Lecture 1

Introduction to Numerical Computing

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Numerical Computing?

Numerical Analysis?

Numerical Computation vs. Symbolic Computation

- Numerical Computation: involve numbers directly
  - manipulate numbers to produce a **numerical** result
- Symbolic Computation: symbols represent numbers
  - manipulate symbols according to mathematical rules to produce a symbolic result

Example (numerical)

$$\frac{(17.36)^2 - 1}{17.36 + 1} = 16.36$$

Example (symbolic)

$$\frac{x^2 - 1}{x + 1} = x - 1$$

Analytic Solution vs. Numerical Solution

- Analytic Solution (a.k.a. symbolic): The exact numerical or symbolic representation of the solution
  - may use special characters such as π, e, or $\tan(83)$
- Numerical Solution: The computational representation of the solution
  - entirely numerical

Example (analytic)

$$\frac{1}{4}$$
$$\frac{1}{3}$$
$$\pi$$
$$\tan(83)$$

Example (numerical)

$$0.25$$
$$0.33333\ldots(?)$$
$$3.14159\ldots(?)$$
$$0.88472\ldots(?)$$

Numerical Computation and Approximation

- Numerical Approximation is needed to carry out the steps in the numerical calculation. The overall process is a numerical computation.

Example (symbolic computation, numerical solution)

$$\frac{1}{2} + \frac{1}{3} + \frac{1}{4} - 1 = \frac{1}{12} = 0.083333333\ldots$$

Example (numerical computation, numerical approximation)

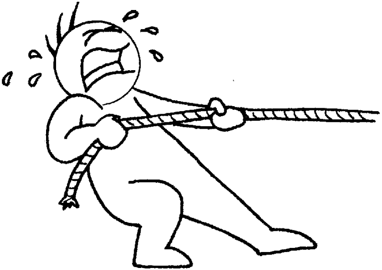
$$0.500 + 0.333 + 0.250 - 1.000 = 0.083$$

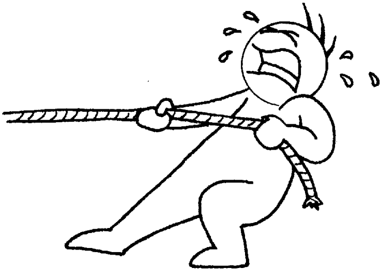
Method vs. Algorithm vs. Implementation

- Method: a general (mathematical) framework describing the solution process
- Algorithm: a detailed description of executing the method
- Implementation: a particular instantiation of the algorithm

- Is it a “good” method?
- Is it a “robust” (or “stable”) algorithm?
- Is it a fast implementation?

The Big Theme





Accuracy

Cost

History: Numerical Algorithms

- date to 1650 BC: The Rhind Papyrus of ancient Egypt contains 85 problems; many use numerical algorithms (T. Chartier, Davidson)

- Approximates π with $(8/9)^2 * 4 \approx 3.1605$

History: Archimedes

- 287-212BC developed the ”Method of Exhaustion”
- Method for determining π
  - find the length of the permieter of a polygon inscribed inside a circle of radius $1/2$
  - find the permiter of a polygon circumscribed outside a circle of radius $1/2$
  - the value of π is between these two lengths

History: Method of Exhaustion

- A circle is not a polygon
- A circle **is** a polygon with an infinite number of sides
- C_n = circumference of an n-sided polygon inscribed in a circle of radius $1/2$
- $\lim_{n\to\infty} = \pi$
- Archimedes deterimined

$$\frac{223}{71} < \pi < \frac{22}{7}$$
$$3.1408 < \pi < 3.1429$$

- two places of accuracy....
- `http://www.pbs.org/wgbh/nova/archimedes/pi.html`

History: Method of Machin

- Around 1700, John Machin discovered the trig identity

$$\pi = 16 \arctan\left(\frac{1}{5}\right) - 4 \arctan\left(\frac{1}{239}\right)$$

- Led to calculation of the first 100 digits of π
- Uses the Taylor series of $\arctan$ in the algorithm

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

- Used until 1973 to find the first Million digits

Numerical Analysis

Definition (Trefethen)

Study of algorithms for the problems of continuous mathematics

We've been doing this since Calculus (and before!)

- Riemann sum for calculating a definite integral
- Newton's Method
- Taylor's Series expansion + truncation

Big Questions

- How algorithms work and how they fail
- Why algorithms work and why they fail

- Connects mathematics and computer science
- Need mathematical theory, computer programming, and scientific inquiry

Numerical Analysis

A Numerical Analyst needs

- computational knowledge (e.g. programming skills)
- understanding of the application (physical intuition for validation)
- mathematical ability to construct a meaningful algorithm

Numerical Analysis

Numerical focus:

Approximation An approximate solution is sought. How close is this to the desired solution?

Efficiency How fast and cheap (memory) can we compute a solution?

Stability Is the solution sensitive to small variations in the problem setup?

Error What is the role of finite precision of our computers?

Numerical Analysis

Why?

- Numerical methods improve scientific simulation
- Some disasters attributable to bad numerical computing (Douglas Arnold)
  - The Patriot Missile failure, in Dharan, Saudi Arabia, on February 25, 1991 which resulted in 28 deaths, is ultimately attributable to poor handling of rounding errors.
  - The explosion of the Ariane 5 rocket just after lift-off on its maiden voyage off French Guiana, on June 4, 1996, was ultimately the consequence of a simple overflow.
  - The sinking of the Sleipner A offshore platform in Gandsfjorden near Stavanger, Norway, on August 23, 1991, resulted in a loss of nearly one billion dollars. It was found to be the result of inaccurate finite element analysis.

I thought we were studying “Numerical Computating”?!

Numerical analysis is the study of numerical computing

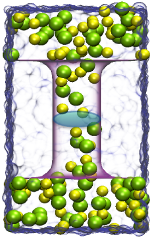
- Numerical Analysis: understanding general behavior of numerical computing
- Numerical Computing: understanding **how** to apply certain methods to solve specific tasks
- As computational scientists, we need to understand the concepts of numerical analysis and implementation aspects of the numerical computing

We thus focus on

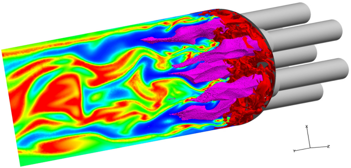
- Matlab implementation
  - fast learning curve
  - quick time-to-production: low development times
  - a major development environment in scientific computing
  - integrated graphics
- Errors in computation
- Specific methods for solving linear and nonlinear systems, root finding, integrating, interpolation, etc.

Applications: Mathematics, Engineering, Computer Science...

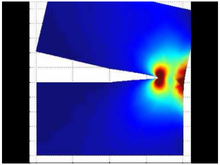
In Engineering



Biomolecular Systems



Rocket Simulations



Crack propagation

Applications: Mathematics, Engineering, Computer Science...

In Computer Science?

- **AI**: transitions, state systems, patterns (eigenvalues, linear algebra)
- **Informatics**: Google matrix, Amazon recommendations (eigenvalues, linear algebra, sparse matrices, iterative methods)
- **Graphics**: image compression, representation of curves/surfaces/lighting (interpolation, differentiation, etc)
- **Security**: ssh (random numbers)
- **Economics/Finance**: modeling/simulation of financial data (monte carlo)
- **Scientific computing**: design of algorithms for high performance/parallel computing.

What is MATLAB?

- both a computing environment and a language
- initially developed as an easy interface to LAPACK: Linear Algebra Package (FORTRAN libraries)
- **MAT**rix **LAB**oratory
- Written in C. For matrix computations, it calls C/Fortran libraries == Fast
- Matlab + “Toolboxes”
  - Symbolic Math Toolbox: mathematical manipulation of symbols
  - Partial Differential Equation Toolbox: tools for solving PDEs in 2-D
  - Statistics Toolbox: statistical data analysis
  - Image processing toolbox: visualization and image analysis
  - Bioinformatics toolbox: computational molecular biology
  - Compiler: application development
  - many many more.
- `http://www.mathworks.com`

Why Matlab?

The Good:

- Fast development times
- no compiling, easy debugging
- accessible syntax and language constructs
- in-house graphics capabilities
- tons of basic ”libraries” or functions available
- many more complicated “toolboxes” can be added

The Bad:

- small coding mistakes can result in slow code
- loops are computationally intensive
- language is limited: no templates etc.

The Ugly:

- proprietary (but the language format is open)
- expensive (but free for UNM students/faculty?)
- the open source substitute, Octave, is not fully compatible

Now, you can fire up Matlab and start the tutorial...