2.29 Numerical Fluid Mechanics Fall 2011 – Lecture 7

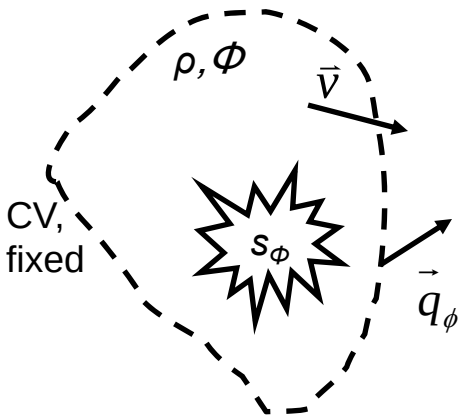
REVIEW of Lecture 6

Material covered in class: Differential forms of conservation laws

- Material Derivative (substantial/total derivative)
- Conservation of Mass
  - Differential Approach
  - Integral (volume) Approach
    - Use of Gauss Theorem
  - Incompressibility
- Reynolds Transport Theorem
- Conservation of Momentum (Cauchy's Momentum equations)
- The Navier-Stokes equations
  - Constitutive equations: Newtonian fluid
  - Navier-stokes, compressible and incompressible

Integral Conservation Law for a scalar ϕ

$$\left\{\frac{d}{dt}\int_{CM}\rho\phi dV=\right\}\boxed{\frac{d}{dt}\int_{CV_{\text{fixed}}}\rho\phi dV+\underbrace{\int_{CS}\rho\phi\,(\vec{v}.\vec{n})dA}_{\substack{\text{Advective fluxes}\\ \text{("convective" fluxes)}}}=\underbrace{-\int_{CS}\vec{q}_{\phi}.\vec{n}\;dA}_{\text{Other transports (diffusion, etc)}}+\underbrace{\sum\int_{CV_{\text{fixed}}}s_{\phi}\;dV}_{\substack{\text{Sum of sources and}\\ \text{sinks terms (reactions, etc)}}}}$$



Applying the Gauss Theorem, for any arbitrary CV gives:

$$\frac{\partial\rho\phi}{\partial t}+\nabla.(\rho\phi\vec{v})=-\nabla.\,\vec{q}_{\phi}+s_{\phi}$$

For a common diffusive flux model (Fick's law, Fourier's law):

$$\vec{q}_{\phi}=-k\nabla\phi$$

Conservative form of the PDE

$$\frac{\partial\rho\phi}{\partial t}+\nabla.\,(\rho\phi\vec{v})=\nabla.\,(k\nabla\phi)+s_{\phi}$$

Strong-Conservative form of the Navier-Stokes Equations ($\phi \Rightarrow \boldsymbol{v}$)

Cons. of Momentum:

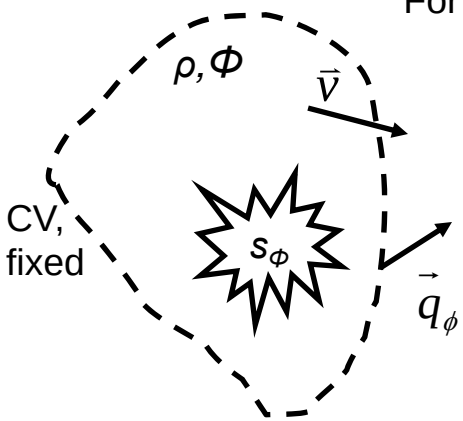
$$\frac{d}{dt}\int_{CV}\rho\vec{v}dV+\int_{CS}\rho\vec{v}(\vec{v}.\vec{n})dA=\underbrace{\int_{CS}-p\,\vec{n}dA+\int_{CS}\vec{\vec{\tau}}.\vec{n}dA+\int_{CV}\rho\vec{g}dV}_{=\sum\vec{F}}$$

Applying the Gauss Theorem gives:

$$=\int_{CV}\left(-\nabla p+\nabla.\vec{\vec{\tau}}+\rho\vec{g}\right)dV$$

For any arbitrary CV gives:

$$\frac{\partial\rho\vec{v}}{\partial t}+\nabla.(\rho\vec{v}\,\vec{v})=-\nabla p+\nabla.\vec{\vec{\tau}}+\rho\vec{g}$$



With Newtonian fluid + incompressible + constant μ:

Momentum: $$\frac{\partial\rho\vec{v}}{\partial t}+\nabla.(\rho\vec{v}\,\vec{v})=-\nabla p+\mu\nabla^2\vec{v}+\rho\vec{g}$$

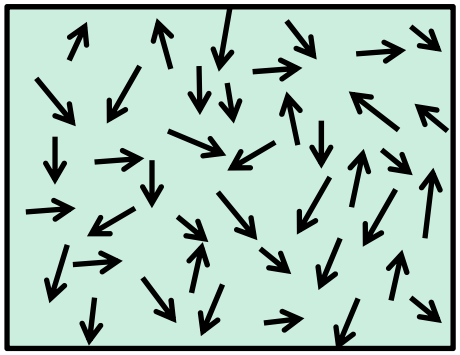
Mass: $$\nabla.\vec{v}=0$$

Equations are said to be in "strong conservative form" if all terms have the form of the divergence of a vector or a tensor. For the ith Cartesian component, in the general Newtonian fluid case:

With Newtonian fluid only: $$\frac{\partial\rho v_i}{\partial t}+\nabla.(\rho v_i\,\vec{v})=\nabla.\left(-p\,\vec{e}_i+\mu\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)\vec{e}_j-\frac{2}{3}\mu\frac{\partial u_j}{\partial x_j}\vec{e}_i+\rho g_i x_i\vec{e}_i\right)$$

Navier-Stokes Equations:
For an Incompressible Fluid with constant viscosity

V(x,y,z)



Fluid Velocity Field

$$\mathbf{V} = \mathbf{i}u + \mathbf{j}v + \mathbf{k}w$$

Hydrostatic Pressure:
$-\rho g z$ for z positive upward

Conservation of Mass

$$\mathrm{div}\mathbf{V} = \nabla \cdot \mathbf{V} = 0$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

Dynamic Pressure $P = P_{actual} - \rho g z$

Navier-Stokes Equation

$$\frac{D\mathbf{V}}{Dt} = \frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V} \cdot \nabla)\mathbf{V} = -\frac{1}{\rho}\nabla P + \nu \nabla^2 \mathbf{V}$$

Density ρ

Kinematic viscosity ν

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z} = -\frac{1}{\rho}\frac{\partial P}{\partial x} + \nu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right)$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + w\frac{\partial v}{\partial z} = -\frac{1}{\rho}\frac{\partial P}{\partial y} + \nu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2}\right)$$

$$\frac{\partial w}{\partial t} + u\frac{\partial w}{\partial x} + v\frac{\partial w}{\partial y} + w\frac{\partial w}{\partial z} = -\frac{1}{\rho}\frac{\partial P}{\partial z} + \nu\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2}\right)$$

Incompressible Fluid

Pressure Equation

Navier-Stokes Equation

$$\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V} \cdot \nabla)\mathbf{V} = -\frac{1}{\rho}\nabla P + \nu \nabla^2 \mathbf{V}$$

Conservation of Mass

$$\nabla \cdot \mathbf{V} = 0$$

Divergence of Navier-Stokes Equation

$$\mathrm{div}(\mathbf{V} \cdot \nabla\ \mathbf{V}) = -\frac{1}{\rho}\nabla^2 P$$

Dynamic Pressure Poisson Equation

$$\Rightarrow \quad \nabla^2 P = -\rho \left\{ \left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial y}\right)^2 + \left(\frac{\partial w}{\partial z}\right)^2 + 2\frac{\partial v}{\partial x}\frac{\partial u}{\partial y} + 2\frac{\partial w}{\partial x}\frac{\partial u}{\partial z} + 2\frac{\partial w}{\partial y}\frac{\partial v}{\partial z} \right\}$$

More general than Bernoulli – Valid for unsteady and rotational flow

Incompressive Fluid
Vorticity Equation

Vorticity

$$\tilde{\omega} \equiv \mathrm{curl}\mathbf{V} \equiv \nabla \times \mathbf{V}$$

Navier-Stokes Equation

$$\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V} \cdot \nabla)\mathbf{V} = -\frac{1}{\rho}\nabla P + \nu \nabla^2 \mathbf{V}$$

curl of Navier-Stokes Equation

$$\frac{D\tilde{\omega}}{Dt} = -(\tilde{\omega} \cdot \nabla)\mathbf{V} + \nu \nabla^2 \tilde{\omega}$$

Inviscid Fluid Mechanics

Euler's Equation

Navier-Stokes Equation: incompressible, constant viscosity

$$\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V} \cdot \nabla)\mathbf{V} = -\frac{1}{\rho}\nabla P + \nu \nabla^2 \mathbf{V}$$

If also inviscid fluid

$$\nu = 0$$

$\Rightarrow$ Euler's Equations

$$\begin{aligned}
\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z} &= -\frac{1}{\rho}\frac{\partial P}{\partial x} \\
\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + w\frac{\partial v}{\partial z} &= -\frac{1}{\rho}\frac{\partial P}{\partial y} \\
\frac{\partial w}{\partial t} + u\frac{\partial w}{\partial x} + v\frac{\partial w}{\partial y} + w\frac{\partial w}{\partial z} &= -\frac{1}{\rho}\frac{\partial P}{\partial z}
\end{aligned}$$

Inviscid Fluid Mechanics

Bernoulli Theorems

Theorem 1

Irrotational Flow, incompressible

$$\nabla \times \mathbf{V} = 0$$

Flow Potential

$$\mathbf{V} = \nabla \phi$$

Define

$$H = \frac{1}{2}|\mathbf{V}|^2 + \frac{P}{\rho}$$

$$\frac{\partial \phi}{\partial t} + H = 0$$

Introduce P_T = Thermodynamic pressure

$$P_T = P - \rho g z$$

$$\boxed{\frac{\partial \phi}{\partial t} + \frac{1}{2}|\mathbf{V}|^2 + \frac{P_T}{\rho} + gz = 0}$$

Theorem 2

Steady, Incompressible, inviscid, no shaft work, no heat transfer

Navier-Stokes Equation

$$\cancel{\frac{\partial \mathbf{V}}{\partial t}} + (\mathbf{V} \cdot \nabla)\mathbf{V} = -\frac{1}{\rho}\nabla P$$

$$\mathbf{V} \times \tilde{\omega} = \nabla H$$

Along stream lines and vortex lines

$$\boxed{\begin{aligned} H &= \frac{1}{2}|\mathbf{V}|^2 + \frac{P}{\rho} \\ &= \frac{1}{2}|\mathbf{V}|^2 + \frac{P_T}{\rho} + gz = \text{const} \end{aligned}}$$

Potential Flows

Integral Equations

Irrotational Flow

$$\nabla \times \mathbf{V} = \mathbf{0}$$

Flow Potential

$$\mathbf{V} = \nabla \phi$$

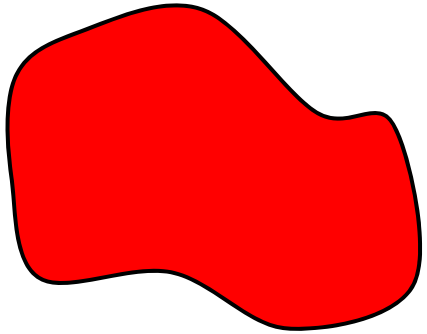
Conservation of Mass

$$\nabla \cdot \mathbf{V} = 0$$

$$\Rightarrow$$

$$\nabla \cdot (\nabla \phi) = 0$$

$$\boxed{\nabla^2 \phi = 0}$$



"Mostly" Potential Flows:

Only rotation occurs at boundaries due to viscous terms

In 2D:

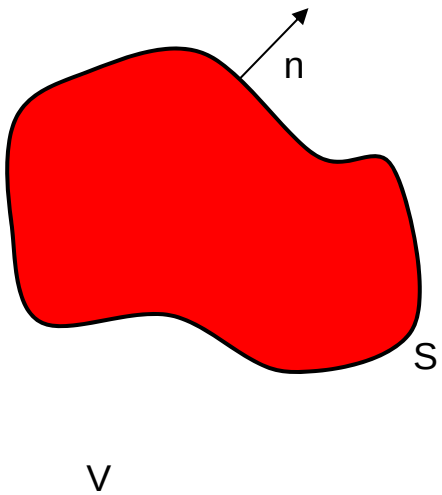
$$\text{Velocity potential}: \quad u = \frac{\partial \phi}{\partial x}, \quad v = \frac{\partial \phi}{\partial y}$$

$$\text{Stream function}: \quad u = \frac{\partial \psi}{\partial y}, \quad v = -\frac{\partial \psi}{\partial x}$$

- Since Laplace equation is linear, it can be solved by superposition of flows, called panel methods
- What distinguishes one flow from another are the boundary conditions and the geometry: there are no intrinsic parameters in the Laplace equation

Potential Flow

Boundary Integral Equations



Green's Theorem

$$\int_S \left[G(\mathbf{x},\mathbf{x}_0)\frac{\partial \phi(\mathbf{x}_0)}{\partial n} - \phi(\mathbf{x}_0)\frac{\partial G(\mathbf{x},\mathbf{x}_0)}{\partial n} \right] dS_0$$

$$= \int_V \left[\phi(\mathbf{x}_0)\nabla^2 G(\mathbf{x},\mathbf{x}_0) - G(\mathbf{x},\mathbf{x}_0)\nabla^2\phi(\mathbf{x}_0) \right] dV_0$$

Green's Function

$$G(\mathbf{x},\mathbf{x}_0) = \frac{1}{r} = \frac{1}{\sqrt{(x-x_0)^2+(y-y_0)^2+(z-z_0)^2}} + \psi(\mathbf{x})$$

Homogeneous Solution

$$\nabla^2\psi = 0$$

$$\nabla^2 G((\mathbf{x},\mathbf{x}_0) = -\delta(\mathbf{x}-\mathbf{x}_0)$$

Boundary Integral Equation

$$\phi(\mathbf{x}) = \int_S \left[G(\mathbf{x},\mathbf{x}_0)\frac{\partial \phi(\mathbf{x}_0)}{\partial n} - \phi(\mathbf{x}_0)\frac{\partial G(\mathbf{x},\mathbf{x}_0)}{\partial n} \right] dS_0 - \int_V \left[G(\mathbf{x},\mathbf{x}_0)\nabla^2\phi(\mathbf{x}_0) \right] dV_0$$

Discretized Integral Equation

$$\sum_{j=0}^{N-1} A_{ij} w_j = B_i$$

Linear System of Equations

$$\overline{\overline{\mathbf{A}}}\mathbf{u} = \mathbf{b}$$

Panel Methods

Systems of Linear Equations

- Motivation and Plans
- Direct Methods for solving Linear Equation Systems
  - Cramer's Rule (and other methods for a small number of equations)
  - Gaussian Elimination
  - Numerical implementation
    - Numerical stability
      - Partial Pivoting
      - Equilibration
      - Full Pivoting
    - Multiple right hand sides, Computation count
    - LU factorization
    - Error Analysis for Linear Systems
      - Condition Number
    - Special Matrices: Tri-diagonal systems
- Iterative Methods
  - Jacobi's method
  - Gauss-Seidel iteration
  - Convergence

Motivations and Plans

- Fundamental equations in engineering are conservation laws (mass, momentum, energy, mass ratios/concentrations, etc)
  - Can be written as " *System Behavior (state variables) = forcing* "
- Result of the discretized (volume or differential form) of the Navier-Stokes equations (or most other differential equations):
  - System of (mostly coupled) algebraic equations which are linear or nonlinear, depending on the nature of the continuous equations
  - Often, resulting matrices are sparse (e.g. banded and/or block matrices)
- Lectures 3 and 4:
  - Methods for solving $f(x)=0$ or $\mathbf{f}(\mathbf{x})=\mathbf{0}$
  - To be used for systems of equations: $\mathbf{f}(\mathbf{x})=\mathbf{b}$, i.e: $\mathbf{f} = \left(f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_n(\mathbf{x}) \right) = \mathbf{b}$
- Here we first deal with solving Linear Algebraic equations:

$$\mathbf{A}\,\mathbf{x} = \mathbf{b} \quad \text{or} \quad \mathbf{A}\,\mathbf{X} = \mathbf{B}$$

Motivations and Plans

- Above 75% of engineering/scientific problems involve solving linear systems of equations
  - As soon as methods were used on computers => dramatic advances
- Main Goal: Learn methods to solve systems of linear algebraic equations and apply them to CFD applications
- Reading Assignment
  - Part III and Chapter 9 of "Chapra and Canale, Numerical Methods for Engineers, 2006."
  - For Matrix background, see Chapra and Canale (pg 219-227) and other linear algebra texts (e.g. Trefethen and Bau, 1997)
- Other References :
  - Any chapter on "Solving linear systems of equations" in CFD references provided.
  - For example: chapter 5 of "J. H. Ferziger and M. Peric, Computational Methods for Fluid Dynamics. Springer, NY, 3rd edition, 2002"

Direct Numerical Methods
for Linear Equation Systems

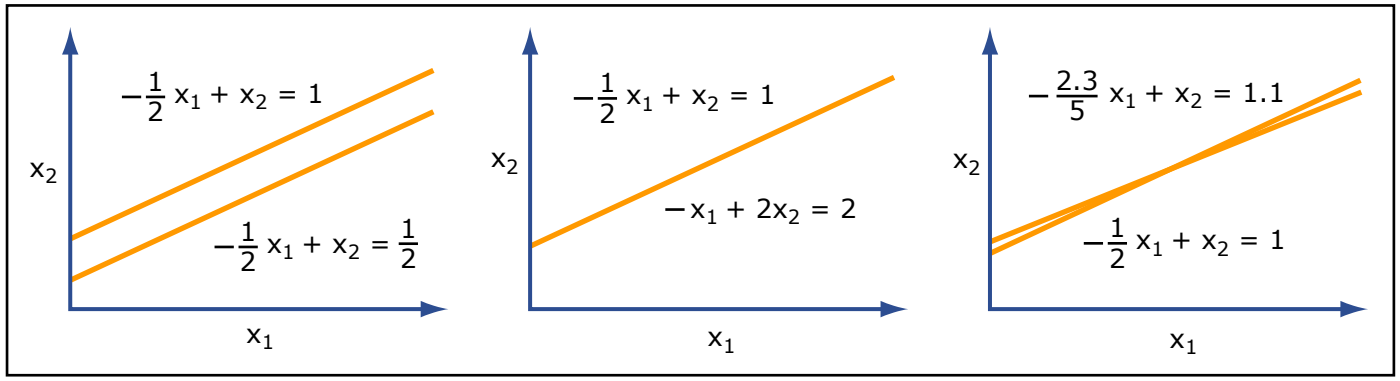
$$\mathbf{A}\,\mathbf{x} = \mathbf{b} \quad \text{or} \quad \mathbf{A}\,\mathbf{X} = \mathbf{B}$$

- Main Direct Method is: Gauss Elimination

  Key idea is simply to "combine equations so as to eliminate unknowns"

- First, let's consider systems with a small number of equations
  - Graphical Methods
    - Two equations: intersection of 2 lines
    - Three equations: intersection of 3 planes
    - Useful to illustrate issues:

      no solution / infinite solutions (singular) or ill-conditioned system



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Direct Methods for Small Systems: Determinants and Cramer's Rule

Linear System of Equations:

$$
\begin{array}{ccccccc}
a_{11}x_1 & a_{12}x_2 & \cdot & \cdot & a_{1n}x_n & = & b_1 \\
a_{21}x_1 & a_{22}x_2 & \cdot & \cdot & a_{2n}x_n & = & b_2 \\
\cdot & \cdot & \cdot & \cdot & \cdot & = & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & = & \cdot \\
a_{n1}x_1 & \cdot & \cdot & \cdot & a_{nn}x_n & = & b_n
\end{array}
$$

Recall, for a 2 by 2 matrix, the determinant is:

$$D = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11}\,a_{22} - a_{21}\,a_{12}$$

Recall, for a 3 by 3 matrix, the determinant is:

$$D = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = a_{11}\begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} - a_{12}\begin{vmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{vmatrix} + a_{13}\begin{vmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{vmatrix}$$

Direct Methods for small systems: Determinants and Cramer's Rule

Cramer's rule:

"Each unknown x_i in a system of linear algebraic equations can be expressed as a fraction of two determinants:

- Numerator is D but with column i replaced by **b**
- Denominator is D

$$x_i = \frac{\begin{vmatrix} a_{11} & \overbrace{b_1}^{\text{i}^{\text{th}}\text{ column}} & a_{1n} \\ & b_2 & \\ & & \\ a_{n1} & b_n & a_{nn} \end{vmatrix}}{D}$$

Example: Cramer's Rule, n=2

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$$

$$\begin{aligned} D &= a_{11}a_{22} - a_{21}a_{12} \\ D_1 &= b_1a_{22} - b_2a_{12} \\ D_2 &= b_2a_{11} - b_1a_{21} \end{aligned}$$

$$x_1 = \frac{D_1}{D} = \frac{b_1a_{22} - b_2a_{12}}{a_{11}a_{22} - a_{21}a_{12}}$$

$$x_2 = \frac{D_2}{D} = \frac{b_2a_{11} - b_1a_{21}}{a_{11}a_{22} - a_{21}a_{12}}$$

Numerical case:

$$\begin{bmatrix} 0.01 & -1.0 \\ 1.0 & 0.01 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 1.0 \\ 1.0 \end{Bmatrix}$$

$$\begin{aligned} x_1 &= \frac{1.0\cdot 0.01 - 1.0\cdot(-1.0)}{0.01\cdot 0.01 - 1.0\cdot(-1.0)} = 1.0099 \\ x_2 &= \frac{1.0\cdot 0.01 - 1.0\cdot 1.0}{0.01\cdot 0.01 - 1.0\cdot(-1.0)} = -0.9899 \end{aligned}$$

Cramer's rule becomes impractical for n>3:

The number of operations is of O(n!)

Direct Methods for large dense systems
Gauss Elimination

- Main idea: "combine equations so as to eliminate unknowns systematically"
  - Solve for each unknown one by one
  - Back-substitute result in the original equations
  - Continue with the remaining unknowns

- General Gauss Elimination Algorithm
  i. Forward Elimination/Reduction to Upper Triangular Systems)
  ii. Back-Substitution

- Comments:
  - Well suited for dense matrices
  - Some modification of above simple algorithm needed to avoid division by zero and other pitfalls

Linear System of Equations

$$
\begin{array}{ccccccc}
a_{11}x_1 & a_{12}x_2 & \cdot & \cdot & a_{1n}x_n & = & b_1 \\
a_{21}x_1 & a_{22}x_2 & \cdot & \cdot & a_{2n}x_n & = & b_2 \\
\cdot & \cdot & \cdot & \cdot & \cdot & = & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & = & \cdot \\
a_{n1}x_1 & \cdot & \cdot & \cdot & a_{nn}x_n & = & b_n
\end{array}
$$

Gauss Elimination

Linear System of Equations

$$
\begin{array}{ccccccc}
a_{11}x_1 & a_{12}x_2 & \cdot & \cdot & a_{1n}x_n & = & b_1 \\
a_{21}x_1 & a_{22}x_2 & \cdot & \cdot & a_{2n}x_n & = & b_2 \\
\cdot & \cdot & \cdot & \cdot & \cdot & = & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & = & \cdot \\
a_{n1}x_1 & \cdot & \cdot & \cdot & a_{nn}x_n & = & b_n
\end{array}
$$

Reduction / Forward Elimination
Step 0

$$a_{ij}^{(1)} = a_{ij}, \quad b_i^{(1)} = b_i$$

$$
\begin{array}{ccccccc}
a_{11}^{(1)}x_1 & a_{12}^{(1)}x_2 & \cdot & \cdot & a_{1n}^{(1)}x_n & = & b_1^{(1)} \\
a_{21}^{(1)}x_1 & a_{22}^{(1)}x_2 & \cdot & \cdot & a_{2n}^{(1)}x_n & = & b_2^{(1)} \\
\cdot & \cdot & \cdot & \cdot & \cdot & = & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & = & \cdot \\
a_{n1}^{(1)}x_1 & \cdot & \cdot & \cdot & a_{nn}^{(1)}x_n & = & b_n^{(1)}
\end{array}
$$

If a_{11} is non zero, we can eliminate x_1 from the remaining equations 2 to (n-1) by multiplying equation 1 with $\frac{a_{i1}}{a_{11}}$ and subtracting the result from equation i .

This leads to the following algorithm for “Step 1”:

Gauss Elimination

Reduction / Forward Elimination
Step 1

$$\left.\begin{aligned} m_{i1} &= \frac{a_{i1}^{(1)}}{a_{11}^{(1)}} \\ a_{ij}^{(2)} &= a_{ij}^{(1)} - m_{i1}a_{1j}^{(1)}, \quad j = 1, \cdots n \\ b_i^{(2)} &= b_i^{(1)} - m_{i1}b_1^{(1)} \end{aligned}\right\} \; i = 2, \cdots n$$

a_{11} is called pivot element:

$$\begin{array}{c} \\ \\ i \downarrow \\ \\ \end{array} \overset{j \rightarrow}{\begin{array}{cccccccc} a_{11}^{(1)}x_1 & a_{12}^{(1)}x_2 & \cdot & \cdot & a_{1n}^{(1)}x_n & = & b_1^{(1)} \\ \boxed{0} & a_{22}^{(2)}x_2 & \cdot & \cdot & a_{2n}^{(2)}x_n & = & b_2^{(2)} \\ \boxed{\cdot} & \cdot & \cdot & \cdot & \cdot & = & \cdot \\ \boxed{\cdot} & \cdot & \cdot & \cdot & \cdot & = & \cdot \\ \boxed{0} & a_{n2}^{(2)}x_2 & \cdot & \cdot & a_{nn}^{(2)}x_n & = & b_n^{(2)} \end{array}}$$

(is called Pivot equation for step 1)

Notes:

- Result of step 1: last (n-1) equations have (n-1) unknowns
- Pivot a_{11} needs to be non-zero

Gauss Elimination

Reduction: Step k

Recursive repetition of step 1 for successively reduced set of (n-k) equations:

$$\left.\begin{aligned} m_{ik} &= \frac{a_{ik}^{(k)}}{a_{kk}^{(k)}} \\ a_{ij}^{(k+1)} &= a_{ij}^{(k)} - m_{ik} a_{kj}^{(k)}, \quad j = k, \cdots n \\ b_i^{(k+1)} &= b_i^{(k)} - m_{ik} b_k^{(k)} \end{aligned}\right\} \; i = k+1, \cdots n$$

The result after completion of step k is:

$$\begin{array}{cccccccc} a_{11}^{(1)} x_1 & a_{12}^{(1)} x_2 & \cdot & \cdot & a_{1n}^{(1)} x_n & = & b_1^{(1)} \\ 0 & a_{22}^{(2)} x_2 & \cdot & \cdot & a_{2n}^{(2)} x_n & = & b_2^{(2)} \\ 0 & \cdot & a_{kk}^{(k)} x_k & \cdot & \cdot & = & \cdot \\ 0 & \cdot & 0 & \cdot & \cdot & = & \cdot \\ 0 & \cdot & 0 & \cdot & a_{nn}^{(k+1)} x_n & = & b_n^{(k+1)} \end{array}$$

First non-zero element on row n: $a_{n,k+1}^{(k+1)} x_k$

Gauss Elimination

Reduction/Elimination: Step k

$$\left.\begin{aligned} m_{ik} &= \frac{a_{ik}^{(k)}}{a_{kk}^{(k)}} \\ a_{ij}^{(k+1)} &= a_{ij}^{(k)} - m_{ik} a_{kj}^{(k)}, \quad j = k, \cdots n \\ b_i^{(k+1)} &= b_i^{(k)} - m_{ik} b_k^{(k)} \end{aligned}\right\} \; i = k+1, \cdots n$$

Reduction: Step (n-1)

$$\begin{array}{cccccccc} a_{11}^{(1)} x_1 & a_{12}^{(1)} x_2 & \cdot & \cdot & a_{1n}^{(1)} x_n & = & b_1^{(1)} \\ 0 & a_{22}^{(2)} x_2 & \cdot & \cdot & a_{2n}^{(2)} x_n & = & b_2^{(2)} \\ 0 & \cdot & \cdot & \cdot & \cdot & = & \cdot \\ 0 & \cdot & 0 & a_{n-1,n-1}^{(n-1)} x_{n-1} & a_{n-1,n}^{(n-1)} x_n & = & b_{n-1}^{(n-1)} \\ 0 & \cdot & \cdot & 0 & a_{nn}^{(n)} x_n & = & b_n^{(n)} \end{array}$$

Result after step (n-1) is an Upper triangular system!

Back-Substitution

$$\begin{aligned} x_n &= b_n^{(n)} / a_{nn}^{(n)} \\ x_{n-1} &= \left(b_{n-1}^{(n-1)} - a_{n-1,n}^{(n-1)} x_n \right) / a_{n-1,n-1}^{(n-1)} \\ &\cdot \quad \cdot \quad \cdot \\ &\cdot \quad \cdot \quad \cdot \\ x_k &= \left(b_k^{(k)} - \sum_{j=k+1}^{n} a_{kj}^{(k)} x_j \right) / a_{kk}^{(k)} \\ &\cdot \quad \cdot \quad \cdot \\ x_1 &= \left(b_1^{(1)} - \sum_{j=2}^{n} a_{1j}^{(1)} x_j \right) / a_{11}^{(1)} \end{aligned}$$

Gauss Elimination: Number of Operations

Reduction/Elimination: Step k

$$\left.\begin{aligned} m_{ik} &= \frac{a_{ik}^{(k)}}{a_{kk}^{(k)}} \\ a_{ij}^{(k+1)} &= a_{ij}^{(k)} - m_{ik}a_{kj}^{(k)}, \quad j = k, \cdots n \\ b_i^{(k+1)} &= b_i^{(k)} - m_{ik}b_k^{(k)} \end{aligned}\right\} \; i = k+1, \cdots n$$

: n-k divisions

: 2 (n-k) (n-k+1) additions/multiplications

: 2 (n-k) additions/multiplications

For reduction, total number of ops is: $\sum_{k=1}^{n-1} 3(n-k) + 2(n-k)*(n-k+1) = 2\left(\frac{n^3}{3} + n^2 - \frac{n}{3}\right) = O(n^3)$

Use: $\sum_{i=1}^{n} i = \frac{n(n+1)}{2}$ and $\sum_{i=1}^{n} i^2 = \frac{n(n+1)(2n+1)}{6}$

Back-Substitution

$$x_k = \left(b_k^{(k)} - \sum_{j=k+1}^{n} a_{kj}^{(k)} x_j\right) / a_{kk}^{(k)}$$

: (n-k-1)+(n-k)+2=2(n-k) +1 additions/multiplications

Hence, total number of ops is: $1 + \sum_{k=1}^{n-1}\left(2(n-k)+1\right) = 1 + (n-1)(n+1) = n^2$ $\quad \left(\sum_{i=1}^{n} i = \frac{n(n+1)}{2}\right)$

(the first 1 before the sum is for x_n)

Grand total number of ops is $O(\frac{2}{3}n^3) = O(n^3)$

- Grows rapidly with n
- Most ops occur in elimination step

:

Gauss Elimination:
Issues and Pitfalls to be addressed

- Division by zero:
  - Pivot elements $a_{k,k}^{(k)}$ must be non-zero and should not be close to zero
- Round-off errors
  - Due to recursive computations and so error propagation
  - Important when large number of equations are solved
  - Always substitute solution found back into original equations
  - Scaling of variables can be used
- Ill-conditioned systems
  - Occurs when one or more equations are nearly identical
  - If determinant of normalized system matrix $\mathbf{A}$ is close to zero, system will be ill-conditioned (in general, if $\mathbf{A}$ is not well conditioned)
  - Determinant can be computed using Gauss Elimination
    - Since forward-elimination consists of simple scaling and addition of equations, the determinent is the product of diagonal elements of the Upper Triangular System

Gauss Elimination: Pivoting

Step k

$$\left.\begin{aligned} m_{ik} &= \frac{a_{ik}^{(k)}}{a_{kk}^{(k)}} \\ a_{ij}^{(k+1)} &= a_{ij}^{(k)} - m_{ik} a_{kj}^{(k)}, \quad j = k, \cdots n \\ b_i^{(k+1)} &= b_i^{(k)} - m_{ik} b_k^{(k)} \end{aligned}\right\} \; i = 2, \cdots n$$

Partial Pivoting by Columns

Row k

Row i

$$\begin{bmatrix} \times & & & & & & \\ 0 & \times & & & & & \\ \cdot & \cdot & \times & & & & \\ \cdot & & 0 & 0 & \times & \times & \times \\ \cdot & & \cdot & \times & & & \\ \cdot & & \cdot & \times & & & \\ \cdot & & \cdot & \times & & & \\ 0 & \cdot & 0 & \times & & & \end{bmatrix} \cdot \bar{\mathbf{x}} = \begin{Bmatrix} \times \\ \cdot \\ \cdot \\ \times \\ \cdot \\ \cdot \\ \cdot \\ \times \end{Bmatrix}$$

Pivot Elements

$$a_{11}^{(1)}, a_{22}^{(2)}, \ldots, a_{nn}^{(n)}$$

Required at each step!

$$\boxed{a_{kk}^{(k)} \neq 0}$$

Gauss Elimination: Pivoting

Reduction
Step k

$$\left.\begin{aligned} m_{ik} &= \frac{a_{ik}^{(k)}}{a_{kk}^{(k)}} \\ a_{ij}^{(k+1)} &= a_{ij}^{(k)} - m_{ik} a_{kj}^{(k)}, \quad j = k, \cdots n \\ b_i^{(k+1)} &= b_i^{(k)} - m_{ik} b_k^{(k)} \end{aligned}\right\} \; i = 2, \cdots n$$

Partial Pivoting by Columns

New Row k

New Row i

$$\begin{bmatrix} \times & & & & & & & \\ 0 & \times & & & & & & \\ \cdot & \cdot & \times & & & & & \\ \cdot & & 0 & \times & \times & \times & \times & \\ \cdot & & \cdot & \times & & & & \\ \cdot & & \cdot & 0 & & & & \\ \cdot & & \cdot & \times & & & & \\ 0 & \cdot & 0 & \times & & & & \end{bmatrix} \cdot \bar{\mathbf{x}} = \begin{Bmatrix} \times \\ \cdot \\ \cdot \\ \times \\ \cdot \\ \cdot \\ \cdot \\ \times \end{Bmatrix}$$

Pivot Elements

$$a_{11}^{(1)}, a_{22}^{(2)}, \ldots, a_{nn}^{(n)}$$

Required at each step!

$$\boxed{a_{kk}^{(k)} \neq 0}$$

Two Solutions:

A. **Partial Pivoting**
   i. Search for largest available coefficient in column below pivot element
   ii. Switch rows k and i

B. **Complete Pivoting**
   i. As for Partial, but search both rows and columns
   ii. Rarely done since column re-ordering changes order of x's, hence more complex code

Gauss Elimination: Pivoting Example

(for division by zero but also reduces round-off errors)

Example, n=2

$$\begin{bmatrix} 0.01 & -1.0 \\ 1.0 & 0.01 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 1.0 \\ 1.0 \end{Bmatrix}$$

Cramer's Rule - Exact

$$x_1 = \frac{1.0 \cdot 0.01 - 1.0 \cdot (-1.0)}{0.01 \cdot 0.01 - 1.0 \cdot (-1.0)} = 1.0099$$

$$x_2 = \frac{1.0 \cdot 0.01 - 1.0 \cdot 1.0}{0.01 \cdot 0.01 - 1.0 \cdot (-1.0)} = -0.9899$$

Relatively close to zero

Direct Gaussian Elimination

$$\begin{bmatrix} 0.01 & -1.0 \\ 1.0 & 0.01 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 1.0 \\ 1.0 \end{Bmatrix} \Rightarrow \begin{Bmatrix} x_1 = 1.01 \\ x_2 = -0.99 \end{Bmatrix}$$

2-digit Arithmetic

$$m_{21} = 100$$

$$a_{21}^{(2)} = 0$$

$$a_{22}^{(2)} = \boxed{0.01} + 100 \simeq 100$$

$$b_2^{(2)} = \boxed{1} - 100 \simeq -100$$

$$x_2 = \boxed{-1}$$

$$x_1 = (1.0 - 1.0)/0.01 = \boxed{0}$$

100% error

1% error

```
n=2
a = [ [0.01 1.0]' [-1.0 0.01]']
b= [1 1]'
r=a^(-1) * b
x=[0 0];
m21=a(2,1)/a(1,1);
a(2,1)=0;
a(2,2) = radd(a(2,2),-m21*a(1,2),n);
b(2)   = radd(b(2),-m21*b(1),n);
x(2)   = b(2)/a(2,2);
x(1)   = (radd(b(1), -a(1,2)*x(2),n))/a(1,1);
x'
```

tbt.m

Gauss Elimination: Pivoting Example

(for division by zero but also reduces round-off errors)

Example, n=2

$$\begin{bmatrix} 0.01 & -1.0 \\ 1.0 & 0.01 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 1.0 \\ 1.0 \end{Bmatrix}$$

Cramer's Rule - Exact

$$x_1 = \frac{1.0 \cdot 0.01 - 1.0 \cdot (-1.0)}{0.01 \cdot 0.01 - 1.0 \cdot (-1.0)} = 1.0099$$

$$x_2 = \frac{1.0 \cdot 0.01 - 1.0 \cdot 1.0}{0.01 \cdot 0.01 - 1.0 \cdot (-1.0)} = -0.9899$$

Partial Pivoting
Interchange Rows

$$\begin{bmatrix} 1.0 & 0.01 \\ 0.01 & -1.0 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 1.0 \\ 1.0 \end{Bmatrix}$$

2-digit Arithmetic

$$m_{21} = 0.01$$

1% error $\quad a_{22}^{(2)} = -1 - 0.0\boxed{001} \simeq -1.0$

$$b_2^{(2)} = 1 - 0.0\boxed{1} \simeq 1.0$$

1% error $\quad x_2 = \boxed{-1}$

$$x_1 = 1 + 0.01 \simeq \boxed{1.0}$$

See tbt2.m

Notes on coding:

- Pivoting can be done in function/subroutine
- Most codes don't exchange rows, but rather keep track of pivot rows (store info in "pointer" vector)

Gauss Elimination: Equation Scaling Example

(normalizes determinant, also reduces round-off errors)

Example, n=2

$$\begin{bmatrix} 0.01 & -1.0 \\ 1.0 & 0.01 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 1.0 \\ 1.0 \end{Bmatrix}$$

Cramer's Rule - Exact

$$x_1 = \frac{1.0 \cdot 0.01 - 1.0 \cdot (-1.0)}{0.01 \cdot 0.01 - 1.0 \cdot (-1.0)} = 1.0099$$

$$x_2 = \frac{1.0 \cdot 0.01 - 1.0 \cdot 1.0}{0.01 \cdot 0.01 - 1.0 \cdot (-1.0)} = -0.9899$$

Multiply Equation 1 by 200

$$\begin{bmatrix} 2.0 & -200 \\ 1.0 & 0.01 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 200.0 \\ 1.0 \end{Bmatrix} \Rightarrow \begin{cases} x_1 = 1.01 \\ x_2 = -0.99 \end{cases}$$

2-digit Arithmetic

$$\begin{aligned} m_{21} &= 0.5 \\ a_{21}^{(2)} &= 0 \\ a_{22}^{(2)} &= 0.01 + 100 \simeq 100 \\ b_2^{(2)} &= 1 - 0.5 \cdot 200 \simeq -100 \\ x_2 &= \boxed{-1} \\ x_1 &= (200 - 200)/2 = \boxed{0} \end{aligned}$$

100% error

1% error

See tbt3.m

Equations must be normalized for partial pivoting to ensure stability

This **Equilibration** is made by normalizing the matrix to unit norm

Element-based Infinity-Norm Normalization

$$||a_{ij}||_\infty = \max_j |a_{ij}| \simeq 1, \quad i = 1, \ldots n$$

Element-based Two-Norm Normalization

$$||a_{ij}||_2 = \sum_{j=1}^{n} a_{ij}^2 \simeq 1, \quad i = 1, \ldots n$$

Note: Examples of Matrix Norms

$$\|A\|_1 = \max_{1\le j\le n} \sum_{i=1}^{m} |a_{ij}|$$ "Maximum Column Sum"

$$\|A\|_\infty = \max_{1\le i\le m} \sum_{j=1}^{n} |a_{ij}|$$ "Maximum Row Sum"

$$\|A\|_F = \left(\sum_{i=1}^{m} \sum_{j=1}^{n} |a_{ij}|^2 \right)^{1/2}$$ "The Frobenius norm"

$$\|A\|_2 = \sqrt{\lambda_{\max}(A^* A)}$$ "The l-2 norm"

Gauss Elimination: Full Pivoting Example
(normalizes determinant, also reduces round-off errors)

Example, n=2

$$\begin{bmatrix} 2.0 & -200 \\ 1.0 & 0.01 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 200.0 \\ 1.0 \end{Bmatrix}$$

Cramer's Rule - Exact

$$x_1 = \frac{1.0 \cdot 0.01 - 1.0 \cdot (-1.0)}{0.01 \cdot 0.01 - 1.0 \cdot (-1.0)} = 1.0099$$

$$x_2 = \frac{1.0 \cdot 0.01 - 1.0 \cdot 1.0}{0.01 \cdot 0.01 - 1.0 \cdot (-1.0)} = -0.9899$$

Interchange Unknowns

$$x_1 = \tilde{x}_2$$

$$x_2 = \tilde{x}_1$$

Pivoting by Rows

$$\begin{bmatrix} -200 & 2.0 \\ 0.01 & 1.0 \end{bmatrix} \begin{Bmatrix} \tilde{x}_1 \\ \tilde{x}_2 \end{Bmatrix} = \begin{Bmatrix} 200.0 \\ 1.0 \end{Bmatrix} \Rightarrow \begin{Bmatrix} \tilde{x}_1 = -0.99 \\ \tilde{x}_2 = 1.01 \end{Bmatrix}$$

2-digit Arithmetic

$$\begin{aligned} m_{21} &= -0.00005 \\ a_{21}^{(2)} &= 0 \\ a_{22}^{(2)} &= 0.01 + 1.0 \simeq 1.0 \\ b_2^{(2)} &= 1 + 0.01 \simeq 1 \\ \tilde{x}_2 &\simeq \boxed{1} \\ \tilde{x}_1 &= (200 - 2)/(-200) \simeq \boxed{-1} \end{aligned}$$

1% error

Full Pivoting

Find largest numerical value in same row and column and interchange

Affects ordering of unknowns (hence rarely done)

Gauss Elimination

Numerical Stability

- Partial Pivoting
  - Equilibrate system of equations
  - Pivoting by Columns
  - Simple book-keeping
    - Solution vector in original order
- Full Pivoting
  - Does not necessarily require equilibration
  - Pivoting by both row and columns
  - More complex book-keeping
    - Solution vector re-ordered

Partial Pivoting is simplest and most common

Neither method guarantees stability due to large number of reccursive computations

Gauss Elimination: Effect of variable transform (variable scaling)

Example, n=2

$$\begin{bmatrix} 0.01 & -1.0 \\ 1.0 & 0.01 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 1.0 \\ 1.0 \end{Bmatrix}$$

Cramer's Rule - Exact

$$x_1 = \frac{1.0 \cdot 0.01 - 1.0 \cdot (-1.0)}{0.01 \cdot 0.01 - 1.0 \cdot (-1.0)} = 1.0099$$

$$x_2 = \frac{1.0 \cdot 0.01 - 1.0 \cdot 1.0}{0.01 \cdot 0.01 - 1.0 \cdot (-1.0)} = -0.9899$$

Variable Transformation

$$x_1 = \tilde{x}_1$$

$$x_2 = 0.01 \cdot \tilde{x}_2$$

$$\begin{bmatrix} 1.0 & -1.0 \\ 1.0 & 0.0001 \end{bmatrix} \begin{Bmatrix} \tilde{x}_1 \\ \tilde{x}_2 \end{Bmatrix} = \begin{Bmatrix} 100.0 \\ 1.0 \end{Bmatrix} \Rightarrow \begin{Bmatrix} \tilde{x}_1 = 1.01 \\ \tilde{x}_2 = -99 \end{Bmatrix}$$

2-digit Arithmetic

1% error

100% error

$$m_{21} = 1.0$$

$$a_{21}^{(2)} = 0$$

$$a_{22}^{(2)} = 0.0001 + 1.0 \simeq 1.0$$

$$b_2^{(2)} = 1 - 100 \simeq -100$$

$$\tilde{x}_2 = \boxed{-100}$$

$$\tilde{x}_1 = 100 - 100 = \boxed{0}$$

Systems of Linear Equations
Gauss Elimination

How to Ensure Numerical Stability

- System of equations must be well conditioned
  - Investigate condition number
    - Tricky, because it can require matrix inversion
  - Consistent with physics
    - E.g. don't couple domains that are physically uncoupled
  - Consistent units
    - E.g. don't mix meter and μm in unknowns
  - Dimensionless unknowns
    - Normalize all unknowns consistently
- Equilibration and Partial Pivoting, or Full Pivoting

2.29 Numerical Fluid Mechanics

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