CS 450: Numerical Analysis

Introduction to Scientific Computing

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1 These slides have been drafted by Edgar Solomonik as lecture templates and supplementary material for the book “Scientific Computing: An Introductory Survey” by Michael T. Heath (slides).
Scientific Computing Applications and Context

- **Mathematical modelling for computational science**  *Typical scientific computing problems are numerical solutions to PDEs*
  - Newtonian dynamics: simulating particle systems in time
  - Fluid and air flow models for engineering
  - PDE-constrained numerical optimization: finding optimal configurations (used in engineering of control systems)
  - Quantum chemistry (electronic structure calculations): many-electron Schrödinger equation

- **Linear algebra and computation**
  - Linear algebra and numerical optimization are building blocks for machine learning methods and data analysis
  - Computer architecture, compilers, and parallel computing use numerical algorithms (matrix multiplication, Gaussian elimination) as benchmarks
Example: Mechanics$^2$

- Newton’s laws provide incomplete particle-centric picture
- Physical systems can be described in terms of degrees of freedom (DoFs)
  - A piston moving up and down requires __________ DoFs
  - 1-particle system requires __________ DoFs
  - 2-particle system requires __________ DoFs
  - 2-particles at a fixed distance require __________ DoFs
- $N$-particle system configuration described by $3N$ DoFs

Course Structure

▶ Complex numerical problems are generally reduced to simpler problems

▶ The course topics will follow this hierarchical structure
Numerical Analysis

- Numerical Problems involving Continuous Phenomena:

- Error Analysis:
Sources of Error

- **Representation of Numbers:**

- **Propagated Data Error:**

- **Computational Error** = $\hat{f}(x) - f(x) = \text{Truncation Error} + \text{Rounding Error}$
Error Analysis

- Forward Error:

- Backward Error:
Visualization of Forward and Backward Error

\[ f(x) = f(\hat{x}) \]
Conditioning

- Absolute Condition Number:

- (Relative) Condition Number:
Posedness and Conditioning

▶ What is the condition number of an ill-posed problem?
Stability and Accuracy

- **Accuracy:**

- **Stability:**
Error and Conditioning

- Two major sources of error: \textit{roundoff} and \textit{truncation} error.
  - roundoff error concerns floating point error due to finite precision
  - truncation error concerns error incurred due to algorithmic approximation, e.g. the representation of a function by a finite Taylor series

- To study the propagation of roundoff error in arithmetic we can use the notion of conditioning.
Floating Point Numbers

- Scientific Notation

- **Significand (Mantissa) and Exponent** Given $x$ with $s$ leading bits $x_0, \ldots, x_{s-1}$
Rounding Error

- Maximum Relative Representation Error (Machine Epsilon)

Demo: Floating point and the Harmonic Series
Demo: Floating Point and the Series for the Exponential Function
Rounding Error in Operations (I)

- Addition and Subtraction

Demo: Catastrophic Cancellation

Activity: Cancellation in Standard Deviation Computation
Rounding Error in Operations (II)

- Multiplication and Division
Exceptional and Subnormal Numbers

- Exceptional Numbers

- Subnormal (Denormal) Number Range

- Gradual Underflow: Avoiding underflow in addition
Floating Point Number Line

\[ \epsilon \cdot 2^{-L} \quad \text{smaller than or equal to the gap between any two floating point numbers, so} \]

\[ fl(a - b) = 0 \iff fl(a) = fl(b) \]

subnormal
\[ 0.x y \cdot 2^{-L} \]

normalized
\[ 1.x y \cdot 2^E, E \in [-L, L] \]