2012 Basic Numerical Analysis

Partial Differential Equations 1: Diffusion Equations

Contents

- The world of errors....
- Explicit and implicit time stepping
- Spatial derivatives
- Heat conduction
- Crank-Nicholson scheme
- von Neumann stability analysis

Implicit method (blackboard)

Stiff equations

$$u' = 998\,u + 1998\,v$$
$$v' = -999\,u + 1999\,v$$

Initial values: $u(0) = 1,\ v(0) = 0$.

By the transformation $u = 2y - z,\ v = -y + z,$

we obtain

$$u = 2\,e^{-x} - e^{-1000x}$$

$$v = -e^{-x} + e^{-1000x}$$

The second term is very sensitive to variation in x.

Round-off errors

The two roots of a quadratic equation

$a\,x^2 + b\,x + c = 0$

are calculated ANALYTICALLY:

$x = (-b \pm \sqrt{b^2 - 4\,ac})/2a$

However, computers do not return

accurate values for, say,

$a = 1.01$, $b = 2718281$, $c = 0.01$. Why ?

Round-off errors

For x = 3.1834 x 10^{-3}

$$1 - \frac{1}{\sqrt{1+x}} = 1.5879 \times 10^{-3}$$

$$= 1 - \frac{1}{\sqrt{1.0032}} = 1 - \frac{1}{1.0016} = 1 - 0.99840 = 0.00160$$

$$= \frac{\sqrt{1+x} - 1}{\sqrt{1+x}} = \frac{1.0016 - 1}{1.0016} = \frac{0.0016}{1.0016} = 0.0015974$$

$$= \frac{x}{1 + x + \sqrt{1+x}} = \frac{0.0031843}{1.0032 + 1.0016} = \frac{0.0031843}{2.0048} = 0.0015879$$

Machine ε

The smallest positive floating point number which a current-generation computer (with IEEE 754) is

2^{-23} = 1.109209.... x 10^{-7} (single precision)

2^{-52} = 2.22044... x 10^{-16} (double precision)

パイこね変換

Choose a value x in between 0 and 1.

If x < 0.5, double the value, i.e. x = 2x.

If x >= 0.5, set x = 2-2x.

Repeat the above procedure.

Discretization and partial difference

$$\frac{d}{dx}f(x) \sim \frac{f(x+h)-f(x)}{h}$$ Forward difference

$$\frac{d}{dx}f(x) \sim \frac{f(x)-f(x-h)}{h}$$ Backward difference

$$\frac{d}{dx}f(x) \sim \frac{f(x+h)-f(x-h)}{2h}$$ Central difference

$$\frac{d^2}{dx^2}f(x) \sim \frac{f(x+h)-2f(x)+f(x-h)}{h^2}$$

Second derivative

2nd order PDEs

Parabolic

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

Diffusion
Heat conduction

Elliptic

Poisson

$$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = S(x, y)$$

Hyperbpolic

Soundwave

$$\frac{\partial^2 f}{\partial t^2} - \frac{\partial^2 f}{\partial x^2} = 0$$

Heat conduction

$$\frac{\partial T(\mathbf{r}, t)}{\partial t} = D \nabla^2 T(\mathbf{r}, t)$$

$$\mathbf{q} = -\kappa \nabla T,$$

1-D problem

In the interval $x_l < x < x_h$, temperature T is given by

$$\frac{\partial T(x,t)}{\partial t} = D\,\frac{\partial^2 T(x,t)}{\partial x^2}$$

Calculate T for the initial condition

$$T(x,t_0) = \exp\left(\frac{-x^2}{4\,D\,t_0}\right)$$

Simple discretization

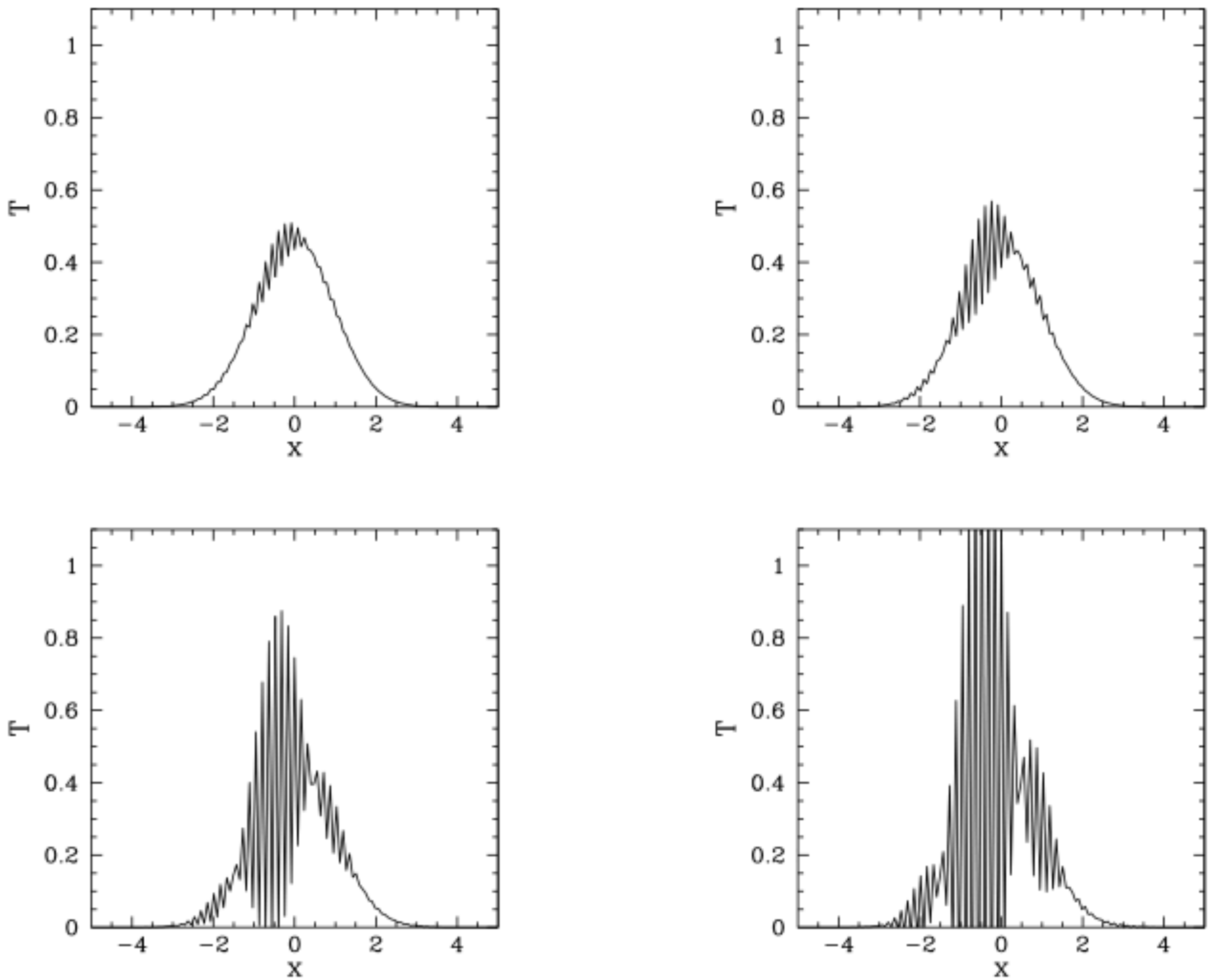
$$\frac{\partial T(x,t)}{\partial t} = D\,\frac{\partial^2 T(x,t)}{\partial x^2}$$

Forward in time, central in space:

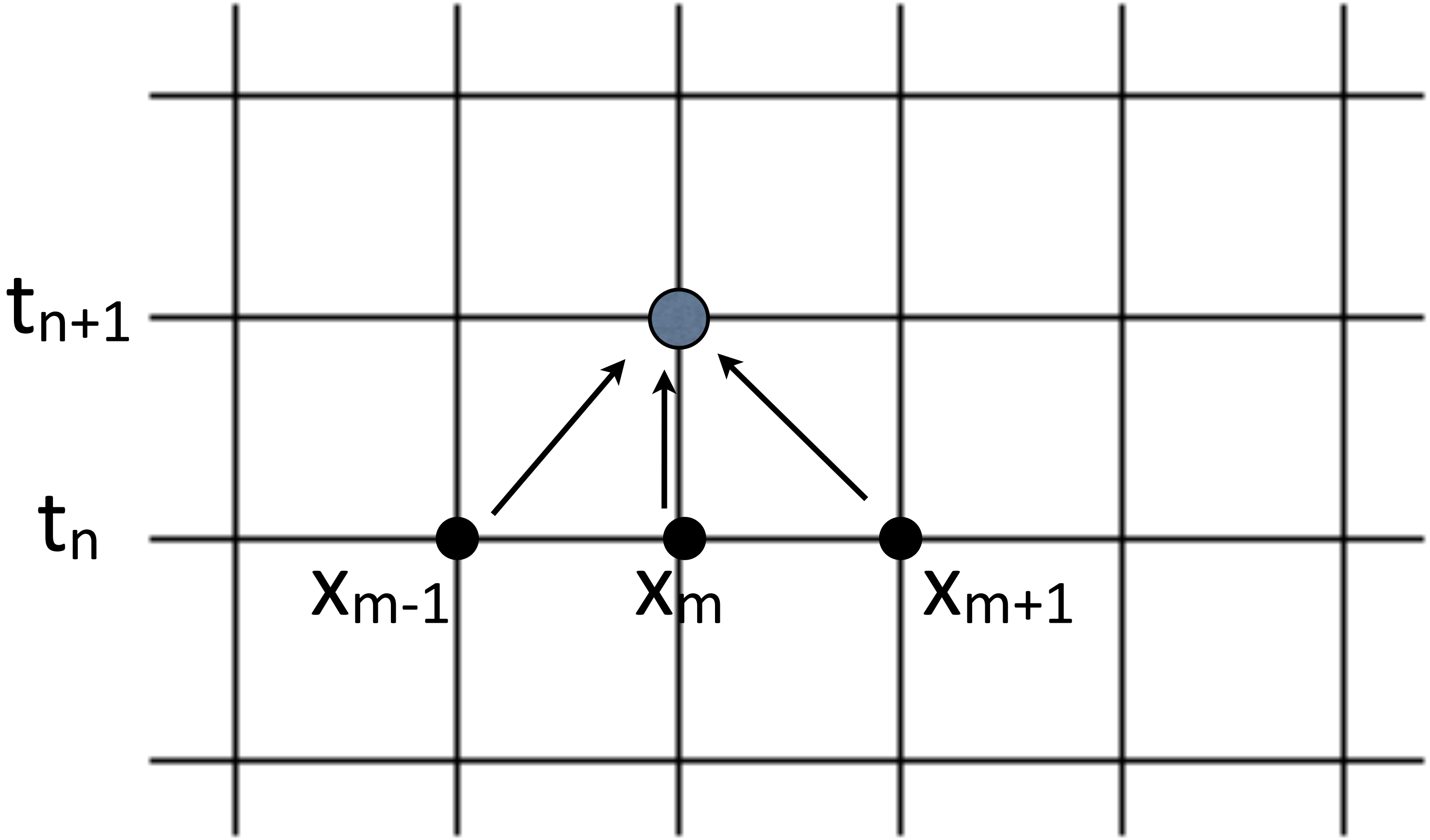
$$\frac{T(t_{n+1},x_m) - T(t_n,x_m)}{\Delta t} = \frac{T(t_n,x_{m+1}) - 2T(t_n,x_m) + T(t_n,x_{m-1})}{h^2}$$

This is an explicit method.

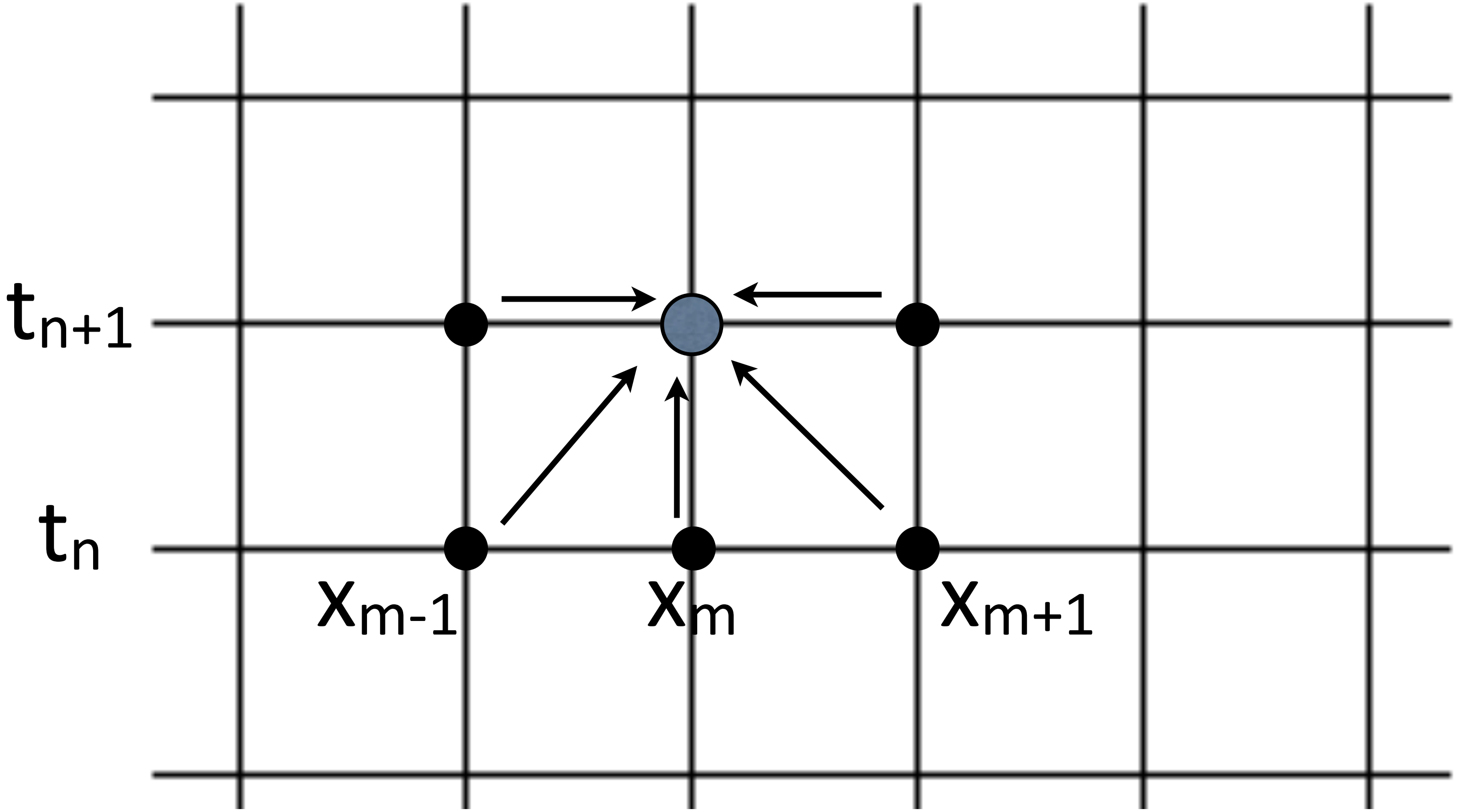
For large Δt:



Stencil for Euler's method



Stencil for Crank-Nicholson



$$\frac{T(x, t_{n+1}) - T(x, t_n)}{\delta t} = \frac{D}{2}\,\frac{\partial^2 T(x, t_n)}{\partial x^2} + \frac{D}{2}\,\frac{\partial^2 T(x, t_{n+1})}{\partial x^2}$$