Materials Discovery 12 (2018) 9–19

Contents lists available at ScienceDirect

Materials Discovery

journal homepage: www.elsevier.com/locate/md

An implementation of ICME in materials information exchanging interfaces[☆]

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ARTICLE INFO

Keywords:
ICME
Interface
Interoperation
Materials database
Implementation

ABSTRACT

The Integrated Computational Materials Engineering (ICME) approach provides a new paradigm for improving the performance of existing materials or discovering and developing new materials. It focuses on developing effective connections between isolated engineering fields, to bring quantitative processing-structure-property relationships and abundant validated data that populate the knowledge base for accelerating the research of new materials while reducing the cost of development. The data exchanging interfaces play a key role in building such ICME connections among different materials models, simulation tools and individual organizations. With implementations of information exchanging interface between different materials database, and interface between database and applications, this article concludes that in building effective ICME applications, 1) standards-compliant interface can improve the exchange efficiency; 2) popular web service enables automated online materials data transfer; 3) customized data interoperation scripts can provide flexibility and productivity.

1. Introduction

From raw materials to final products, the materials are involved in a complicated processing-structure-property relationship. After decades of development, commercial finite element analysis (FEA) and computational fluid dynamics (CFD) tools have enabled quantitative simulation on processing and structure. In contrast, nominal materials properties obtained from traditional mechanical tests or product applications are still the primary material indicators for FEA and CFD software. The integration of material properties, mostly with the simulation softwares only rather than within the complete cycle of material research, material processing and product manufacturing, will definitely lead to conservative designs, longer processing period and costly production [1,2]. To improve the efficiency in manufacturing and shift the culture in materials development, the Integrated Computational Materials Engineering (ICME) was announced by National Academy of Engineering in 2008 [2]. The goal of ICME is to enable the optimization of the materials, manufacturing processes, and component design long before components are fabricated, by integrating the computational processes involved into a holistic system. ICME can be defined as the integration of materials information, captured in computational tools, with engineering product performance analysis and manufacturing-process simulation [2]. It emphasizes on the "I" for integrated and "E" for engineering, and targets on computational materials modeling as its destination. In that report [2], a number of lessons learned from the early applications of ICME approaches were documented. One of them was described as: “Databases are the key to capturing, curating, and archiving the critical information required for development of ICME.” Furthermore, it was emphasized that “for ICME to succeed, it must be embraced as a discipline by the international materials science and engineering community, leading to changes in education, research and information sharing.”

Following that National Academy of Engineering report, in 2011, the 1st World Congress on Integrated Computational Materials Engineering (ICME) was successfully held in Seven Springs, Pennsylvania, USA. Three major topics, modeling processing-microstructure and microstructure-property relationships, and ICME in education were discussed among global professionals. The 2nd World Congress on ICME was held in Salt Lake City, Utah, USA in 2013. Progress in several challenging areas, such as multi-scale modeling,

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[☆] This manuscript has been authored by UT-Battelle, LLC under Contract No. DE-AC05-00OR22725 with the U.S. Department of Energy. The United States Government retains and the publisher, by accepting the article for publication, acknowledges that the United States Government retains a non-exclusive, paid-up, irrevocable, world-wide license to publish or reproduce the published form of this manuscript, or allow others to do so, for United States Government purposes. The Department of Energy will provide public access to these results of federally sponsored research in accordance with the DOE Public Access Plan (http://energy.gov/downloads/doe-public-access-plan).

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https://doi.org/10.1016/j.md.2018.09.001
Received 9 February 2018; Received in revised form 3 July 2018; Accepted 6 September 2018

process optimization, model validation, experimental tools and ICME education were reported. Concerning materials data, challenges and approaches in materials data management, the fundamental databases, the ecosystem, and the applicable tools to support the flow of traceable materials information for ICME were discussed [3–6]. A more recent review article authored by G. Xiong and G. B. Olson [47] has reported further progress in the tools developments, simultaneously D. L. McDowell and S. R. Kalidindi summarized several key elements to develop ICME ecosystem [48]. Although these efforts are absolutely and fundamentally necessary in building the ICME ecosystem, development of materials information standardization and automated data exchange techniques are indispensable as well because ICME cannot be effectively constructed on isolated materials information islands. After decades of accumulation of contents and technology in materials engineering, independent institutes and organizations around the world have developed various individual materials databases, such as the NIMS Materials Database (MatNavi) [7] developed by the Japan National Institute for Material Science (NIMS), the MatDB [8] online materials database developed and supported by the Joint Research Centre (JRC) of the European Commission, and the web-based materials database Gen IV Materials Handbook [9] hosted by Oak Ridge National Laboratory (ORNL), in different scales and formats.

In addition to the traditional materials databases that focus on bulk materials properties, more and more materials data repositories are devoted to materials properties down to the atomic scale, such as MATIN [10], MDF [11], the PRISMS Materials Commons [12], the Citrine database [13], NIST's MDCS and NMRR [14]. Meanwhile, a few collaborative ICME data frameworks have formed and evolved and matured, including the Integrated Collaborative Environment (ICE) developed by AFRL [15] which is based on HUBzero software [16] and its RESTful API, the science and engineering gateway NanoHUB.org [17], the Materials Commons platform [12] from the University of Michigan, and several cloud-based systems like Sumatra [18], the Citrine Informatics [13], and the materials data facility (MDF) [11]. International materials data efforts, such as efforts from the RDA/CODATA Materials Data, Infrastructure & Interoperability Interest Group [19], have never stopped encouraging exchange of computational and experimental materials data through shared online repositories, standardized formats and terminologies and open programming interfaces that are essential to accelerating the development of ICME. The privilege restrictions of data accessing in ICME infrastructure was an obstacle initially because most of the traditional materials data have been isolated and protected for a long time. Recently, along with the development of ICME ecosystem, more and more materials repositories have completely or partially opened their data content to the public or the community for free accessing, such as the MatNavi [7], the MatDB [8], the MATIN [10], MDF [11], etc., which might gradually reduce the difficulty of accessing and sharing materials data. Despite these initial successes, however, the terrain across the ICME frontier still remains largely uncharted, with many hurdles and challenges to overcome for maturation of ICME methodologies [20–27]. Instead of creating new materials database systems, bridging the existing isolated materials repositories might be a cost and time-saving solution with maximum degree of information shared for the development of ICME. The practical approach for consideration would be to promote standards-compliant schemas and ontologies that enable database interoperability through development of data exchange mechanisms, thus allowing participating database systems and applications to largely keep their original terminologies, schemas, and formats, as long as their data can be transferred to each other through a viable means. Therefore, it's not surprise to see that the scope of the Second Workshop on Software Solutions for ICME held in Barcelona in April 2016 was summarized in one word: Interoperability [28].

As case studies in materials information standardization and communication, three data exchanging interface examples are introduced in Section 2,3 and 4 respectively. Section 5 concludes the accomplishments of this article. These examples illustrate the data interoperation between different databases, and data interoperation between database and application as well. Challenges and technical obstacles encountered in these cases, typical or not in ICME infrastructure, along with final resolutions will be described in the following sections. The key contributions of our work in this article include: i) develop information exchanging interface for tensile test in compliance with ISO-6892; ii) implementation of automated online materials data transfer; iii) demonstrate the flexibility and productivity of customized data interoperation scripts that could potentially benefit development of ICME. Through the implementation instances, this article concludes that in building effective ICME applications, 1) standards-compliant interface can improve the exchange efficiency; 2) popular web service enables automated online materials data transfer; 3) customized data interoperation scripts can provide flexibility and productivity. The successful implementation of these interfaces would evolve useful technologies and experiences, and shed light on the data interoperability for ICME infrastructure development.

2. MatDB and gen IV materials handbook

The Online Data and Information Network (ODIN) is hosted by European Commission Joint Research Centre Institute for Energy and Transport (EC-JRC-IET), providing the full cycle of data entry, retrieval and analysis over the Internet, to support European Union projects and network partners in energy and transport research. The facility consists of a collection of online databases organized into four main categories: documents, engineering, nuclear, and product information. The Materials Database (MatDB) [8] is one of the ODIN online databases specialized in the engineering category for materials test data that has a robust data model, comprehensive test support, and an intuitive user interface [30]. The MatDB database covers mechanical properties, thermo-physical properties, and corrosion data of engineering alloys generated in accordance with international material testing standards and recommendations. It contains over 20,000 test results accumulated after decades of development. Eventually, it aims at the direct web-enabled data entry from test machine into database for European Union projects and network partners by using XML (eXtensive Mark-up Language) [31].

Following the early work of ASTM E49 [32], five main entities, namely, Source, Specimen, Condition, Materials and Test Results, form the basis of the MatDB data model [30]. For the purposes of data exchange, the MatDB data model is also manifested as an XML schema definition (XSD). Each entity has sub-schemas with more specifications in different levels, building the whole framework of the database. The hierarchical schemas end with attribute elements, which are the metadata to be assigned with different types of values. In the tree-like MatDB system, the schemas and their sub-schemas build up the branches, while the detailed attributes are leaves at the end. Fig. 1 depicts part of the MatDB structure.

Since the MatDB XML schemas are a representation of data structure of the database application, experimental data can be imported into database efficiently [33]. Reversely, the binary data stored in the system can be exported to external XML data files that are compliant with the MatDB schemas.

The beginning of Gen IV Materials Handbook database system can be traced to 2005, and when its first beta version was released in 2006 [9]. Evolved with the development of Gen IV Nuclear Reactor Systems, the Gen IV Materials Handbook system has been upgraded to Version 5. More details about the Gen IV Materials Handbook system can be found in reference [29].

The entire system of Gen IV Materials Handbook is constructed with several Parts [9]. The early design of the Parts and the interrelationships are illustrated in Fig. 2. The solid black line between two Parts indicates their internal connection, which means an internal hyperlink could be created for two records in different Parts. Each individual Part