Development of Materials Integration System for Structural Materials

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Introduction

The development of computer technology has been remarkably developed in the past decades. Calculations of significantly large simulation models are possible to be done within acceptable calculation time. As a result, it is becoming possible to perform a multiscale analysis with high precision, such as atomistic scale calculation, microstructure prediction, and performance prediction for a macroscopic order. Furthermore, by using data science techniques such as machine learning, which is rapidly developed in recent years, it is becoming possible to comprehensively search materials on computers. It has a potential to make a drastic change in materials development from conventional approaches based on human experience and intuition to the ones with computation and databases.

For materials used in applications requiring extremely high reliability, such as structural materials for transportation equipment, it takes a very long period of time, such as 15 to 20 years, to be applied to actual machines since the beginning of their development.

For this reason, the shortening of the development period has been a big subject to be overcome. In this research, a technology so called Materials Integration (MI) has been under development, which predicts linkages of material processes, microstructure, characteristics, and performance on computer by combining simulations, theoretical models, empirical formulas, and data science. By establishing such technologies, we aim to contribute to a substantial shortening of material development period.

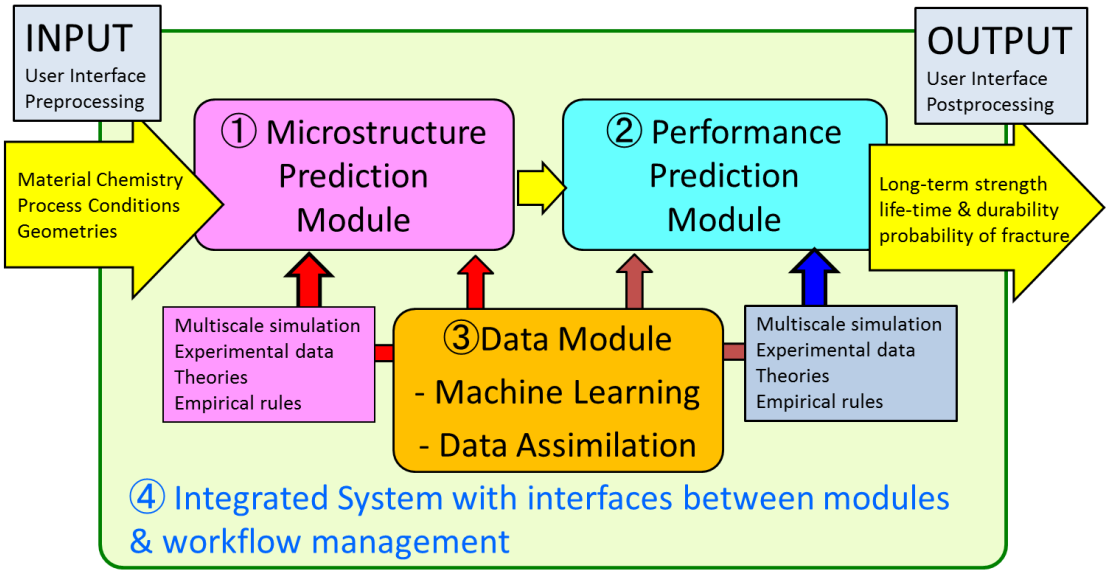

Figure 1: Schematic of Materials Integration (MI) System

Based on the background as described above, we are developing an integrated system to be the platform of Materials Integration technology under the SIP-SM4I project for structural materials (Cross-ministerial

Strategic Innovation Promotion Program, Structural Materials for Innovation) in Japan. In this system, many modules for execution of various analyzes and for derivation of parameters necessary for analysis can be used. And also various general-purpose databases can be used. Furthermore, users can flexibly combine those modules and databases to predict the material performance for their own applications. The schematic of the whole system is shown in the Fig. 1.

Four years have passed since the start of this system development, and the prototype α version has been completed and the launch version 1.0 will be developed in this fiscal year. Basic implementation of analytical flow management technology and data input / output mechanism has been completed and further improvement are under development. Fig. 2 shows the example of the workflow constructed on the system for the prediction of the continuous cooling transformation (CCT) diagram for the carbon steel (NIMS Matnavi database No. 16). By executing the workflow on the system, we can predict the CCT diagram.

In the presentation, we will provide a more detailed overview and an example of utilization of the MI system development.

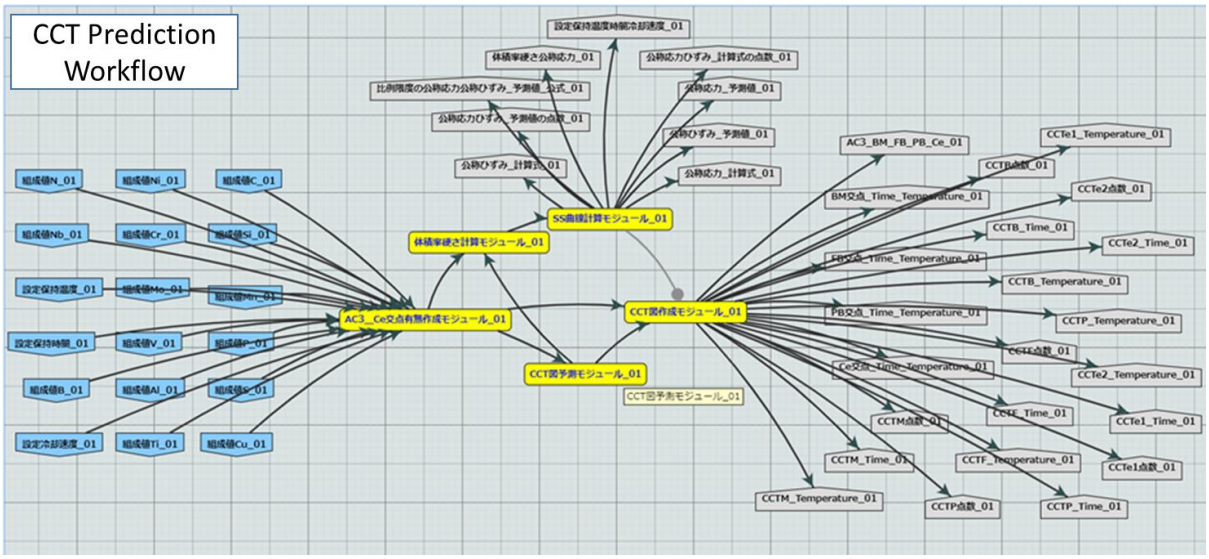

Figure 2: Workflow for the continuous cooling transformation (CCT) diagram

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