

FALL 2025

MEETING #1

Computational Modeling in Engineering and the Sciences

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AGENDA

- Introductions
- Introducing computational modeling
- Goals
- Mentee survey
- Demo: set up Python

**Assignment: Read Konstantinovsky - Mastering the SEIR Model.
We'll discuss next week.**

Introductions

Introductions

- Name
- Major and year
- Something fun you did this summer
- Academic, research, and professional interests

Introducing Computational Modeling

Introducing Computational Modeling

modeling

creating a conceptual representation of a system,
situation, or process, which is used to understand or
predict that thing



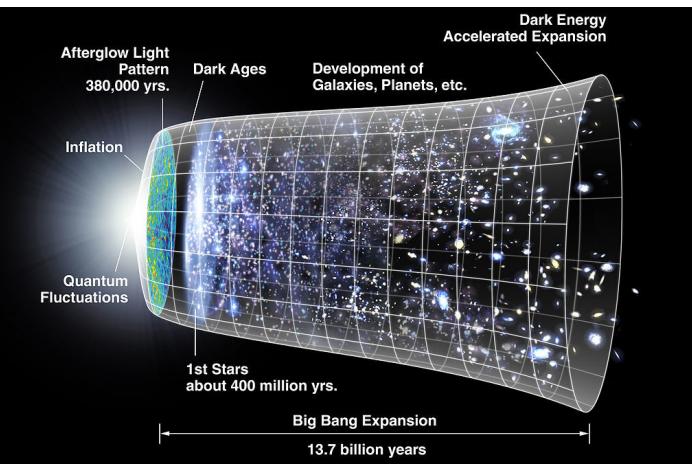
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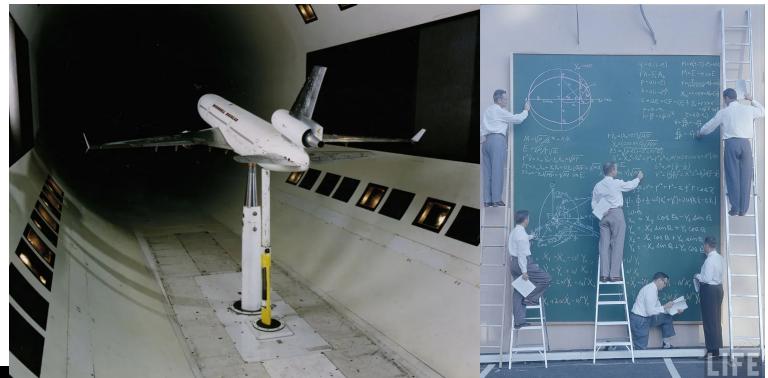
Introducing Computational Modeling



Maybe you want to predict the future



Or understand something that you can't easily test in a lab



Traditionally, your options were relatively limited

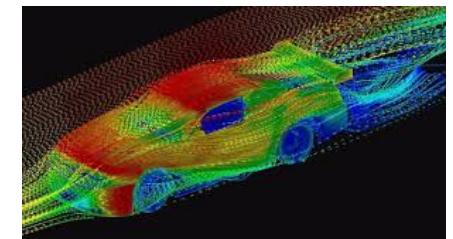
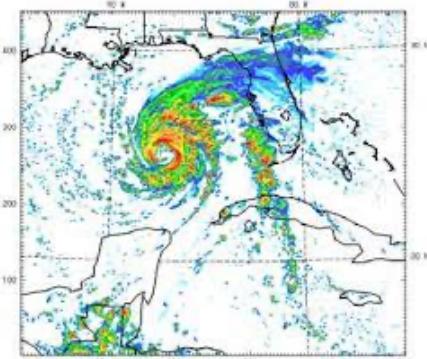
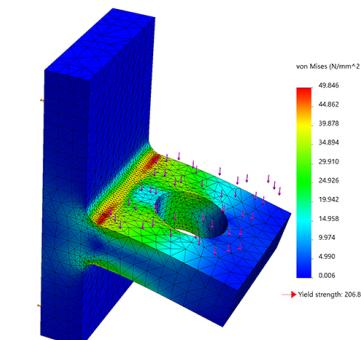
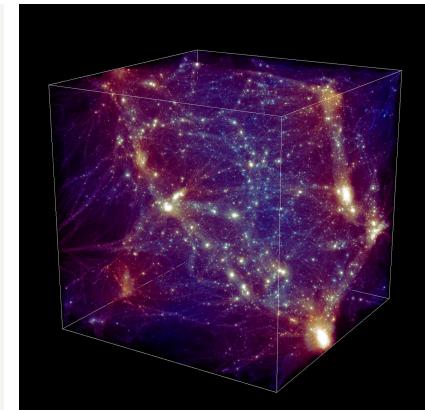
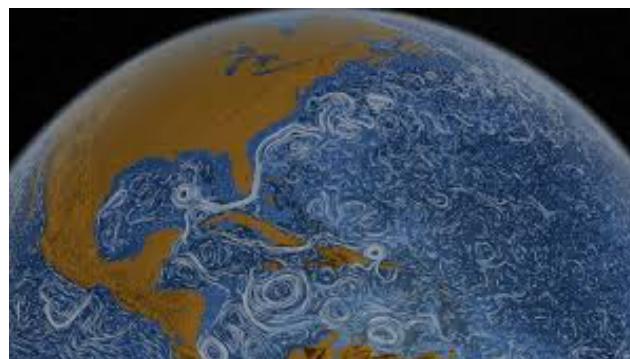
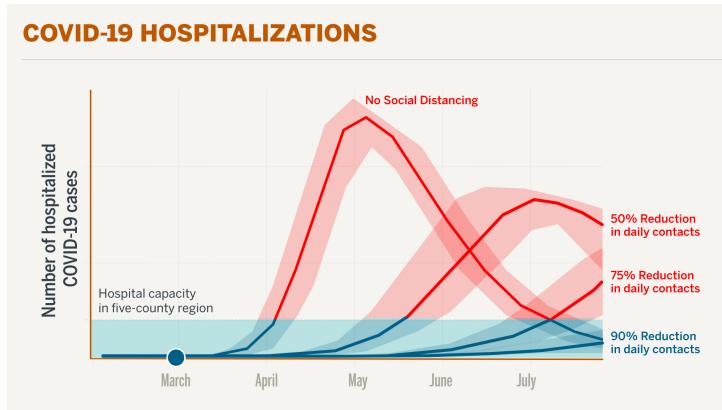
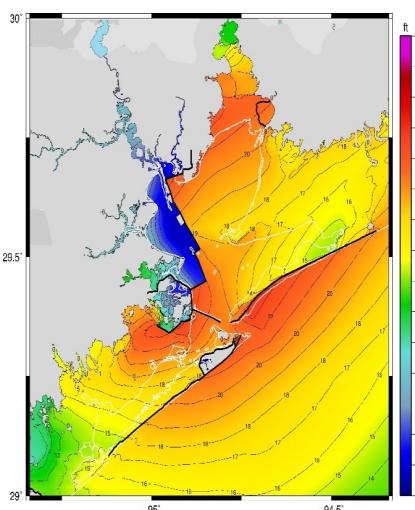
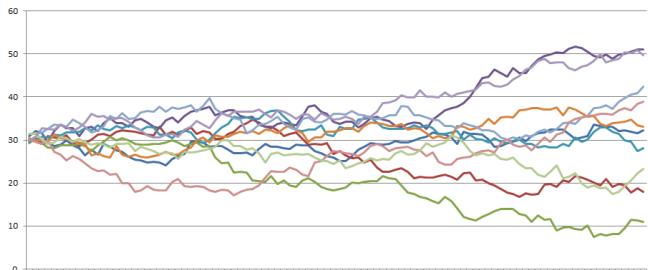


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Introducing Computational Modeling

Computers enable bigger and more complicated models



Introducing Computational Modeling

Computational modeling is very **interdisciplinary**. Computer scientists play an important role in this field of research.

Domain Science

(understanding the thing itself)

Modeling Techniques

(linear algebra, calculus, differential equations, statistics, ML, etc.)

Computer Science

(making computers do big math fast)

Introducing Computational Modeling

Kinds of problems (not comprehensive)

- Forward problems: cause to effect
 - E.g. computational fluid dynamics, COVID forecasting
- Inverse problems: effect to cause
 - E.g. parameter estimation, MRI image reconstruction
- Optimization: finding something that minimizes/maximizes an objective
 - E.g. tumor treatment optimization, best signal to stop a seizure
- Uncertainty quantification: accounting for messy data, uncertain parameters

Introduction to Computational Modeling

Modeling techniques (not comprehensive)

- Differential equations: express how quantities of interest relate to each other using derivatives
 - Solved with FEM, FDM, FVM, spectral methods, etc.
 - E.g. orbital mechanics (ODEs), finite element analysis (PDEs), stock options (stochastic PDEs)
- Data-driven methods: starting with raw data to inform a model, as opposed to principles
 - E.g. regression, statistical fits, machine learning, etc.

Goals

Goals

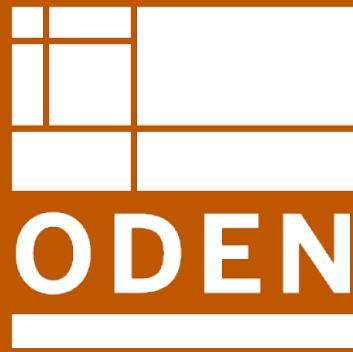
“DiRP is a program to help undergraduate students get involved with computer science research. Mentors can lead reading groups, project groups, or propose their own format.”

- Learn about computational modeling
- Explore research and academia
- Mentorship
- Build up math and coding skills
- “Leave things better than we found them”

See syllabus for details

Mentee Survey

Demo: Set up Python



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