

Overhead Slides for
Chapter 6
of
Fundamentals of
Atmospheric Modeling

by

Mark Z. Jacobson

Department of
Civil & Environmental Engineering
Stanford University
Stanford, CA 94305-4020

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ODEs and PDEs

Ordinary differential equation (ODE)

Equation with one independent variable

Partial differential equation (PDE)

Equation with more than one independent variable

Order

Highest derivative of an equation

Degree

Highest polynomial value of the highest derivative

Initial value problem

Conditions are known at one end of domain but not other

Boundary value problem

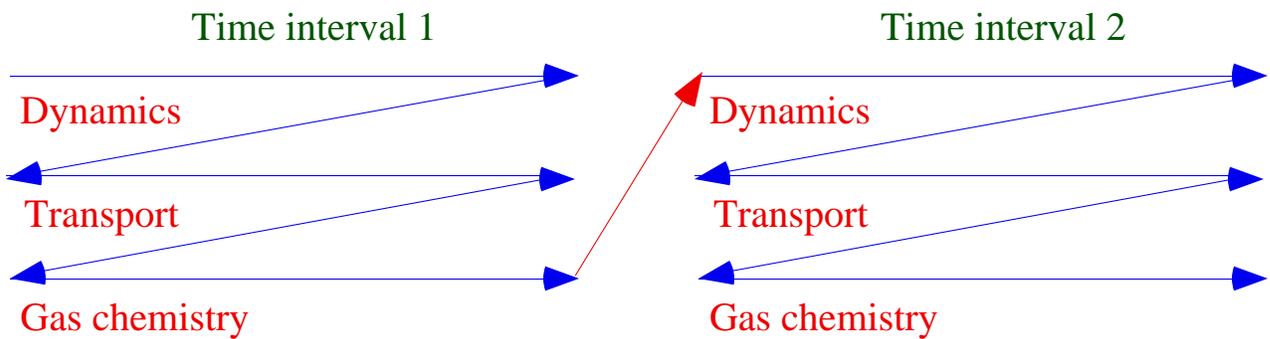
Conditions are known at both ends of domain

Table 6.1. Ordinary and partial differential equations.

	Ordinary Differential Equations	Partial Differential Equations
First-order, first degree	(a) $\frac{dN}{dt} = 16 - 4N^2$	(e) $\frac{N}{t} + \frac{(uN)}{x} = 0$
First-order, first degree	(b) $\frac{dN}{dt} = 3AB - 4NC$	(f) $\frac{u}{t} + u\frac{u}{x} + v\frac{u}{y} = 0$
Second-order, first-degree	(c) $\frac{d^2 N}{dt^2} + \frac{dN}{dt} + 5t = 0$	(g) $\frac{2N}{t^2} + \frac{2N}{x^2} = 3t^2 + x$
Second-order, second-degree	(d) $\frac{d^2 N}{dt^2} + \frac{dN}{dt} + 4 = 0$	(h) $\frac{2N}{t^2} + \frac{N}{x} = t - x$

Operator Splitting

Fig. 6.1. Operator-splitting scheme.



Operator-split advection-diffusion equations

$$\frac{N}{t} + \frac{(uN)}{x} - \frac{K_{h,xx}}{x} \frac{N}{x} = 0 \quad (6.1)$$

$$\frac{N}{t} + \frac{(vN)}{y} - \frac{K_{h,yy}}{y} \frac{N}{y} = 0 \quad (6.2)$$

$$\frac{N}{t} + \frac{(wN)}{z} - \frac{K_{h,zz}}{z} \frac{N}{z} = 0 \quad (6.3)$$

Operator-split external source / sink terms

$$\frac{N}{t} = \sum_{n=1}^{N_{e,t}} R_n \quad (6.4)$$

Consistency, Convergence, Stability

Convergence of finite difference analog

$$\frac{N}{x} = \lim_{x \rightarrow 0} \left\| \frac{N}{x} \right\| \quad (6.6)$$

Consistency

$$\lim_{x \rightarrow 0} \left\| \text{T.E.} \frac{N}{x} \right\| = 0 \quad (6.7)$$

Convergence of overall solution

$$\lim_{x, t \rightarrow 0} \left\| N_{e,x,t} - N_{f,x,t} \right\| = 0 \quad (6.8)$$

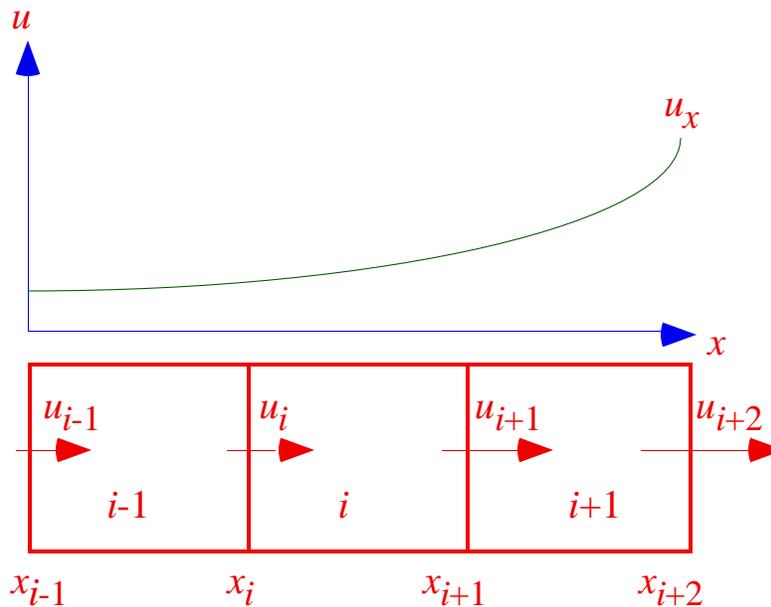
Stability

$$\lim_t \left\| N_{e,x,t} - N_{f,x,t} \right\| < C \quad (6.9)$$

Finite Difference Approximation

Replacement of continuous differential operator (d) with discrete difference analog () written in terms of a finite number of values along a temporal or spatial direction.

Fig. 6.2. Discretization of u_x



Differences at point x_i

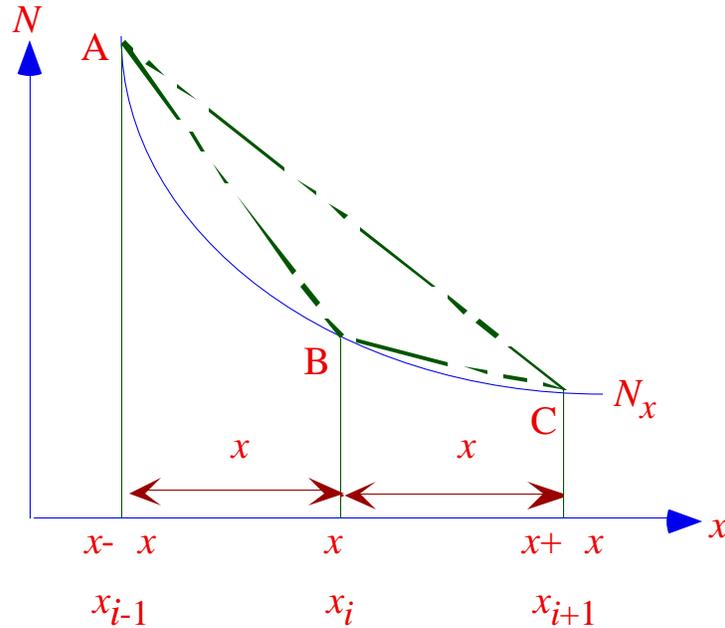
- $\frac{du}{dx} \rightarrow u_i = u_{i+1} - u_{i-1}$ central difference
- $\rightarrow u_i = u_{i+1} - u_i$ forward difference
- $\rightarrow u_i = u_i - u_{i-1}$ backward difference

Central difference approximation to tangent slope at x_i

$$\frac{u}{x} \quad \frac{u_i}{x_i} = \frac{u_{i+1} - u_{i-1}}{x_{i+1} - x_{i-1}} \quad (6.10)$$

Taylor Series Expansions

Fig. 6.3. Central (AC), forward (BC), and backward (AB) approximations to slope of tangent at point B.



Taylor series expansion at point $x + x$

$$N_{x+x} = N_x + x \frac{N_x}{x} + \frac{1}{2} x^2 \frac{2N_x}{x^2} + \frac{1}{6} x^3 \frac{3N_x}{x^3} + \frac{1}{24} x^4 \frac{4N_x}{x^4} + \dots$$

(6.11)

Taylor series expansion at point $x - x$

$$N_{x-x} = N_x - x \frac{N_x}{x} + \frac{1}{2} x^2 \frac{2N_x}{x^2} - \frac{1}{6} x^3 \frac{3N_x}{x^3} + \frac{1}{24} x^4 \frac{4N_x}{x^4} - \dots$$

(6.12)

Finite Difference Approximations

Sum the Taylor series expansions

$$N_{x+\Delta x} + N_{x-\Delta x} = 2N_x + \Delta x^2 \frac{2N_x}{x^2} + \frac{1}{12} \Delta x^4 \frac{4N_x}{x^4} + \dots \quad (6.13)$$

Rearrange

$$\frac{2N_x}{x^2} = \frac{N_{x+\Delta x} - 2N_x + N_{x-\Delta x}}{\Delta x^2} + O(\Delta x^2) \quad (6.14)$$

Truncation error

$$O(\Delta x^2) = -\frac{1}{12} \Delta x^2 \frac{4N_x}{x^4} - \dots \quad (6.15)$$

Second-order central difference approximation of 2nd derivative

$\frac{2N_x}{x^2} - \frac{N_{x+\Delta x} - 2N_x + N_{x-\Delta x}}{\Delta x^2} \quad (6.16)$

Finite Difference Approximations

Subtract the Taylor series expansions

$$N_{x+\Delta x} - N_{x-\Delta x} = 2\Delta x \frac{N_x}{\Delta x} + \frac{1}{3} \Delta x^3 \frac{\partial^3 N_x}{\partial x^3} + \dots \quad (6.17)$$

Rearrange

$$\frac{N_x}{\Delta x} = \frac{N_{x+\Delta x} - N_{x-\Delta x}}{2\Delta x} + O(\Delta x^2) \quad (6.18)$$

Truncation error

$$O(\Delta x^2) = -\frac{1}{6} \Delta x^2 \frac{\partial^3 N_x}{\partial x^3} - \dots \quad (6.19)$$

Second-order central difference approximation of 1st deriv.

$\frac{N_x}{\Delta x} \approx \frac{N_{x+\Delta x} - N_{x-\Delta x}}{2\Delta x} = \frac{N_{i+1} - N_{i-1}}{2\Delta x} \quad (6.20)$

Finite Difference Approximations

First two terms of Taylor series

First-order forward difference approximation of 1st deriv.

$$\frac{N_x}{x} \approx \frac{N_{x+\Delta x} - N_x}{\Delta x} = \frac{N_{i+1} - N_i}{\Delta x} \quad (6.21)$$

First-order backward difference approximation of 1st deriv.

$$\frac{N_x}{x} \approx \frac{N_x - N_{x-\Delta x}}{\Delta x} = \frac{N_i - N_{i-1}}{\Delta x} \quad (6.22)$$

Differencing Time Derivative

Central , forward , and backward difference approximations

$$\frac{N_t}{t} \approx \frac{N_{t+h} - N_{t-h}}{2h} \quad (6.23)$$

$$\frac{N_t}{t} \approx \frac{N_{t+h} - N_t}{h} \quad (6.23)$$

$$\frac{N_t}{t} \approx \frac{N_t - N_{t-h}}{h} \quad (6.23)$$

High Order Approximations

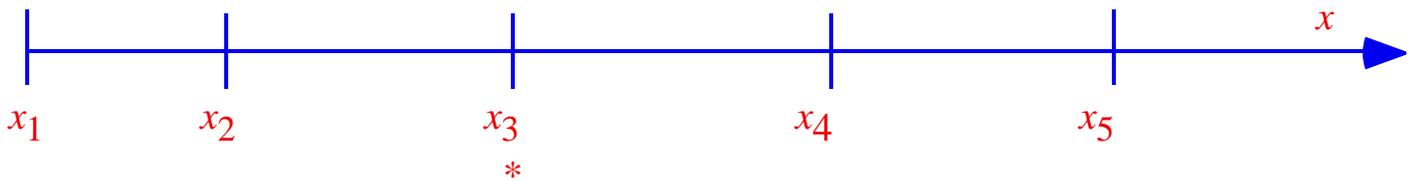
Finite difference approximation of $\frac{d^m N}{dx^m}$

- o Order of derivative = m
- o Approximation expanded across q discrete nodes
- o Minimum number of nodes = $m + 1$
- o Maximum order of approximation = $q - m$

Example

Order of derivative:	$m = 1$
Number of nodes	$q = 5$
---> Order of approximation:	$q - m = 4$

Fig. 6.4. Grid spacing where $q = 5$. Derivative is taken at x_3 .



Distance between two nodes

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

Approximation to the m^{th} derivative across q nodes

$$\frac{d^m N}{dx^m} \approx \sum_{i=1}^q \alpha_i N_i = \alpha_1 N_1 + \alpha_2 N_2 + \dots + \alpha_q N_q \quad (6.24)$$

High Order Approximations

Taylor series expansion for each node about point x_*

$$N_i = N_* + (x_i - x_*) \frac{N_*}{x} + \frac{1}{2} (x_i - x_*)^2 \frac{2N_*}{x^2} + \frac{1}{6} (x_i - x_*)^3 \frac{3N_*}{x^3} + \dots \quad (6.25)$$

Combine (6.24) with (6.25) and gather terms

$$\frac{mN}{x^m} \sum_{i=1}^q N_i = \sum_{i=1}^q N_* + \sum_{i=1}^q (x_i - x_*) \frac{N_*}{x} + \sum_{i=1}^q \frac{1}{2} (x_i - x_*)^2 \frac{2N_*}{x^2} + \dots \quad (6.26)$$

Redefine

$$\sum_{i=1}^q N_i = B_0 N_* + B_1 \frac{N_*}{x} + B_2 \frac{2N_*}{x^2} + \dots \quad (6.27)$$

$$B_n = \sum_{i=1}^q \frac{1}{n!} (x_i - x_*)^n \quad \text{for } n = 0 \dots q - 1 \quad (6.28)$$

- Set $B_n = 0$ for all n , except $n = m$
- Set $B_n = 1$ when $n = m$

Multiply (6.27) through by $n!$ and set matrix (6.29)

$$\begin{matrix} 1 & 1 & 1 & \dots & 1 & & \\ (x_1 - x_*) & (x_2 - x_*) & (x_3 - x_*) & \dots & (x_q - x_*) & 1 & 0!B_0 \\ (x_1 - x_*)^2 & (x_2 - x_*)^2 & (x_3 - x_*)^2 & \dots & (x_q - x_*)^2 & 2 & 1!B_1 \\ \vdots & \vdots & \vdots & & \vdots & 3 & 2!B_2 \\ (x_1 - x_*)^{q-1} & (x_2 - x_*)^{q-1} & (x_3 - x_*)^{q-1} & \dots & (x_q - x_*)^{q-1} & q & (q-1)!B_{q-1} \end{matrix} =$$

Second-Order Central Difference Approximation

Example.

Find second-order central difference approx. to N/x

Order of derivative: $m = 1$

Order of approximation: $q - m = 2$

---> Number of nodes $q = 3$

Set matrix

$$\begin{array}{cccccc} 1 & 1 & 1 & i-1 & 0 & \\ -x & 0 & x & i & = & 1 \\ (-x)^2 & 0 & (x)^2 & i+1 & 0 & \end{array} \quad (6.32)$$

Solve matrix

$$i-1 = -\frac{1}{2x} \quad i = 0 \quad i+1 = \frac{1}{2x}$$

Apply the 's to (6.24)

$$\frac{N}{x} \quad 1N_1 + 2N_2 + 3N_3 = i-1N_{i-1} + iN_i + i+1N_{i+1}$$

Substitute 's to obtain central difference approximation

$\frac{N}{x} \quad \frac{N_{i+1} - N_{i-1}}{2x}$	Table 6.2 (c)
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First-Order Backward Difference Approximation

Example.

Find first-order backward difference approx. to N/x

Order of derivative: $m = 1$
 Order of approximation: $q - m = 1$
 ---> Number of nodes $q = 2$

Set matrix

$$\begin{matrix} 1 & 1 & i-1 & 0 \\ - & x & 0 & i \end{matrix} = \begin{matrix} 0 \\ 1 \end{matrix} \quad (6.30)$$

Solve matrix

$$i-1 = -\frac{1}{x} \qquad i = \frac{1}{x}$$

Applying the 's to (6.24)

$$\frac{N}{x} \quad i-1N_{i-1} + iN_i \quad (6.31)$$

Substitute 's to obtain backward difference approximation

$$\frac{N}{x} \quad \frac{N_i - N_{i-1}}{x} \quad \text{Table 6.2 (a)}$$

Second-Order Backward Difference Approximation

Example

Find second-order backward difference approx. to N/x

Order of derivative: $m = 1$
 Order of approximation: $q - m = 2$
 ---> Number of nodes $q = 3$

Set matrix

$$\begin{matrix} 1 & 1 & 1 & i-2 & 0 \\ -2/x & -x & 0 & i-1 & = & 1 \\ (-2/x)^2 & (-x)^2 & 0 & i & 0 \end{matrix} \quad (6.32)$$

Solve matrix

$$i-2 = \frac{1}{2/x} \quad i-1 = -\frac{2}{x} \quad i = \frac{3}{2/x}$$

Applying the 's to (6.24)

$$\frac{N}{x} \quad i-2N_{i-2} + i-1N_{i-1} + iN_i$$

Substitute 's to obtain backward difference approximation

$\frac{N}{x} \quad \frac{N_{i-2} - 4N_{i-1} + 3N_i}{2/x}$	Table 6.2 (d)
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Higher-Order Approximations

Third-order backward difference ($m = 1, q = 4$)

$$\frac{N}{x} = \frac{N_{i-2} - 6N_{i-1} + 3N_i + 2N_{i+1}}{6x}$$

Table 6.2 (f)

Third-order forward difference ($m = 1, q = 4$)

$$\frac{N}{x} = \frac{-2N_{i-1} - 3N_i + 6N_{i+1} - N_{i+2}}{6x}$$

Table 6.2 (g)

Fourth-order backward difference ($m = 1, q = 5$)

$$\frac{N}{x} = \frac{-N_{i-3} + 6N_{i-2} - 18N_{i-1} + 10N_i + 3N_{i+1}}{12x}$$

Table 6.2 (i)

Fourth-order forward difference ($m = 1, q = 5$)

$$\frac{N}{x} = \frac{-3N_{i-1} - 10N_i + 18N_{i+1} - 6N_{i+2} + N_{i+3}}{12x}$$

Table 6.2 (j)

Fourth-Order Approximations

Discretize around furthest cell

Fourth-order backward diff. scheme ($m = 1, q = 5$)

1	1	1	1	1	$i-4$	0
$-4x$	$-3x$	$-2x$	$-x$	0	$i-3$	1
$(-4x)^2$	$(-3x)^2$	$(-2x)^2$	$(-x)^2$	0	$i-2$	= 0
$(-4x)^3$	$(-3x)^3$	$(-2x)^3$	$(-x)^3$	0	$i-1$	0
$(-4x)^4$	$(-3x)^4$	$(-2x)^4$	$(-x)^4$	0	i	0

$$\frac{N}{x} = \frac{-3N_{i-4} + 16N_{i-3} - 36N_{i-2} + 48N_{i-1} - 25N_i}{12x} \quad \text{Table 6.2 (k)}$$

Fourth-order forward difference ($m = 1, q = 5$)

$$\frac{N}{x} = \frac{25N_i - 48N_{i+1} + 36N_{i+2} - 16N_{i+3} + 3N_{i+4}}{12x} \quad \text{Table 6.2 (l)}$$

Fourth-Order Central Difference Approximations

Fourth-order central difference of N/x ($m = 1, q = 5$)

$$\begin{array}{cccccc}
 1 & 1 & 1 & 1 & 1 & i-2 & 0 \\
 -2x & -x & 0 & x & 2x & i-1 & 1 \\
 (-2x)^2 & (-x)^2 & 0 & (x)^2 & (2x)^2 & i & = 0 \\
 (-2x)^3 & (-x)^3 & 0 & (x)^3 & (2x)^3 & i+1 & 0 \\
 (-2x)^4 & (-x)^4 & 0 & (x)^4 & (2x)^4 & i+2 & 0
 \end{array} \tag{6.33}$$

$$\frac{N}{x} = \frac{N_{i-2} - 8N_{i-1} + 8N_{i+1} - N_{i+2}}{12x} \tag{Table 6.2 (h)}$$

Fourth-order central difference of $2N/x^2$ ($m = 2, q = 5$)

$$\begin{array}{cccccc}
 1 & 1 & 1 & 1 & 1 & i-2 & 0 \\
 -2x & -x & 0 & x & 2x & i-1 & 0 \\
 (-2x)^2 & (-x)^2 & 0 & (x)^2 & (2x)^2 & i & = 2 \\
 (-2x)^3 & (-x)^3 & 0 & (x)^3 & (2x)^3 & i+1 & 0 \\
 (-2x)^4 & (-x)^4 & 0 & (x)^4 & (2x)^4 & i+2 & 0
 \end{array}$$

$$\frac{2N}{x^2} = \frac{-N_{i-2} + 16N_{i-1} - 30N_i + 16N_{i+1} - N_{i+2}}{12x^2} \tag{Table 6.2 (n)}$$

Solutions to the Advection-Diffusion Equation

Species continuity equation in west-east direction

$$\frac{N}{t} + \frac{(uN)}{x} - \frac{K_{h,xx}}{x} \frac{N}{x} = 0 \quad (6.1)$$

CFL stability criterion for advection

$$h < x_{\min}/|u_{\max}|$$

Stability criterion for diffusion

$$h < x_{\min}^2/K_{\max}$$

Forward in time, centered in space (FTCS) solution (6.35)

$$\frac{N_{i,t} - N_{i,t-h}}{h} + \frac{(uN)_{i+1,t-h} - (uN)_{i-1,t-h}}{2x} - K \frac{N_{i+1,t-h} - 2N_{i,t-h} + N_{i-1,t-h}}{x^2} = 0$$

Implicit Solution

Implicit solution (6.36)

$$\frac{N_{i,t} - N_{i,t-h}}{h} + \frac{(uN)_{i+1,t} - (uN)_{i-1,t}}{2x} - K \frac{N_{i+1,t} - 2N_{i,t} + N_{i-1,t}}{x^2} = 0$$

Rearrange and write in tridiagonal matrix form

$$A_i N_{i-1,t} + B_i N_{i,t} + D_i N_{i+1,t} = N_{i,t-h} \quad (6.37)$$

$$A_i = -h \frac{u}{2x} + \frac{K}{x^2} \quad B_i = 1 + h \frac{2K}{x^2} \quad D_i = h \frac{u}{2x} - \frac{K}{x^2}$$

(6.38)

$$\begin{array}{cccccccccccc} B_1 & D_1 & 0 & 0 & \dots & 0 & 0 & 0 & N_{1,t} & N_{1,t-h} & A_1 N_{0,t} \\ A_2 & B_2 & D_2 & 0 & \dots & 0 & 0 & 0 & N_{2,t} & N_{2,t-h} & 0 \\ 0 & A_3 & B_3 & D_3 & \dots & 0 & 0 & 0 & N_{3,t} & N_{3,t-h} & 0 \\ 0 & 0 & A_4 & B_4 & \dots & 0 & 0 & 0 & N_{4,t} & N_{4,t-h} & 0 \\ \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & B_{I-2} & D_{I-2} & 0 & N_{I-2,t} & N_{I-2,t-h} & 0 \\ 0 & 0 & 0 & 0 & \dots & A_{I-1} & B_{I-1} & D_{I-1} & N_{I-1,t} & N_{I-1,t-h} & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & A_I & B_I & N_{I,t} & N_{I,t-h} & D_I N_{I+1,t} \end{array} =$$

(6.39)

Tridiagonal Matrix Solution

Decomposition:

$$\begin{aligned}
 1 &= -\frac{D_1}{B_1} & i &= -\frac{D_i}{B_i + A_i} & i &= 2 \dots I \\
 1 &= \frac{R_1}{B_1} & i &= \frac{R_i - A_i}{B_i + A_i} & i &= 2 \dots I \quad (6.40)
 \end{aligned}$$

Backsubstitution:

$$N_{I,t} = I \quad N_{i,t} = i + i N_{i+1,t} \quad i = I-1, \dots, 1 \quad (6.41)$$

Matrix for solution over a global domain

$$\begin{array}{cccccccccc}
 B_1 & D_1 & 0 & 0 & \dots & 0 & 0 & A_1 & N_{1,t} & N_{1,t-h} \\
 A_2 & B_2 & D_2 & 0 & \dots & 0 & 0 & 0 & N_{2,t} & N_{2,t-h} \\
 0 & A_3 & B_3 & D_3 & \dots & 0 & 0 & 0 & N_{3,t} & N_{3,t-h} \\
 0 & 0 & A_4 & B_4 & \dots & 0 & 0 & 0 & N_{4,t} & N_{4,t-h} \\
 \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & = & \vdots \\
 0 & 0 & 0 & 0 & \dots & B_{I-2} & D_{I-2} & 0 & N_{I-2,t} & N_{I-2,t-h} \\
 0 & 0 & 0 & 0 & \dots & A_{I-1} & B_{I-1} & D_{I-1} & N_{I-1,t} & N_{I-1,t-h} \\
 D_I & 0 & 0 & 0 & \dots & 0 & A_I & B_I & N_{I,t} & N_{I,t-h}
 \end{array} \quad (6.42)$$

$$D_I = D_0$$

$$A_1 = A_{I+1}$$

Crank-Nicolson Scheme

Crank-Nicolson form (6.44)

$$\frac{N_{i,t} - N_{i,t-h}}{h} + \mu_c \frac{(uN)_{i+1,t} - (uN)_{i-1,t}}{2x} + (1 - \mu_c) \frac{(uN)_{i+1,t-h} - (uN)_{i-1,t-h}}{2x} - K \mu_c \frac{N_{i+1,t} - 2N_{i,t} + N_{i-1,t}}{x^2} + (1 - \mu_c) \frac{N_{i+1,t-h} - 2N_{i,t-h} + N_{i-1,t-h}}{x^2} = 0$$

μ_c = Crank-Nicolson parameter

$= 0.5$ --> Crank-Nicolson solution

$= 0.$ --> explicit solution

$= 1$ --> implicit solution

Tridiagonal form

$$A_i N_{i-1,t} + B_i N_{i,t} + D_i N_{i+1,t} = E_i N_{i-1,t-h} + F_i N_{i,t-h} + G_i N_{i+1,t-h} \quad (6.45)$$

$$A_i = -\mu_c h \frac{u}{2x} + \frac{K}{x^2} \quad E_i = (1 - \mu_c) h \frac{u}{2x} + \frac{K}{x^2}$$

$$B_i = 1 + \mu_c h \frac{2K}{x^2} \quad F_i = 1 - (1 - \mu_c) h \frac{2K}{x^2}$$

$$D_i = \mu_c h \frac{u}{2x} - \frac{K}{x^2} \quad G_i = -(1 - \mu_c) h \frac{u}{2x} - \frac{K}{x^2} \quad (6.46)$$

Leapfrog Scheme

$$\frac{N_{i,t} - N_{i,t-2h}}{2h} + \frac{(uN)_{i+1,t-h} - (uN)_{i-1,t-h}}{2x} - K \frac{N_{i+1,t-h} - 2N_{i,t-h} + N_{i-1,t-h}}{x^2} = 0$$

(6.48)

Matsuno Scheme

Prediction step (6.49)

$$\frac{N_{i,est} - N_{i,t-h}}{h} + \frac{(uN)_{i+1,t-h} - (uN)_{i-1,t-h}}{2x} - K \frac{N_{i+1,t-h} - 2N_{i,t-h} + N_{i-1,t-h}}{x^2} = 0$$

Correction step (6.50)

$$\frac{N_{i,t} - N_{i,t-h}}{h} + \frac{(uN)_{i+1,est} - (uN)_{i-1,est}}{2x} - K \frac{N_{i+1,est} - 2N_{i,est} + N_{i-1,est}}{x^2} = 0$$

Heun Scheme

$$\begin{aligned} & \frac{N_{i,t} - N_{i,t-h}}{h} + \frac{1}{2} \frac{(uN)_{i+1,est} - (uN)_{i-1,est}}{2x} - \frac{K}{2} \frac{N_{i+1,est} - 2N_{i,est} + N_{i-1,est}}{x^2} \\ & + \frac{1}{2} \frac{(uN)_{i+1,t-h} - (uN)_{i-1,t-h}}{2x} - \frac{K}{2} \frac{N_{i+1,t-h} - 2N_{i,t-h} + N_{i-1,t-h}}{x^2} = 0 \end{aligned}$$

(6.51)

Adams-Bashforth Scheme

$$\begin{aligned} & \frac{N_{i,t} - N_{i,t-h}}{h} + \frac{3}{2} \frac{(uN)_{i+1,t-h} - (uN)_{i-1,t-h}}{2x} - \frac{3}{2} K \frac{N_{i+1,t-h} - 2N_{i,t-h} + N_{i-1,t-h}}{x^2} \\ & - \frac{1}{2} \frac{(uN)_{i+1,t-2h} - (uN)_{i-1,t-2h}}{2x} + \frac{1}{2} K \frac{N_{i+1,t-2h} - 2N_{i,t-2h} + N_{i-1,t-2h}}{x^2} = 0 \end{aligned}$$

(6.52)

Fourth-Order in Space Equation

Fourth-order central difference explicit solution

$$\frac{N_{i,t} - N_{i,t-h}}{h} + \frac{(uN)_{i-2,t} - 8(uN)_{i-1,t} + 8(uN)_{i+1,t} - (uN)_{i+2,t}}{12 \ x} - K \frac{-N_{i-2,t} + 16N_{i-1,t} - 30N_{i,t} + 16N_{i+1,t} - N_{i+2,t}}{12 \ x^2} = 0$$

(6.53)

Write in Crank-Nicolson and pentadiagonal form

$$A_i N_{i-2,t} + B_i N_{i-1,t} + D_i N_{i,t} + E_i N_{i+1,t} + F_i N_{i+2,t} = R_i N_{i-2,t-h} + Q_i N_{i-1,t-h} + S_i N_{i,t-h} + T_i N_{i+1,t-h} + U_i N_{i+2,t-h}$$

Second-Order Central Difference Form of Diffusion Term

Variable diffusion coefficient, variable grid spacing

$$\frac{1}{x} K \frac{N}{x} = \frac{\frac{K_{i+1/2} (N_{i+1} - N_i)}{x_{i+1} - x_i} - \frac{K_{i-1/2} (N_i - N_{i-1})}{x_i - x_{i-1}}}{x_{i+1/2} - x_{i-1/2}} \quad (6.54)$$

$$K_{i+1/2} = 0.5(K_i + K_{i+1}) \qquad K_{i-1/2} = 0.5(K_{i-1} + K_i)$$

$$x_{i+1/2} = 0.5(x_i + x_{i+1}) \qquad x_{i-1/2} = 0.5(x_{i-1} + x_i)$$

Simplified form

$$\frac{1}{x} K \frac{N}{x} = K_{i-1} N_{i-1} + K_{i,i} N_i + K_{i,i+1} N_{i+1} \quad (6.55)$$

$$K_{i-1} = \frac{2K_{i-1/2}}{(x_i - x_{i-1})(x_{i+1} - x_{i-1})} \quad (6.56)$$

$$K_{i,i} = \frac{-2[(x_{i+1} - x_i)K_{i-1/2} + (x_i - x_{i-1})K_{i+1/2}]}{(x_{i+1} - x_i)(x_i - x_{i-1})(x_{i+1} - x_{i-1})}$$

$$K_{i,i+1} = \frac{2K_{i+1/2}}{(x_{i+1} - x_i)(x_{i+1} - x_{i-1})}$$

Second-Order Central Difference Form of Advection Term

Variable wind speed, variable grid spacing

$$\frac{(uN)}{x} = a_{i-1}(uN)_{i-1} + a_i(uN)_i + a_{i+1}(uN)_{i+1} \quad (6.57)$$

$$a_{i-1} = \frac{(x_{i+1} - x_i) - 2(x_i - x_{i-1})}{(x_i - x_{i-1})(x_{i+1} - x_{i-1})} \quad (6.58)$$

$$a_i = \frac{(x_{i+1} - x_i) - (x_i - x_{i-1})}{(x_{i+1} - x_i)(x_i - x_{i-1})}$$

$$a_{i+1} = \frac{x_i - x_{i-1}}{(x_{i+1} - x_i)(x_{i+1} - x_{i-1})}$$

Coefficients from matrix

$$\begin{array}{ccc} 1 & 1 & 1 \\ -(x_i - x_{i-1}) & 0 & (x_{i+1} - x_i) \\ (x_i - x_{i-1})^2 & 0 & (x_{i+1} - x_i)^2 \end{array} \begin{array}{l} a_{i-1} \\ a_i \\ a_{i+1} \end{array} = \begin{array}{l} 0 \\ 1 \\ 0 \end{array} \quad (6.59)$$

Second-Order Advection-Diffusion Equation With Variable Diffusion Coefficient and Grid Spacing

Crank-Nicolson form

(6.60)

$$\frac{N_{i,t} - N_{i,t-h}}{h} = -\mu_c \left\{ \left[(au - K)N \right]_{i-1} + \left[(au - K)N \right]_i + \left[(au - K)N \right]_{i+1} \right\}_t - (1 - \mu_c) \left\{ \left[(au - K)N \right]_{i-1} + \left[(au - K)N \right]_i + \left[(au - K)N \right]_{i+1} \right\}_{t-h}$$

Write in tridiagonal form

$$A_i N_{i-1,t} + B_i N_{i,t} + D_i N_{i+1,t} = E_i N_{i-1,t-h} + F_i N_{i,t-h} + G_i N_{i+1,t-h}$$

Two Dimensional Solution

Advection-diffusion equation in two dimensions

$$\frac{N}{t} + \frac{(uN)}{x} + \frac{(vN)}{y} - \frac{K_{h,xx}}{x} \frac{N}{x} - \frac{K_{h,yy}}{y} \frac{N}{y} = 0$$

(6.61)

Central difference approximation

$$\begin{aligned} & \frac{N_{i,j,t} - N_{i,j,t-h}}{h} + \frac{(uN)_{i+1,j} - (uN)_{i-1,j}}{2x} + \frac{(vN)_{i,j+1} - (vN)_{i,j-1}}{2y} \\ & - K_{h,xx} \frac{N_{i-1,j} - 2N_{i,j} + N_{i+1,j}}{x^2} + K_{h,yy} \frac{N_{i,j-1} - 2N_{i,j} + N_{i,j+1}}{y^2} = 0 \end{aligned}$$

(6.62)

Solve

$$A_{i,j} N_{i-1,j,t} + B_{i,j} N_{i,j,t} + D_{i,j} N_{i+1,j,t} + E_{i,j} N_{i,j-1,t} + F_{i,j} N_{i,j+1,t} = N_{i,j,t-h}$$

Semi-Lagrangian Method

$$N_{x,t} = N_{x-uh,t-h} \quad (6.63)$$

Finite Element Method

Advection equation at node i

$$\frac{N_i}{t} + \frac{(uN)_i}{x} = 0 \quad (6.64)$$

Trial function = series expansion approximation to N
= linear combination of basis functions

$$N_i \quad \mathbf{N}_i(x) = \sum_j N_j \mathbf{e}_j(x) \quad (6.65)$$

$\mathbf{e}_j(x)$ = basis function

j = trial space

Minimize residual by forcing its weighted average to zero over domain

$$\int_x R_i(x) \mathbf{e}_i(x) dx = 0 \quad (6.66)$$

$\mathbf{e}_i(x)$ = weight function

$\mathbf{e}_i(x) = \mathbf{e}_j(x) \rightarrow$ Galerkin method of weighted residuals

$\mathbf{e}_i(x) \neq \mathbf{e}_j(x) \rightarrow$ Petrov-Galerkin technique

Residual in advection equation

$$R_i(x) = \frac{\mathbf{N}_i(x)}{t} + u \frac{\mathbf{N}_i(x)}{x} - \frac{N_i}{t} + u \frac{N_i}{x} = \frac{\mathbf{N}_i(x)}{t} + u \frac{\mathbf{N}_i(x)}{x} - 0 \quad (6.67)$$

Finite Element Method

Substitute (6.67) and (6.65) into (6.66) (6.68)

$$\begin{aligned}
 & \int_x \frac{N_i(x)}{t} + u \frac{N_i(x)}{x} e_i(x) dx \\
 &= \int_x \frac{N_j}{t} N_j e_j(x) + u \frac{N_j}{x} N_j e_j(x) e_i(x) dx \\
 &= \int_j \frac{N_j}{t} \int_x e_j(x) e_i(x) dx + u \int_j N_j \int_x \frac{de_j(x)}{dx} e_i(x) dx = 0
 \end{aligned}$$

Take time difference of (6.68) over three nodes

$$\begin{aligned}
 & \frac{N_{i-1,t} - N_{i-1,t-h}}{h} \int_{x_{i-1}}^{x_i} e_{i-1}(x) e_i(x) dx + \frac{N_{i,t} - N_{i,t-h}}{h} \int_{x_{i-1}}^{x_{i+1}} e_i(x) e_i(x) dx \\
 & + \frac{N_{i+1,t} - N_{i+1,t-h}}{h} \int_{x_i}^{x_{i+1}} e_{i+1}(x) e_i(x) dx \tag{6.69} \\
 & + u \left[N_{i-1,t} \int_{x_{i-1}}^{x_i} \frac{de_{i-1}(x)}{dx} e_i(x) dx + N_{i,t} \int_{x_{i-1}}^{x_{i+1}} \frac{de_i(x)}{dx} e_i(x) dx \right. \\
 & \left. + N_{i+1,t} \int_{x_i}^{x_{i+1}} \frac{de_{i+1}(x)}{dx} e_i(x) dx \right] = 0
 \end{aligned}$$

Finite Element Method

Define basis functions as chapeau functions

$$e_i(x) = \begin{cases} \frac{x - x_{i-1}}{x_i - x_{i-1}} & x_{i-1} \leq x \leq x_i \\ \frac{x_{i+1} - x}{x_{i+1} - x_i} & x_i \leq x \leq x_{i+1} \\ 0 & \text{all other cases} \end{cases} \quad (6.70)$$

Solve each integral

$$\int_{x_{i-1}}^{x_i} e_{i-1}(x)e_i(x)dx = \int_{x_{i-1}}^{x_i} \frac{x_i - x}{x_i - x_{i-1}} \frac{x - x_{i-1}}{x_i - x_{i-1}} dx = \frac{x_i - x_{i-1}}{6} \quad (6.71)$$

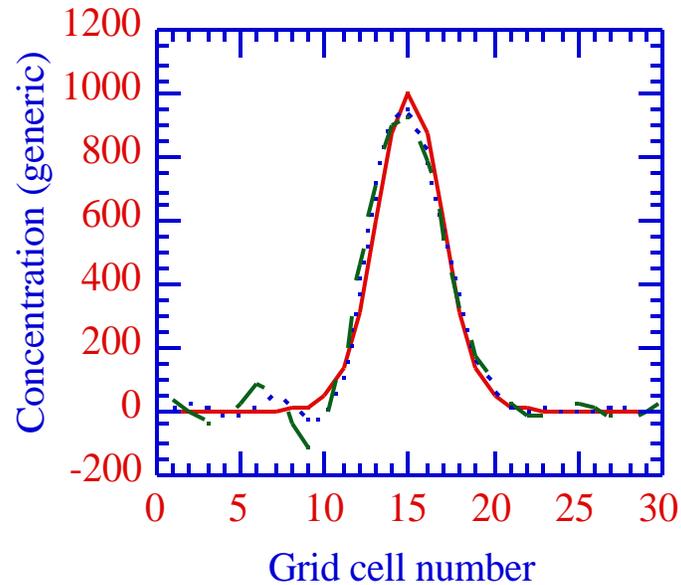
Solution obtained once integrals have been solved

$$\frac{(N_{i-1,t} - N_{i-1,t-h})x_i + (N_{i,t} - N_{i,t-h})2(x_{i+1} + x_i) + (N_{i+1,t} - N_{i+1,t-h})x_{i+1}}{6h} + u \frac{N_{i+1,t} - N_{i-1,t}}{2} = 0 \quad (6.72)$$

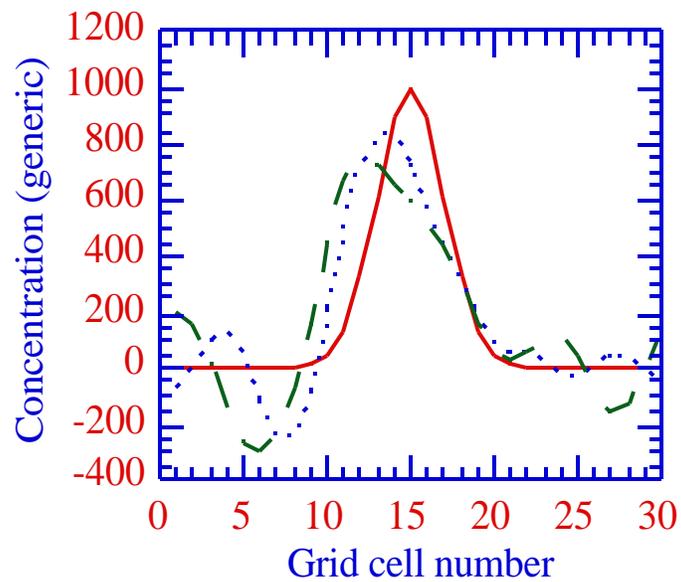
Tests With a Finite Element Method

Fig. 6.7. Preservation of a Gaussian peak during finite element transport after eight revolutions around a circular grid when

(a) $uh|x = 0.02$.



(b) $uh|x = 0.6$.



Pseudospectral Method

Advection equation

$$\frac{N}{t} + u \frac{N}{x} = 0 \quad (6.81)$$

Represent solution with infinite Fourier series

$$N(x,t) = \sum_{k=0} a_k(t) e^{ik2\pi x/L} \quad (6.82)$$

Integrate both sides of (6.82) from 0 to L

$$a_k(0) = \frac{1}{L} \int_0^L N(x,0) e^{-ik2\pi x/L} dx \quad (6.83)$$

Truncate infinite series

$$N(x,t) = \sum_{k=0}^K a_k(t) e^{ik2\pi x/L} \quad (6.84)$$

Pseudospectral Method

Central time-difference approximation of (6.84)

$$\frac{N}{t} = \frac{1}{2h} \sum_{k=0}^K a_{k,t} e^{ik2x/L} - \sum_{k=0}^K a_{k,t-2h} e^{ik2x/L} \quad (6.85)$$

Partial derivative of (6.84) with respect to space

$$\frac{N}{x} = \sum_{k=0}^K \frac{ik2}{L} a_{k,t-h} e^{ik2x/L} \quad (6.86)$$

Substitute (6.85) and (6.86) into (6.81)

$$\frac{1}{2h} \sum_{k=0}^K (a_{k,t} - a_{k,t-2h}) e^{ik2x/L} = -u \sum_{k=0}^K \frac{ik2}{L} a_{k,t-h} e^{ik2x/L} \quad (6.87)$$

Separate into K equations --> solve

$$\frac{a_{k,t} - a_{k,t-2h}}{2h} = -\frac{uik2}{L} a_{k,t-h} \quad (6.88)$$