WISCONSIN
UNIVERSITY OF WISCONSIN–MADISON

UW–Madison Math/CS 714
Methods of Computational Mathematics I

Introduction

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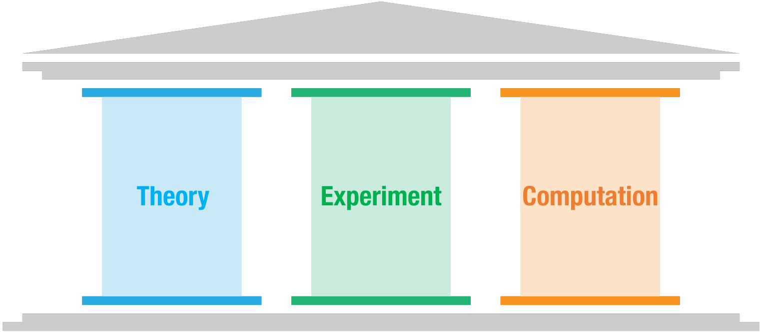
September 4, 2025

Three pillars of scientific discovery
theory, experiment, and computation

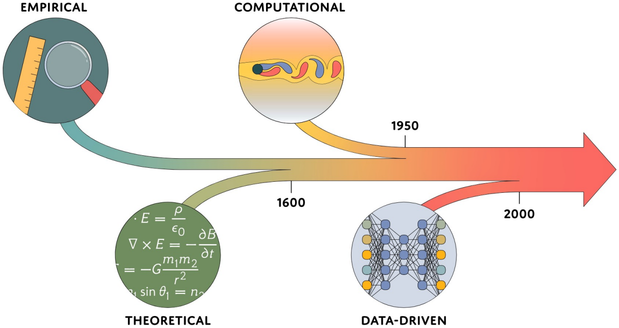
- Computation has been recognized as the “third pillar” of scientific discovery.



Three pillars of scientific discovery

theory, experiment, and computation

- Computation has been recognized as the "third pillar" of scientific discovery.
- *It is also at the core of the emerging* ***data-driven & machine-learning*** *scientific paradigm.*



"Evolution of scientific paradigms." Figure 1.1 from Jovana Andrejevic,
"*Towards data-driven methods for complex systems: Unfolding the crumpling dynamics of thin sheets*", PhD thesis, Harvard University, 2022.

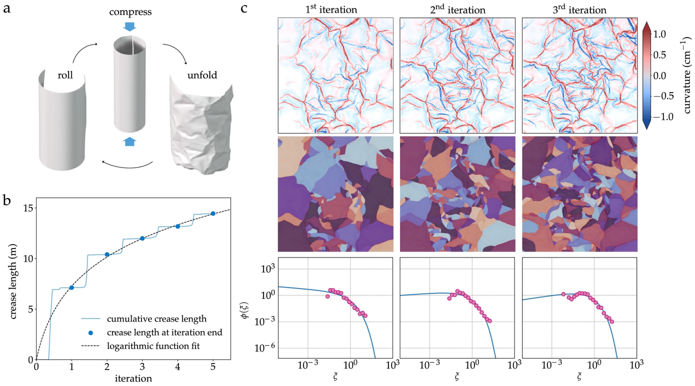
Computational mathematics
an informal definition

- It is the study of mathematical problems that are solved using **computers**.
- It focuses on developing and analyzing numerical algorithms to obtain **approximate** solutions to problems that may be difficult or impossible to solve analytically, or problems that are highly nonlinear or have multi-physics coupling.
- It has many **real-world** applications, including in physics, engineering, finance, and more.

What can we do with computational mathematics?

simulation of crumpled sheets

- A computational model for simulating the large-scale deformation of thin sheets that can serve as an effective tool for data-driven studies of crumpling dynamics.



J. Andrejevic, L. M. Lee, S. M. Rubinstein, and C. H. Rycroft, *A model for fragmentation kinetics of crumpled thin sheets*, Nat. Commun. **12**, 1470 (2021).

What can we do with computational mathematics?

simulation of crumpled sheets

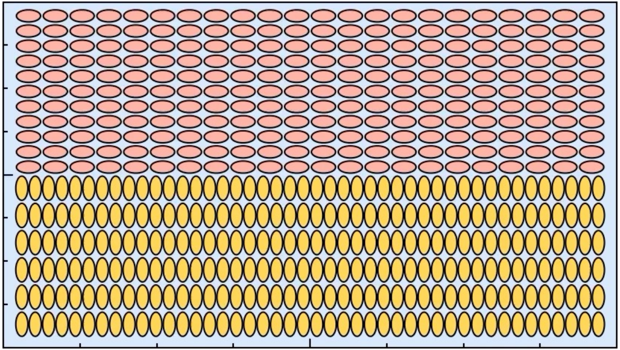
Newton's method, conjugate gradient,
preconditioning, explicit/implicit integration

J. Andrejevic and C. H. Rycroft, *Simulation of crumpled sheets via alternating quasistatic and dynamic representations*, J. Comput. Phys. **471**, 111607 (2022).

What can we do with computational mathematics?

simulation of fluid–structure interaction

- A computational model for simulating interactions between squishy solids and fluids that can be a tool for studying complex suspension and large-deformation under water.

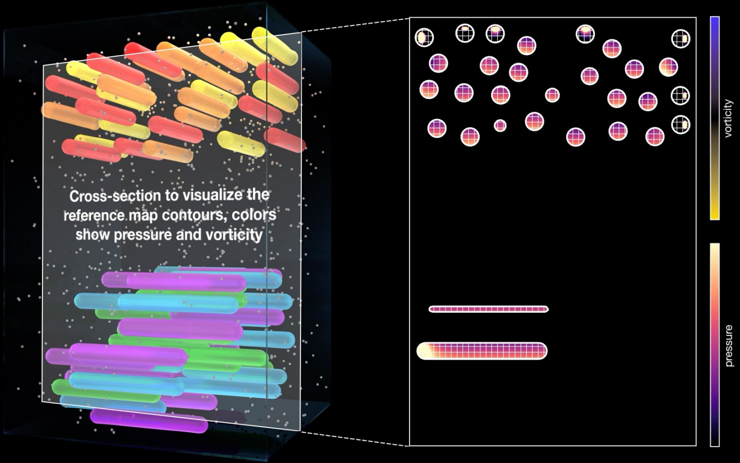


upwinding finite-difference, methods for fluid simulations

Y. Sun and C. H. Rycroft, *A fully-integrated lattice Boltzmann method for fluid–structure interaction*, J. Comput. Phys. **526**, 113774 (2025).

What can we do with computational mathematics?

simulation of fluid–structure interaction

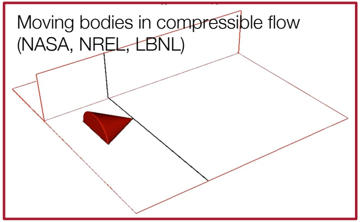


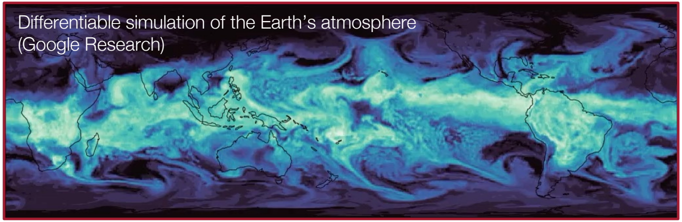
multigrid method, Godunov-type upwinding, projection method

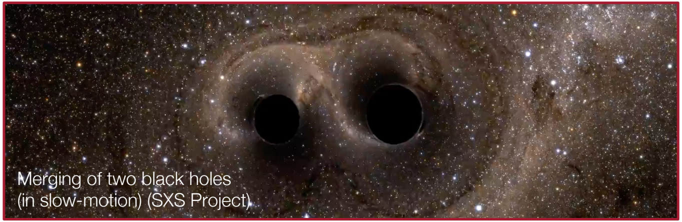
Y. L. Lin, N. J. Derr, and C. H. Rycroft, *Eulerian simulation of complex suspensions and biolocomotion in three dimensions*, Proc. Natl. Acad. Sci. **119**, e2105338118 (2022).

What can we do with computational mathematics?

simulation of more real-world problems







finite volume method

spectral method

Roadmap of the semester

how to approximate solutions to differential equations

Spectral methods

Expand our repertoire for solving PDEs
A similar set up to FD but with spectral convergence via a smart differentiation matrix

Mixed eq.

Navier–Stokes: **hyperbolic** (transport) + **parabolic** (diffusion) + **elliptic** (incompressibility)
Numerical methods specific to simulating incompressible NSEs

FVM

Discretize hyperbolic PDEs via integral formulation for **numerical conservation**
More numerical methods, applications to waves and shocks

Hyperbolic PDEs

New discretizations for **time-dependent, conservative, no SS PDEs** (wave, advection)
Numerical analysis (error, stability, convergence, consistency)

Parabolic PDEs

Extend 2D **elliptic (heat) eq. with time-dependence** with new discretizations
Numerical analysis (error, stability, convergence, stiffness)

IVP ODEs

Begin studying **time-dependent** ODEs
Numerical analysis (error, stability, convergence, stiffness)

Iterative methods

To solve elliptic problems efficiently
How to build descent methods and conjugate gradient

Elliptic PDEs

How to set up 2D FD stencils and linear system (2D heat eq. **w/o time dep.**)
Numerical analysis —> **direct solve is infeasible for both time and memory**

BVP ODEs

How to set up BCs and linear system (1D heat eq.)
How to do numerical analysis (error, stability, convergence, consistency)

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Methods of Computational Mathematics I

Finite difference approximations

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The finite difference method

There are multiple ways to discretize PDEs, and decompose a continuous problem into a finite, discrete one that can be solved numerically on a computer.

The bulk of this course will focus on the finite difference method, which is effective for a wide range of problems.

There are other approaches (*e.g.* finite element method, finite volume method, spectral methods). We will explore some of these, although underlying ideas are often similar.

Finite difference approximations

Let $u : \mathbb{R} \to \mathbb{R}$ be a smooth function, meaning that we can differentiate it several times, and each derivative is a well-defined bounded function over an interval containing a point of interest $\bar{x}$.

Try approximating $u'(\bar{x})$ by a finite difference approximation using only several values of u near $\bar{x}$. Obvious choice is

$$D_+ u(\bar{x}) = \frac{u(\bar{x} + h) - u(\bar{x})}{h}$$

where h is a small value.

Called a *one-sided* approximation, since only evaluated at points with $x \geq \bar{x}$.

Matches the definition of the derivative in the limit as $h \to 0$.

Alternative formula

We could equally use a point in the negative direction, to obtain

$$D_- u(\bar{x}) = \frac{u(\bar{x}) - u(\bar{x} - h)}{h}.$$

An alternative is the *centered approximation*,

$$D_0 u(\bar{x}) = \frac{u(\bar{x} + h) - u(\bar{x} - h)}{2h} = \frac{D_+ u(\bar{x}) + D_- u(\bar{x})}{2}.$$

How accurate are these formulas? How do we derive additional ones?

Truncation errors

The standard approach for error analysis is to perform Taylor series approximations. We have that

$$
\begin{aligned}
u(\bar{x}+h) &= u(\bar{x}) + hu'(\bar{x}) + \frac{h^2}{2}u''(\bar{x}) + \frac{h^3}{6}u'''(\bar{x}) + O(h^4),\\
u(\bar{x}-h) &= u(\bar{x}) - hu'(\bar{x}) + \frac{h^2}{2}u''(\bar{x}) - \frac{h^3}{6}u'''(\bar{x}) + O(h^4).
\end{aligned}
$$

Then

$$
D_+u(\bar{x}) = \frac{u(\bar{x}+h) - u(\bar{x})}{h} = u'(\bar{x}) + \frac{h}{2}u''(\bar{x}) + \frac{h^2}{6}u'''(\bar{x}) + O(h^3).
$$

Leading order term is $O(h)$, so the method is first order accurate.

Truncation errors

From Taylor series expansions

$$u(\bar{x}+h) - u(\bar{x}-h) = 2hu'(\bar{x}) + \frac{h^3}{3}u'''(\bar{x}) + O(h^5)$$

since terms with even powers of h cancel. Hence

$$D_0 u(\bar{x}) - u'(\bar{x}) = \frac{h^2}{6}u'''(\bar{x}) + O(h^4).$$

Leading order term is $O(h^2)$, so the method is second order accurate.

Deriving finite difference approximations

See derivation: method of undetermined coefficients

Second order derivatives

The same approaches can be used to derive higher order formulae. For example, the standard second order centered approximation is

$$D^2u(\bar{x}) = \frac{u(\bar{x}-h) - 2u(\bar{x}) + u(\bar{x}+h)}{h^2}$$
$$= u''(\bar{x}) + \frac{h^2}{12}u^{(4)}(\bar{x}) + O(h^4).$$

Due to cancellation of odd powers of h, this formula is second order accurate.

See derivation: a general formula