

# Fundamentals of Modeling

## Course: Complex Systems Modeling

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# Outline

## 1 Models

- A descriptive definition
- Models in Science and Engineering
- Conclusion
- Exercise
- Solution (suggestion)

## 2 Modeling Approaches and Methodologies

- Simple Models
- Advanced Models
  - Example: Finite Element Method (FEM) Modeling
- Statistical Models
- Classification of Models by State Complexity
- Mathematical Representations



# What is a model?

- Simplified abstraction of reality that allows us to
  - describe
  - understand<sup>1</sup>
  - predict
  - control

reality.

*"Cool, something we actually need as scientists and engineers, right?"*

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<sup>1</sup>esp. via the process of modeling, hypothesis generation and rejection ▶

# Dealing with Reality

- *Science seeks to understand the world by discovering fundamental laws, such as Newton's laws of motion, the ideal gas law, Ohm's law, and the conservation of energy - some you may know*
- *Engineering applies the fundamental laws of nature, like Newton's laws of motion, the ideal gas law, Ohm's law, and the conservation of energy, to design and build solutions for real-world problems.*



# Scientific Effort Cycle

A typical cycle of scientific effort to discover fundamental laws:

- 1 Observe nature.
- 2 Develop a hypothesis that could explain your observations.
- 3 From your hypothesis, make testable predictions through an experiment.
- 4 Carry out the experiment to verify your predictions:
  - **Yes** → Your hypothesis is proven! Uncork a champagne bottle and publish a paper.
  - **No** → Your hypothesis was wrong. Go back to the lab, gather more data, and develop a new hypothesis.

*Many people think this is how science works. But there is at least one thing that is not quite right in the list above. What is it? Can you figure it out?*



# Is This How Science Really Works?

- Consider the steps of the scientific cycle discussed earlier.
- Is science always a straightforward process of proving hypotheses?
- Does a single experiment truly *prove* a hypothesis, or is there more to scientific discovery?



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**Hint:** Science is an iterative process, and *proof* is often more nuanced than a single result.



# The Limits of Scientific Proof

- Supportive evidence from experiments does not "prove" a hypothesis; it only shows that we have failed to disprove it.
- Many believe science can provide absolute proof, but this is not possible. We cannot logically reach the ultimate truth of nature.
- All *laws of nature*, like Newton's laws or the ideal gas law, are well-tested hypotheses.
- These laws gain credibility because scientists have consistently failed to disprove them, but they are not guaranteed to be universally or permanently correct.
- Science remains open to new theories that might better explain nature.





# Science and Engineering: Building and Using Models

- Science builds models of nature, not absolute facts. The *laws of nature* are models that help us understand and predict phenomena.
- Scientists must remember that these models are approximations, not definitive truths.
- Engineering applies these scientific models to design and solve real-world problems, understanding that models have limitations.
- Effective engineering relies on using these models while considering their assumptions and potential inaccuracies.
- Both fields involve continuous refinement as new data and better models emerge.



# All Models Are Wrong, Some Are Useful

*"All models are wrong, but some are useful."*

– George E. P. Box

- Models in science and engineering are simplifications of reality.
- They help us understand complex systems, make predictions, and solve problems.
- The key is to use models appropriately, recognizing their limitations.



# What Is A Good Model? (Part 1)

**Take-Home Message:** A good model is **simple**, **valid**, and **robust**.

## ■ Simplicity:

- A model should be a simpler description of reality, following the principle of Occam's razor: choose the simpler model if two have equal predictive power.
- Eliminate unnecessary parameters and assumptions to focus on the model's core behavior.

## ■ Validity:

- A model's predictions must closely match observations. Check both prediction accuracy and the "face validity" of assumptions.
- Beware of the trade-off between simplicity and validity to avoid overfitting.



# What Is A Good Model? (Part 2)

**Take-Home Message:** A good model is **simple**, **valid**, and **robust**.

## ■ Robustness:

- A robust model's predictions should remain stable even with minor variations in assumptions and parameters.
- Robustness increases trustworthiness and real-world applicability.



## Exercise: Comparing Models of the Solar System

**Task:** Humanity has created various models of the solar system throughout history. Your goal is to investigate these models and compare them in terms of simplicity, validity, and robustness.

### ■ Models to Explore:

- Ptolemy's geocentric model
- Copernicus' heliocentric model
- Kepler's laws of planetary motion
- Newton's law of gravity

**Instructions:** Analyze each model based on the key criteria and be prepared to discuss your findings.

# Criteria for Comparison: Simplicity, Validity, and Robustness

## 1. Simplicity:

- How simple is the model in its assumptions and mathematical formulation?
- Does the model use the minimum number of parameters and variables?

## 2. Validity:

- How well does the model's prediction match observations of planetary motion?
- Is the model's prediction valid across different scenarios and time periods?

## 3. Robustness:

- How sensitive is the model to changes in its assumptions or parameters?
- Does the model remain accurate under minor variations in input values?



# Ptolemy's Geocentric Model

- **Description:** Assumes that the Sun and planets revolve around the Earth in complex circular paths called epicycles.
- **Simplicity:** Complex due to the use of epicycles to explain retrograde motion.
- **Validity:** Could predict planetary positions to some extent but failed to explain them accurately over time.
- **Robustness:** Sensitive to changes in observed planetary motion; required constant adjustments to epicycles.



# Copernicus' Heliocentric Model

- **Description:** Assumes that Earth and other planets revolve around the Sun in circular orbits.
- **Simplicity:** Simpler than Ptolemy's model; eliminates the need for epicycles.
- **Validity:** Provided a more accurate framework but still relied on circular orbits, leading to some inaccuracies.
- **Robustness:** More robust than the geocentric model but still limited by its assumption of circular orbits.





# Kepler's Laws of Planetary Motion

- **Description:** Describes planetary orbits as ellipses with the Sun at one focus; includes laws about orbital speed and periods.
- **Simplicity:** More complex mathematically but simpler in terms of assumptions compared to circular orbits.
- **Validity:** Highly valid; accurately predicts planetary positions and motions.
- **Robustness:** Robust in various contexts; not overly sensitive to minor changes in parameters.



# Newton's Law of Gravity

- **Description:** Proposes that the gravitational force between two objects is proportional to their masses and inversely proportional to the square of their distance.
- **Simplicity:** Uses a single law to describe a wide range of phenomena; conceptually simple, mathematically more complex.
- **Validity:** Extremely valid; matches observations of planetary motion and other gravitational phenomena.
- **Robustness:** Highly robust; predictions hold under various conditions, though it has limitations at very large scales (addressed by Einstein's theory of general relativity).



## Summary and Discussion

- **Ptolemy's Model:** Complex and less valid; lacked robustness.
- **Copernicus' Model:** Simpler and more valid but not entirely robust.
- **Kepler's Model:** Balanced simplicity with validity; robust in predicting planetary motion.
- **Newton's Model:** Simple in concept, highly valid, and robust across many contexts.

**Discussion:** How do these models illustrate the trade-offs between simplicity, validity, and robustness? Which model do you think is the most effective, and why?



# Simple Models in Science and Engineering

## ■ Characteristics:

- Involve a small number of states or variables.
- Use simple mathematical relationships (often linear).

## ■ Examples:

- **Newton's Laws of Motion:** Describe the motion of objects using basic ODEs.
- **Ohm's Law:** Relates voltage, current, and resistance in electrical circuits with a simple linear equation.
- **Ideal Gas Law:** An algebraic model linking pressure, volume, and temperature in gases.

# Advanced Models in Science and Engineering

## ■ Characteristics:

- Involve a large number of states or variables.
- Often described by complex equations, requiring numerical simulations.

## ■ Examples:

### ■ Lotka-Volterra Model:

- Models predator-prey interactions using a system of ODEs.
- Describes population changes over time for two species.

### ■ Epidemic Models (e.g., COVID-19):

- Use systems of ODEs (like SIR models) to simulate virus dynamics.
- Consider factors such as infection rates, recovery, and population movements.

### ■ Climate Models:

- Use PDEs to represent atmospheric dynamics.



# Example Finite Element Method (FEM) Modeling

## ■ Characteristics:

- Breaks down complex structures into smaller, simpler elements.
- Solves PDEs numerically, providing approximate solutions to problems in engineering.

## ■ Applications:

- Structural analysis in civil engineering (e.g., stress and strain in buildings).
- Heat transfer problems in mechanical engineering.
- Fluid dynamics simulations in aerospace engineering.

## ■ Advantages:

- Handles complex geometries, material properties, and boundary conditions.
- Useful for problems with a large number of variables and states.



# Statistical Models in Science and Engineering

## ■ Characteristics:

- Use statistical methods to model data, incorporating randomness and uncertainty.
- Often used in situations with large datasets or where underlying processes are not fully understood.

## ■ Examples:

- **Regression Models:** Linear and logistic regression for predicting trends in data.
- **Machine Learning Models:** Neural networks, decision trees, and clustering algorithms to identify patterns in complex data.

# Classification: Small vs. Large Number of States

## ■ Small Number of States:

- Typically involve a few variables or parameters.
- Examples:
  - Simple harmonic oscillator (single state variable - displacement).
  - Ideal gas law (few parameters - pressure, volume, temperature).

## ■ Large Number of States:

- Require many variables and numerical simulations.
- Examples:
  - Lotka-Volterra predator-prey model (two interacting populations).
  - Epidemic models that account for susceptible, infected, and recovered populations.
  - FEM modeling of stress and strain in complex structures.



- **Ordinary Differential Equations (ODEs):**
  - Describe systems with a small number of states.
  - Examples: Lotka-Volterra model, simple harmonic oscillators.
- **Partial Differential Equations (PDEs):**
  - Used for complex, distributed systems with large numbers of states.
  - Examples: Climate models, fluid dynamics in FEM modeling.
- **Statistical Models:**
  - Incorporate randomness, uncertainty, and large datasets.
  - Examples: Regression models, machine learning algorithms.



# Conclusion: Modeling Approaches and Methodologies (1/3)

## ■ Models as Tools:

- All models, whether simple or complex, serve as tools to understand, predict, and manipulate natural phenomena.

## ■ Diversity of Models:

- **Simple Models:** (e.g., Newton's laws, ideal gas law) provide foundational insights with fewer variables.
- **Advanced Models:** (e.g., Lotka-Volterra, FEM) capture complex interactions and dynamics with greater detail.
- **Statistical Models:** Handle uncertainty and large datasets, essential for fields like machine learning.

# Conclusion: Modeling Approaches and Methodologies (2/3)

## ■ Model Limitations:

- No model perfectly represents reality.
- Each model has assumptions and approximations that define its scope of applicability.

## ■ Modeling Methodologies:

- **ODEs and PDEs:** Describe dynamic systems, essential in fields like physics, biology, and engineering.
- **Numerical Methods (e.g., FEM):** Allow solving complex problems that lack analytical solutions.
- **Statistical Approaches:** Useful for dealing with randomness and data-driven insights.

# Conclusion: Modeling Approaches and Methodologies (3/3)

## ■ Future Perspectives:

- Continuous development of more accurate and computationally efficient models.
- Enhancing our ability to tackle increasingly complex real-world challenges.
- Integration of interdisciplinary knowledge to build more comprehensive models.

## ■ Key Takeaway:

- Models are indispensable tools in science and engineering, but we must always be mindful of their limitations and the assumptions they are built upon.