Lecture 22 Outline

Saturday, November 9, 2019 5:05 PM

Householder Reflections, Stiff Equations

Multistage Methods (Runge-Kutta)

Multistep Methods

- Adams-Bashforth (AB)
- Adams-Moulton (AM)
- Backward Differentiation Formula (BDF)

Boundary Value Problems (BVP)

Householder Reflections

Wednesday, November 13, 2019 1:09 AM

$$\underline{F} = \underline{I} - \frac{2\underline{v}\,\underline{v}^T}{\underline{v}^T\underline{v}}$$

$$\underline{F}\,\underline{F}^T = \left(\underline{I} - \frac{2\underline{v}\underline{v}^T}{\underline{v}^T\underline{v}}\right)\left(\underline{I} - \frac{2\underline{v}\,\underline{v}^T}{\underline{v}^T\underline{v}}\right)^T$$

$$= \underline{I}\,\underline{I}^T - \underline{I}\left(\frac{2\underline{v}\underline{v}^T}{\underline{v}^T\underline{v}}\right)^T - \left(\frac{2\underline{v}\underline{v}^T}{\underline{v}^T\underline{v}}\right)\underline{I}^T$$

$$+ \frac{-2\underline{v}\,\underline{v}^T}{\underline{v}^T\underline{v}}\left(\frac{-2\underline{v}\underline{v}^T}{\underline{v}^T\underline{v}}\right)^T$$

$$= \underline{I} - \frac{2\underline{v}\underline{v}^T}{\underline{v}^T\underline{v}} - \frac{2\underline{v}\underline{v}^T}{\underline{v}^T\underline{v}} + \frac{4\underline{v}\underline{v}^T\underline{v}\underline{v}^T}{(\underline{v}^T\underline{v})^2}$$

$$= \underline{I} - \frac{4\underline{v}\underline{v}^T}{\underline{v}^T\underline{v}} + \frac{4\underline{v}\underline{v}^T}{\underline{v}^T\underline{v}} = \underline{I} \checkmark$$

Stiff ODEs

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Generalize single ODE into the following for two dependent variables $y_1(t)$ & $y_2(t)$

$$\frac{dy_1}{dt} = a_{11} y_1 + a_{12} y_2$$

$$\frac{dy_2}{dt} = a_{21} y_1 + a_{22} y_2$$

with constants $a_{11}, a_{12}, a_{21}, a_{22}$

Let

$$\underline{A} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}, \quad \underline{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

$$\Rightarrow \frac{d\underline{y}}{dt} = \begin{bmatrix} \frac{dy_1}{dt} \\ \frac{dy_2}{dt} \end{bmatrix} \Rightarrow \frac{d\underline{y}}{dt} = \underline{A}\,\underline{y}$$

Assume a solution

$$y_1 = x_1 e^{\lambda t}, \quad y_2 = x_2 e^{\lambda t}$$

$$\frac{dy_1}{dt} = \lambda x_1 e^{\lambda t}, \quad \frac{dy_2}{dt} = \lambda x_2 e^{\lambda t}$$

$$\frac{dy_1}{dt} = \lambda x_1 e^{\lambda t}, \quad \frac{dy_2}{dt} = \lambda x_2 e^{\lambda t}$$

$$\frac{d\underline{y}}{dt} = \underline{A}\,\underline{y}$$

$$\begin{bmatrix} \lambda x_1 \cancel{e^{\lambda t}} \\ \lambda x_2 \cancel{e^{\lambda t}} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} x_1 \cancel{e^{\lambda t}} \\ x_2 \cancel{e^{\lambda t}} \end{bmatrix}$$

$\underline{A}\,\underline{x} = \lambda \underline{x}$ Eigensystem of $\underline{A}$

$\underline{A}\,\underline{x} - \lambda \underline{x} = \underline{0}$ λ: Eigenvalue

$(\underline{A} - \lambda \underline{I})\underline{x} = \underline{0}$ $\underline{x}$: Eigenvector

$$\underline{y}(t) = c_1 \underline{x}_1 e^{-\lambda_1 t} + c_2 \underline{x}_2 e^{-\lambda_2 t}$$

Forward Euler: $\underline{y}_n = (\underline{I} - \underline{A}\,\Delta t)^n \underline{y}_0$

Explicit; Conditionally stable

$$\Delta t < \Delta t_{cr} = \frac{2}{\lambda_1} \quad \text{for } \lambda_1 > \lambda_2 > 0$$

Backward Euler: $\underline{y}_n = (\underline{I} + \underline{A}\,\Delta t)^{-n}\, y_0$

Multistage Methods

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Runge-Kutta Explicit Methods

Example: $\dfrac{dy}{dt} = 4e^{2t} - \dfrac{y}{2}$, $y(0) = 2$

$$y(t) = \frac{40}{12} e^{2t} - \frac{14}{13} e^{-t/2}$$

$$y(3) \cong 33.6771717\ldots$$

Show one step w/ $\Delta t = 1/2$

Forward Euler

$$k_1 = f(t_0, y_0) = 4e^0 - 2/2 = 3$$

$$y_1 = y_0 + \Delta t\, k_1 = 2 + \tfrac{1}{2}(3) = 3.5$$

Midpoint

$$k_1 = 3$$

$$y_{1/2} = y_0 + \tfrac{1}{2}\Delta t\, k_1 = 2.75$$

$$k_2 = f\left(t_0 + \tfrac{1}{2}\Delta t,\ y_0 + \tfrac{1}{2}\Delta t\, k_1\right) = f\left(\tfrac{1}{2}\Delta t,\ y_{1/2}\right)$$

$$= 4e^{2(0.25)} - \frac{2.75}{2} \cong 3.51061$$

$$y_1 = y_0 + \Delta t\, k_2 = 2 + \tfrac{1}{2}(3.51061) \cong 3.75531$$

RK4

$$\left.\begin{aligned} k_1 &= 3 \\ k_2 &= 3.51061 \\ k_3 &= 3.44678 \\ k_4 &= 4.1056 \end{aligned}\right\} \quad y_1 \cong 3.7517$$

Results at $t=3$

Method	$\Delta t = \frac{1}{2}$ (6 steps)		$\Delta t = \frac{1}{4}$ (12 steps)	
	$y(3)$	e	$y(3)$	e
For. Euler	~ 29.6	4.08	~ 31.64	2.03
Midpoint	~ 33.77	9.3×10^{-2}	~ 33.70	2.62×10^{-2}
RK4	~ 33.67	2.81×10^{-3}	~ 33.67	1.75×10^{-4}

Iterations need to have error $< 10^{-3}$

	Time Steps	Calc/Steps	k-evaluations
RK4	9	4	36
Midpoint	65	2	130
For. Euler	24271	1	24271

Multistep Methods

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Multistage methods take several sub-steps in a single time step → low memory but might be slow

Multistep methods use the solution at multiple prior steps → higher memory but lower cost (less derivative evaluations)

Generally, look at $\frac{dy}{dt} = f(t, y)$

Then consider an sth order scheme, such that

$$a_0 y_{n+1} + a_1 y_n + \dots + a_s y_{n+1-s} =$$

$$\Delta t \left[b_0 f(t_{n+1}, y_{n+1}) + b_1 f(t_n, y_n) + \dots + b_s f(t_{n+1-s}, y_{n+1-s}) \right]$$

with $\sum_i a_i = 0$, $\sum_i b_i = 1$

Forward Euler

$$\frac{y_{n+1} - y_n}{\Delta t} = f(t_n, y_n)$$

$$\frac{1}{\Delta t} y_{n+1} - \frac{1}{\Delta t} y_n = f(t_n, y_n)$$

$$y_{n+1} - y_n = \Delta t\, f(t_n, y_n) \Rightarrow a_0 = 1,\ a_1 = -1$$

$b_1 = 1$, all other are 0

The values of $a_0 \to a_s$, $b_0 \to b_s$ determine the particlar scheme

Note: Since one needs y_{n+1}, $a_0 \neq 0$

If $b_0 = 0$, then the method is explicit

If $b_0 \neq 0$, then it is implicit

Three main classes of multistep

1. Adams-Bashforth (AB)
2. Adams-Moulton (AM)
3. Backward Differentiation Formula (BDF)

③ Backward Differentiation Formula (BDF)

① Adams-Bashforth: Explicit schemes

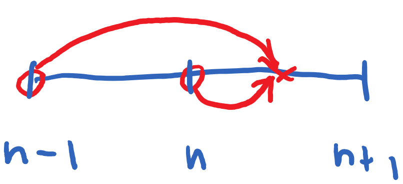
with $a_0 = 1,\ a_1 = -1,\ b_0 = 0,\ b_{i>0} > 0$

$\mathcal{O}(\Delta t)$: $b_1 = 1 \Rightarrow y_{n+1} - y_n = \Delta t\, f(t_n, y_n)$

Forward Euler

$\mathcal{O}(\Delta t^2)$: $b_1 = \frac{3}{2},\ b_2 = -\frac{1}{2}$

$$y_{n+1} - y_n = \Delta t \underbrace{\left[\frac{3}{2} f(t_n, y_n) - \frac{1}{2} f(t_{n-1}, f_{n-1})\right]}_{\approx f(t_{n+1/2},\, y_{n+1/2})}$$



$\mathcal{O}(\Delta t^3)$: $b_1 = \frac{23}{12},\ b_2 = -\frac{4}{3},\ b_3 = \frac{5}{12}$

$\mathcal{O}(\Delta t^4)$: $b_1 = \frac{55}{24},\ b_2 = -\frac{59}{24},\ b_3 = \frac{37}{24},\ b_4 = -\frac{3}{8}$

⋮

Notes:

Higher order schemes need to store more information and also require a bootstrap scheme to get started

How to compute y_1 using $\mathcal{O}(\Delta t^3)$ scheme?

One needs $y_0, \underbrace{y_{-1}, y_{-2}}_{???}$

② Adams-Moulton: Implicit schemes

$a_0 = 1, \quad a_1 = -1, \quad b_0 \neq 0$

$\mathcal{O}(\Delta t)$: $b_0 = 1$ $\qquad y_{n+1} - y_n = \Delta t \, f(t_{n+1}, y_{n+1})$

Backward Euler

$\mathcal{O}(\Delta t^2)$: $b_0 = \frac{1}{2}, \quad b_1 = \frac{1}{2}$

$$y_{n+1} - y_n = \Delta t \left[\frac{1}{2} f(t_{n+1}, y_{n+1}) + \frac{1}{2} f(t_n, y_n) \right]$$

Crank-Nicholson

$\mathcal{O}(\Delta t^3)$: $b_0 = \frac{5}{12}, \quad b_1 = \frac{2}{3}, \quad b_2 = -\frac{1}{12}$

$\mathcal{O}(\Delta t^4)$: $b_0 = \frac{3}{8}$, $b_1 = \frac{19}{24}$, $b_2 = -\frac{5}{24}$, $b_3 = \frac{1}{24}$

$\vdots$

③ Backward Differentiation Formula (BDF)

$b_0 = 1$, $b_{i>0} = 0$

$\mathcal{O}(\Delta t)$: $a_0 = 1$, $a_1 = -1$ Backward Euler

$$y_{n+1} - y_n = \Delta t\, f(t_{n+1}, y_{n+1})$$

$\mathcal{O}(\Delta t^2)$: $a_0 = \frac{3}{2}$, $a_1 = -2$, $a_2 = \frac{1}{2}$

$$\frac{3}{2} y_{n+1} - 2y_n + \frac{1}{2} y_{n-1} = \Delta t\, f(t_{n+1}, y_{n+1})$$

or $$\frac{3/2\, y_{n+1} - 2y_n + 1/2\, y_{n-1}}{\Delta t} = \frac{df}{dt} + \mathcal{O}(\Delta t^2)$$

$\mathcal{O}(\Delta t^3)$: $a_0 = \frac{11}{6}$, $a_1 = -3$, $a_2 = \frac{3}{2}$, $a_3 = -\frac{1}{3}$

Note: BDF of order > 6 is <u>not</u> stable

Boundary Value Problems

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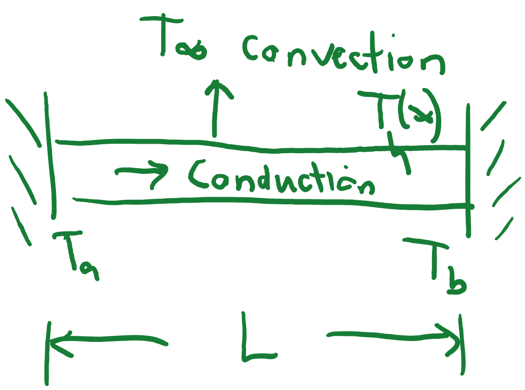
Boundary value problems have conditions specified on the end states

Example: Temperature in a rod with conduction and convection



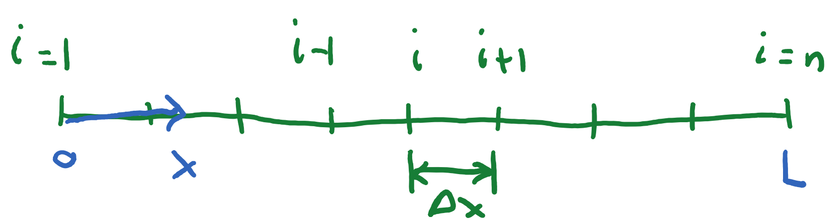
At steady state

$$\frac{d^2T}{dx^2} + h(T - T_\infty) = 0$$

for $0 \leq x \leq L$

with $\underbrace{T(0) = T_a, \quad T(L) = T_b}_{\text{Dirichlet Boundary Conditions (BC)}}$

Discretize on a grid



Substitute finite difference expression for derivatives

Second order central difference $O(\Delta x^2)$

$$\left.\frac{d^2T}{dx^2}\right|_{x_i} \simeq \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2}$$

$$\therefore \frac{d^2T}{dx^2} + h(T_\infty - T) \Rightarrow \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2} + h(T_\infty - T_i) = 0$$

with n grid points having $\Delta x = \frac{L}{n-1}$ uniform spacing

Let $n = 16$, $\Delta x = \frac{L}{15}$

At $i=1 \rightarrow x = 0$, $T_1 = T_a$

At $i=2$

$$\frac{T_3 - 2T_2 + T_1}{\Delta x^2} + h(T_\infty - T_2) = 0$$

or $-T_1 + (2 + \Delta x^2 h)T_2 - T_3 = \Delta x^2 h T_\infty$

At $i=3$

$$-T_2 + (2+\Delta x^2 h)T_3 - T_4 = \Delta x^2 h T_\infty$$

$$\vdots$$

At $i=15$

$$-T_{14} + (2+\Delta x^2 h)T_{15} - T_{16} = \Delta x^2 h T_\infty$$

At $i=16$

$$T_{16} = T_b$$

Write in matrix form

$$\begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & \cdots & 0 \\ -1 & 2+\Delta x^2 h & -1 & 0 & \cdots & \cdots & 0 \\ 0 & -1 & 2+\Delta x^2 h & -1 & \cdots & \cdots & 0 \\ & & & \ddots & & & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 2+\Delta x^2 h & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ \vdots \\ T_{15} \\ T_{16} \end{bmatrix} = \begin{bmatrix} T_q \\ \Delta x^2 h T_\infty \\ \vdots \\ \Delta x^2 h T_\infty \\ T_b \end{bmatrix}$$

$$\underline{A} \qquad \underline{T} = \underline{b}$$

$$\therefore \underline{T} = \underline{A}^{-1} \underline{b} \quad \text{in symbolic form}$$

Perhaps use LU decomposition of $\underline{A}$, along with forward & backward substitution to solve

Consider same problem with Neumann BC at $x = 0$, such that

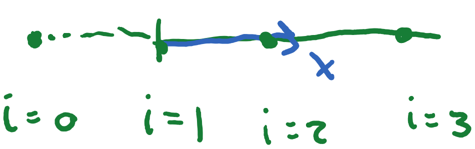
$$\left.\frac{dT}{dx}\right|_{x=0} = a \qquad \text{(specified heat flux)}$$

along with Dirichlet BC at $x = L$

$$\left.T\right|_{x=L} = T_L$$

How to write condition at $x = 0$?

Ghost node



$$-T_0 + (2 + \Delta x^2 h) T_1 - T_2 = \Delta x^2 h T_\infty$$

but $\displaystyle \frac{dT}{dx}(0) \simeq \frac{T_2 - T_0}{2\Delta x} = a$ Central difference $\mathcal{O}(\Delta x^2)$

$$\rightarrow T_0 = T_2 - 2\Delta x\, q$$

$$\therefore -T_2 + 2\Delta x\, q + (2 + \Delta x^2 h) T_1 - T_2 = \Delta x^2 h T_\infty$$

$$\text{or } (2 + \Delta x^2 h) T_1 - 2T_2 = \Delta x^2 h T_\infty - 2\Delta x\, q$$

$$\begin{bmatrix} 2+\Delta x^2 h & -2 & 0 & 0 & \cdots & & 0 \\ -1 & 2+\Delta x^2 h & -1 & 0 & \cdots & & 0 \\ 0 & -1 & 2+\Delta x^2 h & -1 & \cdots & & 0 \\ & & & \ddots & & & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 2+\Delta x^2 h & -1 \\ 0 & 0 & 0 & 0 \cdots & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ \vdots \\ T_{15} \\ T_{16} \end{bmatrix} = \begin{bmatrix} \Delta x^2 h T_\infty - 2\Delta x\, q \\ \Delta x^2 h T_\infty \\ \vdots \\ \\ \Delta x^2 h T_\infty \\ T_b \end{bmatrix}$$

$$\underline{A} \qquad \underline{T} = \underline{b}$$

Solve for $\underline{T} = \underline{A}^{-1} \underline{b}$

In 2D (or 3D), solve PDE

Typical example in 2D

$\nabla^2 u = f$ over a rectangle

Laplacian $\nabla^2 = \nabla \cdot \nabla$

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

For $f = 0 \rightarrow$ Laplace equation

$f \neq 0 \rightarrow$ Poisson equation

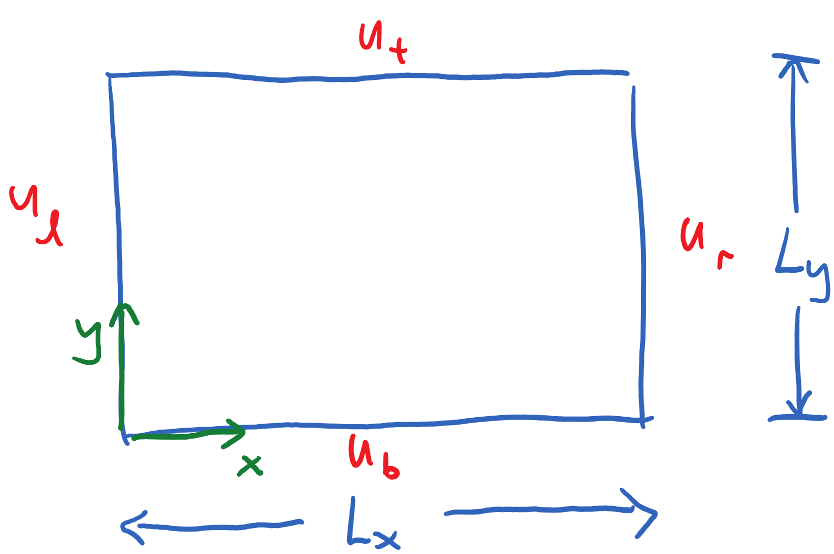
With Dirichlet BCs

$u(0, y) = u_l$ left

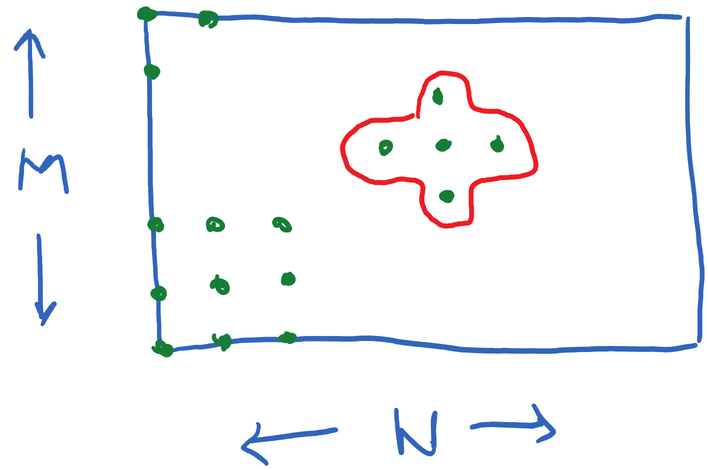
$u(L_x, y) = u_r$ right

$u(x, 0) = u_b$ bottom

$u(x, L_y) = u_t$ top



Create $N \times M$ grid in x and y-directions



Laplace operator produces a stencil that is placed at each interior grid point

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

$$\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta y^2} = f_{i,j}$$

with
$$\left.\begin{aligned} u_{1,j} &= u_l \\ u_{N,j} &= u_r \end{aligned}\right\} \text{ for } j = 1:M$$

$$\left.\begin{aligned} u_{i,1} &= u_b \\ u_{i,M} &= u_t \end{aligned}\right\} \text{ for } i = 1:N$$

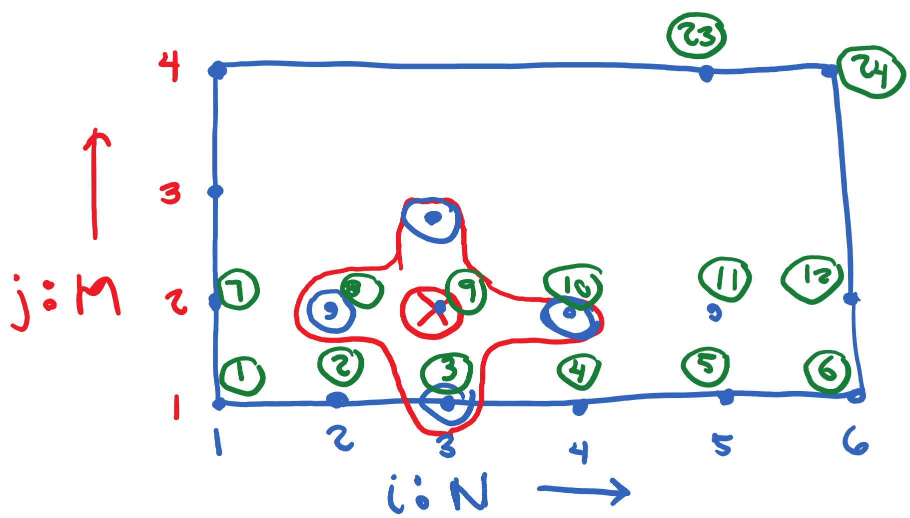
The overall linear system will be $MN \times MN$.

For large M, N, the resulting system matrix will be sparse due to compact stencil

Need a method to organize the data

Row or column ordering. For example,

let $\quad \text{index} = i + (j-1)N$



i	j	$i + (j-1)N$
1	1	1
2	1	2
3	1	3
⋮	⋮	⋮
6	1	6
1	2	7

6	1	6
1	2	7
2	2	8
⋮	⋮	⋮
6	4	24

At $(3,2)$

$$\frac{u_8 - 2u_9 + u_{10}}{\Delta x^2} + \frac{u_{15} - 2u_9 - u_3}{\Delta y^2} = f_9$$