SE 598 – Machine Learning in Material Design

Department of Industrial and Enterprise Systems Engineering
University of Illinois at Urbana-Champaign

Instructor: Yumeng Li, PhD
Course Hours: TR 3:30 -4:50 PM
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Course Description: Growing demands on advanced material systems have challenged scientists to identify new chemical compositions and optimize microstructures and properties over a high-dimensional design space. There has been considerable interest in accelerating the process of material analysis and design through leveraging machine learning, which have revolutionized several areas attributing to its extraordinary capability in pattern reorganization and data mining. In this course, we will explore the benefits of introducing machine learning into material design and how to efficiently integrate machine learning at different level of material analysis and design process for accelerating novel material discovery. The tentative contents that plan to be covered in this course include introduction to computational material simulation, data-driven experimental design, hidden structure identification, data fusion, physics-based machine learning, and adaptive sampling and surrogate modeling. Design applications in energy storage systems, low dimensional materials, polymer based composites and additive manufacturing will be used as case studies for demonstration in this course.

Learning Objectives: After completing this course, students can

- Be familiar with the literature on computational methods for material analysis and design;
- Understand the current challenges in material analysis and design and the opportunities of adopting machine learning techniques
- Develop mathematical models and algorithms for physics-based material simulations and formulate optimization problems for engineer material design;
- Apply machine learning techniques such as physics-based machine learning to address the challenges in the current material simulation methods;
- Solve material design problems involving different length and temporal scales;
- Use date-driven methods to develop multifidelity design models for material design;
- Apply adaptive sampling techniques to enhance the fidelity of computational models for design and improve the efficiency of iterative design process;
- Quantify material simulation uncertainties with statistical models and estimate the model parameters using uncertainty quantification techniques;

References:

- Machine Learning in Materials Science, Keith T. B., Felipe O., Pieremanuele C., American Chemical Society, 2022
- Material Discovery and Design by means of data science and optimal learning, Lookman, T., Eidenbenz, S., Alexander, F. and Barnes, C, Springer Series in Material Science, Volume 280

Prerequisites: Math 241 and IE 300, or per the instructor's approval.

Evaluation: Students are expected to complete their homework/exams on their own. In addition, one term project will be evaluated based on the project report. The evaluation of students' work is the instructor's professional judgment and is **not subject to negotiation.** Incomplete "**I**" will not be given out, unless there are very special circumstances.

Grading: The overall grade of the course will be assembled based on

30%: Homework
35%: Term Project 1
35%: Term Project 2

A+: 97 – 100%	A: 93 – 96%	A-: 90 – 92%
B+: 87 – 89%	B: 83 – 86%	B-: 80 – 82%
C+: 77 – 79%	C: 73 – 76%	C-: 70 – 72%
D+: 67 – 69%	D: 63 – 66%	D-: 60 – 62%

Academic Integrity: We will follow university regulations for academic integrity: (http://admin.illinois.edu/policy/code/). Students who violate academic integrity will receive a "0" on that exam or assignment and may receive an "F" grade in the course. Discussing a homework assignment in a group is encouraged as long as each student writes the answer in his/her own words. Plagiarism is considered a serious violation of academic integrity and will be dealt with utmost severity.

Topical Outline

- Introduction to computational material simulation
- Data and databases
- Data fusion and multifidelity models
- Representation and feature learning
- Neural networks
- Physics-based machine learning
- Adaptive sampling
- Uncertainty quantification
- Material discovery
- Generative modeling