UNITED STATES
NUCLEAR REGULATORY COMMISSION
WASHINGTON, D.C. 20555

FEB 27 1990

MEMO FOR: Ronald L. Ballard, Chief
Geoscience & System Performance Branch, HLWM

FROM: Philip S. Justus, Section Leader
Geology-Geophysics Section
Geosciences & Systems Performance Branch, HLWM

SUBJECT: TRIP REPORT FOR TRAINING COURSE. GROUNDWATER CONTAMINANT TRANSPORT MODELLING, PRINCETON UNIVERSITY, JANUARY 29-31, 1990

Purpose: Training in groundwater flow and transport computer modelling to improve my understanding of finite difference and finite element methods and to enhance my effectiveness as a supervisor of geoscientists who are computer modellers

Course Title: Groundwater Contaminant Transport Modelling

Date/Place: 29-31 January 1990, Dept of Civil Engineering, Princeton University, Princeton, New Jersey

Agenda: See Enclosure 1

Attendees: See Enclosure 2

Instructors: 1). Prof. George Pinder, Dean, College of Engineering, University of Vermont;
2). Prof. Michael Celia, Assistant Professor of Civil Engineering, Princeton;
3). Prof. David Ahlfeld, Assistant Professor, Environmental Research Institute, University of Connecticut.

Course Objectives: 1) provide background in geology, groundwater hydrology and numerical methods necessary to use and understand groundwater transport models, 2) provide participants with a computer code capable of simulating both flow and transport in 3-dimensions, and hands-on experience in its application. These objectives were fulfilled in the three days and nights of classroom discussion and computer lab instruction.

Course Format: about half day discussion of geologic concepts needed to understand formation and structure of groundwater reservoirs, concepts of groundwater flow and contaminant

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transport; about one and a half days discussion of numerical techniques for the solution of differential equations and their utilization in groundwater models, numerical distinctions among finite difference, finite element and alternating direction implicit methods. About a day and a night session on flow and transport modelling, including hands-on use of 1-D and 3-D codes, both with graphic displays of the solutions which allowed instant comparisons of methods and sensitivity studies.

Discussion: The course fulfilled my expectations and provided me with several management tools. It increased my self-confidence in handling and interpreting 3-D flow and transport graphic solutions from computer codes. It provided me with a refresher in differential equations and their use in flow and transport modelling. In particular, the following topics and relationships were discussed at length (see Enclosure 3 excerpted from Handout 1)

Modelling concepts
- Equation formulation (groundwater flow eq)
- Parameter estimation (e.g., permeability)
- Boundary conditions (e.g., constant head specified)
- Initial conditions (e.g., head specified everywhere)
- Hydrodynamic forces (precipitation)
- Equation approximation (e.g., finite elements)
- Equation solution (e.g., gaussian elimination)

Numerical Inputs
- mesh size and geometry
- parameter values (at node or in element)
- time discretization
- simulation time period
- initial potential at each node
- initial concentration(s) at each node
- specified concentration(s) at constant concentration nodes
- specified flux at constant mass flux nodes
- specified potential at constant potential nodes
- specified fluid flux at constant fluid flux nodes
- specified infiltration at constant infiltration nodes (or elements)
- specified discharge at wells
- leakage parameters of fluxes

Basic Idea of Numerical Methods
- solve for an approximate solution

solve for only a finite number of discrete values
solve algebraic equations instead of differential equations

Finite Difference Method
- discrete approximations
- Taylor series, truncation error
- list of standard approximations
- time and space dependence
- stability and convergence

Finite Element Method
- trial function, basis functions
- method of weighted residuals
- finite element method
- time and space dependence
- 2-D elements, non-rectangular elements
- practical considerations

Alternating Direction Methods
- Alternating-direction implicit method

Groundwater Transport Modelling
- Finite difference method (FDM)
- finite element method (FEM)
- wiggles and artificial diffusion
- upstream weighting for FDM, FEM

Princeton Transport Code
- 3-D, FEM, FDM code

Handouts: The following handouts are available in my office for use by any interested person:

1) Groundwater Contaminant Transport Modelling Short Course Lecture Notes, Pinder, Celia, Ahlfeld, Jan 90
2) Chemical Transport by Three Dimensional Groundwater Flows (Manual describing theory and use of the Princeton Transport Code, PTC), Babu and others, Jan 90
3) FEPER (Finite Element Perspective Program) User Documentation, Environ Cor, Jan 90
4) PRECEPT 1: The One-Dimensional Transport Equation, Allen and Dougherty, Jan 90
5) PTC Lab Session and 'Editing Data Files', 1988
6) Computer Methods in Subsurface Flow, Huyakorn and Pinder, Academic Press, 1983
7) Two 3-1/2" Diskettes: PTC-Source, PTC-Graphics (these were distributed for the sole use of each course

participant; a ruling on the legality of my retaining them as an individual is currently under review by OGC)

Benefits: This three day-intensive training improved my skill, confidence and knowledge in computer modeling of groundwater flow and contaminant transport through discussion of theory, numerical methods and hands-on computer lab instruction. Given my improved understanding of the governing equations (including assumptions), the necessary approximations (simplifications) and the limitations of the methods (uncertainties of output due to uncertainties of input and the models themselves), I can enhance the effectiveness of my supervision of geoscientists who model and my management of geoscience licensing issues resolution that involves computer simulations.

Recommendations: I strongly recommend that the course be taken by NRC staff and contractor flow and transport modelers and their supervisors and branch chiefs. It is relevant to our ongoing groundwater flow and radionuclide transport modeling efforts. The superior expertise of the instructors and the focused, well-organized presentation and discussions assure that the time will not be wasted for anyone willing to take the three days to learn and participate.

Philip S. Justus, Section Leader
Geology-Geophysics Section
Geosciences & Systems Performance Branch, HLWM

Enclosures:
As stated

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transport; about one and a half days discussion of numerical techniques for the solution of differential equations and their utilization in groundwater models, numerical distinctions among finite difference, finite element and alternating direction implicit methods. About a day and a night session on flow and transport modelling, including hands-on use of 1-D and 3-D codes, both with graphic displays of the solutions which allowed instant comparisons of methods and sensitivity studies.

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/S/

Philip S. Justus, Section Leader
Geology-Geophysics Section
Geosciences & Systems Performance Branch, HLWM

Enclosures:
As stated

DISTRIBUTION:

Central Files	HLGP r/f	NMSS r/f
RBrowning, HLWM	BJYoungblood, HLWM	JBunting, HLEN
RBallard, HLGP	JLinehan, HLPD	DChery, HLGP
PJustus, HLGP	SCoplan, HLGP	MSilberberg, RES
DBrooks, HLGP	NEisenberg, HLGP	RCodell, HLGP
TMcCartin, RES	JRandall, RES	WFord, HLGP

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ENCLOSURE 1

REVISED COURSE SCHEDULE

GROUNDWATER CONTAMINANT TRANSPORT MODELLING
PRINCETON UNIVERSITY

January 29,30,31, 1990

Monday, January 29

8:30-9:00	**REGISTRATION**
9:00-10:00	**GEOLOGICAL ATTRIBUTES OF GROUNDWATER SYSTEMS** G.F. Pinder
10:00-10:30	Coffee and discussion
10:30-12:00	**BASIC CONCEPTS OF GROUNDWATER FLOW** G.F. Pinder
12:00-1:30	Lunch
1:30-3:00	**BASIC CONCEPTS OF GROUNDWATER TRANSPORT** G.F. Pinder
3:00-3:30	Coffee and discussion
3:30-5:00	**INTRODUCTION TO NUMERICAL METHODS (1)** M.A. Celia
5:00-7:00	Dinner
7:00-8:30	**FIELD CASES** G.F. Pinder

Tuesday, January 30

9:00-10:30	**INTRODUCTION TO NUMERICAL METHODS (2)** M.A. Celia
10:30-11:00	Coffee and discussion
11:00-12:30	**INTRODUCTION TO GROUNDWATER TRANSPORT MODELLING** M.A. Celia
12:30-2:00	Lunch
2:00-3:30	**ONE-DIMENSIONAL TRANSPORT SOLUTIONS** Computer Lab
3:30-4:00	Coffee and discussion
4:00-5:30	**INTRODUCTION TO THE PRINCETON TRANSPORT CODE (PTC)** D.P. Ahlfeld
5:30-7:00	Wine and cheese party

Wednesday, January 31

9:00-10:30	**DATA INPUT TO THE PTC** D.P. Ahlfeld
10:30-11:00	Coffee and discussion
11:00-12:30	**RUNNING THE PTC (1)** Computer Lab
12:30-2:00	Lunch
2:00-5:30	**RUNNING THE PTC (2)** Computer Lab
5:30-7:00	Dinner
7:00-8:30	**RUNNING THE PTC (3)** Optional Computer Lab

ENCLOSURE 2

Groundwater Contaminant Transport Modeling Short Course 1990
List of Participants

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Michael A. Celia
Water Resources Program
Princeton University
Princeton, NJ 08544

David P. Ahlfeld
Environmental Research Institute
University of Connecticut
Storrs, CT

EQUATION FORMULATION

- BALANCE LAWS
  - FLUID CONSERVATION
  - SPECIES CONSERVATION
- CONSTITUTIVE RELATIONSHIPS
  - DARCY'S LAW
  - FICK'S LAW
- THERMODYNAMIC RELATIONSHIPS
  - EQUATION OF STATE

FLUID FLOW

BALANCE EQN

rate of change — porosity mass or density — net outward flux

$$\frac{\partial (n\rho)}{\partial t} + \underset{\sim}{\nabla}\cdot(n\rho \underset{\sim}{V}_f) = 0 \qquad \rho \equiv \rho_f \equiv \text{FLUID DENSITY}$$

CONSTITUTIVE RELATIONSHIP

DARCY'S LAW (most general form)

$$n\underset{\sim}{V}_f = -\frac{\underset{\approx}{k}}{\mu}(\underset{\sim}{\nabla} p + \rho g \underset{\sim}{\nabla} z) \qquad p \equiv p_f \equiv \text{FLUID PRESSURE}$$

$\underset{\approx}{k} \equiv$ INTRINSIC PERMEABILITY

$\mu \equiv$ FLUID VISCOSITY

WHEN $\rho = \rho(p)$

$$n\underset{\sim}{V}_f = -\underset{\approx}{K}\cdot\underset{\sim}{\nabla} h \qquad \underset{\approx}{K} \equiv \frac{\underset{\approx}{k}\rho g}{\mu} \equiv \text{HYDRAULIC CONDUCTIVITY}$$

used interchangeably w/ permeability (k but isn't – note k is w/in $\underset{\approx}{K}$)

$$\begin{bmatrix} nV_{fx} \\ nV_{fy} \\ nV_{fz} \end{bmatrix} = -\begin{bmatrix} K_{xx} & K_{xy} & K_{xz} \\ K_{yx} & K_{yy} & K_{yz} \\ K_{zx} & K_{zy} & K_{zz} \end{bmatrix} \begin{bmatrix} \frac{\partial h}{\partial x} \\ \frac{\partial h}{\partial y} \\ \frac{\partial h}{\partial z} \end{bmatrix}$$

$$nV_{fx} = -K_{xx}\frac{\partial h}{\partial x} - K_{xy}\frac{\partial h}{\partial y} - K_{xz}\frac{\partial h}{\partial z}$$

velocity in X dir.

counterintuitive to have velocity in X f(head in y....)

multiphase flow – non-linear

scalar 0 dim
vector 1 dim
tensor 2-3D (perm is also tensor)

FLUID FLOW

THERMODYNAMIC RELATIONSHIPS

get rid of a variable

$\rho = \rho(p, c)$ $\quad$ $C \equiv$ CONCENTRATION

change in vol as result of change in pressure

$$\frac{\partial(n\rho)}{\partial t} = \frac{d(n\rho)}{dp} \times \frac{\partial p}{\partial t} \equiv S_p \frac{\partial p}{\partial t} \qquad S_p \equiv \text{SPECIFIC STORAGE (PRES.)}$$

$$\frac{\partial(n\rho)}{\partial t} = \frac{d(n\rho)}{dh} \frac{\partial h}{\partial t} \equiv S_h \frac{\partial h}{\partial t} \qquad S_h \equiv \text{SPECIFIC STORAGE (HEAD)}$$

GOVERNING EQUATIONS

only variable not determined in field

$$\boxed{S_p \frac{\partial p}{\partial t} - \underset{\sim}{\nabla} \cdot \frac{\rho \underset{\approx}{k}}{\mu} \cdot (\underset{\sim}{\nabla} p + \rho g \underset{\sim}{\nabla} z) = 0}$$

WITH $\rho = \rho(p)$ ONLY

$$\boxed{S_h \frac{\partial h}{\partial t} - \underset{\sim}{\nabla} \cdot \underset{\approx}{K} \cdot \underset{\sim}{\nabla} h = 0}$$

WITH ISOTROPIC PERMEABILITY, IE. $\underset{\approx}{K} = K \underset{\approx}{I}$

form for analytical eq. for testing

$$S_p \frac{\partial p}{\partial t} - \underset{\sim}{\nabla} \frac{k\rho}{\mu} \cdot (\underset{\sim}{\nabla} p + \rho g \underset{\sim}{\nabla} z) = 0$$

$$S_h \frac{\partial h}{\partial t} - \underset{\sim}{\nabla} K \cdot \underset{\sim}{\nabla} h = 0$$

MASS TRANSPORT

BALANCE LAW ($\rho \equiv \rho^{\alpha}$, $\omega \equiv \omega_k^{\alpha}$, $\underset{\sim}{V} \equiv \underset{\sim}{V}^{\alpha}$, $\underset{\approx}{D} \equiv \underset{\approx}{D}^{\alpha}$, $n \equiv n^{\alpha}$, etc)

$$\underset{①}{\frac{\partial(n\rho\omega)}{\partial t}} + \underset{②}{\underset{\sim}{\nabla}\cdot(\rho\omega V)} - \underset{③}{\underset{\sim}{\nabla}\cdot(n\rho\,\underset{\approx}{D}\cdot\underset{\sim}{\nabla}\omega)} - \underset{④}{n\rho r} - \underset{⑤}{n\rho e(\rho\omega)} - \underset{⑥}{n\rho I} = 0$$

① $\frac{\partial}{\partial t}(n\rho\omega) \equiv$ RATE OF CHANGE OF ω

② $\underset{\sim}{\nabla}\cdot(\rho\omega V) \equiv$ RATE OF CHANGE DUE TO CONVECTION

③ $\underset{\sim}{\nabla}\cdot(n\rho\,\underset{\approx}{D}\cdot\nabla\omega) \equiv$ RATE OF CHANGE DUE TO DISPERSION

④ $n\rho r \equiv$ RATE OF CHANGE DUE TO PRODUCTION RATE r

⑤ $n\rho e(\rho\omega) \equiv$ RATE OF CHANGE DUE PHASE CHANGE $e(\rho\omega)$

⑥ $n\rho I \equiv$ RATE OF CHANGE DUE TO DIFFUSION ACROSS PHASE BOUNDARY I

WHERE

$\omega \equiv$ MASS FRACTION

$\rho \equiv \rho_f$

$\underset{\sim}{V} \equiv \underset{\sim}{V}_f$

$\underset{\approx}{D} \equiv$ DISPERSION COEF.

MASS TRANSPORT

CONSTRAINTS

DEFINE: $\bar{R}_k \equiv \sum_{\alpha=1}^{N} R_k^\alpha = \sum_{\alpha=1}^{N} n^\alpha \rho^\alpha [e^\alpha(\rho\omega_k) + I_k^\alpha]$ $\quad N \equiv$ # OF PHASES α, $M \equiv$ # OF SPECIES k

THEN, CONSERVATION OF REACTING MASS REQUIRES

$$\sum_{k=1}^{M} (n^\alpha \rho^\alpha r_k^\alpha + \bar{R}_k) = 0 \qquad \text{summing over species}$$

AND

$$\sum_{\alpha=1}^{N} n^\alpha \rho_k^\alpha \sum_{k=1}^{M} [e^\alpha(\rho\omega_k) + I_k^\alpha] = 0 \qquad \text{summing over phases}$$

BALANCE OF SOLID AND FLUID

FLUID

convection dispersion

$$\frac{\partial(n\rho\omega)}{\partial t} + \underset{\sim}{\nabla}\cdot(n\rho\omega\underset{\sim}{V}) - \underset{\sim}{\nabla}\cdot(n\rho\underset{\approx}{D}\cdot\underset{\sim}{\nabla}\omega) - n\rho r - n\rho I - n\rho e(\rho\omega) = 0 \quad \Big|_{\substack{\text{phase} = f \\ \text{species} = k}}$$

SOLID

porosity & solid

$$\frac{\partial((1-n)\rho\omega)}{\partial t} - (1-n)\rho r - (1-n)\rho I - (1-n)\rho e(\rho\omega) = 0 \quad \Big|_{\substack{\text{phase} = s \\ \text{species} = k}}$$

COMBINED FLUID AND SOLID

sum of homogeneous reactions

$$\left\{ \begin{aligned} &\frac{\partial}{\partial t}[n\rho_f\omega^f + (1-n)\rho_s\omega^s] + \underset{\sim}{\nabla}\cdot(n\rho_f\omega^f\underset{\sim}{V}) - \underset{\sim}{\nabla}\cdot(n\rho_f\underset{\approx}{D}\cdot\underset{\sim}{\nabla}\omega^f) - [n\rho^f r^f + (1-n)\rho^s r^s] \\ &- [n\rho^f I^f + (1-n)\rho^s I^s] - [n\rho^f e^f(\rho^f\omega^f) + (1-n)\rho^s e^s(\rho^s\omega^s)] = 0 \quad \Big|_{\text{species} = k} \end{aligned} \right.$$

This summing allows k_s to be defined. (see ⓐ)

MASS TRANSPORT

SIMPLIFICATIONS

ASSUME NO HOMOGENEOUS REACTIONS; IE $r=0$

USE: $\bar{R}_k \equiv \sum_{\alpha=1}^{N} n^\alpha \rho^\alpha [e^\alpha(\rho\omega_k) + I_k^\alpha]$

THEN:

(a)

$$\frac{\partial}{\partial t}[n\rho_f\omega^f + (1-n)\rho_s\omega^s] + \underset{\sim}{\nabla}\cdot(n\rho_f\omega^f\underset{\sim}{V}) - \underset{\sim}{\nabla}\cdot(n\rho_f \underset{\approx}{D}\cdot\underset{\sim}{\nabla}\omega^f) + \bar{R} = 0 \Big|_{\text{species}=k}$$

assumes for adsorption get rid of it in * or ignore it.

CONSTITUTIVE RELATIONSHIPS

FREUNDLICH EQUILIBRIUM ISOTHERM $\omega_k^s = \beta_k(\omega_k^f)^{\frac{1}{m}}$ ← experimentally determined

LET: $\beta_k \equiv \rho_f K_{Dk}$; $K_D \equiv$ DISTRIBUTION COEFFICIENT

assume → $\bar{R}_k \equiv 0$; $\kappa \equiv \left(\frac{1-n}{n}\right)\frac{\rho_s\beta_k}{\rho_f} + 1 = \left(\frac{(1-n)}{n}\right)\rho_s K_{Dk} + 1$

$C_k \equiv \rho_f\omega_k^f$

THEN

new, measureable coeff related to K_d

$$* \quad \boxed{\frac{\partial}{\partial t}(n\kappa C) + \underset{\sim}{\nabla}\cdot(nVC) - \underset{\sim}{\nabla}\cdot(n\underset{\approx}{D}\cdot\underset{\sim}{\nabla}C) = 0 \Big|_{\text{species}=k}}$$

LET $D_L \equiv$ LONGITUDINAL DISPERSIVITY, $D_T \equiv$ TRANSVERSE DISPERSIVITY

tensor — $\underset{\approx}{D} = D_{ij} = D_T|V|\delta_{ij} + (D_L - D_T)\frac{V_i V_j}{|V|} + D_d\tau\delta_{ij}$ $\quad i,j = 1,2,3$

$D_d \equiv$ MOLECULAR DIFFUSION; $\tau \equiv$ TORTUOSITY; $\delta_{ij} \equiv$ DELTA FUNCTION

EXAMPLE: $D_{\parallel} = D_T|V| + (D_L - D_T)\frac{V_1 V_1}{|V|} + D_d\tau$

see Adrian Schadegger ref.

ENCLOSURE 3B

INTRODUCTION TO NUMERICAL METHODS

MICHAEL A. CELIA

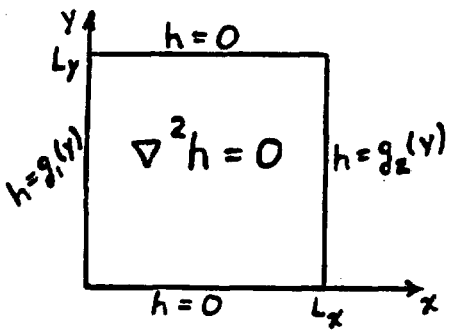
RALPH M. PARSONS LABORATORY
DEPARTMENT OF CIVIL ENGINEERING
MASSACHUSETTS INSTITUTE OF TECHNOLOGY

BASIC IDEA OF NUMERICAL METHODS

- SOLVE FOR AN APPROXIMATE SOLUTION
- SOLVE FOR ONLY A FINITE NUMBER OF DISCRETE VALUES
- SOLVE ALGEBRAIC EQUATIONS INSTEAD OF DIFFERENTIAL EQUATIONS

SIMPLE ANALYTICAL SOLUTION

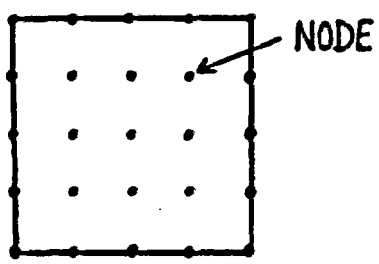
EXAMPLE



$$h(x,y) = \sum_{n=1}^{+\infty} \frac{\sin \mu_n y}{\sinh \mu_n L_x} \left[A_n \sinh \mu_n x + B_n \sinh \mu_n (L_x - x) \right]$$

$$\mu_n \equiv n\pi / L_y$$

NUMERICAL SOLUTION



SOLVE FOR A FINITE NUMBER OF (NODAL) VALUES AS AN APPROXIMATION TO $h(x,y)$.

OUTLINE

I. FINITE DIFFERENCE METHOD

- DISCRETE APPROXIMATIONS
- TAYLOR SERIES, TRUNCATION ERROR
- LIST OF STANDARD APPROXIMATIONS
- EXAMPLE CALCULATION
- TIME AND SPACE DEPENDENCE
- STABILITY AND CONVERGENCE
- REFERENCES

II. FINITE ELEMENT METHOD

- TRIAL FUNCTION, BASIS FUNCTIONS
- METHOD OF WEIGHTED RESIDUALS
- THE FINITE ELEMENT METHOD
- TIME AND SPACE DEPENDENCE
- TWO-DIMENSIONAL ELEMENTS, NON-RECTANGULAR ELEMENTS
- PRACTICAL CONSIDERATIONS
- REFERENCES

III. ALTERNATING DIRECTION METHODS

- ADI METHOD
- REFERENCES

IV. GROUNDWATER TRANSPORT MODELING

- FDM
- FEM
- WIGGLES AND ARTIFICIAL DIFFUSION
- UPSTREAM WEIGHTING FOR FDM AND FEM
- REFERENCES

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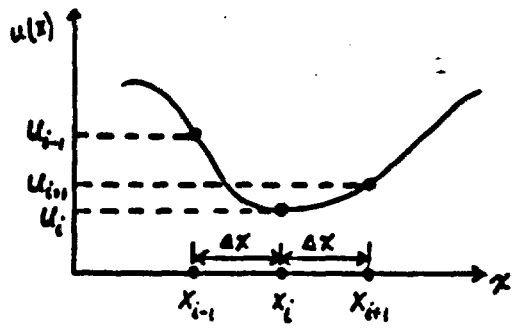
FINITE DIFFERENCE APPROXIMATIONS

BASIC IDEA: APPROXIMATE DERIVATIVES USING DISCRETE VALUES



QUESTION: HOW CAN WE APPROXIMATE $\frac{\partial u}{\partial x}$ AT x_i USING THE DISCRETE VALUES u_{i-1}, u_i, u_{i+1}?

ANSWERS:

1. $\left.\frac{du}{dx}\right|_{x_i} \approx \frac{u_{i+1} - u_i}{\Delta x}$ ("FORWARD DIFFERENCE")

2. $\left.\frac{du}{dx}\right|_{x_i} \approx \frac{u_i - u_{i-1}}{\Delta x}$ ("BACKWARD DIFFERENCE")

3. $\left.\frac{du}{dx}\right|_{x_i} \approx \frac{u_{i+1} - u_{i-1}}{2\Delta x}$ ("CENTRAL DIFFERENCE")

QUESTION: HOW GOOD ARE THESE APPROXIMATIONS?

TAYLOR SERIES

- ASSUMING $u(x)$ AND ITS DERIVATIVES TO BE SUFFICIENTLY SMOOTH, WE CAN EXPAND $u(x)$ IN A TAYLOR SERIES ABOUT AN ARBITRARY POINT X_0 AS

$$\boxed{u(x) = u(x_0) + (x-x_0)\left.\frac{du}{dx}\right|_{x_0} + \frac{(x-x_0)^2}{2!}\left.\frac{d^2u}{dx^2}\right|_{x_0} + \frac{(x-x_0)^3}{3!}\left.\frac{d^3u}{dx^3}\right|_{x_0} + \cdots + \frac{(x-x_0)^n}{n!}\left.\frac{d^nu}{dx^n}\right|_{x_0} + \cdots}$$

ANALYSIS OF F.D. APPROXIMATIONS

- EXPAND $u(x)$ ABOUT NODE POINT X_i

(a) $$u(x_i+\Delta x) = u_{i+1} = u_i + (\Delta x)\left.\frac{du}{dx}\right|_{x_i} + \frac{(\Delta x)^2}{2!}\left.\frac{d^2u}{dx^2}\right|_{x_i} + \frac{(\Delta x)^3}{3!}\left.\frac{d^3u}{dx^3}\right|_{x_i} + \cdots$$

(b) $$u(x_i-\Delta x) = u_{i-1} = u_i - (\Delta x)\left.\frac{du}{dx}\right|_{x_i} + \frac{(\Delta x)^2}{2}\left.\frac{d^2u}{dx^2}\right|_{x_i} - \frac{(\Delta x)^3}{3!}\left.\frac{d^3u}{dx^3}\right|_{x_i} + \cdots$$

$$\Delta x = x_{i+1} - x_i = x_i - x_{i-1}$$

- FORWARD DIFFERENCE

SUBTRACT u_i FROM EQUATION (a)

$$u_{i+1} - u_i = (\Delta x)\left.\frac{du}{dx}\right|_{x_i} + \frac{(\Delta x)^2}{2}\left.\frac{d^2u}{dx^2}\right|_{x_i} + \frac{(\Delta x)^3}{3!}\left.\frac{d^3u}{dx^3}\right|_{x_i} + \cdots$$

$$\boxed{\left.\frac{du}{dx}\right|_{x_i} = \frac{u_{i+1} - u_i}{\Delta x}} - \underbrace{\frac{\Delta x}{2}\left.\frac{d^2u}{dx^2}\right|_{x_i} - \frac{(\Delta x)^2}{6}\left.\frac{d^3u}{dx^3}\right|_{x_i} - \cdots}_{\text{"TRUNCATION ERROR"}}$$

due to cutting off the Taylor Series

$$\boxed{\left.\frac{du}{dx}\right|_{x_i} = \frac{u_{i+1} - u_i}{\Delta x} + O(\Delta x)}$$

"OF ORDER ΔX"

- BACKWARD DIFFERENCE

SUBTRACT EQUATION (b) FROM u_i

$$\boxed{\left.\frac{du}{dx}\right|_{x_i} = \frac{u_i - u_{i-1}}{\Delta x} + O(\Delta x)}$$ (FIRST ORDER)

- CENTRAL DIFFERENCE

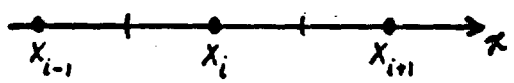
SUBTRACT EQUATION (b) FROM EQUATION (a)

$$\boxed{\left.\frac{du}{dx}\right|_{x_i} = \frac{u_{i+1} - u_{i-1}}{2\,\Delta x} + O((\Delta x)^2)} \qquad \text{(SECOND ORDER)}$$

SECOND ORDER DERIVATIVES

- NEED TO APPROXIMATE $\dfrac{d^2u}{dx^2}$.

- STANDARD APPROXIMATION :



$$\left.\frac{d^2u}{dx^2}\right|_{x_i} = \left.\left[\frac{d}{dx}\left(\frac{du}{dx}\right)\right]\right|_{x_i} \approx \frac{\left.\frac{du}{dx}\right|_{i+1/2} - \left.\frac{du}{dx}\right|_{i-1/2}}{\Delta x}$$

$$\approx \frac{\frac{u_{i+1} - u_i}{\Delta x} - \frac{u_i - u_{i-1}}{\Delta x}}{\Delta x} = \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2}$$

$$\boxed{\left.\frac{d^2u}{dx^2}\right|_{x_i} = \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2} + O((\Delta x)^2)}$$

List of Standard FORMULAE :

$\left.\frac{du}{dx}\right\|_{x_i}$	$\frac{u_{i+1} - u_i}{\Delta x}$	$O(\Delta x)$
	$\frac{u_i - u_{i-1}}{\Delta x}$	$O(\Delta x)$
	$\frac{u_{i+1} - u_{i-1}}{2\,\Delta x}$	$O((\Delta x)^2)$
	$\frac{-u_{i+2} + 4u_{i+1} - 3u_i}{2\,\Delta x}$	$O((\Delta x)^2)$
	$\frac{-u_{i+2} + 8u_{i+1} - 8u_{i-1} + u_{i-2}}{12\,(\Delta x)}$	$O((\Delta x)^4)$
$\left.\frac{d^2u}{dx^2}\right\|_{x_i}$	$\frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2}$	$O((\Delta x)^2)$
	$\frac{-u_{i+2} + 16u_{i+1} - 30u_i + 16u_{i-1} - u_{i-2}}{12\,(\Delta x)^2}$	$O((\Delta x)^4)$

EXAMPLE

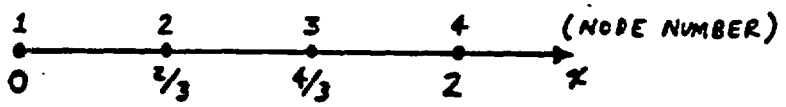
APPROXIMATE THE SOLUTION TO

$$\frac{d^2u}{dx^2} + u = 0 , \qquad 0 \le x \le 2$$

$$u(0) = 0$$
$$u(2) = 1$$

USING THE FINITE DIFFERENCE METHOD.

STEP 1: DISCRETIZE THE DOMAIN



STEP 2: FORMULATE APPROXIMATING EQUATIONS

NODE	EQUATION
1	$u_1 = 0$ (B.C.) boundary condition
2	$\left(\frac{d^2u}{dx^2} + u\right)\Big\|_{x_2} = 0 = \left[\frac{u_1 - 2u_2 + u_3}{(\Delta x)^2} + O(\Delta x^2)\right] + u_2$

$$\frac{u_1 - 2u_2 + u_3}{(\Delta x)^2} + u_2 = 0$$

3 $$\frac{u_2 - 2u_3 + u_4}{(\Delta x)^2} + u_3 = 0$$

4 $$u_4 = 1 \qquad (B.C.)$$

STEP 3: ASSEMBLE EQUATIONS

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & [(\Delta x)^2 - 2] & 1 & 0 \\ 0 & 1 & [(\Delta x)^2 - 2] & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

STEP 4: SOLVE ALGEBRAIC EQUATIONS

NODE	EXACT SOLN.	FD SOLN.
1	0.	0.
2	0.680	0.704 (3.6%)
3	1.069	1.096 (2.5%)
4	1.	1.

% error

APPROXIMATIONS IN SPACE AND TIME

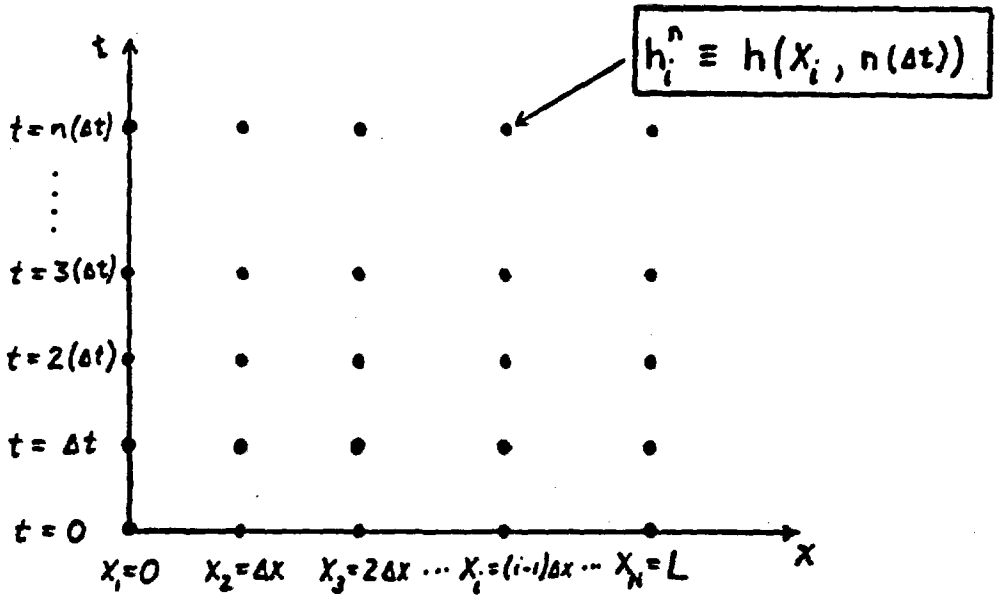
- **EXAMPLE**: TRANSIENT GW FLOW (1-D)

$$S \frac{\partial h}{\partial t} - K \frac{\partial^2 h}{\partial x^2} = 0 , \qquad 0 \le x \le L, \quad t > 0$$

$$h(0,t) = C_1$$
$$h(L,t) = C_2$$

$$h(x,0) = h_0(x)$$

STEP 1: DISCRETIZATION



STEP 2: APPROXIMATING EQUATIONS

- **CLASSIC EXPLICIT APPROXIMATION**

$$\left(S\,\frac{\partial h}{\partial t} - K\,\frac{\partial^2 h}{\partial x^2}\right)\Bigg|_{(x_i\,,\,n\Delta t)} = 0$$

TAYLOR SERIES:

$$\left.\frac{\partial h}{\partial t}\right|_i^n = \frac{h_i^{n+1} - h_i^n}{\Delta t} + O(\Delta t)$$

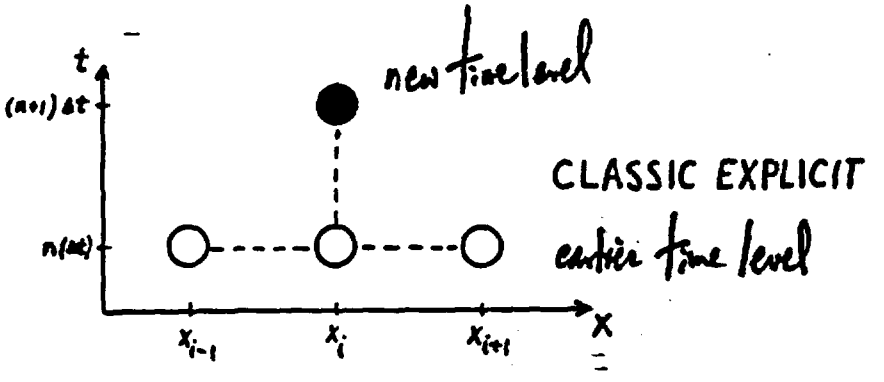
$$\left.\frac{\partial^2 h}{\partial x^2}\right|_i^n = \frac{h_{i+1}^n - 2h_i^n + h_{i-1}^n}{(\Delta x)^2} + O((\Delta x)^2)$$

SO:

$$S\,\frac{h_i^{n+1} - h_i^n}{\Delta t} - K\,\frac{h_{i+1}^n - 2h_i^n + h_{i-1}^n}{(\Delta x)^2} + O(\Delta t, (\Delta x)^2) = 0$$

DEFINE: $\rho = \dfrac{K(\Delta t)}{S\,(\Delta x)^2}$

$$\boxed{h_i^{n+1} = \rho\, h_{i-1}^n + (1-2\rho)\, h_i^n + \rho\, h_{i+1}^n}$$

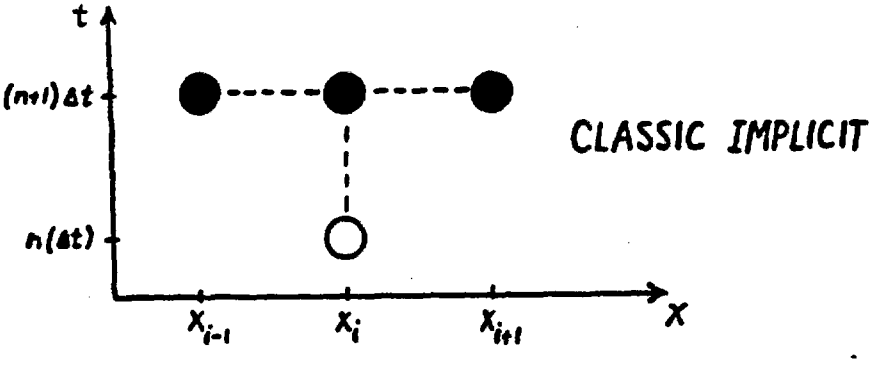


- <u>CLASSIC IMPLICIT APPROXIMATION</u>

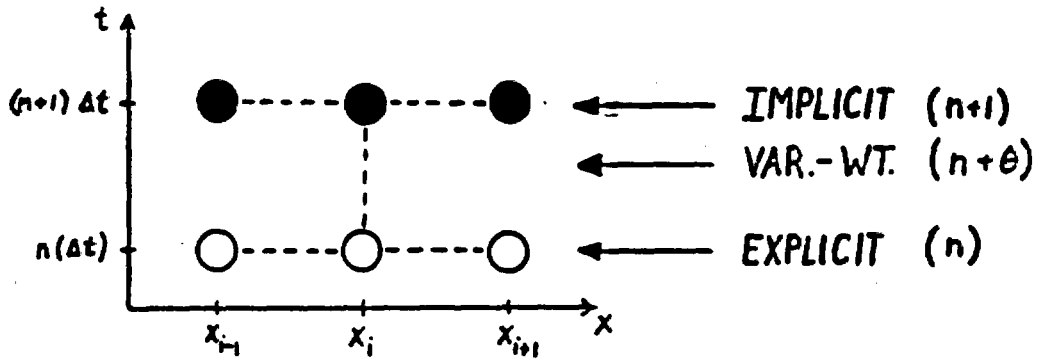
$$\left(S\frac{\partial h}{\partial t} - K\frac{\partial^2 h}{\partial x^2}\right)\Bigg|_i^{n+1} = 0$$

$$S\,\frac{h_i^{n+1}-h_i^n}{\Delta t} - K\,\frac{h_{i+1}^{n+1}-2h_i^{n+1}+h_{i-1}^{n+1}}{(\Delta x)^2} + O(\Delta t,(\Delta x)^2) = 0$$

$$\boxed{-\rho h_{i-1}^{n+1} + (1+2\rho)h_i^{n+1} - \rho h_{i+1}^{n+1} = h_i^n}$$



- **VARIABLY-WEIGHTED APPROXIMATION**



$$\left(S\,\frac{\partial h}{\partial t} - K\,\frac{\partial^2 h}{\partial x^2}\right)\Bigg|_i^{n+\theta} = 0$$

$$\frac{\partial h}{\partial t}\Bigg|_i^{n+\theta} = \frac{h_i^{n+1} - h_i^n}{\Delta t} + O\left((1-2\theta)\Delta t + (\Delta t)^2\right)$$

$$\frac{\partial^2 h}{\partial x^2}\Bigg|_i^{n+\theta} = \frac{h_{i+1}^{n+\theta} - 2h_i^{n+\theta} + h_{i-1}^{n+\theta}}{(\Delta x)^2} + O\left((\Delta x)^2\right)$$

$$h_i^{n+\theta} = \theta h_i^{n+1} + (1-\theta) h_i^n + O\left((\Delta t)^2\right)$$

$$\boxed{\begin{aligned} &-\theta\rho\, h_{i-1}^{n+1} + (1+2\theta\rho)\, h_i^{n+1} - \theta\rho\, h_{i+1}^{n+1} \\ &\qquad = (1-\theta)\rho\, h_{i-1}^n + \left[1 - 2(1-\theta)\rho\right] h_i^n + (1-\theta)\rho\, h_{i+1}^n \end{aligned}}$$

NOTE :

$\theta = 0$	CLASSIC EXPLICIT,	$O(\Delta t, (\Delta x)^2)$
$\theta = 1$	CLASSIC IMPLICIT,	$O(\Delta t, (\Delta x)^2)$
$\theta = 1/2$	CRANK-NICOLSON,	$O((\Delta t)^2, (\Delta x)^2)$

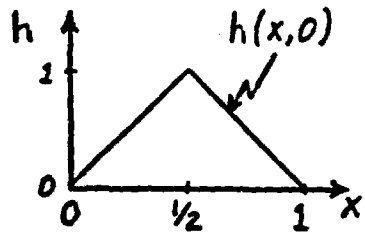
STEP 3: ASSEMBLE EQUATIONS AND SOLVE

EXAMPLE

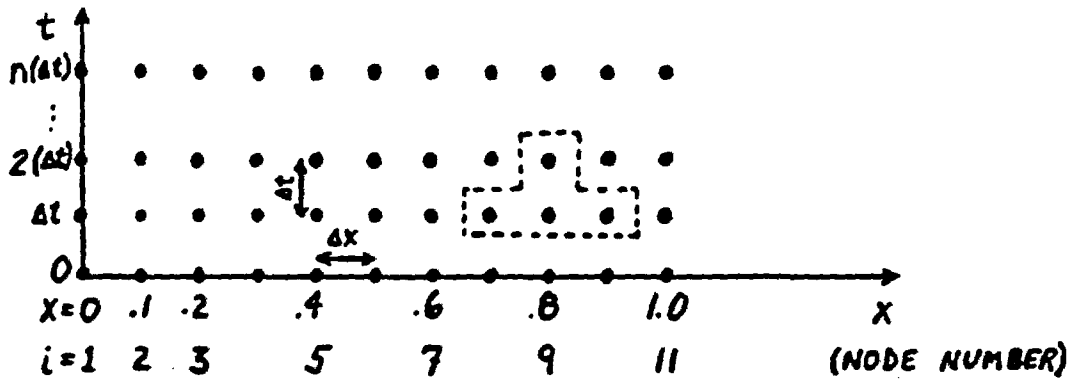
$$\frac{\partial h}{\partial t} - \frac{\partial^2 h}{\partial x^2} = 0 \,, \qquad \begin{array}{l} 0 \le x \le 1 \\ t > 0 \end{array}$$

$$h(0,t) = 0$$
$$h(1,t) = 0$$

$$h(x,0) = \begin{cases} 2x, & 0 \le x \le \tfrac{1}{2} \\ 2(1-x), & \tfrac{1}{2} \le x \le 1 \end{cases}$$



- USE CLASSIC EXPLICIT METHOD ($\theta = 0$)

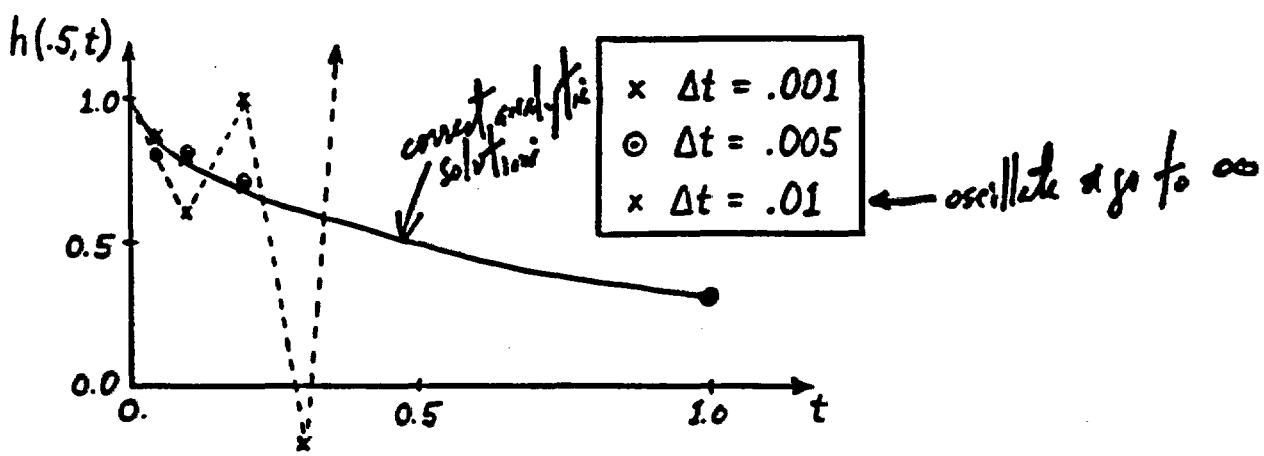


$$\boxed{\begin{array}{c} \Delta X = 0.1 \,, \quad \Delta t = .001, .005, .01 \\ (\rho = 0.1, 0.5, 1.0) \end{array}}$$

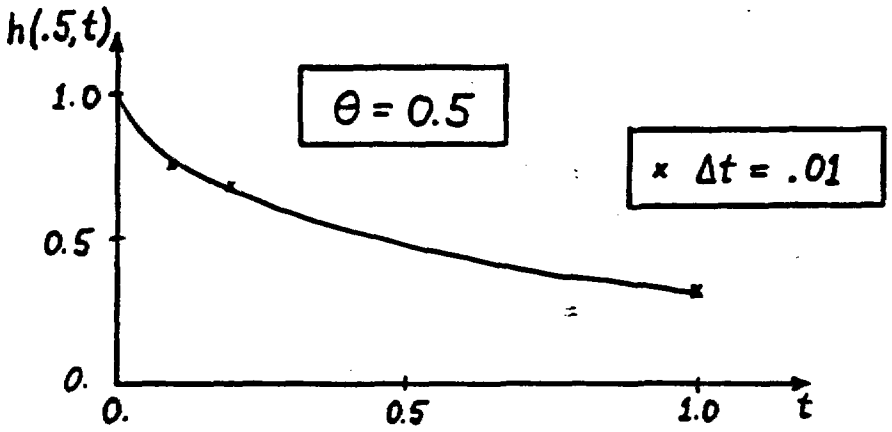
- LET $\Delta t = .001 \quad (\rho = 0.1)$

$$h_i^1 = \rho h_{i-1}^0 + (1-2\rho) h_i^0 + \rho h_{i+1}^0$$

NODE	EQUATION
1	$h_1^1 = 0$ (B.C.)
2	$h_2^1 = 0.1(0) + 0.8(0.2) + 0.1(0.4)$ $= 0.2$
3	$h_3^1 = 0.4$
⋮	
6	$h_6^1 = 0.96$
⋮	
11	$h_{11}^1 = 0$ (B.C.)



this solution is <u>consistent</u>, but <u>unstable</u>



use Crank-Nicholson produces a stable & consistent solution.
x's are on the line of the exact solution.

CONVERGENCE

$$\lim_{\substack{\Delta x \to 0 \\ \Delta t \to 0}} \left| h_{FD} - h_{EXACT} \right| = 0$$

STABILITY

- ERRORS ARE DAMPED OUT (DO NOT GROW) AS THE SOLUTION PROCEEDS IN TIME
- STABILITY IS NECESSARY FOR CONVERGENCE

STABILITY LIMITS

CLASSIC EXPLICIT	$\rho \leq 1/2$
VARIABLY-WEIGHTED	$\rho(1-2\theta) \leq 1/2$
CLASSIC IMPLICIT	ALWAYS STABLE
CRANK-NICOLSON	ALWAYS STABLE

REFERENCES

Ames, W.F., *Numerical Methods for Partial Differential Equations*, Academic Press (Second Edition), 1977. FINITE DIFF - ADV.

Lapidus, L. and G. Pinder, *Numerical Solution of Partial Differential Equations in Science and Engineering*, John Wiley, 1982. } both DIFF & ELEM

Smith, G., *Numerical Solution of Partial Differential Equations*, Oxford University Press, 1965. FINITE DIFF INTRO.

THE FINITE ELEMENT METHOD

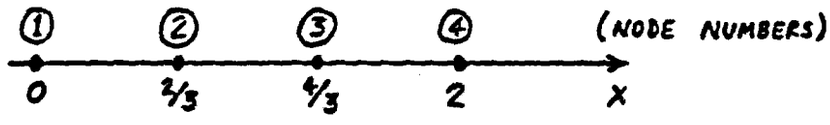
- A DIFFERENT "DISCRETE" APPROXIMATION TO SOLUTIONS OF DIFFERENTIAL EQUATIONS

EXAMPLE

$$\frac{d^2u}{dx^2} + u = 0 \,, \qquad 0 \le x \le 2 \qquad (\Omega \equiv [0,2])$$

$$u(0) = 0$$
$$u(2) = 1$$

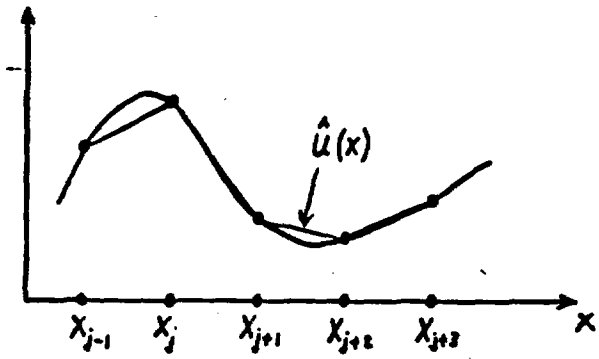
STEP 1: DISCRETIZE DOMAIN



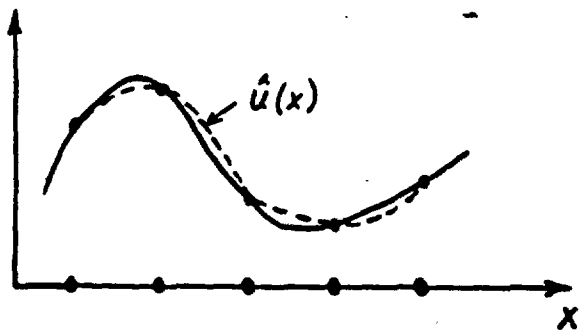
STEP 2: DEFINE TRIAL FUNCTION

TRIAL FUNCTION ≡ SIMPLE FUNCTIONAL REPRESENTATION TO APPROXIMATE $u(x)$

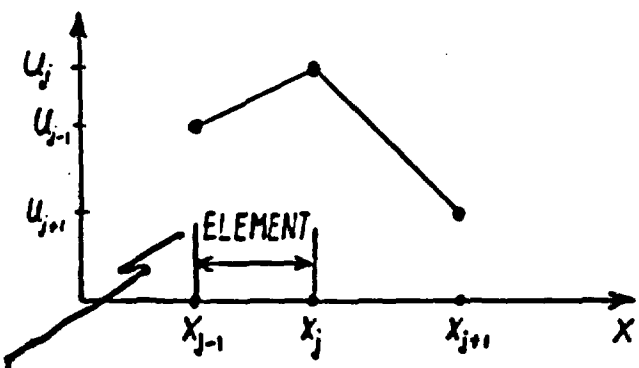
$$= \hat{u}(x)$$



"PIECEWISE LINEAR"



"PIECEWISE QUADRATIC" - for 3 nodes
for 4 nodes - use "cubics"
for n nodes - "polynomials"

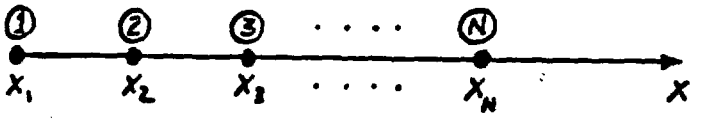


Element:

FOR $X_{j-1} \le x \le X_j$

- $\hat{u}(x)$ DEFINED BY U_{j-1} AND U_j ONLY.
- CONNECT U_{j-1} AND U_j WITH A STRAIGHT LINE
- $\hat{u}^e(x) = U_{j-1}\left(\frac{X_j - X}{\Delta X}\right) + U_j\left(\frac{X - X_{j-1}}{\Delta X}\right)$, $\Delta X = X_j - X_{j-1}$

FOR ENTIRE DOMAIN



$$\boxed{\hat{u}(x) = \sum_{j=1}^{N} U_j \, \phi_j(x)}$$

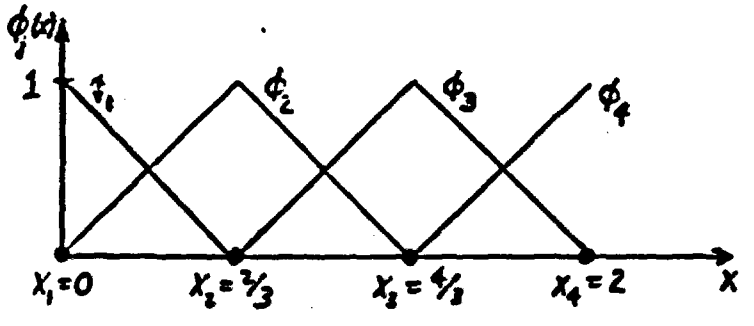
"UNDETERMINED COEFFICIENTS"

"BASIS FUNCTIONS"

$$\phi_j(x) = \begin{cases} \dfrac{x - x_{j-1}}{x_j - x_{j-1}}, & x_{j-1} \le x \le x_j \\[2ex] \dfrac{x_{j+1} - x}{x_{j+1} - x_j}, & x_j \le x \le x_{j+1} \\[2ex] 0, & \text{ALL OTHER } x \end{cases}$$

FOR EXAMPLE PROBLEM

$$\hat{u}(x) = \sum_{j=1}^{4} U_j \, \phi_j(x)$$



"piecewise LaGrange polynomials"

STEP 3: FORM RESIDUAL

$$\text{RESIDUAL} \equiv R(x) = \frac{d^2\hat{u}}{dx^2} + \hat{u} \qquad (\neq 0)$$

STEP 4: FORM APPROXIMATING EQUATIONS

need a weighted average to force to zero residual

- **GENERAL METHOD OF WEIGHTED RESIDUALS**

Ω is the domain

$$\int_\Omega R(x)\, W_i(x)\, dx = 0 , \qquad i = 1, 2, \ldots, M.$$

- **FINITE ELEMENT (GALERKIN) METHOD**

Celia claims this is an algebraic function

CHOOSE $W_i(x) = \phi_i(x)$

$$\boxed{\int_\Omega R(x)\, \phi_i(x)\, dx = 0 , \quad i = 1, 2, \ldots, M.}$$

- **FOR EXAMPLE PROBLEM**

residual

weight function

$$\int_0^2 \left(\frac{d^2\hat{u}}{dx^2} + \hat{u} \right) \phi_i(x)\, dx = 0$$

four unk.

NODE (i)	EQUATION
1	$U_1 = 0 \quad (B.C.)$
2	$\int_0^2 \left[\frac{d^2}{dx^2}\left(\sum_{j=1}^{4} U_j \phi_j(x)\right) + \sum_{j=1}^{4} U_j \phi_j(x)\right]\phi_2(x)\,dx = 0$
	$\sum_{j=1}^{4} U_j \left\{\int_0^2 \left[\frac{d^2\phi_j}{dx^2} + \phi_j\right]\phi_2(x)\,dx\right\} = 0$
3	$\sum_{j=1}^{4} U_j \left\{\int_0^2 \left[\frac{d^2\phi_j}{dx^2} + \phi_j\right]\phi_3(x)\,dx\right\} = 0$
4	$U_4 = 1 \quad (B.C.)$

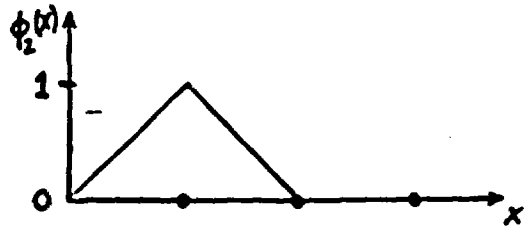
STEP 5: INTEGRATE BY PARTS

$$\int_0^2 \frac{d^2\hat{u}}{dx^2}\phi_i\,dx = \left[\frac{d\hat{u}}{dx}\phi_i\right]_0^2 - \int_0^2 \frac{d\hat{u}}{dx}\frac{d\phi_i}{dx}\,dx$$

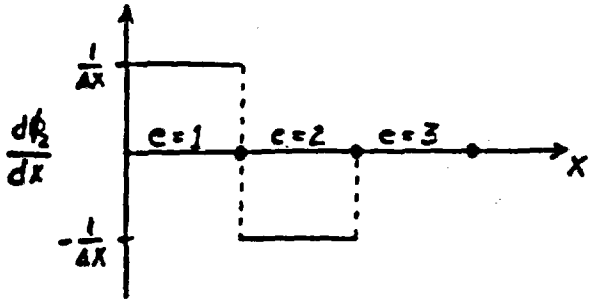
STEP 6: PERFORM INTEGRATIONS

$i = 2$

$$\sum_{j=1}^{4} U_j \left\{\int_0^2 \phi_j \phi_2\,dx - \int_0^2 \frac{d\phi_j}{dx}\frac{d\phi_2}{dx}\,dx\right\} = -\left[\frac{d\hat{u}}{dx}\phi_2\right]_0^2$$



$$\phi_2\Big|_0^2 = \phi_2(2) - \phi_2(0) = 0$$



$$\frac{d\phi_2}{dx} = 0$$ IN ALL ELEMENTS EXCEPT e=1 AND e=2

$$\boxed{\frac{\Delta x}{6}\left[u_1 + 4u_2 + u_3\right] + \frac{u_1 - 2u_2 + u_3}{\Delta x} = 0}$$

the answer, having turned the integration crank.

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ \left(\frac{1}{9}+\frac{3}{2}\right) & \left(\frac{4}{9}-3\right) & \left(\frac{1}{9}+\frac{3}{2}\right) & 0 \\ 0 & \left(\frac{1}{9}+\frac{3}{2}\right) & \left(\frac{4}{9}-3\right) & \left(\frac{1}{9}+\frac{3}{2}\right) \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

STEP 7: SOLVE ALGEBRAIC EQUATIONS

$$(u_1, u_2, u_3, u_4) = (0,\ .6596,\ 1.046,\ 1)$$

NODE	EXACT	FDM	FEM
1	0	0.	0.
2	.6801	.7044 (3.6%)	.6596 (3.0%)
3	1.069	1.096 (2.5%)	1.046 (2.4%)
4	1.	1.	1.

so, it's not clear which method is better

SPACE AND TIME DEPENDENCE

EXAMPLE

time term space term flux term

$$\frac{\partial h}{\partial t} - \frac{\partial^2 h}{\partial x^2} = f(x,t) \qquad 0 \le x \le L, \quad t > 0$$

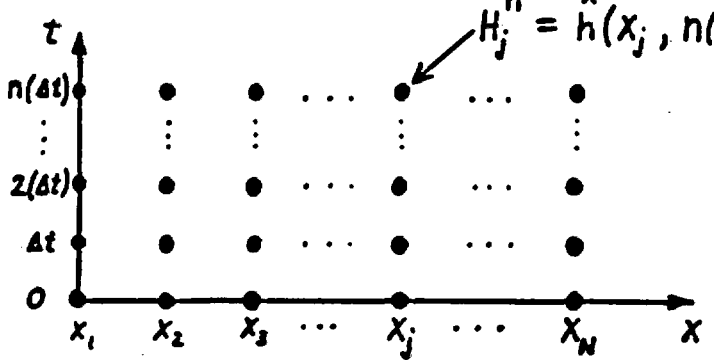
$$h(0,t) = 0$$

$$\frac{\partial h}{\partial x}(L,t) = C$$

$$h(x,0) = h_0(x)$$

STEP 1: DISCRETIZATION

$H_j^n = \hat{h}(x_j, n(\Delta t))$



STEP 2: TRIAL FUNCTION

$$h(x,t) \approx \hat{h}(x,t) = \sum_{j=1}^{N} H_j(t)\, \phi_j(x)$$

UNDETERMINED COEFFS. (TIME DEPENDENT)

BASIS FUNCTIONS

solve for every H_j at every time step

STEP 3: RESIDUAL

$$R(x,t) \equiv \frac{\partial \hat{h}}{\partial t} - \frac{\partial^2 \hat{h}}{\partial x^2} - f(x,t) \qquad (\neq 0)$$

STEP 4: FORM APPROXIMATING EQUATIONS

$$\int_0^L R(x,t)\,\phi_i(x)\,dx = 0\,, \qquad i = 1, 2, \ldots, M.$$

time term space term

$$R(x,t) = \frac{\partial}{\partial t}\left(\sum_{j=1}^{N} H_j(t)\,\phi_j(x)\right) - \frac{\partial^2}{\partial x^2}\left(\sum_{j=1}^{N} H_j(t)\,\phi_j(x)\right) - f(x,t)$$

$$= \sum_{j=1}^{N} \frac{dH_j}{dt}\,\phi_j(x) - \sum_{j=1}^{N} H_j(t)\,\frac{d^2\phi_j}{dx^2} - f(x,t)$$

$$\boxed{\sum_{j=1}^{N}\left[\frac{dH_j}{dt}\int_0^L \phi_j\phi_i\,dx - H_j\int_0^L \frac{d^2\phi_j}{dx^2}\,\phi_i\,dx\right] = \int_0^L f(x,t)\,\phi_i(x)\,dx}$$

STEP 5: APPROXIMATE TIME DERIVATIVE USING FDM

truncation error Crank-Nicolson

$$\left.\frac{dH_j}{dt}\right|^{n+\theta} = \frac{H_j^{n+1} - H_j^n}{\Delta t} + O\left((1-2\theta)\Delta t\,,\,(\Delta t)^2\right)$$

ϕ_j = mass matrix = capacity matrix = "time matrix"

$\frac{d^2\phi_i}{dx^2}$ = stiffness matrix = conductivity matrix = "space matrix"

STEP 6: INTEGRATE BY PARTS

$$\int_0^L \frac{d^2\phi_j}{dx^2}\,\phi_i\,dx = \left(\frac{d\phi_j}{dx}\,\phi_i\right)\Big|_0^L - \int_0^L \frac{d\phi_j}{dx}\,\frac{d\phi_i}{dx}\,dx$$

STEP 7: PERFORM INTEGRATIONS

GENERAL FEM EQUATION (NODE i)

$$\boxed{\begin{aligned}&\left(\tfrac{1}{6}-\theta\rho\right)H_{i-1}^{n+1} + \left(\tfrac{2}{3}+2\theta\rho\right)H_i^{n+1} + \left(\tfrac{1}{6}-\theta\rho\right)H_{i+1}^{n+1} = (\Delta t)\left[\frac{1}{\Delta x}\int_0^L f\phi_i\,dx\right]\\ &+\left[\tfrac{1}{6}+(1-\theta)\rho\right]H_{i-1}^{n} + \left[\tfrac{2}{3}-2(1-\theta)\rho\right]H_i^{n} + \left[\tfrac{1}{6}+(1-\theta)\rho\right]H_{i+1}^{n} - \left[\frac{\partial\hat{h}}{\partial x}\cancelto{0}{\phi_i}\right]_0^L\end{aligned}}$$

VARIABLY-WEIGHTED FD EQUATION (NODE i)

this is for comparison: uses finite differences.

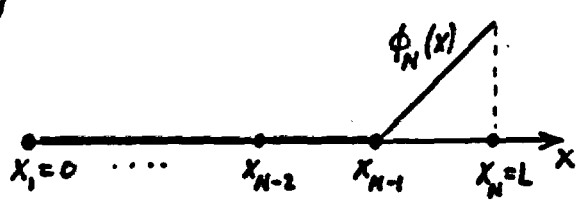
$$\boxed{\begin{aligned}&-\theta\rho\,H_{i-1}^{n+1} + (1+2\theta\rho)H_i^{n+1} - \theta\rho\,H_{i+1}^{n+1} = (\Delta t)\,f|_i\\ &+(1-\theta)\rho\,H_{i-1}^{n} + [1-2(1-\theta)\rho]\,H_i^{n} + (1-\theta)\rho\,H_{i+1}^{n}\end{aligned}}$$

STEP 8: ASSEMBLE EQUATIONS

(LET $\theta = 0$)

NODE	EQUATION	
1	$H_1^1 = 0^-$	first type B.C.
2	$\frac{1}{6} H_1^1 + \frac{2}{3} H_2^1 + \frac{1}{6} H_3^1 = \frac{\Delta t}{\Delta x} \int_0^L f \phi_2 \, dx$	
	$+ \left(\frac{1}{6} + \rho\right) H_1^0 + \left(\frac{2}{3} - 2\rho\right) H_2^0 + \left(\frac{1}{6} + \rho\right) H_3^0$	
$\vdots$	$\vdots$	
N	$\frac{1}{3} H_{N-1}^1 + \frac{2}{3} H_N^1 = \left(\frac{1}{3} + \rho\right) H_{N-1}^0$	second type B.C.
	$+ \left(\frac{2}{3} - \rho\right) H_N^0 - \underbrace{\left[\frac{d\hat{h}}{dx} \phi_N\right]\Big\|_{x = x_N = L}}_{= C \cdot (1)}$	

$$\left(\frac{d\hat{h}}{dx}\Big|_{x=L} = C \; ; \; \phi_N\Big|_{x=L} = 1 \right)$$



STEP 9: SOLVE MATRIX EQUATION

<u>NOTE</u>: STABILITY LIMIT FOR FEM

FOR THE EQUATION

$$S \frac{\partial h}{\partial t} - K \frac{\partial^2 h}{\partial x^2} = 0$$

$\rho \equiv \dfrac{K(\Delta t)}{S\,(\Delta x)^2}$ MUST SATISFY

$$\boxed{\rho(1-2\theta) \leq \frac{1}{6}}$$

PRACTICAL CONSIDERATIONS

1. SPATIALLY VARYING CONDUCTIVITY, K(x)

$$\frac{d}{dx}\left[K(x)\,\frac{dh}{dx}\right] = f(x) \qquad \text{(ST. ST. GW FLOW)}$$

FEM:

$$\int_0^L \underbrace{\left\{\frac{d}{dx}\left(K(x)\frac{d\hat{h}}{dx}\right) - f(x)\right\}}_{R(x)} \phi_i(x)\,dx = 0$$

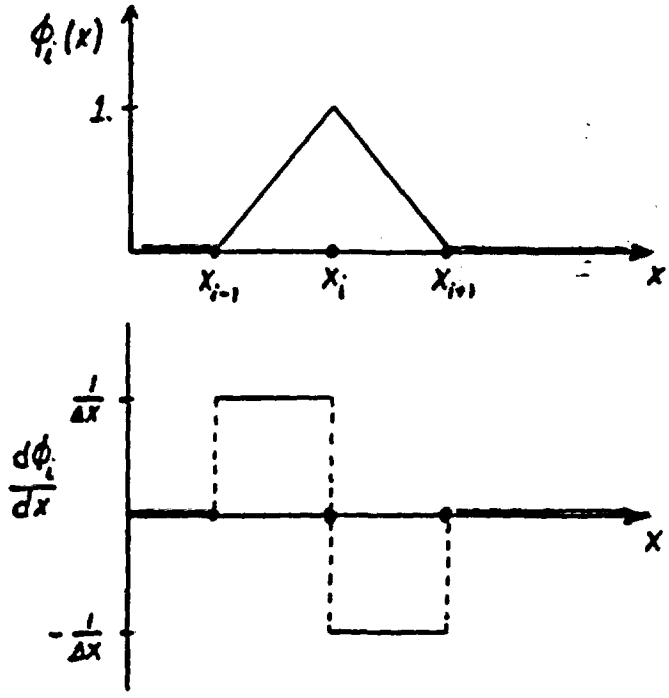
INTEGRATION BY PARTS:

$$\left[K(x)\,\frac{d\hat{h}}{dx}\,\phi_i(x)\right]_0^L - \underbrace{\int_0^L K(x)\,\frac{d\hat{h}}{dx}\,\frac{d\phi_i}{dx}\,dx}_{} = \int_0^L f\phi_i\,dx$$

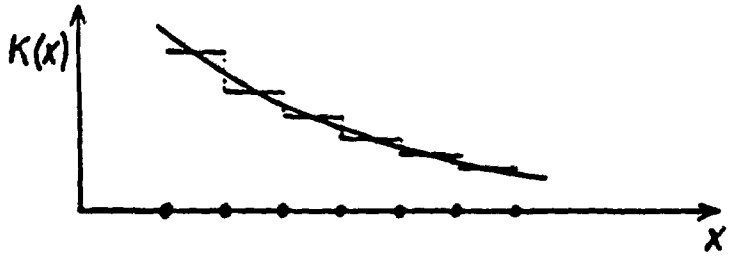
$$= \sum_{j=1}^{N} H_j \int_0^L K(x)\,\frac{d\phi_j}{dx}\,\frac{d\phi_i}{dx}\,dx \qquad (a)$$

ϕ get differentiated + integrated because its a f (space)

RECALL:



- APPROXIMATE K(x) WITH CONSTANT (AVERAGE) VALUES OVER EACH ELEMENT.



- OVER EACH ELEMENT (e)

$$\int_e K(x)\,\frac{d\phi_j}{dx}\,\frac{d\phi_i}{dx}\,dx \approx K^e \int_e \frac{d\phi_j}{dx}\,\frac{d\phi_i}{dx}\,dx \qquad (a)$$

2. POINT SOURCES/SINKS (WELLS)

- RHS $f(x)$ IS $f(x) = Q_w \, \delta(x - x_0)$

  x_0 IS LOCATION OF WELL

  $\delta(x - x_0)$ IS <u>DIRAC DELTA FUNCTION</u> } takes well radius & shrinks it to zero.

<u>RHS OF FEM EQUATION</u>:

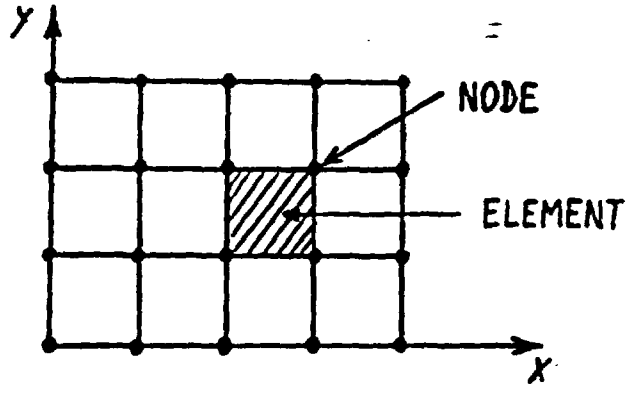
$$\int_0^L f(x)\,\phi_i(x)\,dx = Q_w \int_0^L \phi_i(x)\,\delta(x - x_0)\,dx$$

$$\equiv Q_w \, \phi_i \Big|_{x = x_0}$$

- TYPICALLY LOCATE x_0 AT A NODE
  - ONLY ONE BASIS FUNCTION IS NON-ZERO AT A GIVEN NODE
  - MORE ACCURATE SOLUTIONS

TWO SPACE DIMENSIONS

- STEPWISE PROCEDURE IS EXACTLY THE SAME
- DISCRETIZATION



- TRIAL FUNCTION

$$h(x,y,t) \approx \hat{h}(x,y,t) = \sum_{j=1}^{N} H_j(t)\,\phi_j(x,y)$$

- FE EQUATIONS FOR $S_s \frac{\partial h}{\partial t} - K\left(\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2}\right) = f(x,y,t)$

$$\int_0^{L_y}\int_0^{L_x} \underbrace{\left[S_s \frac{\partial \hat{h}}{\partial t} - K\left(\frac{\partial^2 \hat{h}}{\partial x^2} + \frac{\partial^2 \hat{h}}{\partial y^2}\right) - f\right]}_{\substack{R(x,y) \\ \text{residual}}} \phi_i(x,y)\,dx\,dy = 0$$

- INTEGRATION BY PARTS Green's theorem (multidimensional space)

$$\int_{\Omega} \left(\frac{\partial^2 \hat{h}}{\partial x^2} + \frac{\partial^2 \hat{h}}{\partial y^2} \right) \phi_i(x,y)\, dx\, dy$$

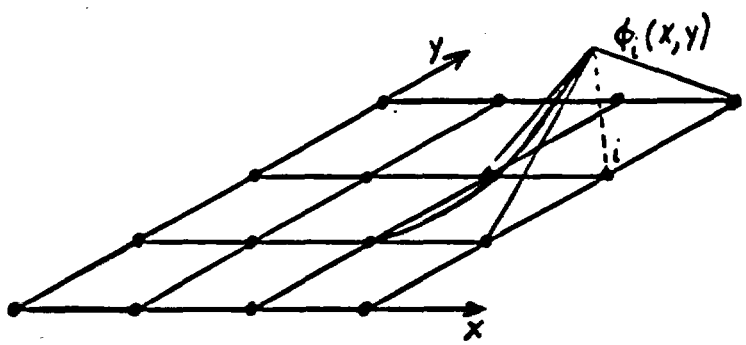
normal flux

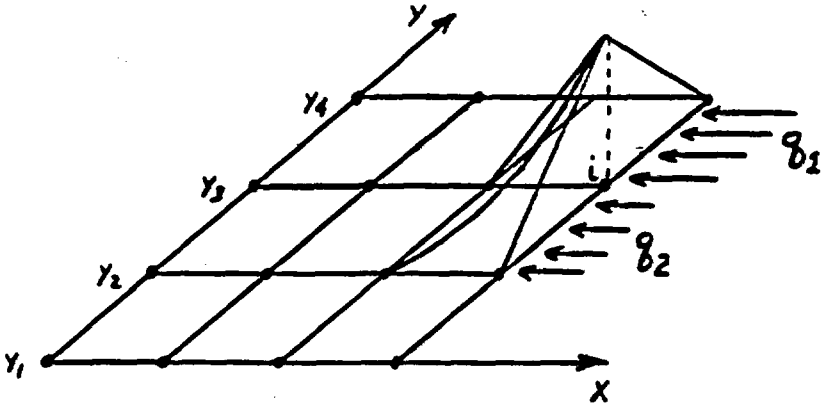
$$= \int_{\partial\Omega} \phi_i \frac{\partial \hat{h}}{\partial n}\, ds - \int_{\Omega} \left(\frac{\partial \hat{h}}{\partial x} \frac{\partial \phi_i}{\partial x} + \frac{\partial \hat{h}}{\partial y} \frac{\partial \phi_i}{\partial y} \right) dx\, dy$$

(BOUNDARY OF Ω)

- SECOND-TYPE BOUNDARY CONDITIONS

  INCORPORATE B.C. THROUGH BOUNDARY INTEGRAL

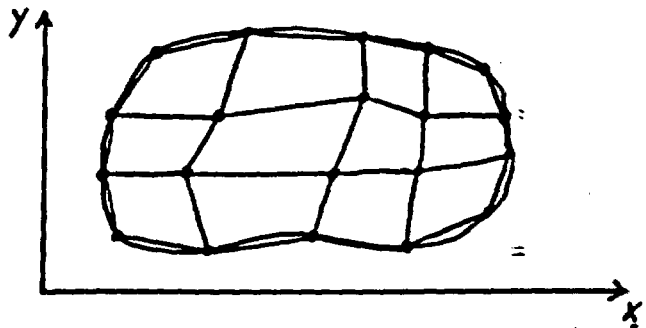




$$K \int_{\partial\Omega} \phi_i \frac{\partial \hat{h}}{\partial n} \, ds = \int_{y_2}^{y_3} (+q_2)\, \phi_i(y)\, dy + \int_{y_3}^{y_4} (+q_1)\, \phi_i(y)\, dy$$

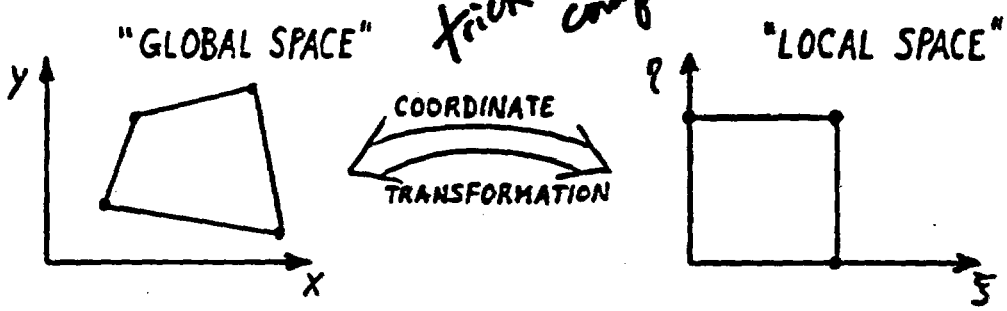
$$= q_2 \left(\frac{y_3 - y_2}{2} \right) + q_1 \left(\frac{y_4 - y_3}{2} \right)$$

NON-RECTANGULAR ELEMENTS



trick to be able to compute irregular polygons

TYPICAL ELEMENT



- DEFINE BASIS FUNCTIONS IN "LOCAL SPACE"

$$\hat{h} = \sum_{j=1}^{N} H_j(t)\, \phi_j(\xi, \eta)$$

- PERFORM INTEGRATIONS IN "LOCAL SPACE"

$$\int_y \int_x F(x,y)\, dx\, dy = \int_\eta \int_\xi F\big(x(\xi,\eta), y(\xi,\eta)\big) \det J \; d\xi\, d\eta$$

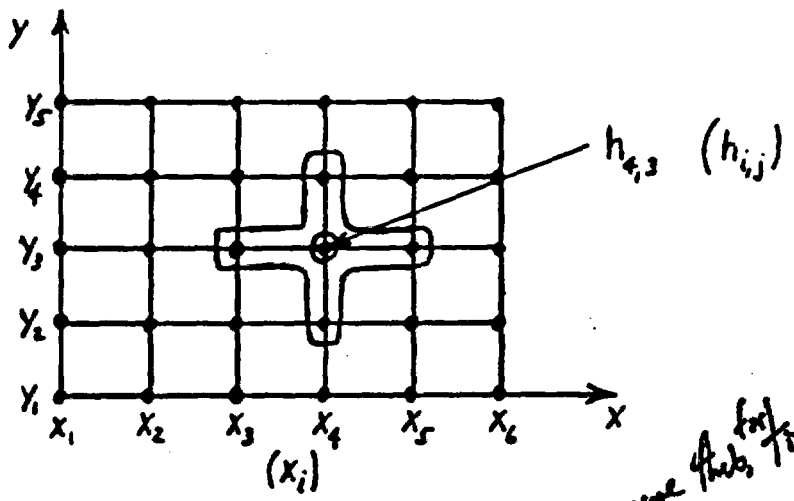
ALTERNATING - DIRECTION METHODS

- ORIGINAL IDEA BY PEACEMAN AND RACHFORD (1955)

tried to solve 2-D problem using 1-D numerics & succeeded.

- CONSIDER 2-D GROUNDWATER FLOW

$$\frac{\partial h}{\partial t} - \frac{\partial^2 h}{\partial x^2} - \frac{\partial^2 h}{\partial y^2} = 0 \,, \qquad \begin{array}{l} 0 \le x \le L_x \\ 0 \le y \le L_y \\ t > 0 \end{array}$$



assume fluids for first-step

STANDARD 2-D FDM (CRANK-NICOLSON):

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

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

TO SOLVE RESULTING MATRIX EQUATION

NUMBER OF OPERATIONS $\propto N^4$

FOR GRID OF $N \times N$ NODES.

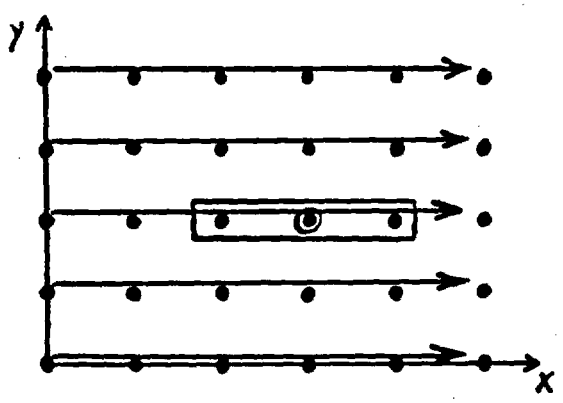
ALTERNATING-DIRECTION IMPLICIT (ADI) METHOD

- GO FROM TIME LEVEL n TO $n+1$ IN TWO STEPS
- EACH STEP INVOLVES ONLY "1-D" MATRIX SOLUTIONS
- STEP 1:

$$\frac{h_{i,j}^{n+\frac{1}{2}} - h_{i,j}^{n}}{\Delta t/2} - \frac{h_{i+1,j}^{n+\frac{1}{2}} - 2h_{i,j}^{n+\frac{1}{2}} + h_{i-1,j}^{n+\frac{1}{2}}}{(\Delta x)^2} = \frac{h_{i,j-1}^{n} - 2h_{i,j}^{n} + h_{i,j+1}^{n}}{(\Delta y)^2}$$

(IMPLICIT IN X, EXPLICIT IN Y)

now can go from 5 unk. to 3-, neighbors on a line

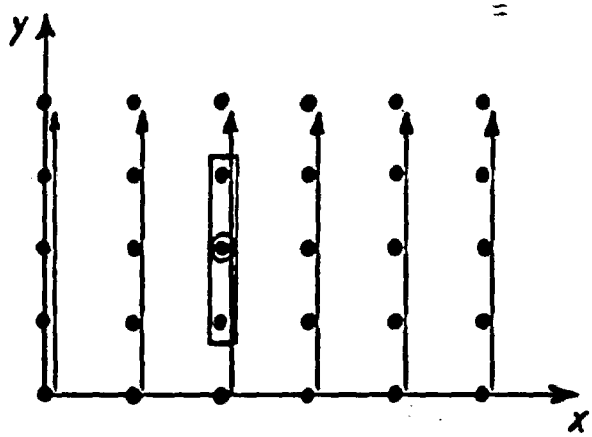


SOLVE FOR $h_{i,j}^{n+1/2}$ AT EVERY NODE.

STEP 2 :

$$\frac{h_{i,j}^{n+1} - h_{i,j}^{n+\frac{1}{2}}}{\Delta t/2} - \frac{h_{i,j-1}^{n+1} - 2h_{i,j}^{n+1} + h_{i,j+1}^{n+1}}{(\Delta x)^2} = \frac{h_{i-1,j}^{n+\frac{1}{2}} - 2h_{i,j}^{n+\frac{1}{2}} + h_{i+1,j}^{n+\frac{1}{2}}}{(\Delta y)^2}$$

(IMPLICIT IN Y, EXPLICIT IN X)



SOLVE FOR $h_{i,j}^{n+1}$ AT EVERY NODE

- GO TO NEXT TIME STEP AND REPEAT PROCEDURE
- TO SOLVE MATRIX EQUATIONS

  NUMBER OF OPERATIONS $\propto N^2$

  FOR GRID OF N×N NODES
- SIGNIFICANT SAVINGS ON STORAGE REQUIREMENTS
- DISADV - introduce an additional error term, but can evaluate it.

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Babu, D.K. and G.F. Pinder, "A Finite Element-Finite Difference Alternating Direction Algorithm for for Three-Dimensional Groundwater Transport," *Advances in Water Resources, 7* (3), 116-119, 1984.

Based on PTC idea.

Celia, M.A. and G.F. Pinder, "An Analysis of Alternating-Direction Methods for Parabolic Equations," ~~accepted for publication,~~ *Numerical Methods for Partial Differential Equations,* 1985. (10)

Douglas, J., Jr. and T. Dupont, "Alternating-Direction Galerkin Methods on Rectangles", in *Numerical Solution of Partial Differential Equations,* Vol. 2, Synspade 1970, B. Hubbard (ed.), Academic Press, 133-214, 1971.

Peaceman, D.W. and H.H. Rachford, "The Numerical Solution of Parabolic and Elliptic Equations," *S.I.A.M. Journal, 3,* 28-41, 1955.

SOLUTIONS OF THE TRANSPORT EQUATION

- EQUATION DESCRIBING MOVEMENT OF DISSOLVED CONTAMINANT (1-D)

$$\frac{\partial c}{\partial t} + V\frac{\partial c}{\partial x} - D\frac{\partial^2 c}{\partial x^2} = 0 , \qquad 0 \le x \le L$$

$$C(0,t) = C_1$$

$$\frac{\partial c}{\partial x}(L,t) = 0$$

$$C(x,0) = C_0(x)$$

C = CONCENTRATION (M/L^3)

V = FLUID VELOCITY (L/T)

D = DIFFUSION COEFF. (L^2/T)

(V, D CONSTANTS)

- FDM APPROXIMATION

$$\left.\frac{\partial c}{\partial t}\right|_i^{n+\theta} = \frac{c_i^{n+1} - c_i^n}{\Delta t} - \frac{1-2\theta}{2}(\Delta t)\left.\frac{\partial^2 c}{\partial t^2}\right|_i^{n+\theta} + O((\Delta t)^2)$$

$$\left.\frac{\partial c}{\partial x}\right|_i^{n+\theta} = \frac{c_{i+1}^{n+\theta} - c_{i-1}^{n+\theta}}{2(\Delta x)} + O((\Delta x)^2)$$

$$\left.\frac{\partial^2 c}{\partial x^2}\right|_i^{n+\theta} = \frac{c_{i+1}^{n+\theta} - 2c_i^{n+\theta} + c_{i-1}^{n+\theta}}{(\Delta x)^2} + O((\Delta x)^2)$$

$$\left.c\right|_i^{n+\theta} = \theta c_i^{n+1} + (1-\theta) c_i^n + O((\Delta t)^2)$$

time derivative space derivative

implicit diff explicit diff

$$\boxed{\begin{aligned} &\frac{c_i^{n+1} - c_i^n}{\Delta t} + V\left[\theta\,\frac{c_{i+1}^{n+1} - c_{i-1}^{n+1}}{2\,\Delta x}\right] - D\left[\theta\,\frac{c_{i+1}^{n+1} - 2c_i^{n+1} + c_{i-1}^{n+1}}{(\Delta x)^2}\right] \\ &= D(1-\theta)\,\frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{(\Delta x)^2} - V(1-\theta)\,\frac{c_{i+1}^n - c_{i-1}^n}{2\,\Delta x} \end{aligned}}$$

THIS IS AN $O(\Delta t^*, (\Delta x)^2)$ APPROXIMATION TO

$$\left.\left(\frac{\partial c}{\partial t} + V\frac{\partial c}{\partial x} - D\frac{\partial^2 c}{\partial x^2}\right)\right|_i^{n+\theta} = 0$$

TRUNCATION ERROR $= \frac{1-2\theta}{2}(\Delta t)\left.\frac{\partial^2 c}{\partial t^2}\right|_i^{n+\theta} + O((\Delta t)^2, (\Delta x)^2)$

- FEM APPROXIMATION

TRIAL FUNCTION

$$\hat{C}(x,t) = \sum_{j=1}^{N} C_j(t)\,\phi_j(x)$$

RESIDUAL

$$R(x,t) = \frac{\partial \hat{C}}{\partial t} + V\frac{\partial \hat{C}}{\partial x} - D\frac{\partial^2 \hat{C}}{\partial x^2}$$

GALERKIN MWR

$$\int_0^L \left(\frac{\partial \hat{C}}{\partial t} + V\frac{\partial \hat{C}}{\partial x} - D\frac{\partial^2 \hat{C}}{\partial x^2}\right)\phi_i(x)\,dx = 0$$

INTEGRATE IN SPACE (PIECEWISE LINEAR ϕ_j's)

$$\frac{1}{6}\frac{dC_{i-1}}{dt} + \frac{2}{3}\frac{dC_i}{dt} + \frac{1}{6}\frac{dC_{i+1}}{dt} + V\frac{C_{i+1} - C_{i-1}}{2\Delta x}$$

$$- D\frac{C_{i+1} - 2C_i + C_{i-1}}{(\Delta x)^2} = 0$$

FINITE DIFFERENCE IN TIME

$$\frac{1}{6}\,\frac{C_{i-1}^{n+1}-C_{i-1}^{n}}{\Delta t}+\frac{2}{3}\,\frac{C_{i}^{n+1}-C_{i}^{n}}{\Delta t}+\frac{1}{6}\,\frac{C_{i+1}^{n+1}-C_{i+1}^{n}}{\Delta t}$$

$$+\,V\,\frac{C_{i+1}^{n+\theta}-C_{i-1}^{n+\theta}}{2\Delta x}-D\,\frac{C_{i+1}^{n+\theta}-2C_{i}^{n+\theta}+C_{i-1}^{n+\theta}}{(\Delta x)^{2}}=0$$

STANDARD

EXAMPLE PROBLEM

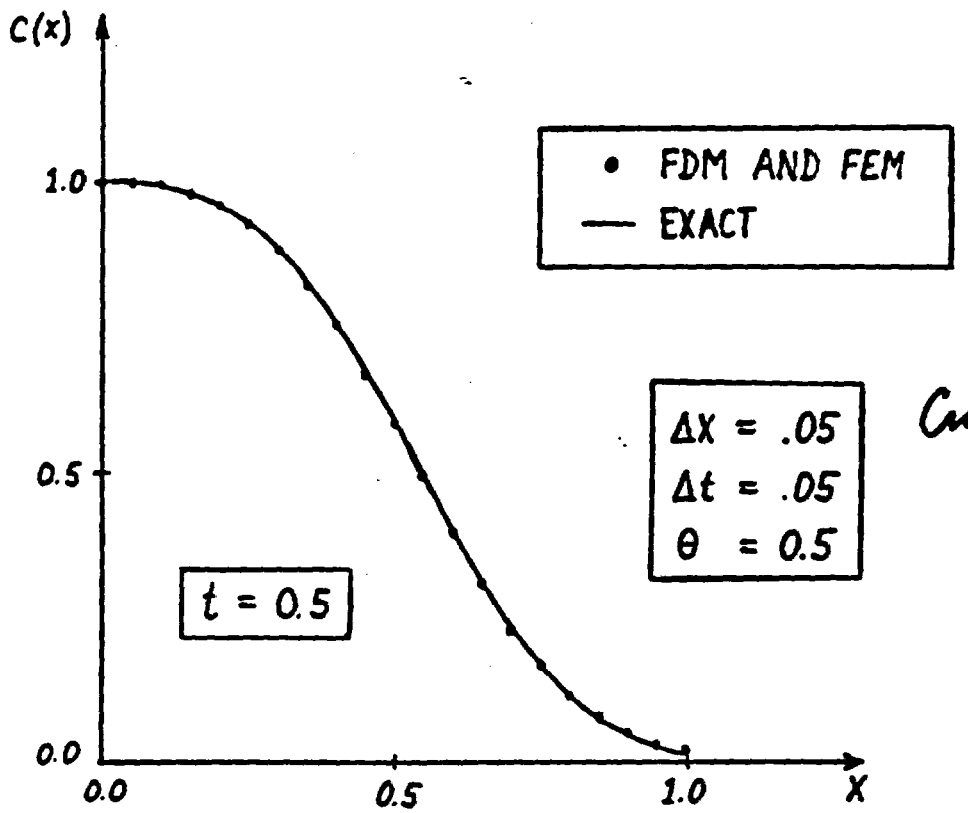
$$\frac{\partial c}{\partial t} + V\frac{\partial c}{\partial x} - D\frac{\partial^2 c}{\partial x^2} = 0, \qquad \begin{array}{l} 0 \le x \le L \\ t > 0 \end{array}$$

$$c(0,t) = 1$$

$$\frac{\partial c}{\partial x}(L,t) = 0$$

$$c(x,0) = 0$$

$D = .05$, $V = 1.0$

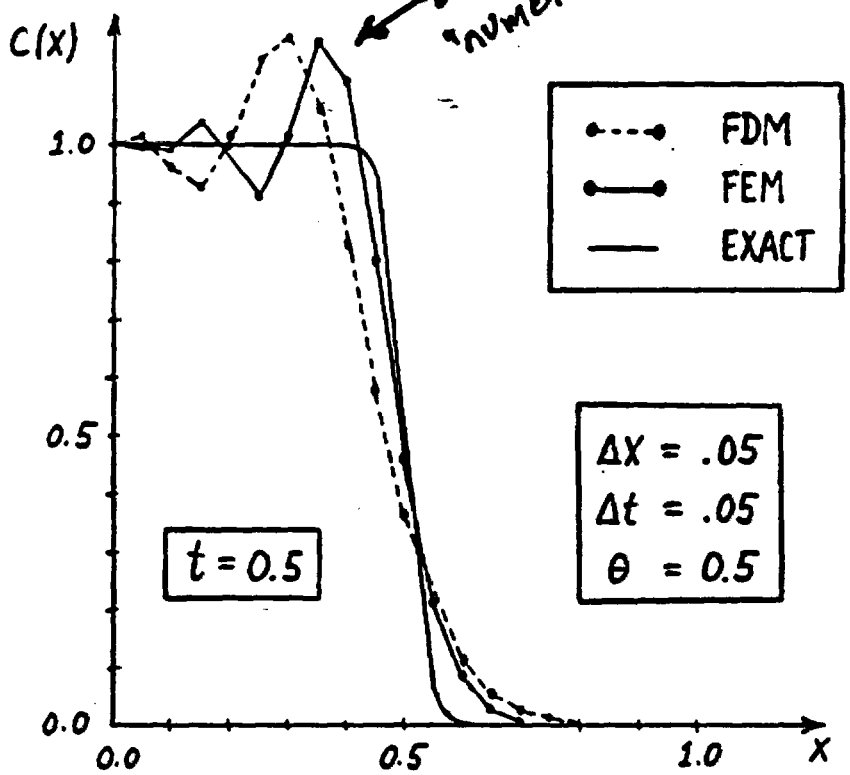


Crank-Nicholson

$$\left(\frac{V(\Delta X)}{D} = 1.0\right)$$

Grid-Peclet number - dimensionless group number

D = .001 , V = 1.0

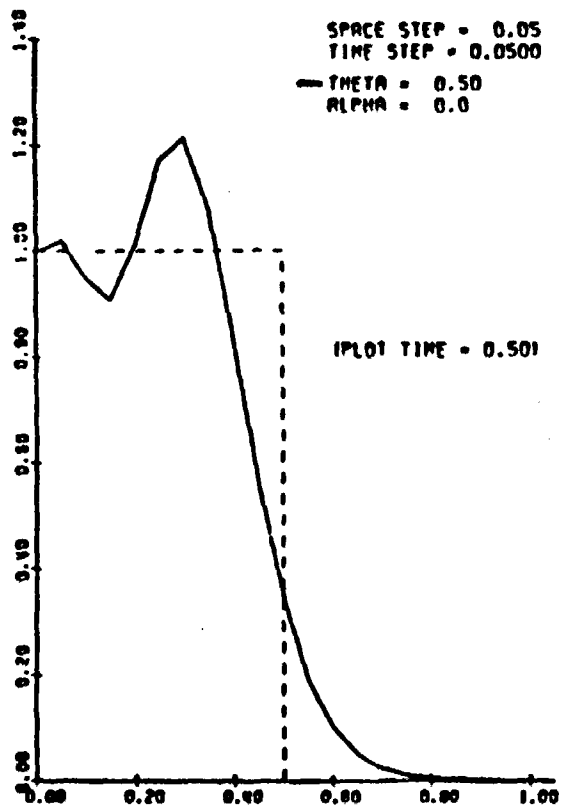


$$\left(\frac{V(\Delta X)}{D} = 50. \right)$$

crank-nicolson

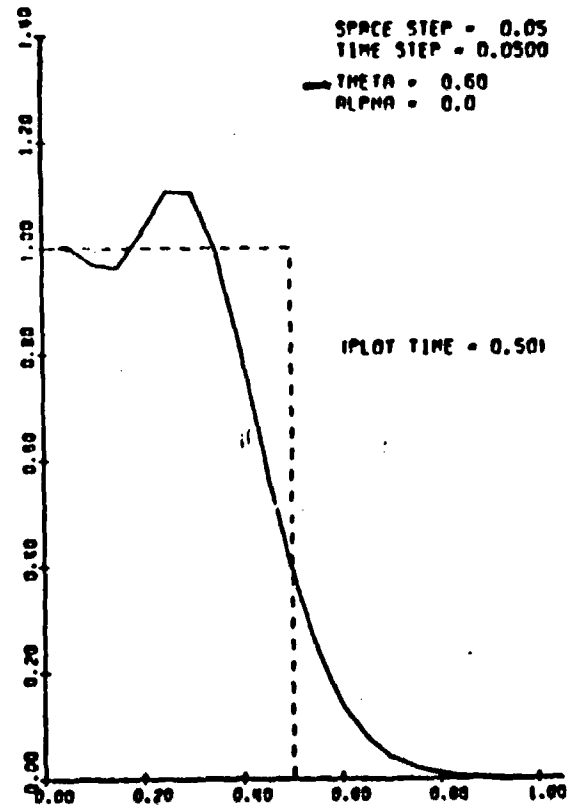
FINITE DIFFERENCE SOLUTION
FOR 1ST ORDER HYPERBOLIC EQUATION

$U_X + U_T = 0$



FINITE DIFFERENCE SOLUTION
FOR 1ST ORDER HYPERBOLIC EQUATION

$U_X + U_T = 0$



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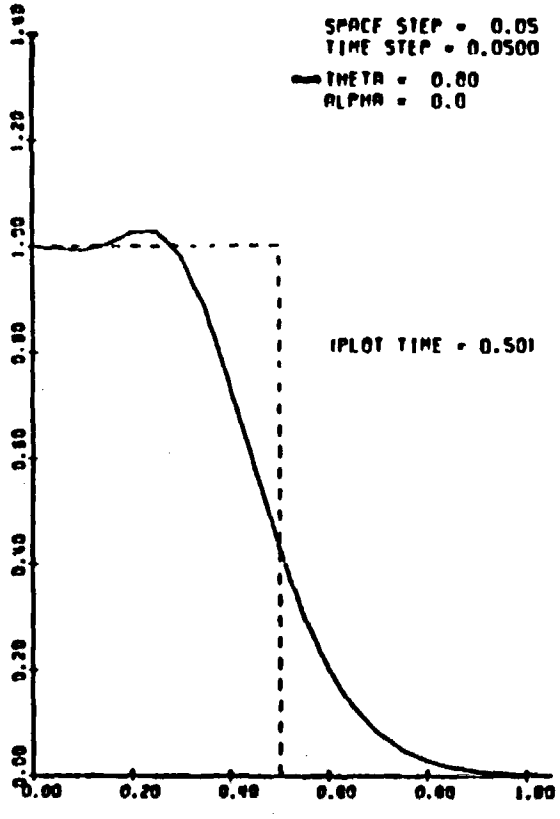
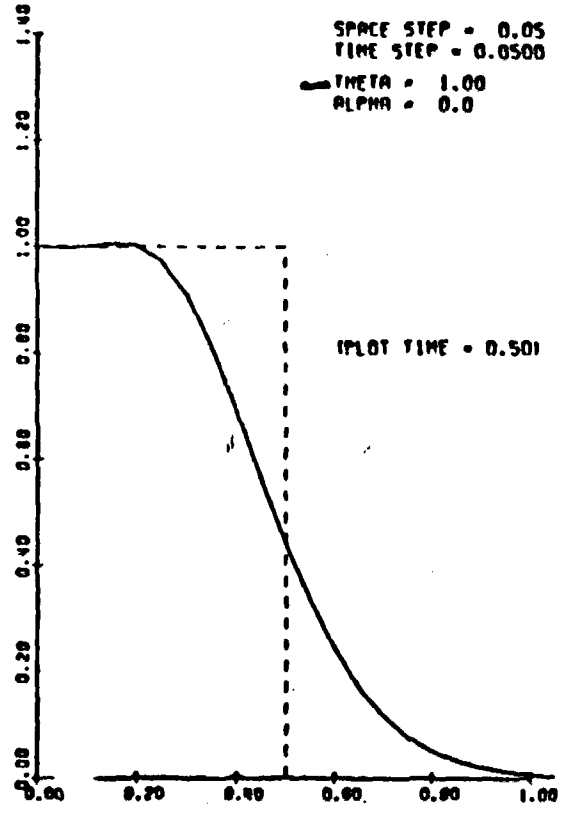


FINITE DIFFERENCE SOLUTION
FOR 1ST ORDER HYPERBOLIC EQUATION

$U_X + U_T = 0$



- CONSIDER AN ALTERNATIVE FD APPROXIMATION

$$\left.\frac{\partial c}{\partial x}\right|_i^{n+\theta} \doteq \frac{C_i^{n+\theta} - C_{i-1}^{n+\theta}}{\Delta x}$$

ALL OTHER APPROXIMATIONS AS BEFORE

"UPSTREAM WEIGHTED" APPROXIMATION

- GENERAL UPSTREAM WEIGHTED FORMULATION

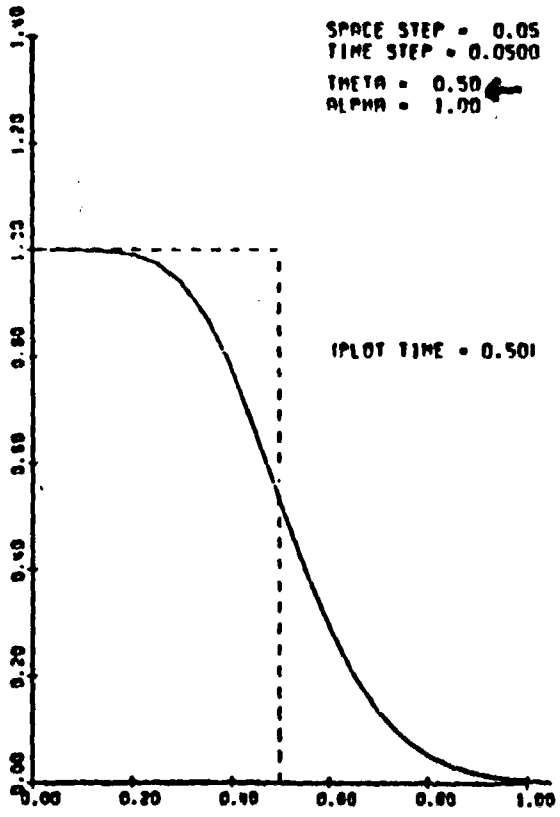
$$\left.\frac{\partial c}{\partial x}\right|_i^{n+\theta} = \alpha \frac{C_i^{n+\theta} - C_{i-1}^{n+\theta}}{\Delta x} + (1-\alpha) \frac{C_{i+1}^{n+\theta} - C_{i-1}^{n+\theta}}{2\Delta x}$$

ALL OTHER APPROXIMATIONS AS BEFORE

α = UPSTREAM WEIGHTING PARAMETER

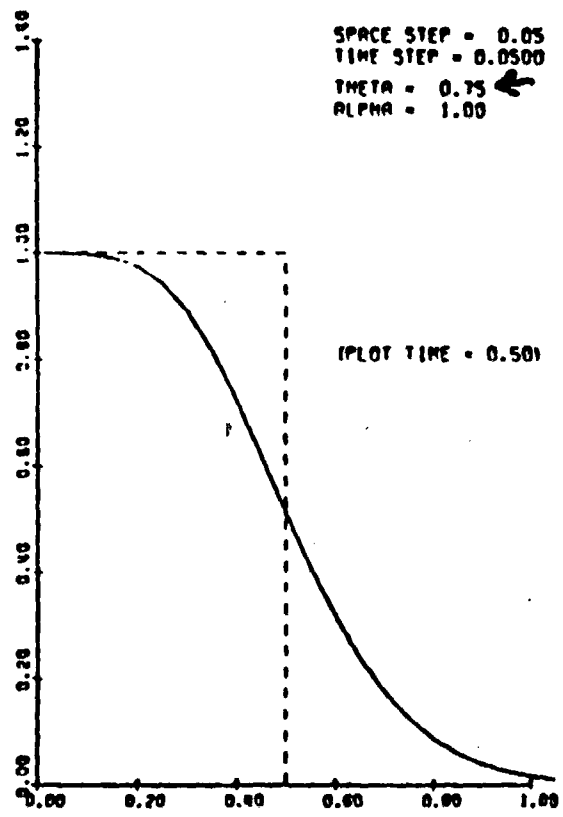
FINITE DIFFERENCE SOLUTION
FOR 1ST ORDER HYPERBOLIC EQUATION

$U_X + U_T = 0$



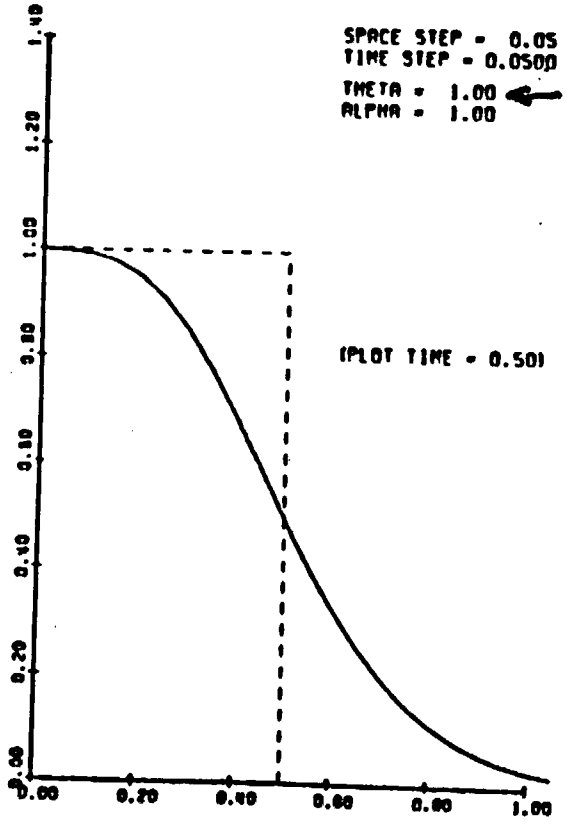
FINITE DIFFERENCE SOLUTION
FOR 1ST ORDER HYPERBOLIC EQUATION

$U_X + U_T = 0$



FINITE DIFFERENCE SOLUTION
FOR 1ST ORDER HYPERBOLIC EQUATION

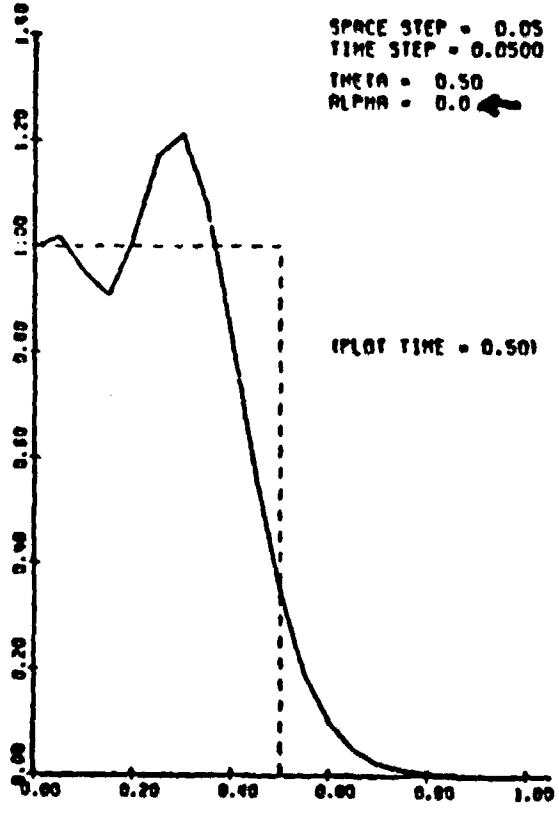
$U_x + U_t = 0$



0% ≡ crank-nicolson

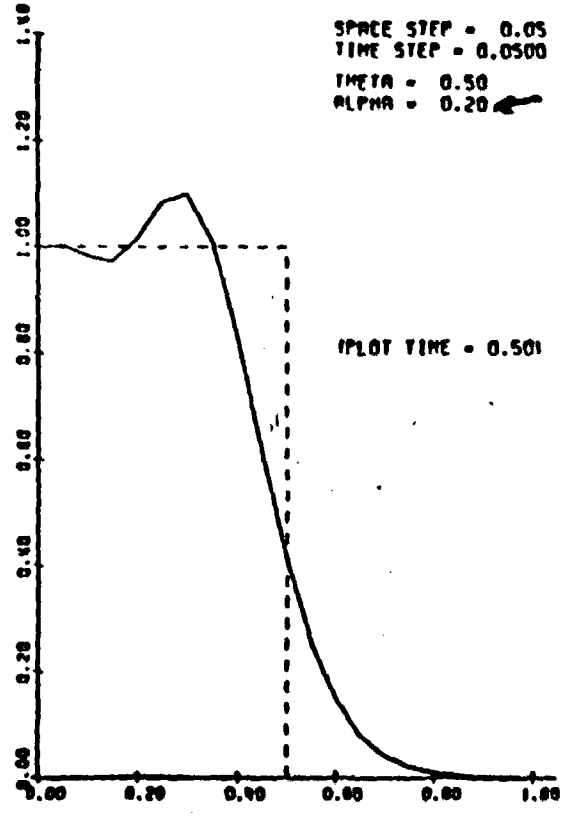
FINITE DIFFERENCE SOLUTION
FOR 1ST ORDER HYPERBOLIC EQUATION

$u_x + u_T = 0$



FINITE DIFFERENCE SOLUTION
FOR 1ST ORDER HYPERBOLIC EQUATION

$u_x + u_T = 0$



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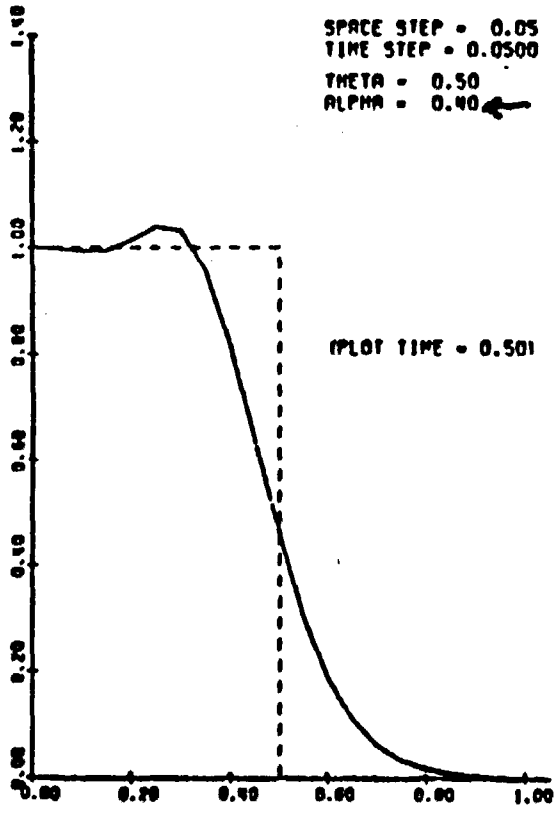

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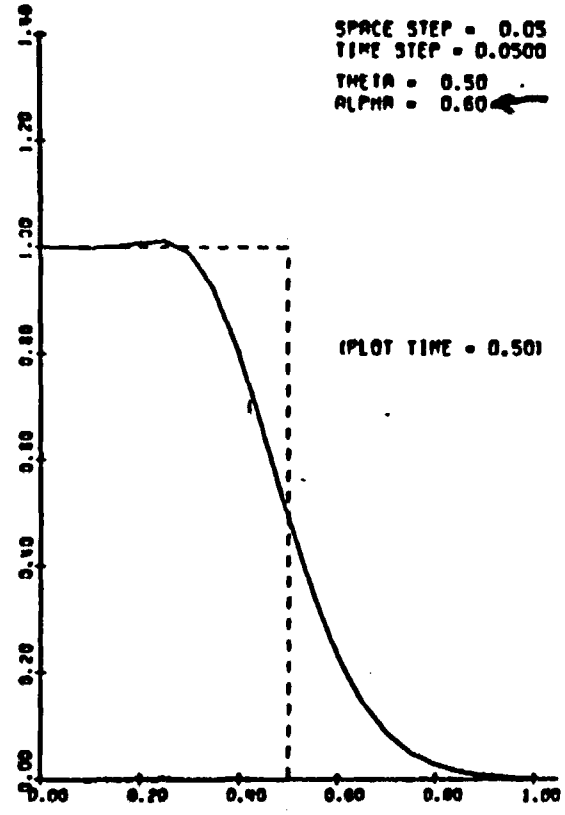

FINITE DIFFERENCE SOLUTION
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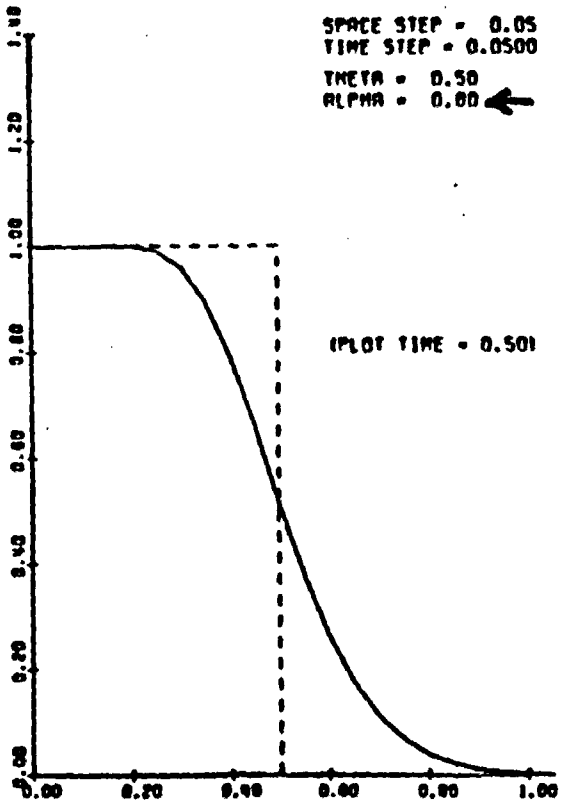
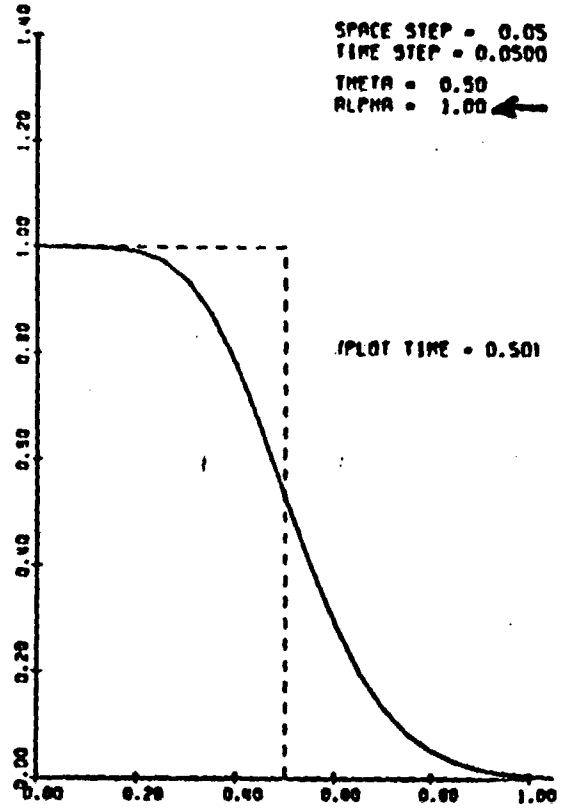
$U_X + U_T = 0$



FINITE DIFFERENCE SOLUTION
FOR 1ST ORDER HYPERBOLIC EQUATION

$U_X + U_T = 0$



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FOR 1ST ORDER HYPERBOLIC EQUATION

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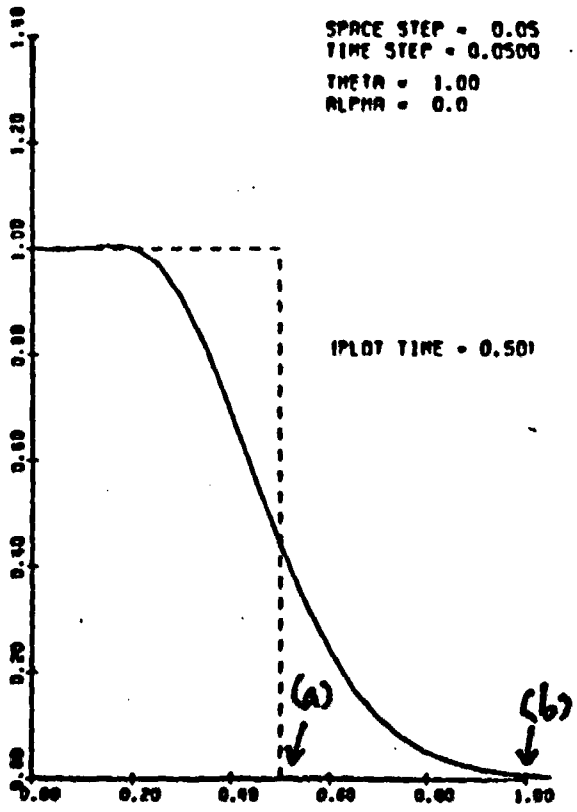

FINITE DIFFERENCE SOLUTION
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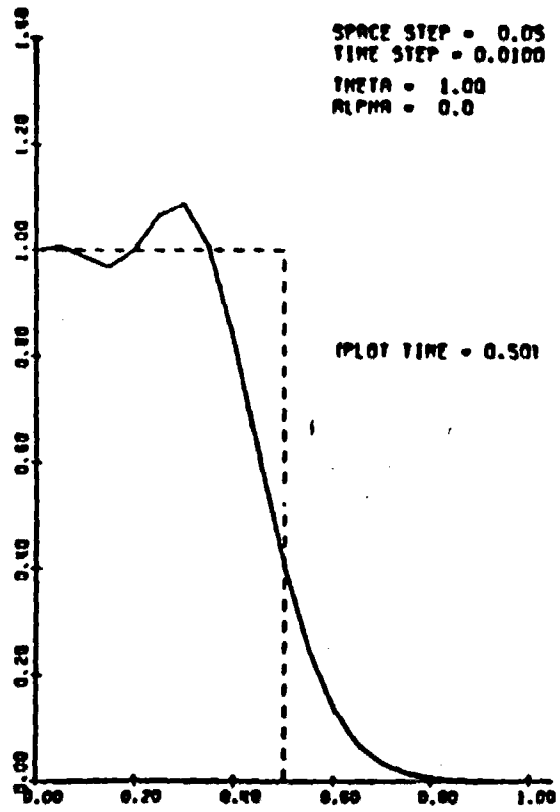
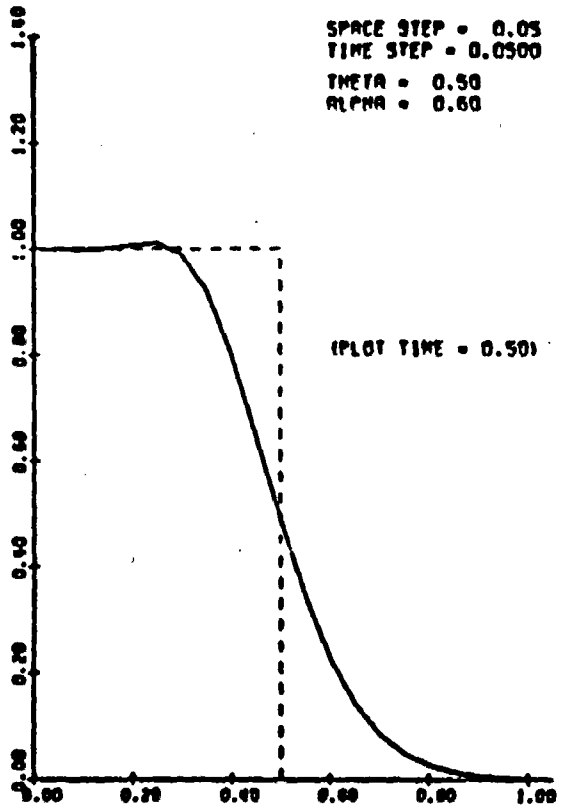


↑
plume front (b)
more than 2x
where it should be (a)

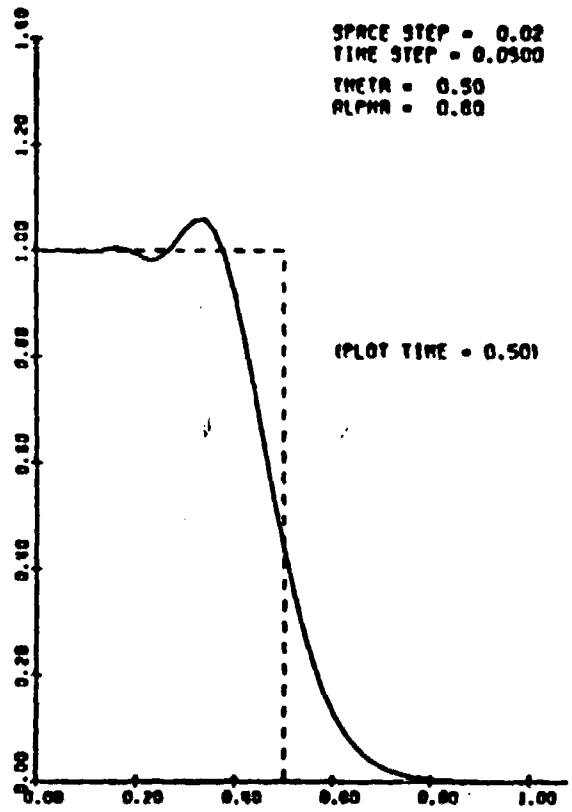
FINITE DIFFERENCE SOLUTION
FOR 1ST ORDER HYPERBOLIC EQUATION

$U_X + U_T = 0$



FINITE DIFFERENCE SOLUTION
FOR 1ST ORDER HYPERBOLIC EQUATION

$U_X + U_T = 0$



GENERAL OBSERVATIONS

1. FEM, FDM SOLUTIONS GOOD FOR LARGE DIFFUSION

2. FOR SOLUTIONS WITH SHARP FRONTS

   A) if $\theta \uparrow$ FROM $0.5 \rightarrow 1.0$ $\Longrightarrow$ MORE SMEARING
   LESS WIGGLES

   B) if $\alpha \uparrow$ FROM $0. \rightarrow 1.0$ $\Longrightarrow$ MORE SMEARING
   LESS WIGGLES

   C) $\Delta t \downarrow$ $\Longrightarrow$ MORE WIGGLES

   D) $\Delta x \downarrow$ $\Longrightarrow$ MORE WIGGLES

GENERAL COMMENTS

Explanation for wiggles & smears

1. LEADING TRUNCATION ERROR TERM FOR FD APPROXIMATION (VARIABLE α, θ) IS:

$$-\left[\frac{\alpha V}{2}(\Delta x)\right]\frac{\partial^2 c}{\partial x^2}\bigg|_i^{n+\theta} + \left[\frac{(1-2\theta)}{2}(\Delta t)\right]\frac{\partial^2 c}{\partial t^2}\bigg|_i^{n+\theta}$$

FD APPROXIMATION IS EQUAL TO:

$$(\text{FD APPROX.}) = \left(\frac{\partial c}{\partial t} + V\frac{\partial c}{\partial x} - D\frac{\partial^2 c}{\partial x^2}\right)\bigg|_i^{n+\theta}$$

$$-\underbrace{\left[\frac{\alpha V}{2}(\Delta x) + \frac{V^2}{2}(2\theta-1)(\Delta t)\right]}_{D^*}\frac{\partial^2 c}{\partial x^2}\bigg|_i^{n+\theta} + \ldots\ldots$$

(A) See my notes V.9, p.12

SO FD EQUATION APPROXIMATES

$$\left[\frac{\partial c}{\partial t} + V\frac{\partial c}{\partial x} - (D+D^*)\frac{\partial^2 c}{\partial x^2}\right]\bigg|_i^{n+\theta} = 0$$

EVEN IF $D=0$, D^* MAY <u>NOT</u> $= 0$

2. "ARTIFICIAL DIFFUSION" $D^* = \alpha \frac{V(\Delta x)}{2} + \frac{V^2}{2}(2\theta - 1)(\Delta t)$

- $\alpha = 0, \quad \theta = 0.5 \Rightarrow D^* = 0$
- $\alpha = 1, \quad \theta = 1.0 \Rightarrow$ LARGEST D^*
- $\uparrow \Delta x$ OR $\uparrow \Delta t \Rightarrow \uparrow D^* \quad (\alpha \neq 0, \theta \neq 0.5)$

nothing to do with physics - totally related to numerical method

3. NOTE THAT

$$\left.\frac{\partial c}{\partial x}\right|_i \approx \alpha \frac{c_i - c_{i-1}}{\Delta x} + (1-\alpha) \frac{c_{i+1} - c_{i-1}}{2\,\Delta x}$$

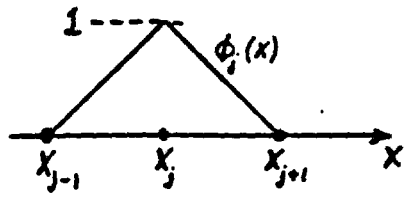
IS EQUIVALENT TO

$$\left.\frac{\partial c}{\partial x}\right|_i \approx \frac{c_{i+1} - c_{i-1}}{2\,\Delta x} - \frac{\alpha(\Delta x)}{2} \underbrace{\left[\frac{c_{i+1} - 2c_i + c_{i-1}}{(\Delta x)^2}\right]}_{\left.\frac{\partial^2 c}{\partial x^2}\right|_i}$$

4. ADD A DIFFUSION TERM DIRECTLY TO THE GOVERNING EQUATION <u>OR</u> ADD DIFFUSION INDIRECTLY BY UPSTREAM WEIGHTING. RESULT IS THE SAME.

UPSTREAM WEIGHTING FOR FINITE ELEMENTS

$$\hat{C}(x,t) = \sum_{j=1}^{N} C_j(t)\,\phi_j(x)$$

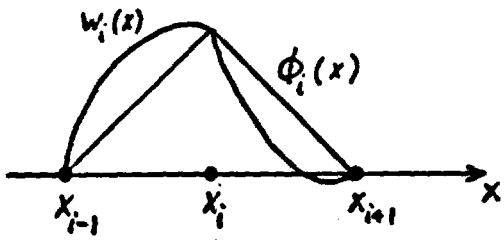


STANDARD FEM

$$\int_0^L \left(\frac{\partial \hat{c}}{\partial t} + V \frac{\partial \hat{c}}{\partial x} - D \frac{\partial^2 \hat{c}}{\partial x^2} \right) \phi_i(x)\, dx = 0$$

UPSTREAM WEIGHTED FEM

$$\int_0^L \frac{\partial \hat{c}}{\partial t} \phi_i\, dx + \int_0^L V \frac{\partial \hat{c}}{\partial x} w_i(x)\, dx - \int_0^L D \frac{\partial^2 \hat{c}}{\partial x^2} \phi_i\, dx = 0$$



$$W_i(x) = \begin{cases} \dfrac{x - x_{i-1}}{\Delta x} - \dfrac{3\alpha (x - x_i)(x - x_{i-1})}{(\Delta x)^2}, & x_{i-1} \le x \le x_i \\ \dfrac{x_{i+1} - x}{\Delta x} + \dfrac{3\alpha (x - x_i)(x - x_{i+1})}{(\Delta x)^2}, & x_i \le x \le x_{i+1} \\ 0, & \text{ALL OTHER } x \end{cases}$$

<u>INTEGRATE FIRST-ORDER SPACE DERIVATIVE</u>

$$\int_0^L V \frac{\partial \hat{c}}{\partial x} W_i(x)\, dx = (\Delta x)\left[\frac{V}{\Delta x}\left(\frac{1-\alpha}{2} C_{i+1} - \alpha C_i - \frac{1+\alpha}{2} C_{i-1}\right)\right]$$

$$= (\Delta x)\left\{\underbrace{V\left[\alpha \frac{C_i - C_{i-1}}{\Delta x} + (1-\alpha)\frac{C_{i+1} - C_{i-1}}{2(\Delta x)}\right]}_{\text{UPSTREAM-WEIGHTED FD APPROXIMATION}}\right\}$$

lots of ways to get upstream weighting — almost all of them look like this

REFERENCES

Gray, W.G. and G.F. Pinder, "An Analysis of the Numerical Solution of the Transport Equation," *Water Resources Research, 12* (3), 547-555, 1976.

Jensen, O.K. and B.A. Finlayson, "Oscillation Limits for Weighted Residual Methods Applied to Convective Diffusion Equations," *Int. J. Numer. Meth. Eng., 15,* 1681-1689, 1980.