

2

Parabolic PDEs

The diffusion equation

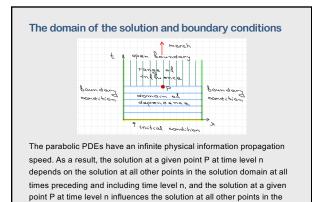
$$\frac{\partial f}{\partial t} = a \frac{\partial^2 f}{\partial^2 x}$$

The diffusion-convection equation

$$\frac{\partial f}{\partial t} = a \frac{\partial^2 f}{\partial^2 x} - b \frac{\partial f}{\partial x}$$

where a is the diffusivity coefficient, and b is the convection velocity.

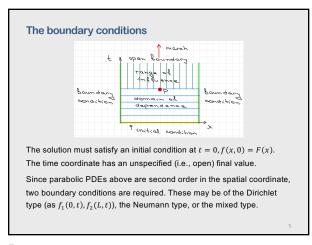
Parabolic PDEs are are initial-boundary-value problems in open domains (open with respect to time or a time-like variable) in which the solution in the domain of interest is marched forward from the initial state, guided and modified by the boundary conditions.



solution domain at all times including and after time level n.



4

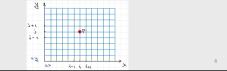


5

Finite-difference method

The finite difference method is a numerical procedure which solves a partial differential equation (PDE) by

- 1. discretizing the continuous physical domain into a discrete finite difference grid,
- 2. approximating the individual exact partial derivatives in the PDE by algebraic finite difference approximations (FDAs),
- substituting the FDAs into the PDE to obtain an algebraic finite difference equation (FDE),
- 4. and solving the resulting algebraic finite difference equations (FDEs)



Part 2: Diffusion equation: explicit methods

 $\frac{\partial f}{\partial t} = a \frac{\partial^2 f}{\partial^2 x}$

7

Explicit methods

The objective of the numerical solution of a parabolic PDE is to march the solution at time level n forward in time to time level n+1.

In view of the infinite physical information propagation associated with parabolic PDEs, the solution at point P at time level n+1 depends on the solution at all of the other points at time level n+1.

Finite difference methods when the solution at point P at time level n+1 depends only on the solution at neighboring points at time level n are called explicit methods. Explicit methods are computationally faster than implicit methods because there is no system of finite difference equations to solve.

However, the finite numerical information propagation speed of explicit methods does not correctly model the infinite physical information propagation speed of parabolic PDEs



8

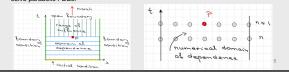
Implicit methods

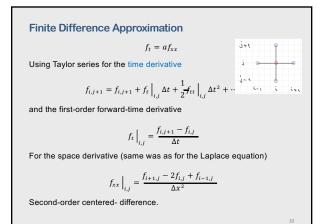
Finite difference methods in which the solution at point P at time level n+1 depends on the solution at neighboring points at time level n+1 as well as the solution at time level n have an infinite numerical information propagation speed. Such finite difference methods are called implicit methods.

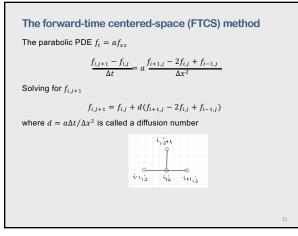
implicit methods appear to be well suited for solving parabolic PDEs, and explicit methods appear to be unsuitable for solving parabolic PDEs.

In actuality, only an infinitesimal amount of physical information propagates at the infinite physical information propagation speed. The bulk of the physical information travels at a finite physical information propagation speed.

Experience has shown that explicit methods as well as implicit methods can be employed to solve parabolic PDEs.







11

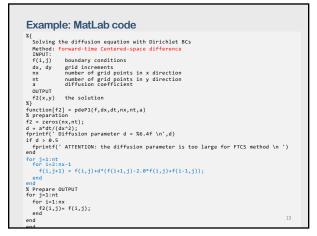
Attention

 $f_{i,j+1} = f_{i,j} + d(f_{i+1,j} - 2f_{i,j} + f_{i-1,j})$

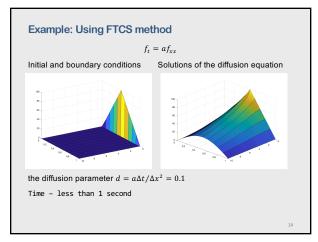
where $d = a\Delta t / \Delta x^2$ is called a diffusion number

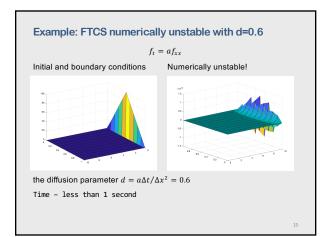
Numerical solutions for $d \ge 1$ are numerically unstable

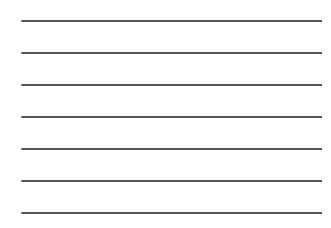
Using von Neuman method* gives that $d \le 0.5$ (at least) for stability.

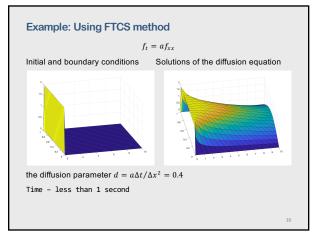




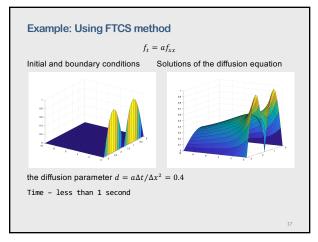












17

Summary for the FTCS

In summary, the forward-time centered-space (FTCS) approximation of the diffusion equation is

- · explicit,
- single step,
- · consistent,
- $O(\Delta t) + O(\Delta x^2)$,
- · conditionally stable,
- · and convergent.

It is somewhat inefficient because the time step varies as the square of the spatial grid size.

The Richardson and Dufort-Frankel methods

The forward-time centered-space(FTCS) approximation of the diffusion equation $f_t = a f_{xx}$ has several desirable features.

It is an explicit, two-level, single-step method.

The finite difference approximation of the spatial derivative is second order. However, the finite difference approximation of the time derivative is only first order.

An obvious improvement would be to use a second-order finite difference approximation of the time derivative.

The Richardson (leapfrog) and Dufort-Frankel methods are two such methods.

19

The Richardson (Leapfrog) methods

Richardson proposed approximating the partial derivative f_t by the three-level second-order centered-difference approximation based on time levels j - 1, j, and j + 1.

$$f_t \Big|_{i,j} = \frac{f_{i,j+1} - f_{i,j-1}}{2\Delta t}$$

Then the diffusion equation

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

 $f_{i,j+1} = f_{i,j-1} + 2d \big(f_{i+1,j} - 2f_{i,j} + f_{i-1,j} \big), \qquad d = a \Delta t / \Delta x^2$

The Richardson method appears to be a significant improvement over the FTCS method because of the increased accuracy of the finite difference approximation of f_t . BUT!!! Since the Richardson method is unconditionally unstable when applied to the diffusion equation, it cannot be used to solve that equation, or any other parabolic PDE

20

The Dufort-Frankel method

Dufort and Frankel (1953) proposed a modification to the Richardson method for the diffusion equation $f_t = a f_{xx}$ which removes the unconditional instability.

 $(1+2d)f_{i,j+1} = (1-2d)f_{i,j-1} + 2d(f_{i+1,j} + f_{i-1,j}).$

However this equation is not a consistent approximation of the diffusion equation as $\Delta t \rightarrow 0, \Delta x \rightarrow 0$.

Due to the inconsistency the Dufort-Frankel method is not an acceptable method for solving the parabolic diffusion equation, or any other parabolic PDE.

Part 3: **Diffusion equation: implicit methods**

 $\frac{\partial f}{\partial t} = a \frac{\partial^2 f}{\partial^2 x}$

22

Implicit methods: Pros and cons.

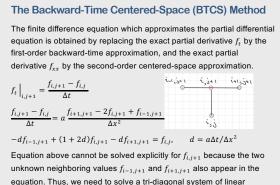
In implicit methods, the finite difference approximations of the individual exact partial derivatives in the partial differential equation are evaluated at the solution time level n + 1.

Implicit difference methods are unconditionally stable. There is no limit on the allowable time step required to achieve a numerically stable solution. There is, of course, some practical limit on the time step required to maintain the truncation errors within reasonable limits, but this is not a stability consideration; it is an accuracy consideration.

Implicit methods do have some disadvantages.

- 1. The solution at a point in the solution time level n + 1 depends on the solution at neighboring points in the solution time level, which are also unknown.
- 2. Additional complexities arise when the partial differential equations are nonlinear.

23



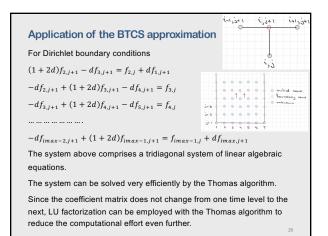
Stability, convergence and consistency.

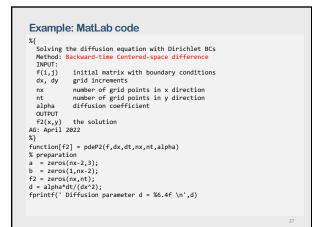
The BTCS approximation of the diffusion equation is consistent and convergent.

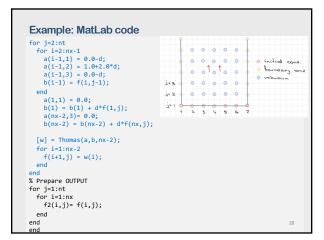
The BTCS method is unconditionally stable. The time step can be much larger than the time step for the FTCS method.

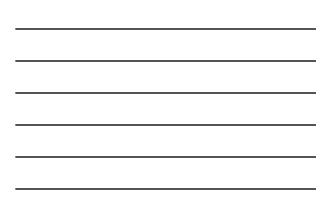
Consequently, the solution at a given time level can be reached with much less computational effort by taking time steps much larger than those allowed for the FTCS method. In fact, the time step is limited only by accuracy requirements.

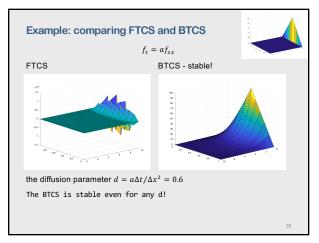
25



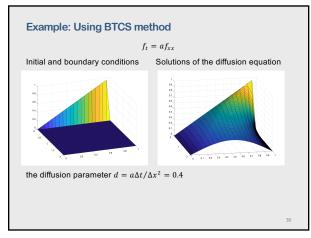




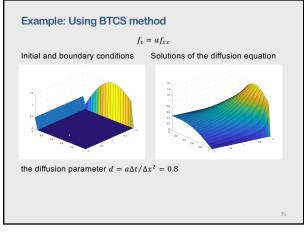




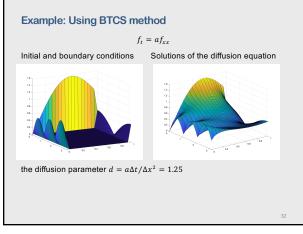












32

Nonlinear PDs and multi-dimensional problems

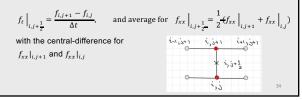
The BTCS method can be used to solve nonlinear PDEs, systems of PDEs, and multidimensional problems.

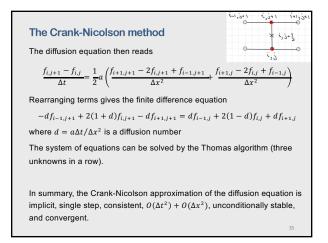
33

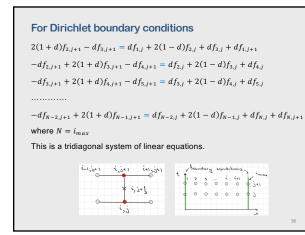
However, in those cases, the solution procedure becomes quite complicated.

The Crank-Nicolson method







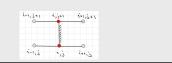


Derivative boundary conditions

The implementation of a derivative boundary condition does not depend on whether the problem is an equilibrium problem or a propagation problem

Consequently, the procedure for implementing a derivative boundary condition for one-dimensional equilibrium problems can be applied directly to one-dimensional propagation problems.

$$f_{i+1,j} = f_{i-1,j} + 2\Delta x f_x$$



37

More on implicit methods

Extensions:

- The derivative boundary conditions see books on numerical methods
 + using ideas similar to elliptical PDEs
- Non-linear equations using Newton's method for solving a system of non-linear equations
- Multidimensional problems
 2D problem yields a system based on a banded penta-diagonal matrix
 Successive-overrelaxation will work for explicit methods
 3D problem use ADI (alternating-direction-implicit) method and AFI (approximate-factorization-implicit) method.

38

38

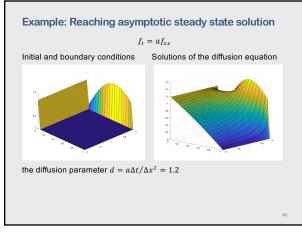
Asymptotic steady-state solution to propagation problems

Marching methods are employed for solving unsteady propagation problems, which are governed by parabolic and hyperbolic partial differential equations. The emphasis in those problems is on the transient solution itself.

Marching methods also can be used to solve steady equilibrium problems and steady mixed (i.e., elliptic-parabolic or elliptic-hyperbolic) problems as the asymptotic solution in time of an appropriate unsteady propagation problem.

Mixed problems present serious numerical difficulties due to the different types of solution domains (closed domains for equilibrium problems and open domains for propagation problems) and different types of auxiliary conditions (boundary conditions for equilibrium problems and boundary conditions and initial conditions for propagation problems).

Consequently, it may be easier to obtain the solution of a steady mixed problem by reposing the problem as an unsteady parabolic or hyperbolic problem and using marching methods to obtain the asymptotic steady state solution.





Part 4: Convection-Diffusion equation

$$\frac{\partial f}{\partial t} = a \frac{\partial^2 f}{\partial^2 x} - b \frac{\partial f}{\partial x}$$

41

The convection-diffusion equation

1D equation

 $f_t = af_{xx} - bf_x$

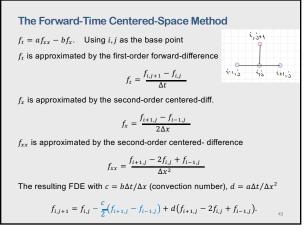
where b is the convection velocity and a is the diffusion coefficient.

The convection-diffusion equation applies to problems in mass transport, momentum transport, energy transport, etc.

The diffusion equation and the convection-diffusion equation are both parabolic PDEs.

However, the presence of the first-order convection term has an influence on the numerical solution procedure.

42





The Forward-Time Centered-Space Method

The forward-time centered-space method applied to the diffusionconvection equation is

- explicit
- two-level
- single-step
- $O(\Delta t) + O(\Delta x^2)$
- conditionally stable criteria $c^2 \le 2d \le 1$ ($c = b\Delta t/\Delta x$, $d = a\Delta t/\Delta x^2$)

convergent

Like most explicit methods applied to convection-diffusion equation, it is somewhat is inefficient, because the time step varies as the square of the spatial grid size $d = a\Delta t/\Delta x^2$

Additional criterion: for accuracy $R = \frac{b\Delta x}{a} \leq 2$ (the cell Peclet or Reynolds number)

44

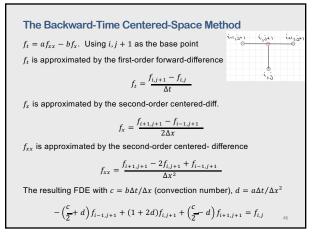
Other forward-time methods

Upwind method: first order $O(\Delta t) + O(\Delta x)$ (fast but not very good)

The Leonard method: $0(\Delta t) + O(\Delta x^2)$ some improvement to FTCS

The DuFort-Frankel method: $\partial(\Delta t) + \partial(\Delta x^2) + O(\Delta t^2/\Delta x^2)$ explicit, three-level, single step and conditionally stable for $c \leq 1$ (for any d). However, a starting method is required for the first step.

The MacCormack method: $O(\Delta t^2) + O(\Delta x^2)$ is explicit, two-level, twostep, conditionally stable. Excellent method for solving convectiondiffusion problem. The method is applied even when *b* and *a* coefficients in $f_t = af_{xx} - bf_x$ are variable coefficients. The method is efficient for solving the non-linear convection-diffusion problem.





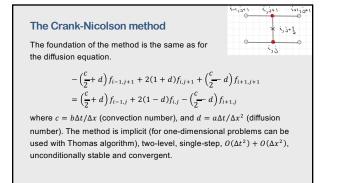
The Backward-Time Centered-Space Method

The forward-time centered-space method applied to the diffusionconvection equation is

- implicit
- two-level
- single-step
- $O(\Delta t) + O(\Delta x^2)$
- · unconditionally stable
- convergent

However, BTCS method becomes considerably more complicated when allied to non-linear PDEs, systems of PDEs and multidimensional problems.

47



48

Other methods

The Keller box method: $\mathit{O}(\Delta t^2) + \mathit{O}(\Delta x^2),$ allows the physical grid spacing to be non-uniform.

The hopscotch method is a combination of FTCS and BTCS methods. It is generally used for two- and three-dimensional problems. The method is conditionally stable $c \leq 1$, and $\partial(\Delta t) + \partial(\Delta x^2)$

49

50

49

SUMMARY for the Parabolic PDEs

Explicit (FTCS) methods

- are conditionally stable and require a relatively small step size in marching direction to satisfy stability criteria.
- nonlinear problems and multidimensional problems can be solved directly by explicit methods

Implicit (BTCS) methods

- are unconditionally stable. The marching step size is restricted by
 accuracy requirements, not stability requirements
- for transient problems, the marching step size cannot be very much larger than for explicit methods