## Numerical Solutions to PDEs

Lecture Notes #11 — Parabolic PDEs Stability, Boundary Conditions; Convection-Diffusion; Variable Coefficients

> Peter Blomgren, \( \text{blomgren.peter@gmail.com} \)

Department of Mathematics and Statistics
Dynamical Systems Group
Computational Sciences Research Center
San Diego State University
San Diego, CA 92182-7720

http://terminus.sdsu.edu/

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A quick introduction to parabolic PDEs: Our model equation is the one-dimensional heat equation.

Exact solutions to the 1D heat equation in infinite space, using the Fourier transform.

The solution corresponds to a damping of the high-frequency content of the initial condition.  $\Rightarrow$  the parabolic solution operator is dissipative.

For t > 0, the solution of the heat equation is infinitely differentiable.

Since parabolic PDEs do not have any characteristics, we need boundary conditions at every boundary. Typically we specify u (fixed temperature, "Dirichlet"), the [normal] derivative  $u_x$ (temperature flux, "Neumann"), or a mixture thereof.





**Numerical Schemes** for  $u_t = bu_{xx} + f$ :

## Forward-Time Central-Space

$$\frac{v_m^{n+1} - v_m^n}{k} = b \frac{v_{m+1}^n - 2v_m^n + v_{m-1}^n}{h^2} + f_m^n$$

Explicit; stable when  $b\mu \leq \frac{1}{2}$ , where  $\mu = \frac{k}{h^2}$ ; order-(1,2); dissipative of order 2.

### **Backward-Time Central-Space**

$$\frac{v_m^{n+1} - v_m^n}{k} = b \frac{v_{m+1}^{n+1} - 2v_m^{n+1} + v_{m-1}^{n+1}}{h^2} + f_m^{n+1}$$

Implicit; unconditionally stable; order-(1,2); dissipative of order 2.





#### Crank-Nicolson

$$\frac{v_m^{n+1} - v_m^n}{k} = \frac{b}{2} \left[ \frac{v_{m+1}^{n+1} - 2v_m^{n+1} + v_{m-1}^{n+1}}{h^2} + \frac{v_{m+1}^n - 2v_m^n + v_{m-1}^n}{h^2} \right] + \frac{1}{2} \left[ f_m^{n+1} + f_m^n \right]$$

Implicit; unconditionally stable; order-(2,2); dissipative of order 2, when  $\mu$  is constant.

## Du-Fort Frankel ("fixed leapfrog")

$$\frac{v_m^{n+1} - v_m^{n-1}}{2k} = b \frac{v_{m+1}^n - (v_m^{n+1} + v_m^{n-1}) + v_{m-1}^n}{h^2} + f_m^n$$

Explicit; unconditionally stable; order-(2,2); dissipative of order 2, when  $\mu$  is constant. It is only consistent if k/h tends to zero as h and k go to zero.





For **hyperbolic** equations we have the following result:

## Theorem (Stability of One-Step Schemes)

A consistent one-step scheme for the equation

$$u_t + au_x + bu = 0$$

is stable if and only if it is stable for this equation when  $\mathbf{b}=\mathbf{0}$ . Moreover, when  $k=\lambda h$ , and  $\lambda$  is a constant, the stability condition on  $g(h\xi,k,h)$  is

$$|g(\theta,0,0)| \leq 1.$$

Similar results do not always apply directly to parabolic equations.



— (6/39)

The problem is that the contribution to the amplification factor from the first derivative is sometimes (often?)  $\mathcal{O}\left(\sqrt{k}\right)$  which is greater than  $\mathcal{O}\left(k\right)$  as  $k \searrow 0$ .

For instance, the forward-time central-space scheme applied to  $u_t = bu_{\rm xx} - {\bf au_x} + {\bf cu}$  gives the amplification factor

$$g = 1 - 4b\mu \sin^2\left(\frac{\theta}{2}\right) - \mathbf{ia}\lambda \sin(\theta) + \mathbf{ck}$$



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The term ck does not affect stability, but the term containing  $\lambda=\sqrt{\mathbf{k}\mu}$  cannot be dropped when  $\mu$  is fixed. In this particular case, we get

$$|g|^2 = \left(1 - 4b\mu \sin^2\left(\frac{\theta}{2}\right)\right)^2 + a^2 \mathbf{k}\mu \sin^2(\theta)$$





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$$|g|^2 = \left(1 - 4b\mu \sin^2\left(\frac{\theta}{2}\right)\right)^2 + \mathbf{a}^2\mathbf{k}\mu \sin^2(\theta)$$

and since the first derivative term gives an  $\mathcal{O}(k)$  contribution to  $|g|^2$ , it does not affect stability. (Strikwerda, p.149) This is also true for the backward-time central-space, and Crank-Nicolson schemes.





The fact that a dissipative one-step scheme for a parabolic equation generates a numerical solution with increased smoothness as  $t\nearrow$  (provided that  $\mu$  is constant) is a key result, so lets show that it is indeed true...

We start with the following theorem

#### **Theorem**

A one-step scheme, consistent with

$$u_t = bu_{xx}$$

that is dissipative of order 2 with  $\mu$  constant satisfies

$$\|v^{n+1}\|_2^2 + ck \sum_{\nu=1}^n \|\delta_+ v^{\nu}\|_2^2 \le \|v^0\|_2^2$$

for all initial data  $v^0$  and n > 0.



## Proof 1 of 2

**Proof:** Let  $c_0$  be such that  $|g(\theta)|^2 \le 1 - c_0 \sin^2\left(\frac{\theta}{2}\right)$  (dissipative scheme of order 2).

Then by

$$\widehat{\mathbf{v}}^{\nu+1}(\xi) = \mathbf{g}(\theta)\widehat{\mathbf{v}}^{\nu}(\xi),$$

we have

$$|\widehat{v}^{\nu+1}(\xi)|^2 = |g(\theta)|^2|\widehat{v}^{\nu}(\xi)|^2 \leq |\widehat{v}^{\nu}(\xi)|^2 - c_0\sin^2\left(\frac{\theta}{2}\right)|\widehat{v}^{\nu}(\xi)|^2;$$

equivalently:

$$|\widehat{v}^{\nu+1}(\xi)|^2 - |\widehat{v}^{\nu}(\xi)|^2 + c_0 \sin^2\left(\frac{\theta}{2}\right) |\widehat{v}^{\nu}(\xi)|^2 \leq 0.$$

Stability





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equivalently:

$$|\widehat{v}^{\nu+1}(\xi)|^2-|\widehat{v}^{\nu}(\xi)|^2+c_0\sin^2\left(\frac{\theta}{2}\right)|\widehat{v}^{\nu}(\xi)|^2\leq 0.$$

By summing this inequality for  $\nu=0,\ldots,n$ , we get (using  $\mu=kh^{-2}$ )

$$|\widehat{v}^{n+1}(\xi)|^2 + \frac{c_0k}{\mu} \sum_{\nu=0}^n \left| \frac{1}{h} \sin\left(\frac{\theta}{2}\right) \widehat{v}^{\nu}(\xi) \right|^2 \leq |\widehat{v}^0(\xi)|^2.$$





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Next we use

$$\left| rac{2\sin\left(rac{ heta}{2}
ight)}{h} \widehat{v}^
u 
ight| = \left| rac{e^{i heta}-1}{h} \widehat{v}^
u 
ight| = \left| \mathcal{F}(\delta_+ v^
u)(\xi) 
ight|.$$





We get

$$|\widehat{v}^{n+1}(\xi)|^2 + ck \sum_{\nu=0}^n |\mathcal{F}(\delta_+ \widehat{v}^{\nu})(\xi)|^2 \le |\widehat{v}^0(\xi)|^2.$$

Integration over  $\xi$  :  $|\widehat{\circ}(\xi)|^2 \rightarrow \|\widehat{\circ}\|^2$  using Parseval's relation :  $\|\widehat{\circ}\|^2 \rightarrow \|\widehat{\circ}\|^2$ 

gives...

$$\|v^{n+1}\|_2^2 + ck \sum_{\nu=0}^n \|\delta_+ v^{\nu}\|_2^2 \le \|v^0\|_2^2$$

which is the inequality in the theorem.  $\Box$ 

Here  $\mathcal{F}(\cdot)$ , denotes the Fourier transform.



We can use the theorem to show that solutions become smoother with time  $\Leftrightarrow$  norms of the high-order differences (approximating high-order derivatives) tend to zero at a faster rate than the norm of u.

Since  $|g(\theta)| \le 1$ , we have  $||v^{\nu+1}||_2 \le ||v^{\nu}||_2$ . We note that  $\delta_+ v$  (being a finite difference) is also a solution to the scheme, therefore we have  $||\delta_+ v^{\nu+1}||_2 \le ||\delta_+ v^{\nu}||_2$ . That is, both the solution and its differences decrease in norm as time increases.

We apply the theorem, and get

$$||v^{n+1}||_2^2 + ct||\delta_+ v^n||_2^2 \le ||v^0||_2^2$$

which shows for nk = t > 0 that  $\|\delta_+ v^n\|_2$  is bounded, and we must have

$$\|\delta_+ v^n\|_2^2 \le \frac{C}{t} \|v^0\|_2^2 \searrow 0$$



The argument can be applied recursively; since  $\delta_+ v^n$  satisfies the difference equations, we find that for nk=t>0, and any positive integer r that  $\delta_+^r v^n$  is also bounded. Thus the solution of the difference scheme becomes smoother as t increases.

It can be shown that if  $v_m^n \to u(t_n, x_m)$  with order of accuracy p, then  $\delta_+^r v_m^n \to \delta_+^r u(t_n, x_m)$  with order of accuracy p.

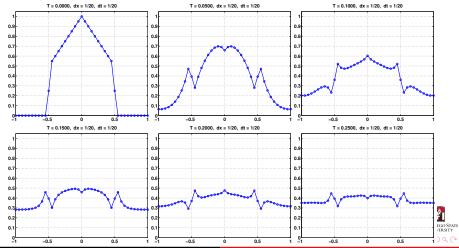
These results hold **if and only if** the scheme is dissipative.





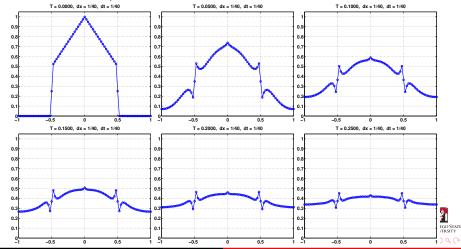
$$dx = 1/20$$
,  $dt = 1/20$ ,  $\mu = 20$ 

**Figure:** The Crank-Nicolson scheme applied to the initial condition in panel #1, with zero-flux boundary conditions. We know that Crank-Nicolson is non-dissipative if  $\lambda$  remains constant (see next slide).



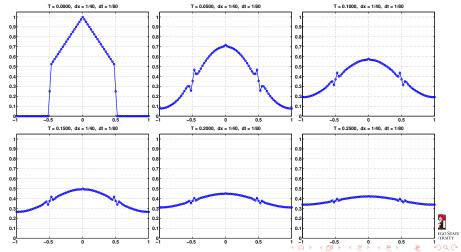
# dx = 1/40, dt = 1/40, $\mu = 40$

**Figure:** The Crank-Nicolson scheme: here we have cut both h and k in half compared with the previous slide. On the next slide we show the result of keeping  $\mu=k/h^2$  constant, in which case the scheme is dissipative.



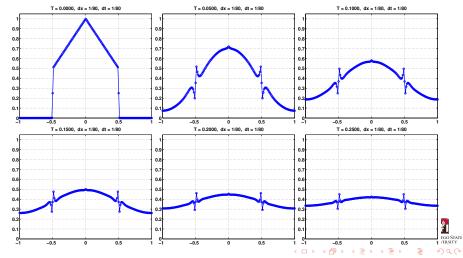
$$dx = 1/40$$
,  $dt = 1/80$ ,  $\mu = 20$ 

**Figure:** The Crank-Nicolson scheme: here, we finally get some damping in the oscillations of the solution. — Dissipation is a convergence result!



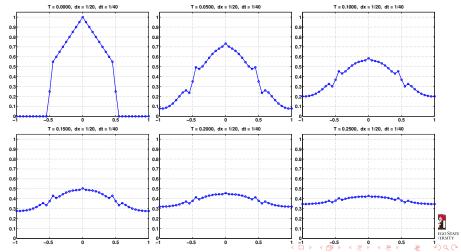
$$dx = 1/80$$
,  $dt = 1/80$ ,  $\mu = 80$ 

**Figure:** Surprisingly(?), refinining in x brings back the over-shoot artefacts.



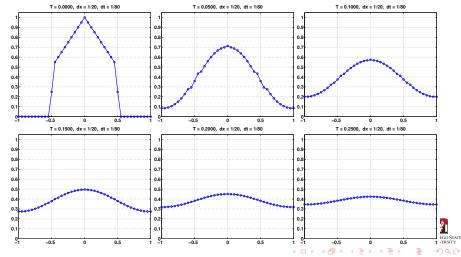
$$dx = 1/20$$
,  $dt = 1/40$ ,  $\mu = 10$ 

**Figure:** Coarsening in x (dx = 1/20, instead of dx = 1/40 lessens the "carrying capacity" of high-frequency content of the grid...



$$dx = 1/20$$
,  $dt = 1/80$ ,  $\mu = 5$ 

Figure: Refining in time lowers  $\mu$ , which reduces oscillations...



Since parabolic problems require boundary conditions at every boundary, there is **less need for "purely" numerical boundary conditions**, compared with hyperbolic problems.

We briefly discuss implementation of the **physical boundary conditions**: — Implementing the Dirichlet (specified values at the boundary points) boundary conditions is straight-forward.

The Neumann (specified flux/derivative) is more of a problem; for instance, **one-sided differences** 

$$\frac{\partial u(t_n,x_0)}{\partial x} \approx \frac{v_1^n - v_0^n}{h}, \quad \frac{\partial u(t_n,x_M)}{\partial x} \approx \frac{v_M^n - v_{M-1}^n}{h}$$

can be used, but these are however only first-order accurate and will degrade the accuracy of higher-order schemes.



## More Accurate Boundary Conditions

Second order one-sided accurate boundary conditions are given by

$$\frac{\partial \textit{u}(\textit{t}_\textit{n},\textit{x}_0)}{\partial \textit{x}} \approx \frac{-\textit{v}_2^\textit{n} + 4\textit{v}_1^\textit{n} - 3\textit{v}_0^\textit{n}}{2\textit{h}}, \quad \frac{\partial \textit{u}(\textit{t}_\textit{n},\textit{x}_M)}{\partial \textit{x}} \approx \frac{\textit{v}_{M-2}^\textit{n} - 4\textit{v}_{M-1}^\textit{n} + 3\textit{v}_M^\textit{n}}{2\textit{h}}$$

It is sometimes useful to use second-order central differences and introduce "ghost-points" for the boundary conditions, *e.g.* 

$$\frac{\partial u(t_n,x_0)}{\partial x} \approx \frac{v_1^n - \textcolor{red}{\mathbf{v_{-1}^n}}}{2h}.$$

How is this useful? — Consider a given flux condition  $u_x(t_n, x_0) = \varphi(t_n)$ , then

$$\frac{v_1^n - \mathbf{v_{-1}^n}}{2h} = \varphi_n \quad \Leftrightarrow \quad \mathbf{v_{-1}^n} = v_1^n - 2h\varphi_n.$$





# More Accurate Boundary Conditions

Now, if we are "leap-frogging" (Du-Fort Frankel style) the scheme can be applied at the boundary (m=0)

$$\frac{v_0^{n+1} - v_0^{n-1}}{2k} = b \frac{v_1^n - (v_0^{n+1} + v_0^{n-1}) + \mathbf{v_{-1}^n}}{h^2} + f_m^n,$$

$$\frac{v_0^{n+1}-v_0^{n-1}}{2k}=b\frac{v_1^n-(v_0^{n+1}+v_0^{n-1})+v_1^n-2h\varphi_n}{h^2}+f_m^n.$$

Ideas like these are commonly used.





Many physical processes are not described by convection (transport, e.g. the one-way wave-equation) or diffusion (e.g. the heat equation) alone.

An oil-spill in the ocean or a river is spreading by diffusion, while being transported by currents; the same goes for your daily multi-vitamin traveling through your bowels and diffusing into your bloodstream.

These physical processes are better described by the **convection-diffusion** equation

$$u_t + \underbrace{a}_{x} u_x = \underbrace{b}_{x} u_{xx},$$

Here a is the **convection speed**, and b is the **diffusion coefficient**.





Numerics, 1 of 3

First, we consider the forward-time central-space scheme

$$\frac{v_m^{n+1}-v_m^n}{k}+a\frac{v_{m+1}^n-v_{m-1}^n}{2h}=b\frac{v_{m+1}^n-2v_m^n+v_{m-1}^n}{h^2},$$

which is first order in time, and second order in space. Since stability requires  $b\mu \leq 1/2$ , we must have  $k \sim h^2$ , so the scheme is second-order overall.





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For convenience, lets assume a>0, define  $\mu=\frac{k}{h^2}$  and  $\alpha=\frac{ha}{2b}=\frac{a\lambda}{2b\mu}$ , we can write the scheme as

$$v_m^{n+1} = (1 - 2b\mu)v_m^n + b\mu(1 - \alpha)v_{m+1}^n + b\mu(1 + \alpha)v_{m-1}^n.$$

Based on previous discussion of parabolic PDEs, we know that  $\|u(t,\cdot)\|_{\infty} \leq \|u(t',\cdot)\|_{\infty}$  if t>t' (the peak-value is non-increasing).





In order to guarantee that the numerical solution of the difference scheme

$$v_m^{n+1} = (1 - 2b\mu)v_m^n + b\mu(1 - \alpha)v_{m+1}^n + b\mu(1 + \alpha)v_{m-1}^n,$$

also is non-increasing, we must have  $\alpha \leq 1$  (and  $b\mu \leq 1/2$ ), when these two conditions are satisfied, we have (let  $v_*^n = \max_m |v_m^n|$ )

$$|v_m^{n+1}| \leq (1-2b\mu)|v_m^n| + b\mu(1-\alpha)|v_{m+1}^n| + b\mu(1+\alpha)|v_{m-1}^n| \leq v_*^n [(1-2b\mu) + b\mu(1-\alpha) + b\mu(1+\alpha)] = v_*^n.$$

So that  $|v_{*'}^{n+1}| \leq |v_*^n|$ , *i.e.* the peak-value of the numerical solution is non-increasing.





The condition  $\alpha \leq 1$ , can be re-written

$$h \leq \frac{2b}{a}$$
,

which is a restriction on the spatial grid-spacing.

The quantity  $\frac{a}{b}$  corresponds to the **Reynolds number** in fluid flow, or the **Peclet number** in heat flow.

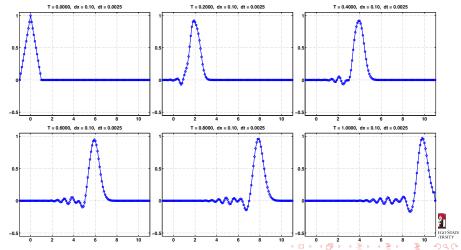
The quantity  $\alpha = \frac{ha}{2b}$  (sometimes  $2\alpha$ ) is often called the **cell Reynolds** number or the **cell Peclet number**.

If the grid-spacing h is too large, then the numerical solution cannot resolve the physics and oscillations occur. These oscillations are **not** due to instability (as long as the stability criterion is satisfied, of course) and do not grow; they are only a result of inadequate resolution.



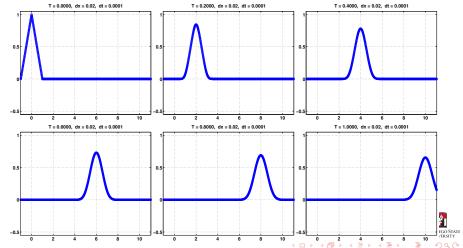
## Example #1

**Figure:** (Forward-Time Central-Space) Convection-diffusion with a=10, b=0.1, h=0.1>0.02, k=0.0025,  $\mu=1/4<1/2$ . We are stable, but have not resolved the physics.



# Example #2

**Figure:** (Forward-Time Central-Space) Convection-diffusion with  $a=10,\ b=0.1,\ h=0.02\leq 0.02,\ k=0.0001,\ \mu=1/4<1/2.$  We are stable, and have resolved the physics.



# Upwind Differences, 1 of 3

In example #2 we had to push the resolution to h = 0.02 (601 points in [-1, 11]) and k = 0.0001 (10001 time-steps in [0, 1]), for a grand total of 6,010,601 space-time grid points. That is a ridiculously high price to pay for such a simple 1D problem!!!

One way to avoid the resolution restriction is to use upwind differencing of the convection term. This corresponds to a switching between backward differencing when a > 0, and forward differencing when a < 0, e.g. only differencing in the direction where the (hyperbolic) characteristics come from:

$$\frac{v_m^{n+1} - v_m^n}{k} + a^+ \left[ \frac{v_m^n - v_{m-1}^n}{h} \right] + a^- \left[ \frac{v_{m+1}^n - v_m^n}{h} \right] = b \frac{v_{m+1}^n - 2v_m^n + v_{m-1}^n}{h^2}$$

or

$$v_m^{n+1} = [1 - 2b\mu(1+\alpha)]v_m^n + b\mu v_{m+1}^n + b\mu(1+2\alpha)v_{m-1}^n$$





# Upwind Differences, 2 of 3

The restriction  $h \leq \frac{2b}{|a|}$  is replaced by

$$2b\mu+|a|\lambda\leq 1,$$

which is much less restrictive when b is small and a large. If we want  $\mu = 1/4$ , i.e.  $k = h^2/4$ , then we must have  $h \leq \frac{4}{3} \left(1 - \frac{b}{3}\right)$ which with a = 10 and b = 0.1 as in the previous examples is 0.38 — 19 times that of the previous restriction.

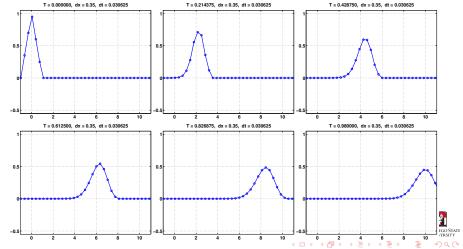
We have, however, also sacrificed the spatial second order accuracy, since the first-order upwind difference is first order.





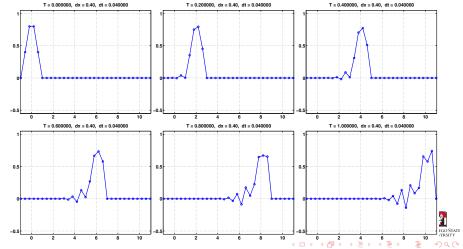
# Example #3

Figure: (Upwinding) Convection-diffusion with  $a=10,\,b=0.1,\,h=0.35\leq0.38,\,k=0.030625,\,\mu=1/4<1/2.$  We are stable, and have resolved the physics.



# Example #4

Figure: (Upwinding) Convection-diffusion with  $a=10,\ b=0.1,\ h=0.40\geq0.38,\ k=0.04,$   $\mu=1/4<1/2.$  We are stable, but have not resolved the physics.



## Upwind Differences, 3 of 3

The upwind scheme

$$\frac{v_m^{n+1} - v_m^n}{k} + a \frac{v_m^n - v_{m-1}^n}{h} = b \frac{v_{m+1}^n - 2v_m^n + v_{m-1}^n}{h^2},$$

can be rewritten in the form

$$\frac{v_m^{n+1}-v_m^n}{k}+a\frac{v_{m+1}^n-v_{m-1}^n}{2h}=\left(b+\frac{ah}{2}\right)\frac{v_{m+1}^n-2v_m^n+v_{m-1}^n}{h^2}.$$

We see that upwinding corresponds to changing the diffusion coefficient, or **adding artificial viscosity** to suppress oscillations.

There has been much debate regarding the value of these artificial-viscosity solutions; clearly they may only give qualitative information about the true solution.

More details on solving the convection-diffusion equation numerically can be found in  $\mathrm{K.W.\ Morton}$ , *Numerical Solution of Convection-Diffusion Problems*, Chapman & Hall, London, 1996.



#### Variable Coefficients

When the diffusivity b is a function of time and space, e.g. of the common form

$$u_t = \left[b(t,x)u_x\right]_x,$$

the difference schemes must be chosen to maintain consistency.

For example, the forward-time central-space scheme for this problem is given by

$$\frac{v_m^{n+1}-v_m^n}{k}=\frac{b(t_n,x_{m+1/2})(v_{m+1}^n-v_m^n)-b(t_n,x_{m-1/2})(v_m^n-v_{m-1}^n)}{h^2}.$$

This scheme is consistent if

$$b(t,x)\mu\leq\frac{1}{2},$$

for all values of (t, x) in the domain of computation...





### Looking Ahead...

- Systems of PDEs in Higher Dimensions.
- Second-Order Equations.
- Analysis of Well-Posed and Stable Problem.
- Convergence Estimates for IVPs.
- Well-Posed and Stable IBVPs.
- Elliptical PDEs and Difference Schemes.
- Linear Iterative Methods.
- The Method of Steepest Descent and the Conjugate Gradient Method.





## The Reynolds Number

### Definition ( $Re_L$ , The Reynolds Number)

$$\operatorname{Re}_{L} = \frac{\rho u L}{\mu} = \frac{u L}{\nu},$$

Symbol	Description	Units
$\rho$	density of the fluid	$kg/m^3$
и	fluid velocity wrt. object	m/s
L	characteristic length	m
$\mu$	fluid dynamic viscosity	$Pa \cdot s$ , or $Ns/m^2$ , or $kg/(m \cdot s)$
$\nu$	fluid kinematic viscosity	$m^2/s$





#### The Péclet Number

#### Definition (Pe<sub>L</sub>, The Péclet Number)

$$Pe_L = \frac{\text{advective transport rate}}{\text{diffusive transport rate}} = \underbrace{\frac{Lu}{D} = \text{Re}_L \, \text{Sc}}_{\text{mass transfer}} = \underbrace{\frac{Lu}{\alpha} = \text{Re}_L \, \text{Pr}}_{\text{heat transfer}}$$

Symbol	Description	Units
Re	Reynolds number	
$\operatorname{Sc}$	Schmidt number	
$\Pr$	Prandtl number	
L	characteristic length	m
и	fluid velocity wrt. object	m/s
D	mass diffusion coefficent	$m^2/s$
$\alpha$	thermal diffusivity	$k/(\rho \cdot c_p)$
k	thermal conductivity	$W/(m \cdot K)$
ho	density	$kg/m^3$
$c_p$	heat capacity	$(\mathrm{kg}\cdot m^2)/(K\cdot s^2)$





#### The Schmidt Number

## Definition (Sc, The Schmidt Number)

$$\mathrm{Sc} = \frac{\mathrm{viscous~diffusion~rate}}{\mathrm{molecular~(mass)~diffusion~rate}} = \frac{\nu}{D} = \frac{\mu}{\rho D}$$

Symbol	Description	Units
ν	kinematic viscosity	$m^2/s$
D	mass diffusivity	$m^2/s$
$\mu$	dynamic viscosity	$kg/(m \cdot s)$ , $Pa \cdot s$ , or $(N \cdot s)/m^2$
$\rho$	density of the fluid	$kg/m^3$





#### The Prandtl Number

### Definition (Pr, The Prandtl Number)

$$\Pr = \frac{\text{viscous diffusion rate}}{\text{thermal diffusion rate}} = \frac{\nu}{\alpha} = \frac{\mu/\rho}{k/(c_p \cdot \rho)} = \frac{c_p \mu}{k}$$

Symbol	Description	Units
$\nu$	kinematic viscosity	$m^2/s$
$\alpha$	thermal diffusivity	$k/(\rho \cdot c_p)$
k	thermal conductivity	$W/(m \cdot K)$
ho	density	$kg/m^3$
$c_p$	heat capacity	$(\mathrm{kg}\cdot m^2)/(K\cdot s^2)$





## A Bunch of physicists and Engineers...

The Reynolds number was introduced by Sir George **Stokes** in 1851, but was named by Arnold **Sommerfeld** in 1908 after Osborne Reynolds (1842 — 1912), who popularized its use in 1883.

- Jean Claude Eugène Péclet (10 February 1793 6
   December 1857), French physicist.
- Osborne Reynolds (23 August 1842 21 February 1912), Irish innovator.
- Ludwig Prandtl (4 February 1875 15 August 1953),
   German engineer.
- Ernst Heinrich Wilhelm Schmidt (1892 1975), German engineer



