# Applied Mathematics 205

## Unit 0. Introduction

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# Scientific Computing

Computation is now recognized as the ”third pillar” of science (along with theory and experiment). Why?

- Practically relevant mathematical models do not have analytical solutions
- Large amounts of data need to be processed automatically
- Modern computers can handle large-scale problems

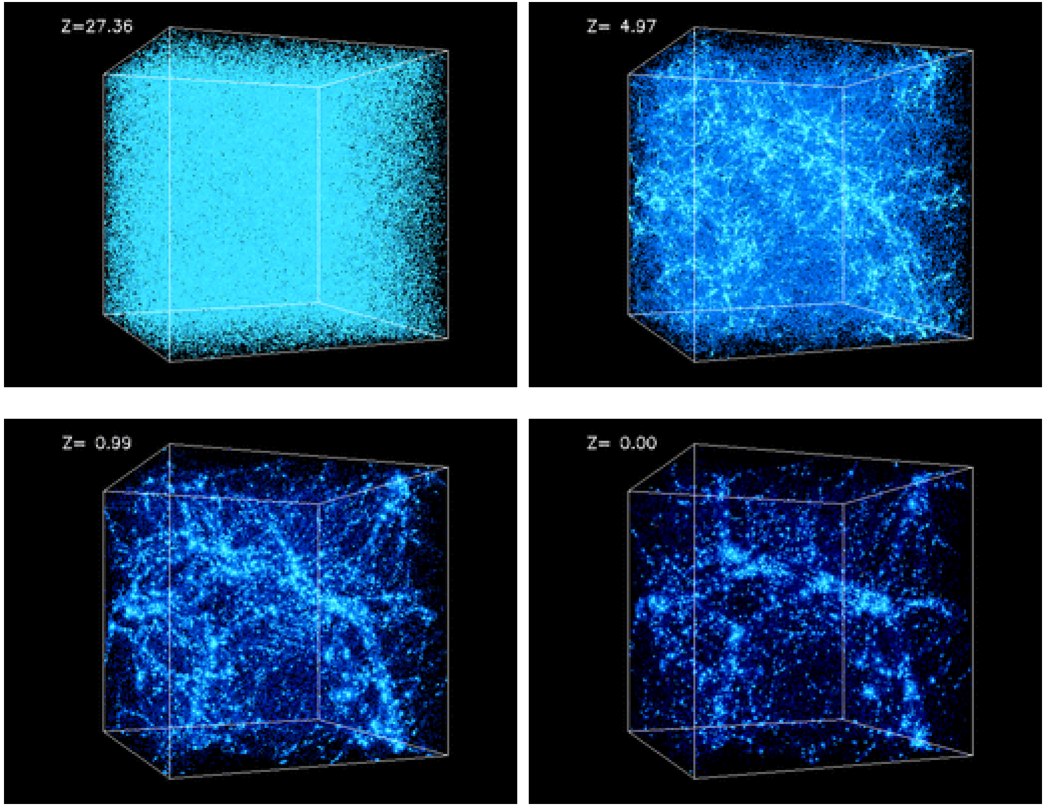
# What is Scientific Computing

- Scientific computing is closely related to numerical analysis
- *"Numerical analysis is the study of algorithms for the problems of continuous mathematics"* [Nick Trefethen, SIAM News, 1992]
- **Continuous mathematics** involves real numbers as opposed to integers
- **Numerical analysis** studies these algorithms
- **Scientific computing** applies them to practical problems
- **Scientific computing** is distinct from Computer Science, which focuses on discrete mathematics (e.g. graph theory)

# Applications of Scientific Computing

# Cosmology

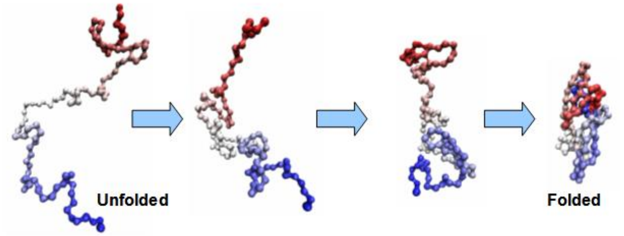
Cosmological simulations to test theories of galaxy formation



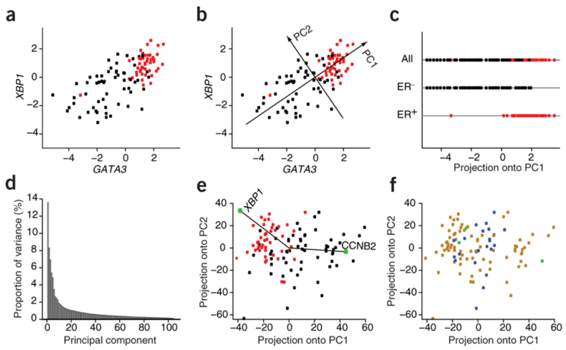

http://cosmicweb.uchicago.edu/filaments.html

# Biology

- Protein folding

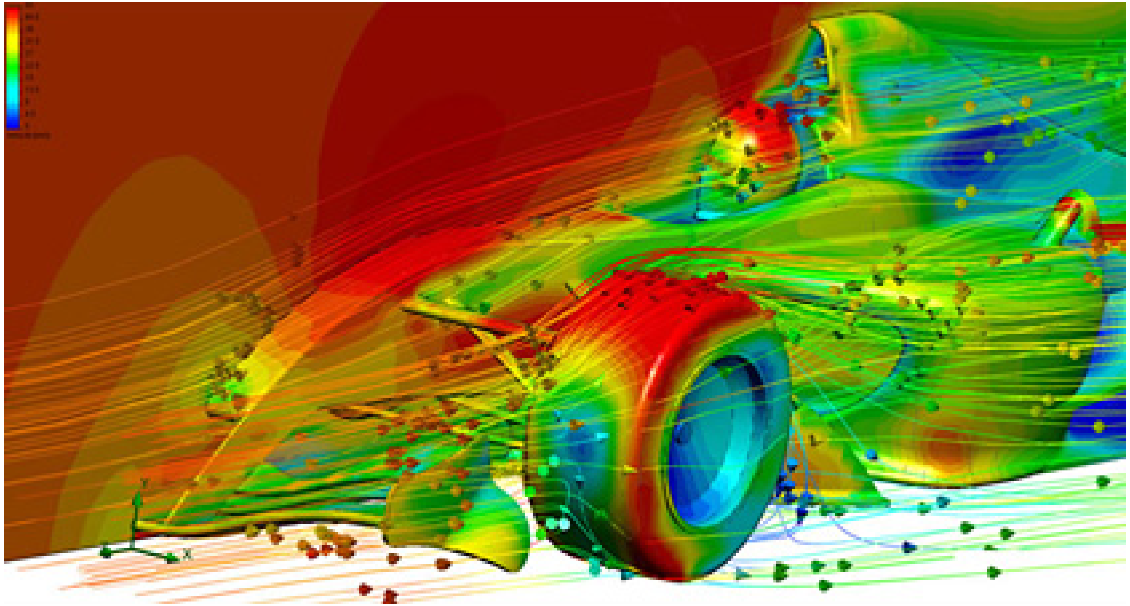



- Statistical analysis of gene expression



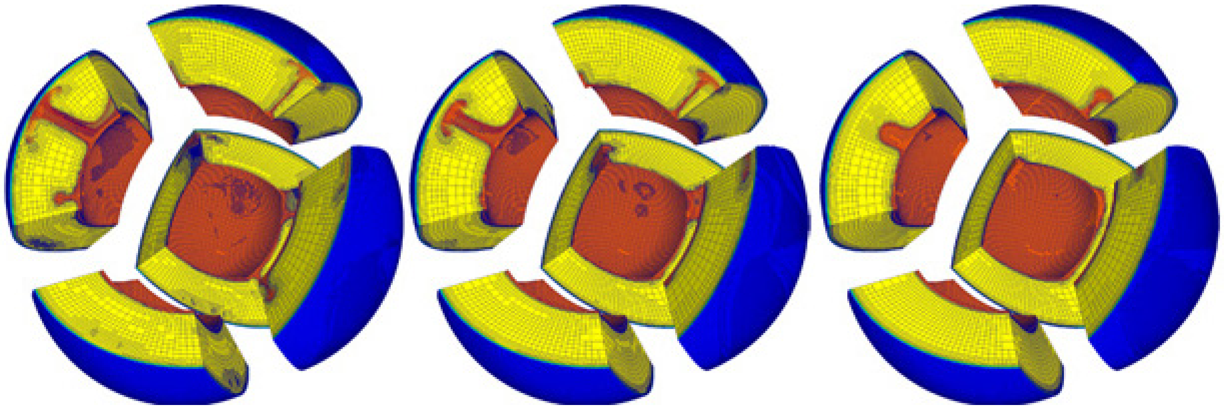
# Computational Fluid Dynamics

- CFD simulations replace or complement wind-tunnel experiments
- Computational geometry is easier to tweak than a physical model
- Simulations provide the entire flow field, not available experimentally



# Geophysics

- Experimental data is only available on Earth's surface
- Simulations help to test models of the interior



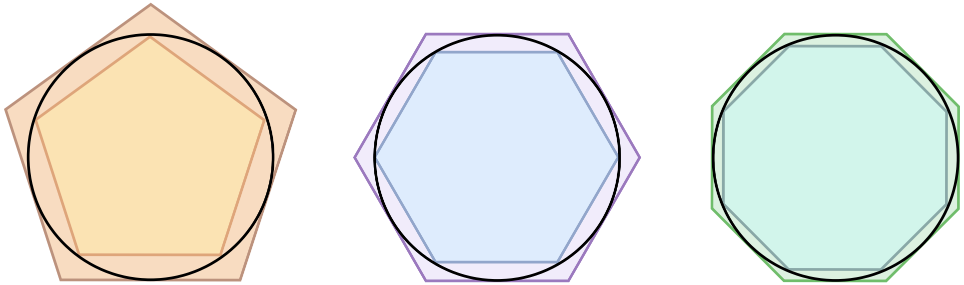
# Calculation of $\pi$

# Calculation of $\pi$

- $\pi$ is the ratio of a circle's circumference to its diameter
- Babylonians (1900 BC): 3.125
- From the Old Testament (1 Kings 7:23):
  *"And he made the molten sea of ten cubits from brim to brim, round in compass, and the height thereof was five cubits; and a lines of thirty cubits did compass it round about"*
  Implies $\pi \approx 3$
- Egyptians (1850 BC): $(\frac{16}{9})^2 \approx 3.16$

# Calculation of $\pi$

- Archimedes (287-212 BC) bounded $\pi$ by perimeters of regular polygons: inscribed and superscribed



- For 96-sided polygon: $\frac{223}{71} < \pi < \frac{22}{7}$ (interval length: 0.00201)
- Example of an infinite process converging to the exact solution
- Provides both the estimate **and** error bounds

# Calculation of $\pi$

- James Gregory (1638-1675) discovers the arctangent series

$$\arctan x = x - \frac{x^3}{3} + \frac{x^5}{5} - \frac{x^7}{7} + \dots$$

- Setting $x = 1$ gives

$$\frac{\pi}{4} = 1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \dots$$

but it converges very slowly

# Calculation of $\pi$

- The arctangent series converges faster for points closer to 0

$$\arctan x = x - \frac{x^3}{3} + \frac{x^5}{5} - \frac{x^7}{7} + \dots$$

- John Machin (1680-1752) observed that

$$\frac{\pi}{4} = 4 \arctan \frac{1}{5} - \arctan \frac{1}{239}$$

  and computed 100 digits of $\pi$

- Derivation
  - $\tan \alpha = \frac{1}{5}$
  - $\tan 2\alpha = \frac{2 \tan \alpha}{1 - \tan^2 \alpha} = \frac{5}{12}$
  - $\tan 4\alpha = \frac{2 \tan 2\alpha}{1 - \tan^2 2\alpha} = \frac{120}{119}$
  - $\tan \left(4\alpha - \frac{\pi}{4}\right) = \frac{\tan 4\alpha - 1}{1 + \tan 4\alpha} = \frac{1}{239}$

# Calculation of $\pi$

Users of Manchin's formula

| | | |
|---|---|---|
| 1706 | John Machin | 100 digits |
| 1719 | Thomas de Lagny | 112 digits |
| 1739 | Matsunaga Ryohitsu | 50 digits |
| 1794 | Georg von Vega | 140 digits |
| 1844 | Zacharias Dase | 200 digits |
| 1847 | Thomas Clausen | 248 digits |
| 1853 | William Rutherford | 440 digits |
| 1876 | William Shanks | 707 digits |

# Sources of Error
# in Scientific Computing

# Sources of Error in Scientific Computing

- There are several sources of error in solving real-world problems
- Some are beyond our control
  (e.g. uncertainty in modeling parameters or initial conditions)
- Some are introduced by our numerical approximations
  - Truncation/discretization error:
    Objects from continuous mathematics need to be discretized
    (finite differences, truncated infinite series...)
  - Rounding error:
    Computers work with finite precision arithmetic

# Sources of Error in Scientific Computing

- It is crucial to understand and control the error introduced by numerical approximation, otherwise the results might be garbage
- This is a major part of Scientific Computing, called error analysis
- Error analysis becomes more important for larger scale problems as errors accumulate
- Most people are familiar with rounding error,
  but discretization error is far more important in practice

# Discretization Error vs. Rounding Error

- Consider a finite difference approximation to $f'(x)$

$$f_{\text{diff}}(x;h) = \frac{f(x+h) - f(x)}{h}$$

- From Taylor series (for $\theta \in [x, x+h]$)

$$f(x+h) = f(x) + hf'(x) + f''(\theta)h^2/2$$

we see that

$$f_{\text{diff}}(x;h) = \frac{f(x+h) - f(x)}{h} = f'(x) + f''(\theta)h/2$$

- Suppose $|f''(\theta)| \leq M$, then bound on discretization error is

$$|f'(x) - f_{\text{diff}}(x;h)| \leq Mh/2$$

# Discretization Error vs. Rounding Error

- But we can't compute $f_{\text{diff}}(x; h)$ in exact arithmetic
- Let $\tilde{f}_{\text{diff}}(x; h)$ denote finite precision approximation of $f_{\text{diff}}(x; h)$
- Numerator of $\tilde{f}_{\text{diff}}$ introduces rounding error $\lesssim \epsilon |f(x)|$
  (on modern computers $\epsilon \approx 10^{-16}$, will discuss this shortly)
- Hence we have the rounding error

$$\left| f_{\text{diff}}(x; h) - \tilde{f}_{\text{diff}}(x; h) \right| \lesssim \left| \frac{f(x+h) - f(x)}{h} - \frac{f(x+h) - f(x) + \epsilon f(x)}{h} \right| = \epsilon |f(x)|/h$$

# Discretization Error vs. Rounding Error

- Then we can bound the total error (discretization and rounding)

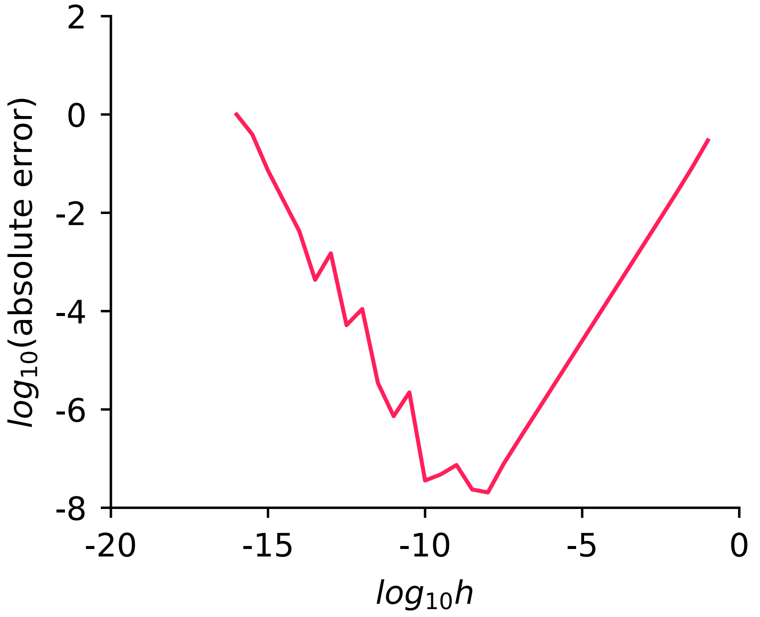
$$\begin{aligned} |f'(x) - \tilde{f}_{\text{diff}}(x;h)| &= |f'(x) - f_{\text{diff}}(x;h) + f_{\text{diff}}(x;h) - \tilde{f}_{\text{diff}}(x;h)| \\ &\le |f'(x) - f_{\text{diff}}(x;h)| + |f_{\text{diff}}(x;h) - \tilde{f}_{\text{diff}}(x;h)| \\ &\le Mh/2 + \epsilon|f(x)|/h \end{aligned}$$

- Since $\epsilon$ is so small, here we expect discretization error to dominate until $h$ gets sufficiently small

# Discretization Error vs. Rounding Error

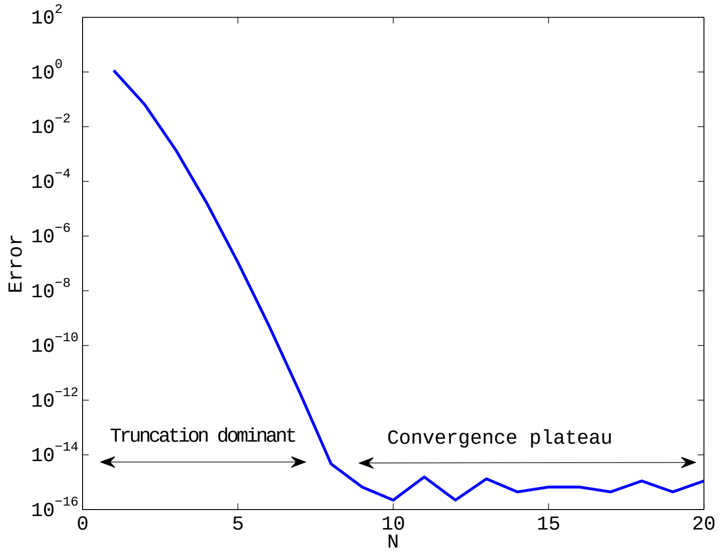
- Consider $f(x) = \exp(5x)$.

  Error of $f_{\text{diff}}(x, h)$ at $x = 1$ as function of $h$



# Discretization Error vs. Rounding Error

- Note that in the finite difference example, we observe error growth due to rounding as $h \to 0$
- A more common situation (that we'll see in Unit 1, for example) is that the error plateaus at around $\epsilon$ due to rounding error



# Absolute vs. Relative Error

- Recall our bound $|f'(x) - \tilde{f}_{\text{diff}}(x;h)| \leq Mh/2 + \epsilon|f(x)|/h$
- This is a bound on Absolute Error

$$\text{Absolute Error} = \text{true value} - \text{approximate value}$$

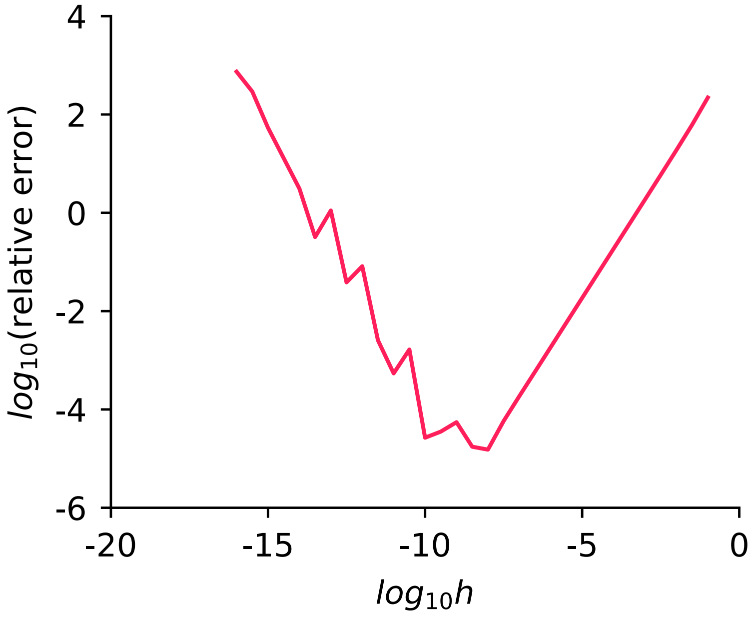
- Generally more interesting to consider Relative Error

$$\text{Relative Error} \equiv \frac{\text{Absolute Error}}{\text{true value}}$$

- Relative error is a dimensionless quantity
- If unknown, true value is replaced with an estimate

# Absolute vs. Relative Error

- For our finite difference example, plotting relative error just rescales the error values



# Convergence Plots

- We have shown several plots of error as a function of a discretization parameter
- In general, these plots are very important in scientific computing to demonstrate that a numerical method is behaving as expected
- To display convergence data in a clear way, it is important to use appropriate axes for our plots

# Convergence Plots

- Most often we will encounter algebraic convergence, where error decreases as $Ch^q$ for some $C, q \in \mathbb{R}$
- Algebraic convergence: If $E = Ch^q$, then

$$\log E = \log C + q \log h$$

- Plotting algebraic convergence on log–log axes asymptotically yields a straight line with slope $q$
- Hence a good way to deduce the algebraic convergence rate is by comparing error to $Ch^q$ on log–log axes

# Convergence Plots

- Sometimes we will encounter exponential convergence, where error decays as $Ce^{-qN}$ as $N \to \infty$
- If $E = Ce^{-qN}$ then

$$\log E = \log C - qN$$

- Hence for exponential convergence, better to use log-linear axes (like the previous "error plateau" plot)

# Numerical Sensitivity

- In practical problems we will always have input perturbations (modeling uncertainty, rounding error)
- Let $y = f(x)$, and denote perturbed input $\hat{x} = x + \Delta x$
- Also, denote perturbed output by $\hat{y} = f(\hat{x})$, and $\hat{y} = y + \Delta y$
- The function $f$ is *sensitive* to input perturbations if $\Delta y \gg \Delta x$
- This is sensitivity inherent in $f$, independent of any approximation (though a numerical approximation $\hat{f} \approx f$ can exacerbate sensitivity)

# Sensitivity and Conditioning

- For a sensitive problem,
  small input perturbation leads to large output perturbation
- Can be made quantitative with the concept of (relative) condition number

$$\text{Condition number} = \frac{|\Delta y / y|}{|\Delta x / x|}$$

- Problems with Condition number $\gg 1$ are called ill-conditioned.
  In such problems, small input perturbations are amplified

# Sensitivity and Conditioning

- Condition number can be analyzed for various problem types (independent of algorithm used to solve the problem). Examples:
  - Function evaluation, $y = f(x)$
  - Matrix multiplication, $Ax = b$ (solve for $b$ given $x$)
  - Linear system, $Ax = b$ (solve for $x$ given $b$)

# Conditioning: Function Evaluation

- Problem: evaluate function, $y = f(x)$
- Perturbed problem: $y + \Delta y = f(x + \Delta x)$
- Change in $x$: $\quad \Delta x$
- Change in $y$: $\quad \Delta y \approx f'(x)\Delta x$
- Condition number is the ratio of relative changes

$$\kappa = \frac{f'(x)\Delta x / f(x)}{\Delta x / x} = \frac{f'(x)x}{f(x)}$$

# Conditioning: Matrix Multiplication

- Problem: multiply matrix and vector, $b = Ax$
- Perturbed problem: $b + \Delta b = A(x + \Delta x) \implies \Delta b = A\Delta x$
- Condition number is

$$\kappa = \frac{\|\Delta b\|/\|b\|}{\|\Delta x\|/\|x\|} = \frac{\|A\Delta x\|}{\|\Delta x\|}\,\frac{\|x\|}{\|Ax\|} = \frac{\|A\Delta x\|}{\|\Delta x\|}\,\frac{\|A^{-1}b\|}{\|b\|}$$

- Matrix norm

$$\|A\| = \max_{v\neq 0} \frac{\|Av\|}{\|v\|}$$

- Condition number $\kappa(A)$ from linear algebra is an upper bound for $\kappa$

$$\kappa = \frac{\|A\Delta x\|}{\|\Delta x\|}\,\frac{\|A^{-1}b\|}{\|b\|} \leq \|A\|\,\|A^{-1}\| = \kappa(A)$$

# Conditioning: Linear System

- Problem: solve linear system $Ax = b$
- Perturbed problem: $A(x + \Delta x) = b + \Delta b \implies A\Delta x = \Delta b$
- Condition number is

$$\kappa = \frac{\|\Delta x\|/\|x\|}{\|\Delta b\|/\|b\|} = \frac{\|\Delta x\|}{\|A\Delta x\|}\,\frac{\|Ax\|}{\|x\|} = \frac{\|A^{-1}\Delta b\|}{\|\Delta b\|}\,\frac{\|Ax\|}{\|x\|}$$

- Matrix norm

$$\|A\| = \max_{v\neq 0} \frac{\|Av\|}{\|v\|}$$

- Condition number $\kappa(A)$ from linear algebra is an upper bound for $\kappa$

$$\kappa = \frac{\|A^{-1}\Delta b\|}{\|\Delta b\|}\,\frac{\|Ax\|}{\|x\|} \leq \|A^{-1}\|\,\|A\| = \kappa(A)$$

# Exercise: Diagonal Matrix

$$A = \begin{pmatrix} d_1 & 0 & 0 \\ 0 & d_2 & 0 \\ 0 & 0 & d_3 \end{pmatrix}$$

- Matrix norm

$$\|A\| = \max_{v \neq 0} \frac{\|Av\|}{\|v\|} = \max(|d_1|, |d_2|, |d_3|)$$

- Condition number

$$\kappa(A) = \|A\| \|A^{-1}\| = \frac{\max(|d_1|, |d_2|, |d_3|)}{\min(|d_1|, |d_2|, |d_3|)}$$

# Stability of an Algorithm

- In practice, we solve problems by applying a numerical method to a mathematical problem, e.g. apply Gaussian elimination to $Ax = b$
- To obtain an accurate answer, we need to apply a stable numerical method to a well-conditioned mathematical problem
- Question: What do we mean by a stable numerical method?
- Answer: Roughly speaking, the numerical method doesn't accumulate error (e.g. rounding error) and produce garbage
- We will make this definition more precise shortly, but first, we discuss rounding error and finite-precision arithmetic

# Code Examples

- From here on, a number of code examples will be provided
- They will be available via Git repository
  github.com/pkarnakov/am205
- Git is one example of version control software, which tracks the changes of files in a software project. Features:
  - Compare files to any previous version
  - Merge changes in the same files by multiple people
  - Not suitable for binary files (Word, PDF, images, videos, etc)
- Note: Avoid storing large binary files in repositories.
  They cannot be removed without rewriting history

# Git

- Git can be installed as a command-line utility on all major systems.
- For authentication, you will need to add an SSH key to your profile at code.harvard.edu
- Follow this guide to generate an SSH key
- To download a copy of the repository, use

```
git clone git@code.harvard.edu:AM205/public.git
```

- Then, at later times, you can type

```
git pull
```

to obtain any updated files. Graphical interfaces for Git are also available

# Finite-Precision Arithmetic

- Key point: we can only represent a finite and discrete subset of the real numbers on a computer.
- The standard approach in modern hardware is to use binary floating point numbers (basically "scientific notation" in base 2),

$$\begin{aligned} x &= \pm(1 + d_1 2^{-1} + d_2 2^{-2} + \ldots + d_p 2^{-p}) \times 2^E \\ &= \pm(1.d_1 d_2 \ldots d_p)_2 \times 2^E \end{aligned}$$

# Finite-Precision Arithmetic

- We store

$$\underbrace{\pm}_{\text{1 sign bit}} \qquad \underbrace{d_1, d_2, \ldots, d_p}_{p \text{ mantissa bits}} \qquad \underbrace{E}_{\text{exponent bits}}$$

- Note that the term bit is a contraction of “binary digit”
- This format assumes that $d_0 = 1$ to save a mantissa bit, but sometimes $d_0 = 0$ is required, such as to represent zero.
- The exponent resides in an interval $L \leq E \leq U$.

# IEEE Floating Point Arithmetic

- Universal standard on modern hardware is IEEE floating point arithmetic (IEEE 754), adopted in 1985
- Development led by Prof. William Kahan (UC Berkeley), who received the 1989 Turing Award for his work

| | **total bits** | $p$ | $L$ | $U$ |
|---|---|---|---|---|
| IEEE single precision | 32 | 23 | -126 | 127 |
| IEEE double precision | 64 | 52 | -1022 | 1023 |

- Note that single precision has 8 exponent bits but only 254 (not 256) different values of $E$, since some exponent bits are reserved to represent special numbers

# Exceptional Values

- These exponents are reserved to indicate special behavior, including values such as Inf and NaN:
  - Inf = "infinity", e.g. $1/0$ (also $-1/0 = -\text{Inf}$)
  - NaN = "not a number", e.g. $0/0$, Inf/Inf

# IEEE Floating Point Arithmetic

- Let $\mathbb{F}$ denote the floating point numbers. Then $\mathbb{F} \subset \mathbb{R}$ and $|\mathbb{F}| < \infty$.
- Question: How should we represent a real number $x$, which is not in $\mathbb{F}$?
- Answer: There are two cases to consider:
  - Case 1: $x$ is outside the range of $\mathbb{F}$ (too small or too large)
  - Case 2: The mantissa of $x$ requires more than $p$ bits.

# IEEE Floating Point Arithmetic

Case 1: $x$ is outside the range of $\mathbb{F}$ (too small or too large)

- Too small:
  - Smallest positive value that can be represented in double precision is $\approx 10^{-323}$
  - For a value smaller than this we get underflow, and the value typically set to 0
- Too large:
  - Largest $x \in \mathbb{F}$ ($E = U$ and all mantissa bits are 1) is approximately $2^{1024} \approx 10^{308}$
  - For values larger than this we get overflow, and the value typically gets set to Inf

# IEEE Floating Point Arithmetic

Case 2: The mantissa of $x$ requires more than $p$ bits

- Need to round $x$ to a nearby floating point number
- Let $\texttt{round} : \mathbb{R} \to \mathbb{F}$ denote our rounding operator
- There are several different options:
  round up, round down, round to nearest, etc
- This introduces a rounding error
  - absolute rounding error $x - \texttt{round}(x)$
  - relative rounding error $(x - \texttt{round}(x))/x$

# Machine Precision

- It is important to be able to quantify this rounding error — it's related to machine precision, often denoted as $\epsilon$ or $\epsilon_{\text{mach}}$
- $\epsilon$ is the difference between 1 and the next floating point number after 1, therefore $\epsilon = 2^{-p}$
- In IEEE double precision, $\epsilon = 2^{-52} \approx 2.22 \times 10^{-16}$

# Rounding Error

- Let $x = (1.d_1 d_2 \ldots d_p d_{p+1})_2 \times 2^E \in \mathbb{R}_+$.
- Then $x \in [x_-, x_+]$ for $x_-, x_+ \in \mathbb{F}$, where $x_- = (1.d_1 d_2 \ldots d_p)_2 \times 2^E$ and $x_+ = x_- + \epsilon \times 2^E$.
- $\texttt{round}(x) = x_-$ or $x_+$ depending on the rounding rule, and hence $|\texttt{round}(x) - x| < \epsilon \times 2^E$
- Also, $|x| \geq 2^E$

# Rounding Error

- Hence we have a relative error of less than $\epsilon$

$$\left|\frac{\texttt{round}(x) - x}{x}\right| < \epsilon$$

- Another standard way to write this is

$$\texttt{round}(x) = x\left(1 + \frac{\texttt{round}(x) - x}{x}\right) = x(1+\delta)$$

where $\delta = \frac{\texttt{round}(x)-x}{x}$ and $|\delta| < \epsilon$

- Hence rounding gives the correct answer to within a factor of $1 + \epsilon$

# Floating Point Operations

- An arithmetic operation on floating point numbers is called a "floating point operation": $\oplus$, $\ominus$, $\otimes$, $\oslash$ versus $+$, $-$, $\times$, $/$
- Computer performance is often measured in Flop/s:
  number of Floating Point OPerations per second
- Supercomputers are ranked based on number of flops achieved in the LINPACK test, which solves dense linear algebra problems
- Currently, the fastest computers are in the 100 petaflop range:
  1 petaflop $= 10^{15}$ floating point operations per second

# Supercomputers

See www.top500.org for an up-to-date list of the fastest supercomputers

TOP500 LIST - JUNE 2022

$R_{max}$ and $R_{peak}$ values are in PFlop/s. For more details about other fields, check the TOP500 description.

$R_{peak}$ values are calculated using the advertised clock rate of the CPU. For the efficiency of the systems you should take into account the Turbo CPU clock rate where it applies.

← 1-100 101-200 201-300 301-400 401-500 →

| Rank | System | Cores | Rmax (PFlop/s) | Rpeak (PFlop/s) | Power (kW) |
|---|---|---|---|---|---|
| 1 | **Frontier** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE<br>DOE/SC/Oak Ridge National Laboratory<br>United States | 8,730,112 | 1,102.00 | 1,685.65 | 21,100 |
| 2 | **Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu<br>RIKEN Center for Computational Science<br>Japan | 7,630,848 | 442.01 | 537.21 | 29,899 |
| 3 | **LUMI** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE<br>EuroHPC/CSC<br>Finland | 1,110,144 | 151.90 | 214.35 | 2,942 |
| 4 | **Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM<br>DOE/SC/Oak Ridge National Laboratory<br>United States | 2,414,592 | 148.60 | 200.79 | 10,096 |

$R_{\text{max}}$ is from LINPACK, $R_{\text{peak}}$ is from clock rate

# Supercomputers

Modern supercomputers are very large, link many processors together with fast interconnect to minimize communication time


Frontier at Oak Ridge is 1102 PFlop/s

# Floating Point Operation Error

- IEEE standard guarantees that for $x, y \in \mathbb{F}$

$$x \circledast y = \texttt{round}(x * y)$$

  where $*$ and $\circledast$ represent one of the four arithmetic operations
- Hence from our discussion of rounding error, it follows that for $x, y \in \mathbb{F}$

$$x \circledast y = (x * y)(1 + \delta)$$

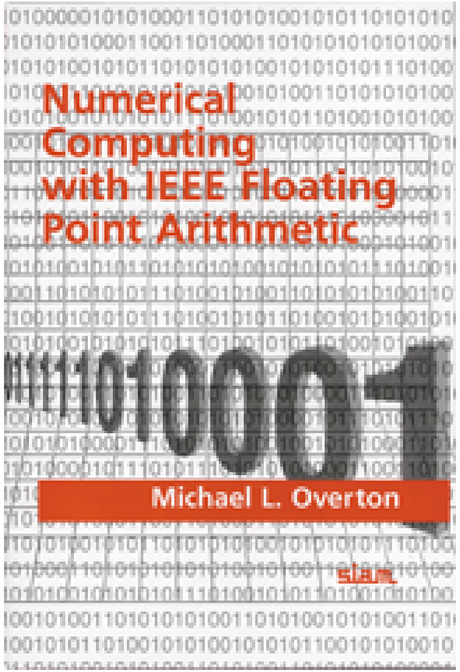
  for some $|\delta| < \epsilon$

# Loss of Precision

- Machine precision can be tested. See [unit0/precision.py]
- Since $\epsilon$ is so small, we typically lose very little precision per operation

# IEEE Floating Point Arithmetic

For more detailed discussion of floating point arithmetic, see:




Michael L. Overton. *Numerical Computing with IEEE Floating Point Arithmetic*. SIAM, 2001 10.1137/1.9780898718072

# Numerical Stability of an Algorithm

- We have discussed rounding for a single operation, but in AM205 we will study numerical algorithms that require many operations
- For an algorithm to be useful, it must be stable in the sense that rounding errors do not accumulate and result in "garbage" output
- More precisely, numerical analysts aim to prove backward stability:
  The method gives the exact answer to a slightly perturbed problem
- For example, a numerical method for solving $Ax = b$ should give the exact answer for $(A + \Delta A)x = (b + \Delta b)$ for small $\Delta A$, $\Delta b$

# Numerical Stability of an Algorithm

- We note the importance of conditioning:
  backward stability doesn't help us if the mathematical problem is ill-conditioned
- For example, if $A$ is ill-conditioned then a backward stable algorithm for solving $Ax = b$ can still give large error for $x$
- Backward stability analysis is a deep subject which we do not cover in detail in AM205
- We will, however, compare algorithms with different stability properties and observe the importance of stability in practice