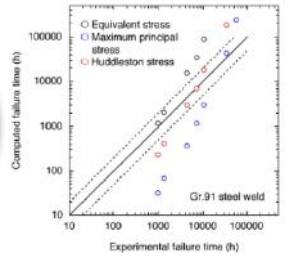


Constitutive law (Machine learning)



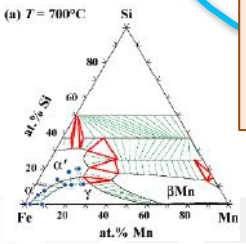
FEM Life time simulation

Life time prediction of a heat-resistant part



Process → **Structure** → **Property** → **Perfor-mance**

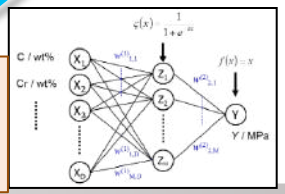
Calphad phase diagram



Empirical rule

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

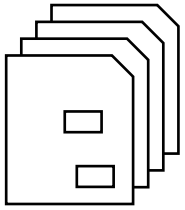
Creep life time (Machine learning)



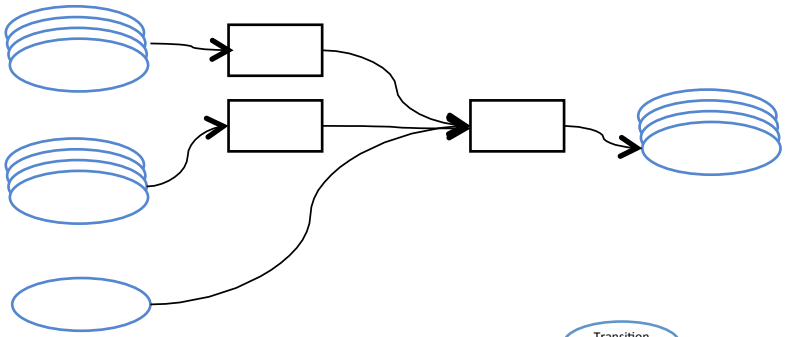
MaDIS NIMS MATERIALS DATA and INTEGRATED SYSTEM

Resources of the MI system

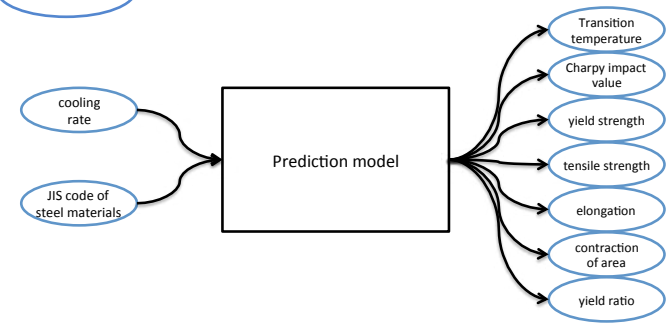
Executed Results



Workflows

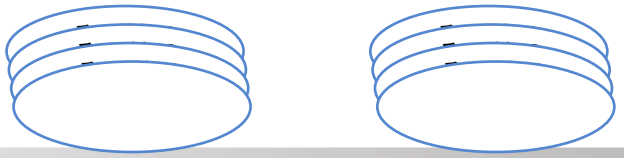


Prediction Models / Modules



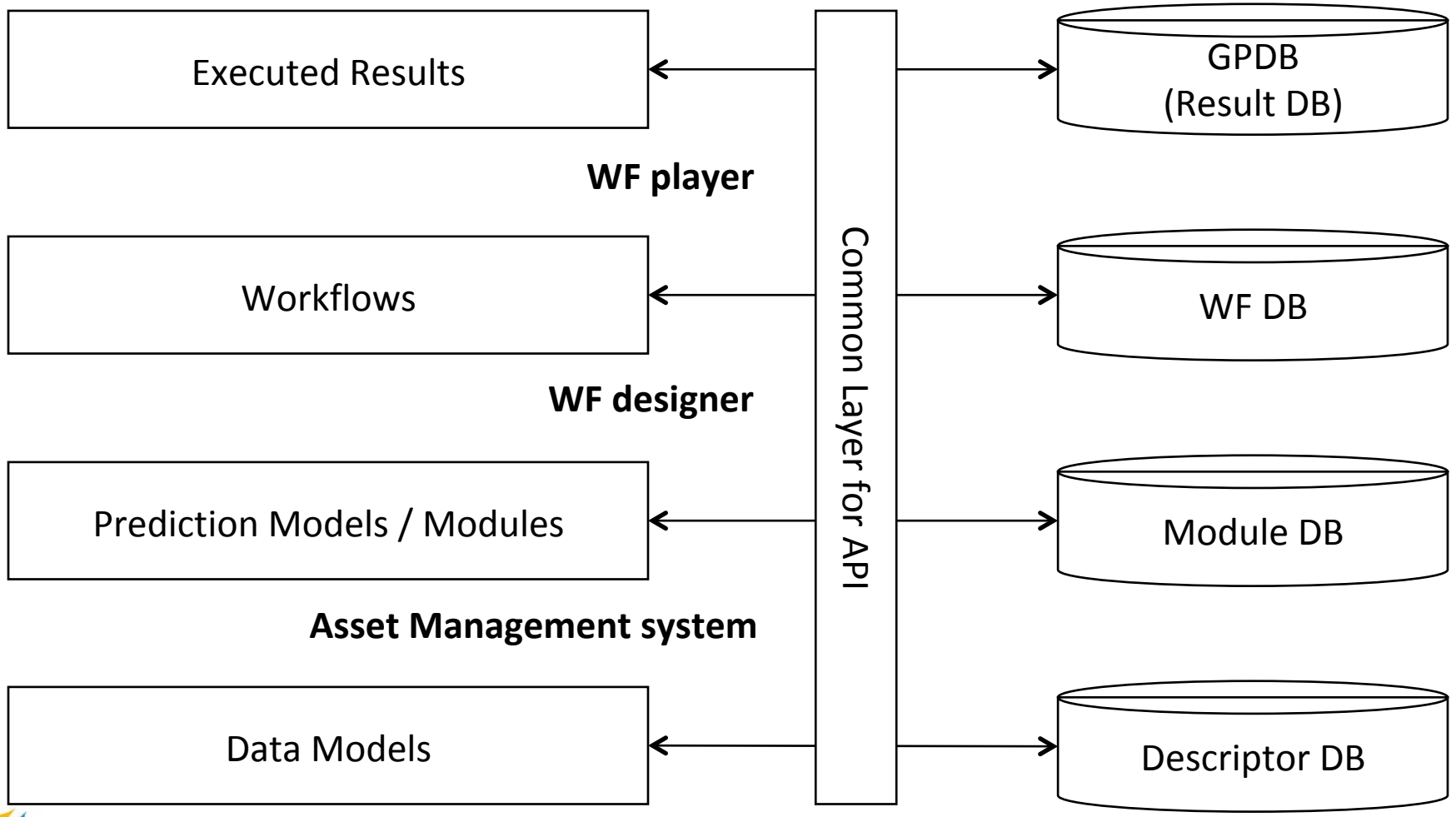
Measurement/Testing/Simulation/Database/etc.

Data Models / Data Instances



Parameters / Physical Quantities/etc.

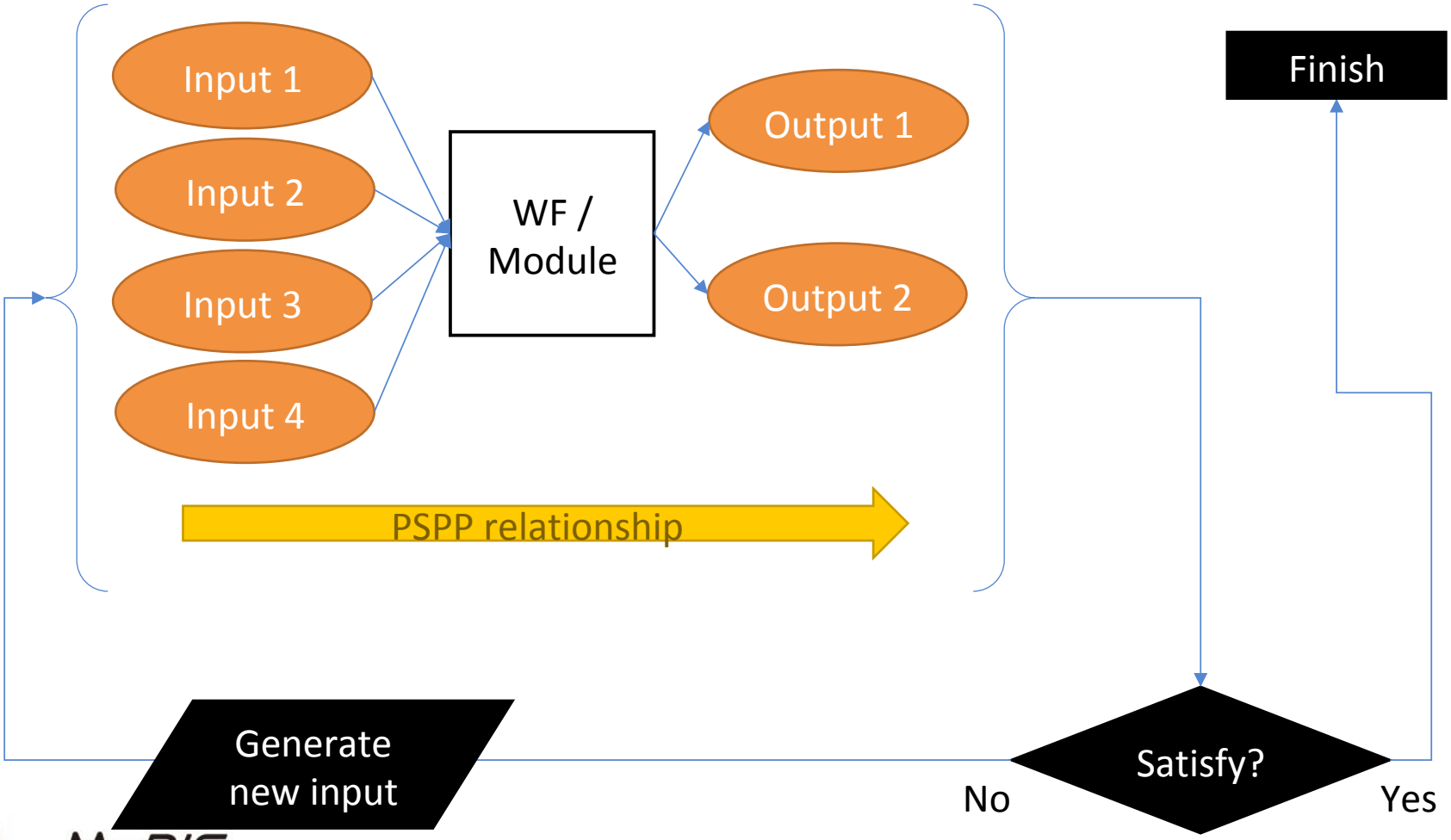
Systems for management of resources



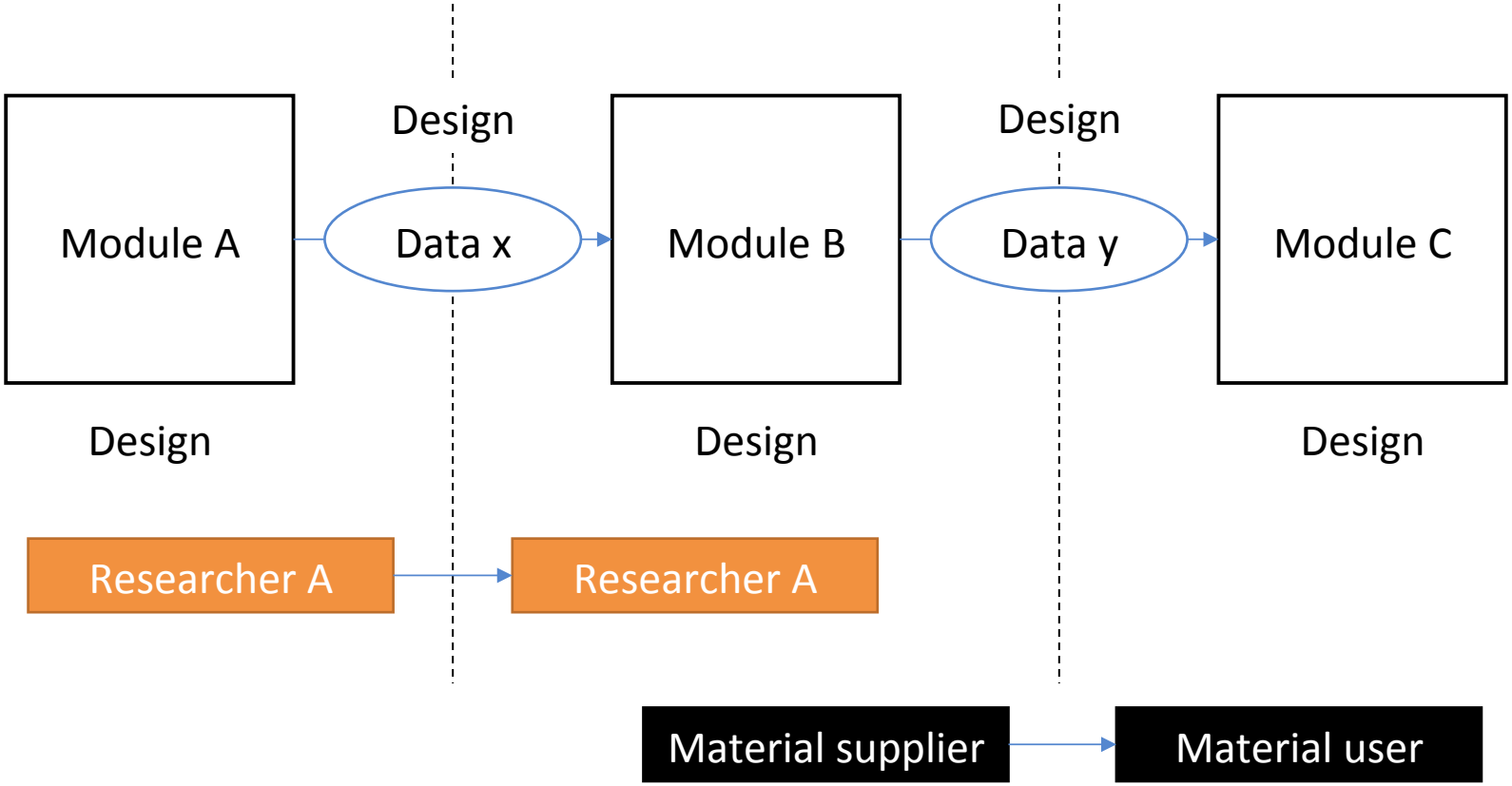
Use cases of the MI system

- **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	● Metadata concerning MSE ● Data schema	● Dictionary editors ● Data curators ● Software owners ● MSE professionals
Prediction models	● I/O relationships	● MSE professionals ● Teachers / students
Executable modules	● Calculation algorithms ● Queries for DBs ● Correlation models generated by ML ● Empirical rules	● Statisticians ● Physicists ● Data collectors ● Software owners ● MSE professionals
Workflows	● Solvers for direct problem along with PSPP	● MSE professionals ● Innovators ● Teachers / students

Use case example 4: e-learning resources

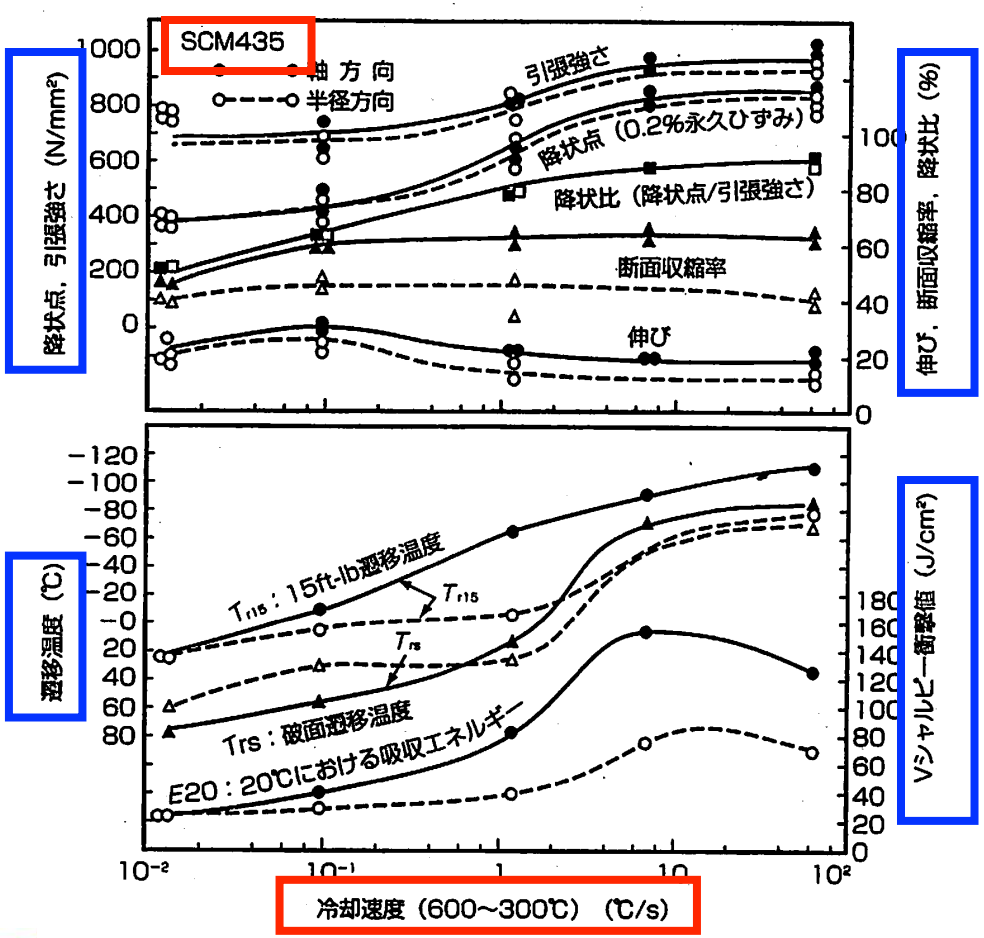


図3.9 焼入冷却速度と620℃焼戻後の機械的性質，靭性値[9]

- 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

Knowledge in the MI system translated from textbooks

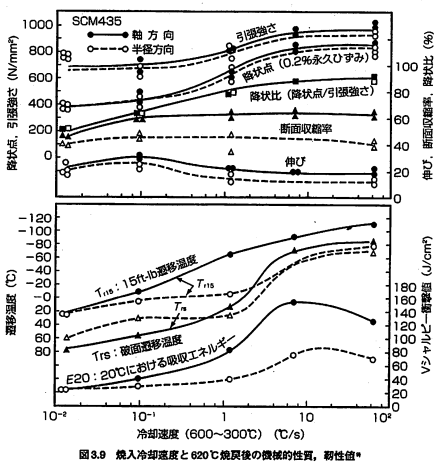
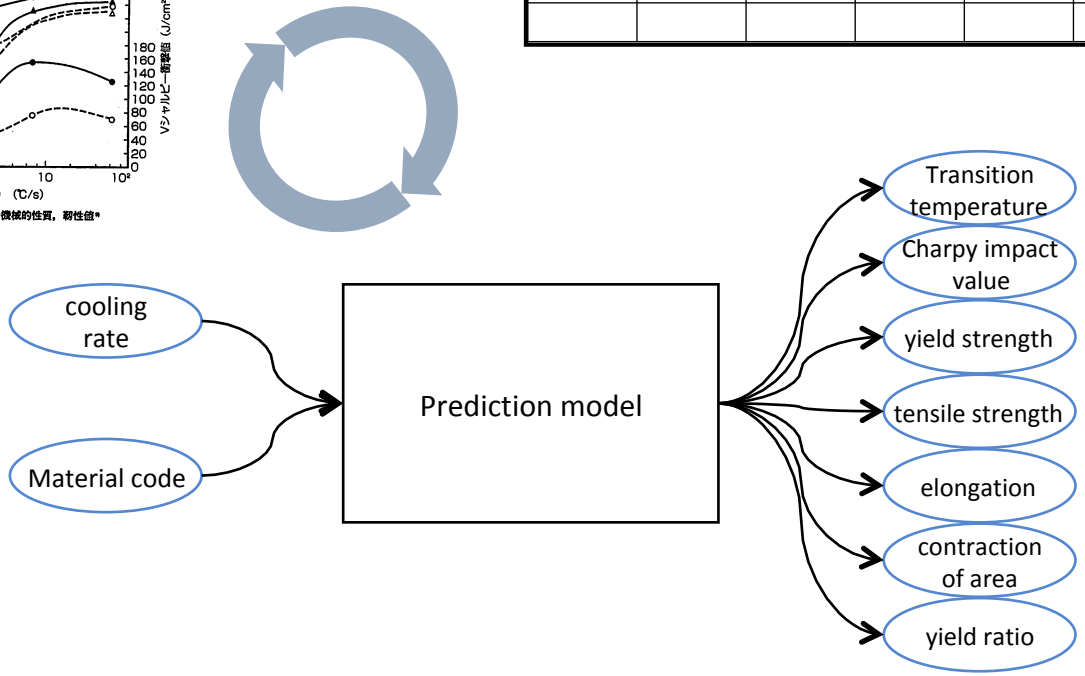


図3.9 焼入冷却速度と620℃焼戻後の機械的性質，靭性値*

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



… **and also it works as resources for e-learning and training**

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 Exelence**
  - 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.