

## The method of lines and general 1D parabolic equations

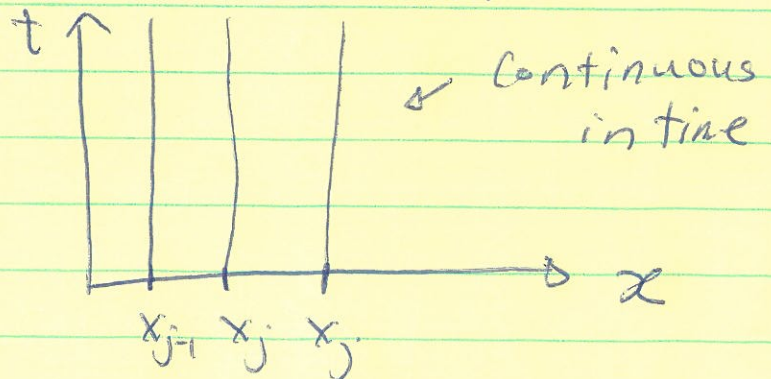
- Method of lines
- general 1D linear PDEs
- divergence form
- nonlinear PDEs
- MOVFIDM

### ▶ The method of lines

- PDEs are discretized simultaneously in time and space.
- Rothe's method: in time first and in space later
- The Method of lines: in space first and in time later

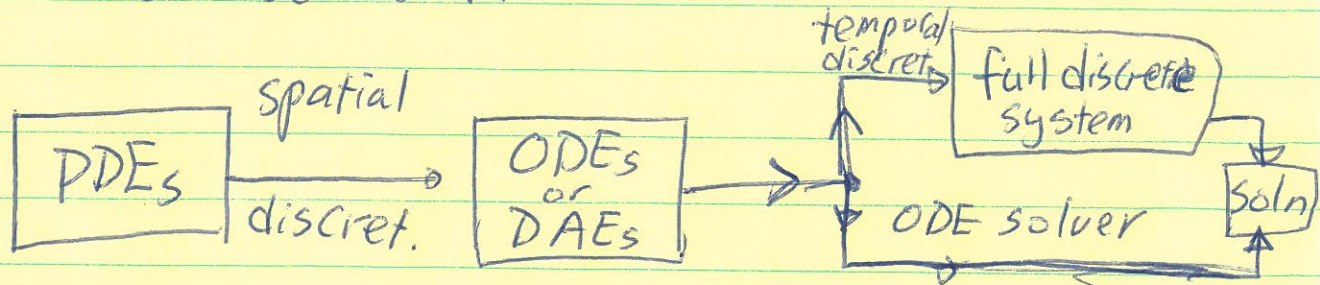
### Advantages of MOL:

- Temporal and spatial discretizations are treated separately. Special attention can be paid to each of them.





- Existing software on ODE integration can be used.



The heat equation (Model problem)

$$\begin{cases} \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \\ u(0,t) = 0, u(1,t) = 0 \end{cases}$$

Let  $u_j(t) \approx u(x_j, t)$

$$\begin{cases} \frac{du_j(t)}{dt} = \frac{1}{\Delta x^2} [u_{j+1}(t) - 2u_j(t) + u_{j-1}(t)] \\ u_0(t) = 0 \\ u_J(t) = 0 \end{cases} \Rightarrow \begin{cases} \frac{d}{dt} u_0(t) = 0 \\ \frac{d}{dt} u_J(t) = 0 \end{cases} \quad j=1, \dots, J-1$$

$$M \frac{d\vec{u}}{dt} = \vec{f}(t, \vec{u})$$

(ODE or DAE system)

They can be solved using existing ODE/DAE codes.



Or: they can be discretized in time to give a full discrete system. For example, Using Implicit Euler, we get

$$\left\{ \begin{aligned} \frac{u_j^{n+1} - u_j^n}{\Delta t} &= \frac{1}{\Delta x^2} [u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}] \\ u_0^{n+1} &= 0 \\ u_J^{n+1} &= 0 \end{aligned} \right.$$

▶ General 1D linear PDEs

$$\left\{ \begin{aligned} \frac{\partial u}{\partial t} &= a(x,t) \frac{\partial^2 u}{\partial x^2} + b(x,t) \frac{\partial u}{\partial x} + c(x,t)u + f(x,t) \\ & \qquad \qquad \qquad x \in (0,1) \\ u(0,t) &= g_0(t) \\ u(1,t) &= g_1(t) \end{aligned} \right.$$

$$\left\{ \begin{aligned} \frac{du_j}{dt} &= \frac{a_j}{\Delta x^2} (u_{j+1} - 2u_j + u_{j-1}) + \frac{b_j}{2\Delta x} (u_{j+1} - u_{j-1}) \\ & \qquad \qquad \qquad + c_j u_j + f_j \\ u_0(t) &= g_0(t) \\ u_J(t) &= g_1(t) \end{aligned} \right.$$



- Treatment of Neumann BC

$$\frac{\partial u}{\partial x}(0,t) = g_0(t)$$

- first order approximation

$$\frac{u_1 - u_0}{\Delta x} = g_0(t) \quad O(\Delta x)$$

- 2nd order approximation - fictitious point

$$x_{-1} = x_0 - \Delta x$$

$$\begin{cases} \frac{u_1 - u_{-1}}{2\Delta x} = g_0(t) \\ \frac{du_0}{dt} = \frac{a_0}{\Delta x^2} (u_1 + 2u_0 + u_{-1}) + \frac{b_0}{2\Delta x} (u_1 - u_{-1}) \\ \quad + c_0 u_0 + f_0 \end{cases}$$

Use these eqns to eliminate  $u_{-1}$ , we get

$$\begin{aligned} \frac{du_0}{dt} &= \frac{a_0}{\Delta x^2} (u_1 - 2u_0 + \underline{u_1 - 2\Delta x g_0(t)}) \\ &\quad + \frac{b_0}{2\Delta x} (u_1 - (u_1 - 2\Delta x g_0(t))) \\ &\quad + c_0 u_0 + f_0 \quad O(\Delta x^2) \end{aligned}$$

- 2nd order approximation - extrapolation



$$\begin{array}{r}
 4x \mid u_1 = u_0 + \Delta x u_x + \Delta x^2 u_{xx} + O(\Delta x^3) \\
 - \mid u_2 = u_0 + 2\Delta x u_x + 4\Delta x^2 u_{xx} + O(\Delta x^3) \\
 \hline
 4u_1 - u_2 = 3u_0 + 2\Delta x u_x + O(\Delta x^3)
 \end{array}$$

$$u_x = \frac{4u_1 - u_2 - 3u_0}{2\Delta x} + O(\Delta x^2)$$

Thus:

$$\frac{4u_1 - u_2 - 3u_0}{2\Delta x} = g_0(t) + O(\Delta x^2)$$



### Divergence form of PDEs

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left( a(x,t) \frac{\partial u}{\partial x} \right)$$

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

better to use this form

$$\frac{du_j}{dt} = \frac{1}{\Delta x^2} \left[ a_{j+1/2} (u_{j+1} - u_j) - a_{j-1/2} (u_j - u_{j-1}) \right]$$

- Symmetric
- diagonally dominant.



### Nonlinear PDEs

Example — Burgers' equation

$$\frac{\partial u}{\partial t} = \underbrace{\varepsilon \frac{\partial^2 u}{\partial x^2}}_{\text{diffusion}} - \underbrace{u \frac{\partial u}{\partial x}}_{\text{convection}}$$

$$\varepsilon = \frac{1}{\text{Re}}$$

Reynolds #



$$\Rightarrow \frac{du_j}{dt} = \frac{\varepsilon}{\Delta x^2} (u_{j+1} - 2u_j + u_{j-1}) - u_j \frac{u_{j+1} - u_{j-1}}{2\Delta x}$$

$$\frac{\partial u}{\partial t} = \varepsilon \frac{\partial^2 u}{\partial x^2} - \frac{\partial}{\partial x} \left( \frac{1}{2} u^2 \right)$$

$$\Rightarrow \frac{du_j}{dt} = \frac{\varepsilon}{\Delta x^2} (u_{j+1} - 2u_j + u_{j-1}) - \frac{1}{4\Delta x} (u_{j+1}^2 - u_{j-1}^2)$$



## MOVFDM

— For 1D system

$$\begin{cases} F(t, x, u, u_x, u_t) = \frac{\partial}{\partial x} G(t, x, u, u_x, u_t) \\ B_l(t, x, u, u_x, u_t) = 0 & a < x < b \\ B_r(t, x, u, u_x, u_t) = 0 & x = a \\ & x = b \end{cases}$$

~~The~~ The user needs to provide

$F$ ,  $G$ ,  $B_l$  and  $B_r$ .

— Central FiD discretization

— ODE15i for time integration



Example Burgers' eqn

$$\begin{cases} \frac{\partial u}{\partial t} = \varepsilon \frac{\partial^2 u}{\partial x^2} - u \frac{\partial u}{\partial x} & x \in (0,1) \\ u(0,t) = 0 \\ u(1,t) = 0 \end{cases}$$

$$\textcircled{1} \quad F = \frac{\partial u}{\partial t}, \quad G = \varepsilon \frac{\partial u}{\partial x} - \frac{1}{2} u^2$$

$$B_e = u_t - 0, \quad B_r = u_t - 0.$$

$$\textcircled{2} \quad F = \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x}, \quad G = \varepsilon \frac{\partial u}{\partial x}$$

$$B_e = u_t - 0, \quad B_r = u_t - 0.$$



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```

function sec1_2_burgersFDM(jmax)
%
% example driver for Burgers' equation in section 1.2.
% it calls movfdm().
)

%
% Copyright (C) 2010 Weizhang Huang and Robert D. Russell
% all rights reserved.
%
% This program is provided "as is", without warranty of any
kind.
% Permission is hereby granted, free of charge, to use this
program
% for personal, research, and education purposes. Distribution
or use
% of this program for any commercial purpose is permissible
% only by direct arrangement with the copyright owner.
%

cpu0=clock;

% job = 1 for solution
% job = 2 for mesh trajectories

job = 1;

%jmax = 41;
npde = 1;
nn = npde*jmax;
)
x=zeros(jmax,1);
u=zeros(npde,jmax);

% define initial solution

x=linspace(0,1,jmax)';
u(1,:)=(sin(2*pi*x)+0.5*sin(pi*x))';
xt=zeros(jmax,1);
ut=zeros(npde,jmax);

% call the moving mesh function
% monitor = 0 (fixed mesh), 1, 2, 3, 4, or 5
% mmpde = 4, 5, 6, 7 (mmpde = 7 ==> modified MMPDE5)
% alpha_type = 1, 2, or 3: (integral def, integral def with
flooring, or alpha = constant)

monitor = 3;
mmpde = 7;
alpha_type = 2;
alpha = 1.0;
reltol=1e-6; abstol=1e-4;

if job==1 % for solution

    tspan = [0 0.2 0.4 0.6 0.8 1.0];
)

[t,X,U]=movfdm(npde,jmax,tspan,x,xt,u,ut,@PDE_F,@PDE_G,@BC_L,@BC
_R,...

```



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```

[],monitor,reltol,abstol,[],mmpde,alpha_type,alpha);
    fprintf('\n cpu time used = %e \n', etime(clock,cpu0));
    % output the solution
    N=size(t,1);
    figure
    labels={};
    marks='+osdv^<>';
    lines1='--:-';
    lines2='- .';
    colors='mkbgrc';
    for n=1:N
        u=U(:,:,n);
        x=X(:,n);
        hold on
        labels{n} = ['t = ' num2str(t(n)) ];
        style=['-' marks(1+rem(n,8))];
        plot(x,u(1,:),'style');%,'LineWidth',2);
    end
    hold off
    legend(labels{:});
    xlabel('x');
    ylabel('u');
    axis([0 1 -1 2]);
    box on;

else % for trajectories

    tspan = [0 1.0];

    [X,U]=movfdm(npde,jmax,tspan,x,xt,u,ut,@PDE_F,@PDE_G,@BC_L,@BC
    _R,...

[],monitor,reltol,abstol,[],mmpde,alpha_type,alpha);
    fprintf('\n cpu time used = %e \n',
etime(clock,cpu0));
    plot(X',t);
    axis([0 1 0 1]);
    xlabel('x')
    ylabel('t')
end

fprintf('cpu time used = %e \n', etime(clock,cpu0));

% -----

function f=PDE_F(t,x,u,ux,ut)
    f(1,:) = ut(1,:);

function f=PDE_G(t,x,u,ux,ut)
    f(1,:) = 1e-4*ux(1,:)-u(1,:).*u(1,)*0.5;

function f=BC_L(t,x,u,ux,ut)
    f(1) = ut(1)-0.0;

function f=BC_R(t,x,u,ux,ut)
    f(1) = ut(1)-0.0;

```



# Lecture 7

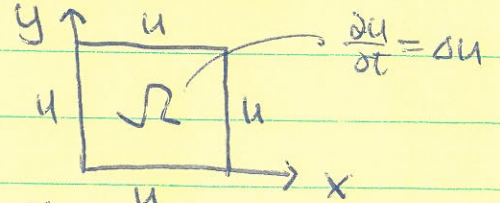
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## FTCS scheme for 2D parabolic PDEs

- Model problem
- Mesh
- FTCS scheme
- local truncation error
- Convergence
- stability

### ▶ The 2D Model problem

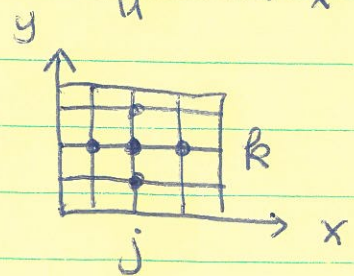
$$\begin{cases} \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \equiv \Delta u & (x,y) \in \Omega = (0,1) \times (0,1) \\ u(x,y,t) = g(x,y,t) & (x,y) \in \partial\Omega \\ u(x,y,0) = u^0(x,y) \end{cases}$$



### ▶ Mesh - Cartesian grid

J subintervals of equal length in x direction

$$x_j = j \Delta x, \quad j=0, 1, \dots, J$$
$$\Delta x = \frac{1}{J}$$



K subintervals of equal length in y direction

$$y_k = k \Delta y, \quad k=0, 1, \dots, K$$

$$\Delta y = \frac{1}{K}$$

N subintervals of equal length in t direction

$$t_n = n \Delta t, \quad n=0, \dots, N \quad \Delta t = \frac{T}{N}$$



▶ FTCS scheme

$$u_{j,k}^n \approx u(x_j, y_k, t_n)$$

$$\left\{ \begin{aligned} \frac{u_{j,k}^{n+1} - u_{j,k}^n}{\Delta t} &= \frac{1}{\Delta x^2} (u_{j+1,k}^n - 2u_{j,k}^n + u_{j-1,k}^n) \\ &+ \frac{1}{\Delta y^2} (u_{j,k+1}^n - 2u_{j,k}^n + u_{j,k-1}^n) \end{aligned} \right.$$

$j = 1, \dots, J-1$   
 $k = 1, \dots, K-1$

$$u_{j,k}^{n+1} = g(x_j, y_k, t_{n+1}), \quad \begin{aligned} j=0 \text{ or } j=J, k=0, \dots, K \\ k=0 \text{ or } k=K, j=1, \dots, J-1 \end{aligned}$$

▶ Local truncation error

The error equation:

$$\frac{e_{j,k}^{n+1} - e_{j,k}^n}{\Delta t} = \frac{1}{\Delta x^2} \delta_x^2 e_{j,k}^n + \frac{1}{\Delta y^2} \delta_y^2 e_{j,k}^n - \tau_{j,k}^n$$

$$\tau_{j,k}^n = \frac{u(x_j, y_k, t_{n+1}) - u(x_j, y_k, t_n)}{\Delta t}$$

$$\begin{aligned} &= \frac{\Delta t}{2} u_{tt}(x_j, y_k, t_n) - \frac{\Delta x^2}{12} u_{xxxx}(x_j, y_k, t_n) \\ &\quad - \frac{\Delta y^2}{12} u_{yyyy}(x_j, y_k, t_n) \end{aligned}$$



$$= O(\Delta t) + O(\Delta x^2) + O(\Delta y^2)$$

► Convergence in  $L^\infty$  norm

$$\|e^n\|_\infty = \max_{j,k} |e_{j,k}^n|$$

If 
$$\Delta t \leq \frac{1}{\frac{2}{\Delta x^2} + \frac{2}{\Delta y^2}}$$

then 
$$\|e^n\|_\infty \leq T \left( \frac{\Delta t}{2} M_{tt} + \frac{\Delta x^2}{12} M_{xxxx} + \frac{\Delta y^2}{12} M_{yyyy} \right)$$

► Stability

— Fourier stability analysis

$$u_{j,k}^n = (\lambda)^n e^{im\pi x_j} e^{i\ell\pi y_k}$$

$$m = 1, \dots, J-1$$

$$\ell = 1, \dots, K-1$$

$$\begin{aligned} \frac{\lambda-1}{\Delta t} &= \frac{1}{\Delta x^2} \left( e^{im\pi\Delta x} - 2 + e^{-im\pi\Delta x} \right) \\ &\quad + \frac{1}{\Delta y^2} \left( e^{i\ell\pi\Delta y} - 2 + e^{-i\ell\pi\Delta y} \right) \end{aligned}$$

$$\begin{aligned} \frac{\lambda-1}{\Delta t} &= \frac{1}{\Delta x^2} \left( 2 \cos(m\pi\Delta x) - 2 \right) \\ &\quad + \frac{1}{\Delta y^2} \left( 2 \cos(\ell\pi\Delta y) - 2 \right) \end{aligned}$$



$$\frac{\lambda-1}{\Delta t} = \frac{4}{\Delta x^2} \sin^2\left(\frac{m\pi\Delta x}{2}\right) - \frac{4}{\Delta y^2} \sin^2\left(\frac{l\pi\Delta y}{2}\right)$$

$$\lambda = 1 - \frac{4\Delta t}{\Delta x^2} \sin^2\left(\frac{m\pi\Delta x}{2}\right) - \frac{4\Delta t}{\Delta y^2} \sin^2\left(\frac{l\pi\Delta y}{2}\right)$$

$|\lambda| \leq 1$  for all  $m=1, \dots, J-1$   
 $l=1, \dots, K-1$

$$\Rightarrow \Delta t \leq \frac{1}{\frac{2}{\Delta x^2} + \frac{2}{\Delta y^2}} \quad \begin{matrix} \text{(CFL)} \\ \text{(Condition)} \end{matrix}$$

-  $L^\infty$  stability analysis

$$\|u^n\|_\infty \leq \|u^0\|_\infty \text{ for all } n$$

$$\Rightarrow \Delta t \leq \frac{1}{\frac{2}{\Delta x^2} + \frac{2}{\Delta y^2}} \quad \text{(CFL)}$$

#



BTCS scheme for 2D parabolic PDEs

- BTCS scheme
- local truncation error, stability, convergence
- Linear system for  $u_{j,k}^{n+1}$  and natural ordering
- ~~Solution~~ Direct solution
- ~~iterative methods~~ techniques for large scale sparse systems

## ▶ BTCS scheme

$$\begin{cases} \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} & \text{in } \Omega \\ u = g & \text{on } \partial\Omega \end{cases}$$

$$\frac{u_{j,k}^{n+1} - u_{j,k}^n}{\Delta t} = \frac{1}{\Delta x^2} \delta_x^2 u_{j,k}^{n+1} + \frac{1}{\Delta y^2} \delta_y^2 u_{j,k}^{n+1}$$

$$j=1, \dots, J-1 \\ k=1, \dots, K-1$$

$$\delta_x^2 u_{j,k}^{n+1} = u_{j+1,k}^{n+1} - 2u_{j,k}^{n+1} + u_{j-1,k}^{n+1}$$

$$\delta_y^2 u_{j,k}^{n+1} = u_{j,k+1}^{n+1} - 2u_{j,k}^{n+1} + u_{j,k-1}^{n+1}$$

$$u_{j,k}^{n+1} = g(x_j, y_k, t_{n+1}) \quad (x_j, y_k) \in \partial\Omega$$



## ► Consistency, stability, and convergence

$$\tau_{j,k}^n = O(\Delta t) + O(\Delta x^2) + O(\Delta y^2)$$

Stability: ( $L^\infty$  and Fourier analysis)

on constraint on choice of  $\Delta t$   
 $\Rightarrow$  unconditionally stable

Convergence:

$$e_{j,k}^n = O(\Delta t) + O(\Delta x^2) + O(\Delta y^2)$$

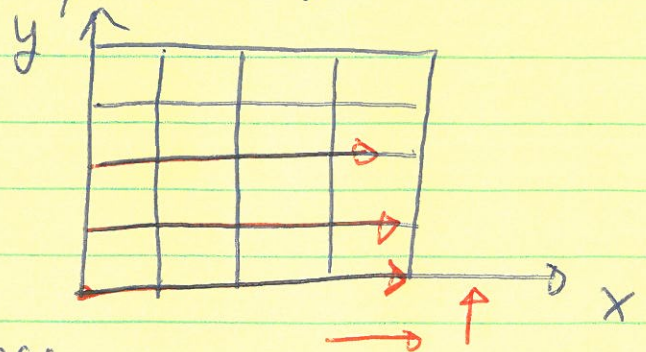
## ► Linear system for $u_{j,k}^{n+1}$ and natural ordering

- BTCS scheme is implicit.

$\Rightarrow \{u_{j,k}^{n+1}, j=1, \dots, J-1, k=1, \dots, K-1\}$  must be solved simultaneously.

- Natural ordering for unknown variables (and for equations):

We need to convert  
 2D array  $u_{j,k}$   
 into 1D array  $\vec{u}$   
 so that we can express  
 the linear system  
 in a matrix form.





$$(j, k) \longrightarrow (j+1)k + j$$

$$u_{j,k} \longrightarrow \vec{u}_{(j+1)k+j}$$

$$\{u_{j,k}\} \longrightarrow (u_{0,0}, u_{1,0}, \dots, u_{J,0}, u_{0,1}, \dots, u_{J,1}, \dots \\ \dots, u_{0,K}, \dots, u_{J,K})$$

- matrix form

$$A \vec{u}^{n+1} = \vec{b}$$

For  $(x_j, y_k) \in \Omega$ :

$$-\frac{\Delta t}{\Delta x^2} (u_{j+1,k}^{n+1} + u_{j-1,k}^{n+1}) - \frac{\Delta t}{\Delta y^2} (u_{j,k+1}^{n+1} + u_{j,k-1}^{n+1})$$

$$+ \left(1 + \frac{2\Delta t}{\Delta x^2} + \frac{2\Delta t}{\Delta y^2}\right) u_{j,k}^{n+1} = u_{j,k}^n$$

$$A_{(j,k), (j,k)} = 1 + \frac{2\Delta t}{\Delta x^2} + \frac{2\Delta t}{\Delta y^2}$$

$$A_{(j,k), (j+1,k)} = -\frac{\Delta t}{\Delta x^2}$$

$$A_{(j,k), (j-1,k)} = -\frac{\Delta t}{\Delta x^2}$$

$$A_{(j,k), (j,k+1)} = -\frac{\Delta t}{\Delta y^2}$$

$$A_{(j,k), (j,k-1)} = -\frac{\Delta t}{\Delta y^2}$$

$$\vec{b}_{(j,k)} = u_{j,k}^n$$



For  $(x_j, y_k) \in \partial\Omega$ :

$$u_{j,k}^{n+1} = g(x_j, y_k, t_{n+1})$$

$$A_{(j,k), (j,k)} = 1$$

$$\vec{b}_{(j,k)} = g(x_j, y_k, t_{n+1})$$

Properties of  $A$ :

(i)  $A$  is pentadiagonal

$$A = \begin{bmatrix} & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \end{bmatrix}_{[(J+1)(K+1)] \times [(J+1) \times (K+1)]}$$

(ii) sparse:

$$\frac{\# \text{ of non-zero entries}}{\# \text{ of entries}} \approx \frac{5(JK)}{(JK)^2} = \frac{5}{JK}$$

small when  $J, K$  large

(iii) diagonally dominant

$$|A_{j,j}| \geq \sum_{k \neq j} |A_{j,k}|$$



Direct solution of the linear system

— Direct solvers (full matrix)



Gaussian elimination, LU decomposition

Cost  $O((JK)^3) = O(J^3K^3)$

— Direct solvers (banded matrix)  
band width =  $J+1$

Cost  $O(J^2(JK)) = O(J^3K)$

$J=K$ , # of operations/sec =  $10^8$

J	$O(J^3K^3)$	CPU(sec)	$O(J^3K)$	CPU(sec)
10	$10^6$	$10^{-2}$	$10^4$	$10^{-4}$
100	$10^{12}$	$10^4$	$10^8$	1
1000	$10^{18}$	$10^{10}$	$10^{12}$	$10^4$

— Direct solvers (sparse matrix)

Example: UMFPACK



► Iterative methods for large scale sparse systems:

— Conventional iterative methods

$$\{u_{j,k}^{n+1,0}\} \rightarrow \{u_{j,k}^{n+1,1}\} \rightarrow \dots$$

$$u_{j,k}^{n+1,i} \rightarrow u_{j,k}^{n+1,i+1} \quad \text{as } i \rightarrow +\infty$$

Jacobi iteration:

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

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

$$j = 1, \dots, J-1 \\ k = 1, \dots, K-1$$

Gauss-seidel iteration

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

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

$$j = 1, \dots, J-1 \\ k = 1, \dots, K-1$$



### SOR (Successive over relaxation)

$$\left\{ \begin{aligned} & -\frac{\Delta t}{\Delta x^2} (u_{j+1,k}^{n+1,i} + u_{j-1,k}^{n+1,i+1}) - \frac{\Delta t}{\Delta y^2} (u_{j,k+1}^{n+1,i} + u_{j,k-1}^{n+1,i+1}) \\ & + \left(1 + \frac{2\Delta t}{\Delta x^2} + \frac{2\Delta t}{\Delta y^2}\right) u_{j,k}^{n+1,*} = u_{j,k}^n \\ & u_{j,k}^{n+1,i+1} = (1-\omega) u_{j,k}^{n+1,i} + \omega u_{j,k}^{n+1,*} \end{aligned} \right.$$

$$\begin{aligned} j &= 1, \dots, J-1 \\ k &= 1, \dots, K-1 \end{aligned}$$

initial guess:

$$u_{j,k}^{n+1,0} = u_{j,k}^n$$

— Krylov Subspace methods + preconditioning techniques

Conjugate gradient (CG)

CR, GMRES, BiCG, BiCGstab, BiCGstab2

preconditioning techniques:

ILU (incomplete LU decomposition)

and many others

— Multigrid (or multilevel) methods

algebraic multigrid methods

(MG, AMG).

#



ADI methods

ADI: alternating direction implicit

- ADI method
- ~~order~~<sup>accuracy</sup> analysis
- stability analysis
- implementation
- limitations

▶ ADI method

Consider BTCS scheme

$$\frac{u_{j,k}^{n+1} - u_{j,k}^n}{\Delta t} = \frac{1}{\Delta x^2} \delta_x^2 u_{j,k}^{n+1} + \frac{1}{\Delta y^2} \delta_y^2 u_{j,k}^{n+1} + O(\Delta t) + O(\Delta x^4) + O(\Delta y^4)$$

$$\left(1 - \frac{\Delta t}{\Delta x^2} \delta_x^2 - \frac{\Delta t}{\Delta y^2} \delta_y^2\right) u_{j,k}^{n+1} = u_{j,k}^n + O(\Delta t^2) + O(\Delta t \Delta x^2) + O(\Delta t \Delta y^2)$$

Introduce increment:

$$u_{j,k}^{n+1} = u_{j,k}^n + \Delta u_{j,k}^n$$

Then, we have



$$\begin{aligned}
 & \left(1 - \frac{\Delta t}{\Delta x^2} \delta_x^2 - \frac{\Delta t}{\Delta y^2} \delta_y^2\right) \Delta u_{j,k}^n \\
 &= \left(\frac{\Delta t}{\Delta x^2} \delta_x^2 + \frac{\Delta t}{\Delta y^2} \delta_y^2\right) u_{j,k}^n \\
 &\quad + O(\Delta t^2) + O(\Delta t \Delta x^2) + O(\Delta t \Delta y^2)
 \end{aligned}$$

Notice that

$$\begin{aligned}
 & \left(1 - \frac{\Delta t}{\Delta x^2} \delta_x^2\right) \left(1 - \frac{\Delta t}{\Delta y^2} \delta_y^2\right) \\
 &= 1 - \frac{\Delta t}{\Delta x^2} \delta_x^2 - \frac{\Delta t}{\Delta y^2} \delta_y^2 + \frac{\Delta t^2}{\Delta x^2 \Delta y^2} \delta_x^2 \delta_y^2
 \end{aligned}$$

Thus

$$\begin{aligned}
 & \left(1 - \frac{\Delta t}{\Delta x^2} \delta_x^2\right) \left(1 - \frac{\Delta t}{\Delta y^2} \delta_y^2\right) \Delta u_{j,k}^n \\
 &= \left(\frac{\Delta t}{\Delta x^2} \delta_x^2 + \frac{\Delta t}{\Delta y^2} \delta_y^2\right) u_{j,k}^n \\
 &\quad + \boxed{\frac{\Delta t^2}{\Delta x^2 \Delta y^2} \delta_x^2 \delta_y^2 \Delta u_{j,k}^n} \quad \text{drop this term?} \\
 &\quad + O(\Delta t^2) + O(\Delta t \Delta x^2) + O(\Delta t \Delta y^2)
 \end{aligned}$$

⇒ ADI scheme:

$$\begin{aligned}
 & \left(1 - \frac{\Delta t}{\Delta x^2} \delta_x^2\right) \left(1 - \frac{\Delta t}{\Delta y^2} \delta_y^2\right) \Delta u_{j,k}^n \\
 &= \left(\frac{\Delta t}{\Delta x^2} \delta_x^2 + \frac{\Delta t}{\Delta y^2} \delta_y^2\right) u_{j,k}^n
 \end{aligned}$$



- (i) The system is much more economic to solve than the BTCS scheme
- (ii) Good stability
- (iii) Good accuracy

### ► Accuracy

We just need to estimate the term dropped:

$$\frac{\Delta t^2}{\Delta x^2 \Delta y^2} \delta_x^2 \delta_y^2 \Delta u_{j,k}^n$$

$$\Delta u_{j,k}^n = u_{j,k}^{n+1} - u_{j,k}^n = O(\Delta t)$$

$$\frac{1}{\Delta x^2} \delta_x^2 u \cong u_{xx} + O(\Delta x^2) = O(1)$$

$$\Rightarrow \frac{\Delta t^2}{\Delta x^2 \Delta y^2} \delta_x^2 \delta_y^2 \Delta u_{j,k}^n = O(\Delta t^3)$$

this order is higher than the local truncation error  $O(\Delta t^2) + O(\Delta t \Delta x^2) + O(\Delta t \Delta y^2)$ .

Thus, the local truncation error for the ADI scheme is

$$\bar{\tau}_{j,k}^n = O(\Delta t) + O(\Delta x^2) + O(\Delta y^2)$$





## Stability

$$u_{j,k}^n = (\lambda)^n e^{im\pi x_j} e^{il\pi y_k}$$

$$\delta_x^2 u_{j,k}^n = -4 \sin^2\left(\frac{m\pi}{2} \Delta x\right) u_{j,k}^n$$

$$\delta_y^2 u_{j,k}^n = -4 \sin^2\left(\frac{l\pi}{2} \Delta y\right) u_{j,k}^n$$

$$\xi \equiv \sin^2\left(\frac{m\pi}{2} \Delta x\right), \quad \eta \equiv \sin^2\left(\frac{l\pi}{2} \Delta y\right)$$

~~Approx~~

$$(1 + \frac{\Delta t}{\Delta x^2} \xi) (1 + \frac{\Delta t}{\Delta y^2} \eta) (\lambda - 1) \quad \underline{0 < \xi, \eta < 1}$$

$$(1 + \frac{4\Delta t}{\Delta x^2} \xi) (1 + \frac{4\Delta t}{\Delta y^2} \eta) (\lambda - 1)$$

$$= -\frac{4\Delta t}{\Delta x^2} \xi - \frac{4\Delta t}{\Delta y^2} \eta$$

$$\lambda = \frac{1 + \frac{16\Delta t^2}{\Delta x^2 \Delta y^2} \xi \eta}{(1 + \frac{4\Delta t}{\Delta x^2} \xi) (1 + \frac{4\Delta t}{\Delta y^2} \eta)}$$

$$|\lambda| \leq 1$$

unconditionally stable!



► Implementation:

$$\begin{aligned} & \left(1 - \frac{\Delta t}{\Delta x^2} \delta_x^2\right) \left(1 - \frac{\Delta t}{\Delta y^2} \delta_y^2\right) \Delta u_{j,k}^n \\ & = \left(\frac{\Delta t}{\Delta x^2} \delta_x^2 + \frac{\Delta t}{\Delta y^2} \delta_y^2\right) u_{j,k}^n \end{aligned}$$

Define

$$v_{j,k} = \left(1 - \frac{\Delta t}{\Delta y^2} \delta_y^2\right) \Delta u_{j,k}^n$$

then

$$\left(1 - \frac{\Delta t}{\Delta x^2} \delta_x^2\right) v_{j,k} = \left(\frac{\Delta t}{\Delta x^2} \delta_x^2 + \frac{\Delta t}{\Delta y^2} \delta_y^2\right) u_{j,k}^n$$

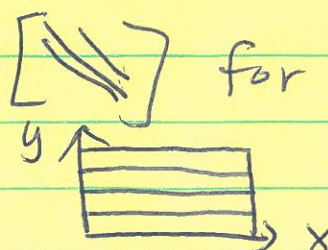
Step 1 X-sweeps

for  $k=1, \dots, K-1$

Solve

$$\begin{cases} \left(1 - \frac{\Delta t}{\Delta x^2} \delta_x^2\right) v_{j,k} = \left(\frac{\Delta t}{\Delta x^2} \delta_x^2 + \frac{\Delta t}{\Delta y^2} \delta_y^2\right) u_{j,k}^n \\ v_{0,k} = \left(1 - \frac{\Delta t}{\Delta y^2} \delta_y^2\right) \Delta u_{0,k}^n \\ v_{J,k} = \left(1 - \frac{\Delta t}{\Delta y^2} \delta_y^2\right) \Delta u_{J,k}^n \end{cases}$$

$$\text{or } \begin{cases} -\frac{\Delta t}{\Delta x^2} v_{j+1,k} + \left(1 + \frac{2\Delta t}{\Delta x^2}\right) v_{j,k} - \frac{\Delta t}{\Delta x^2} v_{j-1,k} \\ = \left(\frac{\Delta t}{\Delta x^2} \delta_x^2 + \frac{\Delta t}{\Delta y^2} \delta_y^2\right) u_{j,k}^n \\ j=1, \dots, J-1 \\ v_{0,k} = \left(1 - \frac{\Delta t}{\Delta y^2} \delta_y^2\right) (u_{0,k}^{n+1} - u_{0,k}^n) \\ v_{J,k} = \left(1 - \frac{\Delta t}{\Delta y^2} \delta_y^2\right) (u_{J,k}^{n+1} - u_{J,k}^n) \end{cases}$$

 for  $(v_{0,k}, v_{1,k}, \dots, v_{J,k})$



Step 2 y-sweeps

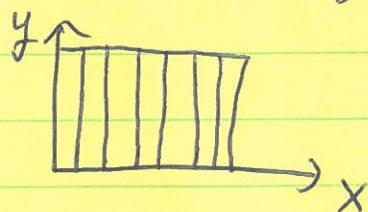
For  $j=1, \dots, J-1$ :

$$\begin{cases} (1 - \frac{\Delta t}{\Delta y^2} \delta_y^2) \Delta U_{j,k}^n = U_{j,k} \\ \Delta U_{j,0}^n = U_{j,0}^{n+1} - U_{j,0}^n \\ \Delta U_{j,K}^n = U_{j,K}^{n+1} - U_{j,K}^n \end{cases}$$

or

$$\begin{cases} -\frac{\Delta t}{\Delta y^2} \Delta U_{j,k+1}^n + (1 + \frac{2\Delta t}{\Delta y^2}) \Delta U_{j,k}^n - \frac{\Delta t}{\Delta y^2} \Delta U_{j,k-1}^n = U_{j,k} \\ \Delta U_{j,0}^n = U_{j,0}^{n+1} - U_{j,0}^n \\ \Delta U_{j,K}^n = U_{j,K}^{n+1} - U_{j,K}^n \end{cases} \quad k=1, \dots, K-1$$

For  $(\Delta U_{j,0}^n, \Delta U_{j,1}^n, \dots, \Delta U_{j,K}^n)$



Step 3

Finally update the soln:

$$U_{j,k}^{n+1} = U_{j,k}^n + \Delta U_{j,k}^n$$

Limitations of ADI

- work only for regular, simple domain
- work only for FID mesh (Cartisian mesh)
- does not work for problems with mixed derivatives

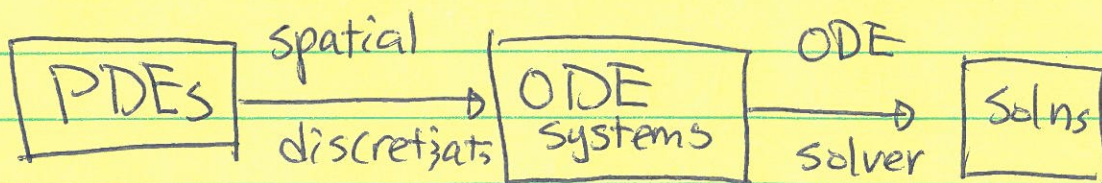
$(1 - \frac{\Delta t}{\Delta x^2} \delta_x^2) (1 - \frac{\Delta t}{\Delta y^2} \delta_y^2)$  can be used as a preconditioner. #



MOL for general 2D problems

- Model PDE
- general PDEs
- PDEs in divergence form

▶ MOL for model PDE



- advantage is that we can focus on the spatial discretization, and leave time discretization, solution of nonlinear equations, and efficient solution of large scale (sparse) systems to the ODE solver:

$$u_{j,k}(t) \approx u(x_j, y_k, t)$$

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

$$\frac{du_{j,k}}{dt} = \frac{1}{\Delta x^2} \delta_x^2 u_{j,k} + \frac{1}{\Delta y^2} \delta_y^2 u_{j,k}$$

$$(x_j, y_k) \in \Omega$$

\* approximation  $u_{j,k} = g(x_j, y_k, t)$ .  $(x_j, y_k) \in \partial \Omega$



$$\Rightarrow M \frac{d\vec{u}}{dt} = \vec{f}(t, \vec{u})$$

$$u_{j,k} \rightarrow \vec{u}_{(j,k)} = \vec{u}_{(j+1)k+j}$$

▶ General 2D parabolic PDEs

$$\begin{aligned} \frac{\partial u}{\partial t} &= d_{11} \frac{\partial^2 u}{\partial x^2} + 2d_{12} \frac{\partial^2 u}{\partial x \partial y} + d_{22} \frac{\partial^2 u}{\partial y^2} \\ &\quad + b_1 \frac{\partial u}{\partial x} + b_2 \frac{\partial u}{\partial y} + cu + f(t, x, y) \\ \frac{d}{dt} u_{j,k} &= d_{11,j,k} \frac{1}{\Delta x^2} \delta_x^2 u_{j,k} + d_{22,j,k} \frac{1}{\Delta y^2} \delta_y^2 u_{j,k} \\ &\quad + 2d_{12,j,k} \frac{1}{4\Delta x \Delta y} (u_{j+1,k+1} - u_{j+1,k-1} \\ &\quad \quad - u_{j-1,k+1} + u_{j-1,k-1}) \\ &\quad + \frac{b_1}{2\Delta x} (u_{j+1,k} - u_{j-1,k}) + \frac{b_2}{2\Delta y} (u_{j,k+1} - u_{j,k-1}) \\ &\quad + c_{j,k} u_{j,k} + f_{j,k} \end{aligned}$$

Nonlinear equations

2D Burgers' equation

$$\frac{\partial u}{\partial t} = \varepsilon \frac{\partial^2 u}{\partial x^2} + \varepsilon \frac{\partial^2 u}{\partial y^2} - u \frac{\partial u}{\partial x} - u \frac{\partial u}{\partial y}$$



(61)

$$\begin{aligned} \frac{du_{j,k}}{dt} &= \frac{\epsilon}{\Delta x^2} \delta_x^2 u_{j,k} + \frac{\epsilon}{\Delta y^2} \delta_y^2 u_{j,k} \\ &\quad - \frac{1}{4\Delta x} (u_{j+1,k}^2 - u_{j-1,k}^2) \\ &\quad - \frac{1}{4\Delta y} (u_{j,k+1}^2 - u_{j,k-1}^2) \end{aligned}$$

▶ PDEs in divergence form

$$\nabla = \begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{bmatrix}$$

$$\frac{\partial u}{\partial t} = \nabla \cdot (\mathbb{D} \nabla u) - \nabla \cdot (\vec{b} u) + cu + f$$

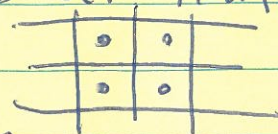
~~Define diffusion fluxes:~~

Define diffusion fluxes:

$$q_1 = d_{11} \frac{\partial u}{\partial x} + d_{12} \frac{\partial u}{\partial y}$$

$$q_2 = d_{21} \frac{\partial u}{\partial x} + d_{22} \frac{\partial u}{\partial y}$$

Approximate these fluxes at half-half points  $(j+\frac{1}{2}, k+\frac{1}{2})$ :



$$\begin{aligned} q_{1, j+\frac{1}{2}, k+\frac{1}{2}} &= d_{11, j+\frac{1}{2}, k+\frac{1}{2}} \frac{1}{2\Delta x} (u_{j+1,k} - u_{j,k} + u_{j+1,k+1} - u_{j,k+1}) \\ &\quad + d_{12, j+\frac{1}{2}, k+\frac{1}{2}} \frac{1}{2\Delta y} (u_{j,k+1} - u_{j,k} + u_{j+1,k+1} - u_{j+1,k}) \end{aligned}$$



$$g_{z, j+\frac{1}{2}, k+\frac{1}{2}} = d_{z1, j+\frac{1}{2}, k+\frac{1}{2}} \frac{1}{2\Delta x} ( \dots )$$

$$+ d_{z2, j+\frac{1}{2}, k+\frac{1}{2}} \frac{1}{2\Delta y} ( \dots )$$

Then

$$\nabla \cdot (\mathbb{D} \nabla u) |_{j,k} = \nabla \cdot (\vec{q}) |_{j,k}$$

$$\approx \left( \frac{\partial q_1}{\partial x} + \frac{\partial q_2}{\partial y} \right) |_{j,k}$$

$$\approx \frac{1}{2\Delta x} \left( q_{1, j+\frac{1}{2}, k+\frac{1}{2}} - q_{1, j-\frac{1}{2}, k+\frac{1}{2}} \right.$$

$$\left. + q_{1, j+\frac{1}{2}, k-\frac{1}{2}} - q_{1, j-\frac{1}{2}, k-\frac{1}{2}} \right)$$

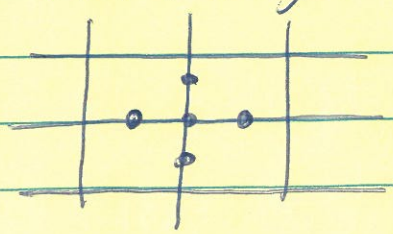
$$+ \frac{1}{2\Delta y} \left( q_{z, j+\frac{1}{2}, k+\frac{1}{2}} - q_{z, j+\frac{1}{2}, k-\frac{1}{2}} \right.$$

$$\left. + q_{z, j-\frac{1}{2}, k+\frac{1}{2}} - q_{z, j-\frac{1}{2}, k-\frac{1}{2}} \right)$$

Define ~~tran~~ convection fluxes:

$$\vec{p} = \vec{b} u$$

Approximate convection fluxes at half-integer and integer-half points





$$p_{1,j+\frac{1}{2},k} = b_{1,j+\frac{1}{2},k} \frac{u_{j+1,k} + u_{j,k}}{2}$$

$$p_{2,j,k+\frac{1}{2}} = b_{2,j,k+\frac{1}{2}} \frac{u_{j,k+1} + u_{j,k}}{2}$$

$$\nabla \cdot (\vec{b}u)_{j,k} = \nabla \cdot \vec{p}_{j,k}$$

$$= \left( \frac{\partial p_1}{\partial x} + \frac{\partial p_2}{\partial y} \right)_{j,k}$$

$$\approx \frac{1}{\Delta x} (p_{1,j+\frac{1}{2},k} - p_{1,j-\frac{1}{2},k})$$

$$+ \frac{1}{\Delta y} (p_{2,j,k+\frac{1}{2}} - p_{2,j,k-\frac{1}{2}})$$

Advantages:

- symmetric
- diagonally dominant

#