

# Introduction to Computational Fluid Dynamics

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## FINITE DIFFERENCES METHOD - part I

### Introduction (very short)

Partial differential equations are widely used in mathematical modelling, many of them coming from different conservation law (particular properties of isolated physical system don't change when the system evolves)

### Examples

- **conservation of mass** (the mass of a closed system remains constant)
- **conservation of energy** (the total amount of energy in an isolated system remains constant, first law of thermodynamics)
- **conservation of linear momentum** (the total momentum of a closed system, which has no interactions with external sources – is constant)
- **conservation of electric charge** (the total electric charge of an isolated system remains constant)

# Introduction to Computational Fluid Dynamics

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Consider the most general form for a 2D linear partial differential equation:

$$a \frac{\partial^2 u}{\partial x^2} + b \frac{\partial^2 u}{\partial x \partial y} + c \frac{\partial^2 u}{\partial y^2} + d \frac{\partial u}{\partial x} + e \frac{\partial u}{\partial y} + fu = g(x, y), \quad (x, y) \in D \subset \mathbf{R}^2$$

where  $a, b, c, \dots$  are constants, and  $g$  a known function. PDE are classified by the main part of the operator:

$$a \frac{\partial^2 u}{\partial x^2} + b \frac{\partial^2 u}{\partial x \partial y} + c \frac{\partial^2 u}{\partial y^2}$$

in elliptic, parabolic and hyperbolic.

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**Elliptic:**  $b^2 - 4ac < 0$

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + Au = g(x, y)$$

where  $A = 0, \pm 1$ .

Particular cases: Laplace ( $A = 0, g = 0$ ), Poisson ( $A = 0, g \neq 0$ )

**Electrostatics:**

$$\begin{cases} -\Delta u(\mathbf{x}) = f(\mathbf{x}), & \mathbf{x} \in \Omega, \\ u(\mathbf{x}) = g(\mathbf{x}), & \mathbf{x} \in \Gamma. \end{cases}$$

$u$  is the electric potential

$f$  is the electric charge density

$g$  is a fixed potential on the boundary (Neumann b.c.  $\Rightarrow$  fixed fluxes)

**Thermostatics:**

$u$  is the temperature

$f$  is the heat source density

$g$  is a fixed temperature on the boundary (Neumann b.c.  $\Rightarrow$  fixed flows)

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---

Helmholtz ( $A = \pm 1$ ,  $g \neq 0$ )

Recall the *wave equation*:

$$\frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} = \frac{\partial^2 u}{\partial t^2}.$$

The wave equation models vibrations in membranes, acoustic waves, certain electro-magnetic waves, and many other phenomena.

Now assume that the time dependence is “time harmonic”:

$$u(\mathbf{x}, t) = v(\mathbf{x}) \cos(\omega t).$$

Then  $\frac{\partial^2 u}{\partial t^2} = -\omega^2 u$  and so the wave equation becomes the *Helmholtz equation*:

$$\frac{\partial^2 v}{\partial x_1^2} + \frac{\partial^2 v}{\partial x_2^2} = -\omega^2 v.$$

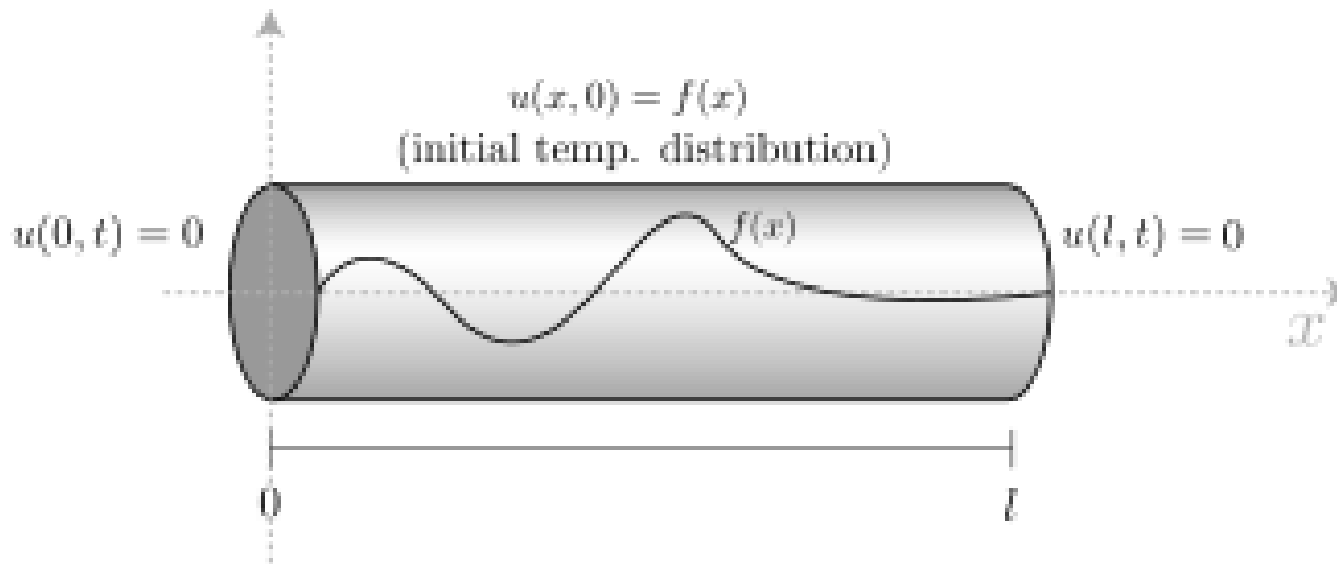
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Parabolic:  $b^2 - 4ac = 0$

$$\frac{\partial u}{\partial x} - \frac{\partial^2 u}{\partial y^2} = g(x, y)$$

(diffusion or heat equation)

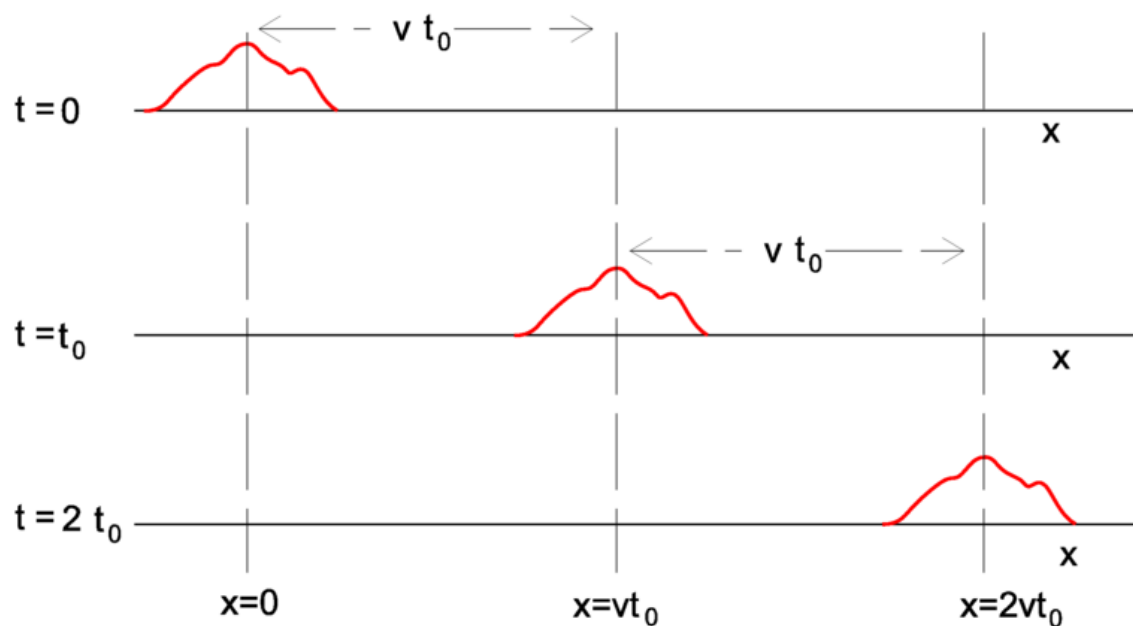


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**Hyperbolic:**  $b^2 - 4ac < 0$

$$\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} + Bu = g(x, y) \quad (\text{III.4})$$

where  $B = 0$  or  $1$ . (  $B = 0$  - wave equation,  $B = 1$  - Klein-Gordon linear equation)



A non-periodic solitary wave traveling along  $x$ -axis to the right with constant speed  $v$ .

At  $t = 0$  the wave is given by the function  $f(x)$  of  $x$ ,  
at  $t=t_0$  by  $f(x-vt_0)$ ,  
etc.

Different types of equations = Different numerical methods

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## Parabolic equations (one spatial variable)

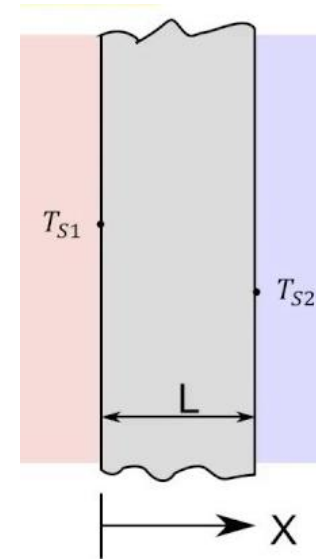
(K.W. Morton, D.F. Mayers, Numerical solution of PDE, 2<sup>nd</sup> ed, Cambridge University Press, New York, 2005)

*Heat equation*

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad t > 0, \quad 0 \leq x \leq 1$$
$$u(0, x) = u^0(x), \quad x \in [0, 1]$$
$$u(t, 0) = u(t, 1) = 0, \quad t > 0$$

Analytic

$$u(x, t) = \sum_{k=1}^{\infty} a_k e^{-(k\pi)^2 t} \sin k\pi x$$
$$a_k = 2 \int_0^1 u^0(x) \sin k\pi x dx$$



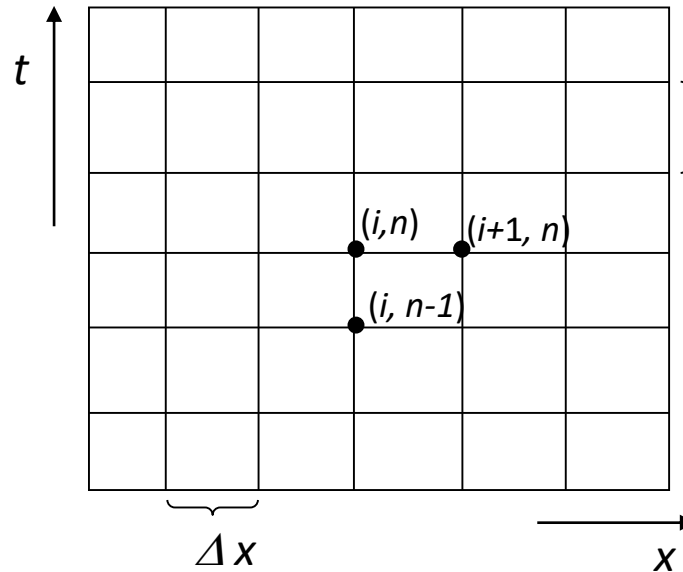
Difficulties: - infinite series,  $a_k$  can be determined for some particular cases

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## *Explicit Scheme*

Domain:  $[0, t_f] \times [0, 1]$  divided in a mesh (grid)



Grid:

$$(x_i = i\Delta x, t_n = n\Delta t), \quad i = 0, 1, \dots, N_x, \quad n = 0, 1, \dots, N_t \quad (\text{III.10})$$

Notation

$$U_i^n \approx u(x_i, t_n) \quad (\text{III.11})$$



# Introduction to Computational Fluid Dynamics

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Derivatives approximation

$$\frac{\partial u}{\partial t}(x_i, t_n) \approx \frac{u(x_i, t_{n+1}) - u(x_i, t_n)}{\Delta t}$$

$$\frac{\partial^2 u}{\partial x^2}(x_i, t_n) \approx \frac{u(x_{i+1}, t_n) - 2u(x_i, t_n) + u(x_{i-1}, t_n))}{(\Delta x)^2}$$

Using the derivatives approximations we get:

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} = \frac{U_{i+1}^n - 2U_i^n + U_{i-1}^n}{(\Delta x)^2} \quad (o)$$

or:

$$U_i^{n+1} = U_i^n + \nu (U_{i+1}^n - 2U_i^n + U_{i-1}^n) \quad (o)$$

where

$$\nu = \frac{\Delta t}{(\Delta x)^2} \quad .$$

Thus, we obtained an explicit method with finite differences.

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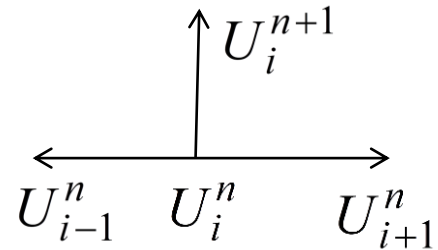
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Using the BC:

$$U_i^0 = u^0(x), \quad i = 1, 2, \dots, N_x - 1$$

$$U_0^n = U_{N_x}^n = 0, \quad n = 0, 1, 2, \dots$$

It is possible to march in time:



Example: For

$$u^0(x) = \begin{cases} x, & x \in \left[0, \frac{1}{2}\right] \\ 1-x, & x \in \left[\frac{1}{2}, 1\right] \end{cases}$$

the analytic solution is given by:  $u(x,t) = \frac{4}{\pi^2} \sum_{k=1}^{\infty} \frac{1}{k^2} \sin\left(\frac{1}{2}k\pi\right) \sin(k\pi x) e^{-(k\pi)^2 t}$

# Introduction to Computational Fluid Dynamics

---

## Matlab program

```
dt=0.0013; dx=0.05;
Nx=1/(dx)+1;
x=0:dx:1;
tf=0.1;
Nt=tf/dt;

Uo=zeros(Nx,1);
Un=zeros(Nx,1);

%initialization
for i=1:round(Nx/2)
    Uo(i)=(i-1)*dx;
end
for i=round(Nx/2):Nx
    Uo(i)=1-(i-1)*dx;
end

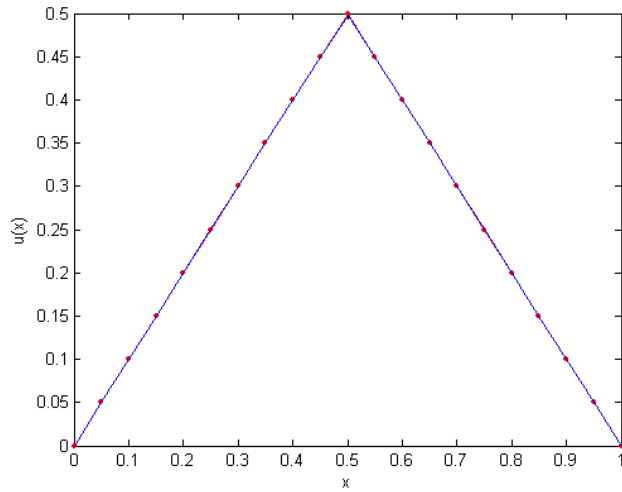
n=0;
while (n<Nt)
    n=n+1;
    for i=2:Nx-1
        Un(i)=Uo(i)+...
            dt/(dx*dx)*(Uo(i-1)-
                2*Uo(i)+Uo(i+1));
        end
        Uo=Un;
    end

    plot(x,Uo,'.-r')
    hold on

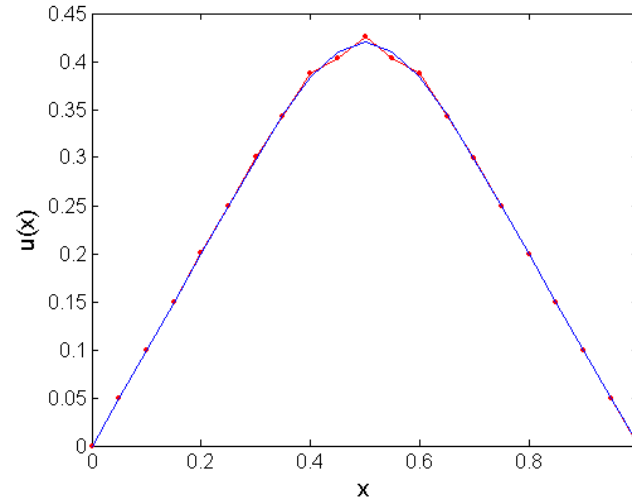
    %analytical solution
    U=HeatAnalytic(x,tf);
    plot(x,U,'b')

    function rez=HeatAnalytic(x,t)
        rez=0;
        for k=1:100
            rez=rez+4/(k*pi)^2*sin(k*pi/2)*
                sin(k*pi*x)*exp(-k^2*pi^2*t);
        end
    end
end
```

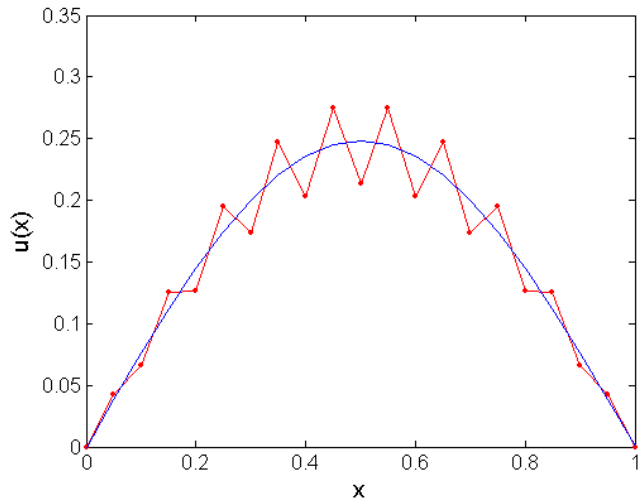
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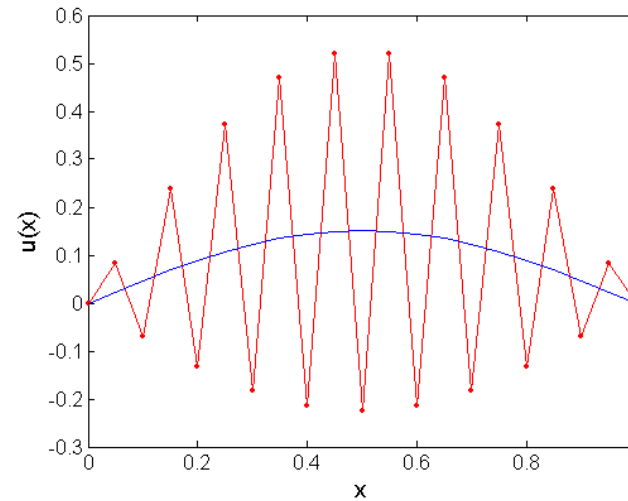
$t = 0$



$t = 0.005$



$t = 0.05$



$t = 0.1$

# Introduction to Computational Fluid Dynamics

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## *Truncation error*

Notations:

- forward differences:

$$\Delta_t u(x, t) = u(x, t + \Delta t) - u(x, t)$$

$$\Delta_x u(x, t) = u(x + \Delta x, t) - u(x, t)$$

- backward differences:

$$\nabla_t u(x, t) = u(x, t) - u(x, t - \Delta t)$$

$$\nabla_x u(x, t) = u(x, t) - u(x - \Delta x, t)$$

- central differences:

$$\delta_t u(x, t) = u\left(x, t + \frac{1}{2}\Delta t\right) - u\left(x, t - \frac{1}{2}\Delta t\right)$$

$$\delta_x u(x, t) = u\left(x + \frac{1}{2}\Delta x, t\right) - u\left(x - \frac{1}{2}\Delta x, t\right)$$

$$\delta_x^2 u(x, t) = u(x + \Delta x, t) - 2u(x, t) + u(x - \Delta x, t)$$

# Introduction to Computational Fluid Dynamics

---

Using Taylor series we have:

$$\begin{aligned}\Delta_t u(x, t) &= u_t \Delta t + \frac{1}{2} u_{tt} (\Delta t)^2 + \frac{1}{6} u_{ttt} (\Delta t)^3 + \dots \\ \delta_x^2 u(x, t) &= u_{xx} (\Delta x)^2 + \frac{1}{12} u_{xxxx} (\Delta x)^4 + \dots\end{aligned}\tag{*}$$

We define the **truncation error** for the scheme:

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} = \frac{U_{i+1}^n - 2U_i^n + U_{i-1}^n}{(\Delta x)^2}$$

the function

$$T(x, t) = \frac{\Delta_t u(x, t)}{\Delta t} - \frac{\delta_x u(x, t)}{(\Delta x)^2}$$

We notice that the above relation is the difference between the left hand term and the right hand term of the numerical scheme where  $U_i^n$  is replaced by  $u(x_i, t_n)$  and operator notation is used.

# Introduction to Computational Fluid Dynamics

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Using (\*) we get:

$$T(x,t) = (u_t - u_{xx}) + \left( \frac{1}{2} u_{tt} \Delta t - \frac{1}{12} u_{xxxx} (\Delta x)^2 \right) + \dots = \frac{1}{2} u_{tt} \Delta t - \frac{1}{12} u_{xxxx} (\Delta x)^2 + \dots$$

where the Taylor expansion of the form:

$$u(x, t + \Delta t) = u(x, t) + u_t \Delta t + \frac{1}{2} u_{tt}(x, \eta) (\Delta t)^2, \quad t \leq \eta \leq t + \Delta t$$

was used. We obtain:

$$T(x,t) = \frac{1}{2} u_{tt}(x, \eta) \Delta t - \frac{1}{12} u_{xxxx}(\xi, t) (\Delta x)^2, \quad t \leq \eta \leq t + \Delta t, \quad x \leq \xi \leq x + \Delta x$$

and if  $u$  and its derivatives are bounded ( $|u_{tt}| < M_{tt}$ ,  $|u_{xxxx}| \leq M_{xxxx}$ ) then we have:

$$|T(x,t)| \leq \frac{1}{2} \Delta t \left( M_{tt} + \frac{1}{6\nu} M_{xxxx} \right) \quad (**)$$

# Introduction to Computational Fluid Dynamics

---

It can be seen that  $T(x,t) \rightarrow 0$  when  $\Delta x, \Delta t \rightarrow 0$  for every  $(x,t) \in (0,1) \times [\tau, t_F)$ . We say that the explicit scheme is **unconditionally consistent** and  $\Delta t$  appears at the power one that the accuracy order is  $O(\Delta t)$  or the scheme is first order accurately.

## *The convergence of the explicit scheme*

Suppose we obtain approximations of the exact solutions for the same initial data for different grids ( $\Delta t \rightarrow 0$  and  $\Delta x \rightarrow 0$ ) but with the same value for the parameter  $\nu = \Delta t / (\Delta x)^2$ .

Will say that the scheme (o) **is convergent** if for every point  $(x^*, t^*) \in (0,1) \times (0, t_F)$

$$x_i \rightarrow x^*, t_n \rightarrow t^* \quad \text{involve} \quad U_i^n \rightarrow u(x^*, t^*)$$

We introduce a superior limit for the truncation error:

$$|T_i^n| \leq \bar{T}$$

where  $T_i^n = T(x_i, t_n)$



# Introduction to Computational Fluid Dynamics

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and the error

$$e_i^n = U_i^n - u(x_i, t_n)$$

But  $U_i^n$  is the approximative solution while  $u(x_i, t_n)$  is the exact solution and using (o) we get:

$$U_i^{n+1} = U_i^n + \nu(U_{i+1}^n - 2U_i^n + U_{i-1}^n)$$

$$u(x_i, t_{n+1}) = u(x_i, t_n) + \nu(u(x_{i+1}, t_n) - 2u(x_i, t_n) + u(x_{i-1}, t_n)) + T_i^n \Delta t$$

and by subtraction we obtain:

$$e_i^{n+1} = e_i^n + \nu(e_{i+1}^n - 2e_i^n + e_{i-1}^n) - T_i^n \Delta t$$

or

$$e_i^{n+1} = (1 - 2\nu)e_i^n + \nu e_{i+1}^n + \nu e_{i-1}^n - T_i^n \Delta t$$

# Introduction to Computational Fluid Dynamics

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Supposing  $\nu \leq \frac{1}{2}$  and considering the maximum of the error for one time step,  $E^n = \max\{|e_i^n|, i = 0, 1, \dots, N_x\}$ , we have:

$$|e_i^{n+1}| = (1 - 2\nu)E^n + \nu E^n + \nu E^n + |T_i^n| \Delta t \leq E^n + \bar{T} \Delta t$$

where in the triangle inequality the modulus notation was dropped. Eq. takes place for  $i = 1, 2, \dots, N_x - 1$  and thus:

$$E^{n+1} \leq E^n + \bar{T} \Delta t$$

From the initial condition we have  $E^0 = 0$  and it is possible to demonstrate by mathematical induction that  $E^n \leq n\bar{T} \Delta t$ .

Using Eq. (\*\*) and taking into account that the final time  $t_F \leq n\Delta t$  we get:

$$E^n \leq \frac{1}{2} \Delta t \left( M_{tt} + \frac{1}{6\nu} M_{xxxx} \right) t_F \rightarrow 0 \text{ when } \Delta t \rightarrow 0$$

# Introduction to Computational Fluid Dynamics

---

A refinement path is a sequence of pairs of mesh sizes,  $\Delta x$  and  $\Delta t$ , each of which tends to zero:

$$MR = \{((\Delta x)_j, (\Delta t)_j), j = 0, 1, \dots, ; (\Delta x)_j \rightarrow 0, (\Delta t)_j \rightarrow 0\}$$

**Theorem:** If a refinement path satisfies  $\nu_j = \frac{(\Delta t)_j}{(\Delta x)_j^2} \leq \frac{1}{2}$  for all sufficiently large values of

$j$  and the positive numbers  $n_j$  and  $i_j$  are such that:

$$n_j(\Delta t)_j \rightarrow t > 0 \quad \text{and} \quad i_j(\Delta t)_j \rightarrow x \in [0, 1]$$

and if  $|u_{xxxx}| \leq M_{xxxx}$  uniformly in  $[0, 1] \times [0, t_F]$  then the approximations  $U_i^{n_j}$  generated by the explicit difference scheme (o) for  $j = 0, 1, 2, \dots$  converge to the solution  $u(x, t)$  of the differential equation uniformly in the region.

# Introduction to Computational Fluid Dynamics

---

Such a convergence theorem is the least that one can expect of a numerical scheme; it shows that arbitrarily high accuracy can be attained by use of a sufficiently fine mesh. Of course, it is also somewhat impractical. As the mesh becomes finer, more and more steps of calculation are required, and the effect of rounding errors in the calculation would become significant and would eventually completely swamp the truncation error.

## *Fourier analysis of the error*

We have already expressed the exact solution of the heat equation as a Fourier series; this expression is based on the observation that a particular set of Fourier modes are exact solutions. In order to study the stability of the scheme (14) we consider the numerical solution in a point  $i\Delta x$  at the time step  $n$  of the form:

$$U_i^n = \lambda^n e^{Ik(i\Delta x)}$$

where  $I = \sqrt{-1}$ .

# Introduction to Computational Fluid Dynamics

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Using this form in (o) and simplifying with  $\lambda^n e^{I k(i\Delta x)}$  we get:

$$\lambda = \lambda(k) = 1 + \nu(e^{I k\Delta x} - 2 + e^{-I k\Delta x}) = 1 - 2\nu(1 - \cos k\Delta x) = 1 - 4\nu \sin^2 \frac{1}{2} k\Delta x$$

where  $\lambda(k)$  is the amplification factor. By taking  $k = m\pi$ , as in the exact solution we can therefore write our numerical approximation in the form

$$U_i^n = \sum_{-\infty}^{\infty} A_m e^{I m\pi(i\Delta x)} [\lambda(m)]^n$$

This equation gives a good approximation to the exact solution of the differential equation given by the Fourier series of the exact solution for small values of  $m$ .

But

$$U_i^{n+1} = \lambda U_i^n$$

In order to limit the truncation error propagation it is necessary that:

$$|\lambda| \leq 1$$

and thus, we obtain:

$$-1 \leq 1 - 4\nu \sin^2 \frac{1}{2} k\Delta x \leq 1 \text{ for every point } k\Delta x$$

# Introduction to Computational Fluid Dynamics

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from where we have the condition: 
$$v = \frac{\Delta t}{(\Delta x)^2} \leq \frac{1}{2} \quad (\Delta)$$

## *The implicit scheme*

Eq.  $(\Delta)$  is a very severe restriction, and implies that very many time steps will be necessary to follow the solution over a reasonably large time interval. If we need good approximations we need small steps in space and the amount of work involved increases very rapidly, since we shall also have to reduce the time step.

In order to avoid this we introduce the scheme

$$(x_i = i\Delta x, t_n = n\Delta t), \quad i = 0, 1, \dots, N_x, \quad n = 0, 1, \dots, N_t)$$

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} = \frac{U_{i+1}^{n+1} - 2U_i^{n+1} + U_{i-1}^{n+1}}{(\Delta x)^2}$$

# Introduction to Computational Fluid Dynamics

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It can be seen that in order to calculate the value of  $U$  at the time step  $t_{n+1}$  it is necessary to march in time starting from the initial condition

$$U_i^0 = u^0(x), \quad i = 1, 2, \dots, N_x - 1$$

and solving a tri-diagonal system of equations:

$$-\nu U_{i-1}^{n+1} + (1 + 2\nu)U_i^{n+1} - \nu U_{i+1}^{n+1} = U_i^n \quad (\text{oo})$$

along with with the boundary conditions

$$U_0^n = U_{N_x}^n = 0, \quad n = 0, 1, 2, \dots$$

In this case we say that the method is implicit and the form of the system is given by:

$$\begin{array}{ccc} U_{i-1}^{n+1} & U_i^{n+1} & U_{i+1}^{n+1} \\ \leftarrow \hspace{1.5cm} \hspace{1.5cm} \hspace{1.5cm} \rightarrow \\ \uparrow \\ U_i^n \end{array}$$

# Introduction to Computational Fluid Dynamics

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$$\begin{bmatrix} 1 & & & & & & & & & & \\ -\nu & 1+2\nu & -\nu & & & & & & & & \\ & \ddots & \ddots & \ddots & & & & & & & \\ & & & -\nu & 1+2\nu & -\nu & & & & & \\ & & & & \ddots & \ddots & \ddots & & & & \\ & & & & & -\nu & 1+2\nu & -\nu & & & \\ & & & & & & & 1 & & & \\ & & & & & & & & & & 1 \end{bmatrix} \times \begin{bmatrix} U_0 \\ U_1 \\ \dots \\ U_i \\ \dots \\ U_{Nx-1} \\ U_{Nx} \end{bmatrix}^{(n+1)} = \begin{bmatrix} 0 \\ U_1 \\ \dots \\ U_i \\ \dots \\ U_{Nx-1} \\ 0 \end{bmatrix}^{(n)}$$

The system can be solved using a known method (e.g. the Thomas algorithm).

We will apply the implicit scheme to the above example, and we will compare the result with the explicit method and with the analytic solution.



# Introduction to Computational Fluid Dynamics

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```
%Matlab program:
dt=0.0013;dx=0.05;
niu=dt/(dx*dx);
Nx=1/(dx)+1;
x=0:dx:1;
tf=0.1;
Nt=tf/dt;

Uo=zeros(Nx,1); Un=zeros(Nx,1);
%initialization
for i=1:round(Nx/2)
    Uo(i)=(i-1)*dx;
end
for i=round(Nx/2):Nx
    Uo(i)=1-(i-1)*dx;
end

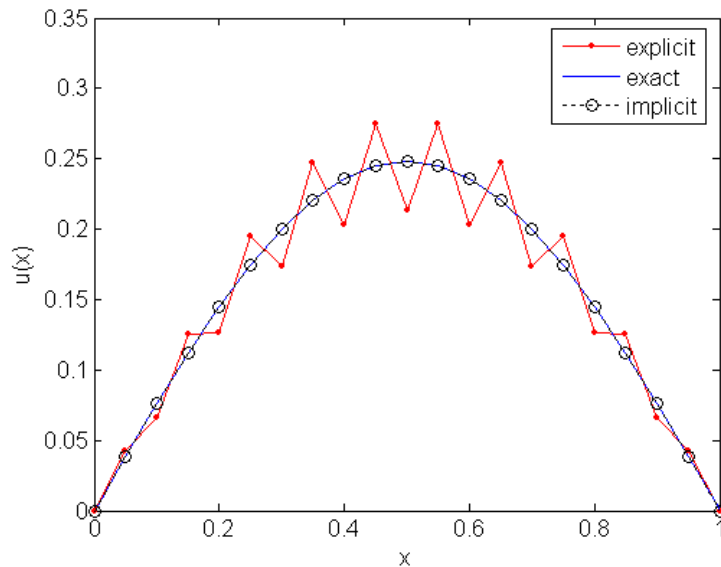
A=zeros(Nx,Nx);b=zeros(Nx,1);

n=0;
while (n<Nt)
    n=n+1;
    A(1,1)=1;b(1)=0;
    for i=2:Nx-1
        A(i,i-1)=-niu;
        A(i,i)=1+2*niu;
        A(i,i+1)=-niu;
        b(i)=Uo(i);
    end
    A(Nx,Nx)=1;b(Nx)=0;
    Un=A\b;
    Uo=Un;
end

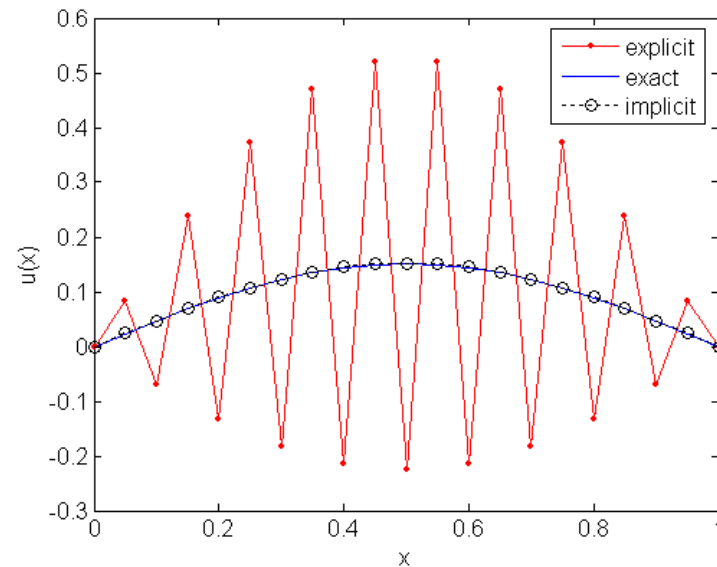
plot(x,Uo,'o:k')
hold on
```

# Introduction to Computational Fluid Dynamics

We used  $\Delta t = 0.0013$  and  $\Delta x = 0.05$ , and the analytic solution (full line), the explicit solution („•”) and the implicit solution („o”) are given. We observe that the implicit solution is stable.



$t = 0.05$



$t = 0.1$

# Introduction to Computational Fluid Dynamics

---

Using again the Fourier mode in the implicit scheme we get:

$$\lambda - 1 = \nu \lambda \left( e^{Ik\Delta x} - 2 + e^{-Ik\Delta x} \right) = -4\nu \lambda \sin^2 \frac{1}{2} k \Delta x$$

or

$$\lambda = \frac{1}{1 + 4\nu \sin^2 \frac{1}{2} k \Delta x}$$

We notice that, we have  $0 < \lambda < 1$  and thus, the implicit method is unconditionally stable.

# Introduction to Computational Fluid Dynamics

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## *Crank-Nicolson method*



*John Crank (1916-2006)*



*Phyllis Nicolson (1917-1968)*

Another method was proposed by Crank and Nicolson in 1947. They use the trapezoidal rule and a central finite difference in space and obtain a scheme of order two:

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} = \frac{1}{2} \left( \frac{U_{i+1}^{n+1} - 2U_i^{n+1} + U_{i-1}^{n+1}}{(\Delta x)^2} + \frac{U_{i+1}^n - 2U_i^n + U_{i-1}^n}{(\Delta x)^2} \right)$$

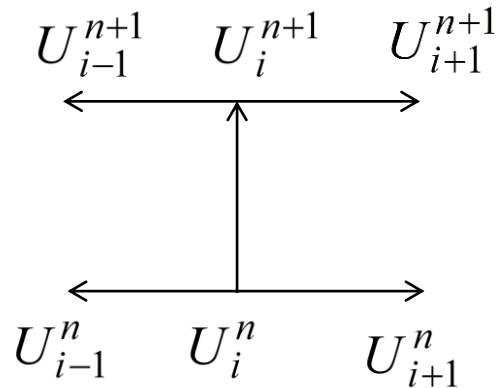
# Introduction to Computational Fluid Dynamics

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The scheme reduces to the following tri-diagonal system of linear equations:

$$-vU_{i+1}^{n+1} + 2(1+v)U_i^{n+1} - vU_{i-1}^{n+1} = vU_{i+1}^n + 2(1-v)U_i^n + vU_{i-1}^n$$

along with the initial and boundary conditions.



We will apply the Crank -Nicolson scheme to the heat equation and we will compare the solution with the analytic solution and that obtained using the implicit scheme.

# Introduction to Computational Fluid Dynamics

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Matlab program:

```
dt=0.0013;dx=0.05;
niu=dt/(dx*dx);
Nx=1/(dx)+1;
x=0:dx:1;
tf=0.1;
Nt=tf/dt;

Uo=zeros(Nx,1); Un=zeros(Nx,1);
%initialization
for i=1:round(Nx/2)
    Uo(i)=(i-1)*dx;
end
for i=round(Nx/2):Nx
    Uo(i)=1-(i-1)*dx;
end

A=zeros(Nx,Nx);b=zeros(Nx,1);

n=0;
while (n<Nt)
    n=n+1;
    A(1,1)=1;b(1)=0;
    for i=2:Nx-1
        A(i,i-1)=-niu;
        A(i,i)=2+2*niu;
        A(i,i+1)=-niu;
        b(i)=niu*Uo(i-1)+
            (2-2*niu)*Uo(i)+niu*Uo(i+1);
    end
    A(Nx,Nx)=1;b(Nx)=0;

    Un=A\b;
    Uo=Un;
end
plot(x,Uo,'o:k')
hold on
```

# Introduction to Computational Fluid Dynamics

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Time	$\ U_{exact} - U_{implicit}\ $	$\ U_{exact} - U_{Crank-Nicolson}\ $
0.00	0	0
0.05	0.000732	0.002992
0.10	0.004491	0.001476
0.20	0.002990	0.000734
0.30	0.001609	0.000342
0.40	0.000785	0.000153
0.50	0.000362	0.000066

We notice that the Crank – Nicolson solution is “better” than the implicit solution.

# Introduction to Computational Fluid Dynamics

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*$\theta$  method*

Following the above described methods we can give a general method:

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} = \theta \frac{U_{i+1}^{n+1} - 2U_i^{n+1} + U_{i-1}^{n+1}}{(\Delta x)^2} + (1 - \theta) \frac{U_{i+1}^n - 2U_i^n + U_{i-1}^n}{(\Delta x)^2}$$

where usually  $0 \leq \theta \leq 1$ .

For  $\theta = 0$  the general method reduces to the implicit scheme, for  $\theta = \frac{1}{2}$  to the Crank-

Nicolson scheme, while for  $\theta = 1$  the implicit scheme is obtained.

Using the  $\theta$  scheme leads like in implicit and Crank-Nicolson schemes to tri-diagonal systems of linear equations.



# Introduction to Computational Fluid Dynamics

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Using the Fourier analysis for the  $\theta$  scheme we get:

$$\lambda - 1 = \nu [\theta \lambda + (1 - \theta)] (e^{I k \Delta x} - 2 + e^{-I k \Delta x}) = \nu [\theta \lambda + (1 - \theta)] \left( -4 \lambda \sin^2 \frac{1}{2} k \Delta x \right)$$

or

$$\lambda = \frac{1 - 4(1 - \theta)\nu \sin^2 \frac{1}{2} k \Delta x}{1 + 4\theta\nu \sin^2 \frac{1}{2} k \Delta x}$$

Because  $\nu > 0$  and  $0 \leq \theta \leq 1$  we always have  $\lambda < 1$ . Thus, the scheme will be unstable for  $\lambda < -1$ , namely

$$1 - 4(1 - \theta)\nu \sin^2 \frac{1}{2} k \Delta x < - \left( 1 + 4\theta\nu \sin^2 \frac{1}{2} k \Delta x \right) \quad \text{or} \quad \nu(1 - 2\theta) \sin^2 \frac{1}{2} k \Delta x > \frac{1}{2}$$

# Introduction to Computational Fluid Dynamics

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Using this equation the stability condition is deduced:

$$\nu(1 - 2\theta) < \frac{1}{2}$$

Then the method is stable for:

- $0 \leq \theta \leq \frac{1}{2}$  and  $\nu \leq \frac{1}{2(1-2\theta)}$
- $\frac{1}{2} \leq \theta \leq 1$  and for every  $\nu$ .

It is possible to show that the truncation error on the node  $(i, n+1/2)$  is given by (see Morton and Meyers, 2005):

$$T_i^{n+1/2} = \left[ \left( \frac{1}{2} - \theta \right) \Delta t u_{xxt} - \frac{1}{12} (\Delta x)^2 u_{xxxx} \right] + \left[ \frac{1}{24} (\Delta t)^2 u_{ttt} - \frac{1}{8} (\Delta t)^2 u_{xxtt} \right] + \dots$$

For  $\theta = \frac{1}{2}$  (Crank-Nicolson case) the truncation error is of the order  $O(\Delta t^2) + O(\Delta x^2)$ , thus the scheme is always second order accurate.