

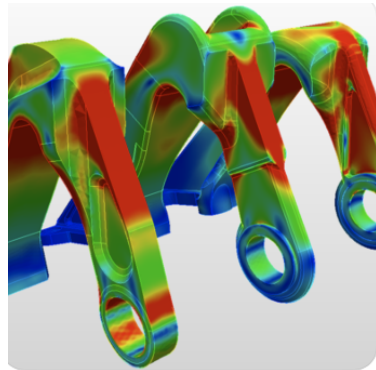
MMAE 450 — Computational Mechanics II

Day 1: Course Introduction & Computational Workflow

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Why Computational Mechanics?

- ▶ Many engineering problems have **no closed-form solution**
- ▶ Computation bridges **theory** and **real systems**
- ▶ Central in:
 - ▶ heat transfer
 - ▶ solid mechanics and dynamics
 - ▶ transport phenomena

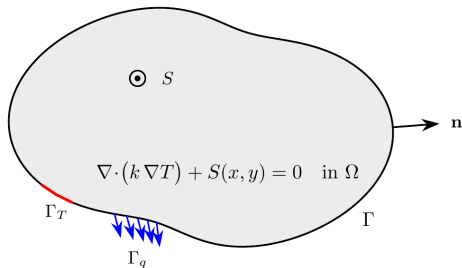


Stress distribution in mechanical part with complex geometry.

What Is Computational Mechanics?

1. Physical system (assumptions + model)
2. Governing equations
3. Numerical approximation (discretization)
4. Computational solution
5. Interpretation and validation

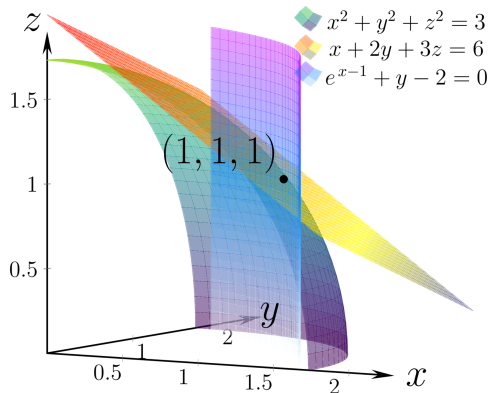
Key message: Computational mechanics is about **models**, not just numbers.



Complex geometry \Rightarrow discretization \Rightarrow
computation

Where This Course Fits

- ▶ Builds on:
 - ▶ calculus
 - ▶ differential equations
 - ▶ linear algebra
- ▶ Develops:
 - ▶ numerical thinking
 - ▶ computational implementation
 - ▶ interpretation of results
- ▶ Prepares you for:
 - ▶ research and modeling
 - ▶ engineering simulation tools
 - ▶ machine learning models and cloud workflows
 - ▶ data analytics



Intersection of nonlinear surfaces representing a system of equations.

What This Course Emphasizes

- ▶ Modeling, not memorization
- ▶ Algorithms, not button-pushing
- ▶ Understanding:
 - ▶ accuracy
 - ▶ stability
 - ▶ limitations and failure modes

We will care *why* methods work—and when they fail.

Tools We Will Use

- ▶ **Python** as the computational language
- ▶ **Jupyter notebooks** for code + math + narrative
- ▶ Core libraries:
 - ▶ NumPy (arrays, linear algebra)
 - ▶ SymPy (symbolic math, derivations)
 - ▶ Matplotlib (plots and visualization)
 - ▶ SciPy (numerical solvers, eigenproblems)
 - ▶ Pandas (data handling and post-processing)
 - ▶ scikit-learn (regression and surrogate models)
 - ▶ PyTorch (physics-informed neural networks)
 - ▶ Cloud workflows for scalable computation

We will briefly review Python and notebooks to ensure everyone is aligned.

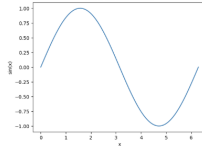
Example 1.1--Python Warm Up

```
[1]: # Import Packages
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from sympy import symbols, Matrix, solve
```

Create a simple NumPy array

```
[2]: x = np.linspace(0, 2*np.pi, 100)
y = np.sin(x)
plt.plot(x, y)
plt.xlabel('x')
plt.ylabel('sin(x)')
plt.title('Plot of the sine function')
plt.show()
```

Plot of the sine function



Create and manipulate a matrix

This command symbolically solves the system $Ax = b$ and returns the solution vector.

```
[3]: A = Matrix([2, 1], [1, 3])
b = Matrix([5, 7])
x = A.LUsolve(b)

[4]: [1]
```

The for loop

```
[5]: for i in range(1, 6):
    print("Square of {} is {}".format(i, i**2))

Square of 1 is 1
Square of 2 is 4
Square of 3 is 9
Square of 4 is 16
Square of 5 is 25
```

Define and call a function

Note: functions are typically placed at the top of the Jupyter notebook after importing packages.

```
[6]: def area_rectangle(a, b):
    return a * b
print(area_rectangle(3, 4))

12
```

Read and write data files

```
[7]: data = {'Name': ['Ava', 'Liam', 'Noah'], 'Score': [92, 85, 88]}
df = pd.DataFrame(data)
df.to_csv('scores.csv', index=False)
df2 = pd.read_csv('scores.csv')
print(df2)

df2.to_csv('names_scores.csv')

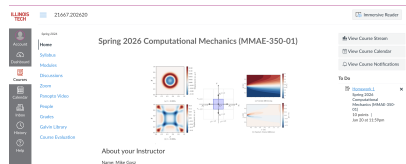
Name Score
```

Why Jupyter Notebooks?

- ▶ Combine: formatted text, equations, executable code, and plots
- ▶ Ideal for:
 - ▶ exploration
 - ▶ verification of derivations
 - ▶ clear communication of results

How the Course Is Structured

- ▶ Weekly modules on Canvas
- ▶ Mix of:
 - ▶ lectures
 - ▶ guided notebooks
 - ▶ homework assignments
- ▶ Two midterms + final exam or final project



A consistent weekly rhythm: learn →
practice → assess

What You Should Do This Week

- ▶ Review the syllabus (PDF)
- ▶ Complete Module 0 setup (Python + environment)
- ▶ Run Notebook 01 and make small edits
- ▶ Start Homework 1 (reflection + small computations)