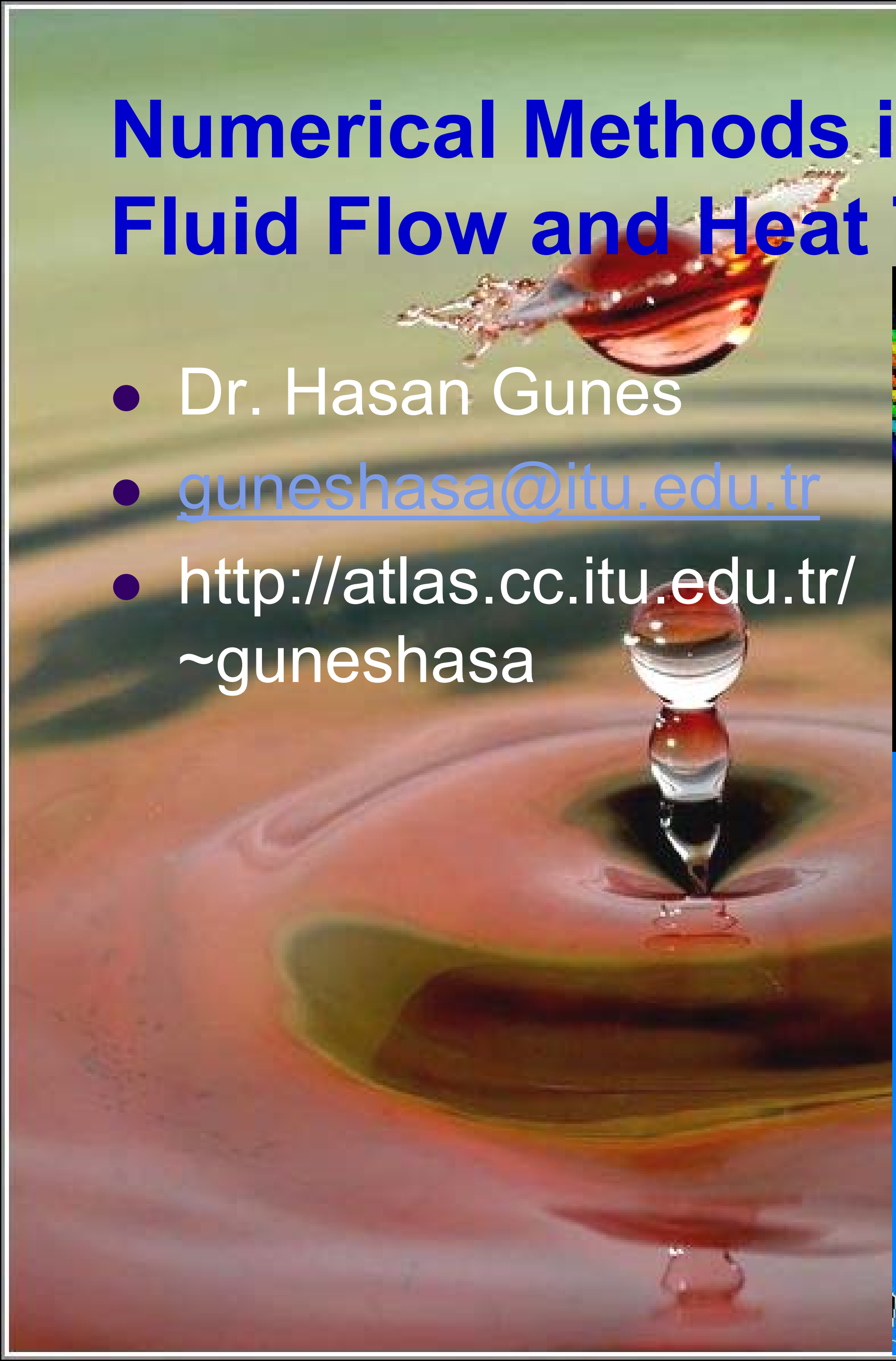
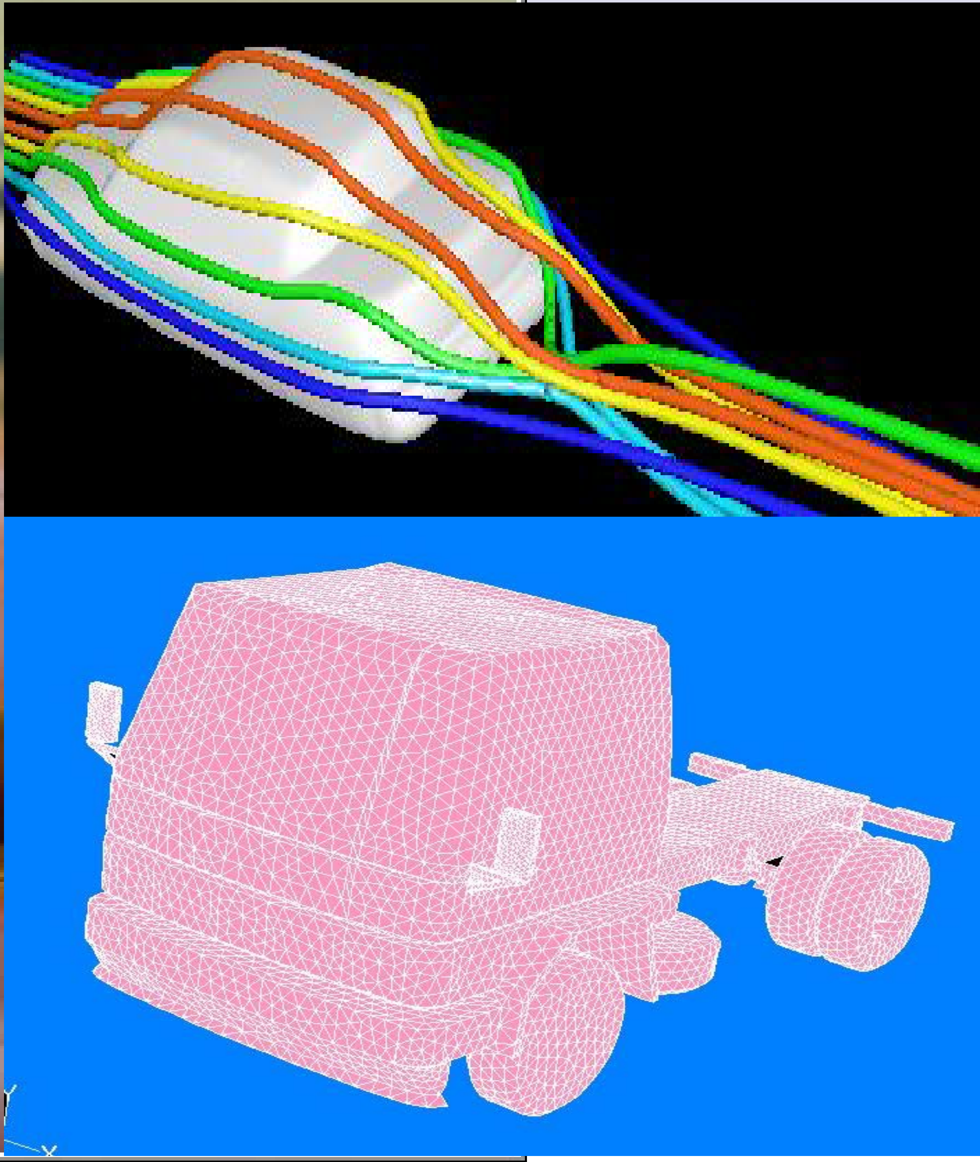
Numerical Methods in Fluid Flow and Heat Transfer



- Dr. Hasan Gunes
- guneshasa@itu.edu.tr
- http://atlas.cc.itu.edu.tr/~guneshasa



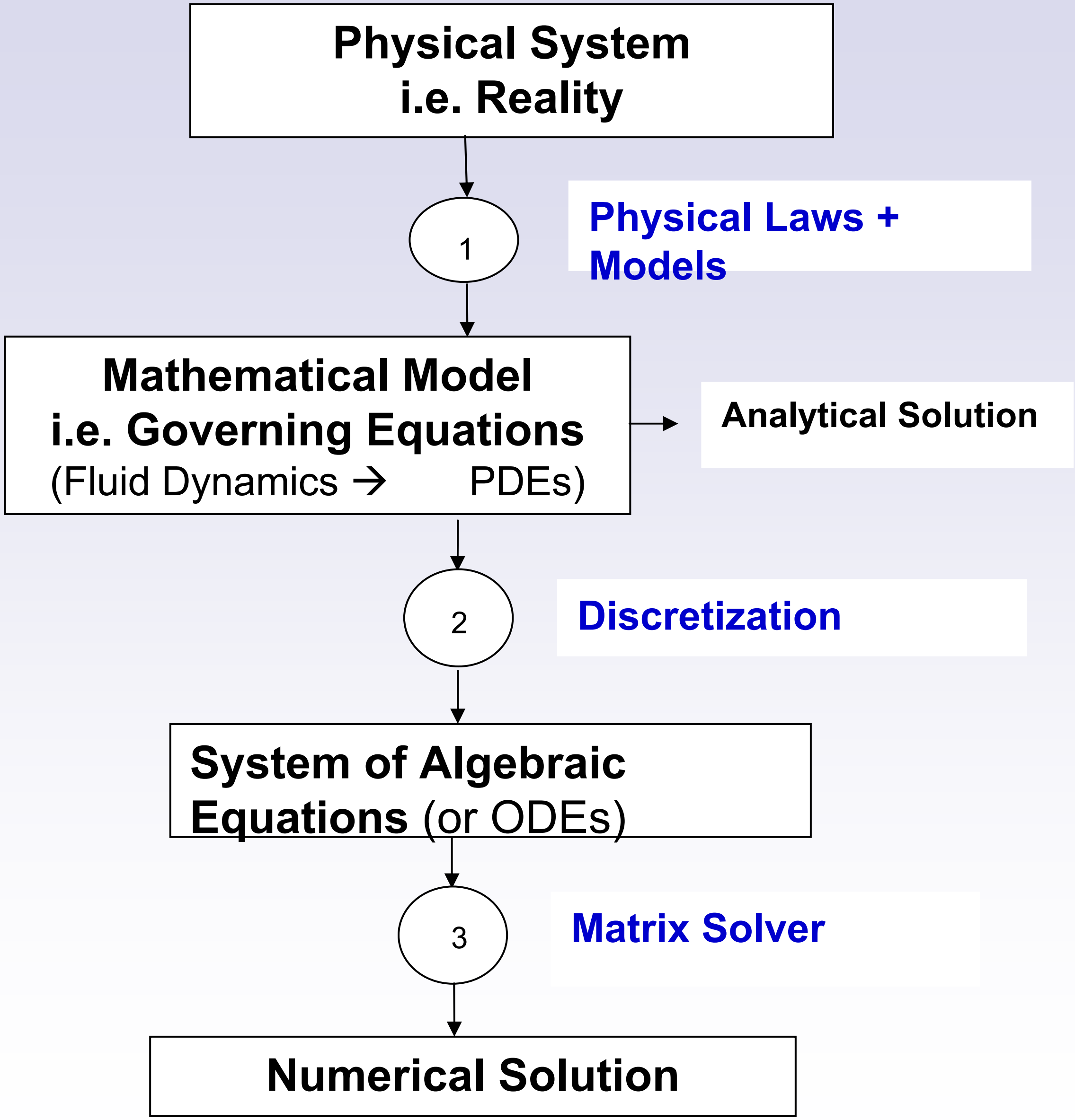
INTRODUCTION

The Scientific Method and Mathematical Modeling

The mathematical formulation of the problem is the reduction of the physical problem to a set of either algebraic or differential equations subject to certain assumptions.

The process of modeling of physical systems in the real world should generally follow the path illustrated schematically in the chart below:

Numerical Solution Procedure



Physical System
i.e. Reality

1

Physical Laws + Models

Mathematical Model
i.e. Governing Equations
(Fluid Dynamics → PDEs)

Analytical Solution

2

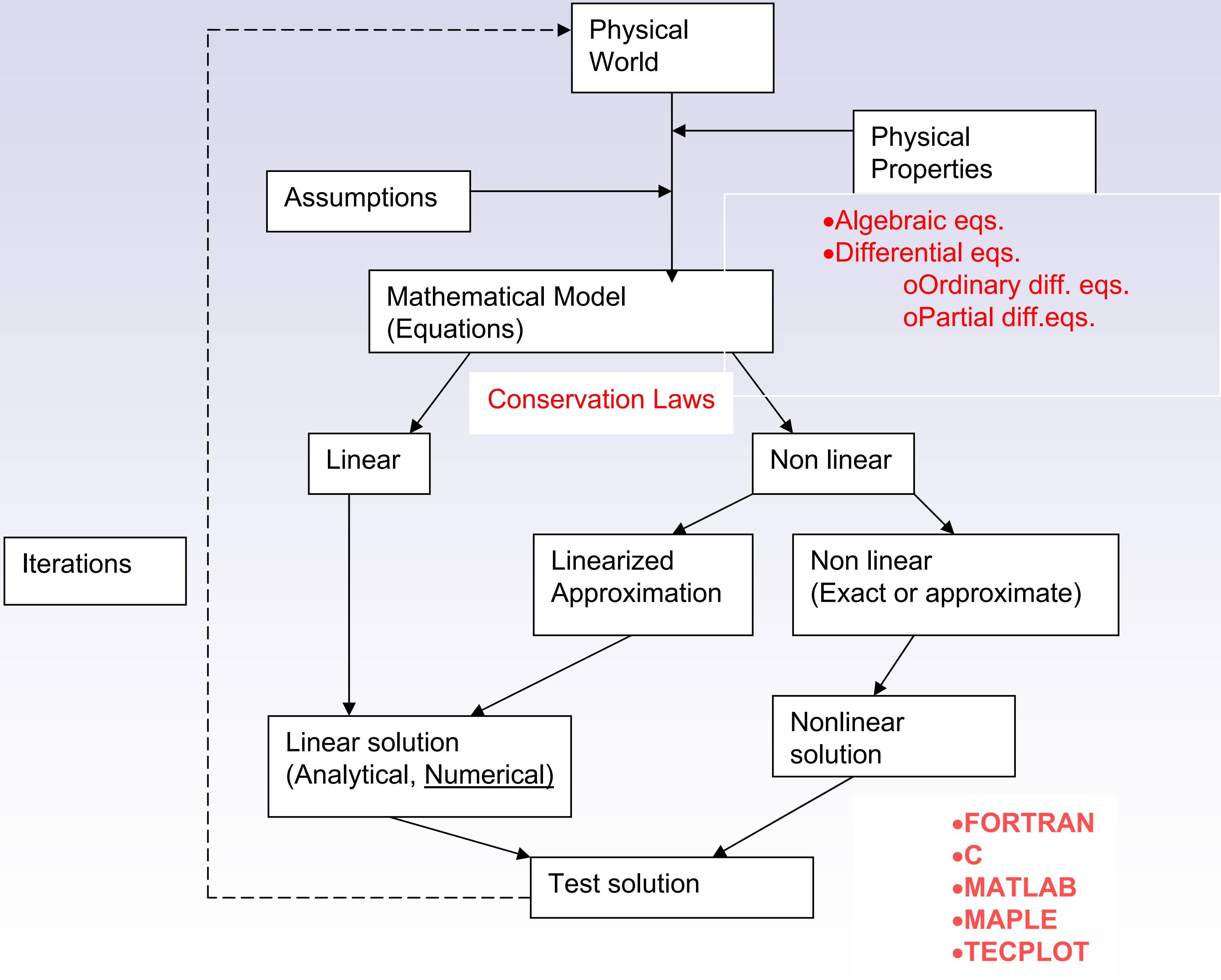
Discretization

System of Algebraic Equations (or ODEs)

3

Matrix Solver

Numerical Solution



Physical World

Physical Properties

Assumptions

Mathematical Model (Equations)

- Algebraic eqs.
- Differential eqs.
  - Ordinary diff. eqs.
  - Partial diff.eqs.

Conservation Laws

Linear

Non linear

Iterations

Linearized Approximation

Non linear (Exact or approximate)

Linear solution (Analytical, Numerical)

Nonlinear solution

Test solution

- **FORTRAN**
- **C**
- **MATLAB**
- **MAPLE**
- **TECPLOT**

Solution Approaches

Three approaches or methods are used to solve a problem in fluid mechanics & heat transfer

1. <u>Experimental methods</u>: capable of being most realistic, experiment required, scaling problems, measurement difficulties, operating costs.
2. <u>Theoretical (analytical) methods</u>: clean, general information in formula form, usually restricted to simple geometry &physics, usually restricted to linear problems.
3. <u>Numerical (CFD) (computational) methods (Simulation)</u>:

- No restriction to linearity
- Complicated physics can be treated
- Time evolution of flow
- Large Re flow

<u>Disadvantages:</u>

- Truncation errors
- Boundary condition problems
- Computer costs
- Need mathematical model for certain complex phenomena

Simulation: The Third Pillar of Science

- Traditional scientific and engineering paradigm:
  1) Do theory or paper design.
  2) Perform experiments or build system.
- Limitations:
  - Too difficult -- build large wind tunnels.
  - Too expensive -- build a throw-away passenger jet.
  - Too slow -- wait for climate or galactic evolution.
  - Too dangerous -- weapons, drug design, climate experimentation.
- Computational science paradigm:
  3) Use high performance computer systems to simulate the phenomenon
     - Base on known physical laws and efficient numerical methods.

Some Particularly Challenging Computations

- Science
  - Global climate modeling
  - Astrophysical modeling
  - Biology: Genome analysis; protein folding (drug design)
- Engineering
  - Crash simulation
  - Semiconductor design
  - Earthquake and structural modeling
- Business
  - Financial and economic modeling
  - Transaction processing, web services and search engines
- Defense
  - Nuclear weapons -- test by simulations
  - Cryptography

Economic Impact of HPC

- Airlines:
  - System-wide logistics optimization systems on parallel systems.
  - Savings: approx. $100 million per airline per year.
- Automotive design:
  - Major automotive companies use large systems (500+ CPUs) for:
    - **CAD-CAM, crash testing, structural integrity and aerodynamics.**
    - **One company has 500+ CPU parallel system.**
- Semiconductor industry:
  - Semiconductor firms use large systems (500+ CPUs) for
    - **device electronics simulation and logic validation**
  - A lot of Savings!!

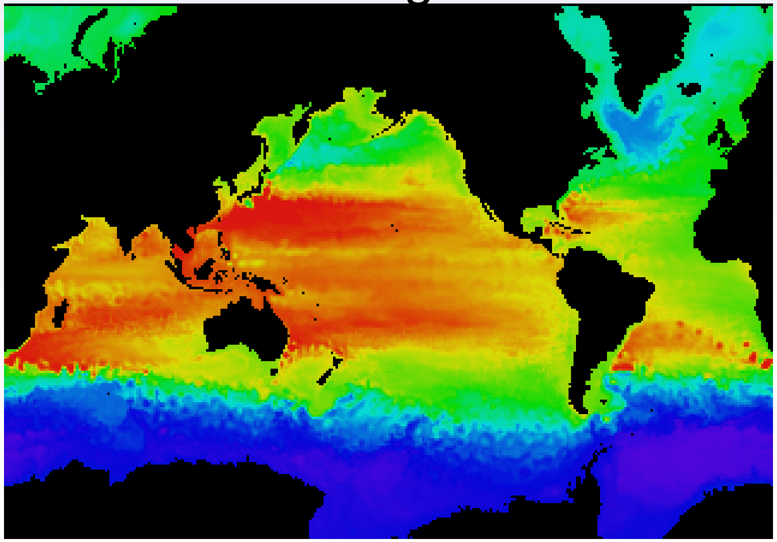
Global Climate Modeling Problem

- Problem is to compute:

  f(latitude, longitude, elevation, time) → temperature, pressure, humidity, wind velocity

- Approach:
  - Discretize the domain, e.g., a measurement point every 1km
  - Devise an algorithm to predict weather at time t+1 given t

- Uses:
  - Predict major events, e.g., Katrina
  - investigate climate change



sea surface temperature output from an eddy resolving ocean model

Source: http://www.epm.ornl.gov/chammp/chammp.html

Global Climate Modeling Computation

- One piece is modeling the fluid flow in the atmosphere
  - Solve Navier-Stokes problem
    - Roughly 100 Flops per grid point with 1 minute timestep
- Computational requirements:
  - To match real-time, need 5x 10^{11} flops in 60 seconds = 8 Gflop/s
  - Weather prediction (7 days in 24 hours) → 56 Gflop/s
  - Climate prediction (50 years in 30 days) → 4.8 Tflop/s
  - To use in policy negotiations (50 years in 12 hours) → 288 Tflop/s
- To double the grid resolution, computation is at least 8x

- Current models are coarser than this
  - ***flops**: **fl**oating-point **op**erations per **s**econd*

Heart Simulation

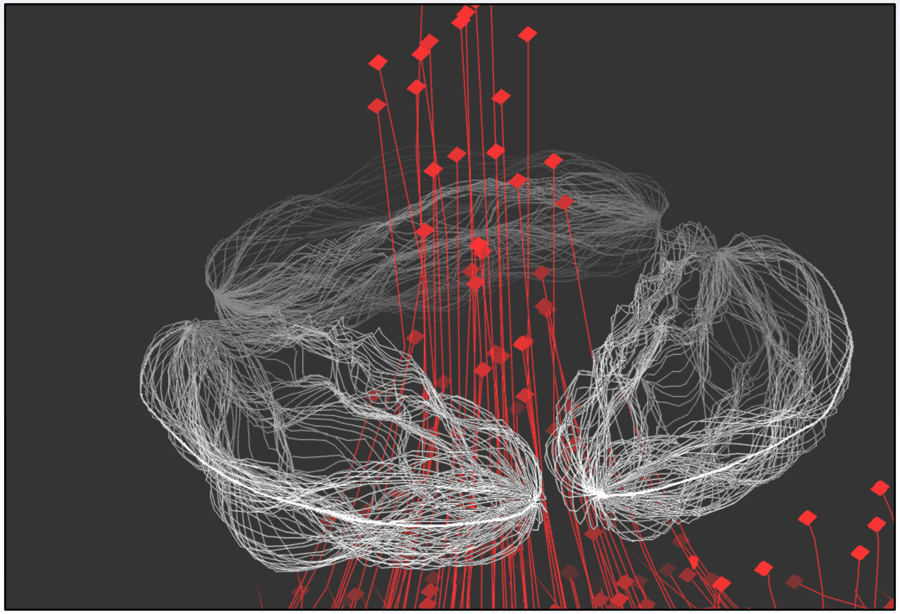
- Problem is to compute blood flow in the heart
- Approach:
  - Modeled as an elastic structure in an incompressible fluid.
    - The “immersed boundary method” due to Peskin and McQueen.
    - 20 years of development in model
    - Many applications other than the heart: blood clotting, inner ear, paper making, embryo growth, and others
- Uses
  - Current model can be used to design artificial heart valves
  - Can help in understand effects of disease (leaky valves)
  - Related projects look at the behavior of the heart during a heart attack
  - Ultimately: real-time clinical work

Heart Simulation Calculation

The involves solving Navier-Stokes equations

- Done on a Cray C90 -- 100x faster and 100x more memory
- Until recently, limited to vector machines

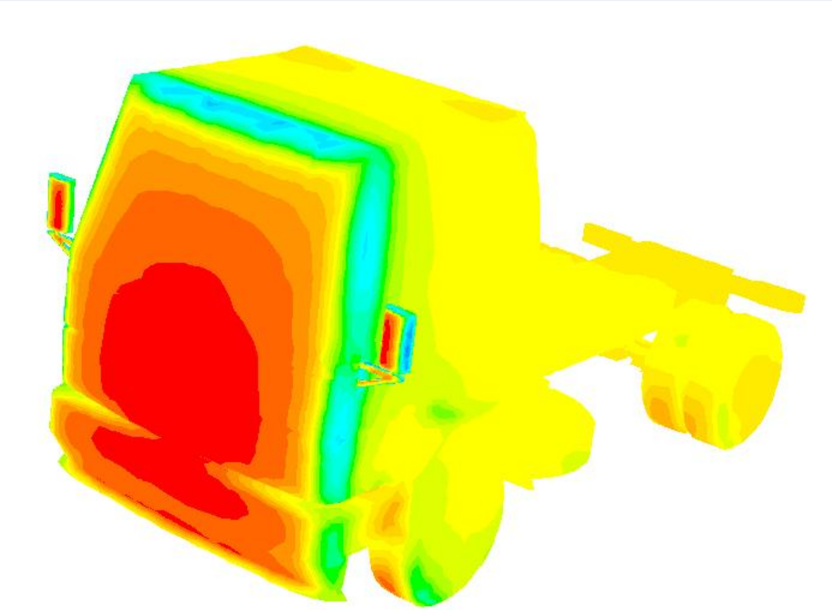
- Needs more features:
    - Electrical model of the heart, and details of muscles, E.g.,
        - Chris Johnson
        - Andrew McCulloch
    - Lungs, circulatory systems

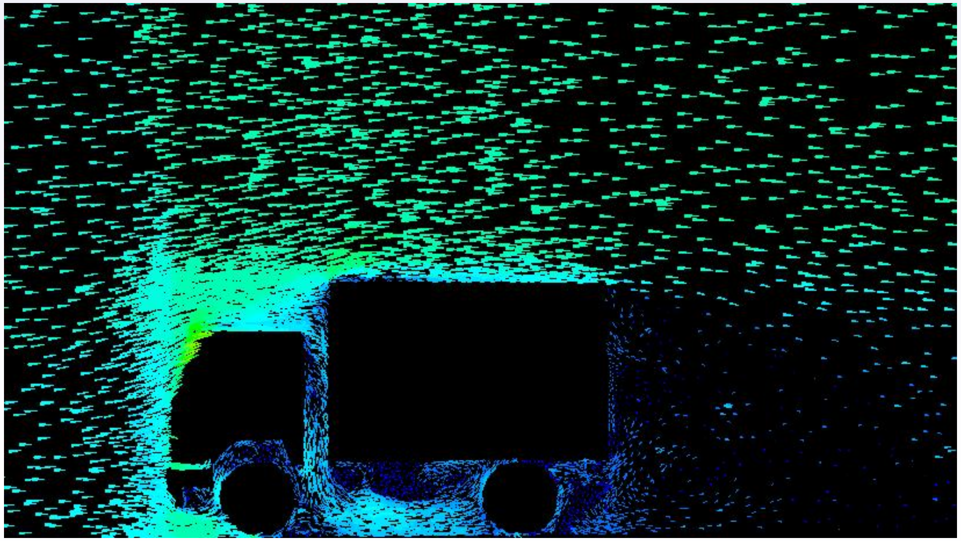


Vehicle Aerodynamics

Flow around a moving truck in a wind tunnel.

- Need to fix the model & blow air at it.
- Floor also has to move at the air speed a difficult task.

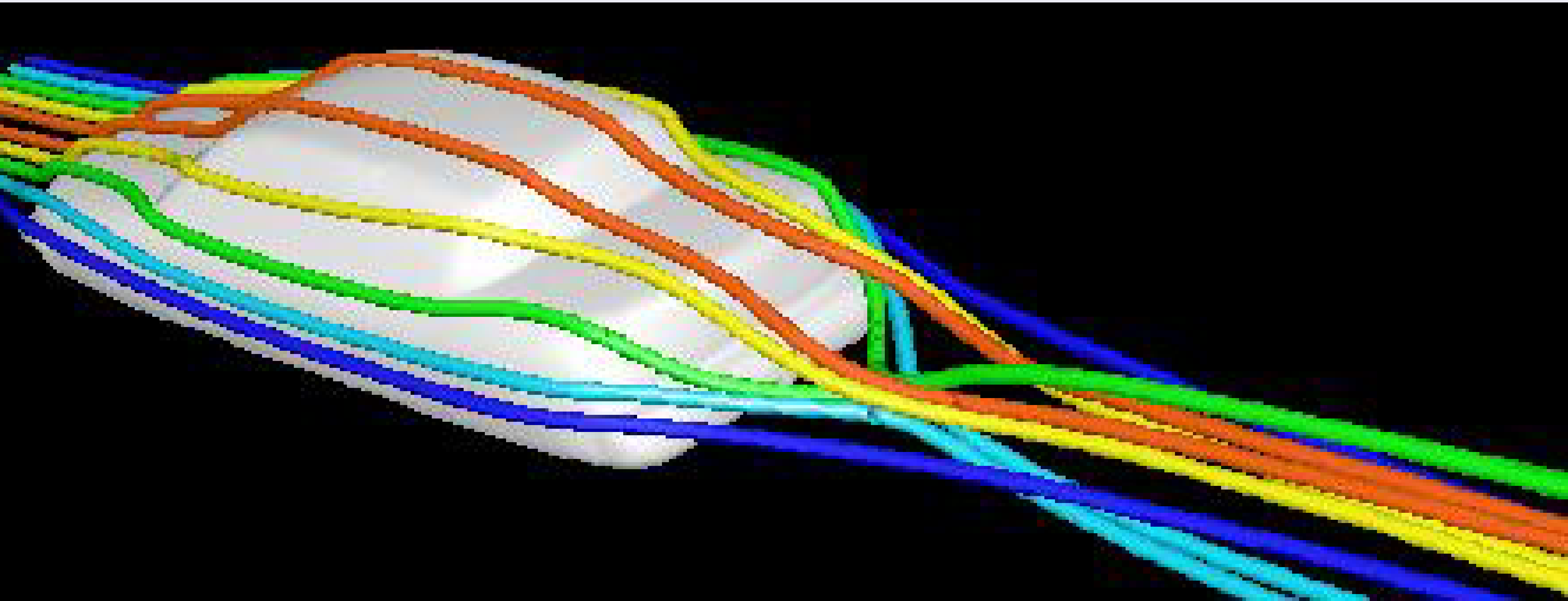




Vehicle Aerodynamics

Flow around a moving car in a wind tunnel.

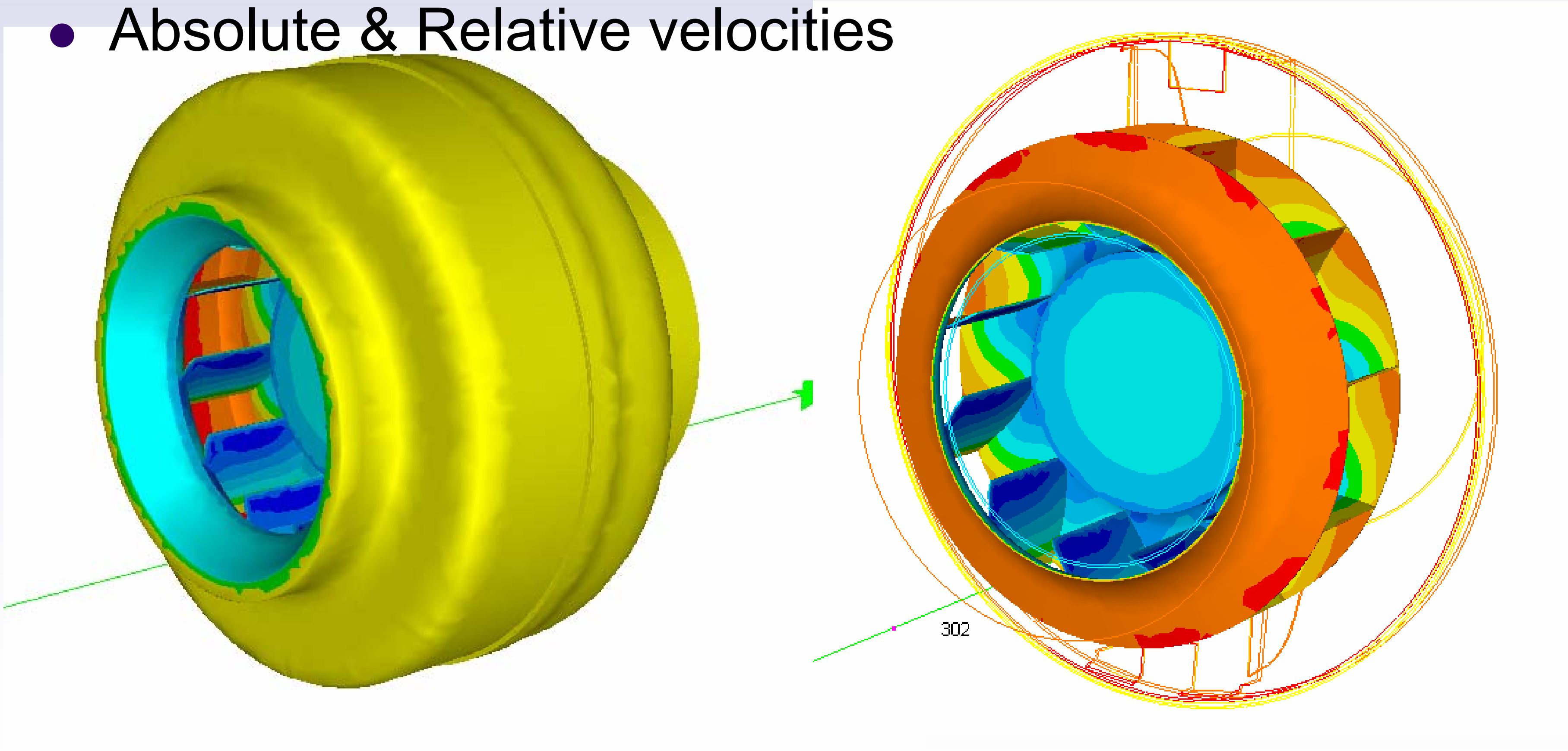
- Drag coefficient, lift coefficient, moment coefficient
- Pathlines/streamlines/streaklines



Turbomachinery analysis

Flow in an inline duct fan

- Need to consider rotating fluid zone.
- Absolute & Relative velocities



CFD: obtain approximate solutions to complex problems numerically.

Need to use a discretization method which approximates the differential equations by a system for algebraic equations, which can then be solved on a computer.

Accuracy of numerical solutions ⟺ quality of discretization

Components of a numerical solution method

1. <u>Mathematical Model:</u>
   Set of PDEs or integro-differantial eqs. and the corresponding boundary conditions.

2. <u>Discretization Method:</u>

- Finite difference
- Finite volume
- Finite element
- Spectral (element) methods
- Boundary element

PDE’s (continuous) → discrete equations (FDE's)

3. Coordinate &Basic Vector System

4. Numerical Grid: grid generation

- Structured (regular) grid
- Block structured grid
- Unstructured grid

Discrete locations at which the variables are to be calculated are defined by
the numerical grid, or mesh.

5. Finite Approximations: approx. used in discretization process is selected

e.g. Finite difference: approximations for the derivatives at the grid points need to be selected

The choice influences:

- Accuracy of approximation
- Developing the solution method
- Coding, debugging, speed of code

Compromise between simplicity easy of implementation,accuracy and computational efficiency has to be made

  - Second order methods in general are used.

6. Solution Method

Discretization yields a large system of linear/non-linear algebraic equations.

Linear equations → Algebraic equation solvers

Non-linear equations → iteration scheme used

i.e. linearize the equations & resulting linear systems are solved by iterative techniques.

Unsteady flows: methods based on marching in time

Steady flows: usually by pseudo-time-marching or equivalent iteration scheme

7. Convergence criteria (for iterative procedures)

Need to set convergence for the iterative method.

Accuracy & efficiency is important

Absolute convergence: $\left| a - a^{*} \right| < \varepsilon(tolerance)$

Relative convergence: $\left| \dfrac{a - a^{*}}{a} \right| < \varepsilon$

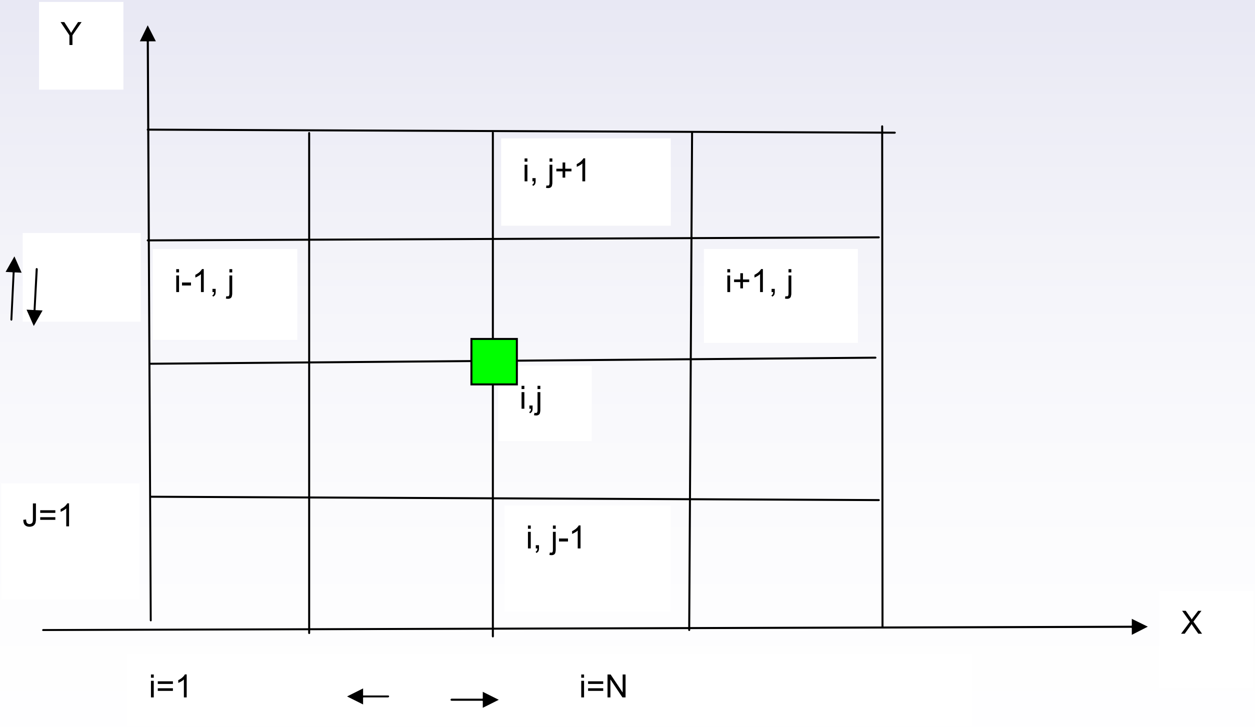
FINITE DIFFERENCE METHODS

Definitions & Remarks

Derivatives in a given PDE are approximated by finite difference relations (using Taylor series expansions)

Resulting approximate eqs. which represent the original PDE, is called a *Finite Difference Equation*. (FDE)

STENCIL



FDE ⇨ algebraic eq. (written for each grid point within the domain)

Objectives:

- study the various schemes to approximate the PDE s by FDE
- explore numerical techniques for solving resulting FDE

Additional Terminology:

1. **Consistency**: a finite dif. approx. of PDE is consistent if the FDE approaches the PDE as the grid size approaches zero.

2. **Stability:** a numerical scheme is said to be stable if any error introduced in the FDE does not grow with the solution of the finite difference equations.

Von Neumann's method: without boundary conditions (BCs)

Conditional stability on some schemes

Time step be smaller than a certain limit.

Under-relaxation needs to be used

i. Temporal problems: stability guaranties that method produces a bounded solution

ii. Iterative methods: stable method does not diverge

It is difficult to do the stability analysis when BCs & non-linearities are present

3. **Convergence:** a finite difference scheme is convergent if the *solution* of the FDE approaches that of the PDE as the grid size approaches zero

4. **Lax's equivalent theorem**: for a FDE which approximates a well-posed, linear initial value problem, the necessary & sufficient condition for convergence is that the FDE must be stable and consistent.

For linear problems which are strongly influenced by BCs.
Stability & convergence of a method are difficult to demonstrate
Thus, we check via numerical experiments (grid refinement)
Grid-independent solutions

Boundedness
Realizability

Accuracy:
Numerical solutions of fluid flow & heat transfer problems are only *approximate* solutions. Involve some kind of error.

Numerical solutions include three kind of errors:
Modeling Errors: difference between actual flow & exact solution of mathematical model
N-S eqs. Represent accurate model of a laminar flow.
Problem with turbulent flows, two-phase flows, combustion etc. simplifying geometry BCs.

Discretization Errors: difference between exact solutions of conservations eqs. & exact solution of algebraic system of eqs. Obtained by discretizing these eqs.(truncation error)

Iteration Errors: difference between the iterative & exact solutions of the algebraic eqs. (round-off error)

THE CONSERVATIVE (DIVERGENT) FORM OF A PDE

PDEs normally represent a physical conservation statement.

Definition:

Coefficients of the derivatives are either constant or if variable, their derivatives do not appear anywhere in the equation. i.e. divergence of physical quantity can be identified in the equation

Example 1: Conservative form of a continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \vec{V} \right) = 0$$

or in Cartesian coordinate system

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0$$

Non conservative form of continuity eq.

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

Example 2: 1-D heat conduction

$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right)$$ Conservative form

$$\rho c \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2} + \frac{\partial k}{\partial x} \frac{\partial T}{\partial x}$$ Non-conservative form

A difference formulation based on a PDE in non-conservative form may lead to numerical difficulties in situations where the coefficients may be discontinuous as in flows containing shock waves.

Dimensionless Equations

$$T = \frac{tV_\infty}{L} \qquad x, y = \left(\frac{x, y}{L}\right) \qquad (u, v) = \left(\frac{u, v}{V_\infty}\right) \qquad P = \frac{p}{\rho_\infty V_\infty^2}$$

L: characteristic length ρ_∞, V_∞ : reference density, velocity

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

$$\frac{\partial V}{\partial t} + (\vec{V} \cdot \nabla)\vec{V} = -\nabla P + \frac{1}{\mathrm{Re}} \nabla^2 \vec{V}$$

Non-conservative form

$$\mathrm{Re} = \frac{\rho_\infty V_\infty L}{\mu_\infty}$$

body force is neglected (Fr if not)

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

$$\frac{\partial V}{\partial t} + (\vec{V} \cdot \nabla)\vec{V} = -\nabla P + \frac{1}{\mathrm{Re}} \nabla^2 \vec{V}$$

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}(u^2 + p) + \frac{\partial}{\partial y}(uv) = \frac{1}{\mathrm{Re}}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)$$

$$\frac{\partial v}{\partial t} + \frac{\partial}{\partial x}(uv) + \frac{\partial}{\partial y}(v^2 + p) = \frac{1}{\mathrm{Re}}\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right)$$

Conservative form

Exercise: Prove that conservative & non-conservative form of NS eqs. are equal to each other.

Important in numerical solution algorithms

1) Primitive-variable solutions, u, v, p

2) Vorticity-Stream Function Formulations, Ω, ψ

2-D $\rho =$ constant

$$\vec{\Omega} = \nabla x \vec{V}$$

$$u = \frac{\partial \Psi}{\partial y}$$

$$v = -\frac{\partial \Psi}{\partial x}$$

CLASSIFICATION OF DIFFERENTIAL EQUATIONS

O.D.E
One independent variable

$$\frac{dy}{dx} = f(x, y)$$

$$y = y(x)$$

P.D.E
More then one independent variable

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

$$u = u(x, y)$$

O.D.E : I.V.P: conditions are specified at one point
B.V.P: conditions are specified at more then one point

e.g. $y'' + \sin t y = \cos t$

$$y(0) = 0 \qquad y'(0) = 0 \Rightarrow IVP$$

$$y(0) = 0 \qquad y(1) = 2 \Rightarrow BVP$$

Solution *procedure* differs between IVP & BVP
Which types of physical phenomena lead to ODEs and PDEs?

Question:
Modeling Concepts:

A. Particle viewpoint: systems described by single particle which moves in space without undergoing any physical changes in position.
e.g. free falling of a solid sphere

- Position of each particle identified solely as a function of time.

In fluid mechanics: Lagrangian description of motion.

ODE of the initial value type is the mathematical description of physical laws formulated by the particle viewpoint.

B. Field Viewpoint:

- Plays a dominant role in fluid mechanics, heat transfer, thermo, optics, and electromagnetism.

- Physical system is regarded as a continuum , i.e., we abandon the notion of large number of individual elementary particles.

CONTINIUM ASSUMPTION

Eulerian description of motion.

- Field quantity is assumed to have a well-defined value at each point in space.
- In general each field quantity can depend on x, y, z, t (4 independent variables).

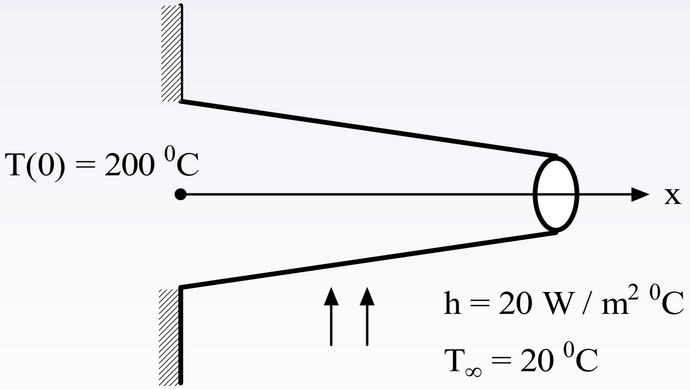
$$\vec{V} = \vec{V}(x, y, z, t) \qquad T = T(x, y, z, t) \qquad P = P(x, y, z, t)$$

Natural mathematical language $\Rightarrow$ PDEs.

C. A third viewpoint:

ODEs often occur in situations which have nothing to do with particles.

Example: Steady state temperature distribution in a fin.



$$P(x) = \frac{1}{A_c} \cdot A'_c(x) \qquad R(x) = -\frac{h}{k} \cdot \frac{A'_s}{A_c}$$

$$\frac{d^2\theta}{dx^2} + P(x)\frac{d\theta}{dx} + R(x)\theta(x) = 0$$

$$T(0) = T_w \quad \theta = T - T_\infty$$

$$T(L) = T_t$$

ODE of the boundary value type is obtained by neglecting the influence of all but one of the independent variables.

ORDINARY DIFFERENTIAL EQUATIONS

A. Initial Value Problems

First order ODE

$$\frac{dy}{dx} = \underbrace{f(x,y)}_{\substack{\text{family of}\\ \text{solutions}}} \Rightarrow \Phi\left(x,y,y'\right) = 0$$

General form

Chose one solution using the initial condition $y(x_0) = y_0$

Exact Solutions

1. Linear equations

$$\frac{dy}{dx} = p(x)y + q(x)$$

$$\int p(x)dx \left\} \begin{array}{l} \text{Evaluated analytically, analytic problems} \\ \text{Not analytically evaluated, not analytic problems (need numerical solution)} \end{array} \right.$$

General Solution is in the form

$$y(x) = e^{\int p(x)dx} \int q(x) e^{-\int pdx} dx + ce^{\int pdx}$$

2. Separable Eqs.

$$\frac{dy}{dx} = F(x)G(y) \qquad \frac{dy}{dx} = xy$$

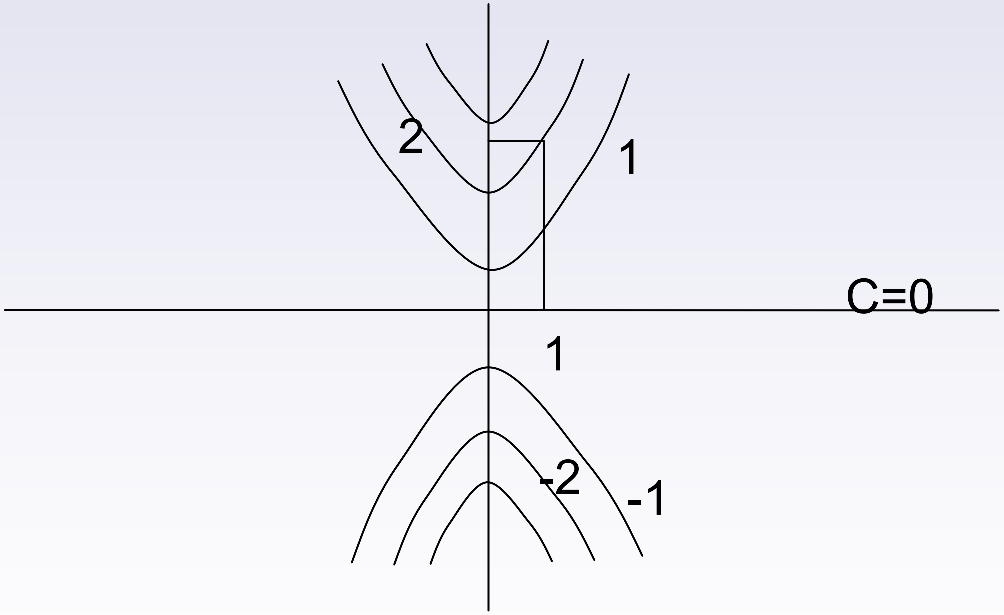
$$\int \frac{dy}{y} = \int x dx \Rightarrow \ln y = \frac{x^2}{2} + c_1$$

$$y(1) = 2$$

$$y = 2e^{\left(x^2+1\right)/2}$$

$$c = \frac{2}{\sqrt{e}}$$

$$y = ce^{x^2/2}$$



3. Exact

$$\frac{dy}{dx} = \frac{M(x,y)}{N(x,y)} \qquad \frac{\partial N}{\partial x} \overset{?}{=} -\frac{\partial M}{\partial y}$$

4. Homogeneous

$$\frac{dy}{dx} = f(x/y) \qquad \frac{y}{x} = p \Rightarrow \frac{dy}{dx} = p + x\frac{dp}{dx}$$

$$p + x\frac{dp}{dx} = f(p) \Rightarrow \int \frac{dp}{f(p) - p} = \int \frac{dx}{x}$$

In general numerical methods are needed for solution

Nth order ODE:

$$a_n y^{(n)} + a_{n-1} y^{(n-1)} + \ldots\ldots\ldots\ldots + a_1 y' + a_0 y = F(t)$$

$$y^{(n)} = \frac{d^n y}{dt^n}, \ldots. \quad \text{or} \quad \frac{d^n y}{dt^n} = f(t, y, \frac{dy}{dt}, \ldots\ldots., \frac{d^{n-1} y}{dt^{n-1}})$$

Theorem: An nth order ODE can be represented as a system of **n first order** ODEs.

Let us define new variables $y_1, y_2, y_3, \ldots\ldots, y_{n+1}$

$$y_1 = t, \quad y_2 = y, \quad y_3 = y', \quad y_4 = y'', \ldots\ldots\ldots, \quad y_n = y^{(n-2)}, \quad y_{n+1} = y^{(n-1)}$$

$$y_1' = 1$$

……….

$$y_2' = y_3 \qquad y_n' = y_{n+1}$$

……….

$$y_3' = y_4 \qquad y'_{n+1} = f(y_1, y_2, y_3, \ldots\ldots y_{n+1})$$

.

.

<u>I.C.s</u> $y_2 = (t_0)$, …, $y_{n+1} = (t_0)$ all specified

<u>In vector relation,</u>

$$\underset{\rightarrow}{Y}' = \underset{\rightarrow}{F}(\underset{\rightarrow}{Y}) \quad \underset{\rightarrow}{Y}(t_0) = y_i$$

$$\underset{\rightarrow}{Y} = (y_1, y_2, \ldots\ldots\ldots, y_{n+1})^T, \quad \underset{\rightarrow}{Y}' = (y'_1, y'_2, \ldots\ldots\ldots, y'_{n+1})^T,$$

$\underset{\rightarrow}{F} = (1, y_3, y_4, \ldots\ldots\ldots, y_{n+1}, f)^T$ T: Transpose.

Eg: $y'' + b(t)y' + c(t)y = d(t) \qquad y' = \frac{dy}{dt} \qquad y(t_0) = y_0 \qquad y'(t_0) = y_1$

Initial Var.	**New Variable**	**Initial Value**	**Dif.Eq.**
y	z_1	y_0	$\frac{dz_1}{dt} = z_2$
y’	z_2	y_1	$\frac{dz_2}{dt} = d(z_3) - d(z_3)z_2 - c(z_3)z_1$
t	z_3	t_0	$\frac{dz_3}{dt} = 1$

$$\frac{dz_3}{dt} = 1$$

$$\frac{dz_1}{dt} = z_2$$

$$\frac{dz_2}{dt} = d(z_3) - d(z_3)z_2 - c(z_3)z_1$$

$$\frac{d\underset{\to}{z}}{dt} = \underset{\to}{f}(\underset{\to}{z})$$

$$\underset{\to}{f} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix} = \begin{bmatrix} z_2 \\ d(z_3) - c(z_3)z_1 - b(z_3)z_2 \\ 1 \end{bmatrix}$$

$$\underset{\to}{z}(t_0) = \begin{bmatrix} y_0 \\ y_1 \\ t_0 \end{bmatrix}$$

Example 2 $x''' = \cos x + \sin x' - e^{x''} + t^2$

$$x(0) = 3$$

$$x'(0) = 7$$

$$x''(0) = 13$$

Old variables	New variables	Initial value	Diff. eq.
t	x_1	0	$x'_1=1$
x	x_2	3	$x'_2=x_3$
x’	x_3	7	$x'_3=x_4$
x’’	x_4	13	$x'_4=\cos x_2+\sin x_3-e^{x4}+x_1^2$

So, corresponding first order system is:

$$\underset{\rightarrow}{x}' = \begin{bmatrix} x_1' \\ x_2' \\ x_3' \\ x_4' \end{bmatrix}, \qquad \underset{\rightarrow}{F} = \begin{bmatrix} 1 \\ x_3 \\ x_4 \\ \cos x_2 + \sin x_3 - e^{x_4} + x_1 \end{bmatrix} \qquad x(0) = \begin{bmatrix} 0 \\ 3 \\ 7 \\ 13 \end{bmatrix}$$

at x_1=0, t=0

Example 3 .

$$x'' = x - y - (3x')^2 + (y')^3 + 6y'' + 2t$$

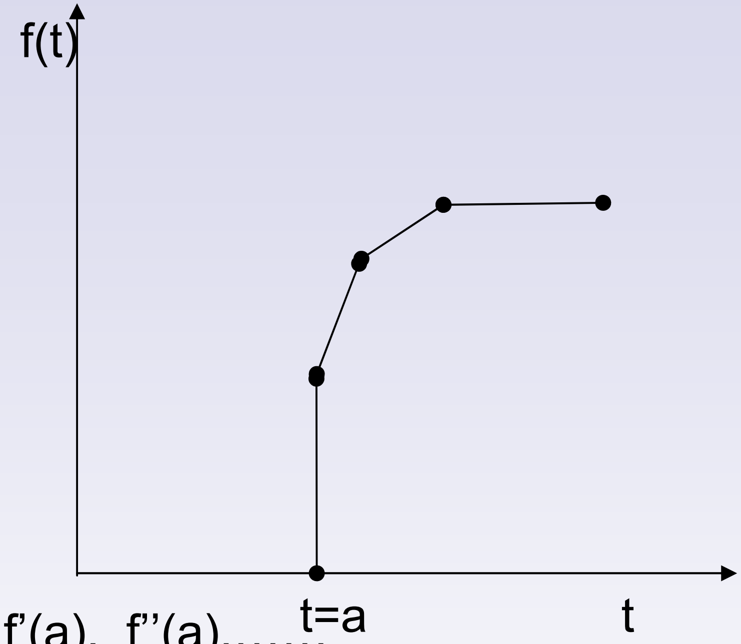
$$y''' = y'' - x' + e^x - t$$

$x(1)=2$, $x'(1)=-4$, $y(1)=-2$, $y'(1)=7$, $y''(1)=6$

Old variables	New variables	Initial value	Diff. eq.
t x x' y y' y''	x_1 x_2 x_3 x_4 x_5 x_6	1 2 -4 -2 7 6	$x'_1=1$ $x'_2=x_3$ $x'_3=x_2-x_4-9x_3^2+x_5^3+6x_6+2x_1$ $x'_4=x_5$ $x'_5=x_6$ $x'_6=x_6-x_3+e^{x2}-x_1$

$$\underset{\rightarrow}{x}(1) = \left[1, \quad 2, \quad -4, -2, \quad 7, \quad 6\right]^T$$

REVIEW OF TAYLOR --DERIVATION



f(a), f’(a), f’’(a),…….

$f(t)=a_0+a_1(t-a)+a_2(t-a)2+\dots\dots\dots+a_n(t-a)n+\dots\dots.$

$a_0=f(a)$
$a_1=f'(a)$

$f'(t)=a_1+2a_2(t-a)+3a_3(t-a)2+\dots\dots\dots+na_n(t-a)n-$
$1+\dots\dots.$

$a_2=(1/2)f''(a)$
$a_3=(1/2*3)f'''(a)$

$f''(t)=2a_2+2*3a_3(t-a)+\dots\dots\dots+n*(n-1)a_n(t-a)n-2+\dots\dots.$

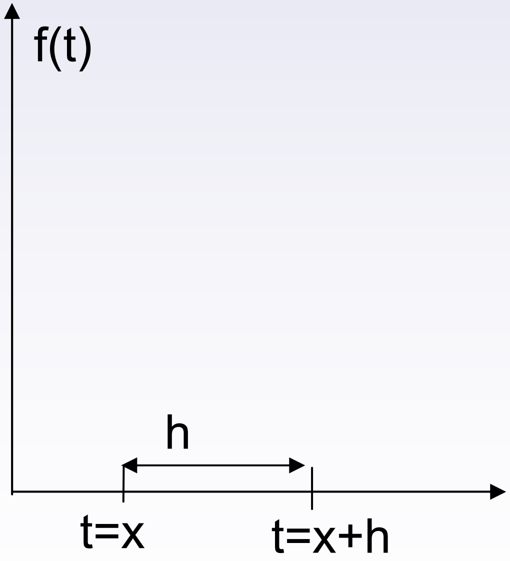
$a_i=f(i)(a)/i!$

Taylor series expansion of f(t) about the point t=a. $f(t) = \sum_{n=0}^{N} \frac{f^{(n)}(a)}{n!}(t-a)^n + E$

For a=0 the series is called **MacLaurin** series.

Truncation: $f(t) = \sum_{n=0}^{N} \frac{f^{(n)}(a)}{n!}(t-a)^n + E$ E: Truncation Error

$$E = \frac{f^{(N+1)}(\xi)}{(N+1)!}(t-a)^{N+1} \qquad a \le \xi \le t$$



$$f(x+h) = \sum_{n=0}^{N} \frac{f^{(n)}(x)}{n!} h^n + E$$

$$E = \frac{f^{(N+1)}(\xi)}{(N+1)!} h^{N+1}$$

$$x \le \xi \le x+h$$

Example: Develop the Taylor series for **Sin (x)** about the point $x = \frac{\pi}{2}$

f(x)=Sin x , f'(x)=Cos x , f''(x)=-Sin x , f'''(x)=-Cos x , fIV(x)=Sin x

$$f(\frac{\pi}{2}) = 1, \ldots\ldots.$$

$$\sin x = 1 - \frac{1}{2!}(x - \pi/_2)^2 + \frac{1}{4!}(x - \pi/_2)^4 - \ldots\ldots\ldots$$

$$f^{(2k+1)}(\pi/_2) = 0 \quad f^{(2k)}(\pi/_2) = (-1)^k \qquad x - \frac{\pi}{2} = h$$

$$\sin(\frac{\pi}{2} + h) = \sum_{k=0}^{N} \frac{(-1)^k}{2k!}(x - \pi/_2)^{2k} + E \qquad \sin x = \sum_{k=0}^{N} \frac{(-1)^k}{2k!}(x - \pi/_2)^{2k} + E$$

Estimate the error for h=10^{-2} $\sum_{k=0}^{1} \frac{(-1)^k}{2k!} h^{2k}$

$$\sin(\frac{\pi}{2} + 0.01) = 1 - \frac{1}{2}10^{-4} = 0.99995$$

$$E\Big| \le \frac{10^{-6}}{3!}$$

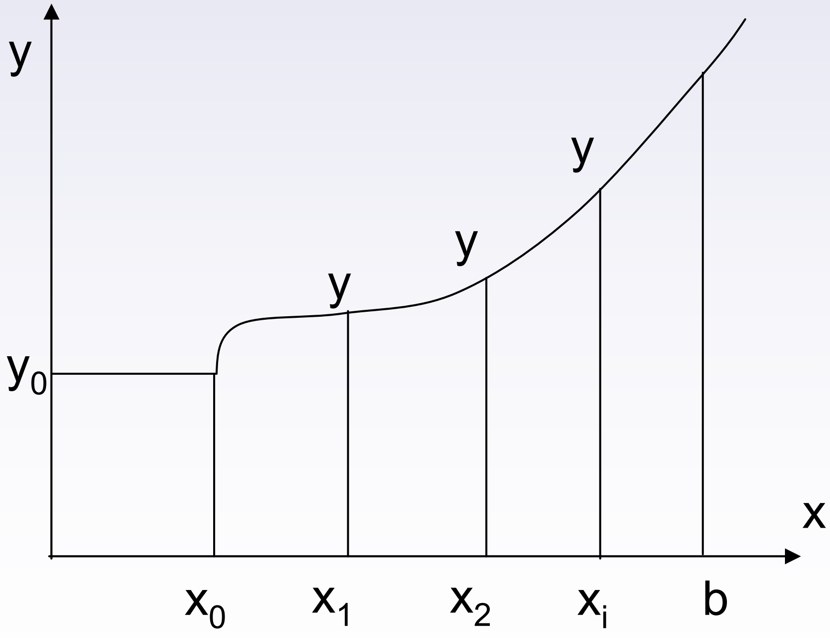
Taylor error formula $E\Big| = \frac{(10^{-2})^3}{3!}\cos\xi$ $\frac{\pi}{2} < \xi < \frac{\pi}{2} + 0.01$ bound-on error

Numerical Solution of ODEs of the Initial Value Type

Taylor's Method:

$$\frac{dy}{dx} = f(x,y) \qquad y(x_0) = y_0 \qquad y(x_0+h) = ?$$

Difference methods or discrete variable methods
Continuous function y(x) is approximated by a set of discrete values yi,



$$y(x_0+h) = y(x_0) + h\left.\frac{dy}{dx}\right|_{x_0} + \frac{h^2}{2!}\left.\frac{d^2y}{dx^2}\right|_{x_0} + \frac{h^3}{3!}\left.\frac{d^3y}{dx^3}\right|_{x_0} + \ldots\ldots$$

$$\left.\frac{dy}{dx}\right|_{x_0} = f(x_0, y_0)$$

$$\frac{d^2y}{dx^2} = \frac{d}{dx}\left(\frac{dy}{dx}\right) = \frac{df}{dx} = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\frac{dy}{dx} = \left[\frac{\partial f}{\partial x} + f\frac{\partial f}{\partial y}\right]_{x_0, y_0}$$

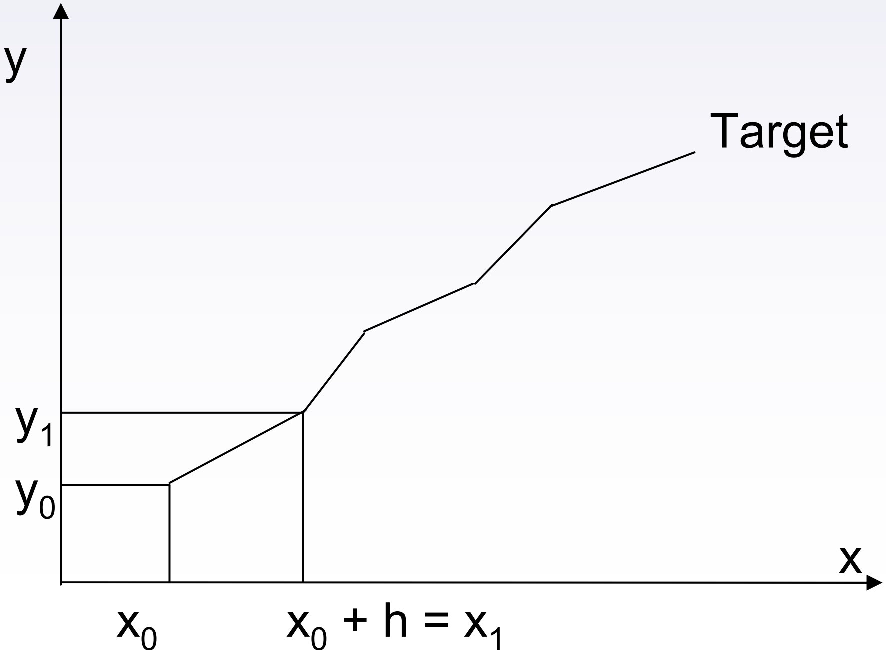
$$f = f(x, y(x))$$

$$\frac{d^3y}{dx^3} = \frac{d}{dx}\left(\frac{d^2y}{dx^2}\right) = \frac{d}{dx}\left[\frac{\partial f}{\partial x} + f\frac{\partial f}{\partial y}\right] = \frac{\partial}{\partial x}\left[\frac{\partial f}{\partial x} + f\frac{\partial f}{\partial y}\right] + f\frac{\partial}{\partial y}\left[\frac{\partial f}{\partial x} + f\frac{\partial f}{\partial y}\right]$$

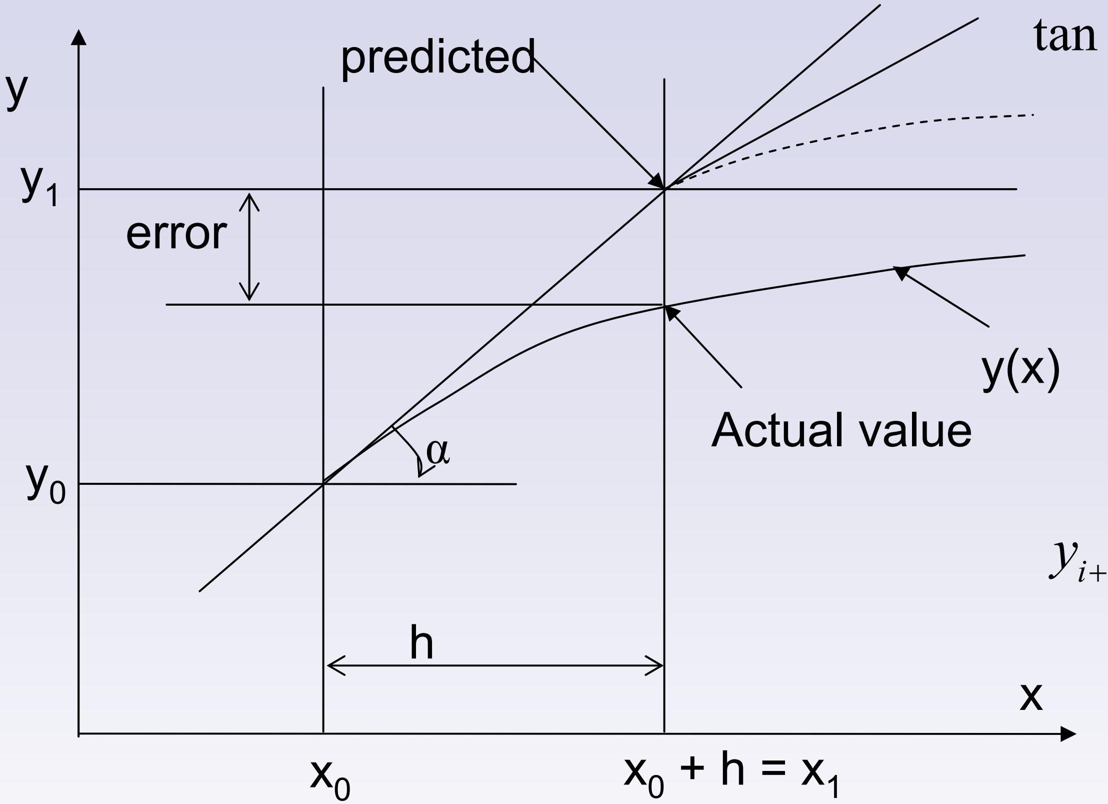
$$= f_{xx} + f_x f_y + ff_{xy} + ff_{xy} + ff_y^2 + f^2 f_{yy}$$

$$\frac{d^2y}{dx^2} = f(x, y, \frac{dy}{dx}) \rightarrow$$ We need $$y(x_0) = y_0$$ $$\& \left(\frac{dy}{dx}\right)_{x_0} = y_1$$

Euler's Method:



$$y(x_0 + h) = y(x_0) + hf(x_0, y_0)$$



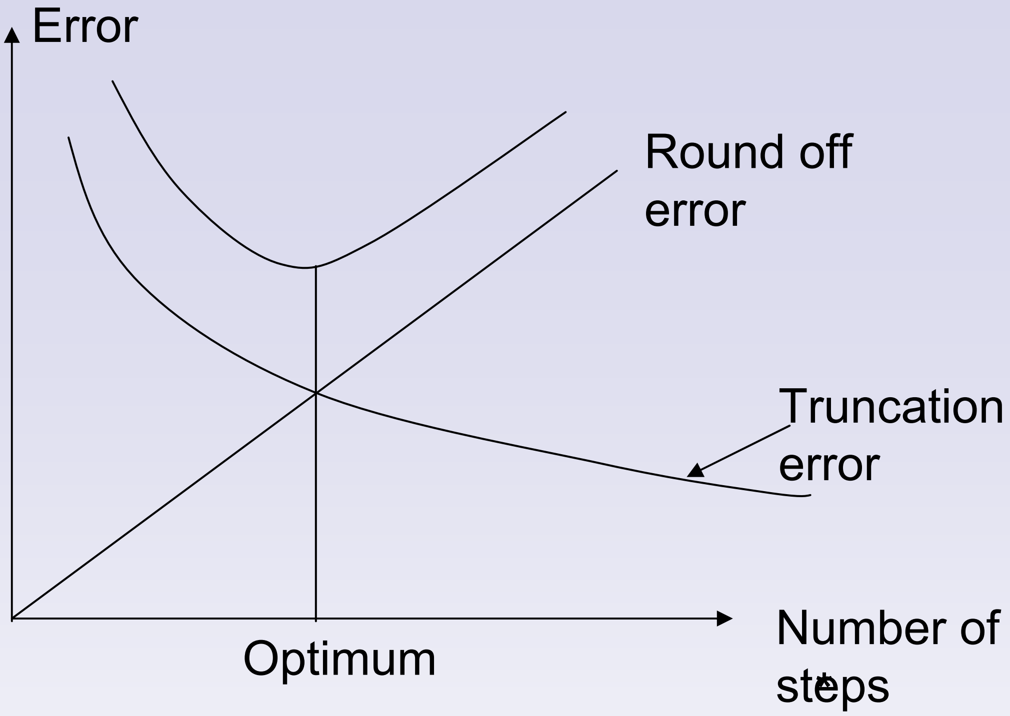
$$\tan\alpha = \frac{dy}{dx} = f(x_0, y_0)$$

$$y_{i+1} = y_i + hf(x_i, y_i)$$

Local truncation error: O(h^2)

Global error: a) Accumulated local error
b) Switching of solution curves
c) Round off error

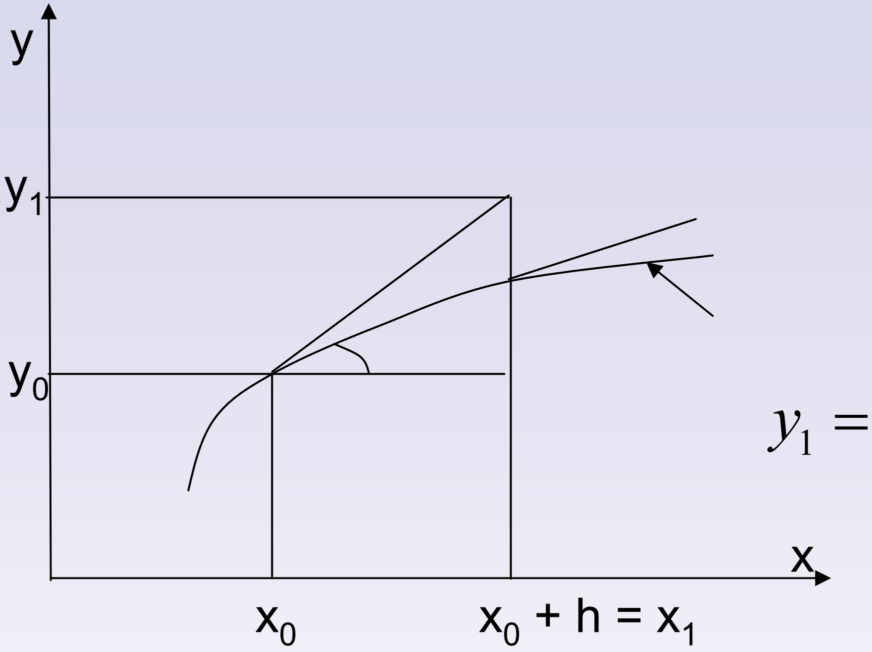
If y_1 has an error $\longrightarrow$ generates wrong value for $f(x_0 + h, y_1)$



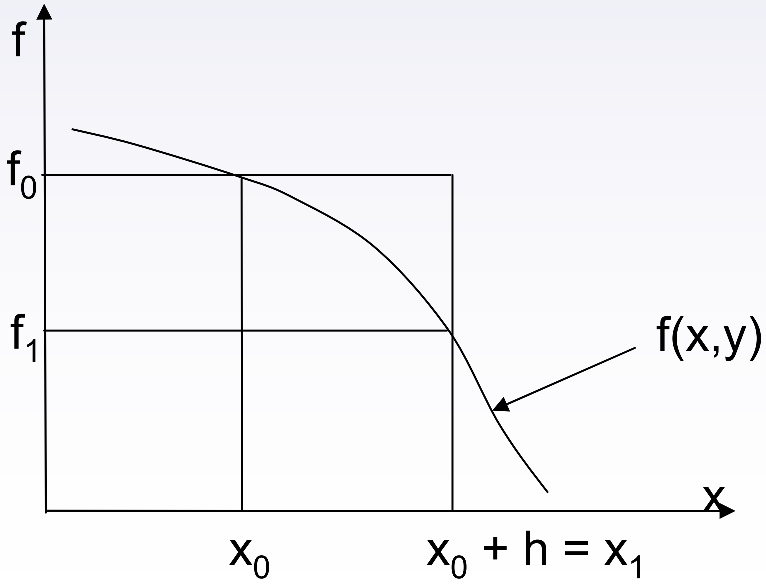
[a,b] interval, at each step the local error

hM=b-a $$y^{(2)}(c_k)\frac{h^2}{2}M = \frac{\left(b-a\right)y^{(2)}h}{2} = Q(h)$$

MODIFIED EULER’S METHOD: HEUN'S METHOD



$$y_1 = y_0 + hf(x_0, y_0)$$



$$\tan\alpha = f(x_0, y_0)$$

$$\frac{dy}{dx} = f(x, y(x))$$

$$y(x_0 + h) = \int_{x=x_0}^{x_0+h} f(x, y(x))dx + y_0$$

slope averaging

$$f_0 = f(x_0, y_0)$$

$$y_1^p = y_0 + hf_0 \qquad \underbrace{y_1^c = y_0 + h\left(\frac{f_0 + f_1}{2}\right)}_{\text{Trapezoidal rule}} \quad (2)$$

$$f_1 = f(x_0 + h, y_1) = f(x_1, y_1)$$

Use Euler as predictor to calculate y$_1$, then calculate f$_1$ & use eq. (2) to correct the result.

TAYLOR’S METHOD:

$$\frac{dx}{dt} = 5xt \quad \text{x(1)=2} \qquad \int \frac{dx}{x} = \int 5tdt \qquad \ln|x| = \frac{5t^2}{2} + C \qquad \ln 2 = \frac{5}{2} + C$$

$$C = -\frac{5}{2} + \ln 2 \qquad \ln\left(\frac{x}{2}\right) = \frac{5}{2}(t^2 - 1) \qquad \frac{x}{2} = e^{5/2(t^2-1)}$$

Taylor series method:

- Not practical to use Taylor’s series expansion method if ***f*** has complicated derivates, therefore,
- No generalized computer program can be constructed
- nth order R-K is an alternative.

$$\frac{d^2y}{dt^2} = 5x + 5xt(5t)$$

$$= 5x + 25xt^2$$

$$= 5x(1+5t^2)$$

$$\frac{d^3y}{dx^3} = 25x(2t) + 5xt\left[5(1+5t^2)\right]$$

$$= 50xt + 25xt + 125xt^3$$

RUNGE-KUTTA METHODS:

- Accurate, stable, easy to program
- Involves only first order derivative evaluation (function itself not derivative)
- Produces results equivalent in accuracy to the higher order Taylor formulas.
- Each R-K method is derived from an appropriate Taylor method.
- Perform several function evaluations at each step to eliminate the necessity to compute the higher derivatives
- Can be constructed for any order.

$$\frac{dy}{dx} = f(x,y) \qquad y(x_0) = y_0 \qquad y(x+h) = y(x) + w_1F_1 + w_2F_2 \qquad w_1, w_2 : weights$$

$$F_1 = hf(x,y)$$

$\alpha = 1 \quad \beta = 1 \quad w_1 = w_2 = \frac{1}{2} \Rightarrow$ MODIFIED EULER

$$F_2 = hf(x+\alpha h, y+\beta F_1)$$

Obtain α, β, w_1, w_2 that the error is the same as in 2nd order Taylor's method.

$$\frac{(\alpha h)^2}{2!} f_{xx} + \frac{(\beta F_1)^2}{2!} f_{yy} + \frac{2(\alpha h)(\beta F_1)}{2!} f_{xy} + Q(h^3)$$

$$F_2 = h\left\{ f(x,y) + \frac{df}{dx}\alpha h + \frac{df}{dy}\beta F_1 + Q(h^2) \right\}$$

Taylor’s series for a function of two variables.

$$y(x+h) = y(x) + w_1 hf + w_2\left[hf + \frac{\partial f}{\partial x}\alpha h^2 + \frac{\partial f}{\partial y}\beta h^2 f \right] + ...$$

$$= y(x) + h(w_1 + w_2)f + w_2 h^2\left[\alpha f_x + \beta f f_y \right] + ...$$

TAYLOR $\rightarrow y(x+h) = y(x) + hf + \frac{h^2}{2!}\left[f_x + f f_y \right] + ...$

$$w_1 + w_2 = 1$$

$$\alpha = \beta = 1$$

$$w_2 = \frac{1}{2}$$

$\Longrightarrow$ **2nd order Runge-Kutta**

4th Order Runge-Kutta: $y_{k+1} = y_k + w_1 F_1 + w_2 F_2 + w_3 F_3 + w_4 F_4$

$$y_{k+1}(x+h) = y_k(x) + \frac{h}{6}(F_1 + 2F_2 + 2F_3 + F_4)$$

$$F_1 = f(x_k, y_k)$$

$$F_2 = f\left(x_k + \frac{h}{2}, y_k + \frac{F_1}{2}\right)$$

$$F_3 = f\left(x_k + \frac{h}{2}, y_k + \frac{F_2}{2}\right)$$

$$F_4 = f\left(x_k + h, y_k + F_3\right)$$

Extensions to systems of differential equations:

$$\frac{dx}{dt} = f(t, x, y)$$

$$\frac{dy}{dt} = g(t, x, y)$$

with

$$x(t_0) = x_0$$

$$y(t_0) = y_0$$

RK4

$$x_{k+1} = x_k + \frac{h}{6}(F_1 + 2F_2 + 2F_3 + F_4) \qquad k = 0,1,2,........MAX$$

$$y_{k+1} = y_k + \frac{h}{6}(G_1 + 2G_2 + 2G_3 + G_4) \qquad h = \frac{b-a}{N}$$

$$F_1 = f(t_k, x_k, y_k)$$

$$G_1 = g(t_k, x_k, y_k)$$

$$F_2 = f\left(t_k + \frac{h}{2}, x_k + \frac{h}{2}F_1, y_k + \frac{h}{2}G_1 \right)$$

$$G_2 = g\left(t_k + \frac{h}{2}, x_k + \frac{h}{2}F_1, y_k + \frac{h}{2}G_1 \right)$$

$$F_3 = f\left(t_k + \frac{h}{2}, x_k + \frac{h}{2}F_2, y_k + \frac{h}{2}G_2 \right)$$

$$G_3 = g\left(t_k + \frac{h}{2}, x_k + \frac{h}{2}F_2, y_k + \frac{h}{2}G_2 \right)$$

$$F_4 = f\left(t_k + h, x_k + hF_3, y_k + hG_3\right)$$

$$G_4 = g\left(t_k + h, x_k + hF_3, y_k + hG_3\right)$$

Örnek: TAYLOR (serisi) yöntemi:

$y' = x^2 + y^2$ y(0)=0 [a=0 , b=1]

n=10 step h= (b-a)/n=0.1

$$y_{i+1} = y_i + h\frac{y_i'}{1!} + \frac{h^2}{2!}y_i'' + \frac{h^3}{3!}y_i'''$$

y’ , y’’ , y’’’ necessary.

+O(h4) Truncation error results from taking finite number of terms in an infinite series.

$$y' = f(x,y) = x^2 + y^2$$

$$y'' = f_x + ff_y = 2x + 2yf = 2x + 2yy'$$

$$y''' = f_{xx} + 2f_{xy}y' + f_{yy}(y')^2 + f_y\left[f_x + ff_y\right] = f_{xx} + 2f_{xy}y' + f_{yy}(y')^2 + f_y y''$$

$$y''' = 2 + 0 + 2(y')^2 + 2yy''$$

x_0=0 , y_0=0 , y_0’=0 , y_0’’=0 , y_0’’’=2

$$y_1 = y_0 + hy_0' + \frac{h^2}{2}y_0'' + \frac{h^3}{3!}y_0''' = \frac{2}{6}(0.1)^3 = 0.3333*10^{-3}$$

x_1=0.1 , y_1=0.333*10^{-3}

$$y_1' \cong 0.01 \quad y_1'' \cong 0.2 \quad y_1''' \cong 2.0003$$

$$y_2 = y_1 + hy_1' + \frac{h^2}{2}y_1'' + \frac{h^3}{3!}y_1''' \cong 0.002667$$

.

.

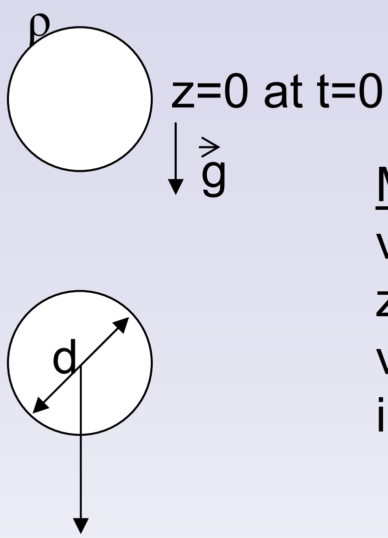
y_5=0.041784 exact value 0.041791

.

.

y_{10}=0.350064 exact value 0.350232

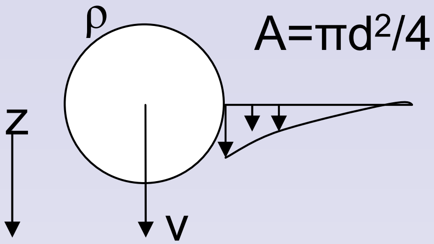
FREE FALLING OF A SOLID SPHERE



$$v = \frac{dz}{dt}$$

Motion of sphere:
v=v(t)=?
z=z(t)=? Displacement
vacuum → only external force is gravitational force but in a fluid additional forces

1. Buoyant force: weight of fluid displaced bt body: $-m_f g \quad -\frac{\pi d^3}{6}\rho_f g$
2. Force on an accelerating body: due to flow field exists for frictionlessflow as well, $-\frac{1}{2}m_f \frac{dv}{dt}$
3. Viscous forces: In real fluid → shear stress on surface



C_D: drag coef.[-]

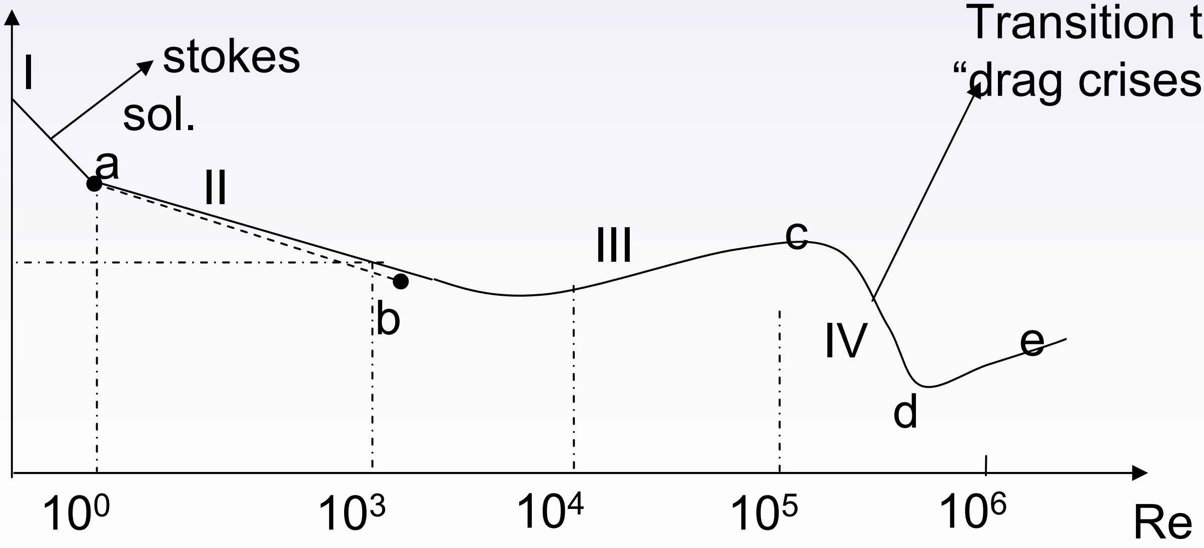
$$F_D \equiv C_D \frac{1}{2} \rho V^2 A$$

F_D:total drag force
A:projected frontal area

Drag due to
1) pressure forces (from drag)
2) friction forces (shear stress)

Valid for ρ = const. Over any body
Viscous fluid flow pg.182 (white)

$C_D = C_D$ (Re, body shape) → dimensional analysis



Transition to turb.
“drag crises”

Rough
surface

I – stoke's solution → $C_D = \frac{24}{\text{Re}}$, Re≤1

II – approx. Fitted curve → $C_D = \frac{24}{\text{Re}^{0.646}}$, 1<Re≤400

III - approx. Const. Drag coef. → $C_D \approx 0.5$, $400<\text{Re}\leq 3\text{x}10^5$

$C_D \approx 0.000366\,\text{Re}^{0.4275}$, $3\text{x}10^5<\text{Re}\leq 2\text{x}10^6$

$C_D \approx 0.18$, $\text{Re}>2\text{x}10^6$

4. Wave drag: M=v(1) M=V/a shock waves cause wave drag.

M<<1 wave drag is neglected
Newton's 2nd Law applied to spherical body.

$$m\frac{dv}{dt} = \underbrace{mg}_{\text{gravit f.}} - \underbrace{m_f g}_{\text{buoyant f.}} - \underbrace{\frac{1}{2}m_f\frac{dv}{dt}}_{\text{force due to accel.}} \underbrace{-\frac{1}{2}\rho_f v\left(\frac{v}{\frac{\pi}{4}d^2}C_D\,\text{Re}\right)}_{\text{viscous force}}$$

ρ: density of sphere
special case:
in a vacuum: $\overline{\rho} = 0$

,A=1 , B=g , C=0

$$\frac{dv}{dt} = \frac{1}{A}\left[B - Cv/V/C_D(\text{Re})\right]$$

$$\frac{dz}{dt} = v$$

$$A = 1 + \frac{1}{2}\overline{\rho} \;\;,\;\; B = \left(1-\overline{\rho}\right)g \;\;,\;\; C = \frac{3}{4}\frac{\overline{\rho}}{d} \;\;,\;\; \overline{\rho} = \frac{\rho_f}{\rho}$$

$$\frac{dz}{dt} = v$$

$$\frac{dv}{dt} = g \rightarrow v = gt + v_0$$

$$\frac{dz}{dt} = gt + v_0 \Rightarrow z = v_0 t + \frac{1}{2} g t^2$$

$$\frac{dz}{dt} = v = g(v)$$

$$\frac{dv}{dt} = \frac{1}{A}\left[B - Cv / V / C_D(\mathrm{Re})\right] = f(v)$$

RK4

$$F_1 = f(v) = \frac{1}{A}[\ ]$$

$$G_1 = g(v) = v$$

$$F_2 = f\left(v + \frac{h}{2}F_1\right)$$

$$G_2 = g\left(v + \frac{h}{2}G_1\right) = v + \frac{h}{2}G_1$$

$$F_3 = f\left(v + \frac{h}{2}F_2\right)$$

$$G_3 = g\left(v + \frac{h}{2}G_2\right) = v + \frac{h}{2}G_2$$

$$F_4 = f(v + hF_3)$$

$$G_4 = g(v + hG_3) = v + hG_3$$

$$v_{k+1} = v_k + \frac{h}{6}\left(F_1 + 2F_2 + 2F_3 + F_4\right)$$

$$z_{k+1} = z_k + \frac{h}{6}\left(G_1 + 2G_2 + 2G_3 + G_4\right)$$

$$[a,b] \equiv [0,10]$$

$$h = \frac{b-a}{N} = \frac{10}{100} = 0.1$$

h:step size
N:number of steps
We are going to march from a to b by step size h.

HW1

$$\frac{dx}{dt} = x' = 1 - y$$

$$\frac{dy}{dt} = y' = x^2 - y^2$$

x(0)=-1.2
y(0)=0
[0,5] , h=0.1 & 0.01
Show the result
Plot phaseportrait

ORDINARY DIFFERENTIAL EQUATIONS OF THE BOUNDARY VALUE TYPE (BVPs)

Finite-difference method (Relaxation method)

Introduction: We will concentrate mainly on second order BVPs since first order problems can be considered as initial value problems.

In practice, some higer order equations occur. When equations of higer order then second occur, we can treat them as a coupled set of second order equations.

Example # 1 A non-linear 4th order equation

$$y^{IV} + y''^{2} + r(x) + y'^{3} + q(x)y = f(x) \qquad (1)$$

$$\left.\begin{array}{l} Let \\ y'' = z \\ z'' + z^{2} + ry'^{3} + qy = f(x) \end{array}\right\} \qquad (2)$$

LINEAR EQUATIONS

Easiest problem: Linear equation function values are specified at the both ends.

Analytical solution: Big difference between the solution of linear&non-linear problems.

Numerical solution: Techniques for linear equations can be easily modified for non-linear problems.

E.g. 2 Boundary Layer Over a Flat Surface:

B.L eqs. reduce an ODE a similarity solution

$$f''' + ff'' = 0$$

$$f(0) = f'(0) = 0$$

$$f'(\infty) = 1$$

$$u = U_\infty f'(\eta) \quad , \quad v = U_\infty x^{1/2} \{\eta f' - f\} \quad , \quad \eta = \frac{y}{\sqrt{x}}$$

Third-order non-linear differential eqs.

- Almost always better to write the equation as a series of first and second order equations.

Let us define $g = f'$

$$g'' + fg' = 0 \quad \text{(A)}$$

$$g = f'$$

or

$$f = \int_0^\eta g d\eta \qquad \text{(B)}$$

numerical integration such as trapezoid rule.

Eqs. (A)&(B) can be solved numerically using an iterative procudure.

- Direct schemes of solution for higer order eqs. (then two) can be unstable.

General second order linear ODE can be written as

$$y'' + p(x)y' + r(x)y = f(x) \qquad (3)$$

- Special cases
- p&r → constant and f(x)=0 → exact analytical solution is obtaained in the form of simple exponentials or sine and cosine solutions
- p&r → constant and f is a special form such as a polynomial, an exponential, or a sine ar cosine function an analytical solution may also be obtained by the method of undetermined coefficient
- f=0 special situations

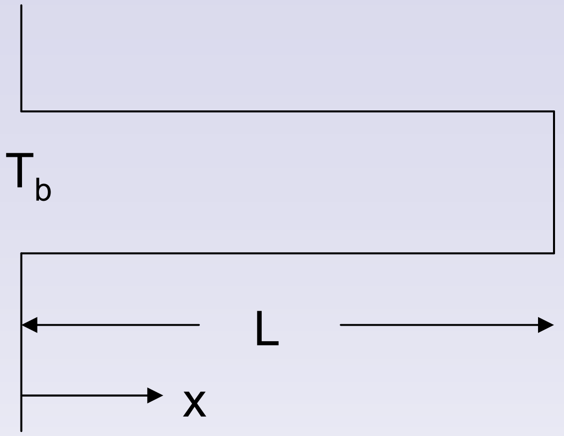
Bessel functions, Legendre functions which satisfy special forms of eq.(3)

- Special situatons are exception rather than the rule
- Need to find ways of computing the solution of eq.(3) numerically

FUNCTIONS VALUES SPECIFID AT THE END POINTS:

2nd order BVP → two conditions need to be specified
These conditions → the function or its derivative or a combination of both.

Example



$$h(T\text{-}T_{\infty}) = k\frac{dt}{dx}$$

$$x = L \rightarrow T = T_t \quad , \quad \frac{\partial T}{\partial x} = 0 \quad \textit{(insulated)}$$

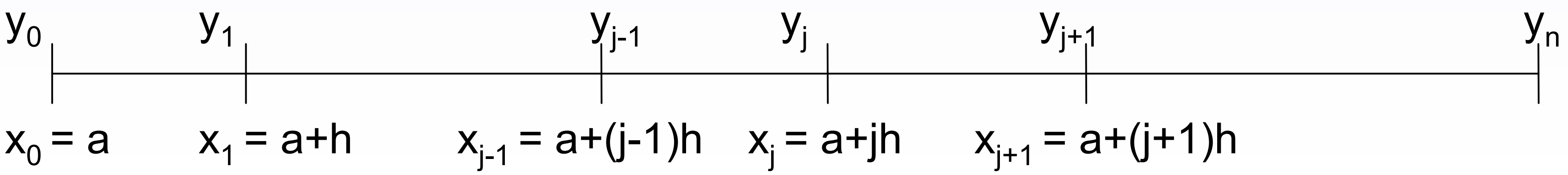
$$y'' + p(x)y' + r(x)y = f(x) \qquad (3)$$

$$y(a) = A$$

$$y(b) = B$$

Wish to solve eq.(3) for x in (a,b) y(x)=?

Range (a,b) is first split into n equal parts of mesh length h and each point is labelled as indicated below.



At a typical point in the mesh at x=xj , we write finite difference representation to eq.(3) as,

$$\frac{y_{j+1}-2y_j+y_{j-1}}{h^2}+p(x_j)\frac{y_{j+1}+y_{j-1}}{2h}+r(x_j)y_j=f(x_j)+\underbrace{\frac{1}{h^2}Cy_j}_{\text{error term}} \qquad (4)$$

Here $y_j = y(x_j)$, $p_j = p(x_j)$

$$y_{j+1}\left(1+\frac{h}{2}p_j\right)+\left(-2+h^2r_j\right)y_j+\left(1-\frac{h}{2}p_j\right)y_{j-1}=h^2f_j+Cy_j \qquad (5)$$

Assuming Cy_j negligible, then, finite difference approximation to eq.(3) at the point x_j = a+jh (j=1,2,..,n-1) is given iby eq.(5)

Example:

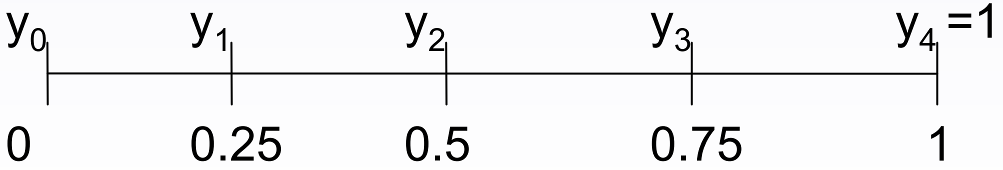
$$y''-y=x$$

For illustration purposes, select h=0.25

P(x)=0 , r(x)=-1 , f(x)=x

$$y(0)=0$$

$$y(1)=1$$



$$y_{j+1}+\left(-2+h^2\right)y_j+y_{j-1}=h^2x_j \qquad x_j=jh \qquad j=1,2,3 \qquad \text{interior points!}$$

$$\left.\begin{aligned} \overbrace{y_0}^{0}-2.0625y_1+y_2&=0.015625\\ y_1-2.0625y_2+y_3&=0.031250\\ y_2-2.0625y_3+\underbrace{y_4}_{1}&=0.046875 \end{aligned}\right\}(6)$$

$y_0=0$, $y_4=1$, Eq.(6) represents 3 equations and 3 unknowns.

Linear systems of equations

- Cramer's rule: few number equations; 3-4
- Gauss elimination: moderate number of equations; 10-50
- Iterative techniques (Jacobi, Gauss Seidel, SOR): large number of equations; 100-1000

Exact solution of $y''-y=x$ $\quad y=\frac{2}{e^2-1}\left(e^{x+1}-e^{-(x-1)}\right)-x$

Comparision

	Numerical	Exact
y_0	0	0
y_1	0.18023	0.17990
y_2	0.38735	0.38682
y_3	0.64993	0.64945
y_4	1.0	1.0

- Good to 3 significant figures of a accuracy even for this large h=0.25
- Agreement will improve as h decreases

Computer Programming

General difference equation

$$y_{j+1}\underbrace{\left(1+\frac{h}{2}p_j\right)}_{b_j}+\underbrace{\left(-2+h^2r_j\right)}_{a_j}y_j+\underbrace{\left(1-\frac{h}{2}p_j\right)}_{c_j}y_{j-1}=\underbrace{h^2 f_j}_{d_j}$$

$b_j y_{j+1}+a_j y_j+c_j y_{j-1}=d_j$ (A) Linear system of eqs.

x_j = a+jh , where j = 1, 2,..., (n-1)

(n-1) eqs. (n-1) unknowns y_1 , y_2 ,..., y_{n-1}
y_0 = A , y_n = B (known from BCs)
need to solve (n-1) linear eqs. in (n-1) unknowns.

Coefficient for the general eq.

$$b_j=\left(1+\frac{h}{2}p_j\right) \quad , \quad c_j=\left(1-\frac{h}{2}p_j\right)$$

$$a_j=\left(-2+h^2r_j\right) \quad , \quad d_j=h^2 f_j$$

Compute and store in one dimensional arrays, $p_j = p(x_j)$, $r_j = r(x_j)$, $x_j = a+jh$

Eq.(A) in obtained by selection of central difference formula to approximate the differential eq.

Advantages

1. Lead to the tri-diagonal matrices
2. Often lead to diagonally dominant matrices

Definition: A matrix of dimension NxN is said to be strictly diagonally dominant if

$$|a_{k,k}| > |a_{k,1}| + \ldots + |a_{k,k-1}| + |a_{k,k+1}| + \ldots + |a_{k,N}| \qquad \text{for k} = 1,2,.., \text{N}$$

Need to have diagonally dominant matrix for convergence!!

TRI-DIAGONAL MATRIX:

All elements other than diagonal, upper and lower diagonal elements of a matrix are zero.

- Note if matrix is tri-diagonal direct method of solution should be the way of solving the matrix.

Let’s write the coefficient matrix

$$\begin{array}{ccccc} a_{11} & a_{12} & a_{13} & . & a_{1N}\\ a_{21} & a_{22} & a_{23} & . & a_{2N}\\ . & . & . & . & .\\ . & . & . & . & .\\ a_{N1} & . & . & . & a_{NN}\end{array}$$

$$\left|a_{3,3}\right| > \left|a_{3,1}\right| + \left|a_{3,2}\right| + \left|a_{3,4}\right| + ... + \left|a_{3,N}\right|$$

Let’s write eq.(A) in open form,

$$\begin{array}{lllllll}
a_1 y_1 + b_1 y_2 & & & & = & d_1 - c_1 y_0 \\
c_2 y_1 + a_2 y_2 + b_2 y_3 & & & & = & d_2 \\
c_3 y_2 + a_3 y_3 + b_3 y_4 & & & & = & d_3 \\
\vdots & & & & & \\
\vdots & & & & & \\
c_k y_{k-1} + a_k y_k + b_k y_{k+1} & & & & = & d_k \\
\vdots & & & & & \\
\vdots & & & & & \\
c_{n-2} y_{n-3} + a_{n-2} y_{n-2} + b_{n-2} y_{n-1} & & & & = & d_{n-2} \\
c_{n-1} y_{n-2} + a_{n-1} y_{n-1} & & & & = & d_{n-1} - b_{n-1} \underbrace{y_n}_{known}
\end{array}$$

- (n-1) eqs. & (n-1) unknowns y_i, i=1,2,..,(n-1)
- y_0 & y_n are known from BCs
- need to eliminate each successive y_i

$$y_1 = \frac{\hat{d}_1 - b_1 y_2}{a_1} \qquad (1')$$

$$c_2 \frac{\hat{d}_1 - b_1 y_2}{a_1} + a_2 y_2 + b_2 y_3 = d_2 \qquad (2)$$

$$\underbrace{\left(a_2 - c_2 \frac{b_1}{a_1} \right)}_{\alpha_2} y_2 + b_2 y_3 = \underbrace{d_2 - c_2 \frac{\hat{d}_1}{a_1}}_{\gamma_2} \qquad (2')$$

$$\alpha_2 y_2 + b_2 y_3 = \gamma_2 \qquad (2'')$$ use (2’’) to eliminate y_2 in (3),

$$y_2 = \frac{\gamma_2 - b_2 y_3}{\alpha_2} \qquad (2''')$$

$$c_3 \left(\frac{\gamma_2 - b_2 y_3}{\alpha_2} \right) + a_3 y_3 + b_3 y_4 = d_3 \qquad (3)$$

$$\underbrace{\left(a_3 - c_3 \frac{b_2}{\alpha_2} \right)}_{\alpha_3} y_3 + b_3 y_4 = \underbrace{d_3 - c_3 \frac{\gamma_2}{\alpha_2}}_{\gamma_3} \qquad (3')$$

$$\alpha_{k+1} = a_{k+1} - \frac{c_{k+1} b_k}{\alpha_k} \qquad (I)$$

Forward elimination, k=1,2,..,(n-1)

$$\gamma_{k+1} = d_{k+1} - \frac{c_{k+1} \gamma_k}{\alpha_k}$$

Recursion relations for α and γ

$$\alpha_k y_k + b_k y_{k+1} = \gamma_k \qquad \text{(kth eq.)}$$

$$y_k = \frac{\gamma_k - b_k y_{k+1}}{\alpha_k} \qquad \text{(II)}$$

Back subtitution k=(n-1),(n-2),..,1

TDMA - Tri-diagonal matrix algorithm.
To obtain values to start the recursion relations off,
Compare (kth) eq. with (1)

$$a_1 y_1 + b_1 y_2 = d_1 - c_1 y_0 \qquad (1)$$

$$\alpha_k y_k + b_k y_{k+1} = \gamma_k \qquad \text{(kth)}$$

$$\alpha_1 = a_1 \quad , \quad \gamma_1 = d_1 - c_1 y_0 = \hat{d}_1 \qquad (*)$$

Summary:
TDMA: Direct process of solution

Step #1: α and γ are calculated using the recursion relations (I) starting from the initial values given in (*)
Called forward elimination k=1,2,..,(n-1)

Step #2: Back substitution using eq.(II) k=(n-1),(n-2),..,1 as y_n = B is known

THE THOMAS ALGORITHM

- more efficient scheme
- numerically stable scheme

Start by calculating two arrays δ and F starting from initial values

$$\delta_0 = y_0 = A$$
$$F_0 = 0$$

Using the recursion relations,

$$F_{k+1} = -\frac{b_{k+1}}{\left(a_{k+1} + c_{k+1}F_k\right)} \quad , \quad \delta_{k+1} = \frac{d_{k+1} - c_{k+1}\delta_k}{\left(a_{k+1} + c_{k+1}F_k\right)} \qquad \text{k} = 0,1,2,..,(\text{n-1})$$

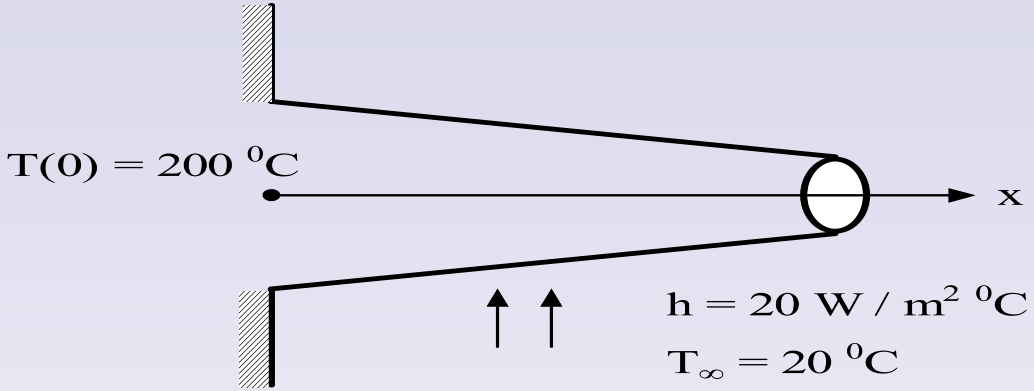
It may be proved by mathematical induction that

$$y_k = F_k y_{k+1} + \delta_k$$
$$y_n = B \quad \text{is known} \;\Rightarrow\; \text{k} = \;(\text{n-1}),(\text{n-2}),.., 2, 1$$

Thomas algorithm is preferred direct method of solution.

```
 subroutine thomas(a, b, c, d, N, y)
              implicit double precision (a-h,o-z)
              dimension a(N), b(N), c(N), d(N)
              dimension F(0:2000), Delta(0:2000),y(0:N)
c             boundary condition #1 at x = 0

             y(0) = 250.0
              Delta(0) = y(0)
              F(0) = 0.0

c             Forward Elimination
      do 5 k = 0, N-1
              F(k+1) = -(b(k+1))/(a(k+1)+c(k+1)*F(k))
              Delta(k+1)=(d(k+1)-c(k+1)*Delta(k))/(a(k+1)+c(k+1)*F(k))
 5    continue
c     derivative boundary condition #2 at x = L (insulation)
              AA =  a(N)
              BB = c(N) + b(N)
      y(N) = (d(N)- BB*Delta(N-1))/(AA+BB*F(N-1))
              print*, y(N)

c            back substitution
      do 6 k = N-1,1,-1
              y(k) = F(k)*y(k+1) + Delta(k)
 6    continue

              return
              end
```

Example of a Boundary Value Problem: Fins or Extended surfaces



$$\frac{d^2T}{dx^2}+\left(\frac{1}{A_c}\frac{dA_c}{dx}\right)\frac{dT}{dx}-\left(\frac{1}{A_c}\frac{h}{k}\frac{dA_s}{dx}\right)\left(T-T_\infty\right)=0$$

$A_c(x)$**: Cross-sectional area**

$A_s(x)$**: Surface area measured from the base.**

Note: if ***$A_c(x)$= const.*** $\Rightarrow$ ***$A_s(x)$= P x***   P: perimeter of cross-section of the fin

$$\frac{d^2T}{dx^2}-\left(\frac{hP}{kA_c}\right)\left(T-T_\infty\right)=0$$

Common boundary conditions

1. T = Tb at x = 0
2. At x = L
    1. dT/dx = 0 (insulated; Neumann condition)
    2. $T = T_L$ (specified temperature; Dirichlet condition)
    3. $T = T_\infty$ (for long fins)

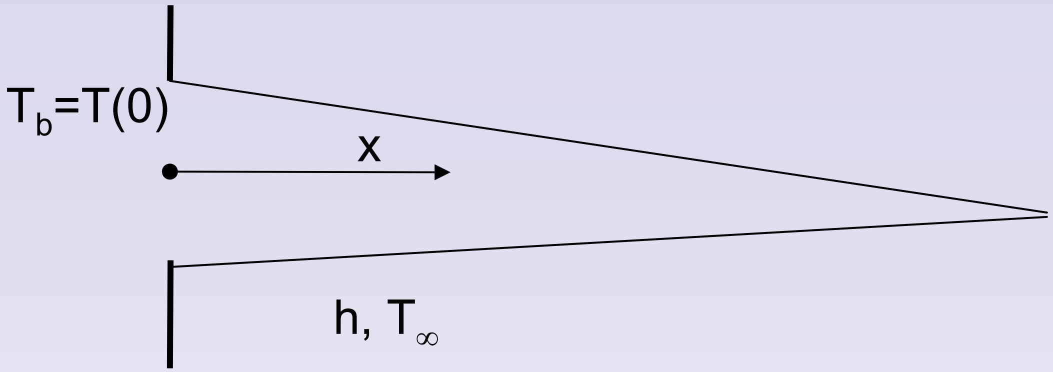
4. $-k\left.\frac{dT}{dx}\right|_{x=L} = -h(T - T_\infty)$ (convection condition; Mixed or Robin condition)

Object of fin analysis

1. Solve for T(x)
2. Compute $q_B = -kA_C(x)\left.\frac{dT}{dx}\right|_{x=0}$ $\Rightarrow$ energy dissipated by the fin

Methods
a) Exact solutions for *$A_c(x)$= const.*
b) Numerical Methods

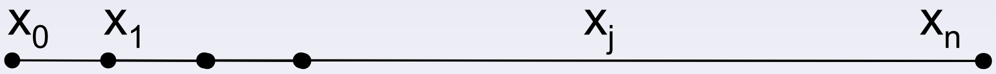
Numerical Solution of fin equation



$$P(x)=\frac{1}{A_c}\frac{dA_c}{dx}$$

$$R(x)=-\frac{h}{kA_c}\frac{dA_s}{dx}$$

$$\theta=T-T_\infty$$



$$\frac{d^2\theta}{dx^2}+P(x)\frac{d\theta}{dx}+R(x)\theta=0$$

$$b_j\theta_{j+1}+a_j\theta_j+c_j\theta_{j-1}=d_j$$ j = 1, 2, …, (n-1)

$$b_j=1+\frac{\Delta x}{2}P_j \quad c_j=1-\frac{\Delta x}{2}P_j \quad a_j=-2+(\Delta x)^2R_j \quad d_j=0$$

a) Specified temperature at x = L **$\theta = \theta_L$ at x = L**
$\theta = \theta_b$ at x = 0

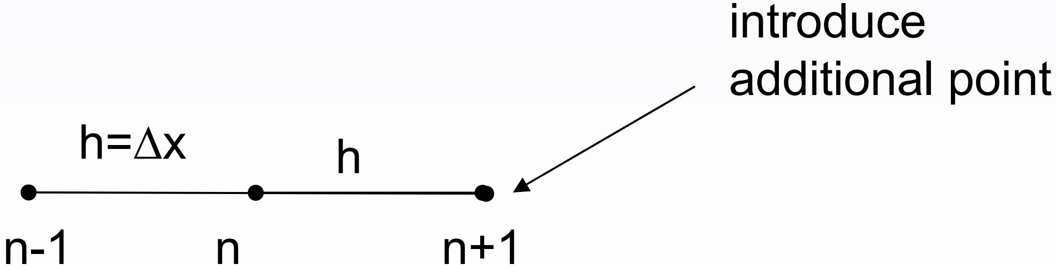
Thomas algorithm is readily applied.
$F_0=0$; $\delta_0 = \theta_0 = \theta_b$

$$F_{k+1} = \frac{-b_{k+1}}{a_{k+1} + c_{k+1}F_k} \qquad \delta_{k+1} = \frac{d_{k+1} - c_{k+1}\delta_k}{a_{k+1} + c_{k+1}F_k}$$

$$\theta_k = F_k\theta_{k+1} + \delta_k$$ k = (n-1),(n-2),…, 2, 1.

b) Convection condition at x = L

$$-k\left.\frac{d\theta}{dx}\right|_{x=L} = -h\theta$$ **at x = L & $\theta = \theta_b$ at x = 0**



Fin equation at x = x_n = L (j = n)

$$b_n\theta_{n+1} + a_n\theta_n + c_n\theta_{n-1} = d_n$$

Convection condition: $$-k\left(\frac{\theta_{n+1} - \theta_{n-1}}{2(\Delta x)}\right) = -h\theta_n$$

Eliminate θ_{n+1}; $$\theta_{n+1} = \theta_{n-1} - \frac{2(\Delta x)h}{k}\theta_n$$

$$\underbrace{\left(a_n - b_n\frac{2(\Delta x)h}{k}\right)}_{A}\theta_n + \underbrace{(c_n + b_n)}_{B}\theta_{n-1} = d_n$$

$$A\theta_n + B\theta_{n-1} = d_n \Rightarrow \theta_n = \frac{d_n - B\theta_{n-1}}{A} \quad (1)$$

$\theta_k = F_k\theta_{k+1} + \delta_k$ k = (n-1),(n-2),…   For k = n-1

$$\theta_{n-1} = F_{n-1}\theta_n + \delta_{n-1} \qquad (2)$$

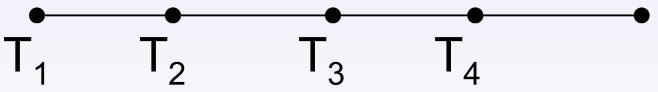
Substitute Eq. (2) into Eq. (1):

$$\theta_n = \frac{d_n - BF_{n-1}\theta_n - B\delta_{n-1}}{A} \quad \Rightarrow \quad (A + BF_{n-1})\theta_n = d_n - B\delta_{n-1}$$

$$\theta_n = \frac{d_n - B\delta_{n-1}}{A + BF_{n-1}}$$

Back substitute as before. Note d_j= 0.

Heat Flux:



$$q_f = -kA_c(0)\left.\frac{dT}{dx}\right|_{x=0}$$

$$\left.\frac{dT}{dx}\right|_{x=0} \cong \frac{T_2 - T_1}{\Delta x}, \quad \text{or} \quad \left.\frac{dT}{dx}\right|_{x=0} \cong \frac{-3T_1 + 4T_2 - T_3}{2(\Delta x)}, \quad \text{or}$$

$$\left.\frac{dT}{dx}\right|_{x=0} \cong \frac{-11T_1 + 18T_2 - 9T_3 + 2T_4}{6(\Delta x)}$$

Non-Linear Equations:

- Methods similar to those used in the linear case can be used

- Obtain a set of non-linear difference eqs. but no general direct methods for solving non-linear algebraic eqs.

i.e. difference eqs. cannot be solved immediately as in the linear case

Standart Approach in Non-linear Case

1. Linearize difference eq. usually by approximating a portion of non-linear terms with a guessed solution
2. Then, solve the linearized dif. eq. with a direct method such as Thomas Algorithm to approximately obtain solution
3. ITERATION needed until two succesive numerical solutions agree at each mesh point to within some tolerance specified

NOTE: Main extra feature of non-linear BVPs is that some iteration is necessary.

EXAMPLE: Unlike the linear case, we cannot write down a general non-linear equation; thus let us illustrate the linearization with an example:

$$y'' + p(x)y^2y' + r(x)y^3 = f(x) \qquad (1)$$

x = a & x = b conditions are specified
Finite difference approximation at x_j to eq.(1)

$$y_{j+1} - 2y_j + y_{j-1} + \frac{h}{2}p_j y_j^2\left(y_{j+1} - y_{j-1}\right) + h^2 r_j y_j^3 = h^2 f_j + \underbrace{Cy_j}_{\text{truncation term}} \qquad (2)$$

Note: Equation (2) is non-linear
To solve eq.(2) , we start off by guessing a solution,

$$y_j^{(0)} \quad , \quad j = 0,1,2,..,n$$

Use above guessed solution to linearize the non-linear terms in eq.(2)

$$y_{j+1}^{(1)} - 2y_j^{(1)} + y_{j-1}^{(1)} + \frac{h}{2}p_j\left\{y_j^{(0)}\right\}^2\left(y_{j+1}^{(1)} - y_{j-1}^{(1)}\right) + h^2 r_j y_j^{(0)^2} y_j^{(1)} = h^2 f_j \qquad (3)$$

Eq.(3) is a linearize eq.& can be solved by a direct method (e.g. Thomas Alg.) to obtain the first solution iterate, $y_j^{(1)}$ j=0,1,2,...,n

Now, test to see wheather $y_j^{(1)}$ is within a specified tolerance of $y_j^{(0)}$ at each internal mesh point; if not repeat the process, but this time using our refined estimate of the solution, $y_j^{(1)}$ to linearize the non-linear terms.

$$y_{j+1}^{(k)} - 2y_j^{(k)} + y_{j-1}^{(k)} + \frac{h}{2} p_j \left\{ y_j^{(k-1)} \right\}^2 \left(y_{j+1}^{(k)} - y_{j-1}^{(k)} \right) + h^2 r_j y_j^{(k-1)^2} y_j^{(k)} = h^2 f_j$$

CONVERGENCE TESTS:

To determine the iteration two basic tests

I. The absolute test

$$\left| y_j^{(k+1)} - y_j^{(k)} \right| < \varepsilon$$

E.g. ε = 10^{-4}

It is not a significant figure test

$$y_m^{(k)} = 3\times 10^{-5} \quad , \quad y_m^{(k)} = 3\times 10^{-5} \quad \text{y is small}$$

Absolute test → convergence occured

But iterates do not agree to even one significant figure

E.g. y_m is large : test may be much more demanding than we wish

y_m = 1234,5678 test asking for 8 significant figures of agreement in successive iterates.

It is not uncommon for the solution of a dif. eq. to contain pivotal values of widely differing in magnitude.

Need a test which takes this into account

II. The Relative Test

$$\left|\frac{y_j^{(k+1)} - y_j^{(k)}}{y_j^{(k+1)}}\right| < \varepsilon \quad \text{or} \quad \left|1 - \frac{y_j^{(k)}}{y_j^{(k+1)}}\right| < \varepsilon$$

Test for significant figures.

If $\varepsilon = 10^{-4}$ two successive iterates must agree to within 4 significant figures at each internal mesh point

Generally gives more satisfactory results

$\left|y_j\right| \geq 10^{-7} \rightarrow$ settle for only testing pivotal values down to a certain minimum magnitude

Falkner-Skan Similarity Solutions

Boundary Layer eqs. (x,y)

Similarity methods → (x,y) → (η)

$$u(x,y) = U(x) f'(\eta) \qquad (1)$$

$$\eta = \frac{y}{\xi(x)}$$

$$\psi(x,y) = U(x)\xi(x) f(\eta) \qquad (2)$$

B.L. eqs.

$$u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}=U\frac{dU}{dx}+\nu\frac{\partial^2 u}{\partial y^2}$$

$$u=\frac{\partial\psi}{\partial y} \quad , \quad v=-\frac{\partial\psi}{\partial x}$$

Substitute (2) in to B.L. eqs. written in terms of ψ and show

$$f'''+\alpha ff''+\beta\left[1-\left(f'\right)^2\right]=0 \quad \text{Falkner-scan eq.}$$

$$\alpha=\frac{\xi}{\nu}\frac{d}{dx}(U\xi) \quad , \quad \beta=\frac{\xi^2}{\nu}\frac{dU}{dx}$$

Flow over a wedge:

α=1 , β=arbitrary

Boundary conditions

$f'(0)=0$ no slip at the wall (u=0)

$f(0)=0$ no slip at the wall (v=0)

$f'(\eta)=1$ as $\eta\to\infty$ B.L. solution merges into the inviscid solution

BVP

$$f''' + ff'' + \beta\left[1-\left(f'\right)^2\right] = 0$$

$$f'(x) = f(0) = 0 \quad , \quad f'(\infty) = 1$$

solve $f(\eta)$ & obtain $f''(0)$

$$\tau_w = A\left(\frac{\mu U_I}{x}\right)^{1/2} f''(0)$$

$$= \mu \frac{\partial u}{\partial y}\bigg|_{y=0}$$

Notes

- Complicated b.c. in $\eta \to \infty$
- Non-linear 3rd order BVP.

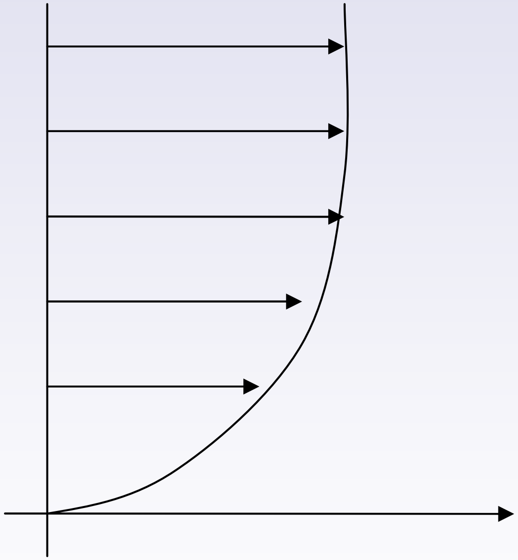
Better to use 2nd order skim,

Let $f'(\eta) = y(\eta) \Rightarrow f(\eta) = \int_0^\eta y(t)dt$

$$y'' + fy' + \beta(1-y^2) = 0 \quad (1)$$

$$f(\eta) = \int_0^\eta y(t)dt \qquad (2) \text{ trapezoid or simpson rule}$$

- Need to iterate
- Use finite difference method not shooting
- β≤-0.19 solution hes multiple solution (do not try)
- guess for y& solve for f by (2)
- use f to solve y by (1)
- iterate until convergence



suggested initial guess for y

$$y = erf\,\eta \quad \text{or} \quad 1 - e^{-\eta^2}$$

Finite difference representation of eq.(1)

$$\frac{y_{i+1}-2y_i+y_{i-1}}{h^2}+f_i\frac{y_{i+1}-y_{i-1}}{2h}-\beta y_i^0 y_i=-\beta \qquad (3)$$

$$y_{i+1}-2y_i+y_{i-1}+f_i\frac{h}{2}\left(y_{i+1}-y_{i-1}\right)-h^2\beta y_i^0 y_i=-h^2\beta \qquad (4)$$

$$y_{i+1}\left[1+f_i\frac{h}{2}\right]+y_i\left[-2-h^2\beta y_i^0\right]+y_{i-1}\left[1-f_i\frac{h}{2}\right]=-h^2\beta \qquad (5)$$

Eq.5 is of the form,

$$b_i y_{i+1}+a_i y_i+c_i y_{i-1}=d_i \qquad (6)$$

Procedure

1. Guess a solution for $y^0(\eta)$

   e.g. $y^0(\eta)=1-e^{-\eta^2}$

2. Solve for $f(\eta)$ from (2)

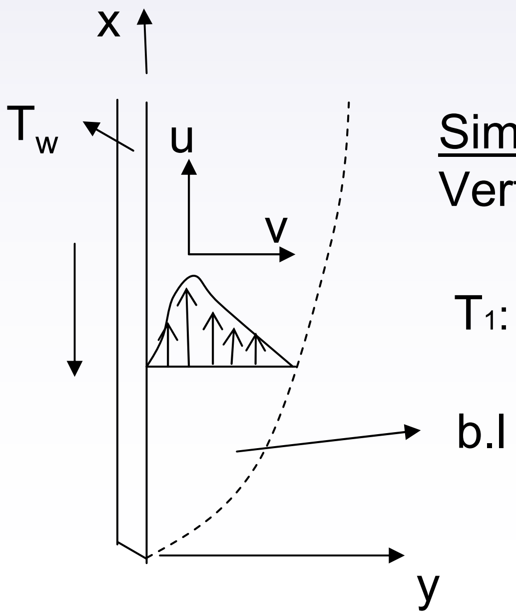
   i.e. $f(\eta_i)=\int_0^{\eta_i} y(t)dt$ trapezoid rule

3. Use $f(\eta_i)$ to solve $y^1(\eta)$ eq.(5) (thomas algorithm)
4. Iterate until convergence

i.e $$\left|\frac{y^{(k)} - y^{(k-1)}}{y^{(k)}}\right| < \varepsilon$$

- Take η = 5-6
- Plot f, f' versus η
- Take β=0,1,&5

LAMINAR NATURAL CONVECTION ON A VERTICAL SURFACE



Similarity solutions:

Vertical surface is held at a uniform surface temperature, T_w .

T_1: ambient fluid temperature

Boundary Layer equations governing the flow

$$\frac{\partial^2 u}{\partial x^2} << \frac{\partial^2 u}{\partial y^2} \quad , \quad v << u \quad , \quad Gr >> 1$$

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

$$u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = \nu\frac{\partial^2 u}{\partial y^2} + \beta g(T - T_1)$$

$$u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y} = \alpha\frac{\partial^2 T}{\partial y^2}$$

$$\nu = \frac{\mu}{\rho} \quad , \quad \alpha = \frac{k}{\rho c_p}$$

B.Cs:

At y=0 , u=v=0 , T=Tw

For large y: u→0 , T→ T1

Velocity & temperature profiles are similar at all values of x.

i.e.

$$\frac{u}{u_r} = func\left(\frac{y}{\delta}\right)$$

$$\frac{T - T_1}{T_w - T_1} = func\left(\frac{y}{\delta}\right)$$

$$u_r = \sqrt{\beta g\left(T_w - T_1\right)x}$$

u_r : reference velocity

δ: measure of both local velocity & thermal b.layer thicknesses

Define a streched variable near the plate

$$\eta = \frac{Gr^{1/4}}{L^{3/4}}\frac{y}{x^{1/4}}$$ which magnifies the thin b.l. region (Gr>>1)

The velocity components are

$$u = \frac{U}{L^{1/4}}x^{1/2}f'(\eta) \quad , \quad v = \frac{UL^{1/4}}{4Gr^{1/4}x^{1/4}}(\eta f' - 3f)$$

$$U = \sqrt{g\beta L(T_w - T_1)}$$

$$\theta(\eta) = \frac{T - T_1}{T_w - T_1}$$

Substituting momentum eq. & energy eq.

$$f''' + \frac{3}{4}ff'' - \frac{1}{2}f'^2 + \overset{\text{driving force}}{\theta} = 0$$

$$\theta'' + \frac{3}{4}\Pr f\theta' = 0$$ Prandtl number

B.Cs

At $y=0\ u=0 \ \Rightarrow\ \eta=0:\ f'=0$ (no-slip)

At $y=0\ v=0 \ \Rightarrow\ \eta=0:\ f=0$ (solid wall)

At $y=0\ T=T_w \ \Rightarrow\ \eta=0:\ \theta=1$ (const. plate temp.)

For large y: $u\to 0 \ \Rightarrow\ \eta\to\infty:\ f'\to 0$ (no motion in the ambient)

For large y: $T\to T_1 \ \Rightarrow\ \eta\to\infty:\ \theta\to 0$

Local nusselt number gives the heat transfer from the plate to the fluid per unit area per unit time

$$Nu_x = -Gr^{1/4}\frac{x^{3/4}}{L^{3/4}}\left.\frac{\partial\theta}{\partial\eta}\right|_{\eta=0}$$

$\theta'(0)$ needs to be numerically calculated

Numerical solution

$$f''' + 3ff'' - 2f'^2 + \theta = 0 \qquad (1)$$

$$\theta'' + 3\Pr f\theta' = 0 \qquad (2)$$

Let f′=y

$$y'' + 3fy' - 2y^2 + \theta = 0$$

$$\theta'' + 3\Pr f\theta' = 0$$

Finite difference representation

$$\frac{y_{i+1}-2y_i+y_{i-1}}{h^2}+3f_i\frac{y_{i+1}-y_{i-1}}{2h}-2y_i^2+\theta_i=0$$

$$y_{i+1}^{(1)}-2y_i^{(1)}+y_{i-1}^{(1)}+f_i\frac{3h}{2}\left(y_{i+1}^{(1)}-y_{i-1}^{(1)}\right)-2h^2y_i^{(0)}y_i^{(1)}+h^2\theta_i=0$$

$$y_{i+1}^{(k)}\underbrace{\left[1+f_i\frac{3h}{2}\right]}_{b_{\mathrm{i}}^{(\mathrm{k})}}+y_i^{(k)}\underbrace{\left[-2-2h^2y_i^{(k-1)}\right]}_{a_{\mathrm{i}}^{(\mathrm{k})}}+y_{i-1}^{(k)}\underbrace{\left[1-f_i\frac{3h}{2}\right]}_{c_{\mathrm{i}}^{(\mathrm{k})}}=\underbrace{-h^2\theta_i}_{\mathrm{d}_{\mathrm{i}}^{(\mathrm{k})}}$$

$$\frac{\theta_{i+1}-2\theta_i+\theta_{i-1}}{h^2}+3\,\mathrm{Pr}\,f_i\frac{\theta_{i+1}-\theta_{i-1}}{2h}=0$$

$$\theta_{i+1}\underbrace{\left(1+f_i\,\mathrm{Pr}\frac{3h}{2}\right)}_{b_i}+\theta_i\underbrace{(-2)}_{a_i}+\theta_{i-1}\underbrace{\left(1-f_i\,\mathrm{Pr}\frac{3h}{2}\right)}_{c_i}=\underbrace{0}_{d_i}$$

<u>Procedure</u>

1. Guess $y^0(\eta)$
2. Find $f(\eta_i)=\int_0^{\eta_i} y(t)dt$ trapezoid rule
3. Use Thomas algorithm to find θ_i

4. Use thomas algorithm to find $y_i^{(1)}$ [using θ_{i} & $y_i^{(0)}$]

5. Iterate until convergence

i.e. $\left|\dfrac{y^{(k)}-y^{(k-1)}}{y^{(k)}}\right|<\varepsilon$ for all i=0,..,N

Notes:

- Infinity about 12
- Use iterative averaging, i.e %50 old, %50 new
- Limit IMAX 100
- provide good initial guess, e.g. $y(\eta)=1-e^{-\eta^2}$

From the derivation of B.L. eqs.

$$\frac{\delta}{x}=\vartheta\left[\frac{1}{Gr_x^{1/4}}\right]$$

$$Gr_x=\frac{\beta g(T_w-T_1)x^3}{\nu^2}$$

Grashof number main parameter in free convection controlling the nature of the motion

$\eta :$ similarity variable

$$\eta = \frac{y}{x} Gr_x^{1/4}$$

$$\frac{u}{\sqrt{\beta g(T_w - T_1)x}} = F'(\eta) \qquad ; \qquad \frac{T - T_1}{T_w - T_1} = \theta(\eta)$$

Following dimensionless variables are introduced

$$U = \frac{u}{\sqrt{\beta g(T_w - T_1)x}} = \left(\frac{ux}{\nu}\right) Gr_x^{-0.5}$$

$$V = \frac{v}{\sqrt{\beta g(T_w - T_1)x}} = \left(\frac{vx}{\nu}\right) Gr_x^{-0.5}$$

$$\text{cont. eq. } V = \frac{1}{4Gr_x^{-0.5}} [\eta F' - 3F]$$

Writing momentum eq. in terms of dimensionless variables

$$U \frac{\partial u}{\partial x} + \frac{U^2}{2x} + V \frac{\partial u}{\partial y} = \nu \frac{\partial^2 u}{\partial y^2} \frac{1}{\sqrt{\beta g(T_w - T_1)x}} + \frac{\theta}{x}$$

Shooting Methods for BVPs

- Make use of techniques that are normally designed to solve IVP.
- Usually 4th order RK methods are used
- Called marching schemes→ march away from the initial data point constructing the solution in a step-by-step manner.

Let us illustrate the approach using an example of a non-linear second order dif. eq.

$$y'' + p(x)yy' + r(x)y^4 = f(x) \qquad (1)$$

$$y(a) = A \quad , \quad y(b) = B \qquad (2)$$

Let us recast the problem as a sequence of two first order equations

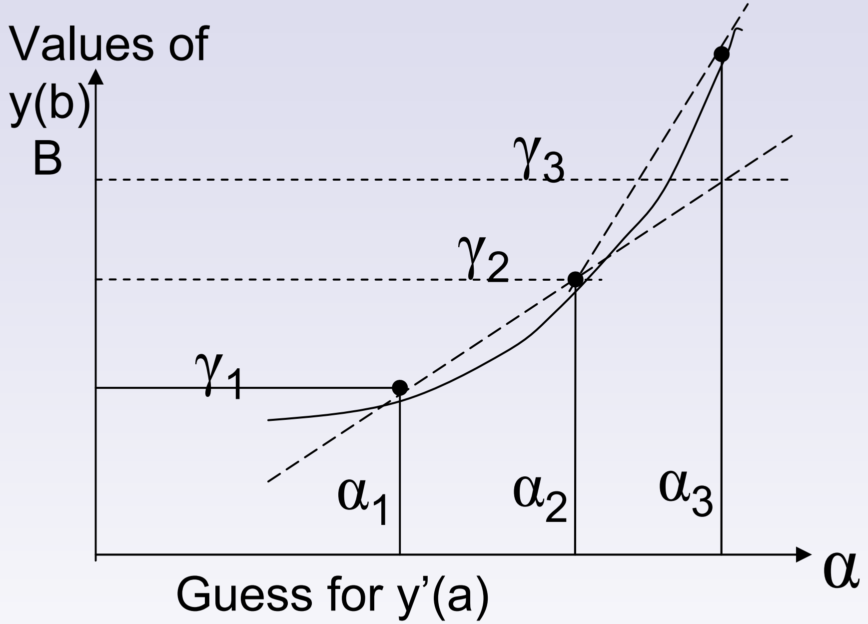
$$\left.\begin{aligned} y' &= z \\ z' &= f(x) - p(x)yz - r(x)y^4 \end{aligned}\right\} \quad (3)$$

Now, if y(a) & z(a)=y'(a) were known, eqs.(3) would define an IVP, and could use a RK4 scheme to construct the solution in a step-by-step manner for values of x>a .

We don't know z(a)=y'(a) & so we GUESS some value for it, $z(a)=\alpha_1$ so the system of two equations (3) may be integrated forward in x as an initial value problem. But, when we reach x=b , y(b)=B will not be, in general, satisfied. Other value $y(b)=\gamma_1$

Problem is to find an intelligent way to go back and adjust the guess for y'(a) so that the condition at x=b will be satisfied.

Select another value of y'(a), say $z(a)=\alpha_2$ and integrate again & produce another value $y(b)=\gamma_2$



The problem is determine where this numerical function intersets the true boundary condition,

$\gamma=B \rightarrow \alpha = ?$ In practice,

Having guessed two values α_1 and α_2 for $z(a)=y'(a)$,

$z(a)=\alpha_1 \rightarrow y(b)=\gamma_1$

$z(a)=\alpha_2 \rightarrow y(b)=\gamma_2$

Equation of the line passing through (α_1, γ_1) & (α_2, γ_2)

$$\frac{\gamma - \gamma_1}{\gamma_1 - \gamma_2} = \frac{\alpha - \alpha_1}{\alpha_1 - \alpha_2} \quad \text{linear interpolation}$$

But we want γ=B so this gives us a revised guess to try for α_3

$$\alpha_3 = \alpha_1 + \frac{(\alpha_1 - \alpha_2)(B - \gamma_1)}{\gamma_1 - \gamma_2} \qquad (4)$$

Use α_3 to start another integration of eq.(3)

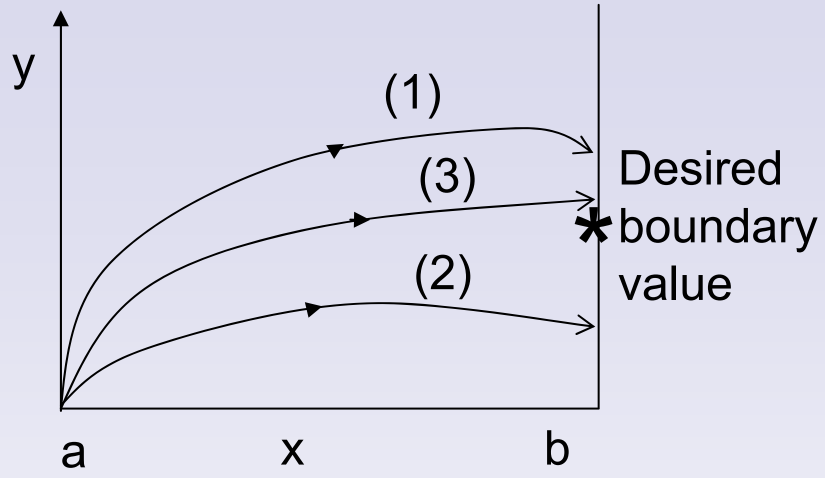
$$y'(a) = z(a) = \alpha_3 \rightarrow y(b) = \gamma_3$$

(α_1, γ_1) , (α_2, γ_2) , (α_3, γ_3) take a line between whichever of the three points have values of γ closes to B, and use this line to obtain a new estimate of z(a)= α_4
Iterate until convergence

$$\left|\alpha_{i+1} - \alpha_i\right| \le \varepsilon \quad \text{tolerance} \quad (5)$$

$$\left|\gamma_{i+1} - B\right| \le \varepsilon$$

Technique is called shooting method
We are adjusting the slope of our “gun” with the objective of hitting the “target” of the true boundary condition at x=b



Comments on this procedure

1. Method may not convergence at all if α_1 & α_2 the initial guesses are not "reasonably" close to the correct value of y(b)=B. Usually some trial&error calculations may be necessary in order to ensure that α_1 & α_2 produce values af γ_1 & γ_2 which are not radically different from B
2. this method is very laborious & almost useless if more than one B.C. must be shot at

E.g.

$$y'' = f(x, y', u, u')$$

$$u'' = g(x, y', u, u')$$

with the B.C.

$$y(a) = A \ , \ y(b) = B$$

$$u(a) = C \ , \ u(b) = D$$

Two values at x=b must be shot at.
Parallel shooting techniques can be used but labourious methods

3. Shooting methods may also fail when the eqs. contain an unwanted solution that may invariably be introduced in the marching procedure.

Example

$$y'' - y = 0$$

general solution $y(x) = A_1 e^{-x} + A_2 e^{x}$

if B.C. are specified such that

$$y(0) = 1 \ , \ y \to 0 \ as \ x \to \infty$$

$$\Rightarrow A_1 = 1, A_2 = 0$$

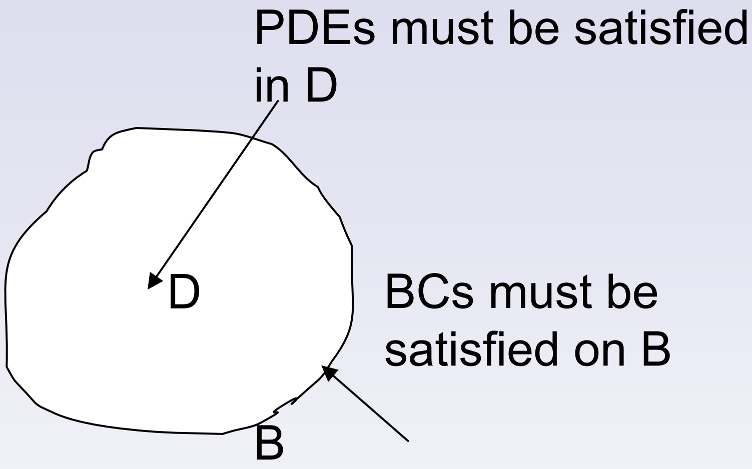
If we try to shoot for the value 0 for large values of x, failure of the scheme will occur abruptly with an overflow due to exp(x) .

- Can solve it by going back & try to adjust the guessed slope if values of y get too large
- But difficult
- Boundary value methods are in general preferable for boundary value problems

PARTIAL DIFFERENTIAL EQUATIONS (PDEs)

Physical classification

Equilibrium Problems: BVPs (Jury problems)

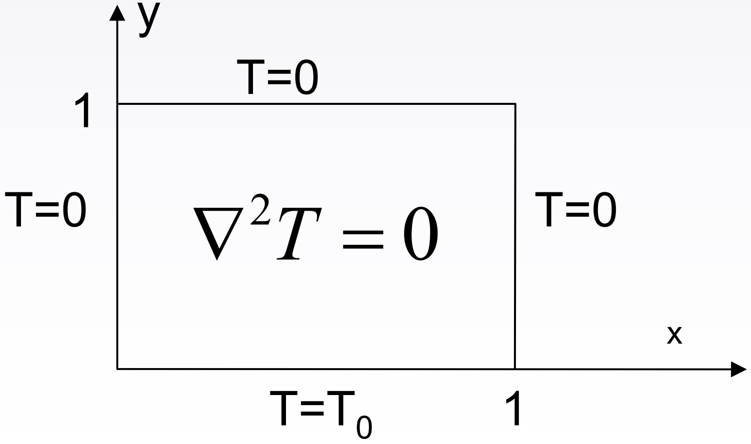


PDEs must be satisfied in D

BCs must be satisfied on B

- Steady state temperature distributions
- Incompressible inviscid flows
- Equilibrium stress distribution in solids

Ex1: Heat conduction in solids in steady state



$$\nabla^2 T = 0$$

Seperation of variables,

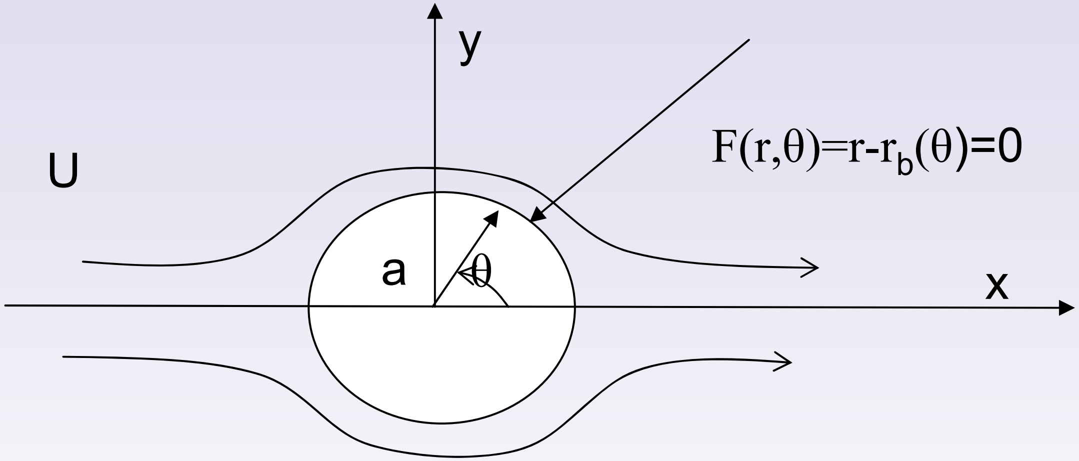
$$T(x,y) = \sum_{n=1}^{\infty} A_n \sin(n\pi x)\sinh\left[n\pi(y-1)\right]$$

$$A_n = \frac{2T_0}{n\pi}\frac{\left[(-1)^n - 1\right]}{\sinh(n\pi)}$$

Ex2: Irrotational flow of an incompressible inviscid fluid is governed by Laplace’s eq.

$$\nabla^2\phi = 0$$

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



B.Cs on surface of cylinder is $\vec{V}.\nabla F = 0$

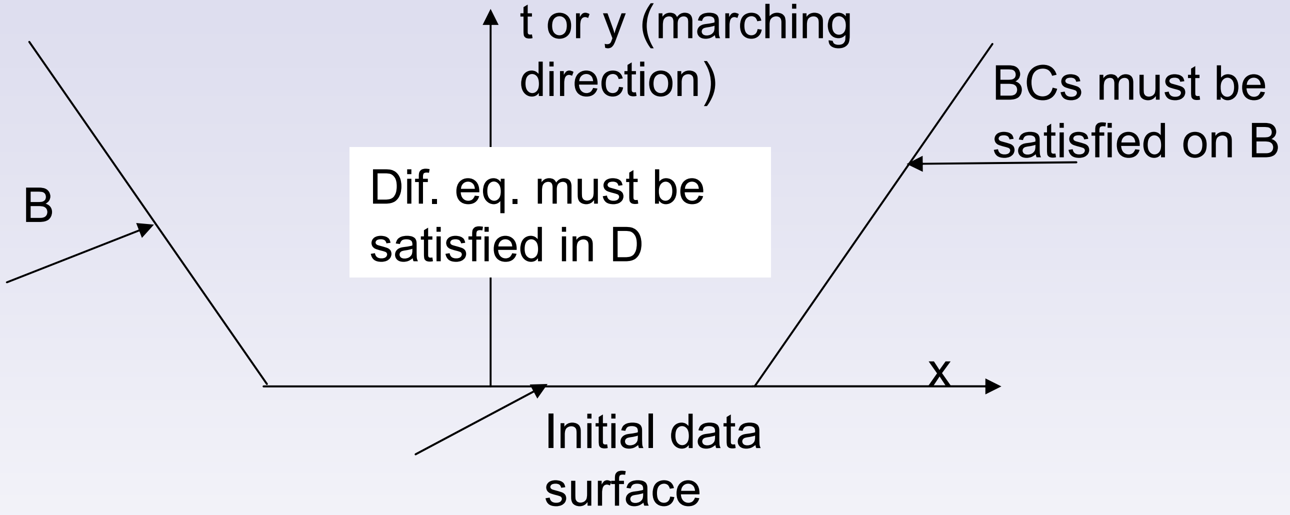
Where F(r,θ)=0 is equation of surface of cylinder.

In addition, velocity must approach free stream value as distance from body becomes large, i.e., as (x,y)→∞ $\nabla\phi = \vec{U}_\infty$

$$\phi = U_\infty x + \frac{K\cos\theta}{\sqrt{x^2+y^2}} = U_\infty x + \frac{Kx}{x^2+y^2}$$

Marching Problems: IVP or IBVP

Marching or propagation problems are transient or transient-like problems



Domain for a marching problem

The solution must be computed by marching outward from initial data surface while satisfying BCs.

Mathematically, these problems are governed by either hyperbolic or parabolic PDEs.

Examples: 1-Dimensional Wave eq. &
1-Dimensional diffusion equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$$

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$

Mathematical Classification of PDEs

Need to examine some mathematical properties of PDEs.

Governing PDEs in Fluid Mech. are quasi-linear

i.e. highest-order derivatives occur linearly

no products or exponentials of the highest-order derivatives.

The general quasi-linear second order PDE in two independent variables is given below

$$A\frac{\partial^2 u}{\partial x^2}+B\frac{\partial^2 u}{\partial x\partial y}+C\frac{\partial^2 u}{\partial y^2}=f$$

Where A,B,C,f may all be functions of x,y, $\frac{\partial u}{\partial x},\frac{\partial u}{\partial y}$ but not allowed to contain second derivatives.

Strict linear case : A,B,C are functions of x and y and f is, at worst, a linear combination of

$\frac{\partial u}{\partial x},\frac{\partial u}{\partial y}$ as well as depending on x & y

If B^2-4AC > 0 → Hyperbolic PDE , Two real distinct characteristics exist at each point in x-y plane

B^2-4AC = 0 → Parabolic PDE , one real characteristic

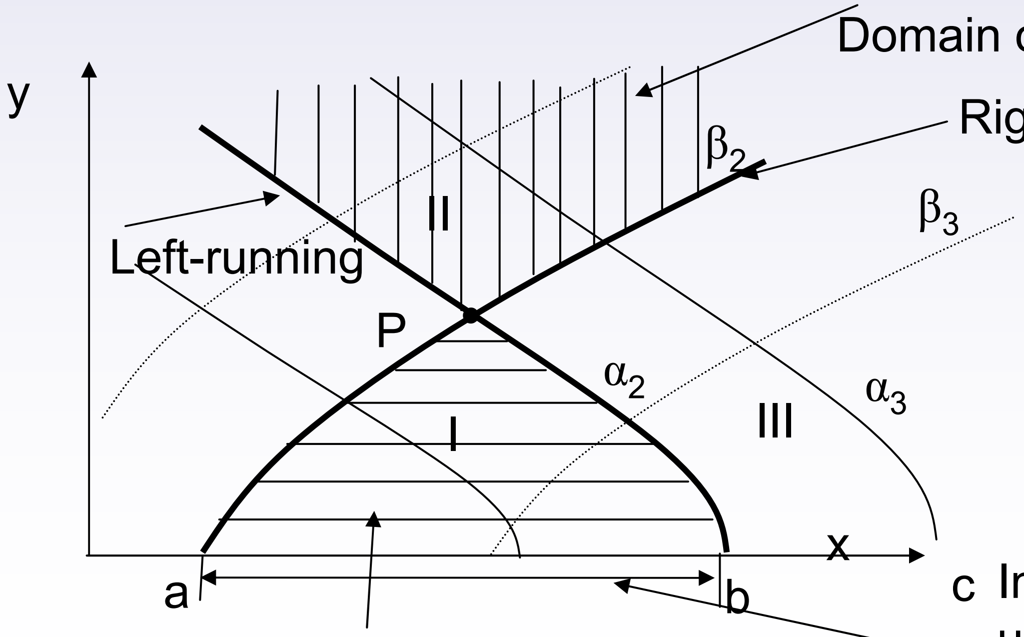
B^2-4AC < 0 → Elliptic PDE , characteristics are imaginary

$$\frac{dy}{dx}=\frac{B\pm\sqrt{B^2-4AC}}{2A}$$

See Tannehill et.al. 1997, page 24 for derivation

Characteristic lines are related to directions in which "information" can be transmitted in physical problems governed by PDEs.

Hyperbolic PDEs with two independent variable x & y



Domain of influence: region influenced by P

Right-running

Left-running

Domain of dependence for P

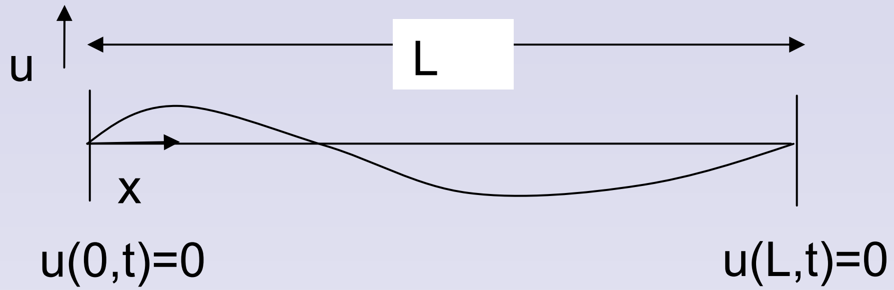
Initial data along the x axis upon which P depends (boundary conditions) α = cont. & β=const. lines represent the two families of characteristics along which signals can propagate

- Observer at point P can feel the effects of what has happened in Region I. The <u>domain of dependence region.</u> Outside Region I, disturbance cannot be felt by P.
- Disturbance created at point P can be felt only in the Region II, i.e. Region II is the domain of influence of point P.

<u>Hyperbolic eqs.</u> domains extend to infinity in the time like coordinate

- Solution can be obtained by “marching forward” in the distance y, starting from the given boundary
- Spatial coordinate may or may not be bounded
- Normally associated with initial value problems
- Typically two initial conditions at t=0 are specified
- If the spatial region is bounded → boundary conditions

Example: Best known example, one dimensional wave eq.

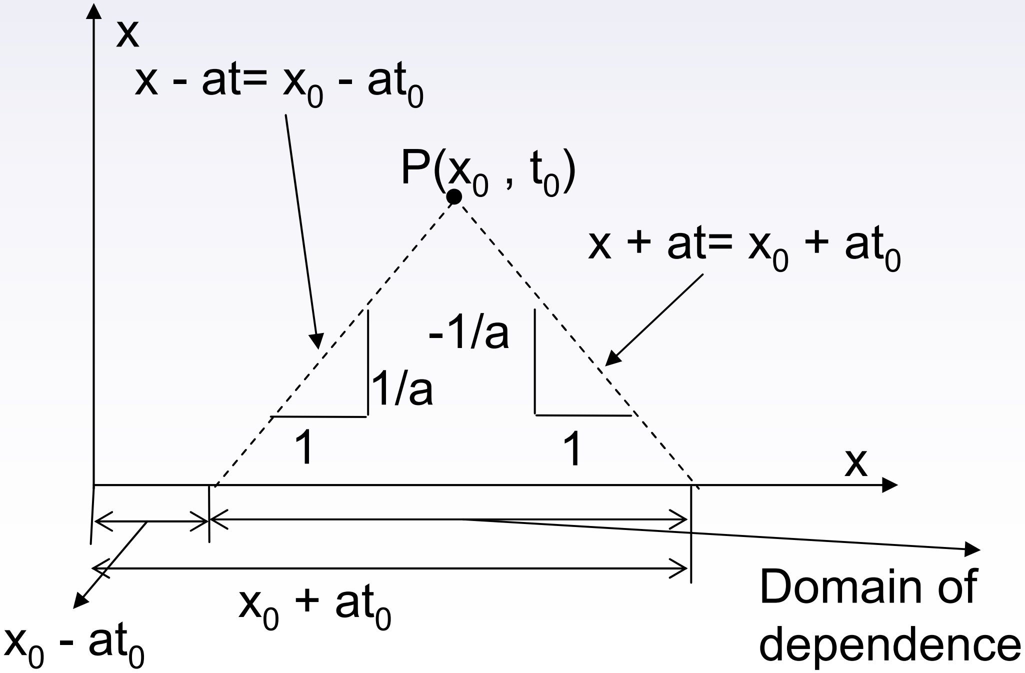


$$\frac{\partial^2 u}{\partial t^2} = a^2 \frac{\partial^2 u}{\partial x^2}$$ $-\infty < x < \infty$

With I.C. $u(x,0)=f(x)$ $A=a^2$, $B=0$, $C=1$

$$\frac{\partial u}{\partial t}(x,0) = g(x)$$

$$\frac{dt}{dx} = \frac{B \pm \sqrt{B^2 - 4AC}}{2A} = \frac{0 \pm \sqrt{0 - 4a^2}}{2a^2} = \pm \frac{1}{a}$$



$x + at = \text{const.} = x_0 – at_0$
$x – at = \text{const.}$

$u(x,t) = F_1(x + ct) + F_2(x - ct)$
D' Alembert solution of wave equation.
$u(x,t)$ at (x_0, t_0) depends only upon initial data contained in the interval.
$x_0 - at_0 \le x \le x_0 + at_0$

$$u(x,t) = \frac{f(x+ct)+f(x\text{-}ct)}{2} + \frac{1}{2a}\int_{x-at}^{x+at} g(\tau)d\tau$$

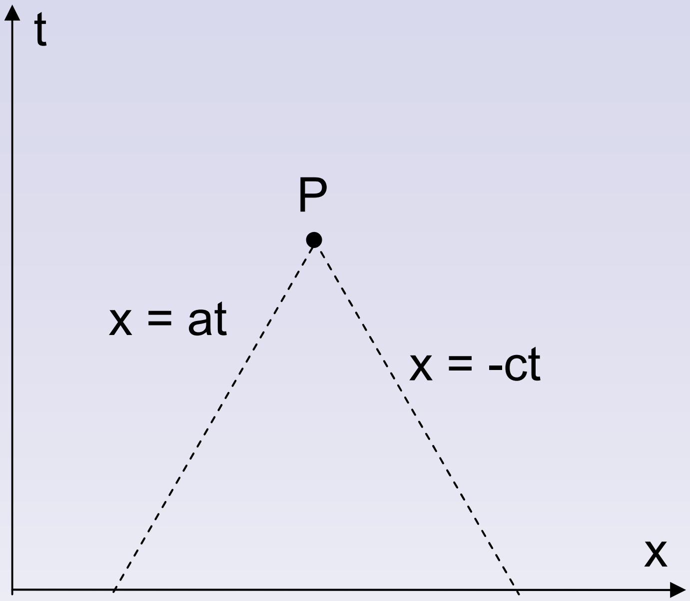
u(x,t) displacement of the string of length L above the equilibrium position
t: time

Initial conditions:
Initial displacements u(x,0) of string; e.g. $u(x,0)=\sin(\pi x/L)$

Initial velocity $\frac{\partial u}{\partial t}(x,0)$ $\quad$ $\text{e.g.}\frac{\partial u}{\partial t}(x,0) = 0 \;\; \text{(released from rest)}$

Find u(x,t) = ? for t>0 all x $\quad u(x,t) = \sin\left(\frac{\pi x}{L}\right)\cos\left(a\frac{\pi x}{L}\right)$

Characteristic lines $\quad x = \begin{cases} \text{at right-running} \\ \text{-at left-running} \end{cases} \frac{dt}{dx} = \pm L$



$x + at = \text{const.} = x_0 + at_0$

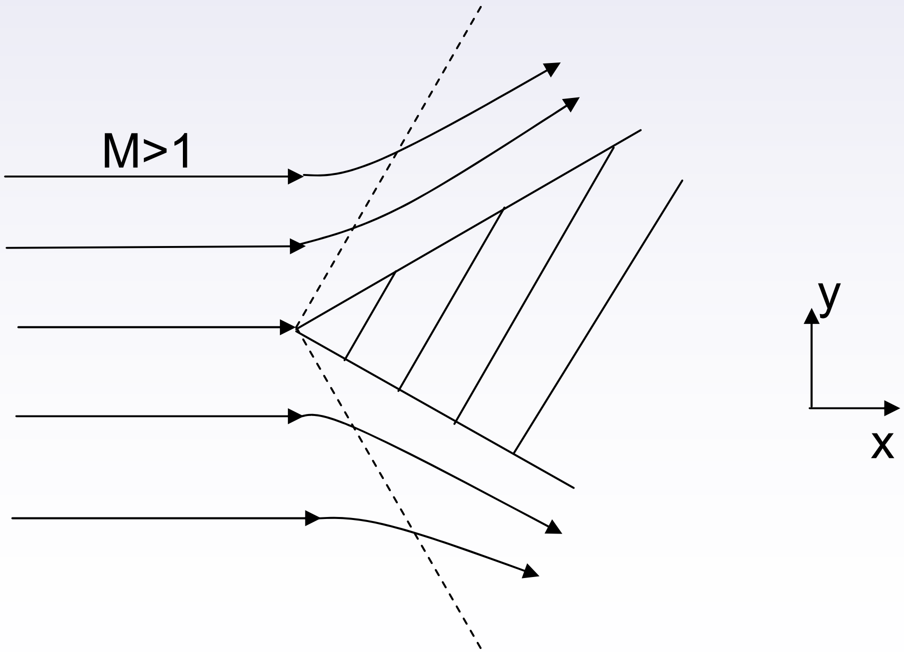
$x - at = \text{const.} = x_0 - at_0$

Fluid Mechanics Examples:

I. Steady, inviscid supersonic flow

$$\left(M^2 - 1\right)\frac{d^2\Phi}{dx^2} - \frac{d^2\Phi}{dy^2} = 0$$

Φ : disturbunce velocity profile



II. Unsteady, inviscid compressible flow

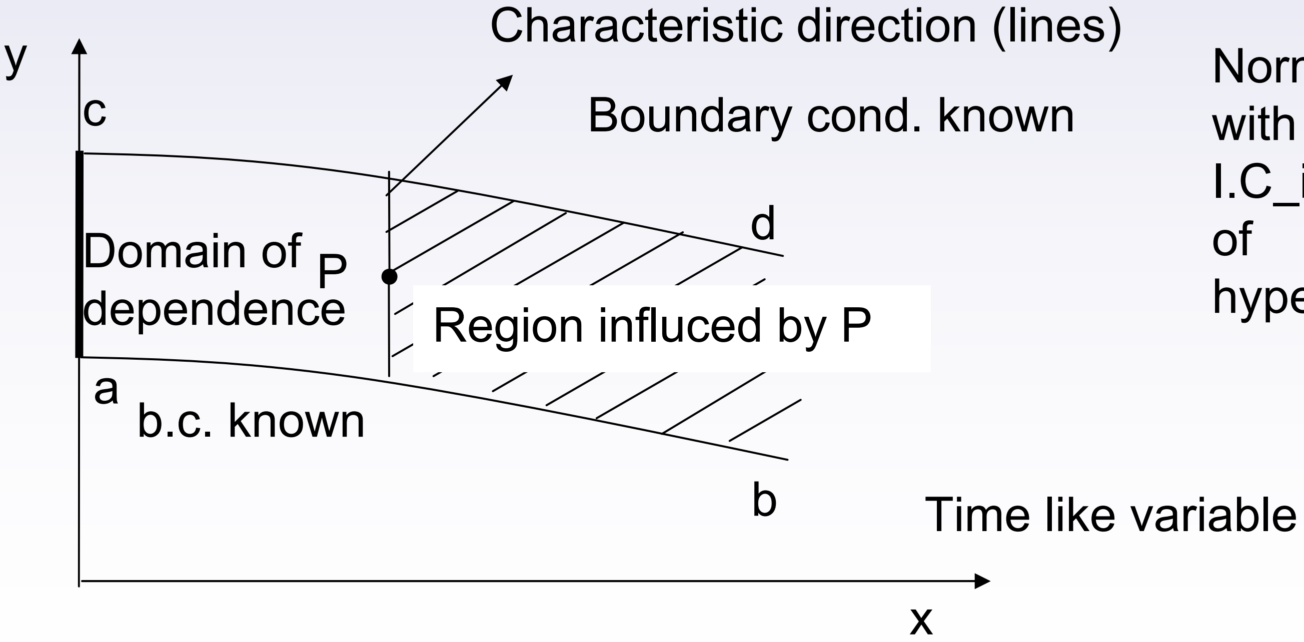
Unsteady 1-D & 2-D inviscid flows → hyperbolic

Time is the marching direction

$$\frac{\partial^2 \phi}{\partial t^2} = c^2 \frac{\partial^2 \phi}{\partial x^2}$$ water-hammer problems wave equation.

Parabolic PDEs

Only one characteristic direction at a point

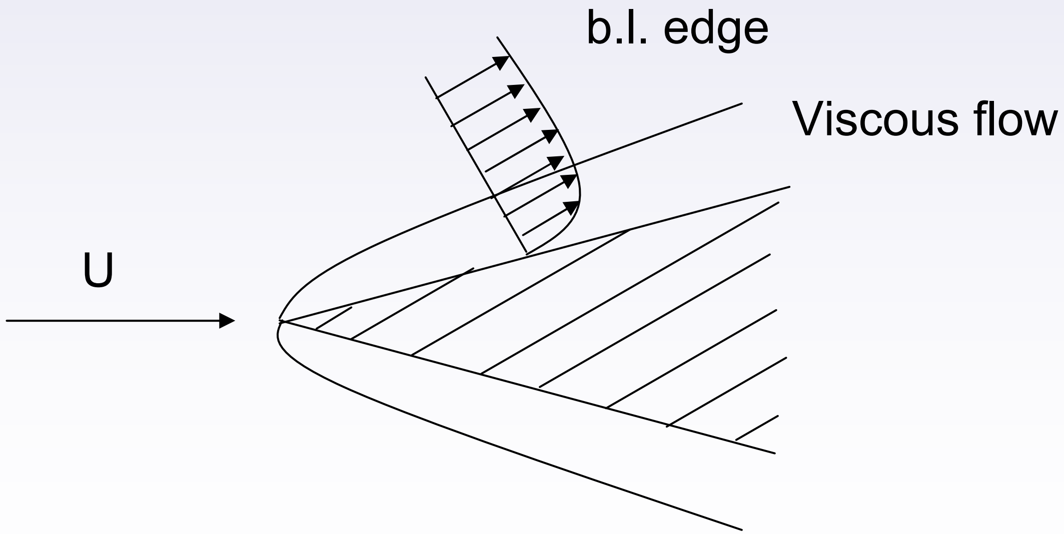


Normally associated with IVPs but only one I.C_is required instead of two (as for hyperbolic eq.)

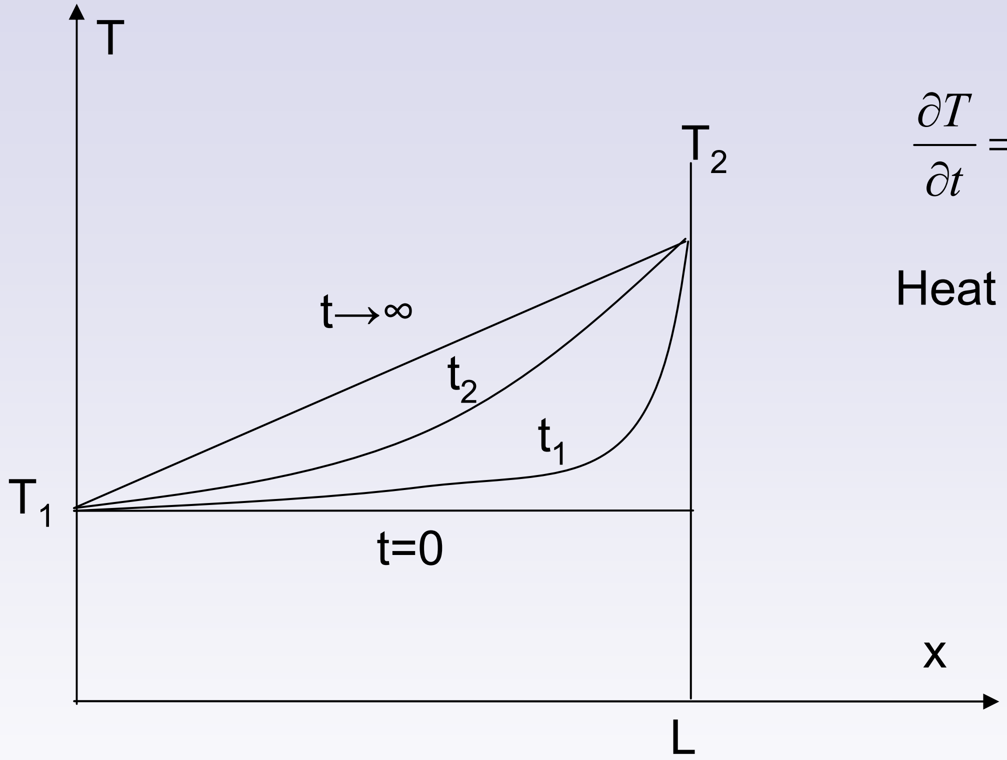
Parabolic equation in two independent variables x & y

- Information at point P influences the entire region on one side of the vertical characteristic and contained by the boundaries
- “marching solutions” applicable

<u>Fluid Mech.</u> B.L. eqs.→ parabolized N-S eqs.



Unsteady heat conduction: the best known example



$$\frac{\partial T}{\partial t} = \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) \qquad \alpha\text{:const.}$$

Heat conduction eq. (diffusion eq.)

$T(x,0)=T_1$=const.
$T(L,t)=T_2$=const.
$T(0,t)=T_1$=const.
$T(x,t)$=?

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

α : thermal diffusity

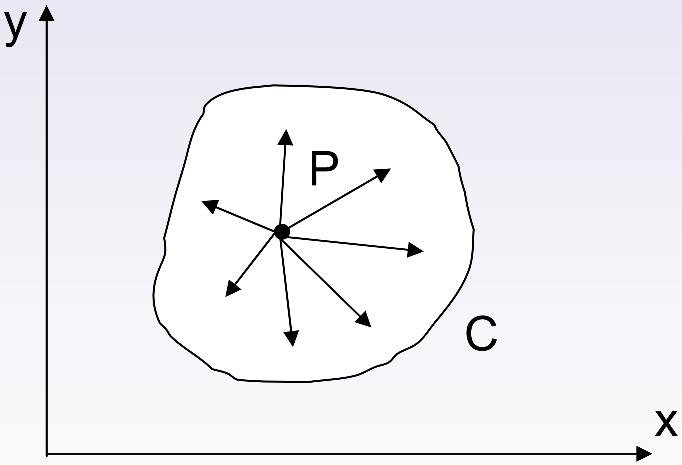
$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial x^2}$$

Elliptic PDEs

Consider an elliptic equation in two independent variables x & y

- Characteristic curves are imaginary
- No preferred direction of propation

i.e. information is propagated everywhere in all directions any disturbance at point P influences the solution everywhere

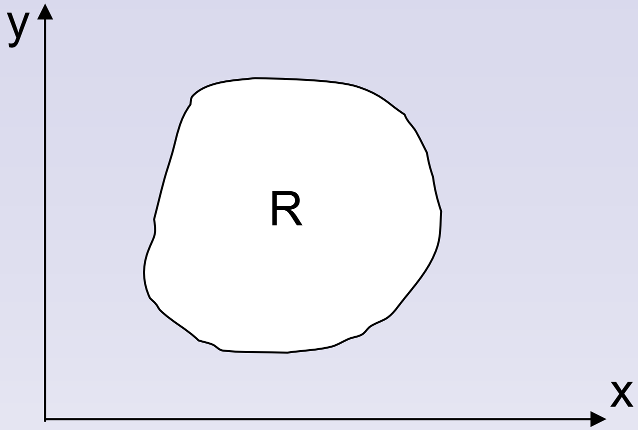


e.g. $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$

Conditions must be specified on closed curve C
u is continious on R+C

Max/Min Property: U_{max} and U_{min} must be on C

Boundary conditions



C. piecewise regular

$$\nabla^2 u = 0$$

I. u=f(x,y) on C.. Dirichlet Problem (unique)

II. $\frac{\partial u}{\partial n} = g(x, y)$ on C: Neumann Probl. (not unique) u must be specified at least one point

III. Combination of u & $\frac{\partial u}{\partial n}$ is known $\frac{\partial u}{\partial n} + Au = B \quad \Rightarrow$ Robin's Probl.

IV. Mixed problems → combination of these conditions on various parts of C

<u>Also</u> can have non-linear conditions e.g. radition

$$\frac{\partial u}{\partial n} + AT^n = B$$

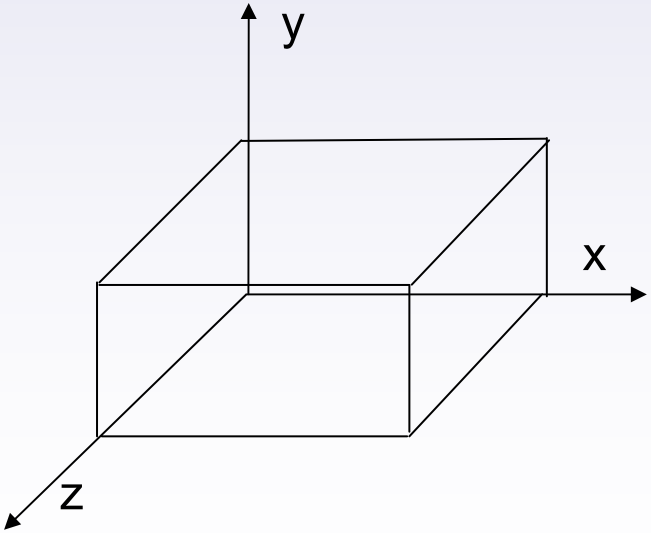
Example:

- Heat conduction in solids. $\nabla^2 T = f(x, y)$

- Steady, subsonic, inviscid
- Incompressible inviscid flow. M→0

$$\nabla^2 \psi = 0 \quad \text{streamlines}$$

$$\text{irrototainal flow } \vec{\omega} = \nabla . \vec{V} = 0$$



$$\cancel{\frac{\partial u}{\partial t}} = \left(\frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right)$$

Steady, Fully-developed velocity profile

$$\cancel{\frac{\partial u}{\partial t}} + \underbrace{u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}}_{\text{convective terms}} = -\frac{1}{\rho}\frac{\partial p}{\partial x} + \nu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)$$

Creeping flow: $\nabla^2 P = 0$

$$\nabla.\vec{V} = 0$$

$$\rho\frac{D\vec{V}}{Dt} = -\nabla P + \mu\nabla^2\vec{V}$$

ρ=const.

$$\rho\left(\frac{\partial \vec{V}}{\partial t} + \cancel{\underbrace{\left(\vec{V}.\nabla\right)}_{0\ \text{non-linear term}}}\,\vec{V}\right) = -\nabla P + \mu\nabla^2\vec{V}$$

Parallel flow, v=w=0 , u≠0

continuity $\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0\rightarrow\frac{\partial u}{\partial x}=0\rightarrow u=u(y,z,t)$

y-comp. $\frac{\partial P}{\partial y}=0$, $\frac{\partial P}{\partial z}=0\rightarrow p=p(x,t)$

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

$\rho\frac{\partial u}{\partial t}=-\frac{\partial P}{\partial x}+\mu\left(\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right)$ Parabolic

Linear differantial equation for u(y,z,t)

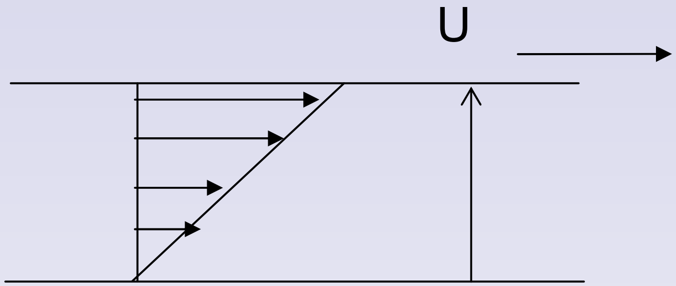
Steady flow → $\frac{\partial u}{\partial t}=0$

$$\underbrace{\nabla^2 u=\frac{1}{\mu}\frac{\partial P}{\partial x}}_{\text{elliptic}}$$

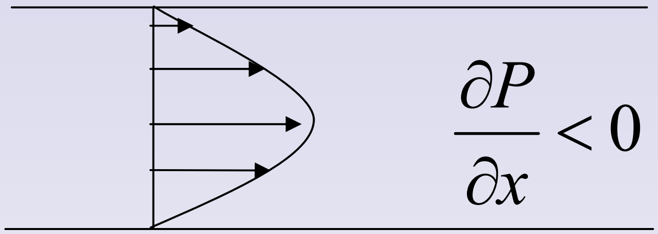
Poisson equation basic differential equation for fully devoloped duct flow.

Ex

I. Coutte flows



II. Poiseuille Flow



$$\frac{\partial P}{\partial x} < 0$$

CREEPING FLOW: Re<<1 , limiting case of very large viscosity

Full N-s , for ρ=const. , μ=const. (steady flow)

$$\rho\left(\frac{\partial\vec{V}}{\partial t}+\left(\vec{V}.\nabla\right)\vec{V}\right)=-\nabla P+\underbrace{\mu\nabla^2\vec{V}}_{\text{viscous force}}$$

$$\left(\vec{V}.\nabla\right)\vec{V}\rightarrow 0 \text{ (inertial force)}$$

$$\nabla P=\mu\nabla^2\vec{V}$$

$$\nabla.\vec{V}=0$$

$$\frac{\partial p}{\partial x}=\mu\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right)$$

Take div($\nabla.$) of the momentum eq.

$$\nabla.(\nabla P) = \nabla^2 P = \nabla.(\mu \nabla^2 \vec{V}) \qquad \mu\text{=const.}$$

$$= \mu \nabla.(\nabla^2 \vec{V}) = \mu \nabla^2 (\nabla \vec{V}) = 0$$

$$\nabla^2 P = 0 \quad \text{Laplace equation}$$

VORTICITY TRANSPORT EQ:

2-D , vorticity-stream function formulation , ρ=const.

$$\nabla.\vec{V} = 0 \qquad (1)$$

$$u = \frac{\partial \psi}{\partial y} \quad , \quad v = -\frac{\partial \psi}{\partial x} \qquad (2)$$

$$\frac{\partial^2 \psi}{\partial x \partial y} - \frac{\partial^2 \psi}{\partial y \partial x} = 0 \qquad (1') \ \text{Identical satisfied}$$

Take the curl $(\nabla \times)$ of the 2-D vector momentum equation

$$\nabla \times \left(\frac{\partial \vec{V}}{\partial t} \right) + \nabla \times \left(\vec{V}.\nabla \right) \vec{V} = \cancel{\nabla \times \vec{g}} - \cancel{\frac{1}{\rho} \nabla \times (\nabla P)} + \nu \nabla \times \left(\nabla^2 \vec{V} \right)$$

Let $\vec{\omega} = \nabla \times \vec{V}$ be vorticity

$$\frac{\partial \vec{\omega}}{\partial t} + \left(\vec{V} . \nabla\right) \vec{\omega} = \nu \nabla^2 \vec{\omega}$$ Vorticity transport equation

$$\vec{\omega} = \omega_z \vec{k} \quad \text{2-D} \; , \; \omega_x = \omega_y = 0$$

$$\frac{\partial \omega_z}{\partial t} + u \frac{\partial \omega_z}{\partial x} + v \frac{\partial \omega_z}{\partial y} = \nu \left(\frac{\partial^2 \omega_z}{\partial x^2} + \frac{\partial^2 \omega_z}{\partial y^2} \right)$$

$$\omega_z = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}$$

$$\frac{D\omega}{Dt} = \nu \nabla^2 \omega \quad \text{2 eqs. 2 unknowns (u,v)}$$

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

$$\omega = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} = -\frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi}{\partial y^2} = -\nabla^2 \psi$$

$$\left.\begin{aligned} \frac{D\omega}{Dt} &= \nu \nabla^2 \omega \\ \nabla^2 \psi &= -\omega \end{aligned}\right\} \omega, \psi \quad \text{formulation, 2-D , } \rho\text{=const.}$$

Irrotational flow (inviscid) , $\vec{\omega} = \nabla \times \vec{V} = 0$

$\nabla^2 \psi = 0$ Laplace eq.

Velocity potential $\vec{\mathrm{V}} = \nabla \phi = \left(\frac{\partial \phi}{\partial x} \vec{i} + \frac{\partial \phi}{\partial y} \vec{j} \right)$

$$\nabla . \vec{\mathrm{V}} = 0 \Rightarrow \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0$$

DISCRETIZATION of PDEs

1. Finite difference methods
2. Finite volume methods
3. Finite element methods
4. Spectral (element) methods
5. Boundary element methods
6. ...

Need to replace a partial derivative with a suitable finite difference quotient

$$u(x, y) \rightarrow \frac{\partial u}{\partial x} = ?$$

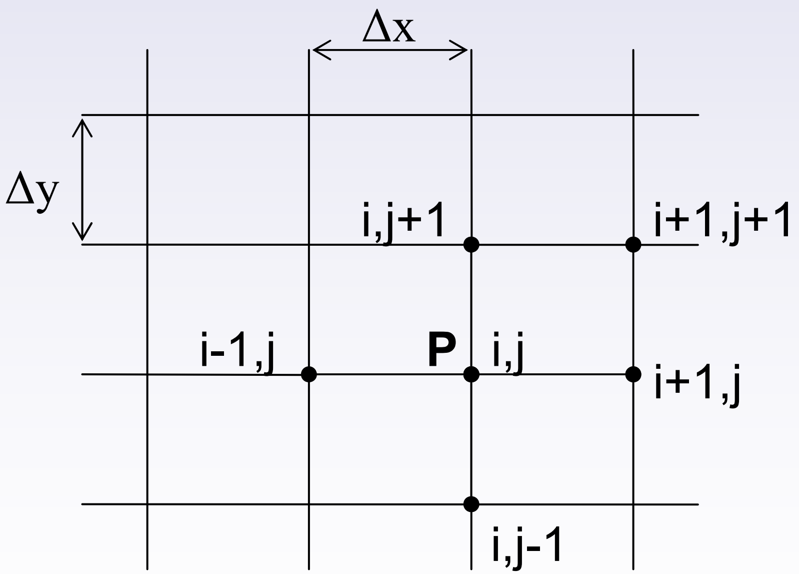
Let $u_{i,j}$ be a component of velocity at point (i,j)

Taylor series expansion for $u_{i+1,j}$, expanded about $u_{i,j}$

$$u_{i+1,j} = u_{i,j} + \left(\frac{\partial u}{\partial x}\right)_{i,j} \Delta x + \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} \frac{(\Delta x)^2}{2!} + \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j} \frac{(\Delta x)^3}{3!} + \ldots \qquad (1)$$

Eq.(1) mathematically an exact expression for $u_{i+1,j}$ if

1. number of terms is infinite
2. $\Delta x \rightarrow 0$



stencil

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \underbrace{\frac{u_{i+1,j} - u_{i,j}}{\Delta x}}_{\text{finite difference represent}} \underbrace{-\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} \frac{\overbrace{\Delta x}^{\text{lowest term in truncation error}}}{2} - \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j} \frac{(\Delta x)^3}{6}}_{\text{truncation error}} - \ldots$$

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} \cong \frac{u_{i+1,j} - u_{i,j}}{\Delta x} - \underbrace{O(\Delta x)}_{\text{terms of order } \Delta \text{x}}$$ First-order forward difference

First-order accurate/Forward difference

Taylor series expansion for $u_{i-1,j}$, expanded about $u_{i,j}$

$$u_{i-1,j} = u_{i,j} + \left(\frac{\partial u}{\partial x}\right)_{i,j} (-\Delta x) + \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} \frac{(-\Delta x)^2}{2!} + \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j} \frac{(-\Delta x)^3}{3!} + \ldots \qquad (2)$$

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i,j} - u_{i-1,j}}{\Delta x} - O(\Delta x)$$ First-order rearward (or backward) difference

Substract eq.(2) from eq.(1)

$$u_{i+1,j} - u_{i-1,j} = 2\left(\frac{\partial u}{\partial x}\right)_{i,j} (\Delta x) + 2\left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j} \frac{(\Delta x)^3}{3!} + \ldots$$

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x} + O(\Delta x^2)$$

Central difference formula, second-order accurate

To obtain second order partial derivatives, **summing eq.(1) & eq.(2)**

$$u_{i+1,j} + u_{i-1,j} = 2u_{i,j} + \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} (\Delta x)^2 + \left(\frac{\partial^4 u}{\partial x^4}\right)_{i,j} \frac{(\Delta x)^4}{12} + \dots$$

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2} + O(\Delta x)^2$$

Central difference formula of second-order accuracy

Similarly,

$$\left(\frac{\partial^2 u}{\partial y^2}\right)_{i,j} = \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{(\Delta y)^2} + O(\Delta y)^2$$

Mixed derivatives:

e.g. $\dfrac{\partial^2 u}{\partial x \partial y}$

differentiate eq.(1) with respect to y,

$$\left(\frac{\partial u}{\partial y}\right)_{i+1,j}=\left(\frac{\partial u}{\partial y}\right)_{i,j}+\left(\frac{\partial^2 u}{\partial x\partial y}\right)_{i,j}\Delta x+\left(\frac{\partial^3 u}{\partial x^2\partial y}\right)_{i,j}\frac{(\Delta x)^2}{2!}+\left(\frac{\partial^4 u}{\partial x^3\partial y}\right)_{i,j}\frac{(\Delta x)^3}{3!}\ldots \qquad (3)$$

differentiate eq.(2) with respect to y,

$$\left(\frac{\partial u}{\partial y}\right)_{i-1,j}=\left(\frac{\partial u}{\partial y}\right)_{i,j}-\left(\frac{\partial^2 u}{\partial x\partial y}\right)_{i,j}\Delta x+\left(\frac{\partial^3 u}{\partial x^2\partial y}\right)_{i,j}\frac{(\Delta x)^2}{2!}-\left(\frac{\partial^4 u}{\partial x^3\partial y}\right)_{i,j}\frac{(\Delta x)^3}{3!}\ldots \qquad (4)$$

Substracting eq.(4) from eq.(3) yields,

$$\left(\frac{\partial u}{\partial y}\right)_{i+1,j}-\left(\frac{\partial u}{\partial y}\right)_{i-1,j}=2\left(\frac{\partial^2 u}{\partial x\partial y}\right)_{i,j}\Delta x+2\left(\frac{\partial^4 u}{\partial x^3\partial y}\right)_{i,j}\frac{(\Delta x)^3}{3!}\ldots$$

$$\left(\frac{\partial u}{\partial y}\right)_{i+1,j}=\frac{u_{i+1.j+1}-u_{i+1.j-1}}{2\Delta y}+O(\Delta y)^2\ldots$$

$$\left(\frac{\partial u}{\partial y}\right)_{i-1,j}=\frac{u_{i-1.j+1}-u_{i-1.j-1}}{2\Delta y}+O(\Delta y)^2\ldots$$

$$\left(\frac{\partial^2 u}{\partial x \partial y}\right)_{i+1,j} = \frac{u_{i+1.j+1} - u_{i+1.j-1} - u_{i-1.j+1} + u_{i-1.j-1}}{4\Delta x \Delta y} + O\left[(\Delta x)^2, (\Delta y)^2\right] \ldots$$

Second order central difference for the mixed derivative.

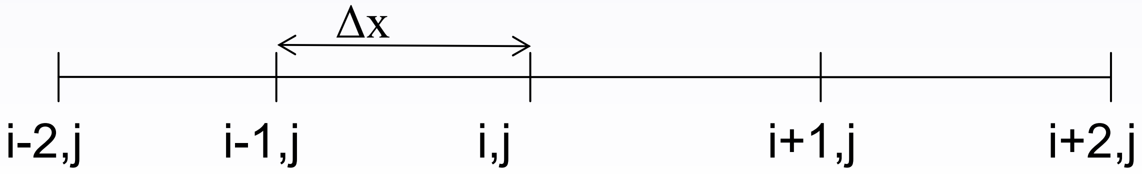
Derived finite difference expressions represent just “tip of the iceberg”.

Higher-order finite difference expressions

e.g. 4th order central difference for $\frac{\partial^2 u}{\partial x^2}$ is

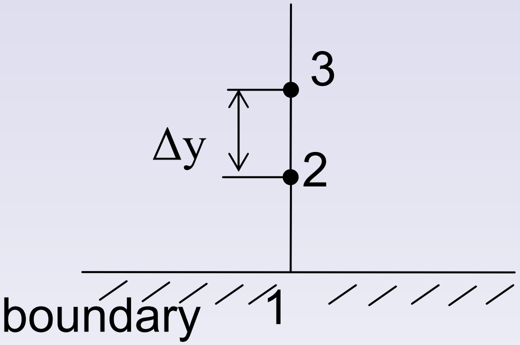
$$\left(\frac{\partial^2 u}{\partial x^2}\right) = \frac{-u_{i+2,j} + 16u_{i+1,j} - 30u_{i,j} + 16u_{i-1,j} - u_{i-2,j}}{12(\Delta x)^2} + O(\Delta x)^4$$

$$u_{i+2,j} = u_{i,j} + \left(\frac{\partial u}{\partial x}\right)_{i,j} \frac{2\Delta x}{1!} + \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} \frac{(2\Delta x)^2}{2!} + \ldots$$



- Information at five grid point is required to form above formula
- Can be derived by represent application of Taylor's series expanded about grid points (i+1,j) , (i,j) , (i-1,j)

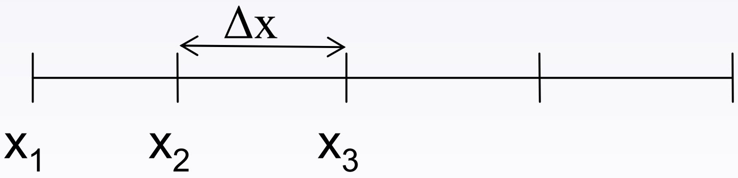
What about at boundary?



$$\left(\frac{\partial u}{\partial y}\right)_1 = \frac{u_2 - u_1}{\Delta y} + O(\Delta y)$$ Forward difference

- But only first-order accurate
- Second-order accuracy is needed

Method of undetermined coefficients (Polynomial approach)



$$\left(\frac{\partial u}{\partial x}\right)_1 = au(x_1) + bu(x_2) + cu(x_3)$$ Forward-difference, **one-sided formulas**

Up to 2nd order polynomials→ exact

$$\left(\frac{\partial u}{\partial x}\right)_1 = au\left(x_1\right)+bu\left(x_2\right)+cu\left(x_3\right)$$

Let $u(x) = 1$, $u'(x) = 0$,

$$0 = a + b + c \qquad (1)$$

$$u(x) = \left(x - x_1\right) \quad , \left(\frac{\partial u}{\partial x}\right)_1 = 1$$

$$1 = 0 + b\left(x_2 - x_1\right) + c\left(x_3 - x_1\right)$$

$$1 = bh + 2hc \qquad (2)$$

3 eqs.& 3 unknowns: a,b,c
(2) & (3)

$$u(x) = \left(x - x_1\right)^2 \quad , \left(\frac{\partial u}{\partial x}\right)_1 = 2\left(x - x_1\right)$$

$$0 = h^2 b + 4h^2 c \qquad (3)$$

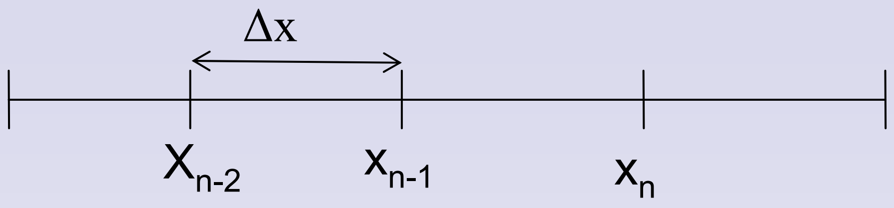
$$c = -\frac{1}{2h} \quad , \quad b = -4c = \frac{2}{h}$$

$$a = -\frac{3}{2h}$$

$$\left(\frac{\partial u}{\partial x}\right)_1 = -\frac{3}{2h}u(x_1) + \frac{4}{2h}u(x_2) - \frac{1}{2h}u(x_3)$$

$$\left(\frac{\partial u}{\partial x}\right)_1 = \frac{-3u(x_1) + 4u(x_2) - u(x_3)}{2h} + O(h^2)$$

Similarly backward-difference

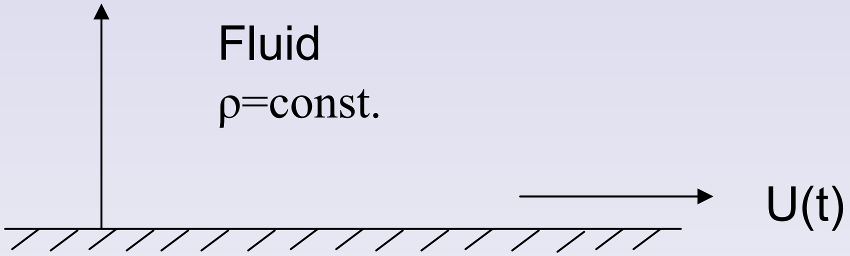


$$\left(\frac{\partial u}{\partial x}\right)_n = \frac{3u(x_n) - 4u(x_{n-1}) + u(x_{n-2})}{2h} + O(h^2)$$

Formulas can be extended for non-equidistance mesh intervals.

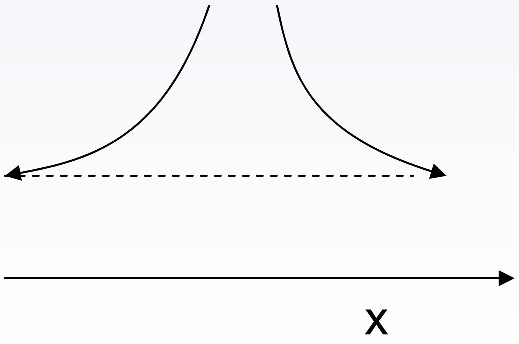
PARABOLIC EQUATIONS:

simplest example in Fluid Mechanics
Stoke’s 1st & 2nd problem



Preferred direction

1. Time – i.e. evolving flow
2. A spatial direction
   e.g. boundary layers, duct flows



$$u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}=\frac{\partial^2 u}{\partial y^2}$$

Unsteady motion of an infinitely extended fluid in response to an infinite plate suddenly set in motion along its own plate.

Incompressible N-S equations reduce to

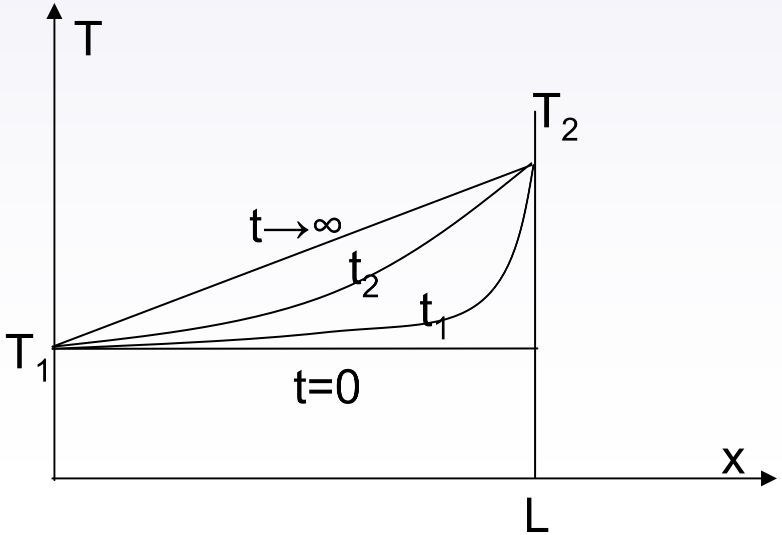
$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial y^2} \quad , \quad \nu = \frac{\mu}{\rho}$$

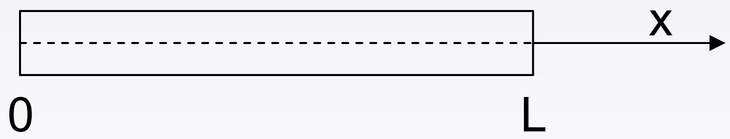
B.C: u(y,t=0)=0
u(y=0,t)=U(t)
u(y→∞,t)→0 (but in numerical computations space coordinates must be finite)

Example:

Unsteady 1-D heat conduction equation.

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial y^2} \quad , \quad \alpha = \frac{k}{\rho c_p}$$





T(x,t) temperature distribution in a rod of length L.

Boundary Conditions

At t=0 u(x,t=0)=f(x) ←specified

For t>0 :

a) u(0,t)=g(t) , u(L,t)=h(t) ends held at specified temperature

b) One end could be insulated

$$\frac{\partial u}{\partial x}(0,t)=0 \quad , \quad \text{or} \quad = f(t) \qquad \text{a specified heat flux}$$

c) $a_1(t)u(0,t)+b_1(t)\frac{\partial u}{\partial x}(0,t)=\gamma(t)$

Problem is to determine u(x,t) for t>0.

Solution evolves in time starting from some initial value

Marching solution with respect to time.

Two methods of solution

a) The method of lines , reduce Partial Differential Equations to a set of Order Differential Equations

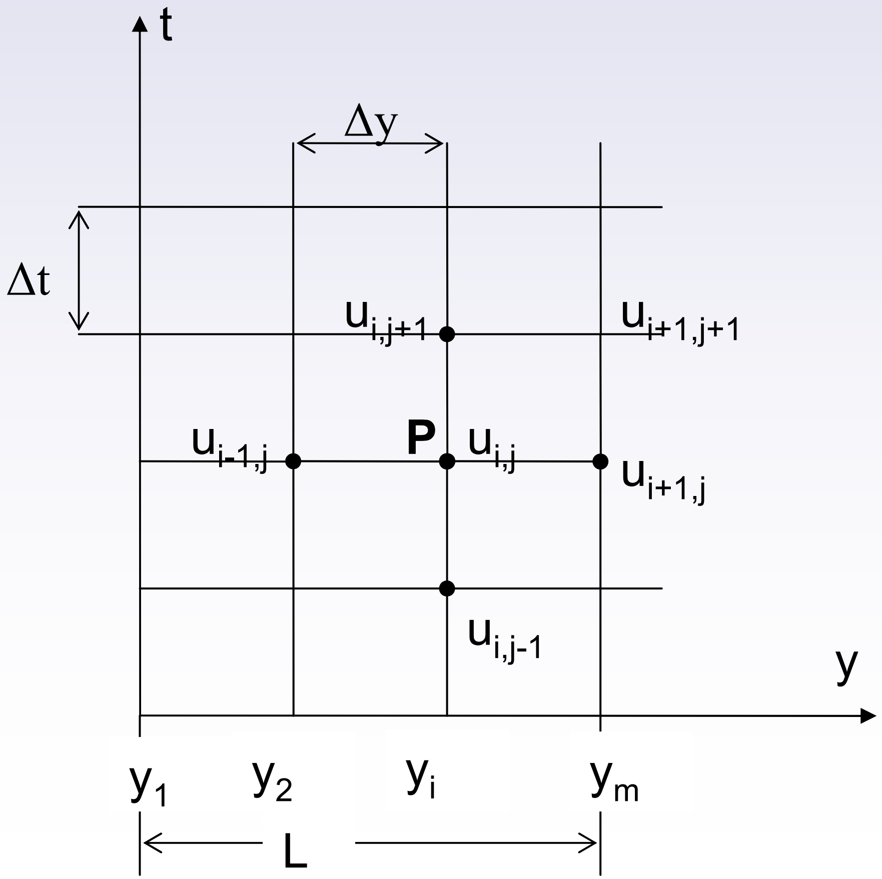
b) **Pure finite difference methods**

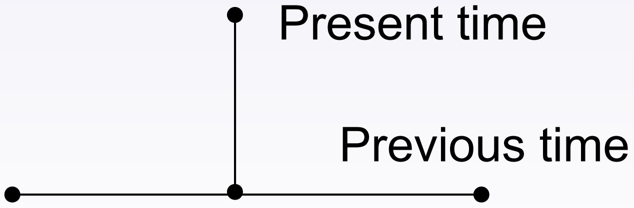
FINITE DIFFERENCE METHODS (explicit, implicit)

PDE is replaced by finite-difference equations at the grid points
This results in algebraic equations called difference equations.

EXPLICIT METHODS

$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial y^2}$$





FTCS

$t_n = n\Delta t$ (uniform time step)

$$\left(\frac{\partial u}{\partial t}\right)_{i,j} = \frac{u_{i,j+1} - u_{i,j}}{\Delta t} - \underbrace{\left(\frac{\partial^2 u}{\partial t^2}\right)_{i,j} \frac{\Delta t}{2}}_{O(\Delta t)} + \ldots.$$

Forward-difference in time

$$\left(\frac{\partial^2 u}{\partial y^2}\right)_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\left(\Delta y\right)^2}$$

Second order <u>central-difference</u> in space

$$\frac{u_{i,j+1} - u_{i,j}}{\Delta t} = \nu \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\left(\Delta y\right)^2} \qquad \text{(A)}$$

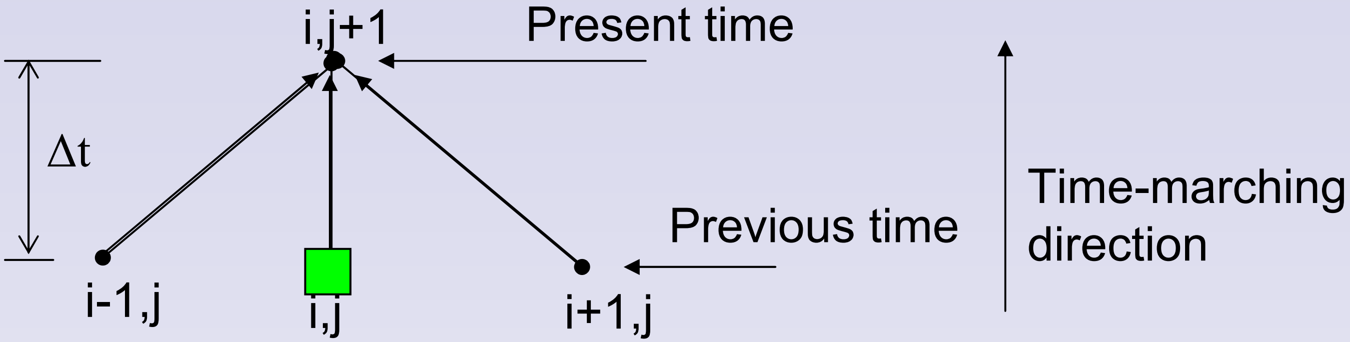
difference equation

After rearragement

$$u_{i,j+1} = u_{i,j} + \nu \frac{\Delta t}{\left(\Delta y\right)^2} \left(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}\right) \qquad \text{(B)}$$

Difference equation (A) is just an approximation for original PDE due to truncation error.
Note: Truncation error for differential equation is $O(\Delta t, (\Delta x)^2)$

Consistency of finite-difference representation of the PDE as Δx→0 & Δt→0 differential equation reduces to original differential equations.



Properties at level (j+1) (present time) to be calculated from values at level j (previous time) Remember that parabolic PDEs lend themselves to a marching solution, here marching variable is time, t

Eq.(B) allows direct calculation of $u_{i,j+1}$ from the known values on the RHS of eq.(B)

Explicit approach: each difference eq. contains only one unknown and therefore can be solved explicitly for this unknown in a straight forward manner.

Comments on this method

- Explicit methods can be very unstable and should be used with caution
- In general, whether the scheme is unstable or not depends on the ratio, $\nu \Delta t / \left(\Delta y \right)^2$
  For a given (Δy), Δt must be less than some limit imposed by stability constraints
- Relatively simple to set up and program

Von Neumann Stability Method: (Fourier method)

Assume solution can be expanded in the form of Fourier Series

Let $u_{i,j} = U_j e^{Iik\Delta y}$

U$_j$: amplitude at t$_j$ and k is the wave number, $I = \sqrt{-1}$

$$u_{i,j+1} = U_{j+1} e^{Iik\Delta y} \quad , \quad u_{i\mp 1} = U_j e^{I(i\pm 1)k\Delta y}$$

Substitute above into finite-difference representation of PDE

$$u_{j+1} e^{Iik\Delta y} = U_j e^{Iik\Delta y} + R\left(U_j e^{I(i-1)k\Delta y} - 2U_j e^{Iik\Delta y} + U_j e^{I(i+1)k\Delta y}\right)$$

$$u_{i,j+1} = U_{i,j} + R\left(U_{i-1,j} - 2U_{i,j} + U_{i+1,j}\right) \quad , \quad R = \nu \frac{\Delta t}{\left(\Delta y\right)^2}$$

$$u_{j+1} = U_j \left[1 + R\left(e^{-Ik\Delta y} - 2 + e^{Ik\Delta y}\right)\right]$$

For a stable solution

$$\left|\frac{U_{j+1}}{U_j}\right| \le 1 \quad , \quad U_j \sim e^{aj\Delta t}$$

$$\cos k\Delta y = \frac{e^{Ik\Delta t} + e^{-Ik\Delta t}}{2}$$

$$U_{j+1} = U_j \underbrace{\left[1 - 2R\left(1 - \cos k\Delta y\right)\right]}_{\lambda\text{:amplification factor}}$$

$$U_{j+1} = U_j \lambda$$

$$\left|\frac{U_{j+1}}{U_j}\right| = \left|\lambda\right| \le 1 \Rightarrow \text{stable solution}$$

$\left|\lambda\right| > 1 \Rightarrow \left|U_{j+1}\right| > \left|U_j\right|$, i.e. amplitude of solution becomes unbounded as j→∞ (time goes to infinity)

$$\left[1 - \underbrace{2R\left(1 - \cos k\Delta y\right)}_{\le 1}\right]^2 \le 1$$

$$-1 + R\left(1 - \cos k\Delta y\right) \le 0$$

coskΔy=-1 → R≤1/2 (for a minimum RHS)

$$R \le \frac{1}{1 - \cos k\Delta y}$$

$$\underbrace{\nu \frac{\Delta t}{\left(\Delta y\right)^2}}_{\text{diffusion}} \le \frac{1}{2}$$

stability criterion for unsteady heat conduction equations.

- Von neumann stability method ignores boundary conditions
- Effect of B.C. can be destabilizing

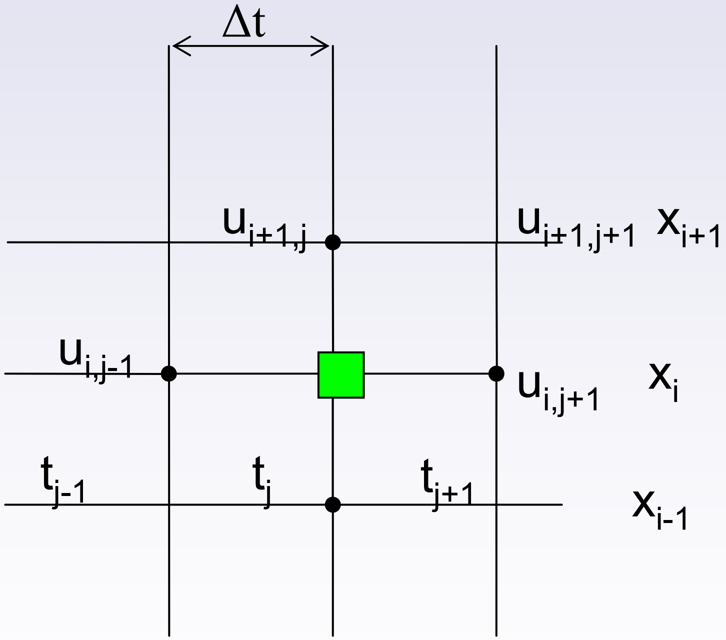
Other Explicit methods:

1. FTCS method $O\left[\Delta t, (\Delta x)^2\right]$
2. Richardson method

Central difference in both time&space derivatives

Approximate at x_i, t_j

$$\frac{u_{i,j+1} - u_{i,j-1}}{2\Delta t} = \alpha \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2}$$



If i know solution on t_j & t_{j-1} have explicit formula

$$u_{i,j+1} = u_{i,j-1} + \frac{2\Delta t \alpha}{(\Delta x)^2}\left(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}\right) \qquad O\left[(\Delta t)^2, (\Delta x)^2\right]$$

Notes:

- In methods like this must keep time step (Δt) uniform
- Starting formula
- Stability analysis UNCONDITIONALLY UNSTABLE CANNOT BE USED TO SOLVE HEAT EQUATION. AVOID THIS

3. DuFort-Frankel method

Variant of Richardson in which

$$u_{i,j} = \frac{1}{2}\left(u_{i,j+1} + u_{i,j-1}\right)$$ for stability

$$\frac{u_{i,j+1} - u_{i,j-1}}{2\Delta t} = \alpha \frac{u_{i+1,j} - \left(u_{i,j+1} + u_{i,j-1}\right) + u_{i-1,j}}{\left(\Delta x\right)^2}$$

$$u_{i,j+1}\left(1 + \frac{2\alpha\Delta t}{\left(\Delta x\right)^2}\right) = \left(1 - \frac{2\alpha\Delta t}{\left(\Delta x\right)^2}\right)u_{i,j-1} + \frac{2\alpha\Delta t}{\left(\Delta x\right)^2}\left(u_{i+1,j} + u_{i-1,j}\right)$$

Notes:

1. Method is unconditionally stable, i.e. for any value of $R = \alpha \frac{\Delta t}{\left(\Delta x\right)^2}$
2. Requires two time levels of storage & uniform time step One step method, starter solution (FTCS) can be used

3. Can be dangerous without a consistency analysis
   Consistency requires that as the step sizes Δx & Δt → 0 , FDE must reduce to original PDE

$$\left\{1+\frac{2\Delta t}{(\Delta x)^2}\right\}u_i^{j+1}=\left\{1-\frac{2\Delta t}{(\Delta x)^2}\right\}u_i^{j-1}+\frac{2\Delta t}{(\Delta x)^2}(u_{i+1}^j+u_{i-1}^j)$$

Show time level as superscript

$$\left\{1+\frac{2\Delta t}{(\Delta x)^2}\right\}\left\{u_i^j+\frac{\partial u}{\partial t}\Delta t+\frac{\partial^2 u}{\partial t^2}\frac{\Delta t^2}{2!}+\ldots\right\}=\left\{1-\frac{2\Delta t}{(\Delta x)^2}\right\}\left\{u_i^j-\frac{\partial u}{\partial t}\Delta t+\ldots\right\}+$$

$$\frac{2\Delta t}{(\Delta x)^2}\left\{u_i^j+\frac{\partial u}{\partial x}\Delta x+\frac{\partial^2 u}{\partial x^2}\frac{\Delta x^2}{2!}+u_i^j-\frac{\partial u}{\partial x}\Delta x+\ldots\right\}$$

$$\frac{\partial u}{\partial t}\Delta t+\frac{\Delta t}{(\Delta x)^2}\frac{\partial^2 u}{\partial t^2}\Delta t^2+O(\Delta t^3)=\frac{\Delta t}{(\Delta x)^2}\frac{\partial^2 u}{\partial x^2}(\Delta x)^2+O(\Delta t,\Delta x^2)$$

$$\frac{\partial u}{\partial t}+\left(\frac{\Delta t}{\Delta x}\right)^2\frac{\partial^2 u}{\partial t^2}=\frac{\partial^2 u}{\partial x^2}+O(\Delta t^2,\Delta x^2)$$

Consistent only if $\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2}+O\left(\Delta t^2,\Delta x^2,\left(\frac{\Delta t}{\Delta x}\right)^2\right)$

$$\frac{\Delta t}{\Delta x} \to 0 \quad \text{as} \quad \Delta x, \Delta t \to 0$$

Otherwise, I am not approximating the eq. I thought I was $\frac{\Delta t}{\Delta x} = 1$ then approximating

$\frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}$ represents a hyperbolic equation!

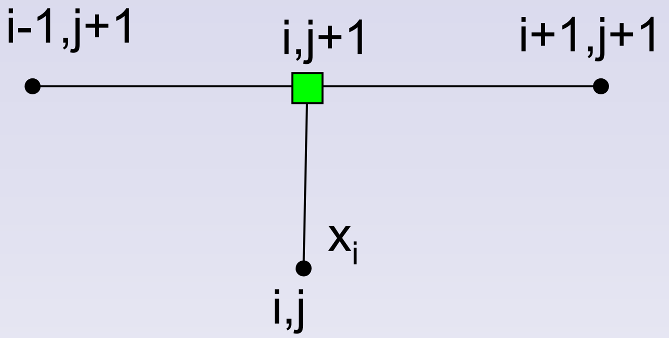
- Show that explicit FTCS method is consistent!

IMPLICIT METHODS:

In implicit method information at the boundaries at the same level does not feed into the computation.

First-order backward difference approximation for time-derivative and second-order central difference approximation for space-derivative

$$\frac{u_{i,j+1} - u_{i,j}}{\Delta t} = \alpha \frac{u_{i+1,j+1} - 2u_{i,j+1} + u_{i-1,j+1}}{(\Delta x)^2} \qquad (1)$$



Present time-unknown

Previous time-known

BTCS Method

In equation (1): 3 unknowns $u_{i-1,j+1}$, $u_{i,j+1}$, $u_{i+1,j+1}$

Thus, it results in a set of coupled finite difference equations all grid points

Rearrange equation (1)

$$\underbrace{\frac{\alpha\Delta t}{(\Delta x)^2}}_{c_i} u_{i-1}^{j+1} - \underbrace{\left(1+2\frac{\alpha\Delta t}{(\Delta x)^2}\right)}_{a_i} u_i^{j+1} + \underbrace{\frac{\alpha\Delta t}{(\Delta x)^2}}_{b_i} u_{i+1}^{j+1} = -\underbrace{u_i^j}_{d_i}$$

3 unknowns in each FDE

Algebraic equations

Coefficient matrix→Tridiagonal→Thomas algorithm (n-1) unknowns

Advantages

$$\underbrace{1}_{c_i} u_{i-1}^{j+1} - \underbrace{\left(2 + 2\frac{(\Delta x)^2}{\alpha \Delta t}\right)}_{a_i} u_i^{j+1} + \underbrace{1}_{b_i} u_{i+1}^{j+1} = -\underbrace{\frac{(\Delta x)^2}{\alpha \Delta t}}_{d_i} u_i^j$$

Now, all the u^{j+1} 's are known except those at the end points u_0 , u_n (known from B.Cs) Identical formulation as in the BVP is applicable

Notes:

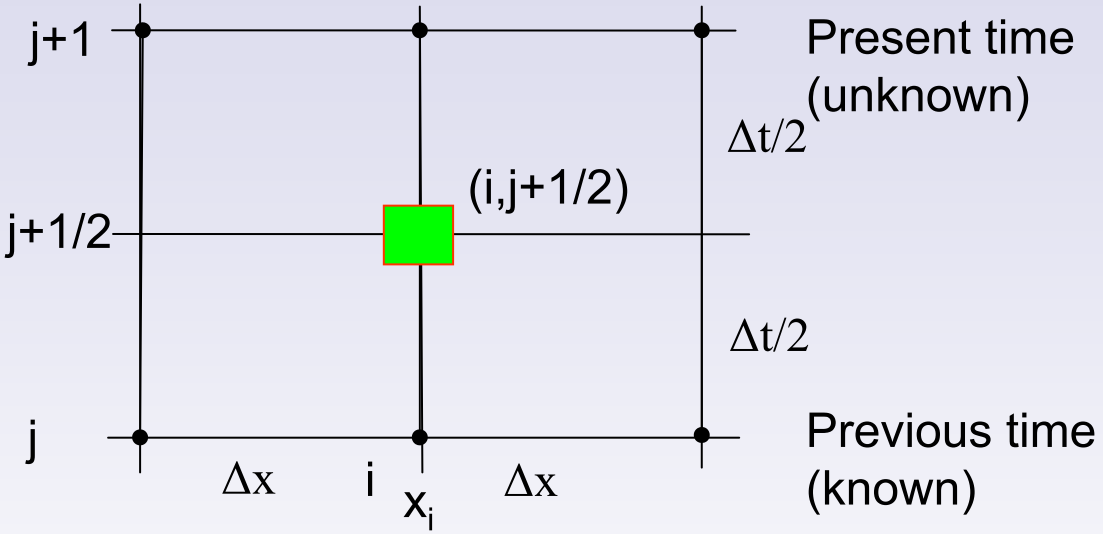
1. Derivative B.C. can be inferred from the section on BVPs
2. Stability problem is removed for this scheme and the method is stable for all values of R (unconditionally stable)
3. Accuracy problem exists in time backward difference $\rightarrow O(\Delta t, \Delta x^2)$
4. Larger step size in time is permitted

Crank-Nicolson Method:

Approximate differential equation at (i,j+1/2); central difference at time levels j & j+1,

$$\frac{u_i^{j+1} - u_i^j}{\Delta t} = \alpha \frac{1}{2}\left[\frac{u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}}{(\Delta x)^2} + \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{(\Delta x)^2}\right]$$

$$\frac{\partial u}{\partial t} = \frac{u_i^{j+1} - u_i^j}{2\left(\frac{\Delta t}{2}\right)}$$ central difference of step Δt/2 , i.e. $(\Delta t)^2$



Unconditionally stable

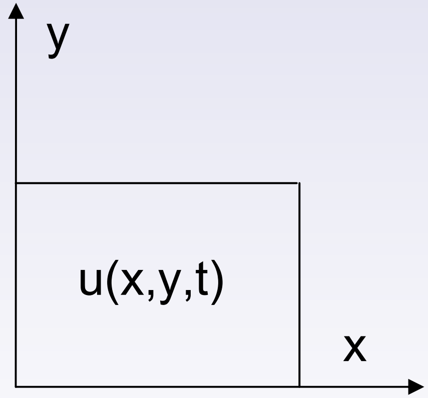
$O\left((\Delta t)^2, (\Delta x)^2\right)$ Second order scheme

$$u_{i+1}^{j+1} - \left(2 + 2\frac{(\Delta x)^2}{\alpha \Delta t}\right) u_i^{j+1} + u_{i-1}^{j+1} = \underbrace{-2\frac{(\Delta x)^2}{\alpha \Delta t} u_i^j - u_{i+1}^j + 2u_i^j - u_{i-1}^j}_{d_j \text{known}}$$

TDMA-Thomas Algorithm

Parabolic equations in two-space coordinates

$$\frac{\partial u}{\partial t} = \alpha\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) \qquad \alpha = \text{const.}$$



On each portion of boundary, we know

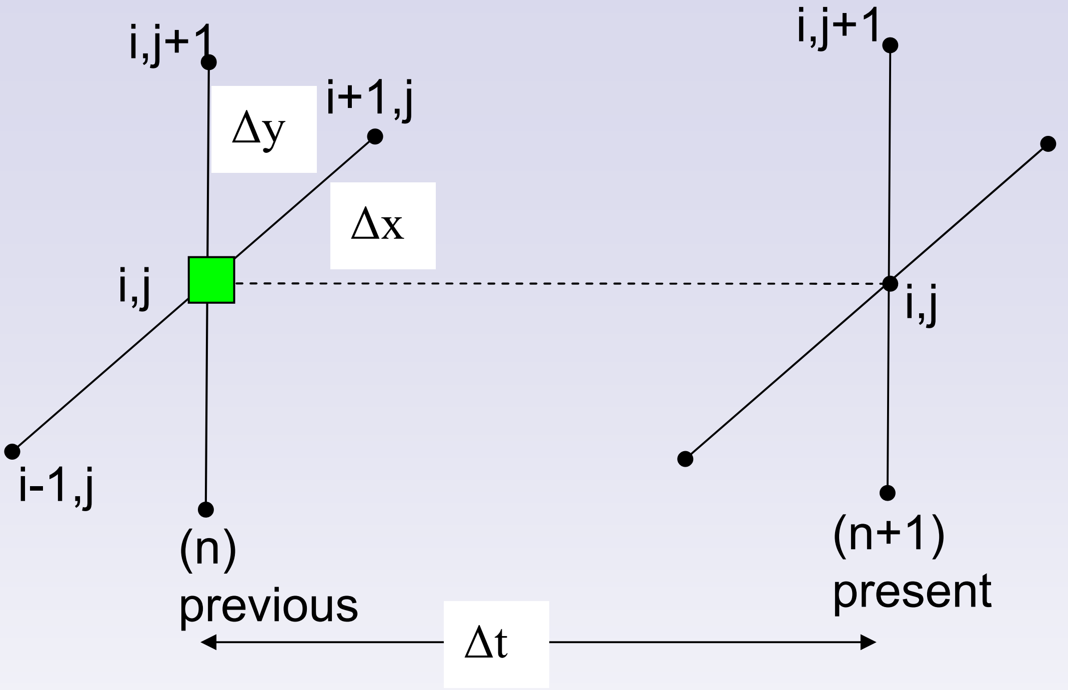
I. u

II. $\frac{\partial u}{\partial n}$

III. $A\frac{\partial u}{\partial n} + Bu$

Explicit method: FTCS

Forward difference in time derivative, central difference in space derivative



$$\frac{u_{i,j}^{n+1}-u_{i,j}^{n}}{\Delta t}=\alpha\left[\frac{u_{i+1,j}^{n}-2u_{i,j}^{n}+u_{i-1,j}^{n}}{(\Delta x)^2}+\frac{u_{i,j+1}^{n}-2u_{i,j}^{n}+u_{i,j-1}^{n}}{(\Delta y)^2}\right]\quad O\left[\Delta t,(\Delta x)^2,(\Delta y)^2\right]$$

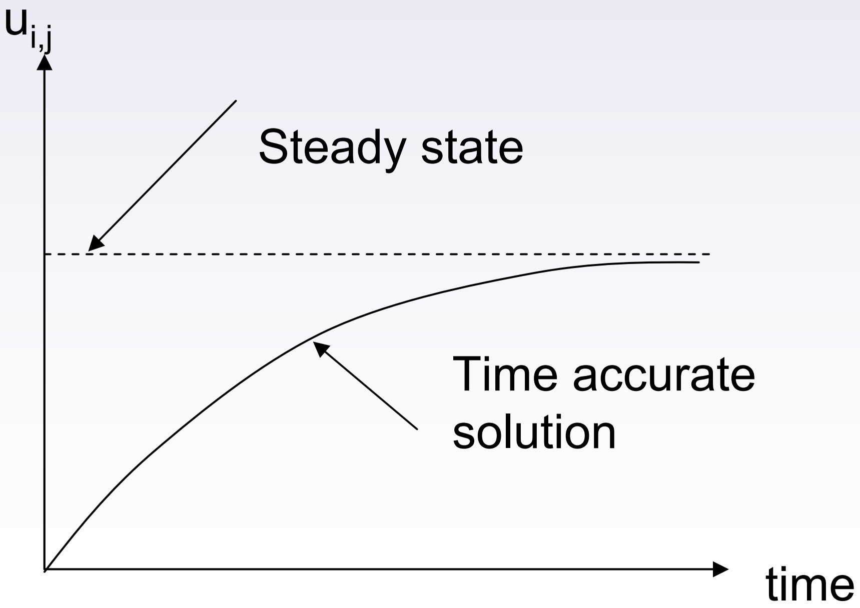
Stability analysis : $\frac{\alpha\Delta t}{(\Delta x)^2}+\frac{\alpha\Delta t}{(\Delta y)^2}\le\frac{1}{2}$

$\Delta x=\Delta y\Rightarrow\frac{\alpha\Delta t}{(\Delta x)^2}\le\frac{1}{4}$ *twice as restrictive as the 1-D case* α=1 & Δx=Δy

$$u_{i,j}^{n+1} = u_{i,j}^{n} + \frac{\Delta t}{(\Delta x)^2}\left[u_{i+1,j}^{n} - 4u_{i,j}^{n} + u_{i-1,j}^{n} + u_{i,j+1}^{n} + u_{i,j-1}^{n}\right]$$

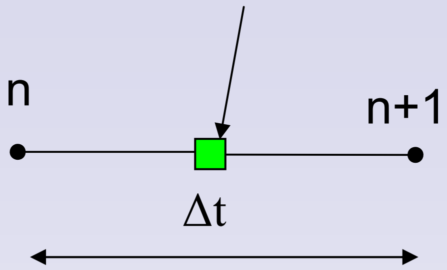
$\frac{\alpha \Delta t}{(\Delta x)^2} \le \frac{1}{4}$ upper limit $\frac{\Delta t}{(\Delta x)^2} = \frac{1}{4}$

$$u_{i,j}^{n+1} = \frac{1}{4}\left[u_{i+1,j}^{n} + u_{i-1,j}^{n} + u_{i,j+1}^{n} + u_{i,j-1}^{n}\right]$$ Five-point formula



Valid solution at any intermediate level

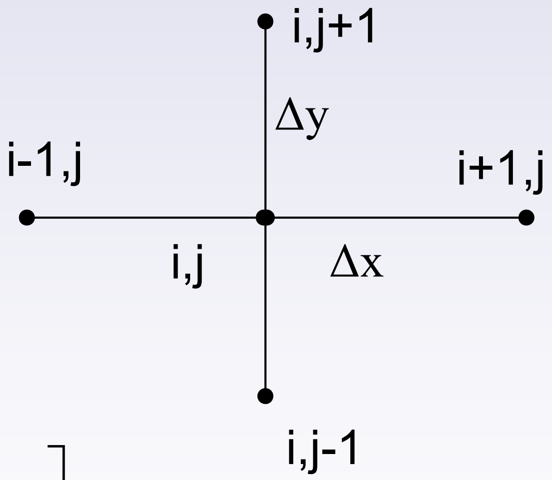
Implicit Method: Crank-Nicolson



$$\frac{\partial u}{\partial t} = \underbrace{\frac{u_{i,j} - u^{*}_{i,j}}{\Delta t}}_{\text{central difference eq. of step } \Delta t/2} + O(\Delta t)^2$$

$u^{n+1}_{i,j} = u_{i,j}$ → unknown (present)

$u^{n}_{i,j} = u^{*}_{i,j}$ → known (previous)



$$\frac{\partial^2 u}{\partial x^2} \cong \frac{1}{2}\left[\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2} + \frac{u^{*}_{i,j+1} - 2u^{*}_{i,j} + u^{*}_{i-1,j}}{(\Delta x)^2}\right] + O(\Delta x)^2$$

$$\frac{\partial^2 u}{\partial y^2} \cong \frac{1}{2}\left[\frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{(\Delta y)^2} + \frac{u^{*}_{i,j+1} - 2u^{*}_{i,j} + u^{*}_{i,j-1}}{(\Delta y)^2}\right] + O(\Delta y)^2$$

$$u_{i+1,j}+u_{i-1,j}+\gamma\left(u_{i,j+1}+u_{i,j-1}\right)-\left(2+2\gamma+\frac{2\left(\Delta x\right)^2}{\Delta t}\right)u_{i,j}=$$

$$-u^*_{i+1,j}-u^*_{i-1,j}-\gamma\left(u^*_{i,j+1}+u^*_{i,j-1}\right)+\left(2+2\gamma-\frac{2\left(\Delta x\right)^2}{\Delta t}\right)u^*_{i,j}$$

where $\gamma=\left(\frac{\Delta x}{\Delta y}\right)^2$ is the ratio of step sizes

Coefficient matrix is *pentadiagonal* (5 unknowns in one-algebraic equation.)
Solve:

1. Gauss-Seidel , SOR (iteration) , iterate until convergence at each time step
2. Alternating Direction Implicit (ADI)

Alternating Direction Implicit (ADI) Method

$$\frac{\partial u}{\partial t}=\alpha\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right)\qquad \text{Marching technique}\qquad (1)$$

u(t+Δt) will be obtained, in some fashion, from the known values of u(t)
Let’s use two-step process: first treat only x derivative implicitly

Step 1:

$$\frac{u_{i,j}^{n+1/2}-u_{i,j}^{n}}{\Delta t}=\alpha\frac{u_{i+1,j}^{n+1/2}-2u_{i,j}^{n+1/2}+u_{i-1,j}^{n+1/2}}{\left(\Delta x\right)^{2}}+\alpha\frac{u_{i,j+1}^{n}-2u_{i,j}^{n}+u_{i,j-1}^{n}}{\left(\Delta y\right)^{2}} \qquad (2)$$

Equation (2) reduces to the tridiagonal form
(n+1/2) : intermediate time

$$b_i u_{i+1,j}^{n+1/2}+a_i u_{i,j}^{n+1/2}+c_i u_{i-1,j}^{n+1/2}=d_i \qquad (2')$$

where

$$b_i=c_i=\frac{\alpha\Delta t}{2\left(\Delta x\right)^{2}} \quad , \quad a_i=-\left(1+\frac{\alpha\Delta t}{\left(\Delta x\right)^{2}}\right)$$

$$d_i=-u_{i,j}^{n}-\frac{\alpha\Delta t}{2\left(\Delta y\right)^{2}}\left(u_{i,j+1}^{n}-2u_{i,j}^{n}+u_{i,j-1}^{n}\right)$$

Eq.(2') yields a solution for $u_{i,j}^{n+1/2}$ for all i, keeping j fixed, via Thomas Algorithm

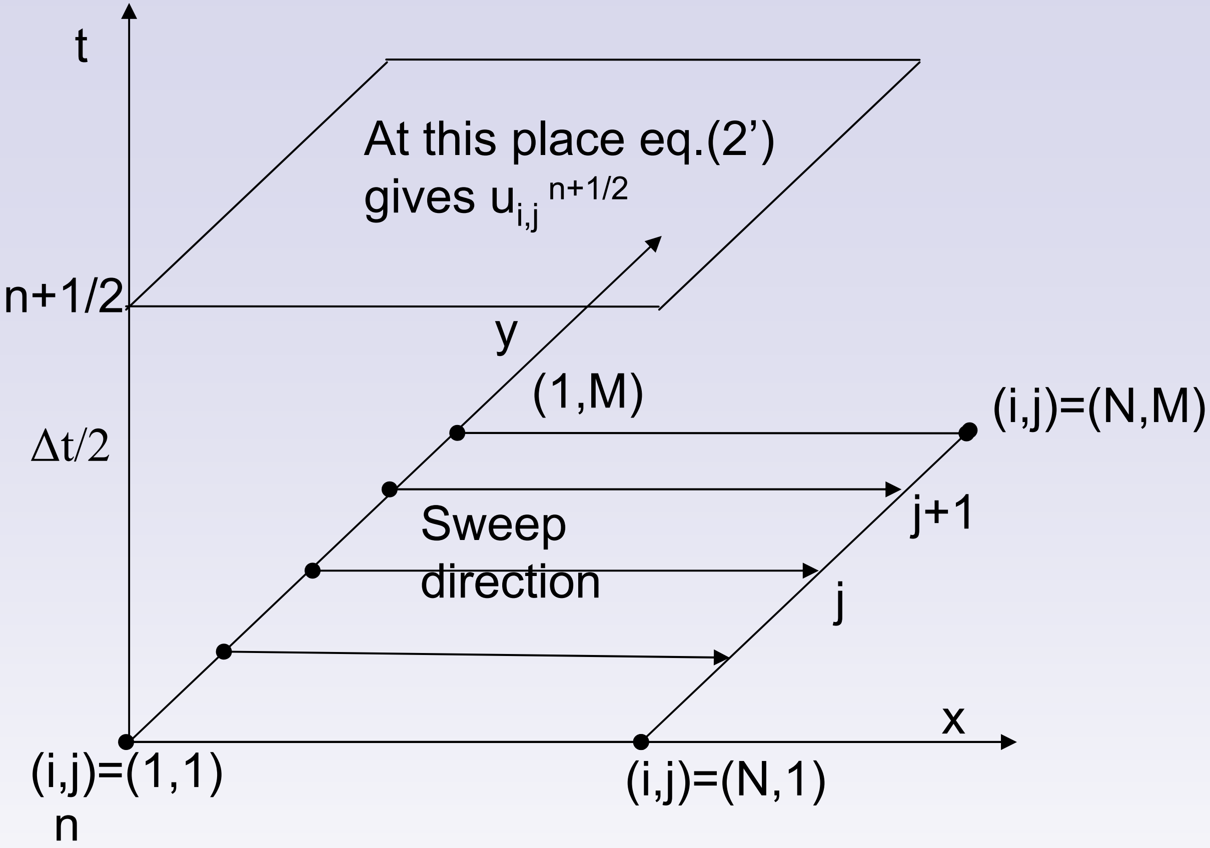
In Eq.(2') first set j=1, and sweep in x (i=1,...,N) to find $u_{i,j=1}^{n+1/2}$

Next, set j=2, and sweep in x (i=1,...,N) to find $u_{i,j=2}^{n+1/2}$

....

M sweeps in x-direction

Need to use Thomas Algorithm M times



At the end of step1 (after M sweeps), the values of u at the intermediate time (t+Δt/2) are known at all grid points: i.e. $u_{i,j}^{n+1/2}$ is known at all (i,j)

Step 2:

Take the solution to the time (t+Δt), using the known values at time (t+Δt/2)
Again replace spatial derivatives with central differences, but this time treat y derivative implicitly

$$\frac{u_{i,j}^{n+1}-u_{i,j}^{n+1/2}}{\Delta t}=\alpha\frac{u_{i+1,j}^{n+1/2}-2u_{i,j}^{n+1/2}+u_{i-1,j}^{n+1/2}}{(\Delta x)^2}+\alpha\frac{u_{i,j+1}^{n+1}-2u_{i,j}^{n+1}+u_{i,j-1}^{n+1}}{(\Delta y)^2} \qquad (3)$$

Eq.(3) reduces to the tridiagonal form

$$b_j u_{i,j+1}^{n+1}+a_j u_{i,j}^{n+1}+c_j u_{i,j-1}^{n+1}=d_j \qquad (3')$$

where

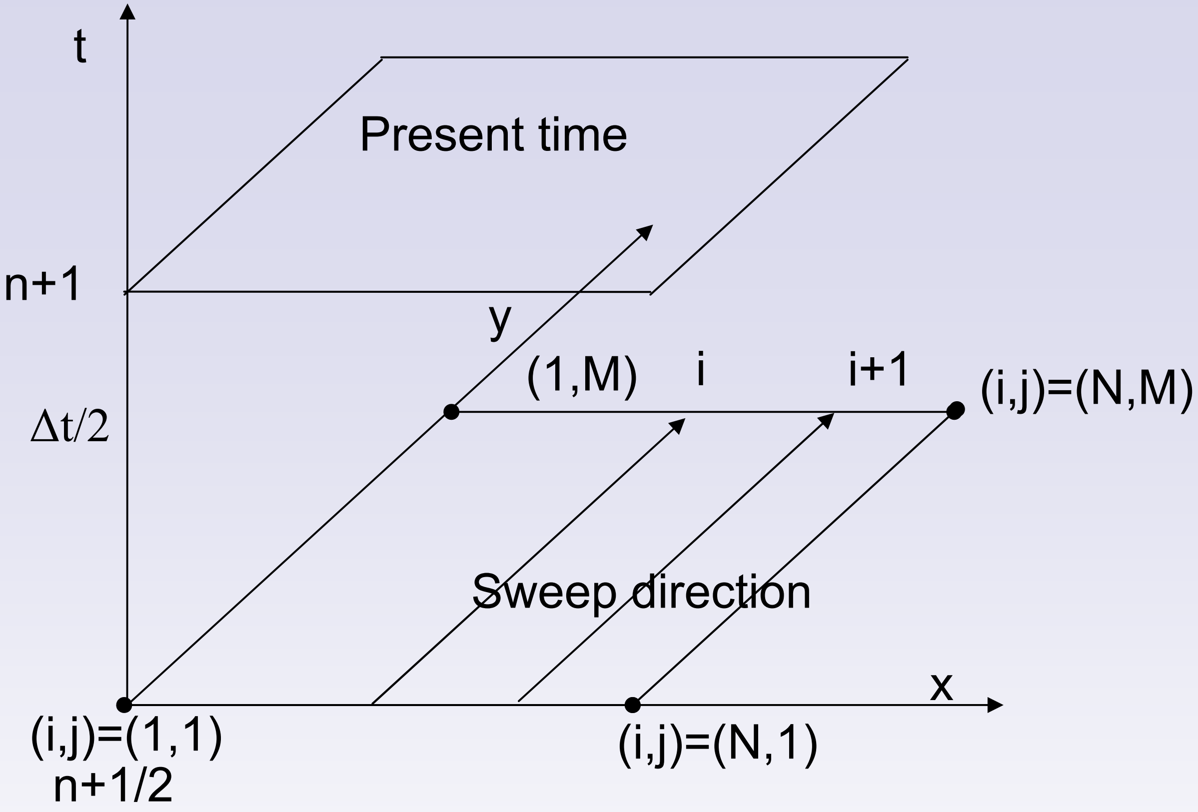
$$b_j=c_j=\frac{\alpha\Delta t}{2(\Delta x)^2} \quad , \quad a_j=-\left(1+\frac{\alpha\Delta t}{2(\Delta x)^2}\right)$$

$$d_j=-u_{i,j}^{n+1/2}-\frac{\alpha\Delta t}{2(\Delta x)^2}\left(u_{i+1,j}^{n+1/2}-2u_{i,j}^{n+1/2}+u_{i-1,j}^{n+1/2}\right)$$

yields a solution for $u_{i,j}^{n+1}$ for all j, keeping i fixed, via Thomas Algorithm

j=1,.....,M	i=1
j=1,.....,M	i=2
	:
....	i=N

N times Thomas Algorithm



Remarks:

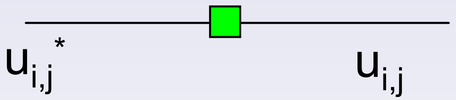
- Involves only tridiagonal forms
- Alternating direction implicit
- Scheme is second-order accurate
- General class of scheme involving splitting of two or more directions in an implicit solution of the governing flow equation to obtain tridiagonal forms
- Approximate factorization
- For 3-D, see the scheme in *Computational Fluid Dynamics for Engineers* Vol.1 Klaus A. Hoffmann & S.T. Chiang pg.90

Approximate Factorization - Factored ADI Method

$$\frac{\partial u}{\partial t} = \alpha\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) \qquad \alpha = 1$$

Sweep 2 directions

Crank-Nicolson



$$\frac{u_{i,j} - u_{i,j}^*}{\Delta t} = \frac{1}{2\Delta x^2}\left\{\delta_x^2 u_{i,j} + \delta_x^2 u_{i,j}^*\right\} + \frac{1}{2\Delta y^2}\left\{\delta_y^2 u_{i,j} + \delta_y^2 u_{i,j}^*\right\} + O\left[(\Delta t)^2, (\Delta x)^2, (\Delta y)^2\right]$$

where

$$\left.\begin{aligned} \delta_x^2 u_{i,j} &= u_{i+1,j} - 2u_{i,j} + u_{i-1,j} \\ \delta_y^2 u_{i,j} &= u_{i,j+1} - 2u_{i,j} + u_{i,j-1} \end{aligned}\right\} \text{compact operators}$$

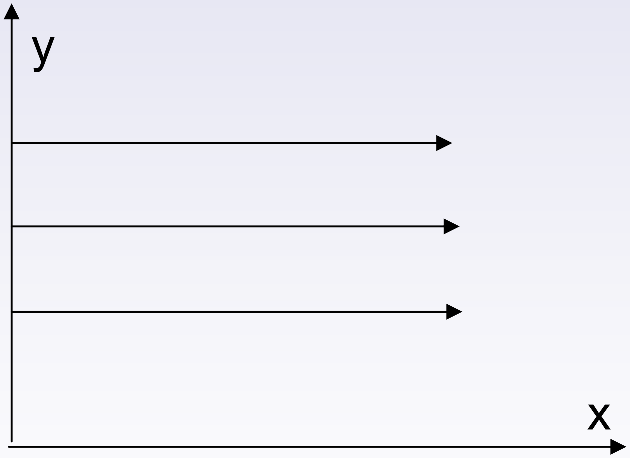
$$u_{i,j}\left\{1 - \frac{\Delta t}{2\Delta x^2}\delta_x^2 - \frac{\Delta t}{2\Delta y^2}\delta_y^2\right\} = \left\{1 + \frac{\Delta t}{2\Delta x^2}\delta_x^2 + \frac{\Delta t}{2\Delta y^2}\delta_y^2\right\}u_{i,j}^*$$

Let $\left\{1-\frac{\Delta t}{2\Delta x^2}\delta_x^2-\frac{\Delta t}{2\Delta y^2}\delta_y^2\right\}=\left\{1-\frac{\Delta t}{2\Delta x^2}\delta_x^2\right\}\left\{1-\frac{\Delta t}{2\Delta y^2}\delta_y^2\right\}+O\left[\left(\Delta t\right)^2\right]$

Define $\hat{u}_{i,j}$ such that

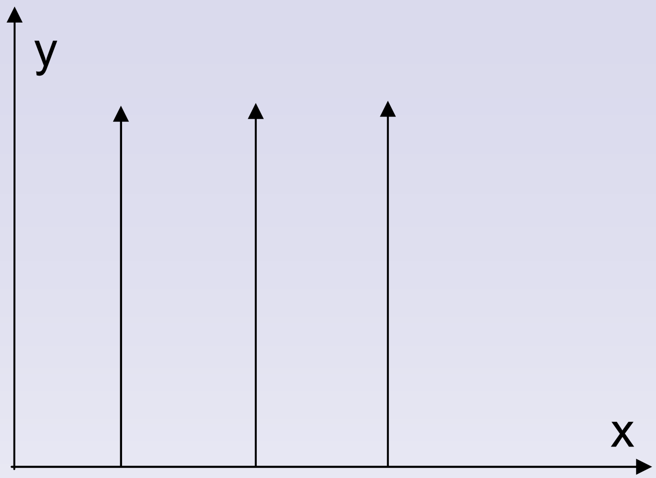
$$\left\{1-\frac{\Delta t}{2\Delta x^2}\delta_x^2\right\}\hat{u}_{i,j}=\left\{1+\frac{\Delta t}{2\Delta x^2}\delta_x^2+\frac{\Delta t}{2\Delta y^2}\delta_y^2\right\}u^*{}_{i,j} \qquad (1)$$

Eq.(1) defines a set tridiagonal matrix problems along constant y lines



$$\hat{u}_{i,j}=\left\{1-\frac{\Delta t}{2\Delta y^2}\delta_y^2\right\}u_{i,j} \qquad (2)$$

Sweep on lines of constant x



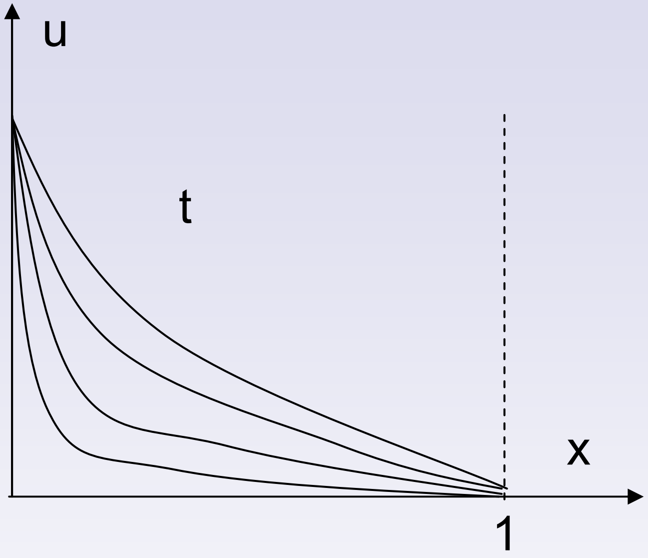
Notes:

1) Use eq.(2) to find values of $\hat{u}$ on vertical boundaries where $u_{i,j}$ known from B.C.s
2) Can reverse order of sweep
3) No iteration
4) Can be extended to higher dimensional problems

Above method is called *Approximate Factorization*

Keller Box Scheme

Implicit scheme for non-uniform meshes



Initially boundary layer near x=0 for small t
Small meshes near x=0
Uniform meshes in x is wasteful
To deal with problem, 2 procedures is possible

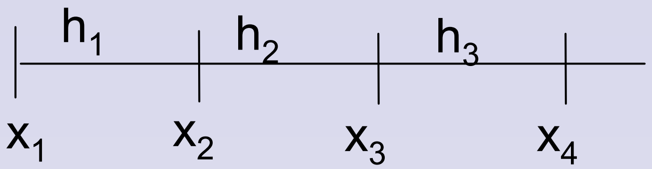
I. Algebraic transformation

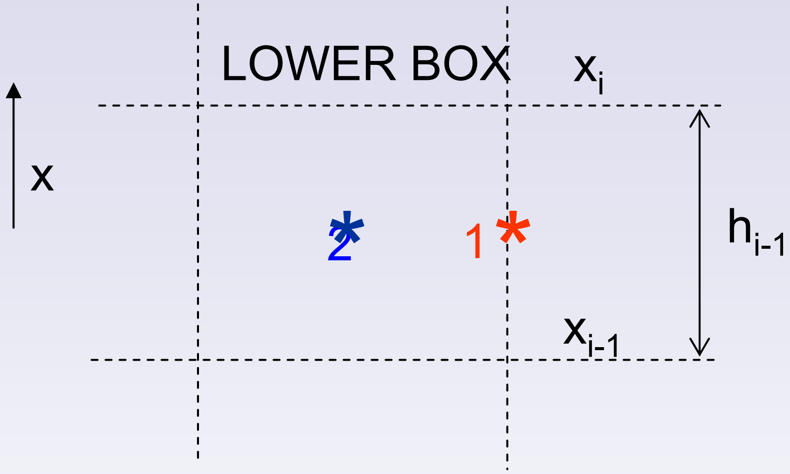
$\xi = x^a$ & then use uniform mesh in ξ $\qquad \xi = \dfrac{x}{\sqrt{t}}$

II. Adopt a method which permits a non-uniform spacing

$$x_i = x_{i-1} + h_{i-1} \qquad \text{i=2,...,N}$$

$$x_1 = 0 \quad , \quad x_{N+1} = 1$$





Sample problem

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t}$$

PROCEDURE

- Reduce the eq(s) to a first order system & write finite difference equations using central differences
- Linearize if they are non-linear
- Obtain matrix for TDMA
- Solve with Thomas Algorithm

$$v = \frac{\partial u}{\partial x} \qquad (1) \qquad , \qquad \frac{\partial v}{\partial x} = \frac{\partial u}{\partial t} \qquad (2)$$

*

$$\frac{u_i - u_{i\text{-}1}}{h_{i\text{-}1}} = v_{i\text{-}1/2} = \frac{1}{2}\left(v_i + v_{i\text{-}1}\right) + O\left(h_{i\text{-}1}\right)^2$$

Approximate eq (1) at

or

$$v_i + v_{i\text{-}1} = \frac{2}{h_{i\text{-}1}}\left(u_i - u_{i\text{-}1}\right) \qquad (3)$$

Approximate eq (2) at box center

$$\frac{\overbrace{v_{i,j-1/2}}^{\text{box center}} - \overbrace{v_{i-1,j-1/2}}^{\frac{1}{2}\left(v_{i-1}+v_{i-1}^{*}\right)}}{h_{i\text{-}1}} = \frac{u_{i-1/2,j} - u_{i-1/2,j-1}}{k}$$

$$v_{i,j-1/2} = \frac{1}{2}\left(v_i^j + v_i^{j-1}\right) = \frac{1}{2}\left(v_i + v_i^{*}\right)$$

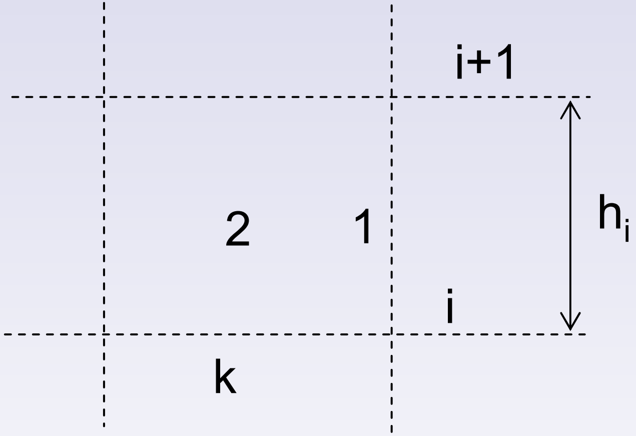
Using simple averages, i.e.

$$\frac{1}{2}\left\{\frac{v_i - v_{i-1}}{h_{i-1}} + \frac{v_i^{*} - v_{i-1}^{*}}{h_{i-1}}\right\} = \frac{1}{2}\left\{\frac{u_i + u_{i-1} - u_i^{*} - u_{i-1}^{*}}{k}\right\} \qquad (4)$$

Eliminate v_{i-1} using (3)

$$\frac{2v_i}{h_{i-1}} - \frac{2}{h^2{}_{i-1}}(u_i - u_{i-1}) + \frac{2v^*{}_i}{h_{i-1}} - \frac{2}{h^2{}_{i-1}}(u_i{}^* - u^*{}_{i-1}) = \frac{u_i - u_{i-1} - u_i{}^* - u^*{}_{i-1}}{k}$$

Upper Box



Same type of approximations & eliminate v_{i+1}

$$-\frac{2v_i}{h_i} + \frac{2}{h^2{}_i}(u_{i+1} - u_i) - \frac{2v^*{}_i}{h_i} - \frac{2}{h^2{}_i}(u_{i+1}{}^* - u^*{}_i) = \frac{u_{i+1} + u_i - u_{i+1}{}^* - u^*{}_i}{k}$$

Eliminate v_i

$$\frac{2}{h_i}(u_{i+1} - u_i) - \frac{2}{h_{i-1}}(u_i - u_{i-1}) - \frac{2}{h_i}(u_{i+1}{}^* - u^*{}_i) - \frac{2}{h_{i-1}}(u_i{}^* - u^*{}_{i-1}) =$$

$$\frac{h_i}{k}(u_{i+1} + u_i - u_{i+1}{}^* - u^*{}_i) + \frac{h_{i-1}}{k}(u_i + u_{i-1} - u_i{}^* - u^*{}_{i-1})$$

Multiply by $h_i/2$ and let

$$\alpha_i = \frac{h_i}{h_{i-1}} \text{ ratio of sizes} \quad , \quad \theta_i = \frac{h_i}{2k} \quad \text{\& system becomes}$$

$$b_i u_{i+1} + a_i u_i + c_i u_{i-1} = d_i$$

$$b_i = 1 - h_i\theta_i \quad , \quad c_i = \alpha_i - h_{i-1}\theta_i$$

$$a_i = -1 - \alpha_i - h_i\theta_i - h_{i-1}\theta_i$$

$$d_i = -u_{i+1}^* + u_i^* + \alpha_i\left(u_i^* - u_{i-1}^*\right) - h_i\theta_i\left(u_{i+1}^* - u_i^*\right) - h_{i-1}\theta_i\left(u_i^* + u_{i-1}^*\right)$$

Thomas Algorithm

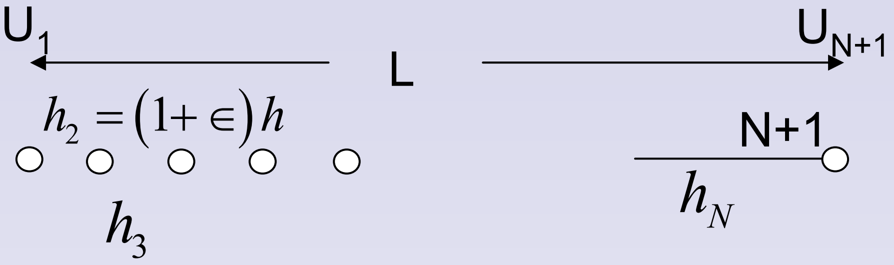
Selection of Mesh:

- Intense variation near x=0
- Small mesh near x=0

$h_1=h$ & progressively increase $h_i = \underbrace{(1+\in)}_{\alpha_i} h_{i-1} \quad i = 2,..,N$

$\in$ is small, e.g. $\in = 0.02$

$$\alpha_i = \alpha = 1 + \in$$



$$h_1 = h \quad \text{given}$$

$$h_3 = (1+\in)^2 h\text{....,}\, h_N = (1+\in)^{N-1} h$$

$$L = h + (1+\in)h + (1+\in)^2 h + \ldots + (1+\in)^{N-1} h$$

$$L = \frac{h}{\in}\left\{(1+\in)^N - 1\right\}$$

3 parameters h, $\in$,N

Select $\mathrm{h}, \in$ such that if you double N, you can compare two solutions!

Additional Features of Linear Equations

$$\frac{\partial u}{\partial t} = \delta(x,t)\frac{\partial^2 u}{\partial x^2} + p(x,t)\frac{\partial u}{\partial x} + r(x,t)u + F(x,t)$$

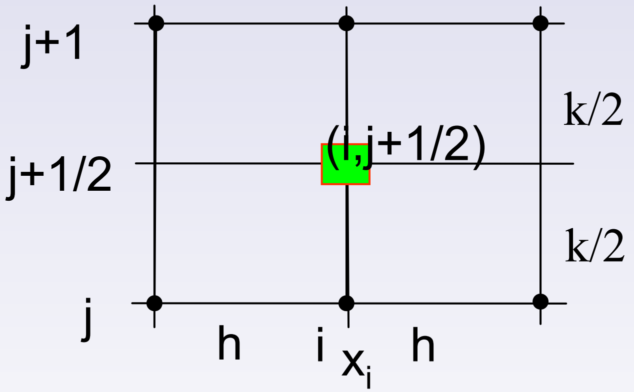
$$\frac{u_i - u_i^*}{k} = \frac{\delta_i^{**}}{2}\left\{\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + \frac{u_{i+1}^* - 2u_i^* + u_{i-1}^*}{h^2}\right\} + \frac{P_i^{**}}{2}\left\{\frac{u_{i+1} - u_{i-1}}{2h} + \frac{u_{i+1}^* - u_{i-1}^*}{2h}\right\} + \frac{r_i^{**}}{2}\left\{u_i + u_i^*\right\} + F_i^{**}$$

e.g. $\delta_i^{**} = \delta(x_i, t^{**})$

$t^{**} = t^* + k/2$

t^* =known time level

t^{**} =intermediate time level



Tridiagonal form

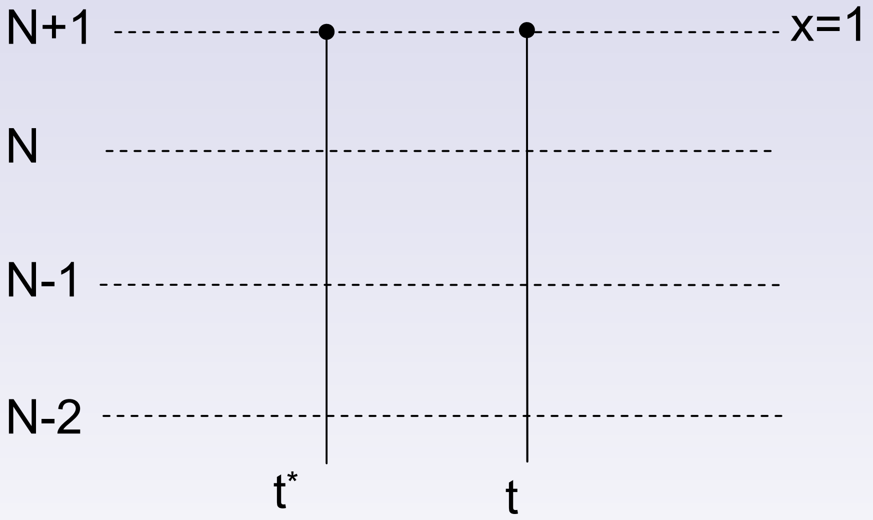
$$b_i = \delta_i^{**} + \frac{h}{2}p_i^{**} \quad , \quad a_i = -2\delta_i^{**} - \frac{2h^2}{2} + h^2 r_i^{**}$$

$$c_i = \delta_i^{**} - \frac{h}{2}p_i^{**} \quad , \quad d_i = \ldots$$

$$b_i u_{i+1} + a_i u_i + c_i u_{i-1} = d_i$$

DERIVATIVE BOUNDARY CONDITIONS

$$\frac{\partial u}{\partial x} = g(t) \qquad \text{x=1} \qquad \& \qquad u(0,t) = A = u_1$$



$$\frac{11u_{N+1} - 18u_N + 9u_{N-1} - 2u_{N-2}}{6h} = g(t)$$

Same procedure, with Thomas algorithm, as in boundary value problems

$$u_{N+1} = \frac{6hg(t) - \left\{\delta_N\left(-18 + 9F_{N-2} - 2F_{N-1}F_{N-2}\right) + \delta_{N-1}\left(9 - 2F_{N-2}\right) + \delta_{N-2}\right\}}{11 - 18F_N + 9F_N F_{N-1} - 2F_N F_{N-1} F_{N-2}}$$

Non-linear Parabolic Equations

Example: Boundary layer type of equation

Burger’s equation

$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial x^2} - u \frac{\partial u}{\partial x}$$

REMARKS

- We prefer Crank-Nicolson scheme
- Difference equations we must solve at each time step are non-linear
- Cannot be solved directly, need to linearize them and iterate at each time step until convergence
- Need to take reasonably small steps in time to ensure accuracy
- The solution at the previous time step provides a convenient first guess for the solution

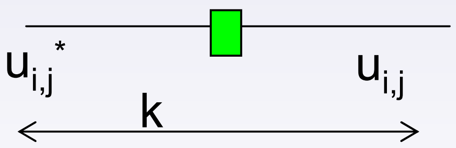
Crank-Nicolson method

$$\frac{u_i - u_i^*}{k} = \frac{1}{2}\left\{\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + \frac{u_{i+1}^* - 2u_i^* + u_{i-1}^*}{h^2}\right\} - \frac{1}{2}u_i^{**}\left\{\frac{u_{i+1} - u_{i-1}}{2h} + \frac{u_{i+1}^* - u_{i-1}^*}{2h}\right\}$$

$$u_i^{**} = \frac{u_i + u_i^*}{2}$$

$$b_i = 1 - \frac{h}{2}u_i^{**}$$

$$a_i = -2 - 2\frac{h^2}{k}$$



$$c_i = 1 + \frac{h}{2}u_i^{**}$$

$$d_i = -\left\{u_{i+1}^* - 2u_i^* + u_{i-1}^*\right\} - \frac{h}{2}u_i^{**}\left\{u_{i+1}^* - u_{i-1}^*\right\} - 2\frac{h^2}{2}u_i^*$$

Notes on non-linear equations

1. Non-linear diff. eqs. must be iterated at each time step
2. At first pass

$$u_i^{**} \simeq u_i^{*}$$

3. Error test

$$\left| 1 - \frac{u_i^{k}}{u_i^{k+1}} \right| < \varepsilon$$

Typically 2-3 steps to satisfy iteration since k is small.

Newton Linearization

$$\frac{h}{2}\left(u_i^{**}\right)\left(u_{i+1}-u_{i-1}\right)$$

$$=\frac{h}{2}\left(\frac{u_i+u_i^{*}}{2}\right)\left(u_{i+1}-u_{i-1}\right)$$

$$=\frac{h}{4}\left[u_i^{*}\left(u_{i+1}-u_{i-1}\right)+u_i\left(u_{i+1}-u_{i-1}\right)\right]$$

$$u_i u_{i+1}=-\bar{u}_i\bar{u}_{i+1}+\bar{u}_i u_{i+1}+u_i\bar{u}_{i+1}$$

$\bar{u}_i \rightarrow$ previous iterate

to start computation: set $\bar{u}_i = u_i^{*}$

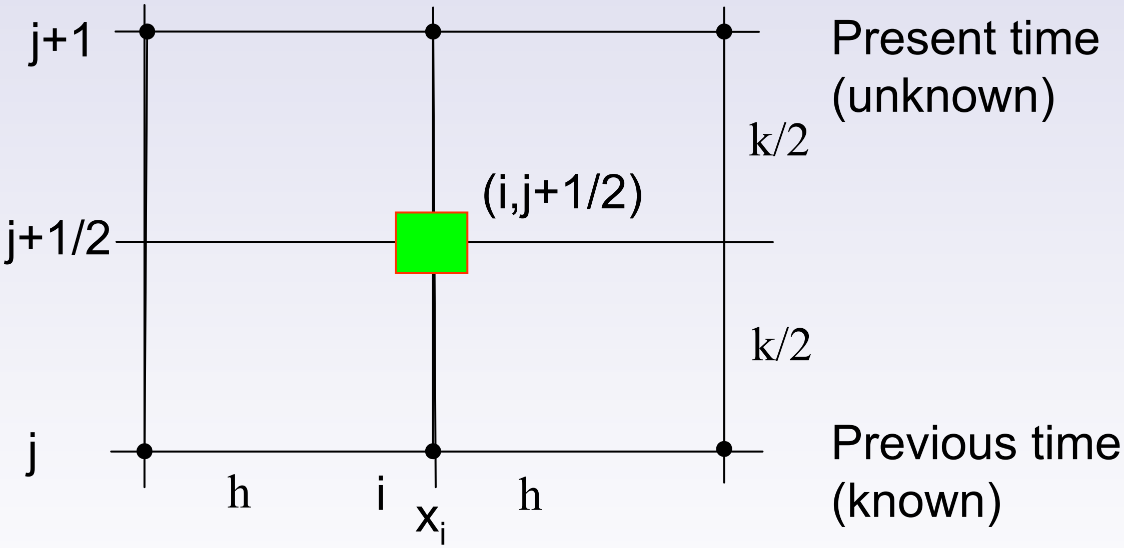
Upwind-Downwind Differencing

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \frac{1}{\mathrm{Re}}\frac{\partial^2 u}{\partial x^2}, \qquad \mathrm{Re} \gg 1$$

$$\tau = \mathrm{Re}\, t$$

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial x^2} - \mathrm{Re}\, u\frac{\partial u}{\partial x}$$

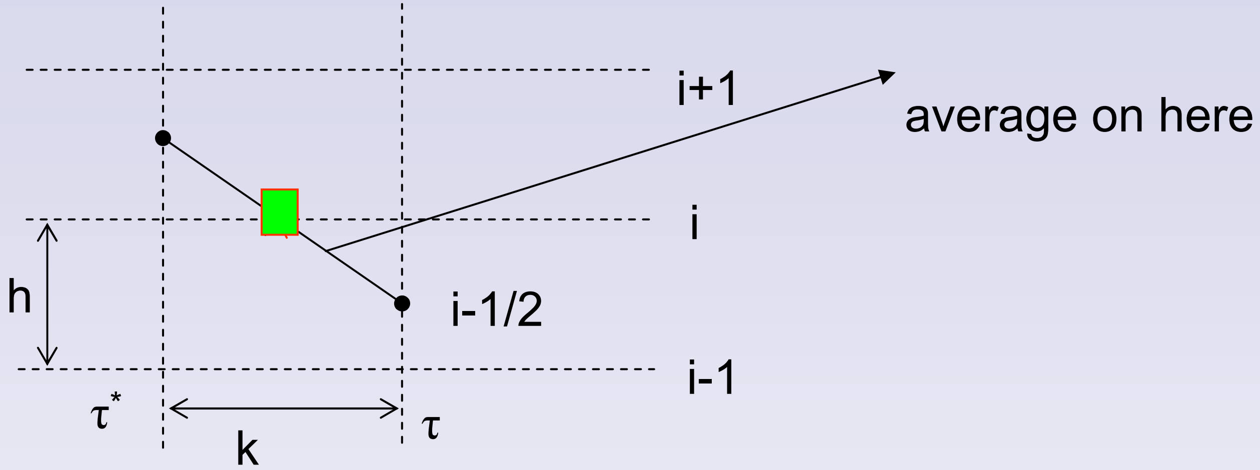
$$\frac{\partial u}{\partial \tau} = \frac{u_i - u_i^*}{k}$$



$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{2}\left\{\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + \frac{u_{i+1}^* - 2u_i^* + u_{i-1}^*}{h^2}\right\}$$

if we use $u_i^{**}\left\{\frac{u_{i+1} - u_{i-1}}{2h} + \ldots.\right\}$ problem with diagonal dominance

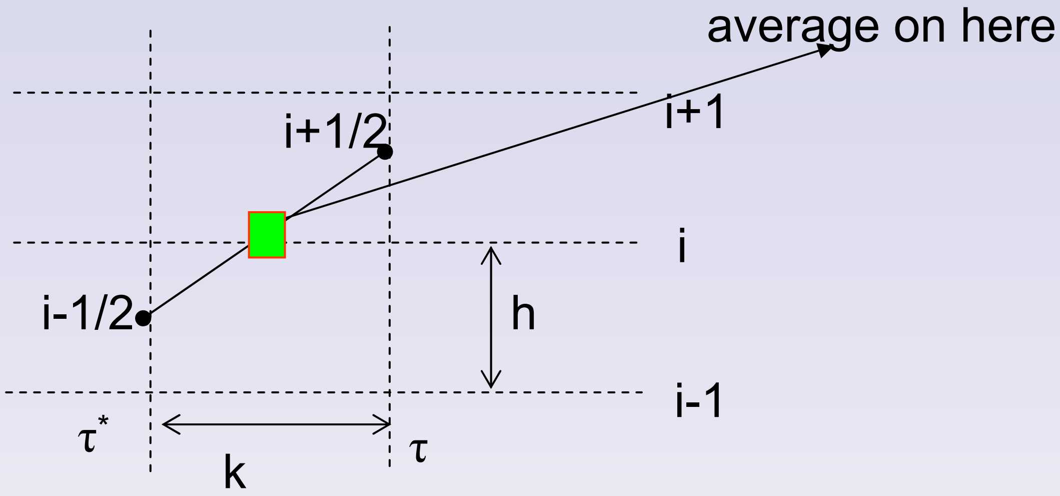
For $u_i^{**} > 0$



$$\frac{\partial u}{\partial x} = \frac{1}{2}\left\{ \left.\frac{\partial u}{\partial x}\right|_{i-1/2} + \left.\frac{\partial u}{\partial x}\right|_{i+1/2}^{*} \right\} + O(k^2)$$

$$= \frac{1}{2}\left\{ \frac{u_i - u_{i-1}}{h} + \frac{u_{i+1}^* - u_i^*}{h} \right\} + O(h^2, k^2)$$

If $u_i^{**} < 0$



$$\frac{\partial u}{\partial x} = \frac{1}{2}\left\{\frac{u_{i+1} - u_i}{h} + \frac{u_i^* - u_{i-1}^*}{h}\right\} + O(h^2, k^2)$$

Difference equations can be written in the following form:

$$u_{i+1} - \left(2 + 2\frac{h^2}{k}\right)u_i + u_{i-1} - h\,\mathrm{Re}\,u_{i+1}^{**}\left\{\begin{matrix} u_i & - & u_{i-1} \\ u_{i+1} & - & u_i \end{matrix}\right\}$$

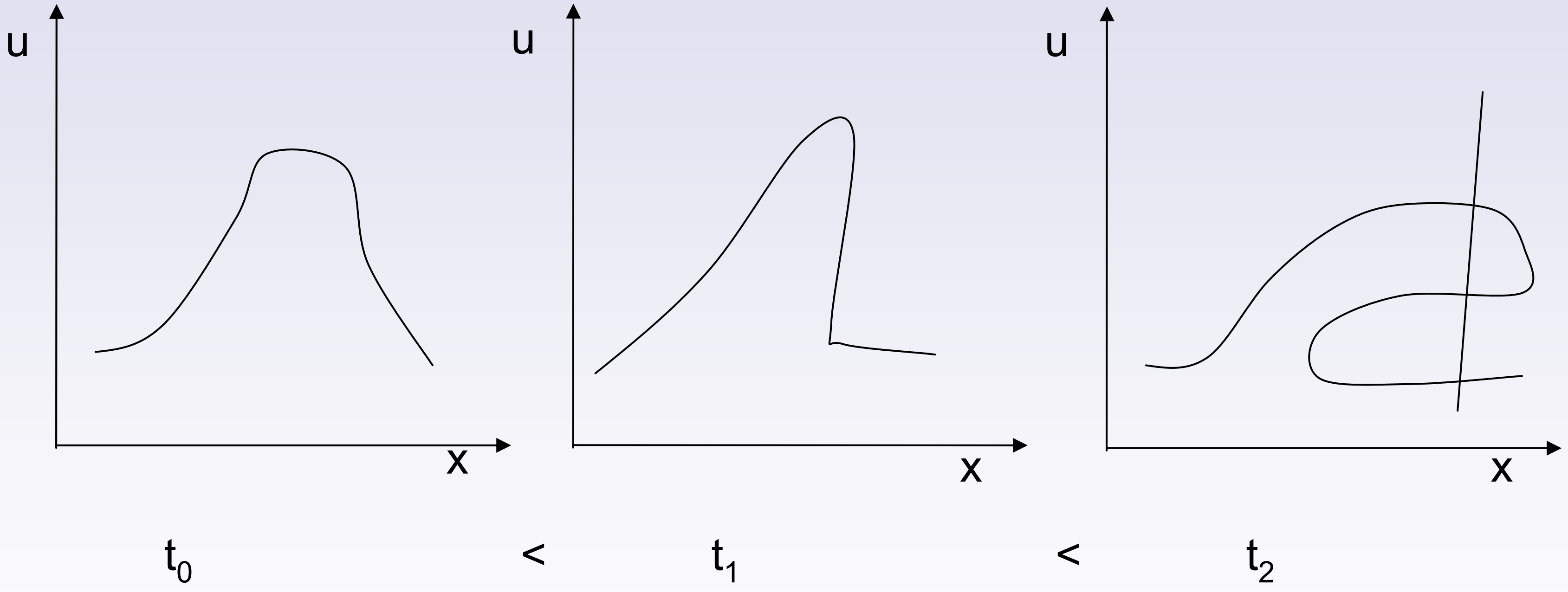
$$= -u_{i+1}^* + \left(2 - 2\frac{h^2}{k}\right)u_i^* - u_{i-1}^* + h\,\mathrm{Re}\,u_i^{**}\left\{\begin{matrix} u_{i+1}^* & - & u_i^* \\ u_i^* & - & u_{i-1}^* \end{matrix}\right\} \begin{matrix} \text{for} & u_i^{**} > 0 \\ \text{for} & u_i^{**} < 0 \end{matrix}$$

Notes:

1. At each time step it may be necessary to average

$$u_i^{(k+1)} = \delta u_i^{(k+1/2)} + (1-\delta) u_i^{(k)} \qquad 0<\delta<1$$

2. Inviscid form (Re→∞) can develop sharp fronts & multiplicity of solution



Viscous form acts to prevent this!

3. “Parabolized Navier-Stokes” eqs. preferred direction in space

$$u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}=-\frac{\partial P}{\partial x}+\frac{1}{\mathrm{Re}}\left\{\underbrace{\cancel{\frac{\partial^2 u}{\partial x^2}}}_{\text{neglect}}+\frac{\partial^2 u}{\partial y^2}\right\}$$

$$u\frac{\partial u}{\partial x}=\frac{1}{\mathrm{Re}}\frac{\partial^2 u}{\partial y^2}-v\frac{\partial u}{\partial y}-\frac{\partial P}{\partial x}$$

& march in x-direction

Factor Algorithm for Navier-Stokes equations

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + p\frac{\partial u}{\partial x} + q\frac{\partial u}{\partial y} + ru + w$$

$$p = p(u,x,y,t) \quad \text{etc.}$$

$$\frac{u_{i,j} - u^*_{i,j}}{k} = \frac{1}{2h_1^2}\left\{\delta_x^2 u_{i,j} + \delta_x^2 u^*_{i,j}\right\} + \frac{1}{2h_2^2}\left\{\delta_y^2 u_{i,j} + \delta_y^2 u^*_{i,j}\right\} +$$

$$\frac{p^{**}}{4h_1}\left\{\mu_x\delta_x u_{i,j} + \mu_x\delta_x u^*_{i,j}\right\} + \frac{Q^{**}}{4h_2}\left\{\mu_y\delta_y u_{i,j} + \mu_y\delta_y u^*_{i,j}\right\} + \frac{R^{**}}{2}\left(u_{i,j} + u^*_{i,j}\right) + w^{**}$$

$$\text{estimate} \quad p^{**} = \frac{1}{2}\left(p + p^*\right)$$

Multiply by 2k & rearrange

$$\left\{2 - kR^{**} - \frac{k}{h_1^2}\delta_x^2 - \frac{kP^{**}}{2h_1}\mu_x\delta_x - \frac{k}{h_2^2}\delta_y^2 - \frac{kQ^{**}}{2h_2}\mu_y\delta_y\right\}u_{i,j} =$$

$$\left\{2 + kR^{**} + \frac{k}{h_1^2}\delta_x^2 + \frac{kP^{**}}{2h_1}\mu_x\delta_x + \frac{k}{h_2^2}\delta_y^2 + \frac{kQ^{**}}{2h_2}\mu_y\delta_y\right\}u_{i,j}^{*} + 2kw^{**}$$

if $\alpha = \dfrac{1}{2 - kR^{**}}$

$$\left\{1 - \frac{\alpha k}{h_1^2}\left[\delta_x^2 + \frac{h_1}{2}P^{**}\mu_x\delta_x\right] - \frac{\alpha k}{h_2^2}\left[\delta_y^2 + \frac{h_2}{2}Q^{**}\mu_y\delta_y\right]\right\}u_{i,j} = D_{i,j}$$

$$D_{i,j} = \alpha\left\{2 + kR^{**} + ...\right\}u_{i,j}^{*} + 2\alpha kw^{**}$$

Factor

$$\left\{1 - \frac{\alpha k}{h_1^2}\left[\delta_x^2 + \frac{h_1}{2}P^{**}\mu_x\delta_x\right]\right\}\left\{1 - \frac{\alpha k}{h_2^2}\left[\delta_y^2 + \frac{h_2}{2}Q^{**}\mu_y\delta_y\right]\right\}u_{i,j} \cong D_{i,j}$$

$$\left\{1 - \frac{\alpha k}{h_1^2}\left[\delta_x^2 + \frac{h_1}{2}P^{**}\mu_x\delta_x\right]\right\}u_{i,j}^{n+1/2} = D_{i,j}$$

Solved in a manner similar to diffusion equation

$$\left\{1 - \frac{\alpha k}{h_1^2}\left[\delta_y^2 + \frac{h_1}{2}Q^{**}\mu_y\delta_y\right]\right\}u_{i,j}^{n+1} = u_{i,j}^{n+1/2}$$

- Iterate

ELLIPTIC PROBLEMS

- Steady state heat conduction equation
- Velocity potential eq. & stream function eq. for incomp., inviscid, irrotational flow

Typical Elliptic equations

Laplace's eq. $\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}=0$ Poisson's eq. $\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}=f(x,y)$

Types of Eqs.

1. Linear: Laplace, Poisson
2. Non-Linear
    a. Linear PDE with non-linear BCs

e.g. $\nabla^2 u = 0 \quad \frac{\partial \mathrm{u}}{\partial \mathrm{n}} = D\left(u^4 - T_\infty^4\right) \quad \text{on C}$

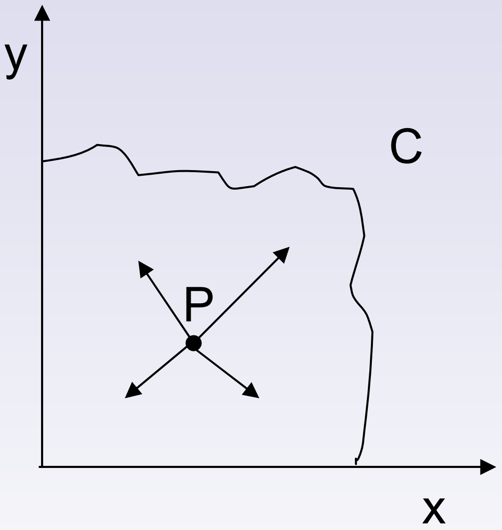
b. Non-Linear PDE

e.g. Navier-Stokes

$$\underbrace{u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}}_{\text{non-linear}}=-\frac{\partial P}{\partial x}+\frac{1}{\mathrm{Re}}\left[\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right]$$

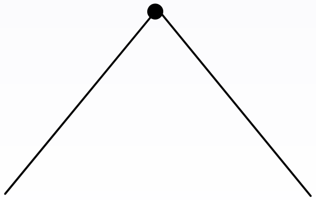
Nature of Solution

a) Any disturbance at a point P influences the solution everywhere
- always necessary to consider solution globally
- in well posed elliptic problems, BCs needed on all boundaries

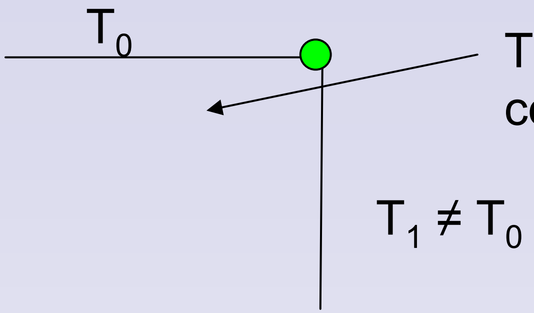


b) Singularities

Discontinuation in the BCs are smoothed out in the interior. No discontinuous behavior in interiour: only in boundary data



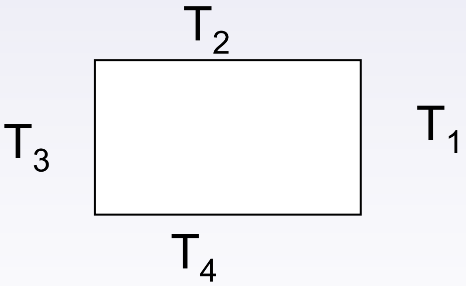
No propagation into interior



Temperature is smooth & continuous

e.g. heat transfer

c) Maximum prensible
For Laplace eq. extrama of function must occur on boundary



$T_0 < T_1 < T_2 < T_3$

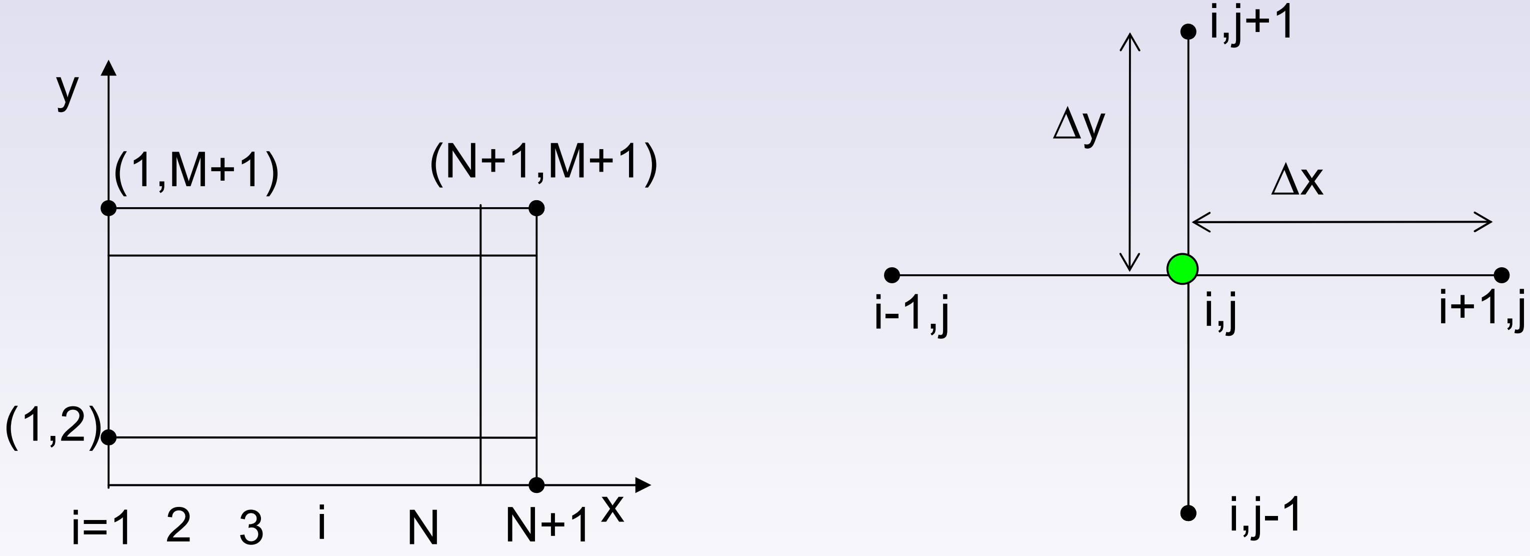
Then, there is no T in interior with
$T < T_0$; $T > T_3$

- Domain Methods: Finite Difference & Finite Element Methods
- Boundary Integral Methods

Finite Difference Formulations:

Start by considering the case where u is known on boundary.
 “Five-point formula” –second order accurate.

Split x interval into N equal points & y into M equal points.



Let us use second – order accurate, central differences at point i,j

$$\nabla^2 u = f(x, y)$$

$$f_{i,j} = f(x_i, y_i)$$

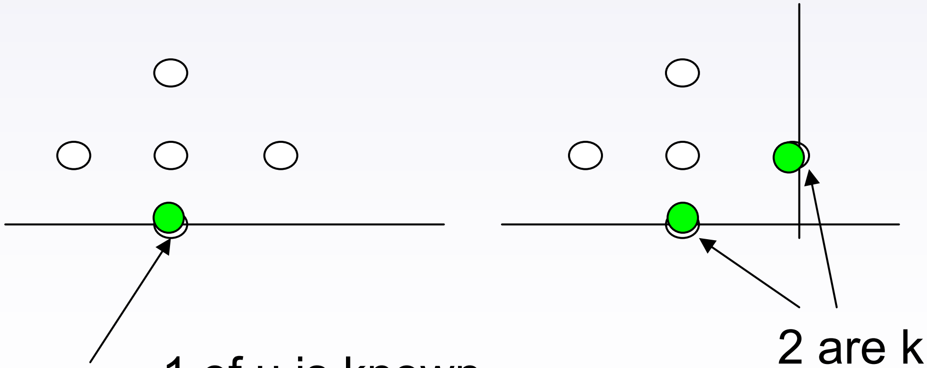
$$\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{k^2} = f_{i,j}$$

$$u_{i+1,j} - 2u_{i,j} + u_{i-1,j} + \gamma\left(u_{i,j+1} - 2u_{i,j} + u_{i,j-1}\right) = h^2 f_{i,j} \qquad (1)$$

$$\gamma = \left(\frac{h}{k}\right)^2$$: ratio of step sizes

Total of (M-1) x (N-1) eqs.

Typically 10000 such eqs. & up



1 of u is known

2 are known

Solution Algorithms:

a) Direct methods
b) Iterative methods

a) Eq.(1) is not tridiagonal

- can be solved with general G.S. elimination based on partial pivoting, or special algorithm which takes into account banded structure of matrix.

•but substantial amount of computation in forward elimination & back substitution
•at around 3000-5000 becomes non-comptetive with iterative methods.
Therefore, usually use iterative methods with elliptic eqs.

ITERATIVE METHODS:

Simple & easy to program

A. Jacobi iteration

Rewrite eq.(1)

$$u_{i,j}^{(k+1)} = \frac{1}{2(1+\gamma)}\left[-h^2 f_{i,j} + u_{i+1,j}^{(k)} + u_{i-1,j}^{(k)} + \gamma u_{i,j+1}^{(k)} + \gamma u_{i,j-1}^{(k)}\right] \quad (2)$$

k:iteration counter

Prodecure:

1. Guess $u_{i,j}$ at every point (k=0) (initial guess) $u_{i,j}^{(0)}$ i=2,..,N , j=2,..,M
2. Apply (2) at every point in the mesh $u_{i,j}$,
   use systematic sweep of mesh
3. Continue until convergence

$$\left| 1 - \frac{u_{i,j}^{(k)}}{u_{i,j}^{(k+1)}} \right| < \in \quad \text{for all i,j}$$

e.g. $\in = 10^{-4}$ → 4 significant figures

Notes:

1. Process is not used in practice because it is too slow

$$e_{i,j}^{n} : \text{error at n}^{\text{th}} \text{ iteration}$$

$$e_{i,j}^{n} = u_{i,j}^{n} - u_{i,j}$$

$$u_{i,j}^{n} : \text{estimate}$$

$$u_{i,j} : \text{true value}$$

$$e_{i,j}^{(n+1)} \approx \rho(J) e_{i,j}^{(n)}$$

$$\rho(J) : \text{ modulus of largest eigenvalue of iteration matrix. } \rho(J) < 1$$

For equal mesh lengths h=k
rectangular regions & Poisson’s eq.

$$\rho(J)=\frac{1}{2}\left\{\cos\left(\frac{\pi}{N+1}\right)+\cos\left(\frac{\pi}{M+1}\right)\right\}$$

i. For coarse meshes, ρ(J) is smaller

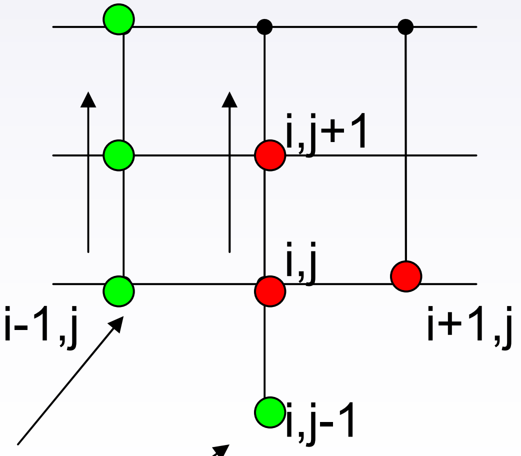
⇨ Fast convergence (but not necessarily correct answers)

ii. Smaller meshes ρ→1 (M, N→∞)

⇨ Slow convergence with finer meshes

B) GAUSS-SEIDEL ITERATION

- Current values of u is used
  - Sweeping on lines of constant x in +y direction



green dots have been computed, therefore use most recent information

$$u_{i,j}^{(k+1)} = \frac{1}{2(1+\gamma)}\left[-h^2 f_{i,j} + u_{i+1,j}^{(k)} + u_{i-1,j}^{(k+1)} + \gamma u_{i,j+1}^{(k)} + \gamma u_{i,j-1}^{(k+1)}\right] \quad (3)$$

Note:

1. No need to hold previous iterate in core
2. Method is much faster than Jacobi
   h=k , rectangular regions, Poisson eq.

$$\rho(G) = \rho^2(J)$$

Analogy between the iterative method & time dependent parabolic equation

2-D unsteady heat conduction

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$$

Remember the Explicit formulation: FTCS

Let Δx=Δy ,

$$u_{i,j}^{n+1} = u_{i,j}^{n} + \frac{\Delta\mathrm{t}}{(\Delta\mathrm{x})^2}\left[u_{i+1,j}^{n} + u_{i-1,j}^{n} + u_{i,j+1}^{n} + u_{i,j-1}^{n} - 4u_{i,j}^{n}\right]$$

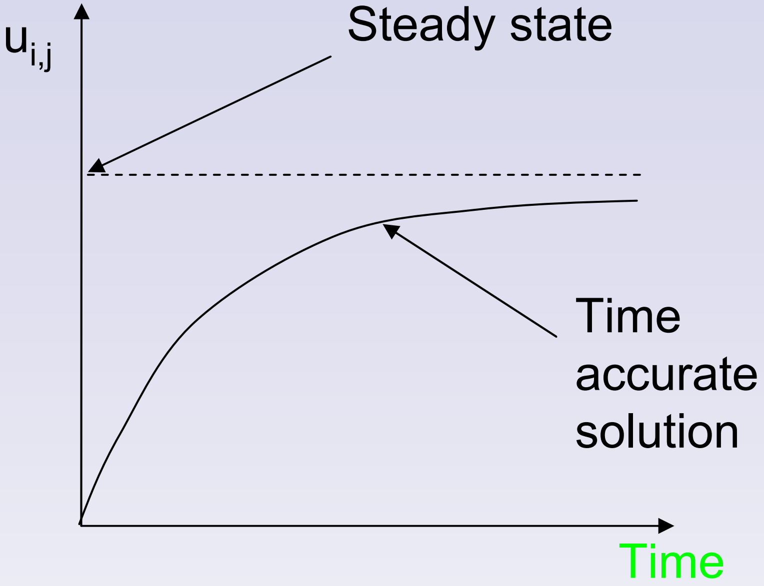
$$\frac{\Delta\mathrm{t}}{(\Delta\mathrm{x})^2} \le \frac{1}{4} \quad \text{upper limit}$$

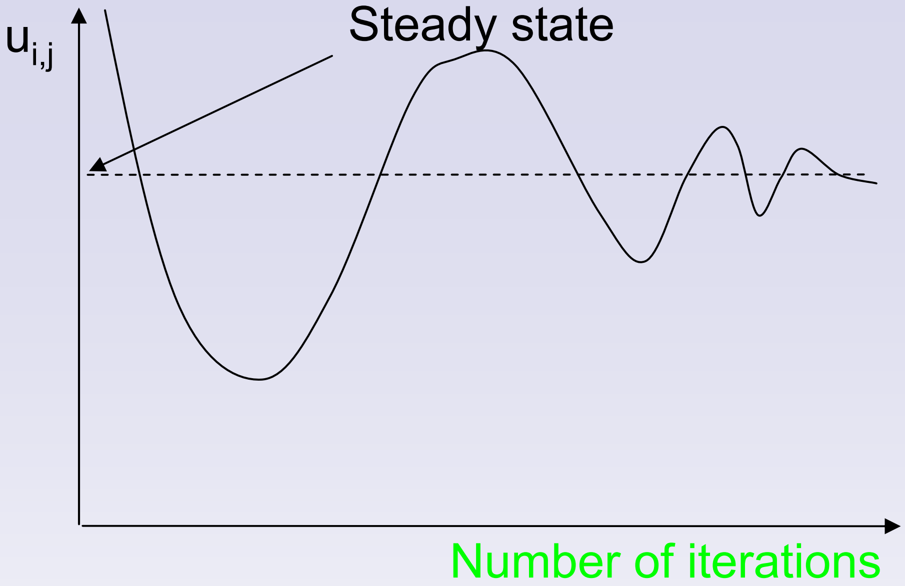
$$u_{i,j}^{n+1} = \frac{1}{4}\left[u_{i+1,j}^{n} + u_{i-1,j}^{n} + u_{i,j+1}^{n} + u_{i,j-1}^{n}\right] \quad \text{(A) FTCS approx. of a parabolic eq.}$$

Now, Jacobi iteration $\gamma = \left(\frac{h}{k}\right)^2 = 1 \quad , \quad \mathrm{f}_{\mathrm{ij}} = 0$

$$u_{i,j}^{k+1} = \frac{1}{4}\left[u_{i+1,j}^{k} + u_{i-1,j}^{k} + u_{i,j+1}^{k} + u_{i,j-1}^{k}\right] \quad \text{(B) Jacobi iteration for an elliptic eq.}$$

- Mathematically (to the computer) the same but the different physical phenomena
- Thus, some techniques used for parabolic eqs. can be extended or modified for elliptic equations





Eq.(A)
Solution is valid at any intermediate time level if imposed initial data & time step represent physics

Eq.(B)
Intermediate solution of eq.(B) has no physical significance ➡ converged, or steady-state solution

C) SUCCESSIVE OVER RELAXATION (SOR)

- Usually faster than G.S for linear problems

Gauss-Seidel iteration

$$u_{i,j}^{(k+1)} = \frac{1}{2(1+\gamma)}\left[-h^2 f_{i,j} + u_{i+1,j}^{(k)} + u_{i-1,j}^{(k+1)} + \gamma\left(u_{i,j+1}^{(k)} + u_{i,j-1}^{(k+1)}\right)\right]$$

adding $u_{i,j}^{(k)}$ -$u_{i,j}^{(k)}$ to RHS & collect terms

$$u_{i,j}^{(k+1)} = u_{i,j}^{(k)} + \frac{1}{2(1+\gamma)}\left[u_{i+1,j}^{(k)} + u_{i-1,j}^{(k+1)} + \gamma\left(u_{i,j+1}^{(k)} + u_{i,j-1}^{(k+1)}\right) - 2(1+\gamma)u_{i,j}^{(k)}\right]$$

$u_{i,j}^{(k)} \rightarrow u_{i,j}^{(k+1)}$ (as solution proceeds)

To accelarate the solution, the bracket term is multiplied by ω, relaxation parameter (factor)

$$u_{i,j}^{k+1} = u_{i,j}^{k} + \frac{\omega}{2(1+\gamma)}\left\{ \qquad \qquad \right\} \quad (*)$$

For convergence 0<ω<2
If 0<ω<1 → under-relaxation (some non-linear problems) (iterative averaging ω≈0.5)
ω=1 : Gauss-Seidel is recovered

Rearrange eq.(*)

$$u_{i,j}^{k+1} = (1-\omega) u_{i,j}^{k} + \frac{\omega}{2(1+\gamma)} \left\{ -h^2 f_{i,j} + u_{i+1,j}^{k} + u_{i-1,j}^{k+1} + \gamma \left(u_{i,j+1}^{k} + u_{i,j-1}^{k+1} \right) \right\}$$

1<ω<2 over-relaxation (best for linear problems)

ω≈1.65

Method of Estimating ω_{opt}

ω_{opt} is related to spectral radius of Gauss-Seidel matrix by

$$\omega_{opt} = \frac{2}{1+\left(1-\rho(G)\right)^{1/2}}$$

Esimate $\rho(G)$ by performing a large number of G.S iterations & estimate $\rho(G)$ from

$$\rho(G) = \lim_{k\to\infty} \frac{\left\| \vec{d}^{(k)} \right\|}{\left\| \vec{d}^{(k-1)} \right\|}$$

$$d_{i,j}^{(k)} = u_{i,j}^{k} - u_{i,j}^{k-1}$$

i. $\left\| \vec{d} \right\| = \sum_i \sum_j \left| u_{i,j}^{k} - u_{i,j}^{k-1} \right|$

ii. $\left\| \vec{d} \right\| = \sqrt{\sum_i \sum_j \left(u_{i,j}^{k} - u_{i,j}^{k-1} \right)^2}$

Special case

Rectangular domain subject to Dirichlet BCs with constant step sizes

$$\omega_{opt} = \frac{2-2\sqrt{1-a}}{a} \quad , \quad a = \left[\frac{\cos\left(\frac{\pi}{N}\right) + \gamma \cos\left(\frac{\pi}{M}\right)}{1+\gamma} \right]^2$$

Derivative Boundary Conditions

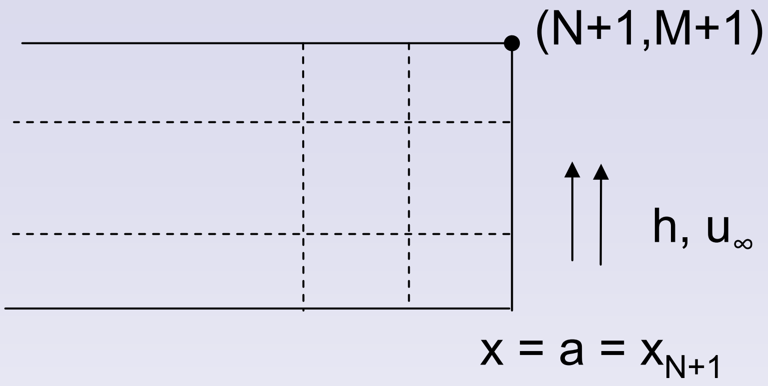
Conduction heat transfer

i. $\frac{\partial u}{\partial n}$ given $\quad \frac{\partial u}{\partial n} = 0$ insulated

$-k^* \frac{\partial u}{\partial n} = q$ specified heat flux

ii. $-k^* \frac{\partial u}{\partial n} = h^* \left(u - u_\infty \right)$ convection conditions

Example: suppose convection on right face.



$$-k^* \frac{\partial u}{\partial n} = h^* \left(u - u_\infty\right) \quad \text{on} \quad x{=}a$$

$$\theta = u - u_\infty$$

$$-k^* \frac{\partial \theta}{\partial n} = h^* \theta$$

Simplest method:

Approximate eq. at nodal points on boundary (x→a-)

At interior nodal points on x = a , j=2,…,M but not at corners j = 1&M+1

$$u_{N+2,j} + u_{N,j} + \gamma\left\{u_{N+1,j+1} + u_{N+1,j-1}\right\} - 2\left(1+\gamma\right)u_{N+1,j} = h^2 f_{ij} \qquad (4)$$

$$\gamma = \left(\frac{h}{k}\right)^2$$

Derivative condition is also valid at x=a, i.e., i=N+1 (on boundary)

$$-k^* \left\{\frac{u_{N+2,j} - u_{N,j}}{2h}\right\} = h^* \left\{u_{N+1,j} - u_\infty\right\} \qquad (5)$$

Use eq.(5) to eliminate $u_{N+2,j}$ in eq.(4).

$$2u_{N,j} + \gamma\left\{u_{N+1,j+1} + u_{N+1,j-1}\right\} - \left(2 + 2\gamma + 2h\alpha\right)u_{N+1,j} = -2h\alpha u_\infty + h^2 f_{ij} \qquad (6)$$

$$\alpha = \left(\frac{h^*}{k^*}\right)$$

Computational Algorithm:

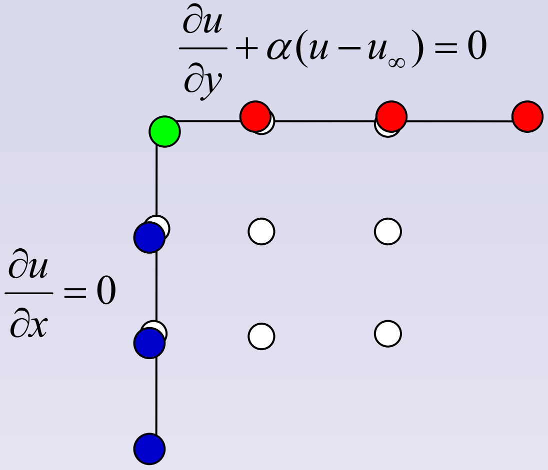
Sweep interior points (G.S) as before plus additional sweep on right face

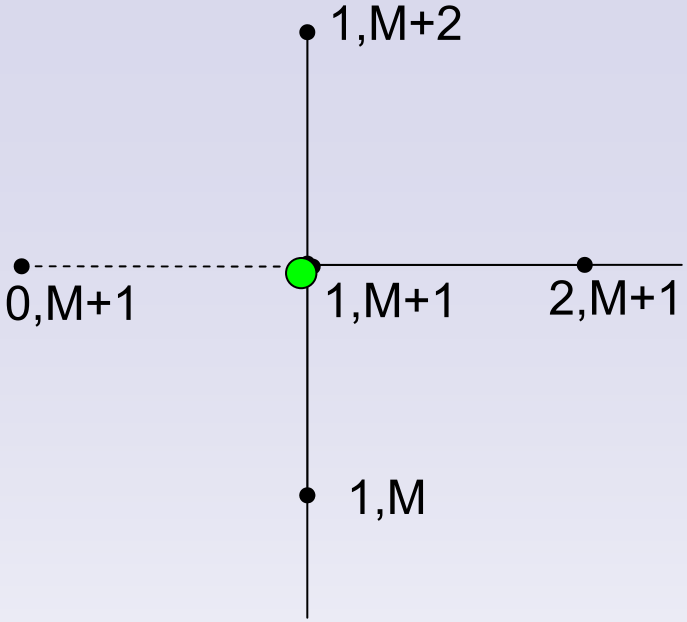
$$u_{N+1,j} = \frac{1}{\left(2 + 2\gamma + 2h\alpha\right)}\left\{2u_{N,j} + \gamma\left(u_{N+1,j+1} + u_{N+1,j-1}\right) + 2h\alpha u_\infty - h^2 f_{ij}\right\} \qquad (7)$$

j=2,..,M

Notes:

1. simplest method but inaccurate
2. additional sweep on any face where derivatives are specified
3. for insulated boundary simply set α=0
4. special care is needed for conditions on adjoining edges





Insulated condition → $u_{0,M+1} = u_{2,M+1}$ (8)

Convective condition

$$u_{1,M+2}-u_{1,M}+2h\alpha\left(u_{1,M+1}-u_\infty\right)=0 \quad (9)$$

Approx. to differential eq. at (1,M+1)

$$u_{2,M+1}-2u_{1,M+1}+u_{0,M+1}+\gamma\left(u_{1,M+1}-2u_{1,M+1}+u_{1,M}\right)=h^2 f_{1,M+1} \quad (10)$$

Eliminate $u_{0,M+1}$ & $u_{1,M+2}$

$$u_{1,M+1}=\frac{1}{\left(2+2\gamma+2h\alpha\gamma\right)}\left\{2u_{2,M+1}+2\gamma u_{1,M}+2\gamma h\alpha u_\infty-h^2 f_{1,M+1}\right\} \quad (11)$$

special eq. for the corner.

Diagonal Dominance

Difference eq.

$$u_{i+1,j}+u_{i-1,j}+\gamma\left(u_{i,j+1}+u_{i,j-1}\right)-\left(2+2\gamma\right)u_{i,j}=h^2 f_{i,j}$$

$$u_{i,j}=\frac{1}{\underbrace{\left(2+2\gamma\right)}_{\text{large \#}}}\left\{-h^2 f_{i,j}+u_{i+1,j}+u_{i-1,j}+\gamma\left(u_{i,j+1}+u_{i,j-1}\right)\right\}$$

Eq. is written in this form so system is diagonally dominant

$$\underset{\sim}{A}\underset{\sim}{x}=\underset{\sim}{b}$$

ith eq. $a_{i1}x_1+a_{i2}x_2+\ldots+a_{ii}x_i+\ldots+a_{im}x_m=b_i$

Diagonally dominant if

$$\left|a_{ii}\right|>\left|a_{i1}\right|+\left|a_{i2}\right|+\ldots+\left|a_{i,i-1}\right|+\left|a_{i,i+1}\right|+\ldots+\left|a_{im}\right|$$

The system is diagonally dominant if all eqs. have this property.
Iteration schemes will converge if the system has this property.

Notes:

1. Our system has

$$|2+2\gamma| = |1| + |1| + |\gamma| + |\gamma|$$

2. If one (or more) not diagonally dominant

   → iteration usually diverge

3. Non-centered differences , → non-diagonally dominant systems.

e.g.

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{ij} = \frac{1}{3h^2}\left\{-3u_{ij} + 12u_{i+1,j} - 15u_{i+2,j} + 3u_{i+3,j}\right\} + O\left(h^3\right)$$

4. For non-linear equations

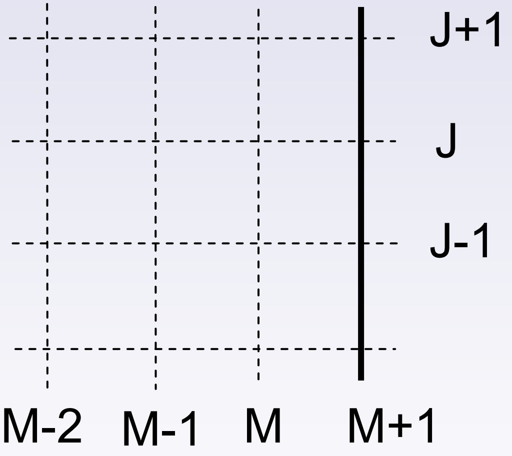
   no guarantee that iterative solution will converge even if diagonally dominant

$$\nabla^2 u + u\frac{\partial u}{\partial x} = 0$$

Improved method for derivative conditions

Higher order approximation for derivative

But must retain diagonal dominance



Sloping difference approximation

$$\frac{\partial u}{\partial x} + \alpha\left(u - u_\infty\right) = 0$$

$$\frac{1}{16}\left\{-2u_{M-2,j} + 9u_{M-1,j} - 18u_{M,j} + 11u_{M+1,j}\right\} + \alpha\left(u_{M+1,j} - u_\infty\right) = 0 + O(h^3)$$

$$u_{M+1,j} = \frac{1}{(11+6\alpha h)}\left\{18u_{M,j} - 9u_{M-1,j} + 2u_{M-2,j} + \alpha u_\infty\right\} + O(h^3) \qquad (13)$$

Substitute into approx. of diff.eq. at i=M

$$u_{i+1,j} \text{-} 2u_{i,j} + u_{i-1,j} + \gamma\left(u_{i,j+1} - 2u_{i,j} + u_{i,j-1}\right) = h^2 f_{i,j} \qquad (1)$$

$$\frac{1}{11+6\alpha h}\left\{18u_{M,j+1} - 9u_{M-1,j} + 2u_{M-2,j} + \alpha u_\infty\right\} + u_{M-1,j} +$$

$$\gamma\left\{u_{M,j+1} + u_{M,j-1}\right\} - (2+2\gamma)u_{M,j} = h^2 f_{ij} \qquad (14)$$

Or

$$\left\{1 \text{-} \frac{9}{11+6\alpha h}\right\}u_{M\text{-}1,j} + \frac{2}{(11+6\alpha h)}u_{M\text{-}2,j} +$$

$$\gamma\left\{u_{M,j+1} - u_{M,j\text{-}1}\right\} \text{-} \left(2+2\gamma \text{-} \frac{18}{11+6\alpha h}\right)u_{M,j} = h^2 f_{M+1,j} \text{-} \frac{\alpha u_\infty}{11+6\alpha h} \qquad (15)$$

Let us check for diagonal dominance of eq.(15) for small h,

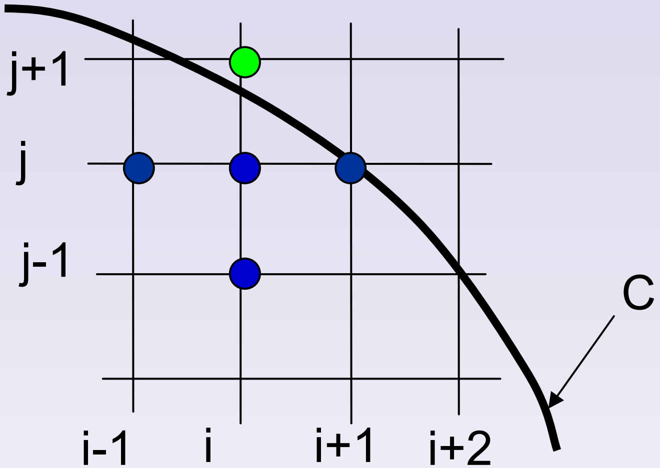
$$2+2\gamma-\frac{18}{11+6\alpha h}\approx\frac{4}{11}+2\gamma$$

$$\left|1-\frac{9}{11+6\alpha h}\right|+\left|\frac{2}{11+6\alpha h}\right|+|\gamma|+|\gamma|\approx\frac{4}{11}+2\gamma$$

Procedure:

1. sweep interior points with the conventional eq.
2. on line adjacent to right boundary use (15)
3. u values on right face, obtained from (13) after convergence

CURVED IRREGULAR BOUNDARIES

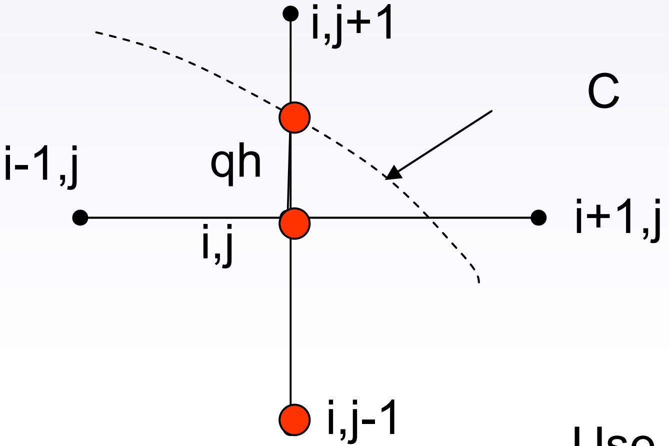


Consider approx. at i,j

$$u_{i+1,j}+u_{i-1,j}+u_{i,j+1}+u_{i,j-1}-4u_{i,j}=h^2 f_{i,j}$$

But $u_{i,j+1}$ is not in interior

Suppose C intersects i



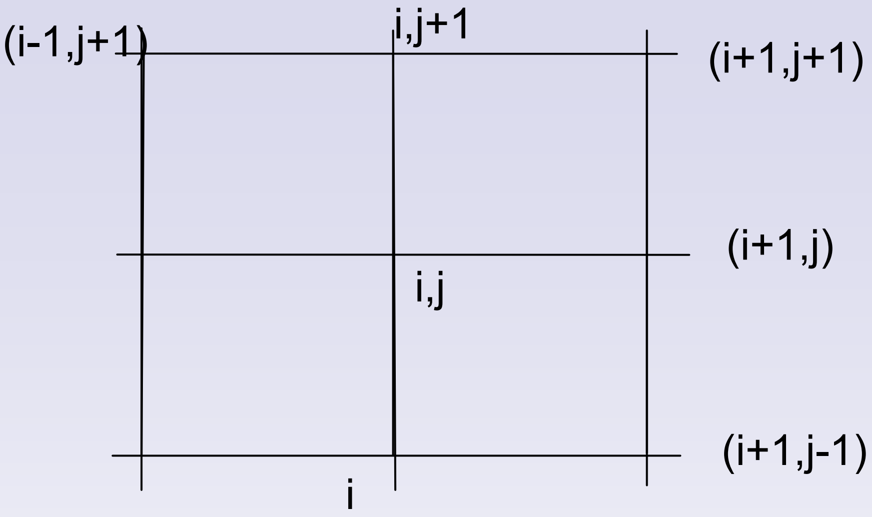
point interpolation on ith mesh line, q<1

$$u_{i,C}=u(x_i,y_i+qh)=\frac{q(q+1)}{2}u_{i,j+1}+$$

$$(1-q^2)u_{i,j}+\frac{q(q-1)}{2}u_{i,j-1}+O(h^3)$$

Use above eq. to eliminate $u_{i,j+1}$

Nine Point Formula For Laplacian (derivation)



Define operators

$$\xi = \frac{\partial}{\partial x} \quad , \quad \eta = \frac{\partial}{\partial y}$$

Hold one variable constant (e.g. x) and consider Taylor Series;

$$u\left(x+h,y\right)=\left(1+h\frac{\partial}{\partial x}+\frac{h^2}{2!}\frac{\partial^2}{\partial x^2}+\ldots\right)u\left(x,y\right)=e^{\xi}u(x,y)$$

Similarly

$$u\left(x, y+h\right) = e^{\eta} u(x, y)$$

Consider the sum

$$S_1 = u_{i+1,j} + u_{i,j+1} + u_{i-1,j} + u_{i,j-1}$$

and

$$S_1 = \left(e^{\xi} + e^{\eta} + e^{-\xi} + e^{-\eta}\right) u(x, y)\Big|_{\substack{x=x_i \\ y=y_j}} \qquad (31)$$

but

$$e^{\xi} + e^{-\xi} + e^{-\eta} + e^{\eta} = 2 + \xi^2 + \frac{\xi^4}{12} + ... + 2 + \eta^2 + \frac{\eta^4}{12} + ...$$

$$= 4 + h^2 \nabla^2 + \frac{h^4}{12}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + ...$$

and equation (31) becomes

$$S_1 = 4u_{i,j} + h^2 \nabla^2 u\Big|_{i,j} + \frac{h^4}{12}\left(\nabla^4 u - 2D^4 u\right)_{i,j} + ... \qquad (32)$$

$$\mathrm{D}^2 = h \frac{\partial^2}{\partial x \partial y} \qquad \nabla^4 = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)^2$$

If we neglect last term in (32) Standard 5 point Formula.

Now consider sum

$$S_2 = u_{i+1,j+1} + u_{i-1,j+1} + u_{i-1,j+1} + u_{i-1,j-1} = \left(e^{\xi+\eta} + e^{-\xi+\eta} + e^{-\xi+\eta} + e^{-\xi-\eta}\right) u(x,y)\Big|_{i,j}$$

$$= \left\{1+\xi+\frac{\xi^2}{2!}+\frac{\xi^3}{3!}+\ldots\right\}\ \left\{2+\eta^2+\frac{\eta^4}{12}+\ldots\right\}+\left\{2+\xi^2+\frac{\xi^4}{12}+\ldots.\right\}\left\{2+\eta^2+\frac{\eta^4}{12}+\ldots\right\}$$

$$= 4+2\left(\xi^2+\eta^2\right)+\left(\frac{\xi^4}{6}+\frac{\eta^4}{6}+\xi^2\eta^2\right)+\ldots$$

$$= 4+2h^2\nabla^2+\frac{h^4}{6}\left(\nabla^4-2D^4+6D^4\right)$$

$$S_2 = u_{i,j}+2h^2\nabla^2 u\Big|_{i,j}+\frac{h^4}{6}\left(\nabla^4 u+4D^4 u\right)_{i,j}+\ldots \qquad (33)$$

To obtain 9 point formula, take 4x32 + 33

$$4S_1+S_2 = 20u_{i,j}+6h^2\nabla^2 u\Big|_{i,j}+\frac{h^2}{12}\nabla^4 u\Big|_{i,j}+\ldots$$

$$\nabla^2 u\Big|_{i,j} = \frac{4S_1+S_2-20u_{i,j}}{6h^2}-\frac{h^2}{12}\nabla^4 u\Big|_{i,j}+O\left(h^4\right) \quad (34)$$

Note Laplace eq. $\nabla^4 u = 0$

$$4S_1+S_2-20u_{i,j} = 0 \qquad (35)$$

- Still diagonally dominant
- Dirichlet conditions, very effective
- Derivative conditions more difficuilt to implement
- Mesh with Δx=h , Δy=k

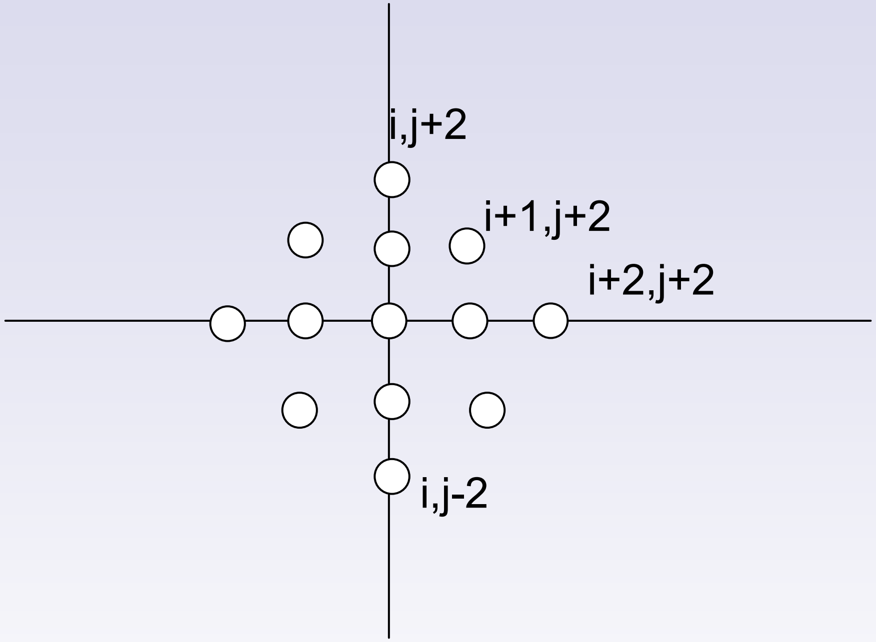
$$u_{i+1,j+1}+u_{i-1,j+1}+u_{i+1,j-1}+u_{i-1,j-1}-\frac{2\left(h^2-5k^2\right)}{h^2+k^2}\left(u_{i+1,j}+u_{i-1,j}\right)$$

$$+\frac{2\left(5h^2-k^2\right)}{h^2+k^2}\left(u_{i,j+1}+u_{i,j-1}\right)-20u_{i,j}=0 \qquad (36)$$

Poisson eq. $\nabla^2 u = f(x,y)$

Then (34) becomes

$$u_{i+1,j+1}+u_{i-1,j+1}+u_{i+1,j-1}+u_{i-1,j-1}-4\left(u_{i+1,j}+u_{i-1,j}+u_{i,j+1}+u_{i,j-1}\right)-20u_{i,j}=6h^2 f_{i,j}+\frac{h^2}{12}\nabla^2 f\Big|_{i,j}$$

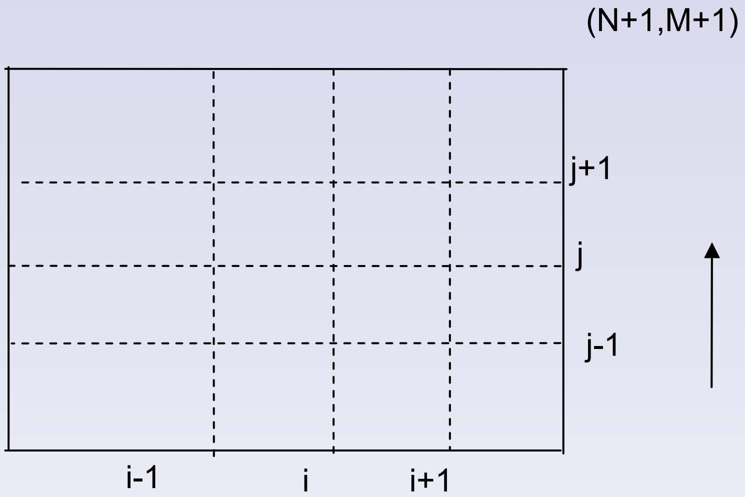


Not diagonally dominant

$$\nabla^2 u\big|_{i,j} = \frac{1}{12h^2}\left\{-60u_{i,j} + 16\left(u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1}\right) - \left(u_{i+2,j} + u_{i-2,j} + u_{i,j+2} + u_{i,j-1}\right)\right\} + O\left(h^2\right)$$

Not good in solving differential equation, not diagonally dominant

ALTERNATING DIRECTION METHODS



Solve along rows at once in the direction y increasing
j th row, assume j+1 & j-1 known

$$u_{i+1,j} - 2(1+\gamma)u_{i,j} + u_{i-1,j} = h^2 f_{i,j} - \gamma u_{i,j+1} - \gamma u_{i,j-1} \qquad (42)$$

i=2,..., N

$u_{1,j}$ & $u_{N,j}$ known (dirichlet BCs)

Thomas algorithm (line by line)

$$u^{(n)}_{i+1,j} - 2(1+\gamma)u^{(n)}_{i,j} + u^{(n)}_{i-1,j} = h^2 f_{i,j} - \gamma u^{(n-1)}_{i,j+1} - \gamma u^{(n)}_{i,j-1} \qquad (43)$$

Gauss-Seidel

Could add SOR

$$u^{(n)}_{i,j} = (1-\omega)\gamma u^{(n-1)}_{i,j} + \omega u^{(n-1/2)}_{i,j} \qquad \text{i=2,..N} \qquad (44)$$

Alternatively we can incorporate SOR factor directly in (43)

$$u_{i,j}^{(n)}=(1-\omega)u_{i,j}^{(n-1)}+\frac{\omega}{2(1+\gamma)}\left\{u_{i+1,j}^{(n)}+u_{i-1,j}^{(n)}+\gamma u_{i,j+1}^{(n-1)}+\gamma u_{i,j-1}^{(n)}\ -h^2 f_{i,j}\right\}$$

rearrange

$$u_{i+1,j}^{(n)}-\frac{2(1+\gamma)}{\omega}u_{i,j}^{(n)}+u_{i-1,j}^{(n)}=-2(1+\gamma)(1-\omega)u_{i,j}^{(n-1)}+h^2 f_{i,j}-\gamma u_{i,j+1}^{(n-1)}-\gamma u_{i,j-1}^{(n)} \qquad (45)$$

Must have diagonally dominance ω≤1+γ
Uniform mesh γ = 1 , ω≤ 2

Note:

. SOR or just straight line relaxation
Number of iterations reduced significantly
But amount of computation comparable

ADI METHODS

- Alternating Direction Implicit
- Alternate sweeps in each of coordinate directions
- One implementation

$$u_{i+1,j} - 2u_{i,j} + u_{i-1,j} = h^2 f_{i,j} - \gamma \left\{ u_{i,j+1} - 2u_{i,j} - u_{i,j-1} \right\} \qquad (47)$$

substract term $\rho u_{i,j}$ to each side

$$u^{(n+1/2)}_{i+1,j} - \left(2+\rho\right) u^{(n+1/2)}_{i,j} + u^{(n+1/2)}_{i-1,j} = h^2 f_{i,j} - \gamma \left\{ u^{(n)}_{i,j+1} - \left(2 - \frac{\rho}{\gamma}\right) u^{n}_{i,j} - u^{(n+1/2)}_{i,j-1} \right\} \qquad (48)$$

ρ accelaration factor

sweeps on line of constant y
then sweep on lines of constant x

$$\gamma u^{(n+1)}_{i,j+1} - \left(2+\gamma\rho\right) u^{(n+1)}_{i,j} + \gamma u^{(n+1)}_{i,j-1} = h^2 f_{i,j} - \left\{ u^{(n+1/2)}_{i+1,j} - \left(2-\rho\right) u^{(n+1/2)}_{i,j} - u^{(n+1)}_{i-1,j} \right\} \qquad (49)$$

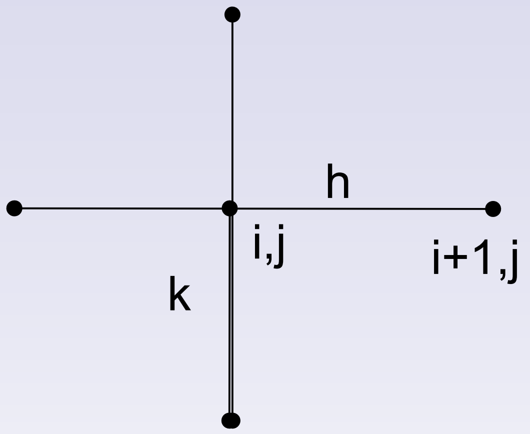
Notes:

1. SOR again on each x or y sweep or after complete sweep
2. $h=k$ $\gamma=1$ optimum value $\rho=2\sin(\text{л}/R)$
   R is largest of $M+1$, $N+1$
3. same problem with SOR of finding wopt

ADI + SOR
20 – 40 % reduction in computation
But programming ADI difficuilt.

Laplace's eq.: $\nabla^2 u = 0$

Five-point formula T.E. $O\left[h^2, k^2\right]$



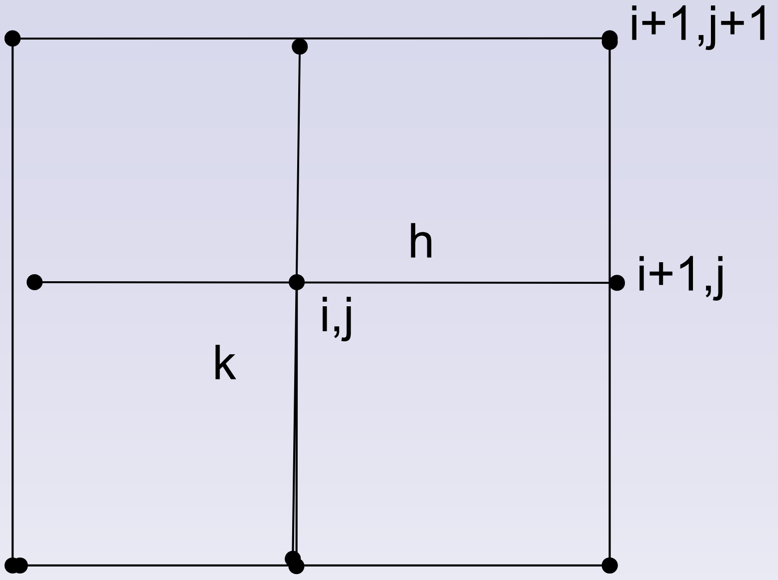
$$\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{k^2} = 0$$

Most common formula

Nine-point formula:

$$u_{i+1,j+1} + u_{i-1,j+1} + u_{i+1,j-1} + u_{i-1,j-1} - 2\frac{h^2 - 5k^2}{h^2 + k^2}\left(u_{i+1,j} + u_{i-1,j}\right) +$$

$$2\frac{5h^2 - k^2}{h^2 + k^2}\left(u_{i,j+1} + u_{i,j-1}\right) - 20u_{i,j} = 0$$



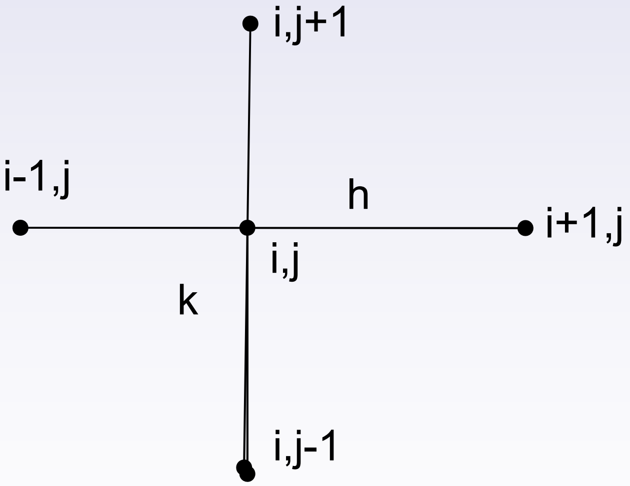
- Diagonally dominant
- Greater accuracy for laplace’s eq.
- $O\left(h^2, k^2\right)$
- But becomes $O\left(h^6\right)$ on a square mesh (h=k)
- T.E may be only $O\left(h^2, k^2\right)$ when applied to a more general elliptic eq. (including Poisson’s eq.) containing other terms
- High accuracy is difficuilt to maintain near boundaries with such schemes
- Dirichlet conditions, very effective
- Derivative conditions, more difficult to implement

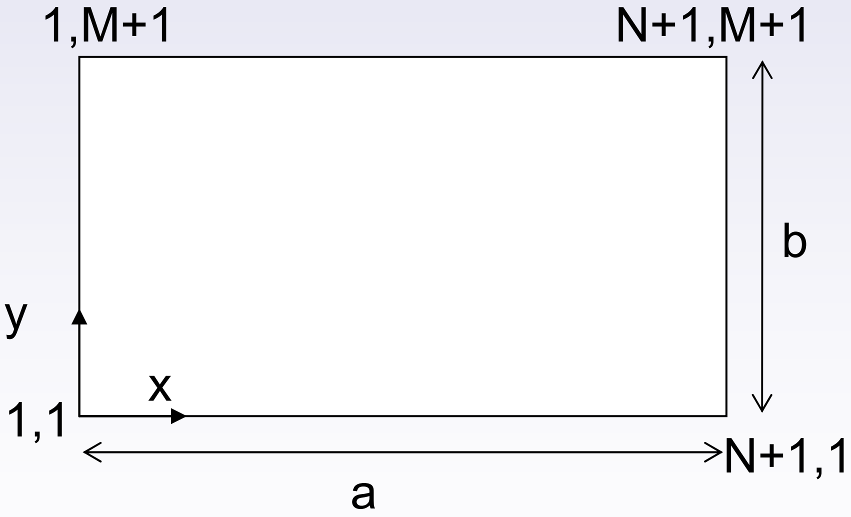
GAUSS-SEIDEL ITERATION FOR POISSON EQUATION

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = f(x, y) \qquad \text{PDE}$$

$$T_{i,j} = \frac{1}{2 + 2\gamma}\left\{- h^2 f_{i,j} + T_{i+1,j} + T_{i-1,j} + \gamma\left(T_{i,j+1} + T_{i,j-1}\right)\right\} \qquad \text{FDE}$$

$$\gamma = \left(\frac{h}{k}\right)^2$$





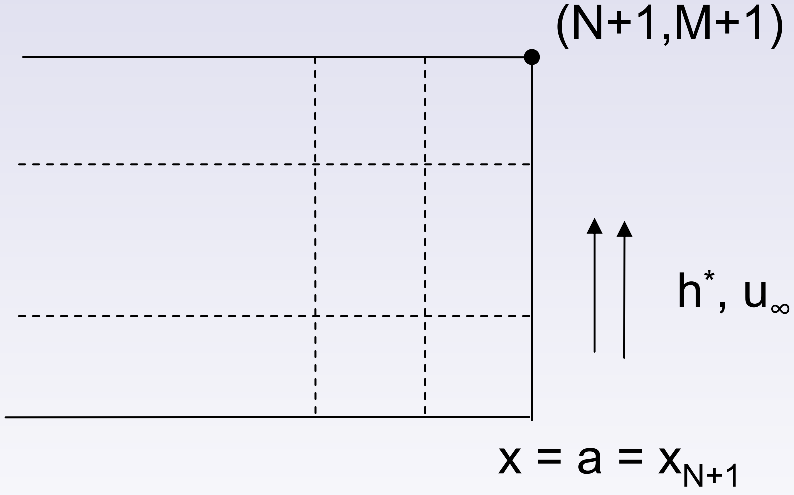
TYPICAL CODE

```
C    SET PROBLEM PARAMETERS & DIMENSIONS
C    a, b, N, M, EPS, ITERMAX, ETC…
     …
C    APPLY BCs for T(I,J)
C    ASSIGN GUESSED INITIAL VALUES T(I,J) FOR ALL INTERNAL POINTS
     …
C    X2=2.0 + 2.0*GAMMA
  100        JC=0
     ITER=ITER+1
     DO 10 I=2,N     !all internal grid points
     DO 10 J=2,M     !all internal grid points
     X1=T(I,J)
     T(I,J)=(-h**2*F(I,J)+T(I,J)+ T(I-1,J)+GAMMA* (T(I,J+1)+ T(I,J-1)))/X2
         IF(T(I,J).EQ.0.0) GO TO 10
         TEST=ABS(1.0-X1/ T(I,J))
         IF(TEST.GT.EPS)JC=1
10   CONTINUE
     IF(ITER.GT.ITERMAX) STOP
     IF (JC.EQ.1) GO TO 100
     ...
```

General formula for $\nabla^2 u = f(x,y)$

$$u_{i,j} = \frac{1}{2(1+\gamma)}\left\{-h^2 f_{i,j} + u_{i+1,j} + u_{i-1,j} + \gamma\left(u_{i,j+1} + u_{i,j-1}\right)\right\} \qquad (1)$$

A. Convection at the right boundary:

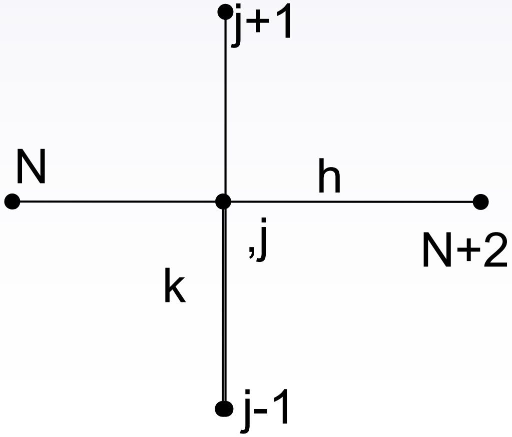


$$-k^* \frac{\partial u}{\partial x} = h^*\left(u - u_\infty\right) \quad \text{on} \quad x=a$$

$$-k^* \frac{\left(u_{N+2,j} - u_{N,j}\right)}{2h} = h^*\left(u_{N+1,j} - u_\infty\right)$$

$$u_{N+2,j} = u_{N,j} - \frac{h^*}{\underbrace{k^*}_{\alpha}} 2h\left(u_{N+1,j} - u_\infty\right)$$

$$u_{N+2,j} = u_{N,j} - \alpha 2h\left(u_{N+1,j} - u_\infty\right)$$



i=N+1 , j=j

$$u_{N+1,j}=\frac{1}{2(1+\gamma)}\left\{-h^2 f_{i,j}+u_{N+2,j}+u_{N,j}+\gamma\left(u_{N+1,j+1}+u_{N+1,j-1}\right)\right\}$$

$$u_{N+1,j}=\frac{1}{2(1+\gamma)}\left\{-h^2 f_{i,j}+2u_{N,j}-2h\alpha\left(u_{N+1,j}-u_{\infty}\right)+\gamma\left(u_{N+1,j+1}+u_{N+1,j-1}\right)\right\}$$

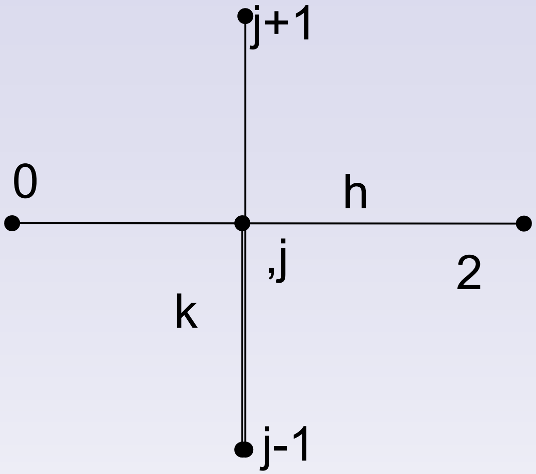
$$u_{N+1,j}=\frac{1}{(2+2\gamma+2h\alpha)}\left\{-h^2 f_{i,j}+2u_{N,j}+\gamma\left(u_{N+1,j+1}+u_{N+1,j-1}\right)+2h\alpha u_{\infty}\right\} \quad \text{j=2,...,M}$$

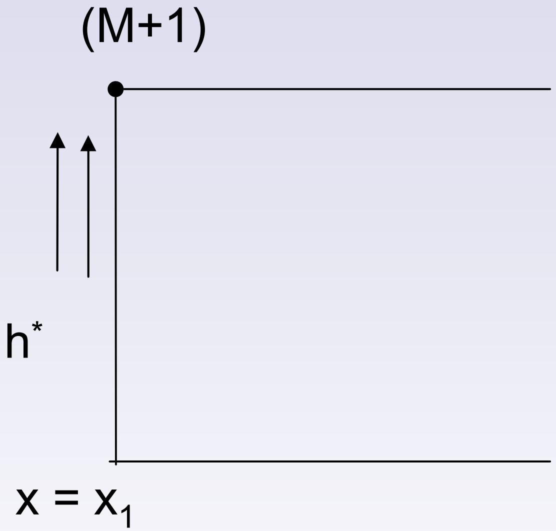
If insulated α=0

B. Convection at the left boundary:

$$-k^{*}\frac{\left(u_{2,j}-u_{0,j}\right)}{2h}=h^{*}\left(u_{1,j}-u_{\infty}\right)$$

$$u_{0,j}=u_{2,j}+2h\alpha\left(u_{1,j}-u_{\infty}\right)$$





i=1 , j=j

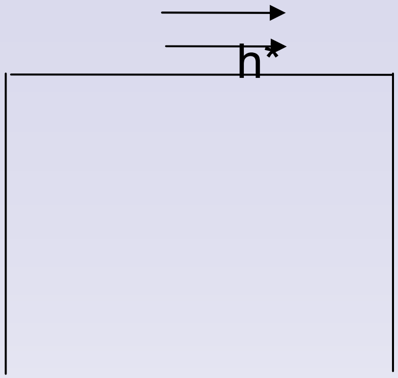
$$u_{1,j}=\frac{1}{2(1+\gamma)}\left\{-h^{2}f_{i,j}+u_{2,j}+u_{0,j}+\gamma\left(u_{1,j+1}+u_{1,j-1}\right)\right\}$$

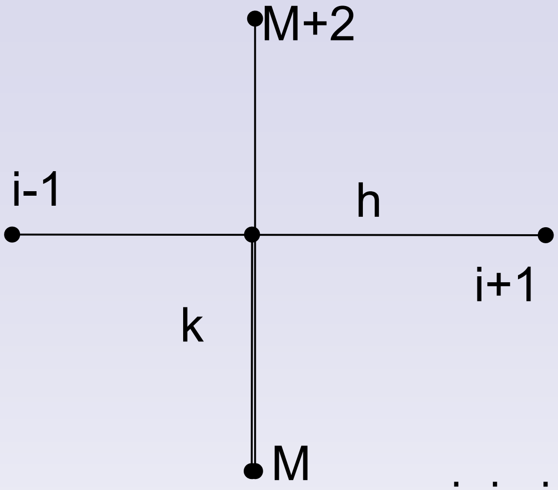
$$u_{1,j}=\frac{1}{2(1+\gamma)}\left\{-h^{2}f_{i,j}+2u_{2,j}+2h\alpha\left(u_{1,j}-u_{\infty}\right)+\gamma\left(u_{1,j+1}+u_{1,j-1}\right)\right\}$$

$$u_{1,j}=\frac{1}{(2+2\gamma-2h\alpha)}\left\{-h^{2}f_{i,j}+2u_{2,j}+\gamma\left(u_{1,j+1}+u_{1,j-1}\right)-2h\alpha u_{\infty}\right\}\quad \text{j=2,...,M}$$

If insulated α=0

C. Convection at the top boundary:





i=i , j=M+1

$$-k^{*}\frac{\left(u_{i,M+2}-u_{i,M}\right)}{2k}=h^{*}\left(u_{i,M+1}-u_{\infty}\right)$$

$$u_{i,M+2}=u_{i,M}-2k\alpha\left(u_{i,M+1}-u_{\infty}\right)$$

$$u_{i,M+1}=\frac{1}{2(1+\gamma)}\left\{-h^{2}f_{i,j}+u_{i+1,M+1}+u_{i-1,M+1}+\gamma\left(u_{i,M+2}+u_{i,M}\right)\right\}$$

$$u_{i,M+1}=\frac{1}{2(1+\gamma)}\left\{-h^{2}f_{i,j}+u_{i+1,M+1}+u_{i-1,M+1}+\gamma\left(2u_{i,M}-2k\alpha\left(u_{i,M+1}-u_{\infty}\right)\right)\right\}$$

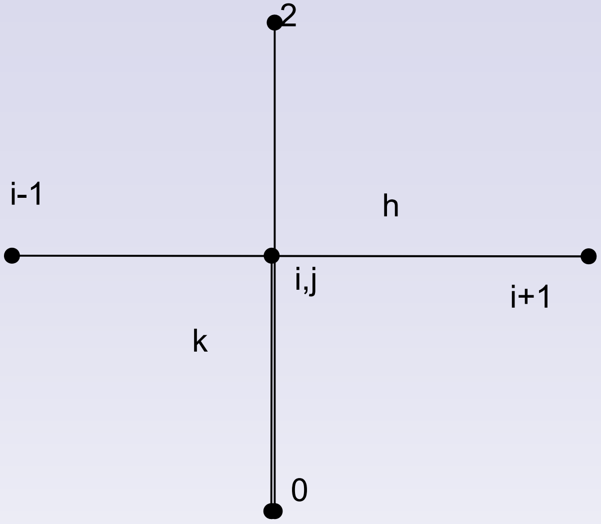
$$u_{i,M+1}(2+2\gamma+\gamma 2k\alpha)=\left\{-h^{2}f_{i,j}+u_{i+1,M+1}+u_{i-1,M+1}+\gamma\left(2u_{i,M}+2k\alpha u_{\infty}\right)\right\}$$

$$u_{i,M+1}=\frac{1}{(2+2\gamma+\gamma 2k\alpha)}\left\{-h^{2}f_{i,j}+u_{i+1,M+1}+u_{i-1,M+1}+\gamma\left(2u_{i,M}+2k\alpha u_{\infty}\right)\right\}$$

D. Convection at the bottom boundary:

$$-k^{*}\frac{\left(u_{i,2}-u_{i,0}\right)}{2k}=h^{*}\left(u_{i,1}-u_{\infty}\right)$$

$$u_{i,0}=u_{i,2}+2k\alpha\left(u_{i,1}-u_{\infty}\right)$$

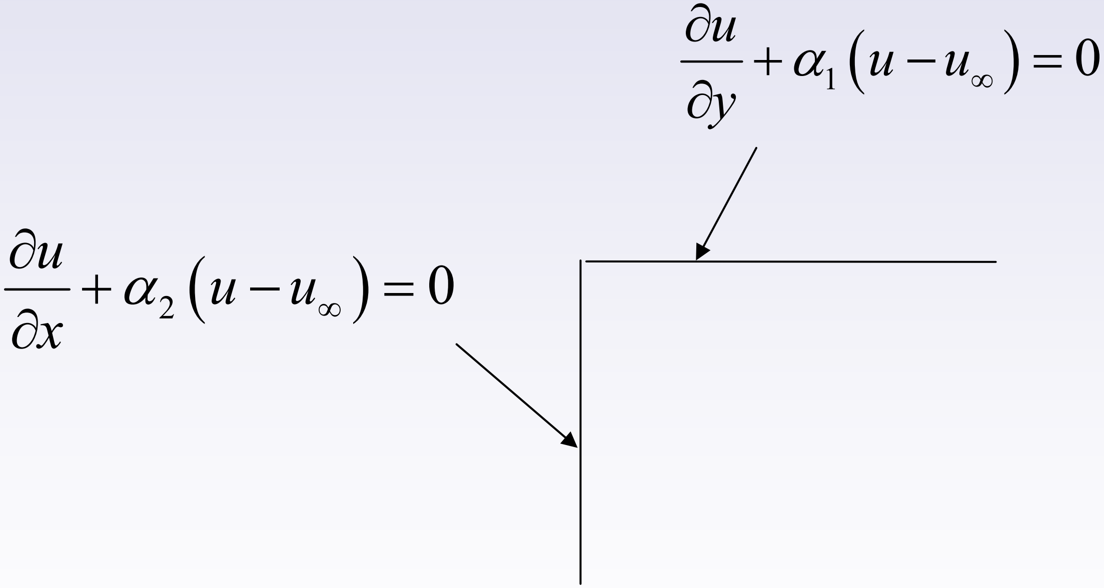


$$u_{i,1}=\frac{1}{2(1+\gamma)}\left\{-h^{2}f_{i,1}+u_{i+1,1}+u_{i-1,1}+\gamma\left(u_{i,2}+u_{i,0}\right)\right\}$$

$$u_{i,M+1}=\frac{1}{2(1+\gamma)}\left\{-h^{2}f_{i,1}+u_{i+1,1}+u_{i-1,1}+\gamma\left(2u_{i,2}+2k\alpha\left(u_{i,1}-u_{\infty}\right)\right)\right\}$$

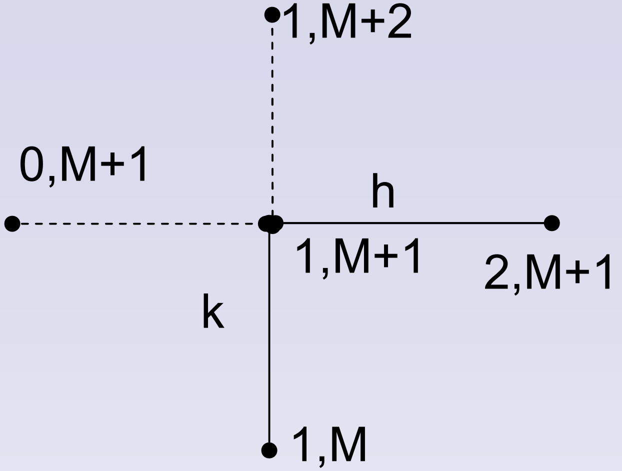
POINT TREATING AT CORNERS

$$\alpha_1 = \frac{h_1}{k} \quad , \quad \alpha_2 = \frac{h_2}{k}$$



$$\frac{\partial u}{\partial y} + \alpha_1 \left(u - u_\infty \right) = 0$$

$$\frac{\partial u}{\partial x} + \alpha_2 \left(u - u_\infty \right) = 0$$



$$-\frac{\left(u_{1,M+2}-u_{1,M}\right)}{2k}=\alpha_1\left(u_{1,M+1}-u_\infty\right)$$

$$u_{1,M+2}=u_{1,M}-2k\alpha_1\left(u_{1,M+1}-u_\infty\right)$$

$$-\frac{\left(u_{2,M+1}-u_{0,M+1}\right)}{2h}=\alpha_2\left(u_{1,M+1}-u_\infty\right)$$

$$u_{0,M+1}=u_{2,M+1}+2h\alpha_2\left(u_{1,M+1}-u_\infty\right)$$

Approx. dif. eq.
i=1 , j=M+1

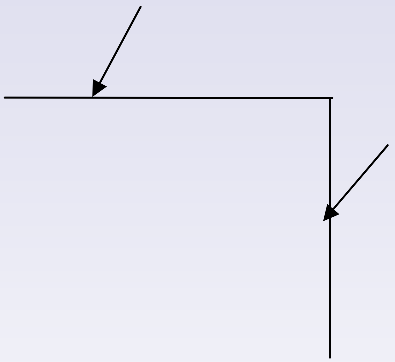
$$u_{1,M+1}=\frac{1}{2(1+\gamma)}\left\{-h^2 f_{1,M+1}+u_{2,M+1}+u_{0,M+1}+\gamma\left(u_{1,M+2}+u_{1,M}\right)\right\}$$

$$(2+2\gamma)u_{1,M+1}=-h^2 f_{1,M+1}+2u_{2,M+1}+2h\alpha_2\left(u_{1,M+1}-u_\infty\right)+\gamma\left(2u_{1,M}-2k\alpha_1\left(u_{1,M+1}-u_\infty\right)\right)$$

$$u_{1,M+1}=\frac{1}{(2+2\gamma+2\gamma k\alpha_1-2h\alpha_2)}\left\{-h^2 f_{1,M+1}+2u_{2,M+1}-2h\alpha_2 u_\infty+\gamma\left(2u_{1,M}+2k\alpha_1 u_\infty\right)\right\}$$

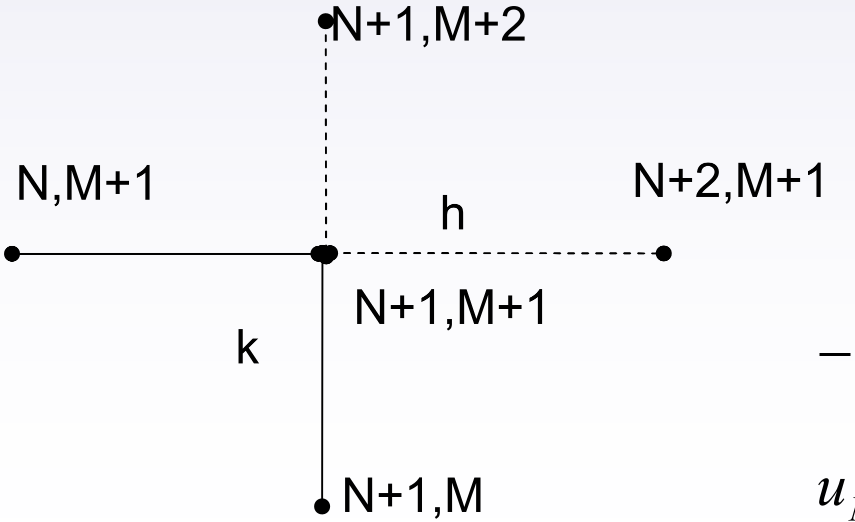
$$\text{if }\frac{\partial \text{u}}{\partial \text{x}}=0\Rightarrow\alpha_2=0$$

$$\alpha_1 = \frac{h_1}{k} \quad , \quad \alpha_2 = \frac{h_2}{k}$$



$$\frac{\partial u}{\partial y} + \alpha_1 \left(u - u_\infty \right) = 0$$

$$\frac{\partial u}{\partial x} + \alpha_2 \left(u - u_\infty \right) = 0$$



$$-\frac{\left(u_{N+1,M+2} - u_{N+1,M}\right)}{2k} = \alpha_1 \left(u_{N+1,M+1} - u_\infty \right)$$

$$u_{N+1,M+2} = u_{N+1,M} - 2k\alpha_1 \left(u_{N+1,M+1} - u_\infty \right)$$

$$-\frac{\left(u_{N+2,M+1}-u_{N,M+1}\right)}{2h}=\alpha_2\left(u_{N+1,M+1}-u_\infty\right)$$

$$u_{N+2,M+1}=u_{N,M+1}-2h\alpha_2\left(u_{N+1,M+1}-u_\infty\right)$$

Approx. dif. eq.

i=1 , j=M+1

$$u_{N+1,M+1}=\frac{1}{2(1+\gamma)}\left\{-h^2 f_{N+1,M+1}+u_{N+2,M+1}+u_{N,M+1}+\gamma\left(u_{N+1,M+2}+u_{N+1,M}\right)\right\}$$

$$(2+2\gamma)u_{N+1,M+1}=-h^2 f+2u_{N,M+1}-2h\alpha_2\left(u_{N+1,M+1}-u_\infty\right)+\gamma\left(2u_{N+1,M}-2k\alpha_1\left(u_{N+1,M+1}-u_\infty\right)\right)$$

$$u_{N+1,M+1}(2+2\gamma+2\gamma k\alpha_1+2h\alpha_2)=\left\{-h^2 f+2u_{N,M+1}+2h\alpha_2 u_\infty+\gamma\left(2u_{N+1,M}+2k\alpha_1 u_\infty\right)\right\}$$

CONVECTIVE TERMS

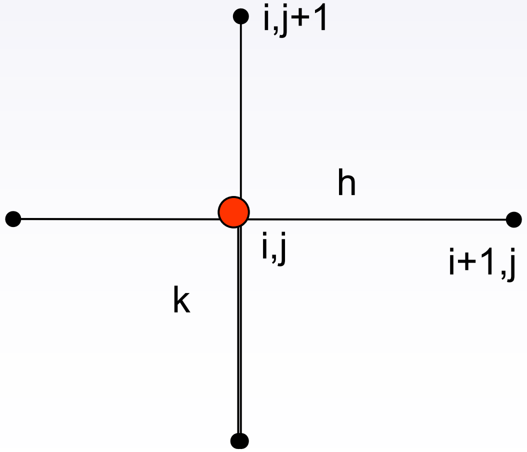
Navier-Stokes problems:

Example: 2-D , Steady Burgers equation

$$\mathrm{Re}\left\{u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}\right\}=\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2} \qquad (50)$$

$$\mathrm{Re}\left\{u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}\right\}=\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2} \qquad (51)$$

Standart Central Difference:



- Similar to N-S but do not include pressure gradient
- Coupled equations so iteration between equations are necessary

Approximating (50),

$$\mathrm{Re}\left\{u_{i,j}\left(\frac{u_{i+1,j}-u_{i-1,j}}{2h}\right)+v_{i,j}\left(\frac{u_{i,j+1}-u_{i,j-1}}{2k}\right)\right\}=\frac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{h^2}+\frac{u_{i,j+1}-2u_{i,j}+u_{i,j-1}}{k^2} \qquad (50)$$

Multiply by h^2 , $\gamma=\dfrac{h^2}{k^2}$

$$u_{i+1,j}+u_{i-1,j}+\gamma u_{i,j+1}+\gamma u_{i,j-1}-2(1+\gamma)u_{i,j}-\mathrm{Re}\frac{h}{2}\left\{u_{i,j}\left(u_{i+1,j}-u_{i-1,j}\right)+v_{i,j}\gamma^{1/2}\left(u_{i,j+1}-u_{i,j-1}\right)\right\}=0 \quad (52)$$

Now non-linear algebraic eq.

Most Common Approach

Linearize by guessing selected coefficients

1st derivative term in (52)

$$u^{(n)}_{i+1,j}\left\{1-\frac{h\,\mathrm{Re}}{2}u^{(n-1)}_{i,j}\right\}+u^{(n)}_{i-1,j}\left\{1+\frac{h\,\mathrm{Re}}{2}u^{(n-1)}_{i,j}\right\}$$

$$+u^{(n)}_{i,j+1}\left\{\gamma-\frac{\mathrm{Re}}{2}\gamma^{1/2}hv^{(n-1)}_{i,j}\right\}+u^{(n)}_{i,j-1}\left\{\gamma+\frac{\mathrm{Re}}{2}\gamma^{1/2}hv^{(n-1)}_{i,j}\right\}-2(1+\gamma)u^{(n)}_{i,j}=0 \quad (53)$$

Typical code involves Gauss-Seidel

```
A1 = 0.5*RE*H
G = H*H/(AK*AK)
A2 = 2.0*(1+G)
GR = SQRT(G)
DO 10 I = 2, N1
DO 10 J = 2, M1
B1 = 1.0 –A1*U(I,J)
B3 = 2.0 – B1
B2 = G - A1*G2*V(I,J)
B4 = 2.0*G – B2
U(I,J) = (U(I+1,J)*B1+ U(I-1,J)*B3+ U(I,J+1)*B2+ U(I,J-1)*B4)/A2
V(I,J) = ….
END DO
END DO
```

Notes:

1. We could use SOR but often divergence
2. Often we must use under-relaxation as Re increases

$$u_{i,j}^{(n)} = \omega u_{i,j}^{(n)} + (1-\omega) u_{i,j}^{(n-1)}$$

$\omega = 0.5$ & reduce

if $\omega < 0.01$, not worth continuing

3. can use ADI
4. mesh restrictions

need (53) to be diagonally dominant

$$\text{p}=\frac{h\text{Re}}{2}u_{i,j} \quad , \quad \text{q}=\gamma^{1/2}\frac{h\text{Re}}{2}v_{i,j}$$

$$|1-p|+|1+p|+|\gamma-p|+|\gamma+p|\le 2(1+\gamma)$$

Suppose p>1 $|1-p|+|1+p|$=2p>2

& not diagonally dominant

select h,k $|p|<1$, $|q|<\gamma$

$$i.e.\left|\frac{h}{2}\text{Re}\,u_{i,j}\right|<1 \quad , \quad \left|\frac{h}{2}\text{Re}\,v_{i,j}\right|<\gamma^{1/2}$$

But difficult to select a priori
i.$u_{i,j}$ unknown , always try to non-dimensionalize so $0\le|u_{i,j}|<1$

ii. as Re inreases , smaller & smaller mesh sizes

Possible Acceleration?

Newton linearization

Consider term like (52)

$$u_{i,j}\left(u_{i+1,j}-u_{i-1,j}\right) \qquad (54)$$

Instead of taking $u_{i,j}$ from previous iterate, use

$\tilde{u}_{i,j}\left(estimate\right)\ \ u^T_{i,j}=\tilde{u}_{i,j}+\delta u_{i,j}$

δ:assumed small

In (54)

$$\left(\tilde{u}_{i,j}+\delta u_{i,j}\right)\left(\tilde{u}_{i+1,j}+\delta u_{i+1,j}-\tilde{u}_{i-1,j}-\delta u_{i-1,j}\right)$$

$$\approx \tilde{u}_{i,j}\tilde{u}_{i+1,j}+\delta u_{i,j}\tilde{u}_{i+1,j}+\tilde{u}_{i,j}\delta u_{i+1,j}+\ldots-\ldots$$

$$=\tilde{u}_{i,j}\tilde{u}_{i+1,j}+\tilde{u}_{i+1,j}\left(u_{i,j}-\tilde{u}_{i,j}\right)+\tilde{u}_{i,j}\left(u_{i+1,j}-\tilde{u}_{i+1,j}\right)+\ldots$$

$$=-\tilde{u}_{i,j}\tilde{u}_{i+1,j}+\tilde{u}_{i+1,j}u_{i,j}+\tilde{u}_{i,j}u_{i+1,j}-\left\{-\tilde{u}_{i,j}\tilde{u}_{i-1,j}+\tilde{u}_{i-1,j}u_{i,j}+\tilde{u}_{i,j}u_{i-1,j}\right\} \qquad (55)$$

Danger, must be close to solution or divergence

Damping

UPWIND-DOWNWIND DIFFERENCES
(FORWARD-BACKWARD ALGORITHM)

As Re increases, difficult to reduce mesh to maintain diagonal dominance
Need to consider difference in local flow direction

Consider term $u\dfrac{\partial u}{\partial x}$

If $a)\quad u_{i,j} > 0$

$$u\frac{\partial u}{\partial x} = u_{i,j}^{(n-1)}\left\{\frac{u_{i,j} - u_{i-1,j}}{h}\right\} + O(h) \qquad (56)$$

$b)\quad u_{i,j} < 0$

$$u\frac{\partial u}{\partial x} = u_{i,j}^{(n-1)}\left\{\frac{u_{i+1,j} - u_{i,j}}{h}\right\} + O(h) \qquad (57)$$

Similarly for $v\dfrac{\partial u}{\partial y}$

$a)\quad v_{i,j} > 0$

$$v\frac{\partial u}{\partial y} = v_{i,j}^{(n-1)}\left\{\frac{v_{i,j} - v_{i,j-1}}{k}\right\} + O(k) \qquad (58)$$

$b)\quad v_{i,j} < 0$

$$v\frac{\partial u}{\partial y} = v_{i,j}^{(n-1)}\left\{\frac{v_{i,j+1} - v_{i,j}}{k}\right\} + O(k) \qquad (59)$$

Consider first approximate to x derivatives & denote values of $u_{i,j}$, $v_{i,j}$ from last iteration with $u^*{}_{i,j}$, $v^*{}_{i,j}$

$$T_1 = \frac{\partial^2 u}{\partial x^2} - \mathrm{Re}\, u \frac{\partial u}{\partial x}$$

$$= \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} - \mathrm{Re} \frac{u^*_{i,j}}{h} \begin{cases} u_{i,j} - u_{i-1,j}, & u^*_{i,j} > 0 \\ u_{i+1,j} - u_{i,j}, & u^*_{i,j} < 0 \end{cases}$$

or

$$h^2 T_1 = u_{i+1,j} + u_{i-1,j}\left(1 + h\,\mathrm{Re}\, u^*_{i,j}\right) - u_{i,j}\left(2 + h\,\mathrm{Re}\, u^*_{i,j}\right) \qquad u^*_{i,j} > 0$$

$$= u_{i+1,j}\left(1 - h\,\mathrm{Re}\, u^*_{i,j}\right) + u_{i-1,j} - u_{i,j}\left(2 - h\,\mathrm{Re}\, u^*_{i,j}\right) \qquad u^*_{i,j} < 0$$

Note:

Diagonally dominant for all Re

For y derivatives

$$T_2 = \frac{\partial^2 u}{\partial y^2} - \mathrm{Re}\, v \frac{\partial u}{\partial y}$$

$$= \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{k^2} - \mathrm{Re} \frac{v^*_{i,j}}{k} \begin{cases} u_{i,j} - u_{i,j-1}, & v^*_{i,j} > 0 \\ u_{i,j+1} - u_{i,j}, & v^*_{i,j} < 0 \end{cases}$$

$$or$$

$$h^2 T_2 = u_{i,j+1} + u_{i,j-1}\left(1 + k\,\mathrm{Re}\, v^*_{i,j}\right) - u_{i,j}\left(2 + h\,\mathrm{Re}\, v^*_{i,j}\right) \qquad v^*_{i,j} > 0$$

$$= u_{i,j+1}\left(1 - k\,\mathrm{Re}\, v^*_{i,j}\right) + u_{i,j-1} - u_{i,j}\left(2 - k\,\mathrm{Re}\, v^*_{i,j}\right) \qquad v^*_{i,j} < 0$$

Approximating to differential equation (50)

$$\mathrm{Re}\left\{u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}\right\} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \qquad (50)$$

$$h^2 T_1 + \frac{h^2}{k^2} T_2 = 0$$

$$h^2 T_1 + \gamma T_2 = 0 \qquad (62)$$

or in the form

$$b_1 u_{i+1,j} + b_2 u_{i,j+1} + b_3 u_{i-1,j} + b_4 u_{i,j-1} - b_0 u_{i,j} = 0 \quad (63)$$

where

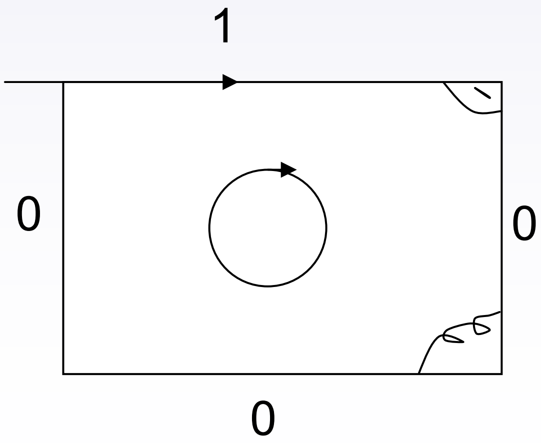
$$b_1 = 1 \quad , \quad b_3 = 1 + h \operatorname{Re} u^*_{i,j} \qquad u^*_{i,j} > 0$$

$$= 1 - h \operatorname{Re} u^*_{i,j} \quad , \quad b_3 = 1 \qquad u^*_{i,j} < 0$$

$$b_2 = \gamma \quad , \quad b_4 = \gamma \left(1 + k \operatorname{Re} v^*_{i,j} \right) \qquad v^*_{i,j} > 0$$

$$= \gamma \left(1 + k \operatorname{Re} v^*_{i,j} \right) \quad , b_4 = \gamma \qquad v^*_{i,j} < 0$$

$$b_0 = 2 + h \operatorname{Re} \left| u^*_{i,j} \right| + \gamma \left(2 + h \operatorname{Re} \left| v^*_{i,j} \right| \right)$$



Simplified driven cavity problem

$$u \frac{\partial u}{\partial x} = \frac{1}{\operatorname{Re}} \left\{ \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right\}$$

Typical code changes

```
F1 = h*Re
F2 = k*Re
DO 10 I  = 2, N1
DO 10 J = 2, M1
X1 = U(I,J)
X2 = V(I,J)
X3 = 1 + F1*ABS(X1)
X4 = G*(1.0 + F2*ABS(X2))
IF (X1.GT.0.0) THEN
B1 = 1.0
B3 = X3
ELSE
B1 = X3
B3 = 1.0
END IF
IF (X2.GT.0.0) THEN
B2 = G
B4 = X4
ELSE
B2 = X4
B4 = G
END IF
B0 = X3 + 1.0 + X4 + G
U(I,J) = (U(I+1,J)*B1+U(I-1,J)*B3+U(I,J+1)*B2 + U(I,J-1)*B4)/B0
Convergence test
END DO
END DO
```

DEFERRED CORRECTION

Upwind/downwind differencing , diagonally dominant ,
Convergence but accuracy problem

Central difference

$$\frac{\partial u}{\partial x}=\frac{u_{i+1,j}-u_{i-1,j}}{2h}+O(h^2) \qquad (64)$$

$$\frac{\partial u}{\partial x}=\frac{u_{i,j}-u_{i-1,j}}{h}+C_{x^+}+O(h^2)$$

$$=\frac{u_{i+1,j}-u_{i,j}}{h}+C_{x^-}+O(h^2) \qquad (65)$$

Choose correction C_x^+ & C_x- so (64) & (65)

$$C_{x^+}=\frac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{2h}$$

$$C_{x^-}=-\frac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{2h} \qquad (66)$$

Similar expressions for $\dfrac{\partial u}{\partial y}$

$$\frac{\partial u}{\partial y}=\frac{u_{i,j}-u_{i,j-1}}{k}+C_{y^+}+O(k^2) \qquad (67)$$

$$=\frac{u_{i,j+1}-u_{i,j}}{h}+C_{y^-}+O(k^2)$$

$$C_{y^+}=-C_{y^-}=\frac{u_{i,j+1}-2u_{i,j}+u_{i,j-1}}{2k} \qquad (68)$$

Difference equations become

$$b_1u_{i+1,j}+b_2u_{i,j+1}+b_3u_{i-1,j}+b_4u_{i,j-1}-b_0u_{i,j}=d_{i,j} \qquad (69)$$

$$d_{i,j}=-\frac{hu^*_{i,j}}{2}\left\{u_{i+1,j}-2u_{i,j}+u_{i-1,j}\right\}-\frac{h^2}{2k}v^*_{i,j}\left\{u_{i,j+1}-2u_{i,j}+u_{i,j-1}\right\} \qquad (70)$$

Implementation

1) perform several iteration with $d_{i,j}=0$
2) evaluate $d_{i,j}$ at each point in mesh & add to right side of (69)
3) perform several iterations with $d_{i,j}$ constant
4) return to (2)

COMPUTATION OF FORCED CONVECTION WITH CONSTANT FLUID PROPERTIES

If flow properties are constant, flow field is independent of temperature distribution. Continuity & momentum eqs.

$$\nabla.\vec{V} = 0$$

$$\rho \frac{D\vec{V}}{Dt} = \rho\left[\frac{\partial \vec{V}}{\partial t} + \left(\vec{V}.\nabla\right)\vec{V}\right] = \vec{F} - \nabla P + \mu \nabla^2 \vec{V} \qquad (1)$$

Using characteristic velocity U and length L, and time is non-dimensionalized with L/U ,

$$\tau = \frac{t}{L/U}$$

Dimensionless eq.

$$\frac{\partial \vec{V}}{\partial \tau} + \left(\vec{V}.\nabla\right)\vec{V} = \frac{\vec{F}\rho g L}{\rho U^2} - \nabla P + \frac{1}{\mathrm{Re}} \nabla^2 \vec{V}$$

$$\mathrm{Re} = \frac{UL}{\nu}$$

$\mathrm{Fr} = \frac{\mathrm{U}^2}{gL}$ when gravitational field is considered as the body force term

Two basic approaches:

1. **Primitive variables**: velocities & pressure are the unknown dependent parameters (direct approach)
2. **Stream function-Vorticity variables**: use the derived variables ψ&ω to solve the problem

Temperature field is considered after velocity field is obtained!

(ψ-ω) approach:

2-D flow , ρ = constant

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

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

Note: continuity eq. is identically satisfied.
Taking curl of (1) , vorticity eq. is obtained

$$\frac{\partial \vec{\omega}}{\partial \tau}+\vec{V}.\nabla\vec{\omega}=\left(\vec{\omega}.\nabla\right)\vec{V}+\nu\nabla^2\vec{\omega}$$

$$\text{Inviscid flow } \rightarrow \nu=0 \ , \ \vec{\mathrm{F}}=0, \nabla\times\nabla P=0 \ \text{(show!)}$$

$$\text{Vorticity is defined } \nabla\times\vec{V}=\vec{\omega}$$

$$\text{Here } \left(\vec{\omega}.\nabla\right)\vec{V}=0 \text{ for 2-D flow since}$$

ω_z : perpendicular to plane of flow (only non-zero comp. of vorticity for 2-D flow)

$$\frac{\partial \vec{\omega}}{\partial \tau} + \vec{V}.\nabla\vec{\omega} = \frac{D\omega_z}{D\tau} = 0$$

vorticity is preserved for steady inviscid flow!

Steady flow, ω_z along a streamline

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

$$\omega_z = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} = -\frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi}{\partial y^2}$$

$$\nabla^2\psi = -\omega_z$$

i. **For irrotational flow:** $\nabla^2\psi = 0$ (Laplace eq.)

Velocity potential may also be used

$$\vec{V} = \nabla\phi \rightarrow \nabla^2\phi = 0 \quad \text{(continuity eq.)}$$

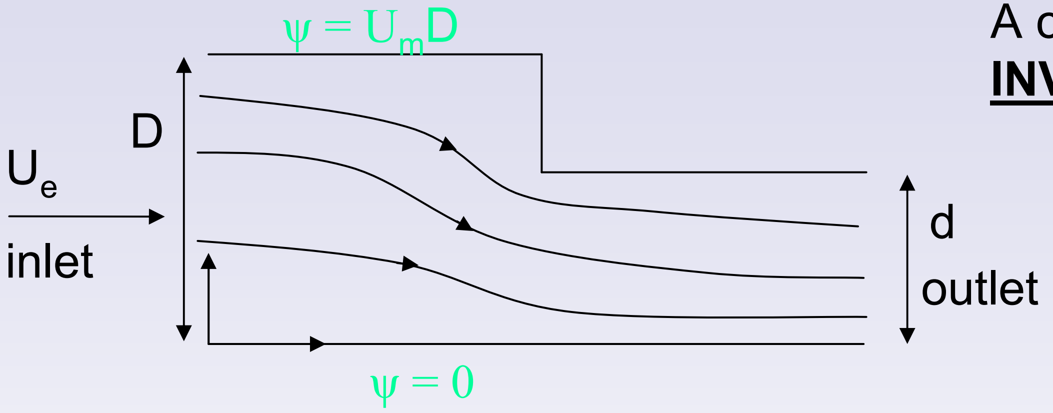
ii. **For rotational flow** $\nabla^2\psi = -\omega_z$

Analitical solutions for the inviscid or potential flow in simple configurations exist.

Numerical Solution

Elliptic problem → ψ must be specified at the boundaries

Example:



A channel of varying area

INVISCID FLOW

Channel is much wider in the third direction so; 2-D flow in (x,y) plane may be considered.

Velocity at the outlet is taken uniform (long narrow passage) ρ=const. (inlet volume flow rate = outlet volume flow rate)

Consider two cases for velocity at the inlet U_e

Case I: U_e = const. = U_m : uniform flow at inlet

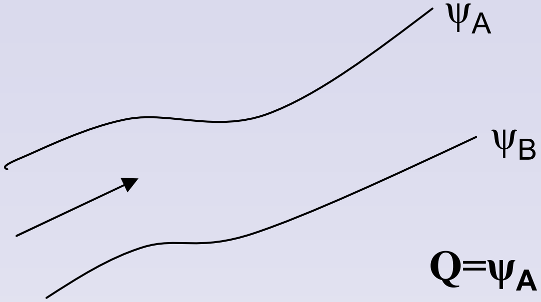
Case II: $U_e = \pi/2\ U_m \sin \pi y/D$: fully developed laminar flow

U_m : average of velocity distribution at the inlet

Flow rate in both cases is $U_m D$

$$Q=\int_0^D \frac{\pi}{2}U_m \sin\frac{\pi}{D}y\,dy$$

$$U_m D=\psi_{\text{upper wall}}-\psi_{\text{lower wall}}$$



$Q=\psi_A-\psi_B$

Boundary conditions for ψ

A. INLET

$$u=\frac{\partial\psi}{\partial y}\quad,\quad v=-\frac{\partial\psi}{\partial x}$$

$$\frac{\partial\psi}{\partial y}=u_e\quad,\quad\frac{\partial\psi}{\partial x}=0\rightarrow\psi\neq\psi(x)$$

$$\psi=U_e y+c$$

Take ψ=0 at y=0 → c=0

$\psi=\mathrm{U_e}y$

i. $\psi=U_m y$

ii. $\psi=U_m\frac{D}{2}\left(1-\cos\frac{\pi y}{D}\right)$: $\frac{\partial\psi}{\partial y}=\frac{\pi}{2}U_m\sin\frac{\pi y}{D}$

B. UPPER WALL

$\psi = U_m D$ for both cases indicates the same volume flow rate

C. EXIT $\psi = \dfrac{D}{d} U_m y$

VORTICITY FOR THE CASES AT INLET

i. $\omega_z = \dfrac{\partial v}{\partial x} - \dfrac{\partial u}{\partial y} = 0$

ii. $\omega_z = -\dfrac{\pi^2}{2D} U_m \cos \dfrac{\pi y}{D} = \dfrac{\pi^2 \psi}{D^2} - \dfrac{\pi^2 U_m}{2D} \neq 0$

Vorticity in preserved in inviscid flow

Governing eqs.

i. $\omega_z = 0$

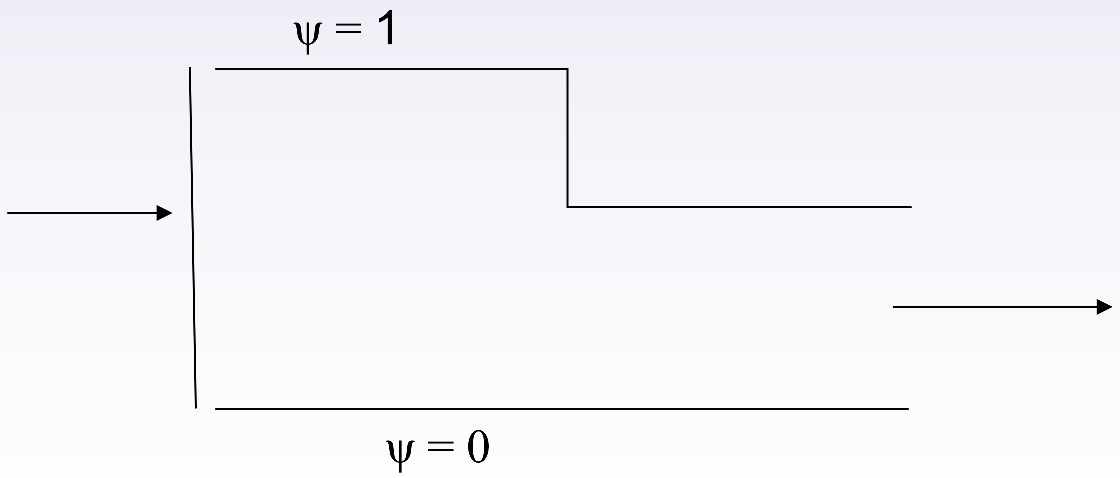
ii. $\omega_z = \dfrac{\pi^2 \psi}{D^2} - \dfrac{\pi^2 U_m}{2D}$

Non-dimensionalize for general results

$$X = \frac{x}{D} \quad , \quad Y = \frac{y}{D} \quad , \quad \Psi = \frac{\psi}{U_m D}$$

i. $$\frac{\partial^2 \Psi}{\partial X^2} + \frac{\partial^2 \Psi}{\partial Y^2} = 0$$

ii. $$\frac{\partial^2 \Psi}{\partial X^2} + \frac{\partial^2 \Psi}{\partial Y^2} = \pi^2 \left(\frac{1}{2} - \Psi \right) = f(\Psi)$$



Inlet

i. $\Psi = Y \quad \left(\underbrace{\mathrm{U_m} D\Psi}_{\psi} = U_m \underbrace{YD}_{y} \right)$

ii. $\Psi = \frac{1}{2}\left(1 - \cos \pi Y\right)$

At outlet distribution for both cases

$$\Psi = \frac{D}{d} Y$$

Poisson eq.

$$\left(\delta_x^2 + \delta_y^2\right)\Psi = f(\Psi)$$

G.S iteration scheme

$$\Psi_{\mathrm{i,j}}^{\mathrm{n+1}} = \frac{1}{2\left(1+\gamma\right)}\left[\Psi_{\mathrm{i+1,j}}^{\mathrm{n}} + \Psi_{\mathrm{i\text{-}1,j}}^{\mathrm{n+1}} + \gamma\left(\Psi_{\mathrm{i,j+1}}^{\mathrm{n}} + \Psi_{\mathrm{i,j\text{-}1}}^{\mathrm{n+1}}\right) - \left(\Delta x\right)^2 f\left(\Psi_{i,j}^{n}\right)\right] - f\left(\Psi_{i,j}^{n}\right)$$

SOR is possible $\Psi_{\mathrm{i,j}}^{\mathrm{n+1}} = \left(1-\omega\right)\Psi_{\mathrm{i,j}}^{\mathrm{n}} + \omega\, \Psi_{\mathrm{i,j}}^{\mathrm{n+1}}$

Having obtained streamlines or lines of constant Ψ
Velocity components

$$u_{i,j} = \frac{\Psi_{i,j+1} - \Psi_{i,j-1}}{2\Delta y}$$

$$v_{i,j} = \frac{\Psi_{i-1,j} - \Psi_{i+1,j}}{2\Delta x}$$

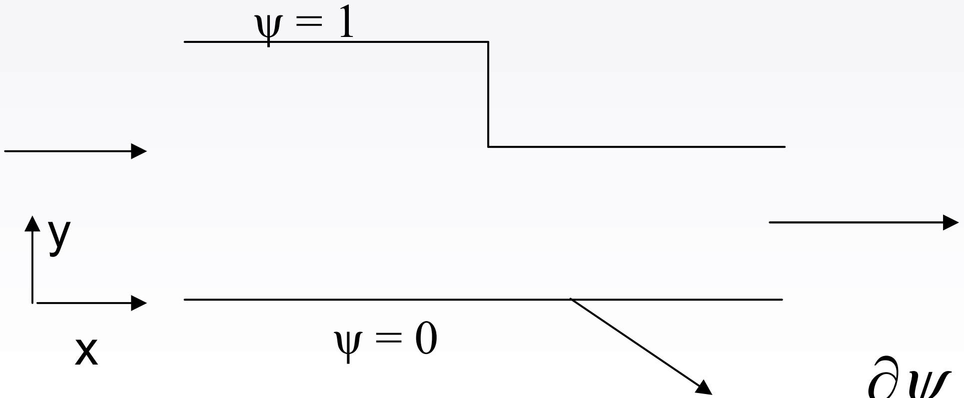
Note: inviscid flow (viscous terms neglected)

⇨ order of governing momentum equation drops from two to one

Only one physical cond. wrt velocity field can be satisfied at boundaries

i.e., slip is allowed parallel to walls & normal velocity component is taken zero

Constant value of ψ obtained along the wall.



$$u = \frac{\partial \psi}{\partial y} \neq 0 \quad , \quad v = -\frac{\partial \psi}{\partial x} = 0$$

Pressure field

$$p + \frac{1}{2}\rho V^2 = \text{const.}$$

V: flow speed at a point

$$V_{i,j} = \sqrt{u_{i,j}^2 + v_{i,j}^2}$$

$p_{i,j}$ is obtained & employed in B.L eqs.

Vorticity-Stream Function Formulation: pg.650

$$\vec{\Omega} = \nabla \times \vec{V} \quad \rightarrow \quad \text{2-D} \quad \rightarrow \quad \Omega_z = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}$$

$$\text{2-D Flow} \rightarrow u = \frac{\partial \psi}{\partial y}, v = -\frac{\partial \psi}{\partial x}$$

$$\left.\begin{array}{l} \dfrac{\partial \Omega}{\partial t} + u\dfrac{\partial \Omega}{\partial x} + v\dfrac{\partial \Omega}{\partial y} = \nu\left(\dfrac{\partial^2 \Omega}{\partial x^2} + \dfrac{\partial^2 \Omega}{\partial y^2}\right) \\ \dfrac{\partial^2 \psi}{\partial x^2} + \dfrac{\partial^2 \psi}{\partial y^2} = -\Omega \end{array}\right\} \text{dimensional}$$

$$\text{non-dimensional } \nu = \frac{1}{\text{Re}}$$

$$\Omega^* = \frac{\Omega L}{U_\infty} \; , \; \psi^* = \frac{\psi}{U_\infty L} \; , \; u^* = \frac{u}{U_\infty} \; , \; x^* = \frac{x}{L} \; , \; t^* = \frac{tU_\infty}{L} \; ,$$

1. N-S eqs. ; mixed elliptic-parabolic system of eqs. $\vec{V}, P$ simultaneous solution

2. Vorticity-stream function formulation: $\omega - \psi$ formulation

- Incompressible N-S eqs. are decoupled into one elliptic eq. & one parabolic eq.
- can be solved sequentially

- $\omega - \psi$ formulation does not include the pressure term

  i.e., velocity is determined first → pressure is found next

  - It is best for 2-D flows
  - B.Cs on vorticity need to be specified.(lack of physical B.Cs on vorticity)

$$-\left(\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2}\right) = 2\left(\frac{\partial u}{\partial y}\frac{\partial v}{\partial x} - \frac{\partial u}{\partial x}\frac{\partial v}{\partial y}\right)$$

$$\nabla^2 P = 2\left[\frac{\partial^2 \psi}{\partial x^2}\frac{\partial^2 \psi}{\partial y^2} - \left(\frac{\partial^2 \psi}{\partial x \partial y}\right)^2\right] \text{ dimensionless form}$$

Vorticity-stream function formulation $\omega - \psi$

A. Vorticity-transport equation (parabolic)

$$\frac{\partial \Omega}{\partial t} + u\frac{\partial \Omega}{\partial x} + v\frac{\partial \Omega}{\partial y} = \frac{1}{\mathrm{Re}}\left(\frac{\partial^2 \Omega}{\partial x^2} + \frac{\partial^2 \Omega}{\partial y^2}\right) \qquad (1)$$

B. Stream function eq. (elliptic)

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = -\Omega \qquad (2)$$

Numerical Algorithms

a. Unsteady flows:

1. Any scheme developed for parabolic eqs.
2. Any scheme developed for elliptic eqs.

b. Steady flows:

I.
$$u\frac{\partial \Omega}{\partial x}+v\frac{\partial \Omega}{\partial y}=\frac{1}{\mathrm{Re}}\left(\frac{\partial^2 \Omega}{\partial x^2}+\frac{\partial^2 \Omega}{\partial y^2}\right) \qquad (3)$$

$$\nabla^2\psi=-\Omega$$

Two elliptic eqs.
can be solved by iterative scheme. e.g. G.S or upwind-downwind differencing

II. Unsteady equations are solved until steady state
Total computation time may be too excessive

III. Pseudo-transient approach

$$\frac{\partial \psi}{\partial t}-\left(\frac{\partial^2 \psi}{\partial x^2}+\frac{\partial^2 \psi}{\partial y^2}+\Omega\right)=0 \qquad \text{Two parabolic eqs.}$$

Vorticity-transport equation

A. Explicit: FTCS scheme

$$\frac{\Omega_{i,j}^{n+1}-\Omega_{i,j}^{n}}{\Delta t}+u_{i,j}^{n}\frac{\Omega_{i+1,j}^{n}-\Omega_{i-1,j}^{n}}{2\Delta x}+v_{i,j}^{n}\frac{\Omega_{i,j+1}^{n}-\Omega_{i,j-1}^{n}}{2\Delta y}=$$

$$\frac{1}{\text{Re}}\left\{\frac{\Omega_{i+1,j}^{n}-2\Omega_{i,j}^{n}+2\Omega_{i-1,j}^{n}}{\left(\Delta x\right)^{2}}+\frac{\Omega_{i,j+1}^{n}-2\Omega_{i,j}^{n}+2\Omega_{i,j-1}^{n}}{\left(\Delta y\right)^{2}}\right\} \qquad (4)$$

DuFort-Frankel:

$$\frac{\partial\Omega}{\partial t}=\frac{\Omega_{i,j}^{n+1}-\Omega_{i,j}^{n-1}}{2\Delta t}$$

$$\Omega_{i,j}^{n}=\frac{\Omega_{i,j}^{n+1}+\Omega_{i,j}^{n-1}}{2}$$

- Use of an upwind differencing scheme may be appropriate for convection dominated flows

B. Implicit: Approximate Factorization for efficiency for multi-dimensional problems.

ADI formulation: two-step process; treat x der. implicitly & y der. implicitly.

$$\frac{\Omega_{i,j}^{n+1/2}-\Omega_{i,j}^{n}}{\Delta t/2}+u_{i,j}^{n}\frac{\Omega_{i+1,j}^{n+1/2}-\Omega_{i-1,j}^{n+1/2}}{2\Delta x}+v_{i,j}^{n}\frac{\Omega_{i,j+1}^{n}-\Omega_{i,j-1}^{n}}{2\Delta y}=$$

$$\frac{1}{\mathrm{Re}}\left\{\underbrace{\frac{\Omega_{i+1,j}^{n+1/2}-2\Omega_{i,j}^{n+1/2}+2\Omega_{i-1,j}^{n+1/2}}{\left(\Delta x\right)^{2}}}_{\delta_{xx}^{n+1/2}\Omega_{ij}}+\underbrace{\frac{\Omega_{i,j+1}^{n}-2\Omega_{i,j}^{n}+2\Omega_{i,j-1}^{n}}{\left(\Delta y\right)^{2}}}_{\delta_{yy}^{n+1/2}\Omega_{ij}}\right\} \qquad (5a)$$

$$\frac{\Omega_{i,j}^{n+1}-\Omega_{i,j}^{n+1/2}}{\Delta t/2}+u_{i,j}^{n+1/2}\frac{\Omega_{i+1,j}^{n+1/2}-\Omega_{i-1,j}^{n+1/2}}{2\Delta x}+v_{i,j}^{n+1/2}\frac{\Omega_{i,j+1}^{n+1}-\Omega_{i,j-1}^{n+1}}{2\Delta y}=$$

$$\frac{1}{\mathrm{Re}}\left\{\underbrace{\frac{\Omega_{i+1,j}^{n+1/2}-2\Omega_{i,j}^{n+1/2}+2\Omega_{i-1,j}^{n+1/2}}{\left(\Delta x\right)^{2}}}_{\delta_{xx}^{n+1/2}\Omega_{ii}}+\underbrace{\frac{\Omega_{i,j+1}^{n+1}-2\Omega_{i,j}^{n+1}+2\Omega_{i,j-1}^{n+1}}{\left(\Delta y\right)^{2}}}_{\delta_{yy}^{n+1}\Omega_{ij}}\right\} \qquad (5b)$$

In eq.(5b) can use $u_{i,j}^{n}$ & $v_{i,j}^{n}$ instead of (n+1/2) time level

➡ No need to solve ψ at level (n+1/2)

➡ Computation time reduced

With this argument, eqs. 5a&5b becomes,

$$(5a)\quad \Rightarrow\quad -\frac{1}{2}\underbrace{\left(\frac{1}{2}c_x+d_x\right)}_{A_x}\Omega^{n+1/2}_{i-1,j}+\underbrace{\left(1+d_x\right)}_{B_x}\Omega^{n+1/2}_{i,j}+\frac{1}{2}\underbrace{\left(\frac{1}{2}c_x-d_x\right)}_{C_x}\Omega^{n+1/2}_{i+1,j}=D_x$$

$$(5b)\quad \Rightarrow\quad -\frac{1}{2}\underbrace{\left(\frac{1}{2}c_y+d_y\right)}_{A_y}\Omega^{n+1}_{i,j-1}+\underbrace{\left(1+d_y\right)}_{B_y}\Omega^{n+1}_{i,j}+\frac{1}{2}\underbrace{\left(\frac{1}{2}c_y-d_y\right)}_{C_y}\Omega^{n+1}_{i,j+1}=D_y$$

where $c_x=u\dfrac{\Delta t}{\Delta x}$, $c_y=v\dfrac{\Delta t}{\Delta y}$ Courant numbers

$d_x=\dfrac{1}{\mathrm{Re}}\dfrac{\Delta t}{(\Delta x)^2}$, $d_y=\dfrac{1}{\mathrm{Re}}\dfrac{\Delta t}{(\Delta y)^2}$ Diffusion numbers

$$D_x=\frac{1}{2}\left(\frac{1}{2}c_y+d_y\right)\Omega^{n}_{i,j-1}+\left(1-d_y\right)\Omega^{n}_{i,j}+\frac{1}{2}\left(-\frac{1}{2}c_y+d_y\right)\Omega^{n}_{i,j+1}$$

$$D_y=\frac{1}{2}\left(\frac{1}{2}c_x+d_x\right)\Omega^{n+1/2}_{i-1,j}+\left(1-d_x\right)\Omega^{n+1/2}_{i,j}+\frac{1}{2}\left(-\frac{1}{2}c_x+d_x\right)\Omega^{n+1/2}_{i+1,j}$$

$$A_x \Omega_{i-1,j}^{n+1/2} + B_x \Omega_{i,j}^{n+1/2} + C_x \Omega_{i+1,j}^{n+1/2} = D_x \qquad (6a)$$

$$A_y \Omega_{i,j-1}^{n+1} + B_y \Omega_{i,j}^{n+1} + C_y \Omega_{i,j+1}^{n+1} = D_y \qquad (6b)$$

Tri-diagonal matrix algorithm Thomas Algorithm

Stream Function Equation

$$\nabla^2 \psi = -\Omega$$

- Any numerical scheme for elliptic eq. is applicable, e.g., G.S.

$$\psi_{i,j}^{k+1} = \frac{1}{2(1+\gamma)}\left[(\Delta x)^2 \Omega_{i,j}^{k} + \psi_{i+1,j}^{k} + \psi_{i-1,j}^{k+1} + \gamma\left(\psi_{i,j+1}^{k} + \psi_{i,j-1}^{k+1}\right)\right] \qquad (7)$$

$$\gamma = \left(\frac{\Delta x}{\Delta y}\right)^2$$

Procedure

i. Computation begins with the solution of vorticity eq. (6-a,b) within the domain (ψ fixed) Perform limited number of iterations (5-10)

ii. Vorticity in eq.(7) is updated and the eq.(7) is solved for ψ . Iterate on $\nabla^2\psi = -\Omega$

(new values of ψ (5-10))

iii. Repeat the process untill the desired solution is reached.
B.C relation for Ω to find new vorticity values

Boundary Conditions

- Body surface
- Far-field
- Symmetry line
- Inflow
- Outflow

$$\Omega_{i,1} = 2\left[\frac{\psi_{i,1} - \psi_{i,2}}{\left(\Delta y\right)^2}\right] + O\left(\Delta y\right)$$

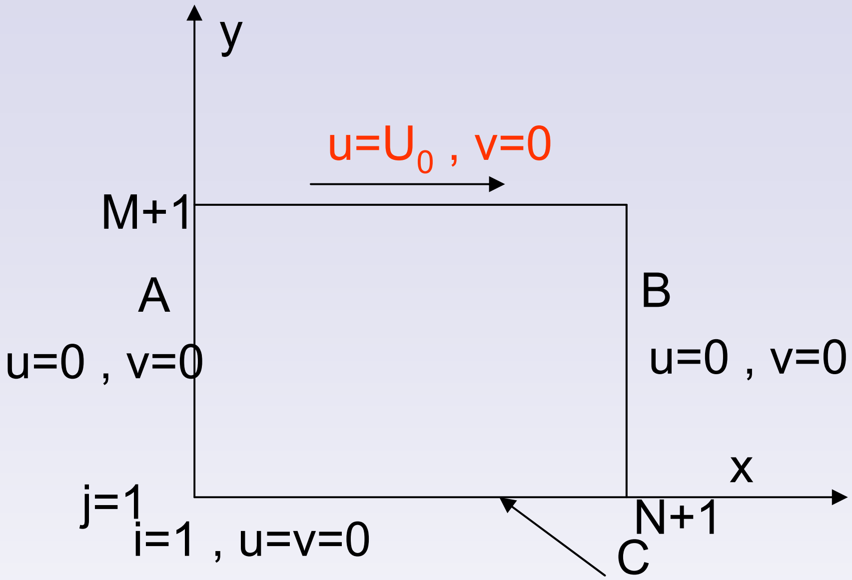
use under-relaxation here

$$\Omega_{i,1}^{k+1} = \left(1-\lambda\right)\Omega_{i,1}^{k} + \lambda\ \Omega_{i,1}^{k+1}$$

check convergence

return to (ii)

Body Surface B.Cs: Driven cavity problem



Looks as if too much information for ψ & not enough info for Ω

Answer:

a) ψ =0 (constant) for $\nabla^2\psi = -\Omega$

b) $\frac{\partial \psi}{\partial n}$ ← used to construct conditions on Ω

Example: BCs at the left wall. u=v=0 at x=0

$$\left.\begin{aligned} u &= \frac{\partial \psi}{\partial y} = 0 \\ v &= -\frac{\partial \psi}{\partial x} = 0 \end{aligned}\right\} \psi = \text{const. (arbitrary)} \qquad \text{(B1)}$$

on x=0 ψ & $\frac{\partial \psi}{\partial \text{x}}$ known but not Ω

Use stream function eq. to find B.Cs for vorticity; i.e. $\nabla^2 \psi = -\Omega$ on the left wall. i=1 , j=j

Thom's method:

$$\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2}\right)_{1,j} = -\Omega_{1,j} \qquad \text{(B2)}$$

Along A (left wall) $\Rightarrow$ $\left.\frac{\partial^2 \psi}{\partial y^2}\right|_{1,j} = 0$ (ψ is constant along y)

$$\left.\frac{\partial^2 \psi}{\partial x^2}\right|_{1,j} = -\Omega_{1,j} \qquad \text{(B3)}$$

To obtain an expression for the second-derivative in eq. above, use Taylor Series expansion

$$\psi_{2,j} = \psi_{1,j} + \left.\frac{\partial \psi}{\partial x}\right|_{1,j} \Delta x + \left.\frac{\partial^2 \psi}{\partial x^2}\right|_{1,j} \frac{(\Delta x)^2}{2} + \ldots \qquad \text{(B4)}$$

Along boundary A, v=0

$$v_{1,j} = -\left.\frac{\partial \psi}{\partial x}\right|_{1,j} = 0$$

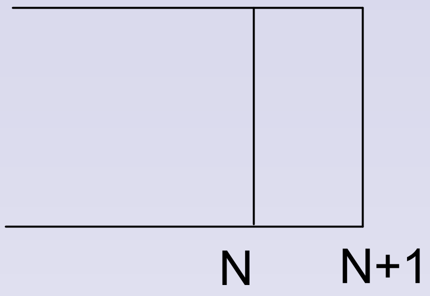
$$\psi_{2,j} = \psi_{1,j} + \left.\frac{\partial^2 \psi}{\partial x^2}\right|_{1,j} \frac{(\Delta x)^2}{2} + O(\Delta x)^3$$

$$\left.\frac{\partial^2 \psi}{\partial x^2}\right|_{1,j} = \frac{2(\psi_{2,j} - \psi_{1,j})}{(\Delta x)^2} + O(\Delta x) \qquad \text{(B5)}$$

Substitute (B5) into (B3)

$$\Omega_{1,j} = \frac{2(\psi_{1,j} - \psi_{2,j})}{(\Delta x)^2} + O(\Delta x) \qquad \text{(B6)}$$

Similarly, for right wall B & bottom wall C:



$$\psi_{N,j} = \psi_{N+1,j} - \cancel{\frac{\partial \psi}{\partial x}}\Bigg|_{N+1,j} \Delta x + \frac{\partial^2 \psi}{\partial x^2}\Bigg|_{N+1,j} \frac{(\Delta x)^2}{2}$$

$$\frac{2\left(\psi_{N,j} - \psi_{N+1,j}\right)}{(\Delta x)^2} + O(\Delta x) = \frac{\partial^2 \psi}{\partial x^2}\Bigg|_{N+1,j}$$

B: $\Omega_{N+1,j} = -\dfrac{\partial^2 \psi}{\partial x^2}\Bigg|_{N+1,j} = \dfrac{2\left(\psi_{N+1,j} - \psi_{N,j}\right)}{(\Delta x)^2}$

C: $\Omega_{i,1} = -\dfrac{\partial^2 \psi}{\partial y^2}\Bigg|_{i,1} = \dfrac{2\left(\psi_{i,1} - \psi_{i,2}\right)}{(\Delta y)^2}$

II.Method:

$$(\mathrm{B3}) \Rightarrow \quad \frac{\partial^2 \psi}{\partial x^2}\Bigg|_{1,j} = -\Omega_{1,j} \Rightarrow \frac{\psi_{2,j} - 2\psi_{1,j} + \psi_{0,j}}{(\Delta x)^2} + O(\Delta x)^2 = -\Omega_{1,j}$$

$$\psi_{0,j} = ? \quad v_{1,j} = -\frac{\partial \psi}{\partial x}\Bigg|_{1,j} = -\frac{\psi_{2,j} - \psi_{0,j}}{2\Delta x} + O(\Delta x)^2 = 0 \Rightarrow \psi_{2,j} = \psi_{0,j} + O(\Delta x)^3$$

$$\Omega_{1,j} = \frac{2\left(\psi_{1,j} - \psi_{2,j}\right)}{(\Delta x)^2} + O(\Delta x)$$

Now suppose upper boundary moving with a specified velocity, U_0

$$\psi_{i,j-1} = \psi_{i,j} - \underbrace{\left.\frac{\partial \psi}{\partial y}\right|_{i,j}}_{U_0 \ (j=M+1)} \Delta y + \left.\frac{\partial^2 \psi}{\partial y^2}\right|_{i,j} \frac{(\Delta y)^2}{2!} + \ldots$$

j=M+1

$$\psi_{i,M} = \psi_{i,M+1} - U_0 \Delta y - \Omega_{i,M+1} \frac{(\Delta y)^2}{2} + O(\Delta y)^3$$

$$\left.\frac{\partial^2 \psi}{\partial y^2}\right|_{i,M+1} + \cancel{\left.\frac{\partial^2 \psi}{\partial x^2}\right|_{i,M+1}} = -\Omega_{i,M+1}$$

$$\Omega_{i,M+1} = \frac{2(\psi_{i,M+1} - \psi_{i,M})}{(\Delta y)^2} - \frac{2U_0}{\Delta y} + O(\Delta y)$$

$$\text{Note that} \rightarrow U_0 = 0 \Rightarrow \Omega_{i,M+1} = \frac{2(\psi_{i,M+1} - \psi_{i,M})}{(\Delta y)^2}$$

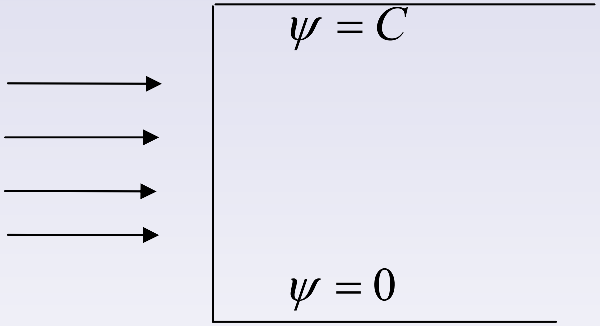
A second order equivalent of (B6) is given

$$\Omega_{1,j} = \frac{\psi_{3,j} - 8\psi_{2,j} + 7\psi_{1,j}}{2(\Delta x)^2} + O(\Delta x)^2$$

- Higher order implementation of B.Cs, in general, will increase the accuracy of solution , but it may cause instabilities for high Reynolds number flow

$$\psi_{i,M+1} = \frac{-\psi_{i,M+1} + 8\psi_{i,M} - 7\psi_{i,M-1}}{2(\Delta y)^2} - \frac{3U_o}{\Delta y}$$

INFLOW: u is specified



Inlet velocity profile u = u(x,y) at x = x_0 then

$$u = \frac{\partial \psi}{\partial y} \rightarrow \psi(x_0, y) = \int_0^{y_0} u(x_0, y)dy$$

$$u = \frac{\partial \psi}{\partial y}, v = -\frac{\partial \psi}{\partial x}$$

i. Values of ψ along the inflow are specified

$$u = U_0 \rightarrow \frac{\partial \psi}{\partial y} = U_0 \rightarrow \psi = U_0 y$$

ii. Its values is determined from the interiour

$$v = 0 \rightarrow \left.\frac{\partial \psi}{\partial x}\right|_{1,j} = 0 \Rightarrow -3\psi_{1,j} + 4\psi_{2,j} - \psi_{3,j} = 0; \quad \psi_{1,j} = \frac{1}{3}\left[4\psi_{2,j} - \psi_{3,j}\right]$$

Vorticity at the inflow:

a. $$\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}\right)_{1,j}=-\Omega_{1,j}$$

$$\Omega_{1,j}=\frac{2\left(\psi_{1,j}-\psi_{2,j}\right)}{\left(\Delta x\right)^2}-\frac{\psi_{1,j+1}-2\psi_{1,j}+\psi_{1,j-1}}{\left(\Delta y\right)^2}$$

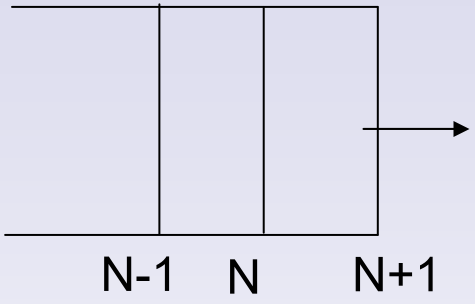
b. $$\Omega_{i,j}=\frac{\partial v}{\partial x}-\frac{\partial u}{\partial y}=\left(-\frac{\partial^2\psi}{\partial x^2}+\frac{\partial u}{\partial y}\right)_{i,j}$$

specified u is directly used to evaluate Ω & set i=1

$$\Omega_{1,j}=\underbrace{\frac{-3\psi_{1,j}+4\psi_{2,j}-\psi_{3,j}}{\left(\Delta x\right)^2}}_{\text{second order forward dif.}}-\underbrace{\frac{u_{1,j+1}-u_{1,j-1}}{2\Delta y}}_{\text{second order central dif.}}$$

OUTFLOW: value of streamfunction is usually extrapolated from the interior solution.

Utilizing $\frac{\partial \psi}{\partial x} = 0$ second-order backward approximation



$$\frac{\partial \psi}{\partial x} = 0$$

$$(v = 0)$$

$$\left.\frac{\partial \psi}{\partial x}\right|_{N+1,j} = 0 = \frac{3\psi_{N+1,j} - 4\psi_{N,j} + \psi_{N-1,j}}{2\Delta x}$$

$$\psi_{N+1,j} = \frac{1}{3}\left(4\psi_{N,j} - \psi_{N-1,j}\right)$$

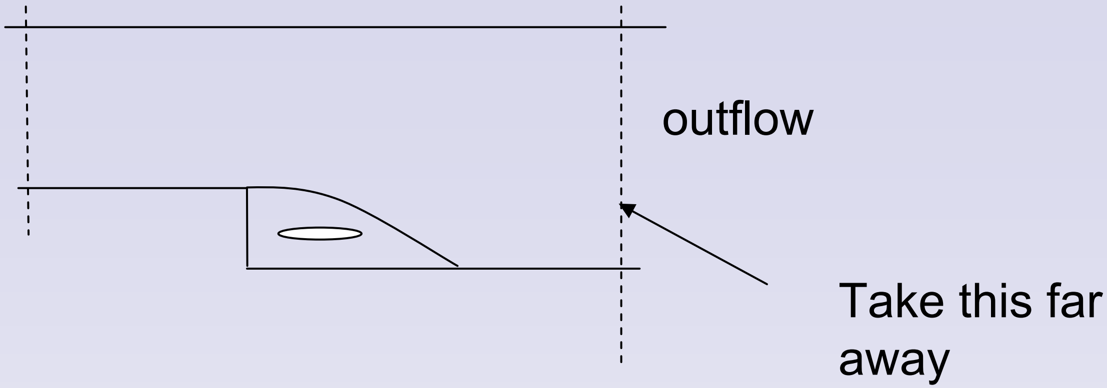
The condition $\frac{\partial^2 \psi}{\partial x^2} = 0$ is also used

Second-order backward approx.

$$\psi_{N+1,j} = \frac{1}{2}\left(\psi_{N-2,j} - 4\psi_{N-1,j} + 5\psi_{N,j}\right)$$

First-order backward approximation

$$\psi_{N+1,j} = -\psi_{N-1,j} + 2\psi_{N,j}$$



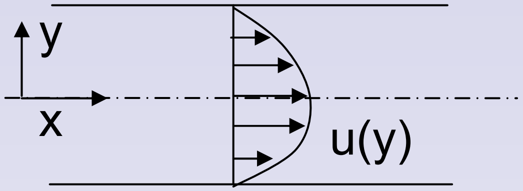
As with the inflow B.C vorticity at outlet can be determined by numerous methods,
Examples:

$$\Omega_{N+1,j} = \frac{2\left(\psi_{N+1,j} - \psi_{N,j}\right)}{\left(\Delta x\right)^2} - \frac{\left(\psi_{N+1,j+1} - 2\psi_{N+1,j} + \psi_{N+1,j-1}\right)}{\left(\Delta y\right)^2}$$

Simple extrapolation may be used for which one sets

$$\frac{\partial \Omega}{\partial x} = 0 \Rightarrow \Omega_{N+1,j} = \frac{1}{3}\left(4\Omega_{N,j} - \Omega_{N-1,j}\right)$$

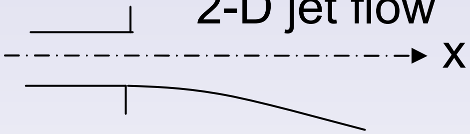
SYMMETRY BOUNDARIES:



v=0 ,

v=0 , $\frac{\partial u}{\partial y} = 0 \Rightarrow \Omega = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} = 0$

$$\text{u symmetric} \rightarrow \frac{\partial u}{\partial y} = 0$$



2-D jet flow

Stream function

$$V_r = \frac{1}{r}\frac{\partial \psi}{\partial \theta} \quad , \quad V_\theta = -\frac{\partial \psi}{\partial r}$$

$$\Omega = \nabla \times \vec{V} = \frac{\partial V_\theta}{\partial r} + \frac{V_\theta}{r} - \frac{1}{r}\frac{\partial V_r}{\partial r} \qquad (*)$$

Vorticity transport:

$$\nabla^2 \psi = -\Omega$$

B.Cs

$$\text{as } r \to \infty \qquad V_r = \frac{1}{r}\frac{\partial \psi}{\partial \theta} \to \cos\theta$$

$$V_\theta = -\frac{\partial \psi}{\partial r} \to -\sin\theta$$

$\psi \sim r\sin\theta$ as $r \to \infty$

$\Omega = 0$ (*) as $r \to \infty$

$$\text{on r=1} \qquad V_r = \frac{1}{r}\frac{\partial \psi}{\partial \theta} = 0 \to \psi = 0 \text{ on r=1}$$

$$V_\theta = -\frac{\partial \psi}{\partial r} = 0 \qquad \frac{\partial \psi}{\partial r} = 0 \text{ on r=1}$$

Boundary Conditions For Vorticity

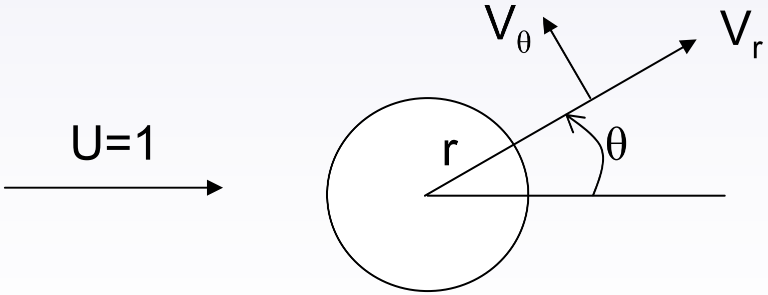
$$\nabla^2 \psi = -\Omega$$

$$u\frac{\partial \Omega}{\partial x} + v\frac{\partial \Omega}{\partial y} = \frac{1}{\mathrm{Re}}\left\{\frac{\partial^2 \Omega}{\partial x^2} + \frac{\partial^2 \Omega}{\partial y^2}\right\}$$

Stream function:

$$V_r = \frac{1}{r}\frac{\partial \psi}{\partial \theta} \quad , \quad V_\theta = -\frac{\partial \psi}{\partial r} \qquad (71)$$

$$\Omega = \nabla \times \vec{V} = \frac{\partial V_\theta}{\partial r} + \frac{V_\theta}{r} - \frac{1}{r}\frac{\partial V_r}{\partial \theta} \qquad (72)$$



governing eq. i) Vorticity transport

ii) $\nabla^2 \psi = -\Omega$

Boundary conditions for cylindrical coordinates

i)

$$\text{as r} \rightarrow \infty \quad V_r = \frac{1}{r}\frac{\partial \psi}{\partial \theta} \rightarrow \cos\theta$$

$$V_\theta = -\frac{\partial \psi}{\partial r} \rightarrow -\sin\theta$$

$$\psi \approx r\sin\theta \quad \text{as} \quad \text{r} \rightarrow \infty$$

And from (72)

$$\Omega \rightarrow 0 \quad \text{as} \quad \text{r} \rightarrow \infty$$

$$\psi \,\&\, \Omega \quad \text{known}$$

ii) $\text{on r} = 1 \quad V_r = \frac{1}{r}\frac{\partial \psi}{\partial \theta} = 0 \qquad \psi = 0 \quad \text{on r=1}$

$$V_\theta = -\frac{\partial \psi}{\partial r} = 0 \qquad \frac{\partial \psi}{\partial r} = 0$$

$$\psi, \ \frac{\partial \psi}{\partial r} \quad \text{known but not } \Omega$$

Pressure Equation:

$$\nabla^2 P = 2\rho\left[\left(\frac{\partial^2\psi}{\partial x^2}\right)\left(\frac{\partial^2\psi}{\partial y^2}\right)-\left(\frac{\partial^2\psi}{\partial x\partial y}\right)\right] = S \quad \text{(P1)}$$

see page 652 for derivation

Second-order difference representation

$$S_{i,j} = 2\rho_{i,j}\left[\left(\frac{\psi_{i+1,j}-2\psi_{i,j}+\psi_{i-1,j}}{(\Delta x)^2}\right)\left(\frac{\psi_{i,j+1}-2\psi_{i,j}+\psi_{i,j-1}}{(\Delta y)^2}\right)-\left(\frac{\psi_{i+1,j+1}-\psi_{i+1,j-1}-\psi_{i-1,j+1}+\psi_{i-1,j-1}}{4\Delta x\Delta y}\right)^2\right] \quad \text{(P2)}$$

Note: For a steady flow problem, the pressure equation is only solved once, i.e. after steady-state values of ω&ψ have been computed.

If only wall pressures are desired, no need to solve poisson eq. over entire flow field.

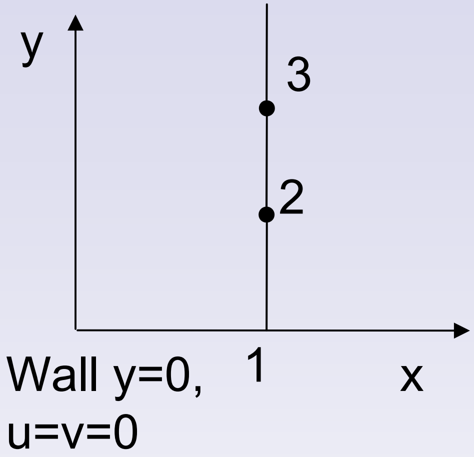
Pressure dist. on airfoil
turbine blades, etc.

$$\rho\left(u\cancel{\frac{\partial u}{\partial x}}+\cancel{v}\frac{\partial u}{\partial y}\right)=-\frac{\partial P}{\partial x}+\mu\left(\cancel{\frac{\partial^2 u}{\partial x^2}}+\frac{\partial^2 u}{\partial y^2}\right)$$

$$\left.\frac{\partial P}{\partial x}\right|_{\text{wall}}=\mu\left.\frac{\partial^2 u}{\partial y^2}\right|_{\text{wall}}$$

$$\left.\frac{\partial P}{\partial x}\right|_{\text{wall}}=-\mu\left.\frac{\partial \Omega}{\partial y}\right|_{\text{wall}} \qquad \text{(P3)}$$

$$\Omega\big|_{\text{wall}}=\left.\cancel{\frac{\partial v}{\partial x}}\right|_{\text{wall}}-\left.\frac{\partial u}{\partial y}\right|_{\text{wall}}$$



$$\frac{P_{i+1,1}-P_{i-1,1}}{2\Delta x}=-\mu\left(\frac{-3\Omega_{i,1}+4\Omega_{i,2}-\Omega_{i,3}}{2\Delta y}\right) \qquad \text{(P4)}$$

- In order to apply (P4) the pressure must be known for at least one point on the wall surface.
- Then pressure at adjacent point can be determined using a first order, one-sided difference formula for $\frac{\partial P}{\partial x}$ in (P4)
- Thereafter, use eq.(P4) to find pressure at all other wall points.

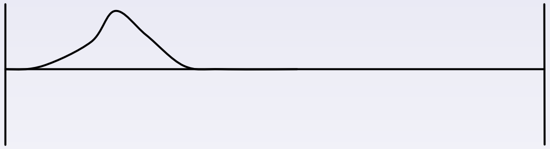
HYPERBOLIC EQUATIONS:

- Method of characteristics: paths of propagation of physical disturbance, inviscid supersonic flow fields: mach lines are characteristics of the flow, difficult to use for 3-D problems and problems with non-linear terms

- Finite difference formulations

Model equation: First order wave equation (linear if a =const.)

$$\frac{\partial u}{\partial t}+a\frac{\partial u}{\partial x}=0 \quad , \quad \text{a>0 (speed of sound)} \quad (1)$$



I.C. u(x,t=0) = f(x) initial disturbance

B.Cs x=0 u(0,t)=0 no-displacement

x=L u(L,t)=0 at boundaries

Explicit Formulations:

1. Euler's FTCS method:

$$\frac{u_i^{n+1}-u_i^n}{\Delta t}=-a\frac{u_{i+1}^n-u_{i-1}^n}{2\Delta x} \qquad O\left(\Delta t,\left(\Delta x\right)^2\right) \qquad (2)$$

Von Neumann stability analysis shows it is unconditionally unstable.

2. The Lax method:

In FTCS method: replace u_i^n with an average value

$$u_i^n = \frac{1}{2}\left(u_{i+1}^n + u_{i-1}^n\right) \qquad (3)$$

$$\frac{\partial u}{\partial t} = \frac{u_i^{n+1} - \frac{1}{2}\left(u_{i+1}^n + u_{i-1}^n\right)}{\Delta t} \qquad (4)$$

Substituting (2) & (4) into (1), we have

$$u_i^{n+1} = \frac{u_{i+1}^n + u_{i-1}^n}{2} - a\frac{\Delta t}{\Delta x}\frac{u_{i+1}^n - u_{i-1}^n}{2} \qquad (5)$$

Von Neumann stability analysis

Assume an error of the form $\in_m (x,t) = e^{bt} e^{ik_m x}$ & substitute in (5),

amplification factor becomes

Note: the error also satisfies the differential eq.

$$\left|\frac{\in_i^{n+1}}{\in_i^n}\right| \leq 1$$ stable solution

$$e^{bt} = \cos(k_m \Delta x) - iC\sin(k_m \Delta x)$$

where $C = a\dfrac{\Delta t}{\Delta x}$

the stability requirement is $\left|e^{bt}\right| \leq 1$

$C = a\dfrac{\Delta t}{\Delta x} \leq 1$ Courant number (CFL condition) (6)

important stability requirement for hyperbolic eqs.

3. Midpoint Leapfrog method

second-order central differencing for both time&space derivatives

$$\frac{u_i^{n+1} - u_i^{n-1}}{2\Delta t} = -a\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} \qquad O\left((\Delta \mathrm{t})^2, (\Delta x)^2\right) \qquad (7)$$

Method is stable when C ≤ 1

- Two sets of initial values are required to start the solution,
- a starter scheme is needed (affects the order of accuracy of the method),
- large increase in computer storage.

4. The Lax-Wendroff method:

The L-W method is derived from Taylor series expansion of the dependent variable as follows

$$u(x,t+\Delta t) = u(x,t) + \frac{\partial u}{\partial t}\Delta t + \frac{\partial^2 u}{\partial t^2}\frac{(\Delta t)^2}{2!} + O(\Delta t)^3 \qquad (8)$$

or in terms of indices

$$u_i^{n+1} = u_i^n + \frac{\partial u}{\partial t}\Delta t + \frac{\partial^2 u}{\partial t^2}\frac{(\Delta t)^2}{2!} + O(\Delta t)^3 \qquad (9)$$

Now consider the model eq.

$$\frac{\partial u}{\partial t} = -a\frac{\partial u}{\partial x} \qquad (10)$$

$$\frac{\partial^2 u}{\partial t^2} = -a\frac{\partial}{\partial t}\left(\frac{\partial u}{\partial x}\right) = -a\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial t}\right) = a^2\frac{\partial^2 u}{\partial x^2} \qquad (11)$$

Substituting (10) & (11) into (9) produces

$$u_i^{n+1} = u_i^n + \left(-a\frac{\partial u}{\partial x}\right)\Delta t + \frac{(\Delta t)^2}{2}a^2\frac{\partial^2 u}{\partial x^2}$$

Use central differencing of second order for the spatial derivatives

$$u_i^{n+1} = u_i^n - a\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x}\Delta t + \frac{1}{2}a^2\left(\Delta t\right)^2\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\left(\Delta x\right)^2}$$

Lax-Wendroff method $O\left[\left(\Delta t\right)^2, \left(\Delta x\right)^2\right]$

Stability analysis shows → explicit method is stable for C ≤ 1

Implicit Formulations

1. Euler’s BTCS method:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -\frac{a}{2\Delta x}\left[u_{i+1}^{n+1} - u_{i-1}^{n+1}\right]$$

$$\frac{1}{2}Cu_{i-1}^{n+1} - u_i^{n+1} - \frac{1}{2}Cu_{i+1}^{n+1} = -u_i^n \qquad \left[\Delta t, \left(\Delta x\right)^2\right]$$

TDMA

2. Crank-Nicolson method:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -\frac{a}{2}\left[\frac{u_{i+1}^{n+1} - u_{i-1}^{n+1}}{2\Delta x} + \frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x}\right]$$

$O\left[\left(\Delta t\right)^2, \left(\Delta x\right)^2\right]$ TDMA

SOLUTION OF EULER'S EQUATIONS

Lax-Wendroff Technique

- Explicit
- Particularly suited to marching solutions: hyperbolic & parabolic eqs.

Example: Time-marching solution of an inviscid flow using unsteady Euler eqs.
For ***unsteady, 2-D inviscid*** flow eqs. (HYPERBOLIC IN TIME)

Continuity: $$\frac{\partial \rho}{\partial t} = -\left(\rho \frac{\partial u}{\partial x} + u \frac{\partial \rho}{\partial x} + \rho \frac{\partial v}{\partial y} + v \frac{\partial \rho}{\partial y} \right) \quad (1)$$ no boundary forces

x-mom: $$\frac{\partial u}{\partial t} = -\left(u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + \frac{1}{\rho} \frac{\partial P}{\partial x} \right) \quad (2)$$

y-mom: $$\frac{\partial v}{\partial t} = -\left(u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + \frac{1}{\rho} \frac{\partial P}{\partial y} \right) \quad (3)$$

Energy: $$\frac{\partial e}{\partial t} = -\left(u \frac{\partial e}{\partial x} + v \frac{\partial e}{\partial y} + \frac{P}{\rho} \frac{\partial u}{\partial x} + \frac{P}{\rho} \frac{\partial v}{\partial y} \right) \quad (4)$$

C_v: specific heat at constant volume
e: internal energy, we have thermodynamic relation
e=e(T,P)
For perfect gas with constant specific heat ⟹ $e(T)=c_vT$
Eqs. (1) to (4) are hyperbolic with respect to time

Taylor series expansion in time

$$\rho_{i,j}^{n+1} = \rho_{i,j}^{n} + \left(\frac{\partial \rho}{\partial t}\right)_{i,j}^{n} \Delta t + \left(\frac{\partial^2 \rho}{\partial t^2}\right)_{i,j}^{n} \frac{(\Delta t)^2}{2!} + \ldots \qquad (5)$$

If flow field at time level n is known,

⇨ Eq.(5) gives the new flow field at time (n+1)→t+Δt

if $\left(\frac{\partial \rho}{\partial t}\right)_{i,j}^{n}$ & $\left(\frac{\partial^2 \rho}{\partial t^2}\right)_{i,j}^{n}$ are found $\rho_{i,j}^{n+1}$ can be calculated explicitly, from eq.(5)

Analogous Taylor series for all other dependent variables can be written as follows:

$$u_{i,j}^{n+1} = u_{i,j}^{n} + \left(\frac{\partial u}{\partial t}\right)_{i,j}^{n} \Delta t + \left(\frac{\partial^2 u}{\partial t^2}\right)_{i,j}^{n} \frac{(\Delta t)^2}{2!} + \ldots \qquad (6)$$

$$v_{i,j}^{n+1} = v_{i,j}^{n} + \left(\frac{\partial v}{\partial t}\right)_{i,j}^{n} \Delta t + \left(\frac{\partial^2 v}{\partial t^2}\right)_{i,j}^{n} \frac{(\Delta t)^2}{2!} + \ldots \qquad (7)$$

$$e_{i,j}^{n+1} = e_{i,j}^{n} + \left(\frac{\partial e}{\partial t}\right)_{i,j}^{n} \Delta t + \left(\frac{\partial^2 e}{\partial t^2}\right)_{i,j}^{n} \frac{(\Delta t)^2}{2!} + \ldots \qquad (8)$$

Using spatial derivatives (second-order central dif.) from eq.(1)

$$\left(\frac{\partial\rho}{\partial t}\right)_{i,j}^{n} = -\left(\rho_{i,j}^{n}\frac{u_{i+1,j}^{n}-u_{i-1,j}^{n}}{2\Delta x}+u_{i,j}^{n}\frac{\rho_{i+1,j}^{n}-\rho_{i-1,j}^{n}}{2\Delta x}+\rho_{i,j}^{n}\frac{v_{i,j+1}^{n}-v_{i,j-1}^{n}}{2\Delta y}+v_{i,j}^{n}\frac{\rho_{i,j+1}^{n}-\rho_{i,j-1}^{n}}{2\Delta y}\right) \qquad (9)$$

In (9), all quantities on RHS are known.

Differentiate eq.(1) with respect to time $\left(\frac{\partial^2\rho}{\partial t^2}\right)_{i,j}^{n} = ?$

$$\left(\frac{\partial^2\rho}{\partial t^2}\right)_{i,j}^{n} = -\left(\rho\frac{\partial^2 u}{\partial x\partial t}+\frac{\partial u}{\partial x}\frac{\partial\rho}{\partial t}+u\frac{\partial^2\rho}{\partial x\partial t}+\frac{\partial\rho}{\partial x}\frac{\partial u}{\partial t}+\rho\frac{\partial^2 v}{\partial y\partial t}+\frac{\partial v}{\partial y}\frac{\partial\rho}{\partial t}+v\frac{\partial^2\rho}{\partial y\partial t}+\frac{\partial\rho}{\partial y}\frac{\partial v}{\partial t}\right) \qquad (10)$$

$\frac{\partial^2 u}{\partial x\partial t}$ =?

Differentiate eq.(2) wrt x;

$$\frac{\partial^2 u}{\partial x\partial t} = -u\frac{\partial^2 u}{\partial x^2}+\left(\frac{\partial u}{\partial x}\right)^2+v\frac{\partial^2 u}{\partial x\partial y}+\frac{\partial u}{\partial y}\frac{\partial v}{\partial x}+\frac{1}{\rho}\frac{\partial^2 P}{\partial x^2}-\frac{1}{\rho^2}\frac{\partial P}{\partial x}\frac{\partial\rho}{\partial x} \qquad (11)$$

In eq.(11) all terms on RHS are expressed as second-order, central dif. eqs. at time level n:

$$\left(\frac{\partial^2 u}{\partial x \partial t}\right)^n_{i,j} = -u^n_{i,j}\frac{u^n_{i+1,j}-2u^n_{i,j}+u^n_{i-1,j}}{(\Delta x)^2}+\left(\frac{u_{i+1,j}-u_{i-1,j}}{2\Delta x}\right)^2 +$$

$$v^n_{i,j}\frac{u^n_{i+1,j+1}+u^n_{i-1,j-1}-u^n_{i-1,j+1}-u^n_{i+1,j-1}}{4(\Delta x)(\Delta y)}+\frac{u^n_{i,j+1}-u^n_{i,j-1}}{2\Delta y}\,\frac{v^n_{i+1,j}-v^n_{i-1,j}}{2\Delta x}+$$

$$\frac{1}{\rho_{i,j}}\,\frac{P^n_{i+1,j}-2P^n_{i,j}+P^n_{i-1,j}}{(\Delta x)^2}-\frac{1}{\left(\rho^n_{i,j}\right)^2}\,\frac{P^n_{i+1,j}-P^n_{i-1,j}}{2(\Delta x)}\,\frac{\rho^n_{i+1,j}-\rho^n_{i-1,j}}{2(\Delta x)} \tag{12}$$

In eq.(12) all terms on RHS are known.

Continuing with the evaluation of eq.(10), a number for $\frac{\partial^2 \rho}{\partial x \partial t}$ is found by differentiating eq.(1) wrt x & replacing all derivatives on RHS with second-order central differences, similar to eq.(12).

$\frac{\partial^2 v}{\partial y \partial t}$ → differentiate eq.(3) wrt y

$\frac{\partial^2 \rho}{\partial y \partial t}$ → differentiate eq.(1) wrt y

$\frac{\partial u}{\partial t}, \frac{\partial v}{\partial t}$ → central difference; eqs.(2) & (3) , respectively.

Finally;

$\left(\frac{\partial^2 \rho}{\partial t^2}\right)_{i,j}^{n}$ is calculated from eq.(10)

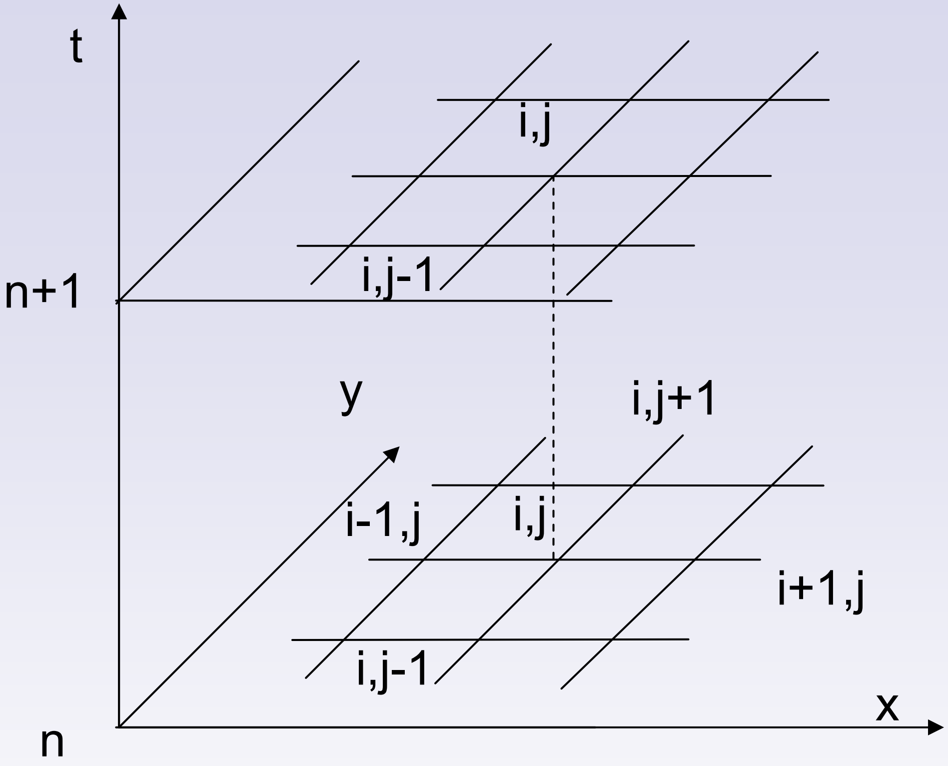
From eq.(5) $\rho_{i,j}^{n+1}$ is known

For the remaining flow-field variables, $u_{i,j}^{n+1}, v_{i,j}^{n+1}, e_{i,j}^{n+1}$ repeat the above procedure

$$u_{i,j}^{n+1} = f\left(u_{i,j}^{n}, u_{i,j+1}^{n}, u_{i,j-1}^{n}, u_{i+1,j}^{n}, u_{i-1,j}^{n}\right)$$

Remarks on Lax-Wendroff

- second-order accuracy in both space & time
- Algebra is lengthy


t
i,j
i,j-1
n+1
y
i,j+1
i-1,j
i,j
i+1,j
i,j-1
x
n

MACCORMACK'S TECHNIQUE

- A variant of Lax-Wendroff approach
- But much simpler in its application
- Explicit finite-difference (second-order accurate in time&space)
- First introduced in 1969

Consider again the Euler eqs. given in eqs.(1) to (4)
Assume that flow field at each grid point is known at time level n

$$\rho_{i,j}^{n+1} = \rho_{i,j}^{n} + \left(\frac{\partial \rho}{\partial t}\right)_{av} \Delta t \qquad (13)$$

Where $\left(\frac{\partial \rho}{\partial t}\right)_{av}$ representative mean value of $\frac{\partial \rho}{\partial t}$ between times t & t+Δt, i.e. time levels n and (n+1)

$\left(\frac{\partial \rho}{\partial t}\right)_{av}$ is to be calculated so as to preserve second-order accuracy without the need to calculate values of the second time derivative $\left(\frac{\partial^2 \rho}{\partial t^2}\right)_{i,j}^{n}$

Similar relations for the other flow-field variables,

$$u_{i,j}^{n+1} = u_{i,j}^{n} + \left(\frac{\partial u}{\partial t}\right)_{av} \Delta t \qquad (14)$$

$$v_{i,j}^{n+1} = v_{i,j}^{n} + \left(\frac{\partial v}{\partial t}\right)_{av} \Delta t \qquad (15)$$

$$e_{i,j}^{n+1} = e_{i,j}^{n} + \left(\frac{\partial e}{\partial t}\right)_{av} \Delta t \qquad (16)$$

Use the predictor-corrector philosophy as follows

Predictor step: in the continuity eq.(1), replace the spatial derivatives of the RHS with FORWARD differences

$$\left(\frac{\partial \rho}{\partial t}\right)_{i,j}^{n} = -\left(\rho_{i,j}^{n} \frac{u_{i+1,j}^{n} - u_{i,j}^{n}}{\Delta x} + u_{i,j}^{n} \frac{\rho_{i+1,j}^{n} - \rho_{i,j}^{n}}{\Delta x} + \rho_{i,j}^{n} \frac{v_{i,j+1}^{n} - v_{i,j}^{n}}{\Delta y} + v_{i,j}^{n} \frac{\rho_{i,j+1}^{n} - \rho_{i,j}^{n}}{\Delta y}\right) \qquad (17)$$

Obtain a predicted value of density, $\overline{\rho}^{n+1}$ from the first two terms of a Taylor series;

$$\underbrace{\overline{\rho}_{i,j}^{n+1}}_{\substack{\text{predicted value of density} \\ \text{(only first-order accurate)}}} = \rho_{i,j}^{n} + \left(\frac{\partial \rho}{\partial t}\right)_{i,j} \Delta t \qquad (18)$$

A similar fashion, predicted values of u,v&e can be obtained.

$$\overline{u}_{i,j}^{n+1} = u_{i,j}^{n} + \left(\frac{\partial u}{\partial t}\right)_{i,j} \Delta t \qquad (19)$$

$$\overline{v}_{i,j}^{n+1} = v_{i,j}^{n} + \left(\frac{\partial v}{\partial t}\right)_{i,j} \Delta t \qquad (20)$$

$$\overline{e}_{i,j}^{n+1} = e_{i,j}^{n} + \left(\frac{\partial e}{\partial t}\right)_{i,j} \Delta t \qquad (21)$$

Forward differences for the spatial derivatives

Corrector step:

First obtain a predicted value of the time derivative at time t+Δt , $\left(\frac{\partial \overline{\rho}}{\partial t}\right)_{i,j}^{n+1}$

by substituting the predicted values of ρ, u and v into the RHS of continuity eq., replacing the spatial derivatives with BACKWARD differences.

$$\left(\frac{\partial \overline{\rho}}{\partial t}\right)_{i,j}^{n+1} = -\left(\overline{\rho}_{i,j}^{n+1} \frac{\overline{u}_{i,j}^{n+1} - \overline{u}_{i-1,j}^{n+1}}{\Delta x} + \overline{u}_{i,j}^{n+1} \frac{\overline{\rho}_{i,j}^{n+1} - \overline{\rho}_{i-1,j}^{n+1}}{\Delta x} + \overline{\rho}_{i,j}^{n+1} \frac{\overline{v}_{i,j}^{n+1} - \overline{v}_{i,j-1}^{n+1}}{\Delta y} + \overline{v}_{i,j}^{n+1} \frac{\overline{\rho}_{i,j}^{n+1} - \overline{\rho}_{i,j-1}^{n+1}}{\Delta y}\right) \qquad (22)$$

In eq.(13)

$$\left(\frac{\partial\rho}{\partial t}\right)_{av} = \frac{1}{2}\left[\underbrace{\left(\frac{\partial\rho}{\partial t}\right)^{n}_{i,j}}_{\text{from eq.(17)}} + \underbrace{\left(\frac{\partial\bar{\rho}}{\partial t}\right)^{n+1}_{i,j}}_{\text{from eq.(22)}}\right]$$

$$\rho^{n+1}_{i,j} = \rho^{n}_{i,j} + \left(\frac{\partial\rho}{\partial t}\right)_{av}\Delta t \qquad (13) \qquad \text{repeated}$$

Same accuracy as the Lax-Wendroff method

- Simpler (no need to evaluate second derivative $\left(\frac{\partial^2\rho}{\partial t^2}\right)^{n}_{i,j}$

- Also possible to ose backward differences on the predictor and forward differences on the corrector

Remarks:

- Lax-Wendroff & MacCormack techniques can be applied to VISCOUS FLOWS as well
- Space marching possible instead of time-marching step
- Viscous Flows → governed by Navier-Stokes eqs.
- Steady N-S → partially elliptic
- Lax-Wendroff & MacCormack techniques are NOT appropriate for the solution of elliptic PDEs

- Unsteady N-S → mixed parabolic & elliptic behavior
  L-W & MacCormack techniques ARE suitable
  The approach is the same
  Predictor - Corrector
  Forward differences & backward differences; for convective terms only

Viscous terms should be centrally differenced on both the predictor&corrector steps!!

Incompressible N-S eqs.

- Can be derived in a sraightforward fashion from the compressible N-S eqs. (set ρ=const. $\nabla . \vec{V} = 0$

But numerical solution of incompressible eqs. cannot be obtained in a straightforward fashion from a numerical technique developed for the compressible eqs.

Eg. Compressible N-S eqs. using a time-marching MacCormack's technique, explicit time step Δt is restricted by stability condition.

$$\Delta t \le \frac{1}{\frac{|u|}{\Delta x}+\frac{|v|}{\Delta y}+a\sqrt{\frac{1}{(\Delta x)^2}+\frac{1}{(\Delta y)^2}}}$$

For compressible flow, speed of sound *a* is finite.
Above eq. gives a finite value of Δt for numerical solution
For an incompressible flow, a is theoretically infinite, i.e above eq. gives Δt=0!!
Something else must be done! SIMPLE-pressure correction algorithm.

Incompressible N-S eqs.

- Primative variable formulation
- Governing equations are a mixed elliptic-parabolic system of eqs. which are solved simultaneously.

Unknowns; $\vec{V}, P$

- There is no direct link for pressure between continuity&momentum equations.
  (i.e. no eqs. for pressure!)
  Two mathematical manipulations are used to establish a connection.
  1. P equation for pressure is introduced
  2. Introduction of artificial compressibility into continuity eq.
- Specification of b.conditions for pressure may be difficuilt
- Extension to 3-D is straightforward

Poisson eq. for pressure:

Used for computation of pressure field

- In lieu of continuity eq.

Conservative form of x & y components of momentum eq.

$$\frac{\partial u}{\partial t}+\frac{\partial}{\partial x}\left(u^2\right)+\frac{\partial P}{\partial x}+\frac{\partial}{\partial y}\left(uv\right)=\frac{1}{\mathrm{Re}}\nabla^2 u \qquad (1)$$

$$\frac{\partial v}{\partial t}+\frac{\partial}{\partial x}\left(uv\right)+\frac{\partial}{\partial y}\left(v^2\right)+\frac{\partial P}{\partial y}=\frac{1}{\mathrm{Re}}\nabla^2 v \qquad (2)$$

Differentiate eq.(1) wrt x & differentiate eq.(2) wrt y and add two resulting eqs.
After arrangment

$$\frac{\partial^2 P}{\partial x^2}+\frac{\partial^2 P}{\partial y^2}=-\frac{\partial D}{\partial t}-\frac{\partial^2}{\partial x^2}\left(u^2\right)-2\frac{\partial^2}{\partial x\partial y}(uv)-\frac{\partial^2}{\partial y^2}\left(v^2\right)+\frac{1}{\text{Re}}\left[\frac{\partial^2}{\partial x^2}(D)+\frac{\partial^2}{\partial y^2}(D)\right] \qquad (3)$$

$$\text{D}=\frac{\partial}{\partial x}+\frac{\partial}{\partial y}$$

For ρ=const. , D=0!
However,due to numerical considerations, keep the term in (3) to prevent error accumulation in process of iterative solution of eq.

Artificial Compressibility:
Continuity eq. is modified by inclusion of a time-dependent term,

$$\frac{\partial P}{\partial t}+\frac{1}{\tau}\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}\right)=0 \qquad (4)$$

τ: artificial compressibility of fluid

compressibility ~ pseudo-speed of sound, a

$$\tau=\frac{1}{a^2}\rightarrow a^2=\frac{P}{\rho}$$

Steady, incompressible N-S eqs. (2-D cartesian coord.)

$$\frac{\partial P}{\partial t}+a^2\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}\right)=0 \qquad (5)$$

$$\frac{\partial u}{\partial t}+\frac{\partial}{\partial x}\left(u^2+P\right)+\frac{\partial}{\partial y}\left(uv\right)=\frac{1}{\mathrm{Re}}\left(\nabla^2 u\right) \qquad (6)$$

$$\frac{\partial v}{\partial t}+\frac{\partial}{\partial x}\left(uv\right)+\frac{\partial}{\partial y}\left(v^2+P\right)=\frac{1}{\mathrm{Re}}\left(\nabla^2 v\right) \qquad (7)$$

Solution on Regular Grid

To facilitate application of finite dif. formulations, eqs (5)-(7) are written in a flux vector form as

$$\frac{\partial Q}{\partial t}+\frac{\partial E}{\partial x}+\frac{\partial F}{\partial y}=\frac{1}{\mathrm{Re}}\left[N\right]\nabla^2 Q \qquad (8)$$

$$\mathrm{Q}=\begin{bmatrix}\mathrm{P}\\ \mathrm{u}\\ \mathrm{v}\end{bmatrix},\quad \mathrm{E}=\begin{bmatrix}a^2u\\ u^2+P\\ uv\end{bmatrix},\quad \mathrm{F}=\begin{bmatrix}a^2v\\ uv\\ v^2+P\end{bmatrix},\quad \mathrm{N}=\begin{bmatrix}0&0&0\\ 0&1&0\\ 0&0&1\end{bmatrix}$$

Eq.(8) non-linear systems of eqs.

- Explicit formulation of non-linear eqs. can be formulated with no difficulty
- Implicit formulations: a linearization procedure must be introduced

See CFD for Engineers Vol.I, Klaus A.Hoffman & S.T.Chiang

<u>Use of Poisson Equation for Pressure:</u>

Instead of eq.(4), use eq.(3) Poisson eq. for pressure..

<u>Procedure:</u> use eq.(3) to evaluate pressure at (n+1) time level.

Then, eqs. (1)&(2) [Mom. Eqs.] are solved for values of un+1 & vn+1 respectively.

To solve eq.(3) an iterative scheme is usually used.

For example; G-S

$$P_{i,j}^{k+1} = \frac{1}{2\left(1+\gamma\right)}\left[P_{i+1,j}^{k} + P_{i-1,j}^{k+1} + \gamma\left(P_{i,j+1}^{k} + P_{i,j-1}^{k+1}\right)\right] + (RHS)_{i,j}$$

$(RHS)_{i,j}$: central difference formula discretized eq. of RHS of (3)

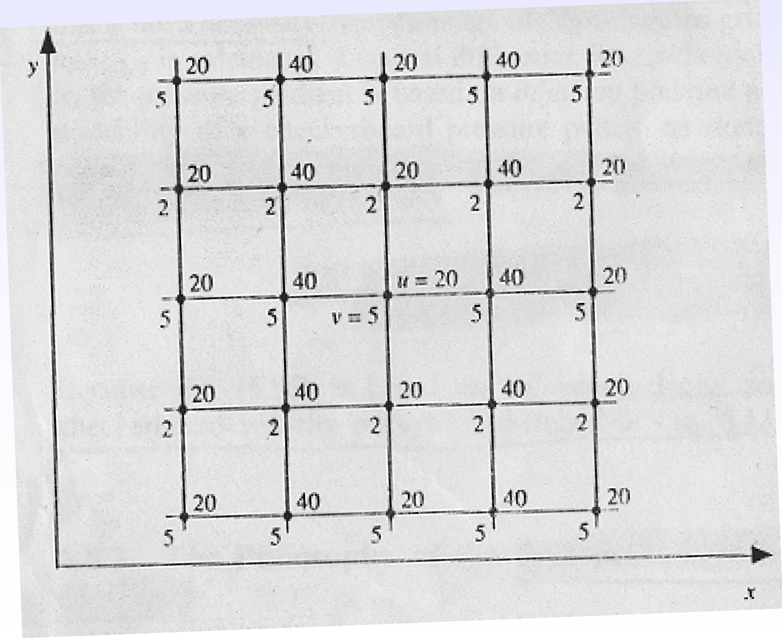
Numerical Solution of Incompressible N-S equations:

Need for a **staggered** grid:

Continuity equation: $$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0$$

$$\frac{u_{i+1,j}-u_{i-1,j}}{2\Delta x}+\frac{v_{i,j+1}-v_{i,j-1}}{2\Delta y}=0$$

Consider ***Checkerboard*** Velocity Distribution; **u: 20,40,20,,, ; v: 5,2,5,...**



Discrete velocity distribution shown satisfies central difference form of the continuity equation.

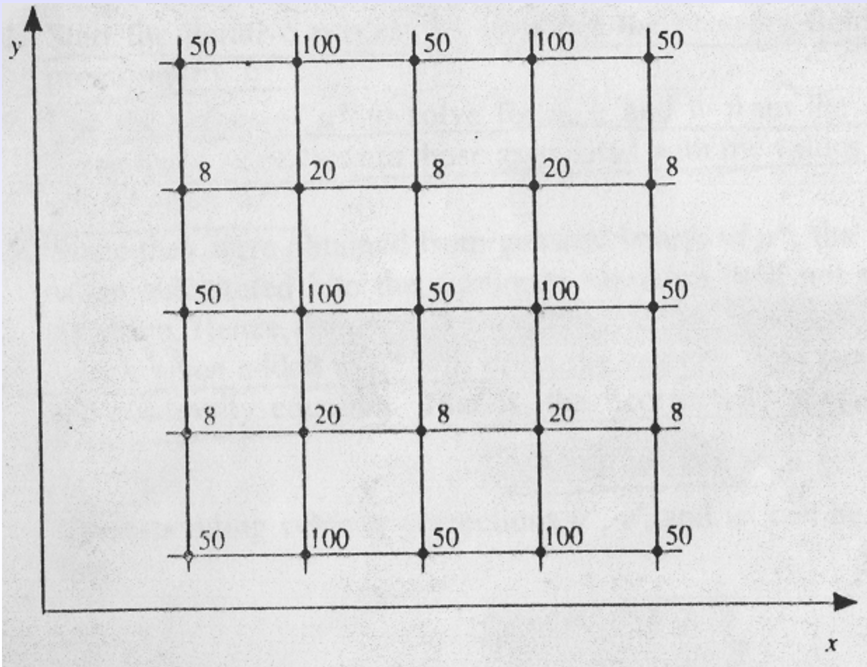
Physically nonsense!

This problem does not occur for *compressible* flow, because inclusion of density variation in the continuity equation wipe out the checkerboard pattern after first time step.

Consider the pressure gradient in Navier-Stokes equations:

$$\frac{\partial p}{\partial x} = \frac{p_{i+1,j} - p_{i-1,j}}{2\Delta x} \quad ; \qquad \frac{\partial p}{\partial y} = \frac{p_{i,j+1} - p_{i,j-1}}{2\Delta y}$$

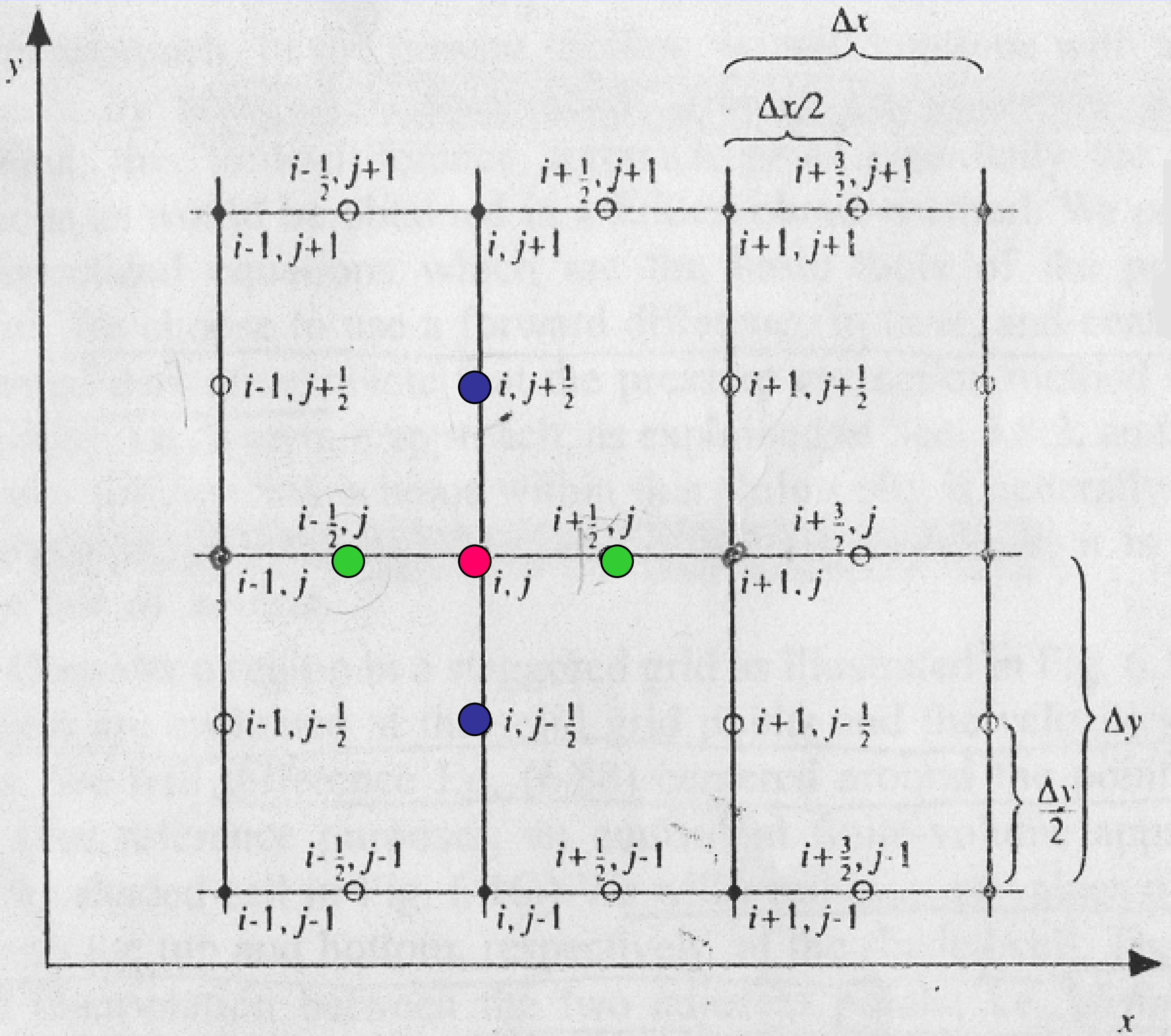
Pressure field dicretized in below mesh, would not be *felt* by the Navier-Stokes equations→**effectively uniform pressure in x & y.**



To fix the potential problem:

-Upwind differences instead of central differences

-Maintain central differencing but **stagger** the grid.



Solid grid points:p

(i-1,j),(i,j),(i+1,j),

(i,j+1),(i,j-1),…

Open grid points:u,v

(i-1/2,j),(i+1/2,j),

(i,j+1/2),(i,j-1/2)…

u is calculated at:

(i-1/2,j),(i+1/2,j)…

v is calculated at:

(i,j+1/2),(i,j-1/2)…

- Pressure and velocities are calculated at *different* grid points.
- Open grid points are shown equidistant between solid grid points but this is not a necessity.
- Central difference expression for continuity equation centered around point **(i,j)** becomes :

$$\frac{u_{i+1/2,j} - u_{i-1/2,j}}{\Delta x} + \frac{v_{i,j+1/2} - v_{i,j-1/2}}{\Delta y} = 0$$

-Because this equation is based on adjacent velocity points, possibility of a checkerboard velocity pattern is eliminated.

Pressure Correction Method

-Basically an *iterative* approach

-Innovative physical reasoning used to construct next iteration from previous iteration results.

Procedure:

1) Start by guessing pressure field (p^*)

2) Usr p^* to solve u,v,w from momentum equations. Denote them u^*, v^*, w^*

3) Since u^*, v^*, w^* were obtained from guessed values,they will not necessarily satisfy continuity equation. Using continuity equation, construct a pressure correction p' which when added to p^* ,will bring velocity field more into agreement with the continuity equation. "Corrected" pressure p:

$$p = p^* + p' \qquad (1)$$

Velocity corrections u',v',w' can be obtained from p'

$$u = u^* + u' \qquad (2)$$

$$v = v^* + v' \qquad (3)$$

$$w = w^* + w' \qquad (4)$$

4)Designate new value of p on the LHS as the new value of p^*

Return to step 2, repeat the process until veloity field satisfies continuity equation.

The Pressure Correction Formula

-How to calculate/find a formula for pressure correction, p' ?

-For simplicity: consider 2D flow & neglect body forces

x & y momentum equations for an incomp. viscous flow in ***conservation form***:

$$\frac{\partial(\rho u)}{\partial t}+\frac{\partial(\rho u^2)}{\partial x}+\frac{\partial(\rho uv)}{\partial y}=-\frac{\partial p}{\partial x}+\mu\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right) \qquad (5)$$

$$\frac{\partial(\rho v)}{\partial t}+\frac{\partial(\rho vu)}{\partial x}+\frac{\partial(\rho v^2)}{\partial y}=-\frac{\partial p}{\partial y}+\mu\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}\right) \qquad (6)$$

-The conservation form follows directly from the model of an infinitely small volume fixed in space→Finite difference form of momentum equations will be somewhat akin to dicretized equations obtained from a finite volume approach.

-Formulation of pressure correction method by *Patankar and Spalding* involved finite volume approach using conservation form of the governing PDEs.

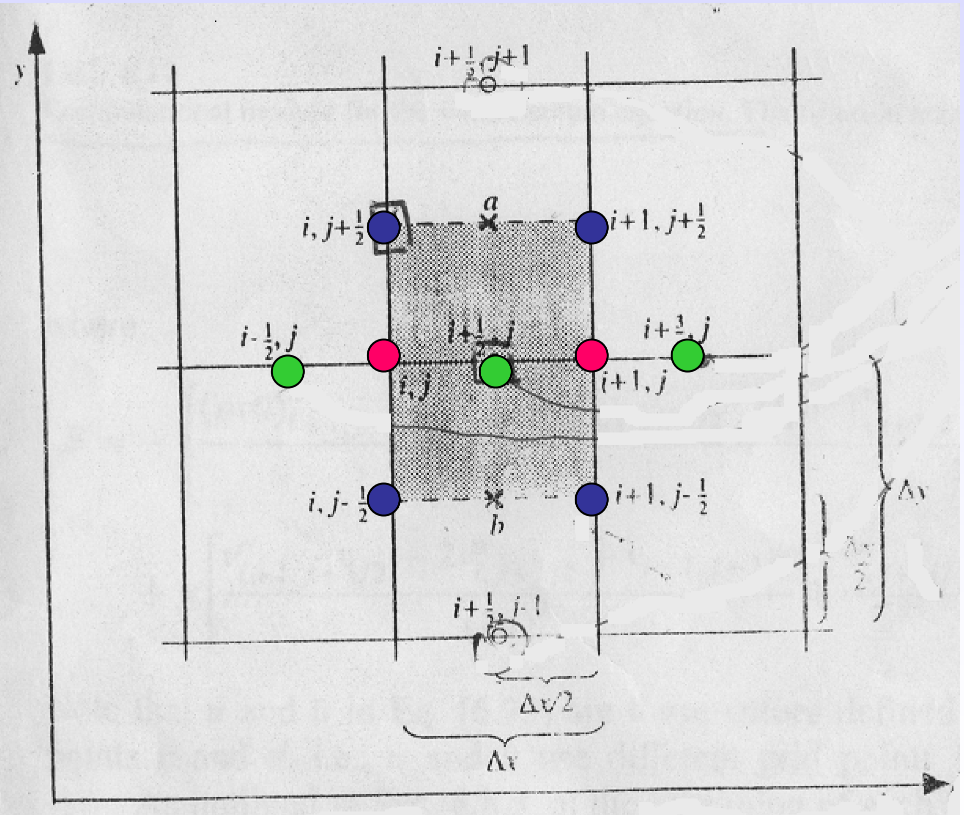
-We choose “forward difference” in time and “central difference” for spatial derivatives

-The scheme is not the only approach,just a reasonable choice.

-Recall: ***red grid points:p**

***yellow grid points:u, blue grid points: v**

-We will difference x momentum equation centered around (i+1/2,j)



Average values of “v” at points a and b (top and bottom)

At point a: $\bar{v}_{j+1/2} \equiv \frac{1}{2}(v_{i,j+1/2} + v_{i+1,j+1/2})$

At point b: $v_{j-1/2} \equiv \frac{1}{2}(v_{i,j-1/2} + v_{i+1,j-1/2})$

Centered around point (i+1/2,j) ,a difference representation of ***x momentum*** equation:

$$\frac{(\rho u)_{i+1/2,j}^{n+1}-(\rho u)_{i+1/2,j}^{n}}{\Delta t}=-\left[\frac{(\rho u^2)_{i+3/2,j}^{n}-(\rho u^2)_{i-1/2,j}^{n}}{2\Delta x}+\frac{(\rho u\bar{v})_{i+1/2,j+1}^{n}-(\rho uv)_{i+1/2,j-1}^{n}}{2\Delta y}\right]$$

$$-\frac{p_{i+1,j}^{n}-p_{i,j}^{n}}{\Delta x}+\mu\left[\frac{u_{i+3/2,j}^{n}-2u_{i+1/2,j}^{n}+u_{i-1/2,j}^{n}}{(\Delta x)^2}+\frac{u_{i+1/2,j+1}^{n}-2u_{i+1/2,j}^{n}+u_{i+1/2,j-1}^{n}}{(\Delta y)^2}\right]$$

Difference equation representing x momentum equation

$$\boxed{(\rho u)_{i+1/2,j}^{n+1}=(\rho u)_{i+1/2,j}^{n}+A\Delta t-\frac{\Delta t}{\Delta x}(p_{i+1,j}^{n}-p_{i,j}^{n})} \qquad (7)$$

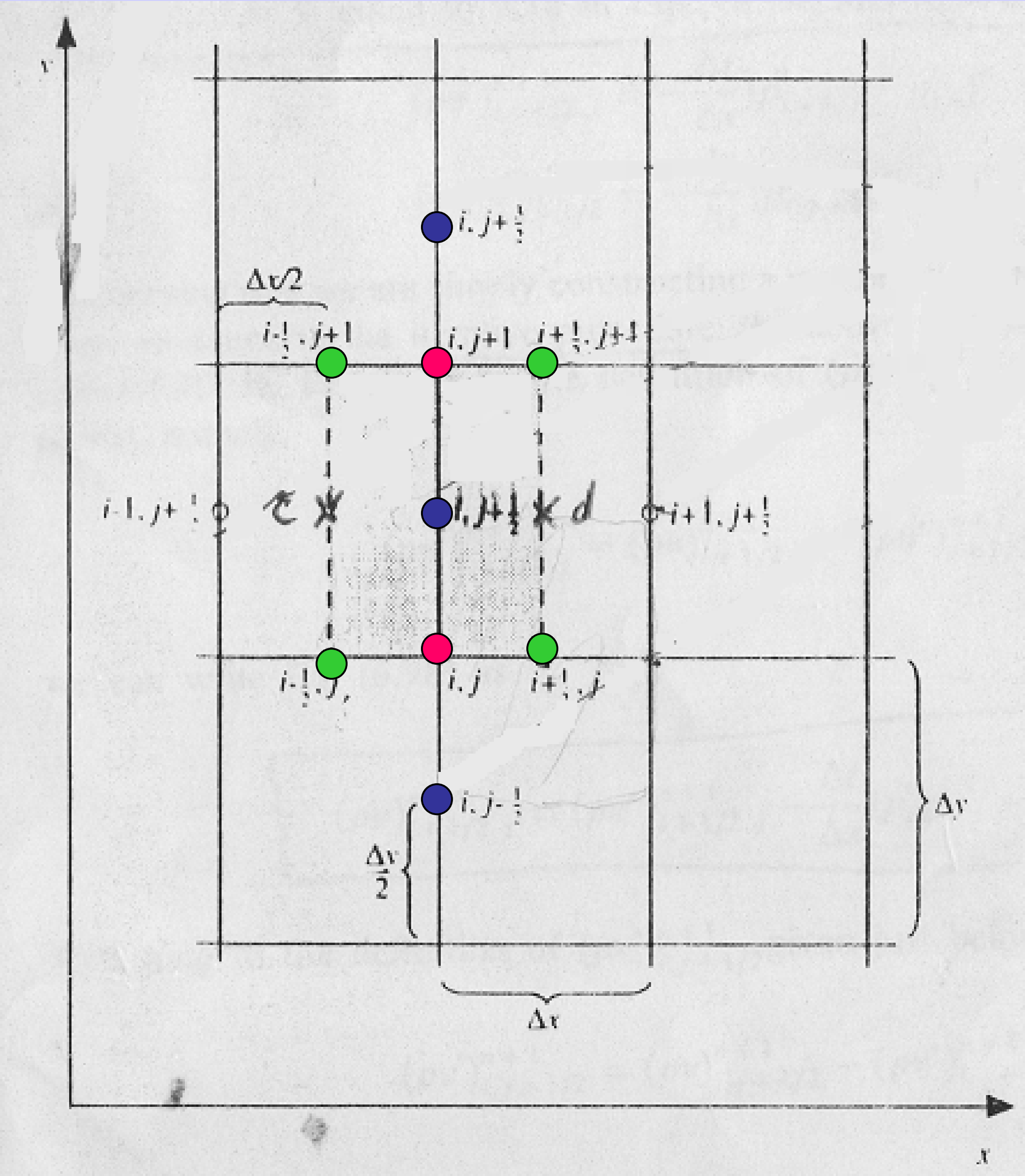
$$A=-\left[\frac{(\rho u^2)_{i+3/2,j}^{n}-(\rho u^2)_{i-1/2,j}^{n}}{2\Delta x}+\frac{(\rho u\bar{v})_{i+1/2,j+1}^{n}-(\rho uv)_{i+1/2,j-1}^{n}}{2\Delta y}\right]$$

$$+\mu\left[\frac{u_{i+3/2,j}^{n}-2u_{i+1/2,j}^{n}+u_{i-1/2,j}^{n}}{(\Delta x)^2}+\frac{u_{i+1/2,j+1}^{n}-2u_{i+1/2,j}^{n}+u_{i+1/2,j-1}^{n}}{(\Delta y)^2}\right]$$

$Note:$ $\bar{v}$ and v use different grid points than those for u.

Centered around point (i,j+1/2) ,a difference representation of y momentum equation:

Average values of “u” at c and d (left and right sides)



At point c: $u=\frac{1}{2}(u_{i-1/2,j}+u_{i-1/2,j+1})$

At point d: $\overline{u}=\frac{1}{2}(u_{i+1/2,j}+u_{i+1/2,j+1})$

Using forward difference in time,central differences in space:

Difference equation representing y momentum equation becomes

$$\boxed{(\rho v)^{n+1}_{i,j+1/2} = (\rho v)^{n}_{i,j+1/2} + B\Delta t - \frac{\Delta t}{\Delta x}(p^{n}_{i,j+1} - p^{n}_{i,j})} \qquad (8)$$

$$B = -\left[\frac{(\rho v\bar{u})^{n}_{i+1,j+1/2} - (\rho v u)^{n}_{i-1,j+1/2}}{2\Delta x} + \frac{(\rho v^{2})^{n}_{i,j+3/2} - (\rho v^{2})^{n}_{i,j-1/2}}{2\Delta y}\right]$$

$$+\mu\left[\frac{v^{n}_{i+1,j+1/2} - 2v^{n}_{i,j+1/2} + v^{n}_{i-1,j+1/2}}{(\Delta x)^{2}} + \frac{v^{n}_{i,j+3/2} - 2v^{n}_{i,j+1/2} + u^{n}_{i,j-1/2}}{(\Delta y)^{2}}\right]$$

$Note:$ $\bar{u}$ and u use different grid points than those for v.

At the beginning of each new iteration, p=p*
Equation 7 and 8 become respectively:

$$(\rho u^*)^{n+1}_{i+1/2,j} = (\rho u^*)^{n}_{i+1/2,j} + A^* \Delta t - \frac{\Delta t}{\Delta x}(p^*_{i+1,j} - p^*_{i,j}) \tag{9}$$

$$(\rho v^*)^{n+1}_{i,j+1/2} = (\rho v^*)^{n}_{i,j+1/2} + B^* \Delta t - \frac{\Delta t}{\Delta x}(p^*_{i,j+1} - p^*_{i,j}) \tag{10}$$

If p* were correct, u* would be true velocity.

Substracting equation (9) from (7):

$$(\rho u')^{n+1}_{i+1/2,j} = (\rho u')^{n}_{i+1/2,j} + A' \Delta t - \frac{\Delta t}{\Delta x}(p'_{i+1,j} - p'_{i,j})^{n} \tag{11}$$

Substracting equation (10) from (8):

$$(\rho v')^{n+1}_{i,j+1/2} = (\rho v')^{n}_{i,j+1/2} + B' \Delta t - \frac{\Delta t}{\Delta x}(p'_{i,j+1} - p'_{i,j}) \tag{12}$$

-Equations (11) and (12) are x and y momentum equations in terms of pressure corrections p’,u’,v’ defined by (1) ,(2) and (3).

-We are in a position to obtain a formula for the pressure correction p’ by insisting that the *velocity field must satisfy the continuity equation*.

-However, pressure correction method is an iterative approach

→there is no inherent reason why the formula designed to predict p’ from one iteration to the next be physically correct.

-We are concerned with only two aspects:

1) Formula for p’ must yield the values that ultimately lead th the proper, converged solution
2) In the limit of converged solution,the formula for p’ must reduce to the physically correct continuity equation.

When this convergence is achieved, p’→0, and the formula for p’ reduce to the physically correct continuity equation.

Can use a formula with a ***numerical artifice !***

Let us arbitrarily set A', B', $(\rho u')^n, (\rho v')^n$ equal to zero in (11) and (12)

$$(\rho u')_{i+1/2,j}^{n+1} = -\frac{\Delta t}{\Delta x}(p'_{i+1,j} - p'_{i,j})^n \qquad (13)$$

$$(\rho v')_{i,j+1/2}^{n+1} = -\frac{\Delta t}{\Delta y}(p'_{i,j+1} - p'_{i,j})^n \qquad (14)$$

we are simply constructing a *numerical artifice* which will provide some guidance in the iterative procedure. Do not worry much !

Definition of $(\rho u')_{i+1/2,j}^{n+1}$

$$(\rho u')_{i+1/2,j}^{n+1} = (\rho u)_{i+1/2,j}^{n+1} - (\rho u^*)_{i+1/2,j}^{n+1}$$

Equation (13) becomes:

$$(\rho u)_{i+1/2,j}^{n+1} = (\rho u^*)_{i+1/2,j}^{n+1} - \frac{\Delta t}{\Delta x}(p'_{i+1,j} - p'_{i,j})^n \qquad (15)$$

Definition of $(\rho v')^{n+1}_{i,j+1/2}$

$$(\rho v')^{n+1}_{i,j+1/2} = (\rho v)^{n+1}_{i,j+1/2} - (\rho v^*)^{n+1}_{i,j+1/2}$$

Equation (14) becomes:

$$(\rho v)^{n+1}_{i,j+1/2} = (\rho v^*)^{n+1}_{i,j+1/2} - \frac{\Delta t}{\Delta y}(p'_{i,j+1} - p'_{i,j})^n \qquad (16)$$

Returning to continuity equation:

$$\frac{\partial(\rho \mathrm{u})}{\partial \mathrm{x}} + \frac{\partial(\rho v)}{\partial y} = 0$$

And writing corresponding central difference equations around (i,j)

$$\frac{(\rho \mathrm{u})_{\mathrm{i+1/2,j}} - (\rho \mathrm{u})_{\mathrm{i\text{-}1/2,j}}}{\Delta x} + \frac{(\rho v)_{\mathrm{i,j+1/2}} - (\rho v)_{\mathrm{i,j\text{-}1/2}}}{\Delta y} = 0 \qquad (17)$$

Substituting (15) and (16) in (17):

$$\boxed{ap'_{i,j} + bp'_{i+1,j} + bp'_{i-1,j} + cp'_{i,j+1} + cp'_{i,j-1} + d = 0} \qquad (18)$$

$$a = 2\left[\frac{\Delta t}{(\Delta x)^2} + \frac{\Delta t}{(\Delta y)^2}\right] \qquad b = -\frac{\Delta t}{(\Delta x)^2} \qquad c = -\frac{\Delta t}{(\Delta y)^2}$$

$$d = \frac{1}{\Delta x}\left[(\rho u^*)_{i+1/2,j} - (\rho u^*)_{i-1/2,j}\right] + \frac{1}{\Delta y}\left[(\rho v^*)_{i,j+1/2} - (\rho v^*)_{i,j-1/2}\right]$$

Pressure correction formula

$$ap'_{i,j}+bp'_{i+1,j}+bp'_{i-1,j}+cp'_{i,j+1}+cp'_{i,j-1}+d=0 \quad (18)$$

-Elliptic behaviour,consistent with the fact that a pressure disturbance will propagate everywhere throughout an incompressible flow.

-Thus, equation (18) can be solved for p’ by means of a numerical relaxation technique, like Gauss-Seidel iteration

During the course of the iterative process,u* and v* define a velocity field that does not satisfy the continuity equation ;hence in (18) , $d \neq 0$ for all but the last iteration.
-d is a *mass source* therm.
-Theoretically d=0 for the last iteration.

-Although a mathemetical artifice was used to obtain (18),in the last iterative step we can construe (18) as being a proper physical statement of the conservation of mass.

The pressure correction formula (18) is a central difference formulation of the Poisson equation in terms of pressure correction p'.

$$\frac{\partial^2 p'}{\partial x^2} + \frac{\partial^2 p'}{\partial y^2} = Q \qquad (19)$$

-If second partial derivatives in (19) are replaced by central differences, and

-If $Q = \frac{d}{(\Delta t \Delta x)}$ Then equation (18) is obtained.

Notes:-Pressure correction formula is nothing than a diiference equation representing Poisson equation for p'.

-Poisson equation is elliptic;which mathematically verifies elliptic behaviour of pressure correction formula

The Numerical Procedure:The SIMPLE Algorithm

-Following description is the essence of the SIMPLE algorithm as seth forth in Patankar.

-SIMPLE: Semi-implicit method for pressure linked equations.

-Semi implicit refers to our arbitrary setting of $A', B', (\rho u')^n, (\rho v')^n$ equal zero in (11) and (12) allowing the pressure correction formula(18),to have p' appearing at only 4 grid points.

-If this artifice had not been used,resulting pressure correction formula would have included velocities at neighboring grid points.

-These velocities are influenced by pressure corrections in their neighborhood, and resulting pressure correction formula would have reached much further into the flow field.
→ Results in "fully implicit" equation

Step by step procedure for SIMPLE algortihm:

1)Guess values of $(p^*)^n$ at all the pressure grid points.

Also arbitrarly set values of $(\rho u^*)^n$ and $(\rho v^*)^n$ at proper velocity grid points.

-Here we are considering the grid points internal to the flow field; not boundaries.

2)Solve for $(\rho u^*)^{n+1}$ from equation (9) and $(\rho v^*)^{n+1}$ from (10) at all internal points.

3)Substitute these values of $(\rho u^*)^{n+1}$ and $(\rho v^*)^{n+1}$ into (18), and solve for p' at all internal points.

4)Calculate p^{n+1} obtained in all internal points from equation (1)

$$p^{n+1} = (p^*)^n + p'$$

5)The values of p^{n+1} obtained in step 4 are used to solve the momentum equations.

For this,we designate p^{n+1} obtained above as the new values of $(p^*)^n$ to be inserted in (9) and (10)

Return to step 2 ;repeat until convergence.

Reasonable criterion is when mass source term "d" aprroaches zero.

-When convergence is achieved,velocity distribution is obtained which satisfies continuity equation.

-Equation (18) is to aim the iteration process in such a direction that when the velocity distribution is calculated from the momentum equations,it will eventually converge to correct distribution which satisfies continuty equation.

-Eq. (5) and (6) are the unsteady momentum equations,and hence the corresponding difference equations (7) and (8) utilize the standart superscript notation ,”n” for a given time level and n+1 for the next time level.

-However,no problem, because pressure correction method is deisgned for “steady “ flow,and we obtain this via an iterative process.

-*Sequential iteration steps* ,with no significance to any real transient variation.

-Δt is a parameter which has some effect on the speed at which convergence is achieved.

-Eq. (18) may diverge in some cases:

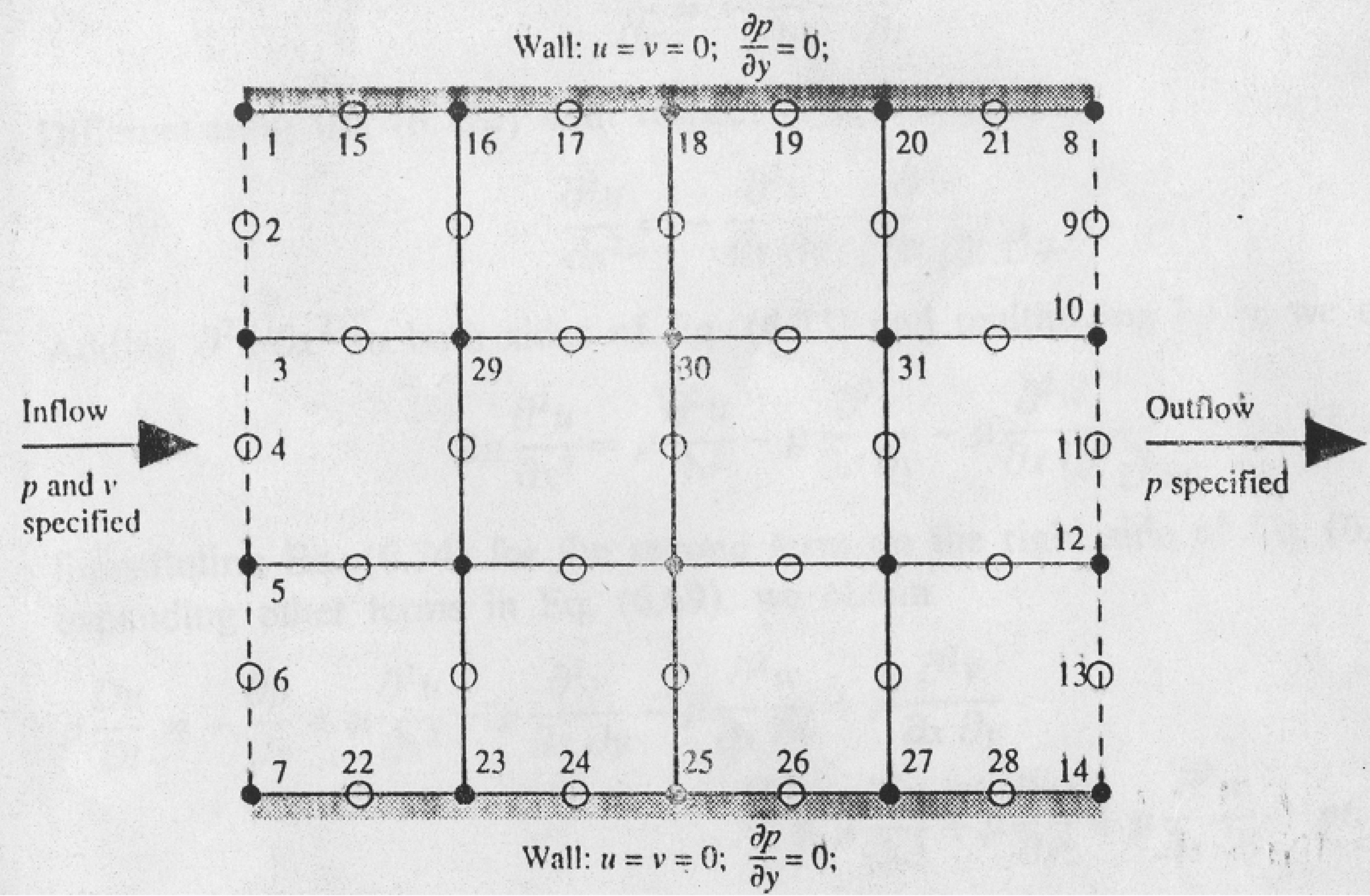
Patankar suggests using some underrelaxation in such cases:

Instead of using the equation in step 4 , use:

$$p^{n+1} = (p*)^n + \alpha_p p'$$

where α is an underrelaxation factor;a value of 0.8 is suggested.

Boundary Conditions For the Pressure Correction Method



1)At inflow boundary,p and v are specified and u is allowed to float.

$$p'_1 = p'_3 = p'_5 = p'_7 = 0$$

Then p' is zero at the inflow boundary.

2)At the outflow boundary,p is specified and u and v are allowed to float.

$$p'_8 = p'_{10} = p'_{12} = p'_{14} = 0$$

3) At the walls,the viscous,no slip condition holds at the wall.

$$u_{15} = u_{17} = u_{19} = u_{21} = u_{22} = u_{24} = u_{26} = u_{28} = 0$$

Since (18) is elliptic,and is solved by relaxation technique,a boundary condition associated with p' must be specified over the *complete* boundary containing the computational domain.

A condition associated with p' at walls derived as:

-Evaluate y momentum equation at the wall where u=v=0

$$\left(\frac{\partial p}{\partial y}\right)_w = \mu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right)_w \qquad (19)$$

In equation (19),since $v_w = 0, \left(\partial^2 v / \partial x^2\right)_w = 0.$

Also near vicinity of the wall,v is small: $\left(\partial^2 v / \partial y^2\right)_w = 0$

So: $$\left(\frac{\partial p}{\partial y}\right)_w = 0 \qquad (20)$$

Discretizing (20):

$p_1 = p_3 \qquad p_{16} = p_{29} \qquad p_5 = p_7$ etc.

Grid Generation

Introduction:

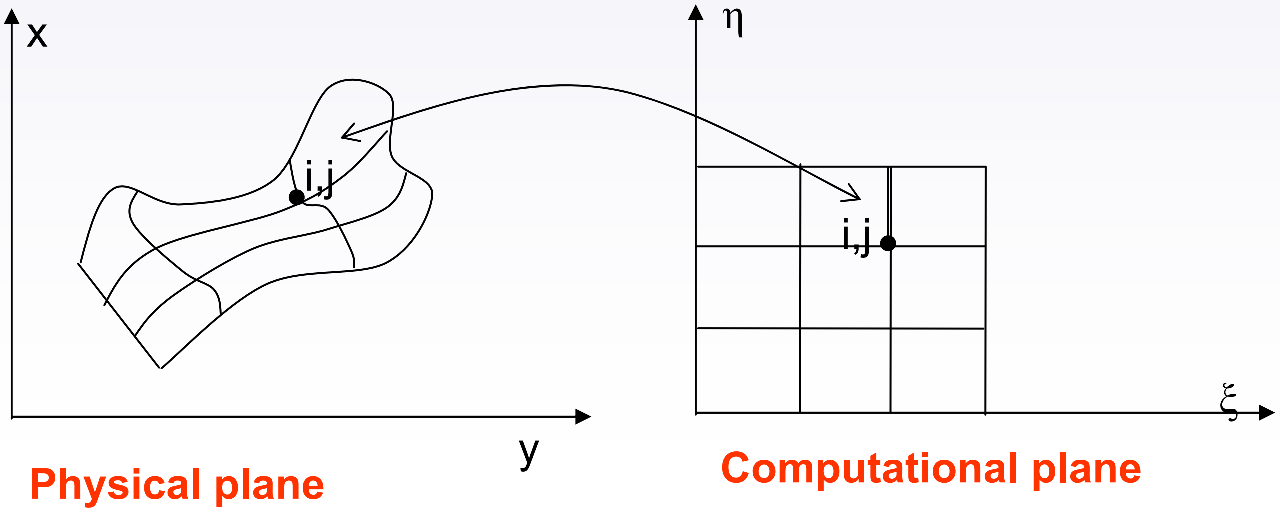
- Have assumed rectangular domain
- Any curved domain can be mapped to rectangle
- Flow in curved passage

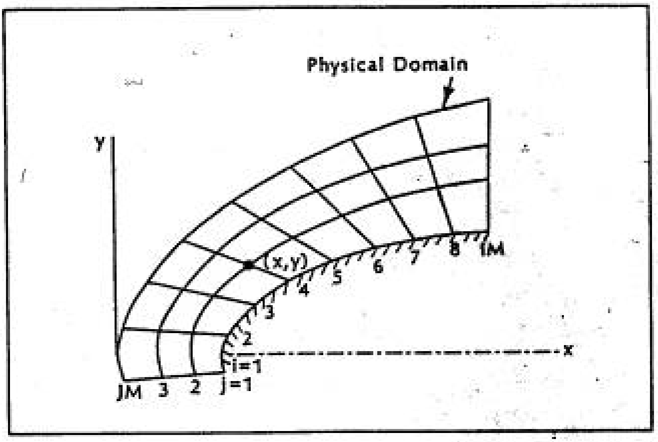
Transformation of governing partial differential equations.

Mapping

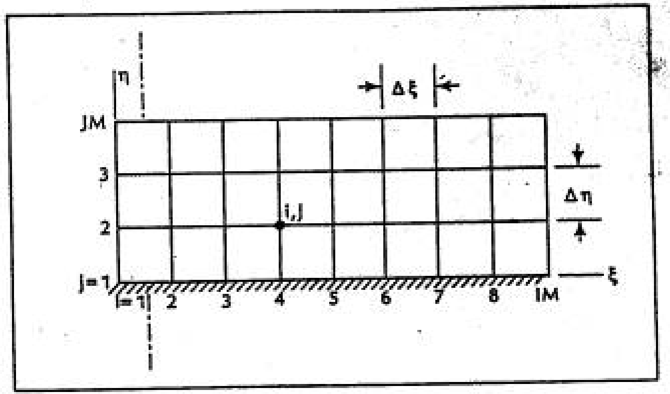
$$\xi = \xi(x, y)$$
$$\eta = \eta(x, y)$$

Relations between physical and computational planes





1



2

Computational domain.

Main issue: how to find the location of the grid points in the physical domain

(x,y): physical coordinates
(ξ,η): computational coordinates

$$\frac{\partial}{\partial x} = \frac{\partial \xi}{\partial x}\frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial x}\frac{\partial}{\partial \eta} \qquad (1)$$

$$\frac{\partial}{\partial y} = \frac{\partial \xi}{\partial y}\frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial y}\frac{\partial}{\partial \eta}$$

$$\frac{\partial \xi}{\partial x}, \frac{\partial \xi}{\partial y}, \frac{\partial \eta}{\partial x}, \frac{\partial \eta}{\partial y} \text{ called metrics of transformation}$$

Example:

$$\frac{\partial u}{\partial x} + c\frac{\partial u}{\partial y} + y = 0 \quad \text{(A)} \quad \text{original PDE}$$

$$\xi = \xi(x, y)$$

$$\eta = \eta(x, y)$$

$$\frac{\partial u}{\partial x} = \frac{\partial u}{\partial \xi}\xi_x + \frac{\partial u}{\partial \eta}\eta_x \quad ; \quad \frac{\partial u}{\partial y} = \frac{\partial u}{\partial \xi}\xi_y + \frac{\partial u}{\partial \eta}\eta_y$$

$$\left(\xi_x + c\xi_y\right)\frac{\partial u}{\partial \xi} + \left(\eta_x + c\eta_y\right)\frac{\partial u}{\partial \eta} + y\left(\xi, \eta\right) = 0 \quad \text{(B) transformed PDE}$$

- Equation (B) is solved on a uniform grid in the computational plane
- Relationship between physical and computational planes are given by the metrics of transformation, i.e. ξx , ξy , ηx , ηy .

Notes:

1. Form and type of the transformed equation remains the same as the original partial differential equation.

2. $\xi_x = \frac{\partial \xi}{\partial x} \cong \frac{\Delta \xi}{\Delta x}$ i.e. metrics represent the ratio of are lengths in the computational plane to that of the physical plane.

Computation of metrics

$$d\xi = \xi_x dx + \xi_y dy \qquad (2)$$

$$d\eta = \eta_x dx + \eta_y dy$$

or in a compact form,

$$\begin{pmatrix} d\xi \\ d\eta \end{pmatrix} = \begin{pmatrix} \xi_x & \xi_y \\ \eta_x & \eta_y \end{pmatrix} \begin{pmatrix} dx \\ dy \end{pmatrix} \qquad (3)$$

To transform back to physical plane,
or reversing the role of independent variables, i.e.

$$x = x(\xi, \eta)$$

$$y = y(\xi, \eta)$$

$$dx = x_\xi d_\xi + x_\eta d_\eta \quad ; \quad dy = y_\xi d_\xi + y_\eta d_\eta$$

$$\begin{pmatrix} dx \\ dy \end{pmatrix} = \begin{pmatrix} x_\xi & x_\eta \\ y_\xi & y_\eta \end{pmatrix} \begin{pmatrix} d_\xi \\ d_\eta \end{pmatrix} \quad (4)$$

Compare 4 with 3

$$\begin{pmatrix} \xi_x & \xi_y \\ \eta_x & \eta_y \end{pmatrix} = \begin{pmatrix} x_\xi & x_\eta \\ y_\xi & y_\eta \end{pmatrix}^{-1}$$

$$\xi_x = \frac{1}{J} y_\eta \quad , \quad \xi_y = -\frac{1}{J} x_\eta$$

$$\eta_x = -\frac{1}{J} y_\xi \quad , \quad \eta_y = \frac{1}{J} x_\xi \qquad (6)$$

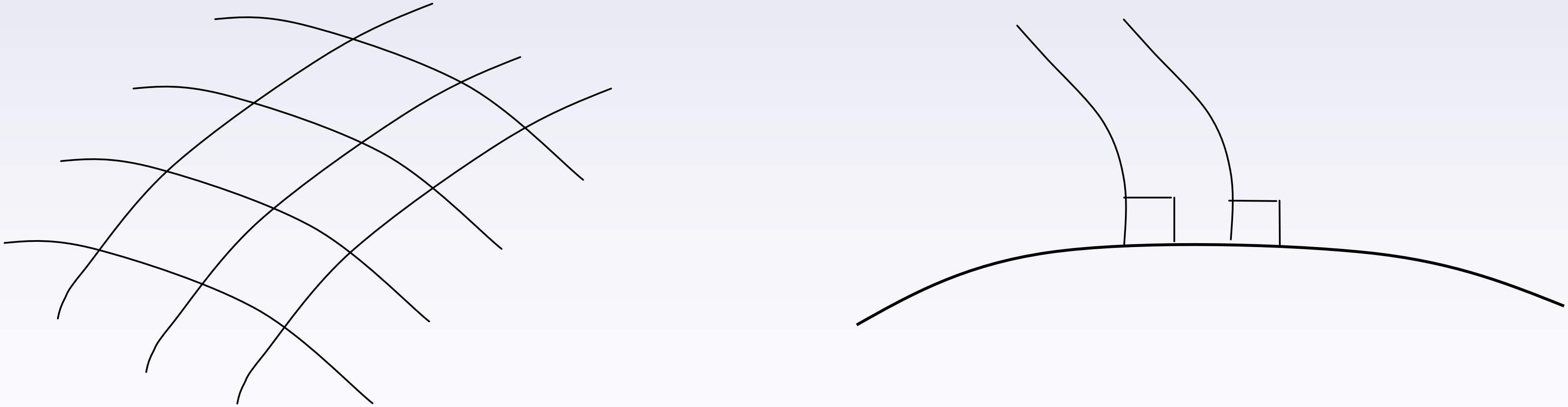
$J = x_\xi y_\eta - y_\xi x_\eta$ = Jacobian of transformation

J: ratio of areas (volumes in 3-D) of computational space to that of physical space.

In determining the grid points (mapping) following requirements are necessary.

Notes:

1. Mapping must be one-to-one. J≠0
2. Want smoothness in grid distribution (smooth behavior of metrics)
3. May want to cluster points in certain regions of physical spaces
4. May want orthogonality in grid, at least in certain regions. Excessive grid skewness should be avoided.



Methods of Grid Generation

1. Conformal mapping (based on complex variables), not extendible to 3-D
2. Algebraic Methods
3. Solution of Differential Equations (Partial differential equations)

Fixed Grid, independent of solution.
Adaptive Grid, evolves as a result of solution of flow equations (high gradients).

Algebraic Methods

Example: Figure 3&4 : half difusser

$$\xi = x \quad , \quad \eta = y / \underbrace{f(x)}_{\substack{represents \\ upper\ boundary}} \qquad (7)$$

$$x = \xi \quad , \quad y = \left\{ H_1 + \frac{H_2 - H_1}{L} \xi \right\} \eta \qquad (8)$$

Known functions are used in one, two or three dimensions to take arbitrary shaped physical regions into a rectangular computational domain

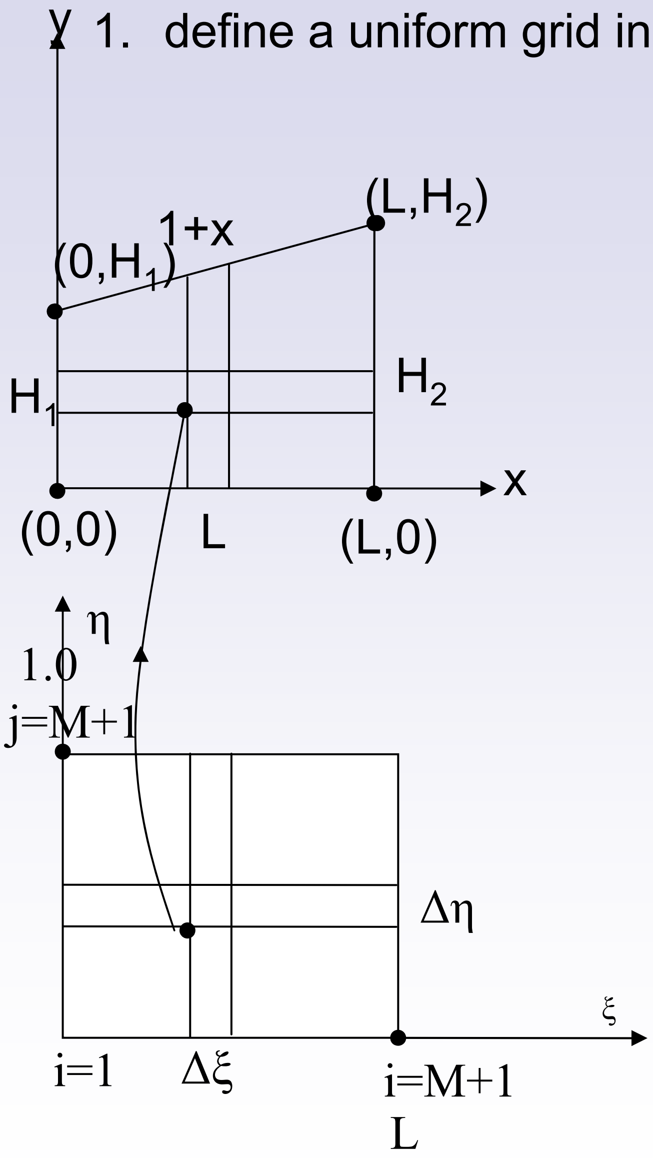
To generate grid

1. Define a uniform grid in ξ,η plane
2. Corresponding points in physical plane found from (8)

Metrics and Jacobian of transformation must be evaluated before any transformed Partial Differential Equations can be solved.

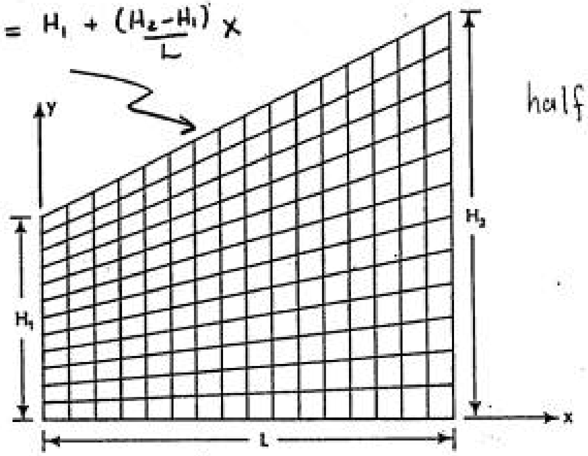
Example:
Generation of Grid: Algebraic Grid

1. define a uniform grid in ξ,η plane



ALGEBRAIC METHODS: simplest grid generation technique

$y = f(x) = H_1 + \frac{(H_2 - H_1)}{L} x$



half of diffuser

Physical plane

3

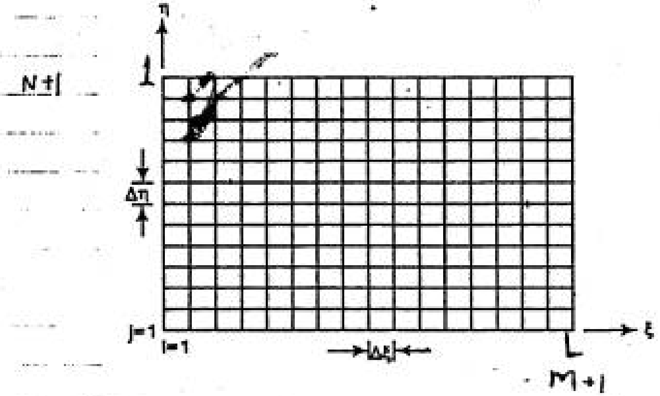
Inverse,

$$\xi = x \quad , \quad \eta = y/f(x) \qquad ⑦$$

$$x = \xi \quad , \quad y = \left\{ H_1 + \frac{(H_2 - H_1)}{L} \text{[illegible]} \right\} \eta \qquad ⑧$$

Algebraic equations (interpolation schemes)

Computational plane



4

Analytical calculation of metrics

$$\xi_x = 1 \quad , \quad \xi_y = 0$$

$$\eta_x = -\frac{y f'(x)}{f^2(x)} = \frac{-\left(\frac{H_2 - H_1}{L}\right)\eta}{\left\{H_1 + \left(\frac{H_1 - H_2}{L}\right)\xi\right\}^2}$$

$$\eta_y = \frac{1}{f(x)} = \frac{1}{\left\{H_1 + \left(\frac{H_2 - H_1}{L}\right)\xi\right\}}$$

To numerically find metrics

for interval points $\begin{cases} x_\xi\big|_{i,j} = \dfrac{x_{i+1,j} - x_{i-1,j}}{2\Delta\xi} \\ x_\eta\big|_{i,j} = \dfrac{x_{i,j+1} - x_{i,j-1}}{2\Delta\eta}, \end{cases}$ $\quad etc.\ y_\xi, y_\eta$

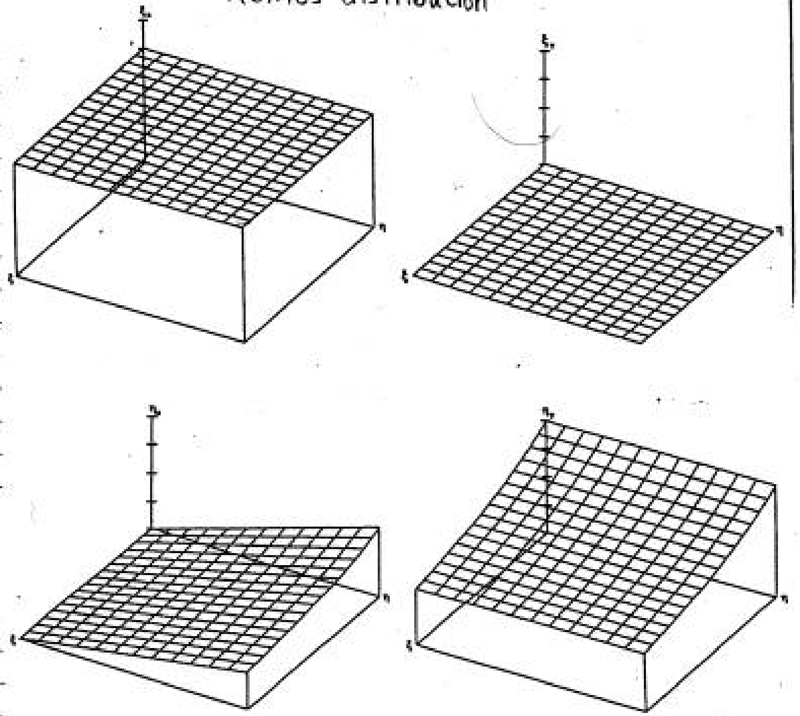
evaluate $J = x_\xi y_\eta - y_\xi x_\eta$

evaluate $\xi_x, \xi_y, \eta_x, \eta_y$ from (6)

derivatives at boundaries are evaluated with forward or backward 2nd order approximation

$$j = 1; \ \ x_\eta\big|_{i,1} = \frac{-3x_{i,1} + 4x_{i,2} - x_{i,3}}{2\Delta\eta}$$

Metrics distribution



Note: smooth distribution

Clustering Techniques

- consider a duct

Clustering Techniques

To cluster near bottom (Consider duct problem)

$$\xi = x$$

$$\eta = 1 - \frac{\log\left\{\dfrac{\beta + 1 - y/H}{\beta - 1 + y/H}\right\}}{\log\left(\dfrac{\beta+1}{\beta-1}\right)} \qquad 1 < \beta < \infty$$

β: clustering parameter

as $\beta \rightarrow 1$ more grid points near y=0

Inverse

$$x = \xi$$

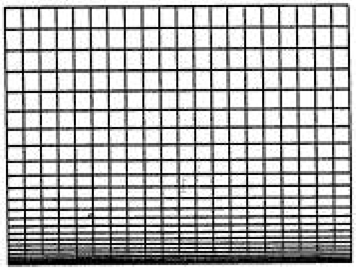
$$y = H\left\{\frac{(\beta+1) - (\beta-1)\left\{\dfrac{\beta+1}{\beta-1}\right\}^{1-\eta}}{\left(\dfrac{\beta+1}{\beta-1}\right)^{1-\eta} + 1}\right\}$$

Metrics

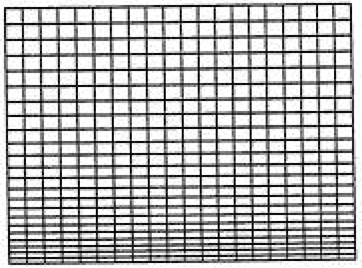
$$\xi_x = 1 \ , \quad \eta_x = 0$$

$$\xi_y = 0 \ , \quad \eta_y = \frac{2\beta}{H\left\{\beta^2 - \left(1 - y/H\right)^2 \left\{\log\left(\dfrac{\beta+1}{\beta-1}\right)\right\}\right\}}$$

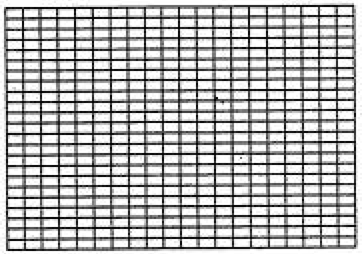
Clustering near bottom



(a) $\beta = 1.05$



(b) $\beta = 1.2$



(c) Computational domain.

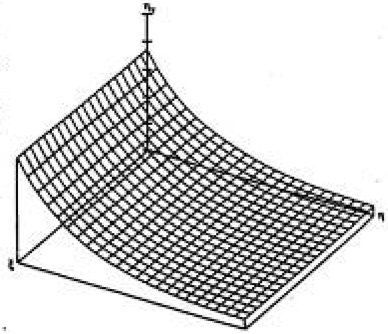
$$\xi = x$$

$$\tilde{\eta} = 1 - \frac{\ln\left\{\frac{\beta+1-y/H}{\beta-1+y/H}\right\}}{\ln\left(\frac{\beta+1}{\beta-1}\right)}$$

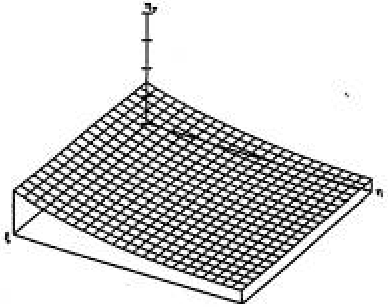
(21 x 24) grid

β : clustering parameter

as $\beta \to 1$, more grid points near $y=0$.



$\beta = 1.05$



$\beta = 1.2$

Grid is suitable for boundary layer type computations where grid clustering near surface is required.

Clustering on both walls

$$\xi = x$$

$$\eta = \alpha + (1-\alpha)\frac{\log\left\{\dfrac{\beta+(2\alpha+1)\dfrac{y}{H}-2\alpha}{\beta-(2\alpha+1)\dfrac{y}{H}+2\alpha}\right\}}{\log\left(\dfrac{\beta+1}{\beta-1}\right)}$$

$\alpha = 0$ clustering at y=H

$\alpha = 1/2$ clustering equally at y=0 , H

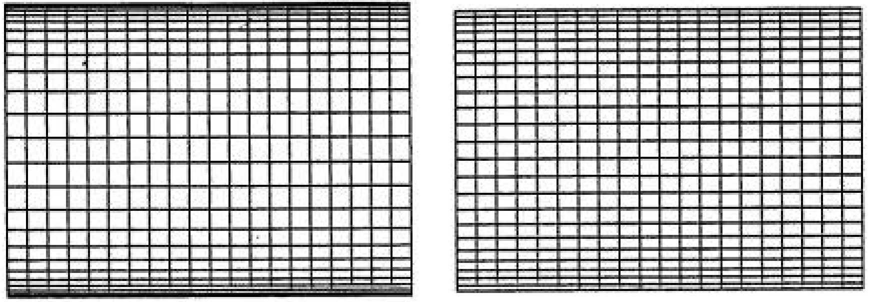
CLUSTERING ON BOTH WALLS

$\alpha = 0$ clustering at $y = H$

$\alpha = \frac{1}{2}$ " equally at $y = 0, H$

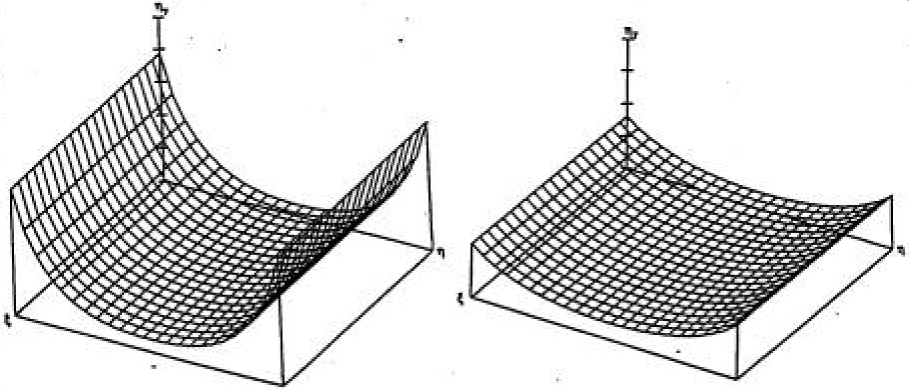
$$\xi = x$$

$$\eta = \alpha + (1-\alpha)\frac{\ln\left\{\dfrac{\beta + (2\alpha+1)\frac{y}{H} - 2\alpha}{\beta - (2\alpha+1)\,y/H + 2\alpha}\right\}}{\ln\left(\dfrac{\beta+1}{\beta-1}\right)}$$



(a) $\beta = 1.05$, $\alpha = 1/2$ (b) $\beta = 1.2$, $\alpha = 1/2$

Physical Grid



Metric distributions for the grids above.

Clustering in Interior

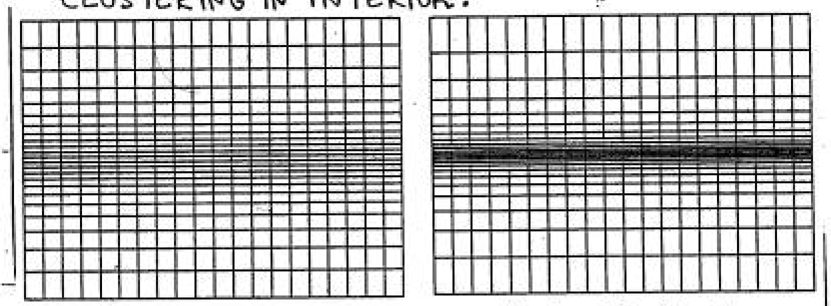
$$\xi = x$$

$$\eta = A + \frac{1}{\beta}\sinh^{-1}\left\{\left(\frac{y}{D} - 1\right)\sinh(\beta A)\right\}$$

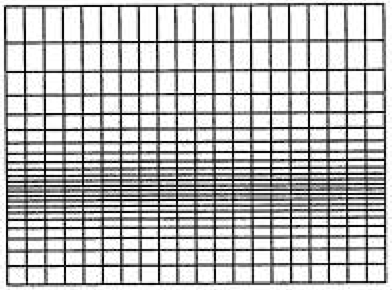
$$A = \frac{1}{2\beta}\log\left\{\frac{1 + \left(e^{\beta} - 1\right)(D/H)}{1 + \left(e^{-\beta} - 1\right)(D/H)}\right\}$$

D is where clustering desired

CLUSTERING IN INTERIOR:



(a) $D = H/2, \quad \beta = 5$ (b) $D = H/2, \quad \beta = 10$



(c) $D = H/4, \quad \beta = 5$

Grids

$$\xi = x$$

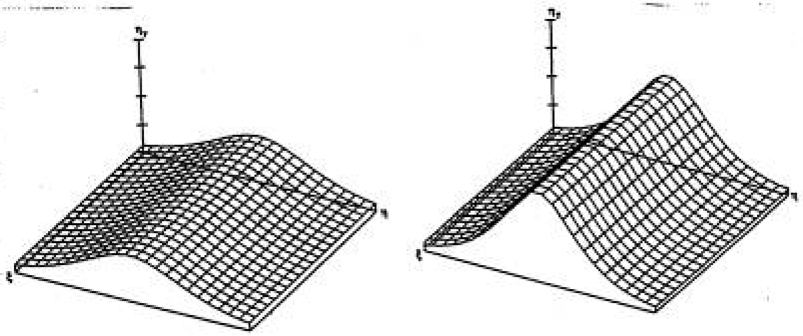
$$\eta = A + \frac{1}{\beta}\sinh^{-1}\left[\left(\frac{y}{D} - 1\right)\sinh(\beta A)\right]$$

$$A = \frac{1}{2\beta}\ln\left[\frac{1 + (e^{\beta} - 1)(D/H)}{1 + (e^{-\beta} - 1)(D/H)}\right]$$

$$0 < \beta < \infty$$

D is where clustering desired

$\beta = 0$: no clustering



(a) (b)

Metrics

Remarks on Algebraic Methods

Advantages:

1. fast computationally
2. metrics can be evaluated analytically, avoiding numerical errors
3. clustering easy

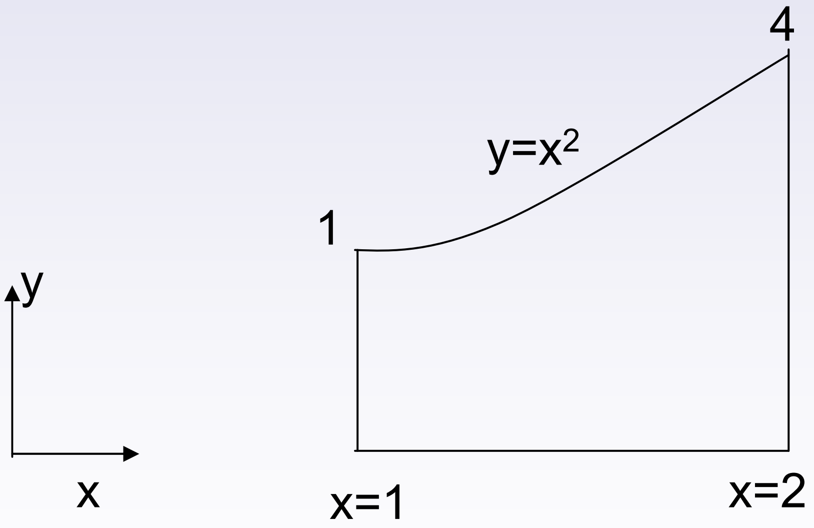
Disadvantages

1. smoothness and skewness hard to control
2. discontinuities at boundary may propogate into interior,
   → errors due to sudden changes in metrics.

Algebraic methods (continued)

Example:

Body fitted mesh is desired to solve for the flow in a divergent nozzle.



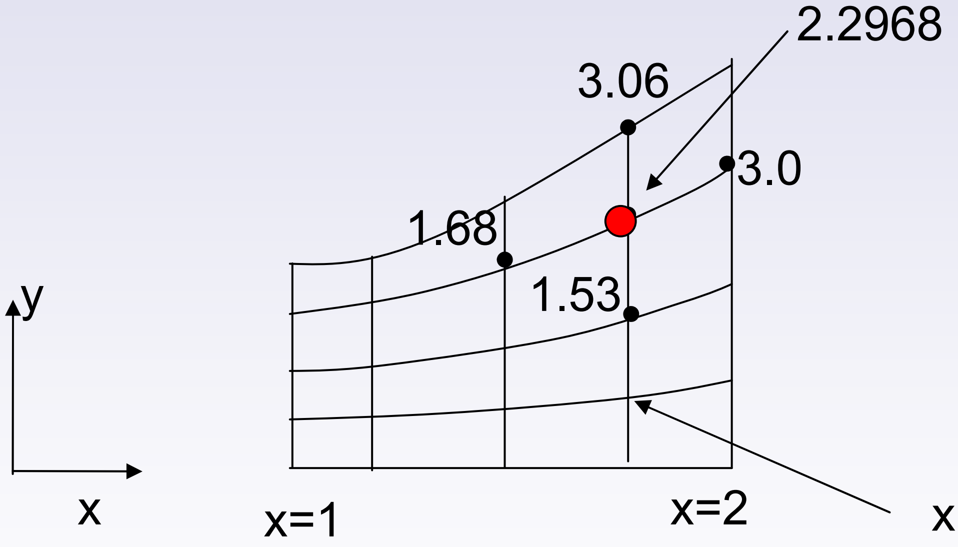
$y=x^2 \quad 1 \leq x \leq 2$

Nozzle geometry

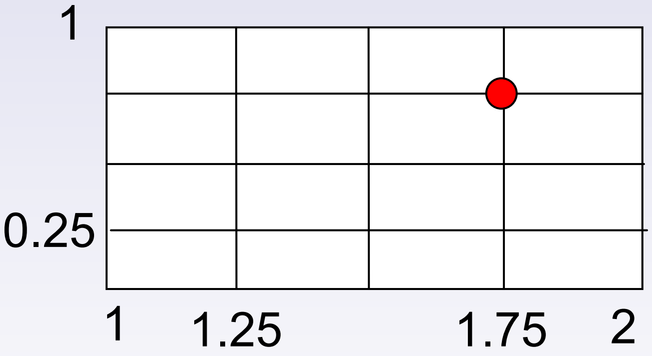
Equally spaced increments in x direction $\xi = x$

Uniform division in the y direction $\eta = \frac{y}{y_{max}} = \frac{y}{x^2}$

Y_{max} : nozzle boundary equation.



$x = \xi$
$y = \eta \xi^2$
physical coordinates



$\Delta\xi = 0.25$, $\Delta\eta = 0.25$

Metrics of transformation $\xi_x = 1$, $\xi_y = 0$

$$\eta_x = -2\frac{y}{x^3} \quad , \quad \eta_y = \frac{1}{x^2} = \frac{1}{\xi^2} \quad = -\frac{2\eta}{\xi}$$

If numerical methods are used to generate required transformation use second-order finite difference

$$\xi_x = \frac{y_\eta}{J} \quad , \quad \xi_y = -\frac{x_\eta}{J} \quad , \quad \eta_x = -\frac{y_\xi}{J} \quad , \quad \eta_y = -\frac{x_\xi}{J}$$

$$J = x_\xi y_\eta - y_\xi x_\eta$$

Example:

Select point (1.75 , 2.2969) = (x,y)

$$\eta_x = -2\frac{\eta}{x^3} = -2\frac{0.75}{1.75} = -0.85714 \quad \text{analytical}$$

Numerical calculation

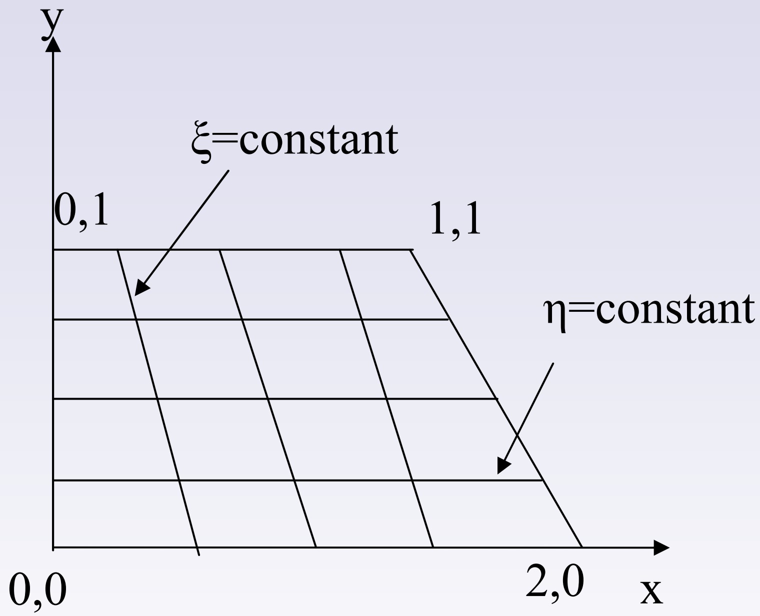
$$\eta_x = -2\frac{y_\xi}{J} \quad , \quad J = \underbrace{x_\xi}_{1} y_\eta \text{ - } y_\xi x_\eta = y_\eta = \frac{y_{a+1} - y_{a\text{-}1}}{2\Delta\eta}$$

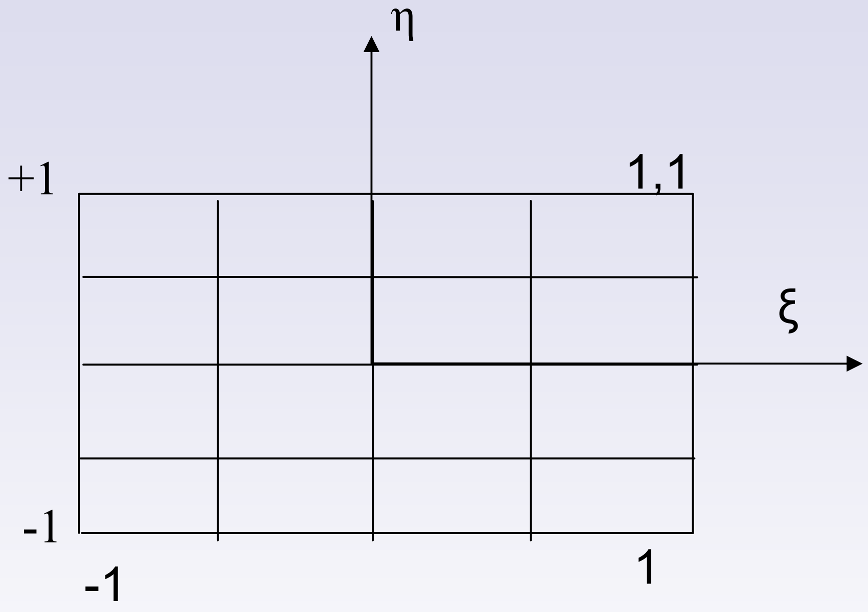
$$y_\eta = \frac{3.0625 - 1.53125}{2(0.25)} = 3.06250$$

$$y_\xi = \frac{3 - 1.6875}{2(0.25)} = 2.625 \rightarrow \eta_x = -0.85714$$

not always the same for many problems

NORMALIZING TRANSFORMATION





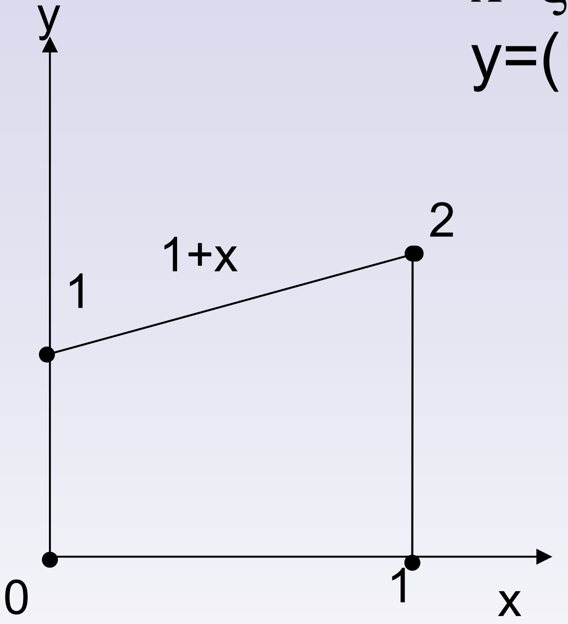
$$x = \left(\frac{1+\xi}{2}\right)\left(\frac{3-\eta}{2}\right) \qquad (\xi,\eta) = (1,1) \Rightarrow (x,y) = (1,1)$$

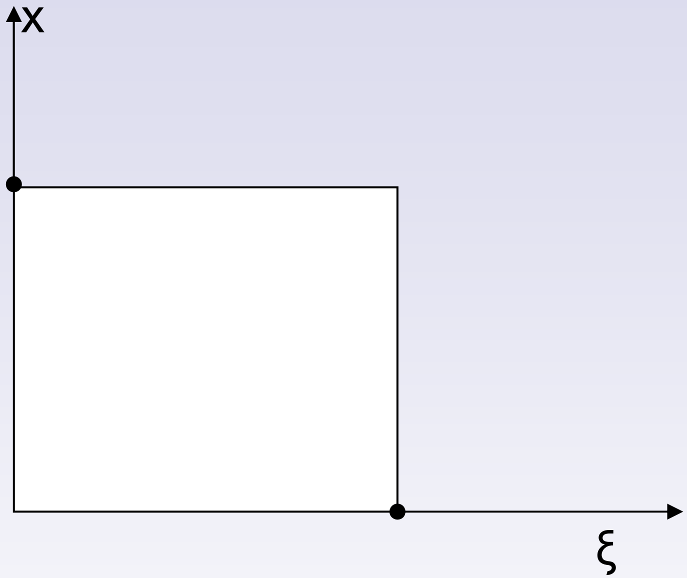
$$y = \frac{\eta+1}{2} \qquad (\xi,\eta) = (-1,1) \Rightarrow (x,y) = (0,1)$$

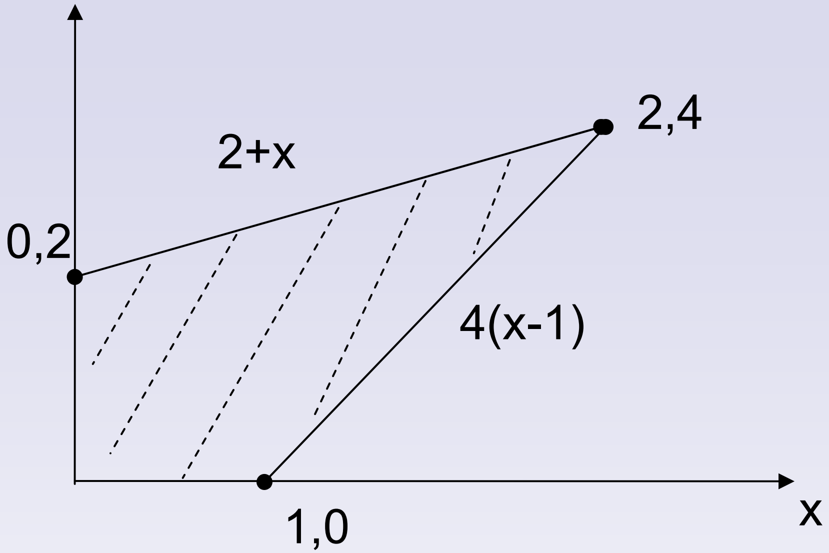
Any quadrilateral physical domain can be transformed into a rectangle in computational space by use of a normalizing transformation.

$x = \xi$

$y = (1 + \xi)\,\eta$







$$x = a\xi + b\eta + c\eta\xi \qquad x = \xi(1+\eta)$$

$$y = d\xi + e\eta + f\eta\xi \qquad y = 2\eta\left(1+\xi\right)$$

Example:

$$\left.\begin{aligned} x_1 &= \xi^2 \\ x_2 &= \xi^2 \end{aligned}\right\} \Rightarrow \begin{aligned} x &= \xi^2 \\ y &= \left(1+\xi^2\right)\eta \end{aligned}$$

Most problems, boundaries are not analytic functions but are simply prescribed as a set of data points.
Boundaries must be approximated by a curve fitting procedure to employ algebraic mappings.
Tension splines, avoids wiggless in boundary

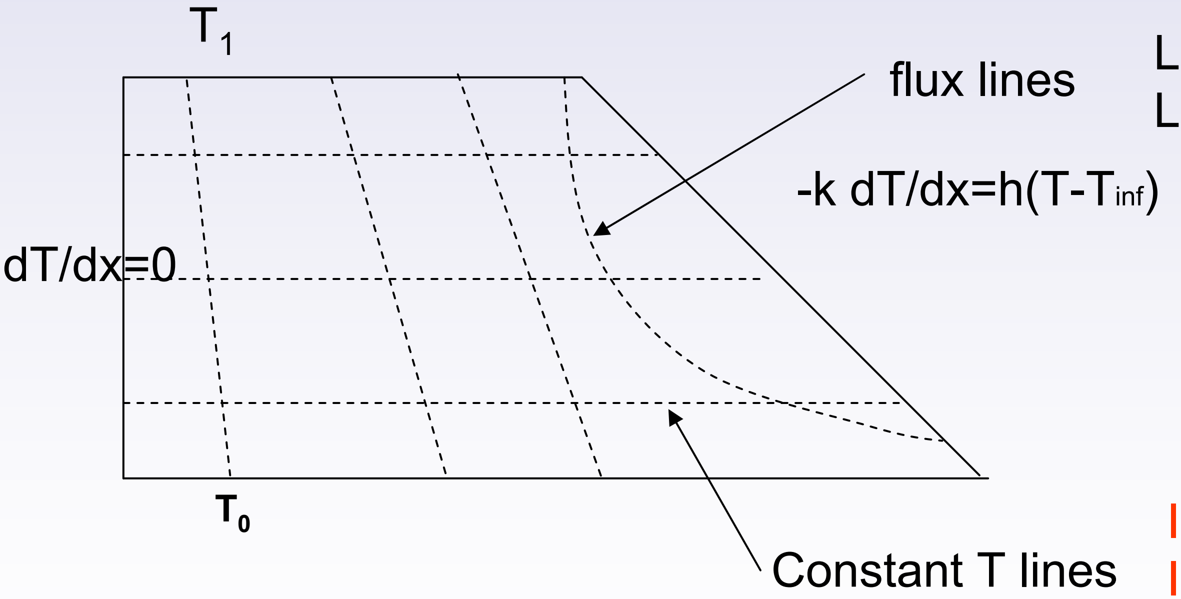
Algebraic mappings summary

- direct
- analytical evaluation of metrics
- can be applied to 3D problems straightforward way
- some ingenuity is required for a proper grid

Elliptic Grid Generators

For situations where all physical boundaries specified
Smoother grid

Example:
Heat conduction in a solid



Looks like a good grid
Let ξ, η satisfy Laplace’s equation.

$$\xi_{xx} + \xi_{yy} = 0$$

$$\eta_{xx} + \eta_{yy} = 0 \qquad (9)$$

Iterative scheme is used to solve
Isothermal lines, grid lines

(ξ,η) coordinates in computational space
(x,y) coordinates in phsical space

To transform equations (9) dependent and independent variables are interchanged see Appendix E

$$ax_{\xi\xi} - 2bx_{\xi\eta} + cx_{\eta\eta} = 0 \qquad (10)$$

$$ay_{\xi\xi} - 2by_{\xi\eta} + cy_{\eta\eta} = 0 \qquad (11)$$

$$a = x_{\eta}^{2} + y_{\eta}^{2}$$

$$b = x_{\xi}x_{\eta} + y_{\xi}y_{\eta}$$

$$c = x_{\xi}^{2} + y_{\xi}^{2} \qquad (12)$$

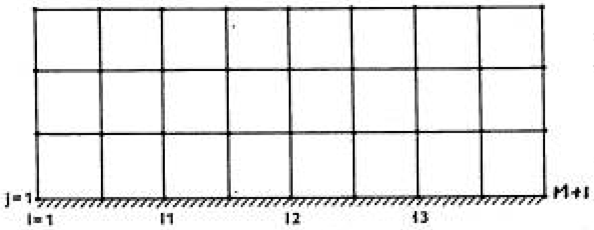
System of equations (10)-(11) is solved in computational domain (ξ,η) to provide grid point locations in physical space (x,y)

Eqs. (10) – (12) is a set of coupled non-linear elliptic equations

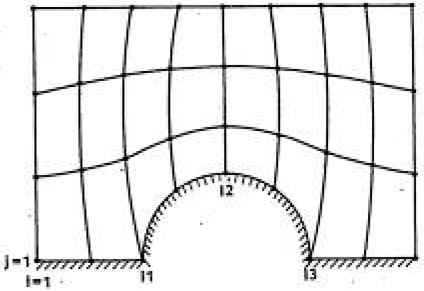
⇨ Solve numerically ,

⇨ linearization procedure is necessary

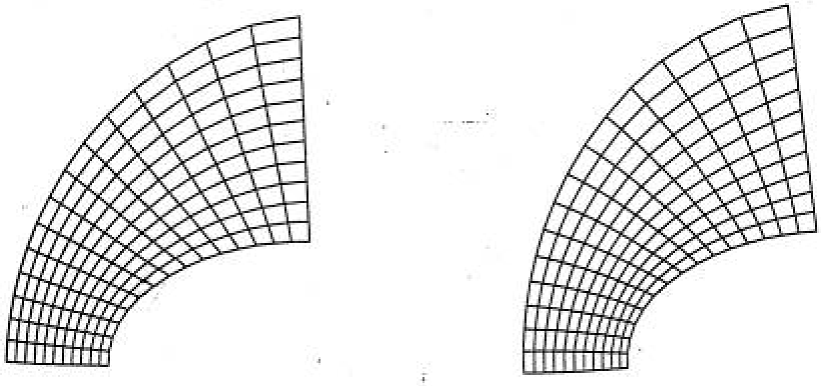
a,b,c are evaluated at the previous iteration level.



Computational Plane



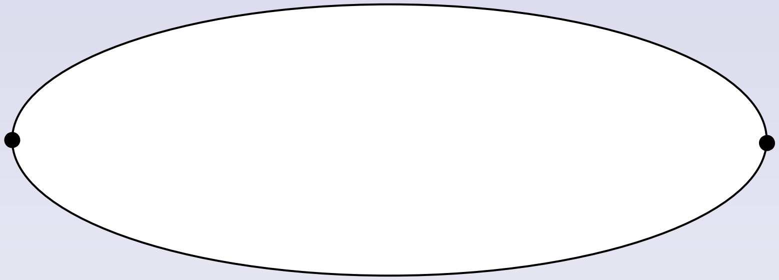
10 Physical Plane



11 Starting algebraic grid

Grid from elliptic solver

Simply-Connected Domain:



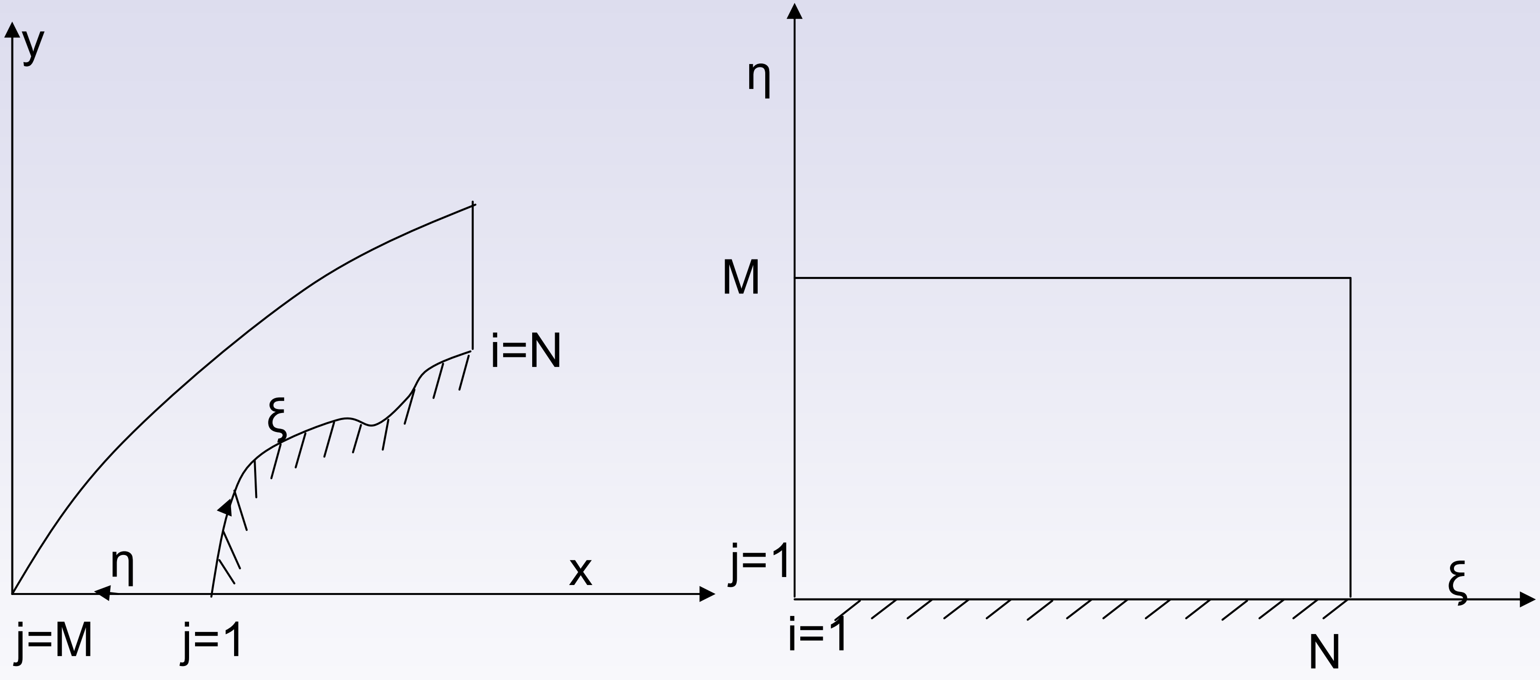
Any contour connecting 2 points can be deformed without passing out of region. Domain which is reducible & can be contracted to a point,

i.e, no object within the domain

Procedure:

1. start with test grid generated by same algebraic method
   this defines at every point in computational and physical space an estimate of $x(\xi,\eta)$, $y(\xi,\eta)$
2. discretize (10)-(11) linearize by calculating a,b,c, and hold constant.

Simply-Connected Domain: Example



Example:

$$a=\left\{\frac{x_{i,j+1}-x_{i,j-1}}{2\Delta\eta}\right\}^2+\left\{\frac{y_{i,j+1}-y_{i,j-1}}{2\Delta\eta}\right\}^2$$

discretization of (10)

$$\text{a}\left\{\frac{x_{i+1,j}-2x_{i,j}+x_{i-1,j}}{(\Delta\xi)^2}\right\}-2b\left\{\frac{x_{i+1,j+1}-x_{i+1,j-1}-x_{i-1,j-1}+x_{i-1,j+1}}{4\Delta\eta\Delta\xi}\right\}+c\left\{\frac{x_{i,j+1}-2x_{i,j}+x_{i,j-1}}{(\Delta\eta)^2}\right\}=0 \quad (13)$$

Can write similar equation for y (replace x by y)

Iterate Gauss-Seidel and update a,b,c from time to time
Note grid on boundaries of physical plane must be specified

If Gauss-Seidel iterative scheme is used, equation (13) is arranged as

$$2\left[\frac{a}{(\Delta\xi)^2}+\frac{c}{(\Delta\eta)^2}\right]x_{i,j}=\frac{a}{(\Delta\xi)^2}\left[x_{i+1,j}+x_{i-1,j}\right]+\frac{c}{(\Delta\eta)^2}\left[x_{i,j+1}+x_{i,j-1}\right]$$

$$-\frac{b}{2\Delta\xi\Delta\eta}\left[x_{i+1,j+1}-x_{i+1,j-1}-x_{i-1,j-1}+x_{i-1,j+1}\right]$$

$$2\left[\frac{a}{(\Delta\xi)^2}+\frac{c}{(\Delta\eta)^2}\right]x_{i,j}=\frac{a}{(\Delta\xi)^2}\left[x_{i+1,j}+x_{i-1,j}\right]+\frac{c}{(\Delta\eta)^2}\left[x_{i,j+1}+x_{i,j-1}\right]$$

$$-\frac{b}{2\Delta\xi\Delta\eta}\left[x_{i+1,j+1}-x_{i+1,j-1}-x_{i-1,j-1}+x_{i-1,j+1}\right]$$

For $y_{i,j}$

$$2\left[\frac{a}{(\Delta\xi)^2}+\frac{c}{(\Delta\eta)^2}\right]y_{i,j}=\frac{a}{(\Delta\xi)^2}\left[y_{i+1,j}+y_{i-1,j}\right]+\frac{c}{(\Delta\eta)^2}\left[y_{i,j+1}+y_{i,j-1}\right]$$

$$-\frac{b}{2\Delta\xi\Delta\eta}\left[y_{i+1,j+1}-y_{i+1,j-1}-y_{i-1,j-1}+y_{i-1,j+1}\right]$$

İterate until convergence,

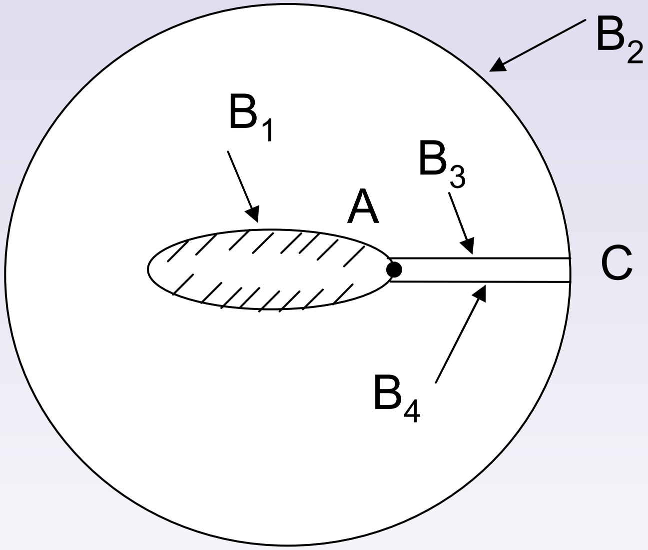
Example:

$$E_x=\sum_{\substack{i=2\\j=2}}^{N,M}\left|x_{i,j}^{k+1}-x_{i,j}^{k}\right| \quad , \; E_y=\ldots$$

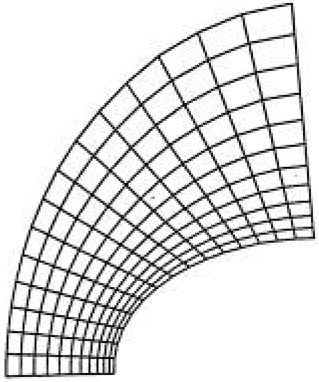
$$E_T=E_x+E_y<\varepsilon$$

Double-Connected Domain:

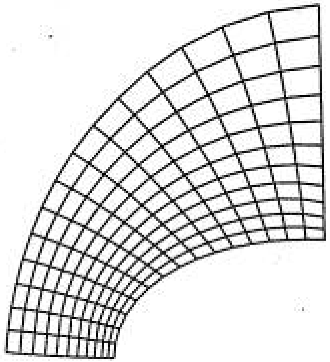
Domain is not reducible. i.e. domain includes one configuration within region of interest



Can be rendered simply-connected by introducing a suitable branch cut



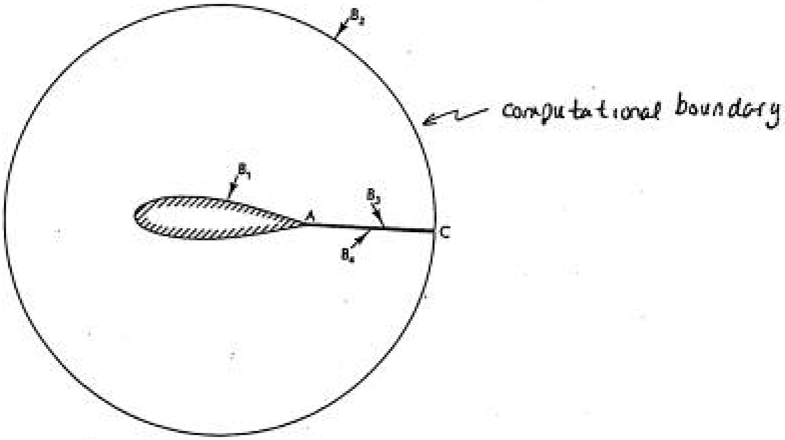
Algebraic



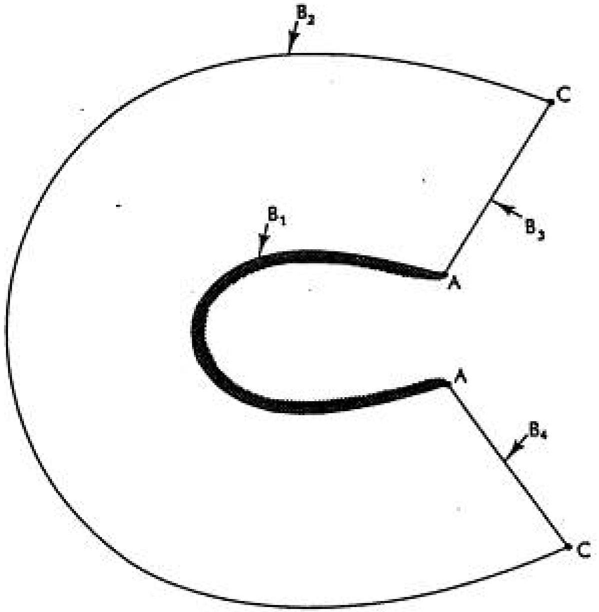
Elliptic

eg. Clustering near lower boundary

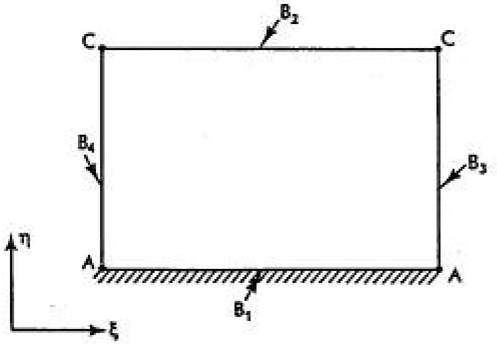
ubly Connected Domains



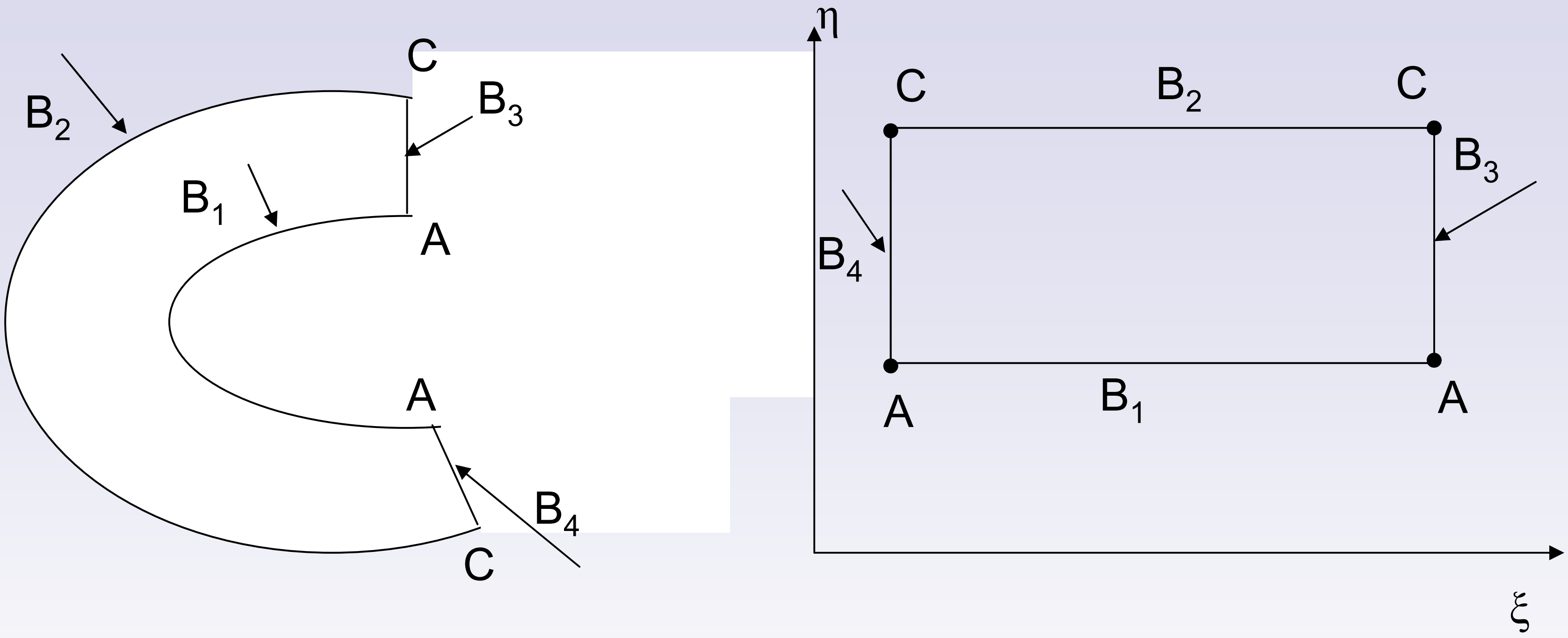
Physical plane



Unwrapping of Doubly Connected Region (C grids)



Unwrap the domain



Computational domain (uniform grid)
i.e. location of every grid point (ξ,η) is known.

Employ Elliptic Grid Generation to determine grid points in physical space. Equations (10) & (11) need to be solved.

➡ Similar procedure Gauss-Seidel

Difference, ➡ treatment of grid points on B_3&B_4 , i.e. on the branch cut.

Location of grids along line AC must be updated. Compute new values of $x_{1,j}$ and $y_{1,j}$ after each iteration.

Note: It is not necessary to compute $x_{N,j}$ and $y_{N,j}$ since grid lines i=1 & i=N are coincident.

$x_{N,j} = x_{1,j}$ and $y_{N,j} = y_{1,j}$

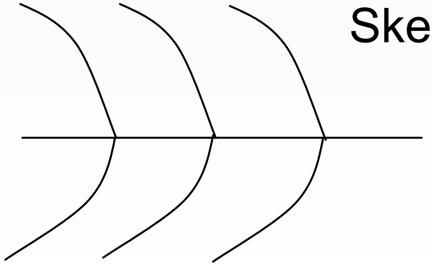
Gauss-Seidel Formulation

$$x_{1,j} = \frac{\left\{ \frac{a}{(\Delta\xi)^2}\left[x_{2,j} + x_{N-1,j}\right] + \frac{c}{(\Delta\eta)^2}\left[x_{1,j+1} + x_{1,j-1}\right] - \frac{b}{2\Delta\xi\Delta\eta}\left[x_{2,j+1} - x_{2,j-1} - x_{N-1,j-1} + x_{N-1,j+1}\right] \right\}}{2\left[\frac{a}{(\Delta\xi)^2} + \frac{c}{(\Delta\eta)^2}\right]} \quad (14)$$

similarly,

$$y_{1,j} = \frac{\{\ \}}{..}.. \quad (15)$$

Use equation (14) & (15) after each iteration to find new location of grid points on the branch cut.



Skewness in grid

If grid points on branch cut are kept fixed, highly skewed grids at branch cut are obtained!!

Example: airfoil,

$$y = \frac{t}{0.2}\left(0.2969x^{1/2} - 0.126x - 0.3516x^2 + ... + x^4\right)$$

max thickness of chord

$$\Delta\text{x}=\frac{\text{c}}{\frac{(\text{N}+1)}{2}-1}$$

N:odd, symmetry of grid points

Circle

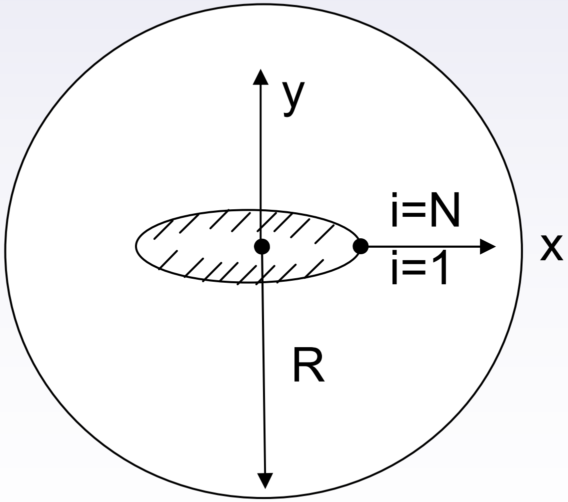
$$\Delta\delta=\frac{2\pi}{\text{N-1}}$$

$$\delta(i)=i*\Delta\delta$$

$$x(i,M)=R*\cos(\delta(i))$$

$$y(i,M)=-R*\sin(\delta(i))$$

Doubly-connected region



GRID CONTROL:

1. clustering in different regions

$$\xi_{xx} + \xi_{yy} = P(\xi,\eta)$$

$$\eta_{xx} + \eta_{yy} = Q(\xi,\eta)$$

P,Q: sources of sinks

Can show

$$ax_{\xi\xi} - 2bx_{\xi\eta} + cx_{\eta\eta} = -\frac{1}{J^2}\left\{\mathrm{P}x_{\xi} + Qx_{\eta}\right\}$$

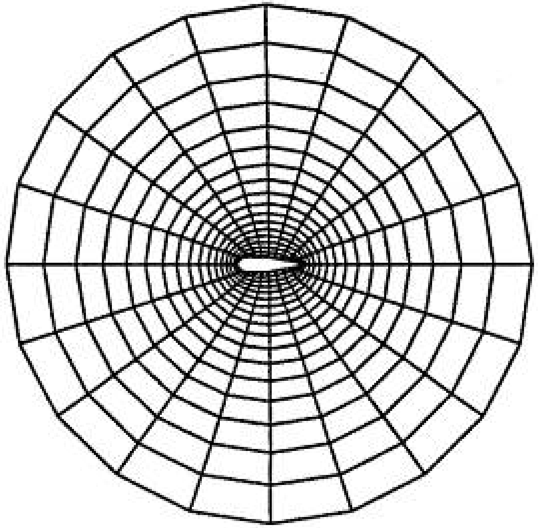
$$ay_{\xi\xi} - 2by_{\xi\eta} + cy_{\eta\eta} = -\frac{1}{J^2}\left\{\mathrm{Py}_{\xi} + Qy_{\eta}\right\}$$

P,Q complicated functions

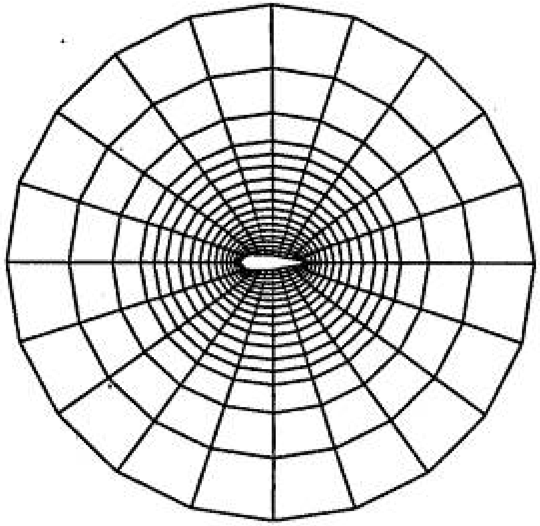
Thonson, JF., Warsi, Z.U.A, & Mastin, C.W.
Numerical Grid Generation
North Holland, 1985

SOFTWARES Gridgen, Eagle, Gambit, ...

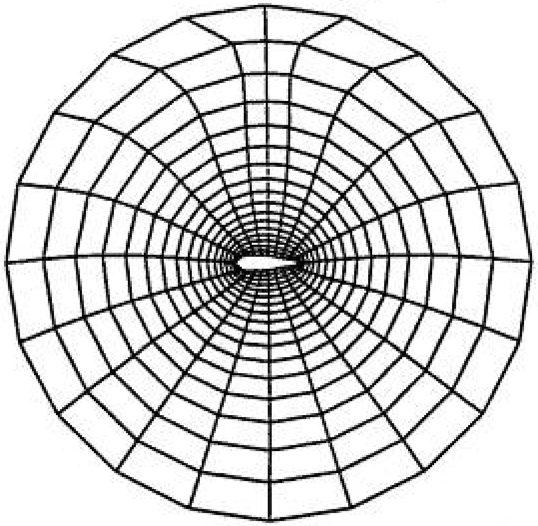
2. orthogonally at surface
   Steger, J.L & Sorenson, R.L.



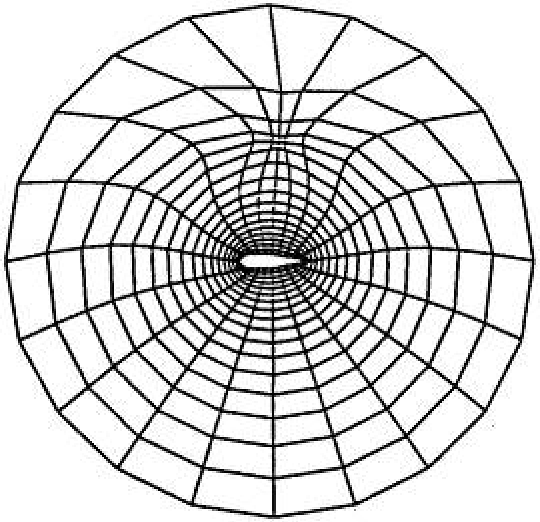
a. $P = 0, Q = 0$



b. Clustering at $j = 14$



c. Clustering at $i = 16$



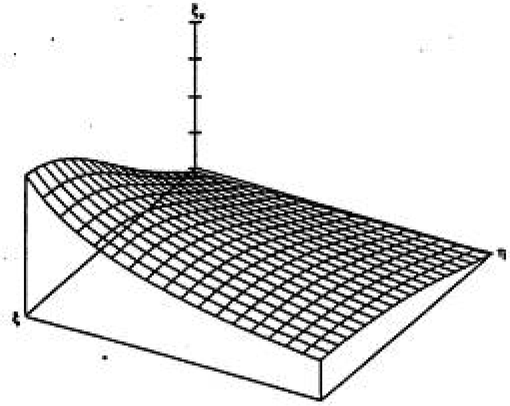
d. Clustering at $i = 16$, $j = 14$

PDE Techniques (summary)

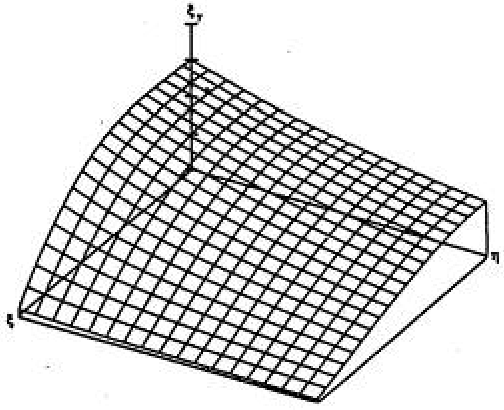
- PDEs are used to create the grid system
- A system of PDEs is solved for the location of the grid points in physical domain
- Computational domain is a rectangular shape with uniform grid spacing

PDE Methods

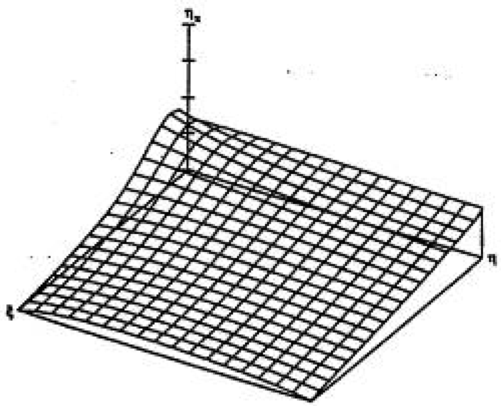
1. elliptic
2. parabolic
3. hyperbolic



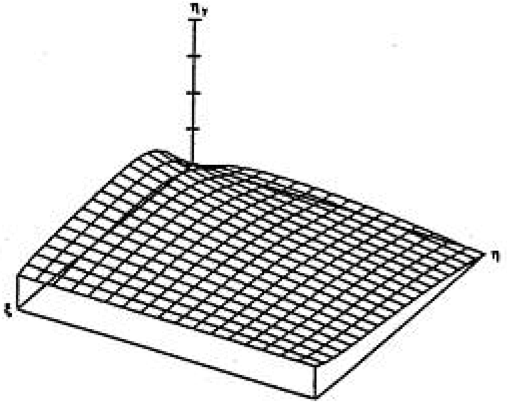
(a)



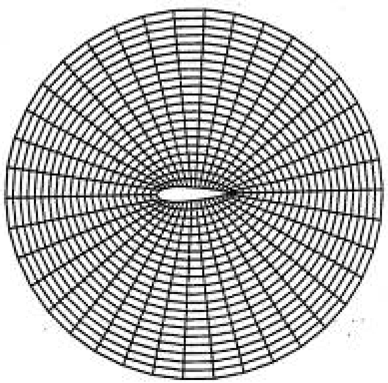
(b)



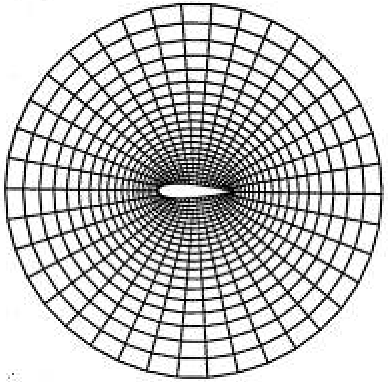
(c)



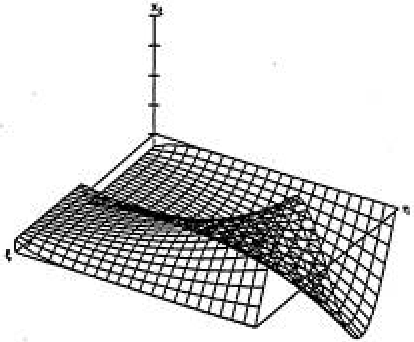
(d)

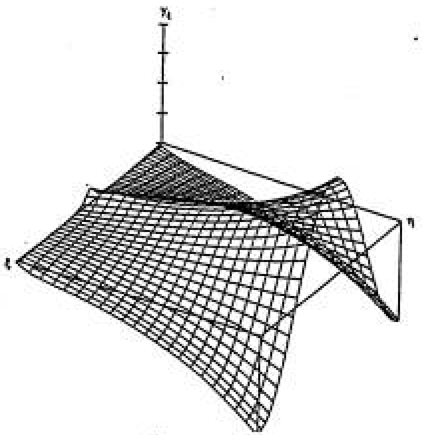


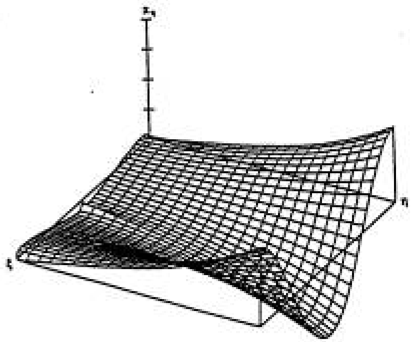
Algebraic mesh

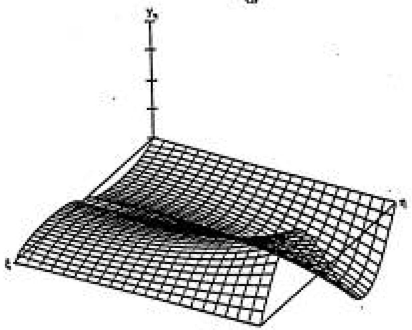


Elliptic mesh

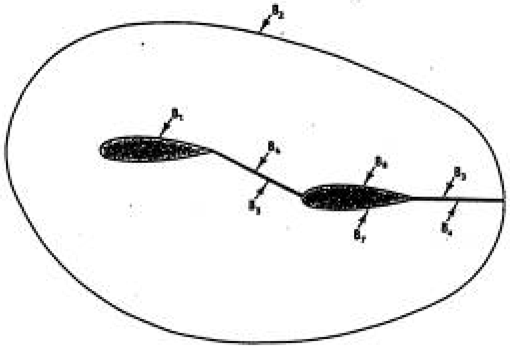


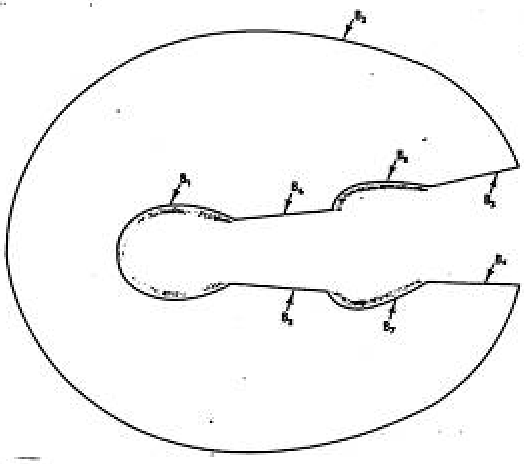


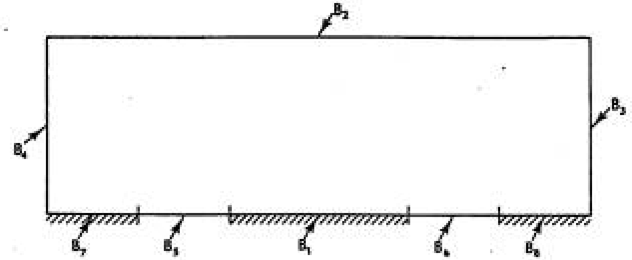


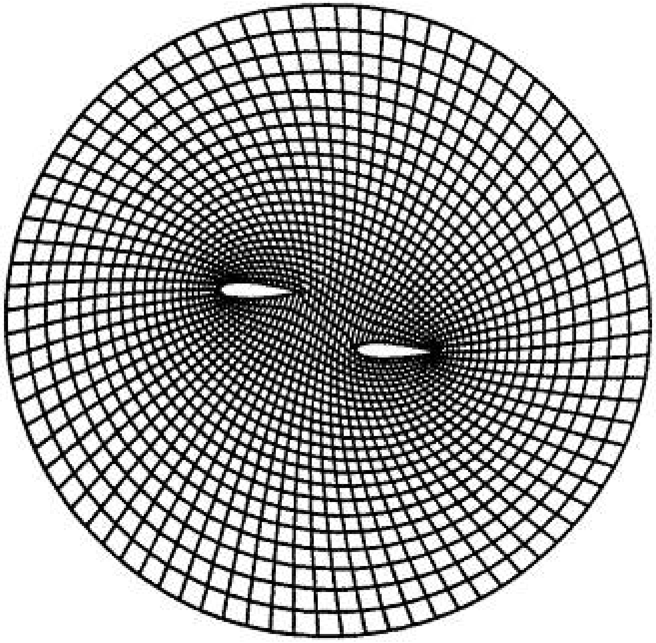


Multiply - Connected Regions

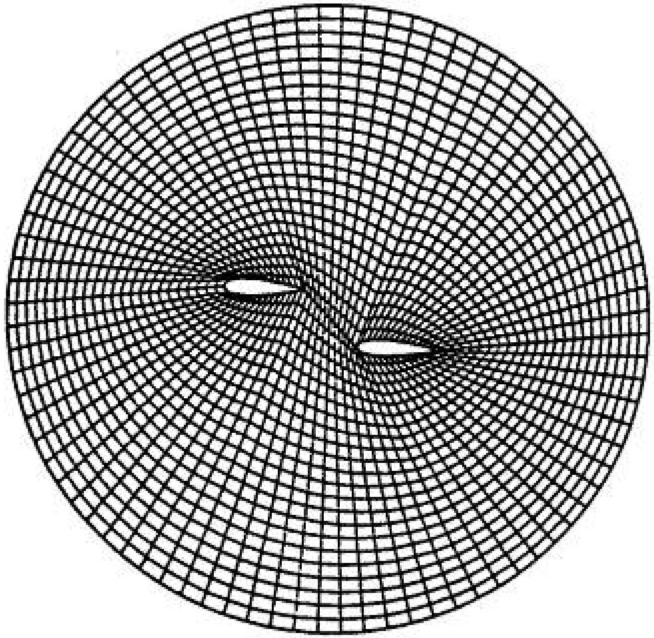




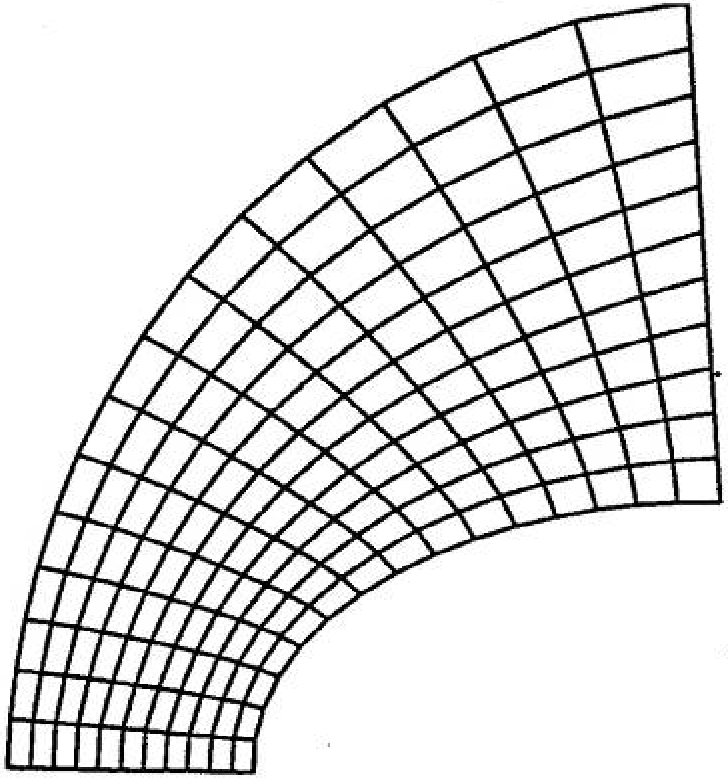




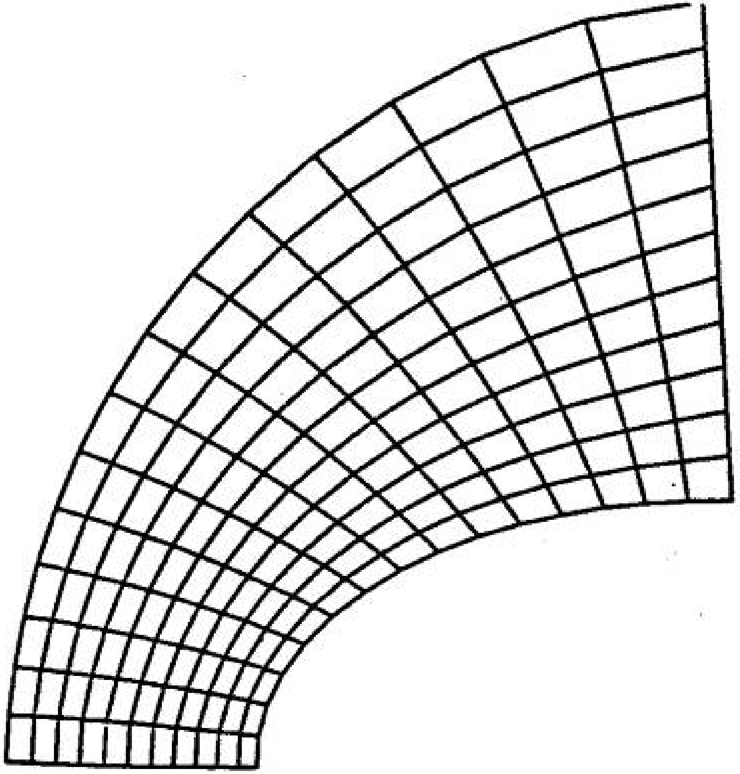
Elliptic
(smooth distribution of grid points
& original branch cuts reshaped)



Algebraic (straight rays, equal spacing



Orthogonal grid
at Surface



No orthogonality condition