Numerical Solutions to PDEs

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

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Spring 2018

Outline

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Last Time

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.

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Last Time

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.

Last Time

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 μ is constant.

Du-Fort Frankel ("fixed leapfrog")

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

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

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Lower Order Terms and Stability

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 $\mathbf{b = 0}$.** *Moreover, when $k = \lambda h$, and λ 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.

Lower Order Terms and Stability

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 $\mathcal{O}(k)$ as $k \searrow 0$.

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

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

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

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

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.

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Dissipation and Smoothness

The fact that a dissipative one-step scheme for a parabolic equation generates a numerical solution with increased smoothness as $t \nearrow$ (provided that μ 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

$$u_t = b u_{xx},$$

that is dissipative of order 2 with μ constant satisfies

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

for all initial data v^0 and $n \geq 0$.

Dissipation and Smoothness

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

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

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:

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

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

$$|\widehat{v}^{n+1}(\xi)|^2 + \frac{c_0 k}{\mu} \sum_{\nu=0}^{n} \left| \frac{1}{h} \sin\left(\frac{\theta}{2}\right) \widehat{v}^{\nu}(\xi) \right|^2 \leq |\widehat{v}^{0}(\xi)|^2.$$

Next we use

$$\left| \frac{2\sin\left(\frac{\theta}{2}\right)}{h} \widehat{v}^{\nu} \right| = \left| \frac{e^{i\theta} - 1}{h} \widehat{v}^{\nu} \right| = \left| \mathcal{F}(\delta_+ v^{\nu})(\xi) \right|.$$

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Dissipation and Smoothness — Proof 2 of 2

We get

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

Integration over ξ	:	$\left\|\, \widehat{\circ}(\xi) \,\right\|^2$	$\to$	$\|\, \widehat{\circ} \,\|^2$
using Parseval's relation	:	$\|\, \widehat{\circ} \,\|^2$	$\to$	$\|\circ\|^2$

gives...

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

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

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

Dissipation and Smoothness

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

We apply the theorem, and get

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

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

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

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Dissipation and Smoothness

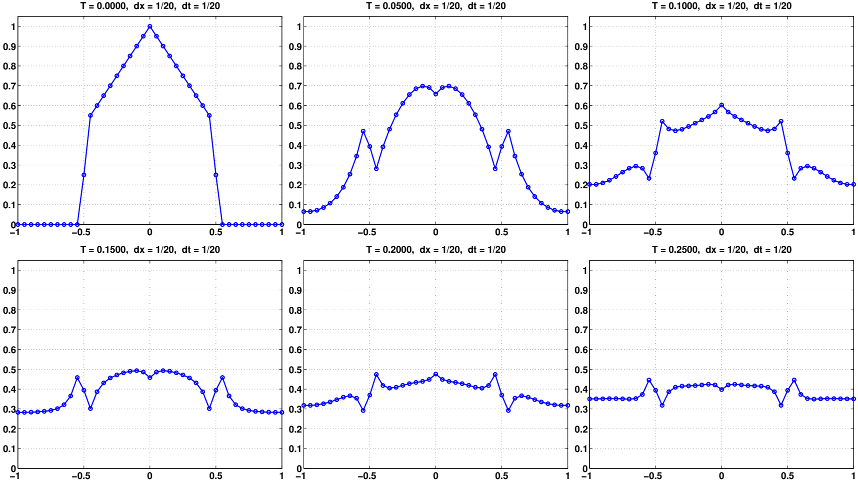
The argument can be applied recursively; since $\delta_+ v^n$ satisfies the difference equations, we find that for $nk = t > 0$, and any positive integer r that $\delta_+^r v^n$ is also bounded. Thus the solution of the difference scheme becomes smoother as t increases.

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.

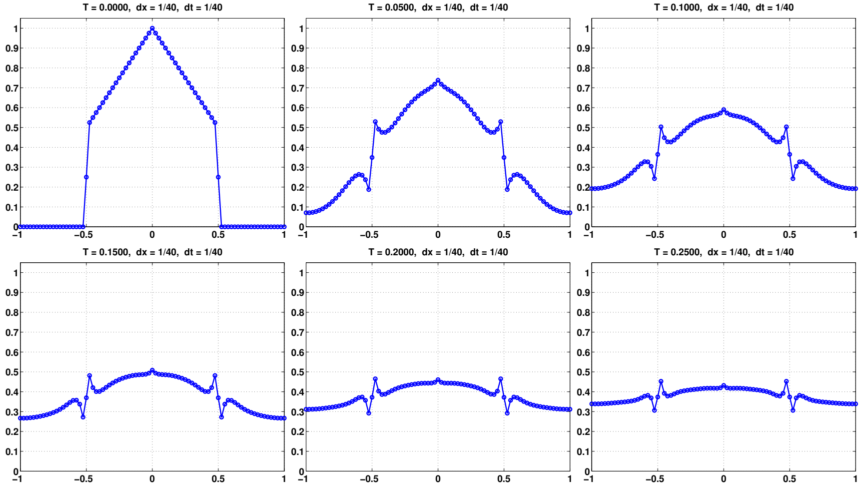
Example: Crank-Nicolson $dx = 1/20,\ dt = 1/20,\ \mu = 20$

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 λ remains constant (see next slide).



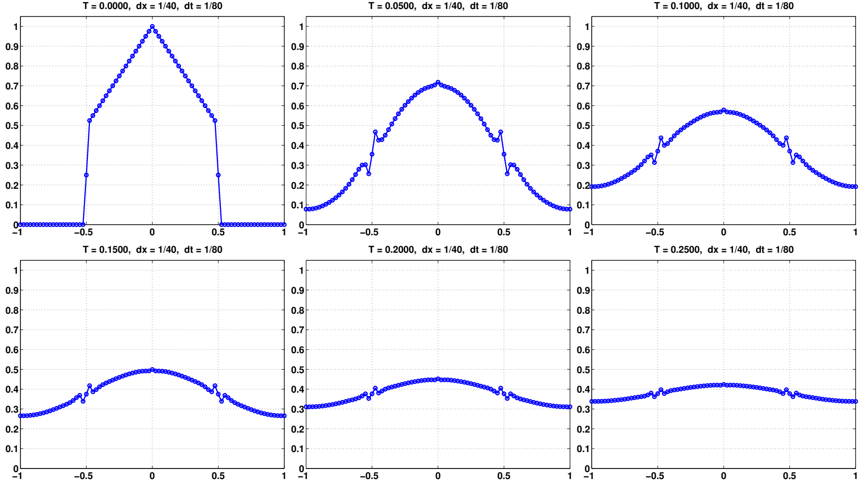
Example: Crank-Nicolson $dx = 1/40,\ dt = 1/40,\ \mu = 40$

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.



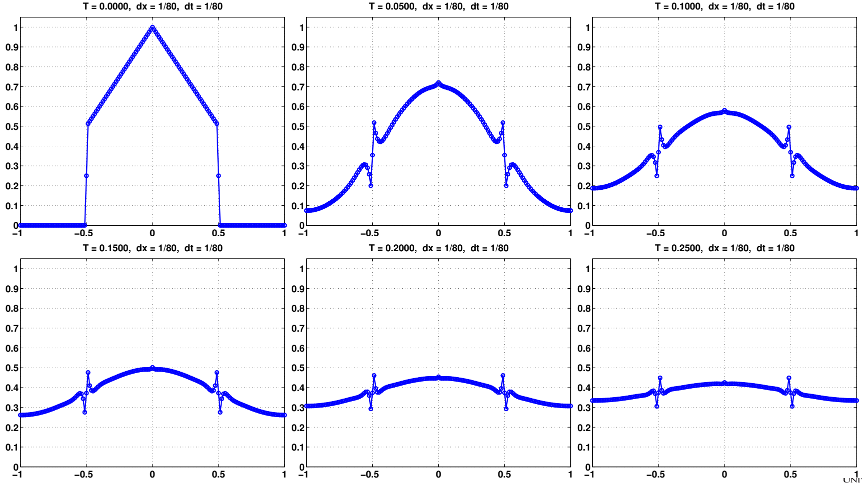
Example: Crank-Nicolson $dx = 1/40,\ dt = 1/80,\ \mu = 20$

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



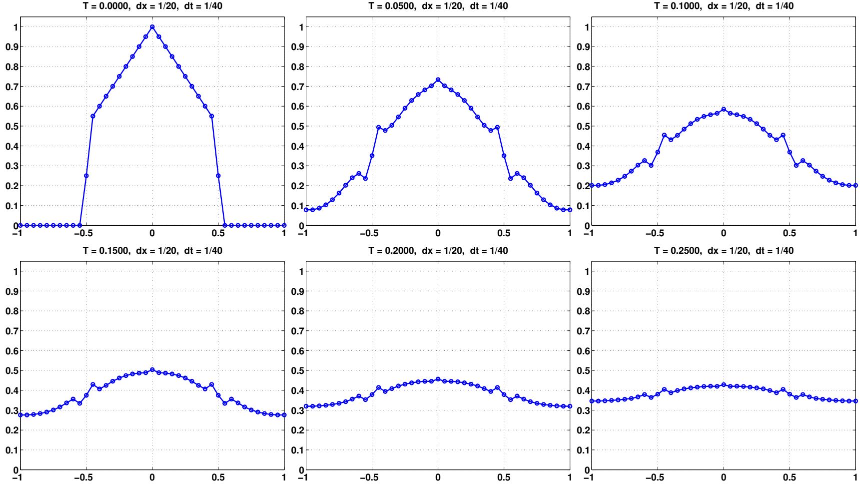
Example: Crank-Nicolson $dx = 1/80,\ dt = 1/80,\ \mu = 80$

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



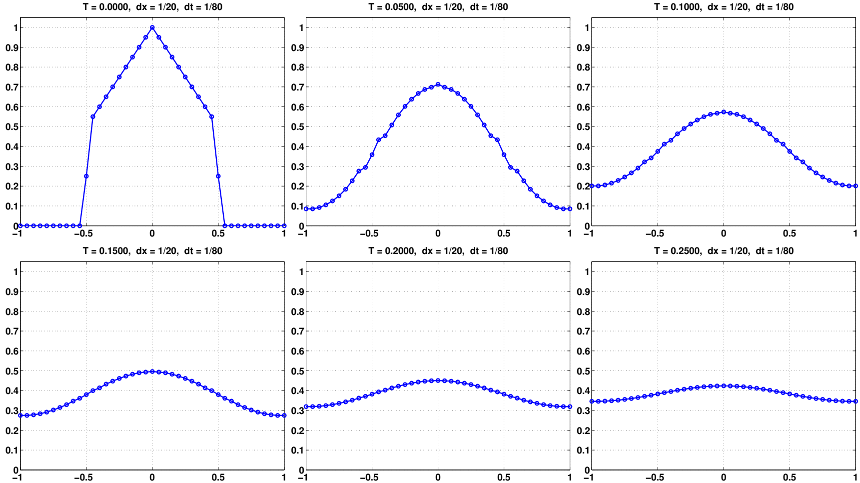
Example: Crank-Nicolson $dx = 1/20,\ dt = 1/40,\ \mu = 10$

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



Example: Crank-Nicolson $dx = 1/20,\ dt = 1/80,\ \mu = 5$

Figure: Refining in time lowers μ, which reduces oscillations...



Boundary Conditions (Again)

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.

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More Accurate Boundary Conditions

Second order one-sided accurate boundary conditions are given by

$$\frac{\partial u(t_n, x_0)}{\partial x} \approx \frac{-v_2^n + 4v_1^n - 3v_0^n}{2h}, \quad \frac{\partial u(t_n, x_M)}{\partial x} \approx \frac{v_{M-2}^n - 4v_{M-1}^n + 3v_M^n}{2h}$$

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

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

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

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

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More Accurate Boundary Conditions

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

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

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

Ideas like these are commonly used.

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The Convection-Diffusion Equation

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

$$u_t + a u_x = b u_{xx},$$

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

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The Convection-Diffusion Equation

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.

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).

The Convection-Diffusion Equation

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 $\alpha \le 1$ (and $b\mu \le 1/2$), when these two conditions are satisfied, we have (let $v_*^n = \max_m |v_m^n|$)

$$\begin{aligned} |v_m^{n+1}| &\le (1-2b\mu)|v_m^n| + b\mu(1-\alpha)|v_{m+1}^n| + b\mu(1+\alpha)|v_{m-1}^n| \\ &\le v_*^n\left[(1-2b\mu) + b\mu(1-\alpha) + b\mu(1+\alpha)\right] = v_*^n. \end{aligned}$$

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

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The Convection-Diffusion Equation

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

The quantity $\alpha = \frac{ha}{2b}$ (sometimes 2α) 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.

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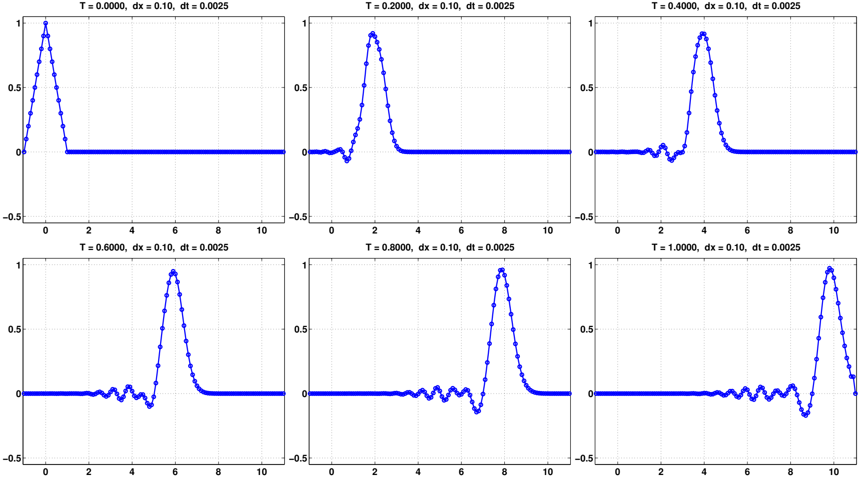
The Convection-Diffusion Equation — Example #1

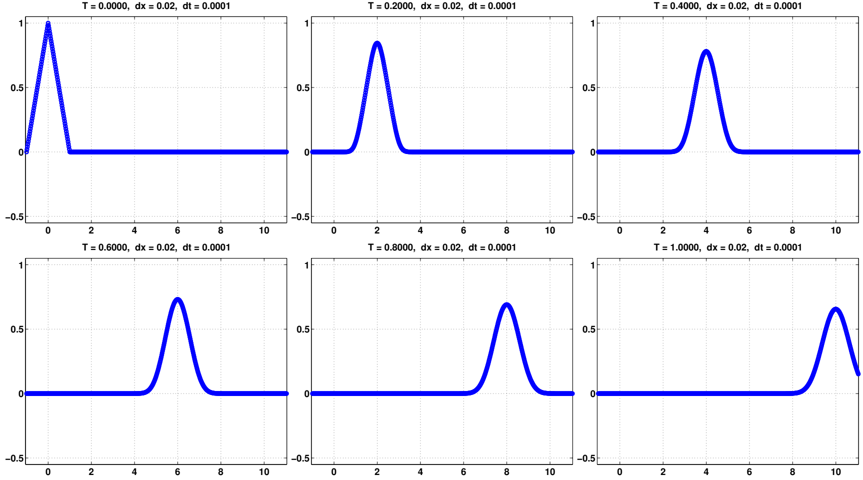
Figure: (Forward-Time Central-Space) Convection-diffusion with $a = 10$, $b = 0.1$, $h = 0.1 > 0.02$, $k = 0.0025$, $\mu = 1/4 < 1/2$. We are stable, but have not resolved the physics.



The Convection-Diffusion Equation

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.



The Convection-Diffusion Equation — 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

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

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The Convection-Diffusion Equation — 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 $h \leq \frac{4}{a}\left(1 - \frac{b}{2}\right)$ 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.

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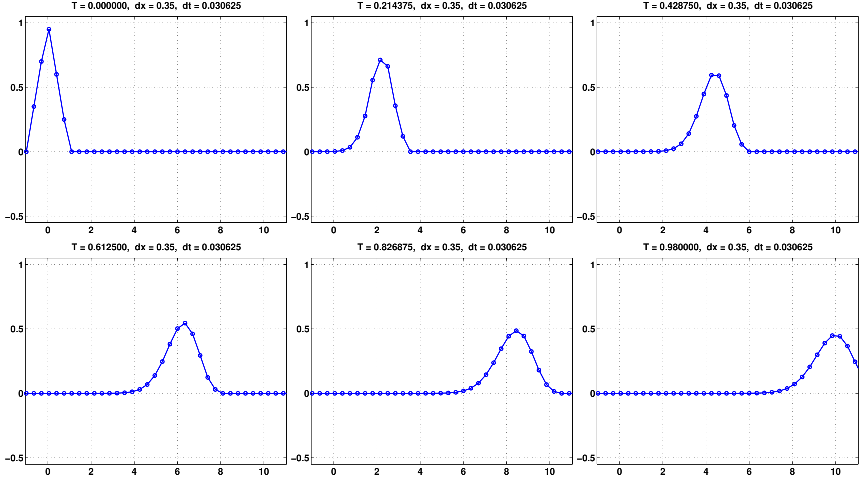
The Convection-Diffusion Equation

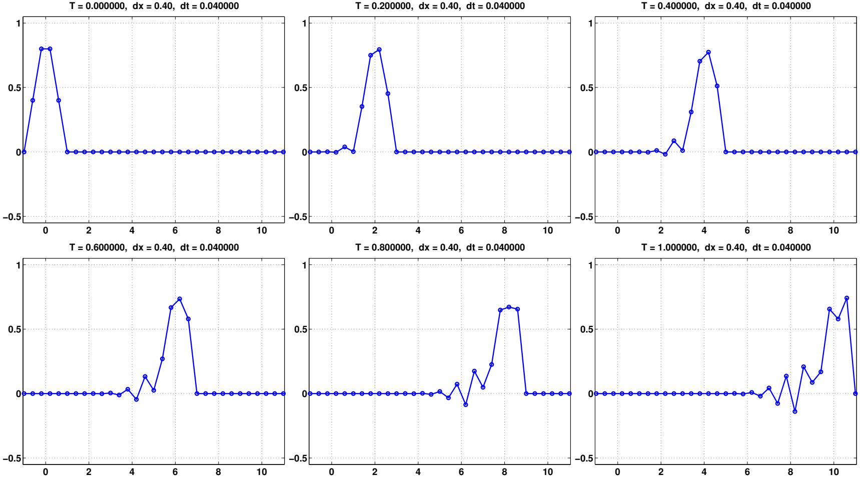
Example #3

Figure: (Upwinding) Convection-diffusion with $a = 10$, $b = 0.1$, $h = 0.35 \leq 0.38$, $k = 0.030625$, $\mu = 1/4 < 1/2$. We are stable, and have resolved the physics.



The Convection-Diffusion Equation — Example #4

Figure: (Upwinding) Convection-diffusion with $a = 10$, $b = 0.1$, $h = 0.40 \geq 0.38$, $k = 0.04$, $\mu = 1/4 < 1/2$. We are stable, but have not resolved the physics.



The Convection-Diffusion Equation — 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 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.

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The Reynolds Number

Definition (Re_L, The Reynolds Number)

$$\mathrm{Re}_L = \frac{\rho u L}{\mu} = \frac{u L}{\nu},$$

Symbol	Description	Units
ρ	density of the fluid	kg/m^3
u	fluid velocity wrt. object	m/s
L	characteristic length	m
μ	fluid dynamic viscosity	$\mathrm{Pa}\cdot s$, or $\mathrm{N}s/m^2$, or $\mathrm{kg}/(m\cdot s)$
ν	fluid kinematic viscosity	m^2/s

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The Péclet Number

Definition (Pe_L, The Péclet Number)

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

Symbol	Description	Units
Re	Reynolds number	
Sc	Schmidt number	
Pr	Prandtl number	
L	characteristic length	m
u	fluid velocity wrt. object	m/s
D	mass diffusion coefficent	m^2/s
α	thermal diffusivity	$k/(\rho \cdot c_p)$
k	thermal conductivity	$W/(m \cdot K)$
ρ	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)

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

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

The Prandtl Number

Definition (Pr, The Prandtl Number)

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

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

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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

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