MEC-E1070 - Selection of Engineering Materials, Lecture, 4.9.2023-13.10.2023

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Grade	**3.00** out of 3.00 (**100**%)

Question 1

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Why is material modeling used widely nowadays?

Definition: A material model, or constitutive model, is a mathematical representation of the expected behavior of a given material in response to a physical phenomenon [1] (applied force, temperature, material phase evolution etc). Examples are Linear Elastic model (Hooke's law), the Plastic model (von Mises criterion, crystal plasticity, enHill48), damage models, cleavage/ductile fracture models (eMBW), composite and laminate material models, etc

Why is material modeling (MM) used widely nowadays?
1. Predictive Capabilities: MM allows engineers to predict the behavior of materials under various operating conditions without the need for extensive experimental testing. This can save time and resources. For example, crystal plasticity model can predict stress strain curve without conducting tensile testing
2. Design Optimization: Engineers can use MM to optimize designs for specific applications. For instance, aeronautics and aerospace requires higher performance and efficiency while ensuring maximum reliability and controlling costs. MM plays a central role in achieving those objectives [2]
3. Understanding Complex Phenomena: Some material behaviors, especially at the atomic or molecular level, are difficult to observe directly. Modeling provides insights into these behaviors, helping researchers understand mechanisms like hydrogen diffusion and phase transformations.
4. Integration into Computational methods: these MMs are highly optimized on various softwares, which enables large scale simulations and efficient automation workflow.

References:
[1] https://www.sciencedirect.com/topics/engineering/material-model
[2] https://www.hindawi.com/journals/ijae/2018/6296145/

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Question 2

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What is the typical material modeling software?

Many MM softwares belong to the class of CEA (Computer-aided engineering) to deal with tasks related to engineering analysis. Most commercial CAE softwares support FEA (Finite Element Analysis) feature, which can derive material properties under different deformation schemes. The typical softwares falling into this type include Abaqus, Ansys, Siemens NX and CreoPTC. MATLAB, while a proprietary programming language, also supports a wide variety of MM simulation. There are many other softwares developed independently by many researchers and became open source. Some of them are:

1. MSC Marc: A nonlinear finite element analysis software used to simulate complex material behaviors and interactions.

2. MOOSE (Multiphysics Object-Oriented Simulation Environment): An open-source computational framework that provides a high-level interface for solving fully coupled systems of nonlinear partial differential equations.

3. DREAM3D (Digital Representation Environment for the Analysis of Microstructure in 3D): A software tool for reconstructing, processing, and analyzing 3D microstructure data, particularly useful for materials science applications.

4. DAMASK (Düsseldorf Advanced Material Simulation Kit): A simulation toolkit for multiscale modeling of crystalline materials, focusing on the mechanical behavior of metallic materials.

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Question 3

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Any ideas to use machine learning models to boost the material modeling and material design?

Machine learning (ML) techniques enable us to infer relationships from a large amount of input data. Physical sciences have been quite behind to utilize the power of ML, even though their computational implementation is suited to modern simulation techniques already [1]. As a result, right now MM can greatly benefit from a number of ML applications, such as materials discovery and MM design that promise to accelerate development of novel technologies.

Some of the key points in applied ML for MM and material design are:
1. Neural networks: Obtain nonlinear correlation between material properties and material behavior. Neural networks are proven to model any types of functions (no matter how complex it is).
2. Graph neural networks: material and pattern discovery
3. K-clustering: can be used to categorize materials based on their properties or behaviors
4. Dimensionality reduction techniques: find which properties are the most likely cause of the observed behavior.
5. Compressed sensing can be used to reconstruct microstructural images or patterns from limited data, especially in techniques like electron microscopy or tomography.
5. Derivative-free optimization algorithm to find the optimum to a material design problem, such as Genetic algorithms and Particle Swarm optimization. They are usually coupled with a surrogate model like neural networks or polynomial functions.
6. Bayesian optimization: Nonparametric optimization algorithm with the same purpose above, but with the surrogate model as the Gaussian Process.

Reference:
[1] https://courses.aalto.fi/s/course/a053X000012QxjwQAC/machine-learning-for-materials-science-d?language=en_US

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