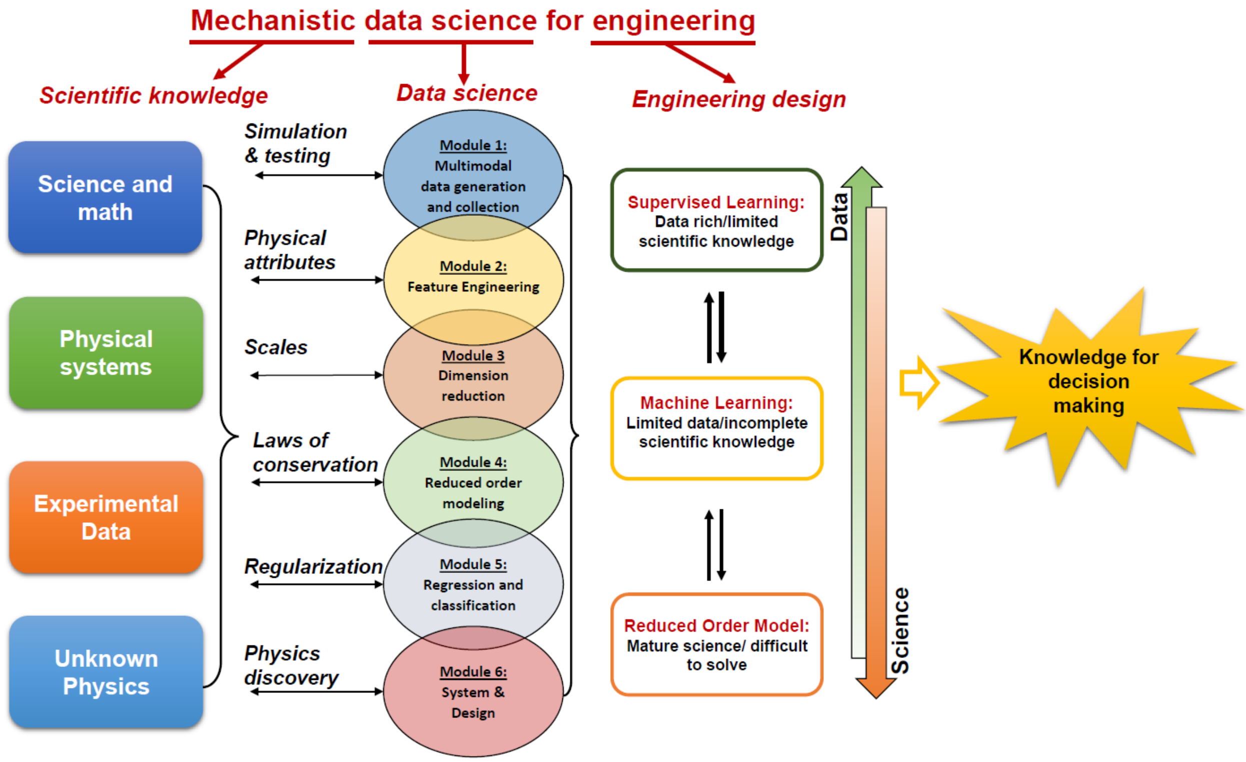
Course ME395 – Mechanistic Data Science for Engineering

Instructor: Wing Kam Liu, w-liu@northwestern.edu, Tech A326, 847-491-7094
Meet on TU and TH 9:30-11:00, place TBD
Who should take the class: Senior and graduate engineering students

Goals:
We introduce mechanistic data science for engineering through the integration of scientific knowledge, such as physics and mechanics through six basic data science concepts: *multimodal data generation and collection, feature engineering, dimension reduction, reduced order modeling, regression, and classification*. These concepts will be applied through the use of Matlab and Python for engineering applications.



Syllabus

Module 1 (Multimodal data generation and collection): (1 week)
Learn the basics of multimodal data generation and collection. Relevant examples will be taken from civil, mechanical, and biomedical engineering, advanced manufacturing, materials science, nanoscience, etc.
Homework 1: reading assignment on multimodal data generation and collection; *write a report on multimodal data generation and collection in area of student's interest.*

Module 2 (Feature Engineering): (1.5 weeks/2.5 weeks)
Learn how to apply basic functional transformations, Fast Fourier Transformation, Wavelet Analysis, and related software/libraries to extract meaningful features from scientific and engineering data.
Homework 2: Application of feature engineering to scientific and engineering analysis

a. *Transform features from temperature history of a process (e.g. Additive Manufacturing or any other time dependent process) using wavelet and Fourier transformation.*
b. *Convert microstructural images to a distribution function.*
c. *Extract spine geometry from DICOM (Digital Imaging and Communications in Medicine) images.*

<u>Module 3 (Dimension reduction):</u> (1.5 weeks/4 weeks)
Learn the basic fundamentals of K-means clustering, Self-Organizing Maps, Gaussian mixture clustering, and related software/libraries on datasets.
Homework 3: Compression of high dimensional engineering data using clustering
a. *Clustering similar element values from Finite Element simulation results of an engineering part*
b. *Using clustering to analyze a micrograph of a material system*
c. *Clustering the atomic trajectory from Molecular Dynamics simulations*
d. *Clustering in a microstructure using stress or strain distribution, the dataset for a microstructure stress/strain distribution will be provided.*

<u>Module 4 (Reduced ordering modeling):</u> (1.5 weeks/5.5 weeks)
Develop a basic understanding of the fundamentals of Principal Component Analysis (PCA), Singular Value Decomposition, Empirical Mode Decomposition, and related software on datasets.
Homework 4: Using data-driven reduced order model for prediction in engineering analysis
a. *Reducing the distribution from HW 2 (b) to a few principal components*
b. *Reducing the history data from HW 2 (a) to a few empirical modes.*
c. *Using principal components to represent the composition of an alloy.*
d. *PCA analysis of microstructure stress/strain distribution (reconstruction of the stress/strain distribution with few principle components and calculate the error)*
Midterm projects: digital thread of the three concepts projects

<u>Module 5 (Regression and classification):</u> (2.5 weeks/8.0 weeks)
Develop a basic understanding of the fundamentals and related software of Linear and Non-linear regression, Feedforward Neural Network, Decision tree, Random Forest, K-nearest neighbor, Bayesian Neural Network.
Homework 5: Using deep learning tools for regression with engineering data
a. *Using the principal components from one of the selected HW 3 to regress and find the mechanical properties of composite materials by neural network or random forest.*
b. *Using linear or non-linear regression to relate the compositions of alloy (from principal components of HW 4(c)) to mechanical properties from Molecular Dynamics.*
c. *Using CNN to relate the mechanical properties of AM parts with wavelet analysis from HW 2(a). (students will have time to submit this HW after module 5 is complete)*

<u>Module 6 (System and Design):</u> (2 weeks/10 weeks)

Apply the six concepts using Convolutional Neural Network, Logistic Regression, and Optimization methods and techniques discussed in previous modules. The system and design will be illustrated for multiple engineering applications.
Final projects: integration of the five concepts for system analysis and design.

Grading: Attendance (15%) Homework assignments (20%), midterm (30%), and final projects (35%)

Grading will be based on homework assignments, a midterm project, and a final project
Homework: there will be one homework set for each of the five modules.
Homework will be due 1 week after assignment.
Midterm project: The midterm project will be based on the integration of modules 1 - 3 proposed by the students.
The midterm project will be due 2 weeks after assignment.
Final project: The final project will be a scientific or engineering application of the integration of all five modules discussed in the class.
The final project will be due during finals week.