5.4 The Heat Equation and Convection-Diffusion

The wave equation conserves energy. The heat equation $u_t = u_{xx}$ dissipates energy. The starting conditions for the wave equation can be recovered by going backward in time. The starting conditions for the heat equation can never be recovered. Compare $u_t = cu_x$ with $u_t = u_{xx}$, and look for pure exponential solutions $u(x,t) = G(t)\, e^{ikx}$:

Wave equation: $\boldsymbol{G' = ickG}$ $\quad G(t) = e^{ickt}$ has $|G| = 1$ (conserving energy)

Heat equation: $\boldsymbol{G' = -k^2G}$ $\quad G(t) = e^{-k^2t}$ has $G < 1$ (dissipating energy)

Discontinuities are immediately smoothed out by the heat equation, since G is exponentially small when k is large. This section solves $u_t = u_{xx}$ first analytically and then by finite differences. The key to the analysis is the beautiful ***fundamental solution*** starting from a point source (delta function). We will show in equation (7) that this special solution is a bell-shaped curve:

$$\boldsymbol{u(x,t) = \frac{1}{\sqrt{4\pi t}}\, e^{-x^2/4t}} \quad \text{comes from the initial condition} \quad u(x,0) = \delta(x)\,. \tag{1}$$

Notice that $u_t = cu_x + du_{xx}$ has convection and diffusion at the same time. The wave is smoothed out as it travels. This is a much simplified linear model of the nonlinear Navier-Stokes equations for fluid flow. The relative strength of convection by cu_x and diffusion by du_{xx} will be given below by the Peclet number.

The **Black-Scholes equation** for option pricing in mathematical finance also has this form. So do the key equations of environmental and chemical engineering.

For difference equations, explicit methods have stability conditions like $\Delta t \le \frac{1}{2}(\Delta x)^2$. This very short time step is more expensive than $c\Delta t \le \Delta x$. **Implicit methods** can avoid that stability condition by computing the space difference $\Delta^2 U$ at the new time level $n+1$. This requires solving a linear system at each time step.

We can already see two major differences between the heat equation and the wave equation (and also one conservation law that applies to both):

1. ***Infinite signal speed.*** The initial condition at a single point *immediately* affects the solution at all points. The effect far away is not large, because of the very small exponential $e^{-x^2/4t}$ in the fundamental solution. But it is not zero. (A wave produces no effect at all until the signal arrives, with speed c.)

2. ***Dissipation of energy.*** The energy $\frac{1}{2}\int (u(x,t))^2\, dx$ is a *decreasing* function of t. For proof, multiply the heat equation $u_t = u_{xx}$ by u. Integrate uu_{xx} by parts with $u(\infty) = u(-\infty) = 0$ to produce the integral of $-(u_x)^2$:

Energy decay
$$\frac{d}{dt}\int_{-\infty}^{\infty} \frac{1}{2}u^2\, dx = \int_{-\infty}^{\infty} uu_{xx}\, dx = -\int_{-\infty}^{\infty} (u_x)^2\, dx \le 0\,. \tag{2}$$

3. ***Conservation of heat*** (analogous to conservation of mass):

Heat is conserved $$\frac{d}{dt}\int_{-\infty}^{\infty} u(x,t)\,dx = \int_{-\infty}^{\infty} u_{xx}\,dx = \Big[u_x(x,t)\Big]_{x=-\infty}^{\infty} = 0\,. \qquad (3)$$

Analytic Solution of the Heat Equation

Start with **separation of variables** to find solutions to the heat equation:

$$\text{Assume } u(x,t) = G(t)E(x). \quad \text{Then } u_t = u_{xx} \text{ gives } G'E = GE'' \text{ and } \frac{G'}{G} = \frac{E''}{E}\,. \qquad (4)$$

The ratio G'/G depends only on t. The ratio E''/E depends only on x. Since equation (4) says they are equal, they must be constant. This produces a useful family of solutions to $u_t = u_{xx}$:

$$\frac{E''}{E} = \frac{G'}{G} \quad \text{is solved by} \quad \boldsymbol{E(x) = e^{ikx}} \text{ and } \boldsymbol{G(t) = e^{-k^2 t}}\,.$$

Two x-derivatives produce the same $-k^2$ as one t-derivative. We are led to exponential solutions of $e^{ikx}e^{-k^2t}$ and to their linear combinations (integrals over different k):

General solution $$\boldsymbol{u(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \widehat{u}_0(k)e^{ikx}e^{-k^2t}\,dx.} \qquad (5)$$

At $t = 0$, formula (5) recovers the initial condition $u(x,0)$ because it inverts the Fourier transform $\widehat{u}_0$ (Section 4.4.) So we have the analytical solution to the heat equation—not necessarily in an easily computable form! This form usually requires two integrals, one to find the transform $\widehat{u}_0(k)$ of $u(x,0)$, and the other to find the inverse transform of $\widehat{u}_0(k)e^{-k^2t}$ in (5).

Example 1 Suppose the initial function is a bell-shaped Gaussian $u(x,0) = e^{-x^2/2\sigma}$. Then the solution remains a Gaussian. The number σ that measures the width of the bell increases to $\sigma + 2t$ at time t, as heat spreads out. This is one of the few integrals involving e^{-x^2} that we can do exactly. Actually, we don't have to do the integral.

That function $e^{-x^2/2\sigma}$ is the impulse response (fundamental solution) at time $t = 0$ to a delta function $\delta(x)$ that occurred earlier at $t = -\frac{1}{2}\sigma$. So the answer we want (at time t) is the result of starting from that $\delta(x)$ and going forward a total time $\frac{1}{2}\sigma + t$:

Widening Gaussian $$u(x,t) = \frac{\sqrt{\pi(2\sigma)}}{\sqrt{\pi(2\sigma + 4t)}}\, e^{-x^2/(2\sigma+4t)}\,. \qquad (6)$$

This has the right start at $t = 0$ and it satisfies the heat equation.

The Fundamental Solution

For a delta function $u(x,0) = \delta(x)$ at $t = 0$, the Fourier transform is $\widehat{u}_0(k) = 1$. Then the inverse transform in (5) produces $u(x,t) = \frac{1}{2\pi}\int e^{ikx}e^{-k^2t}\,dk$ One computation of this u uses a neat integration by parts for $\partial u/\partial x$. It has three -1's, from the integral of ke^{-k^2t} and the derivative of ie^{ikx} and integration by parts itself:

$$\frac{\partial u}{\partial x} = \frac{1}{2\pi}\int_{-\infty}^{\infty}(e^{-k^2t}k)(ie^{ikx})\,dk = -\frac{1}{4\pi t}\int_{-\infty}^{\infty}(e^{-k^2t})(xe^{ikx})\,dk = -\frac{xu}{2t}\,. \qquad (7)$$

This linear equation $\partial u/\partial x = -xu/2t$ is solved by $u = ce^{-x^2/4t}$. The constant $c = 1/\sqrt{4\pi t}$ is determined by the requirement $\int u(x,t)\,dx = 1$. (This conserves the heat $\int u(x,0)\,dx = \int \delta(x)\,dx = 1$ that we started with. It is the area under a bell-shaped curve.) The solution (1) for diffusion from a point source is confirmed:

Fundamental solution from $u(x,0) = \delta(x)$

$$u(x,t) = \frac{1}{\sqrt{4\pi t}}\,e^{-x^2/4t}\,. \qquad (8)$$

In two dimensions, we can separate x from y and solve $u_t = u_{xx} + u_{yy}$:

Fundamental solution from $u(x,y,0) = \delta(x)\delta(y)$

$$u(x,y,t) = \left(\frac{1}{\sqrt{4\pi t}}\right)^2 e^{-x^2/4t}\,e^{-y^2/4t}\,. \qquad (9)$$

With patience you can verify that $u(x,t)$ and $u(x,y,t)$ do solve the 1D and 2D heat equations (Problem ____). The zero initial conditions away from the origin are correct as $t \to 0$, because $e^{-c/t}$ goes to zero much faster than $1/\sqrt{t}$ blows up. And since the total heat remains at $\int u\,dx = 1$ or $\iint u\,dx\,dy = 1$, we have a valid solution.

If the source is at another point $x = s$, then the response just shifts by s. The exponent becomes $-(x-s)^2/4t$ instead of $-x^2/4t$. If the initial $u(x,0)$ is a *combination* of delta functions, then by linearity the solution is the same combination of responses. But every $u(x,0)$ is an integral $\int \delta(x-s)\,u(s,0)\,ds$ of point sources! So the solution to $u_t = u_{xx}$ is an integral of the responses to $\delta(x-s)$. Those responses are fundamental solutions starting from all points $x = s$:

Solution from any $u(x,0)$

$$u(x,t) = \frac{1}{\sqrt{4\pi t}}\int_{-\infty}^{\infty} u(s,0)\,e^{-(x-s)^2/4t}\,ds\,. \qquad (10)$$

Now the formula is reduced to one infinite integral—but still not simple. And for a problem with boundary conditions at $x = 0$ and $x = 1$ (the temperature on a finite interval, much more realistic), we have to think again. Similarly for an equation $u_t = (c(x)u_x)_x$ with variable conductivity or diffusivity. That thinking probably leads us to finite differences.

I see the solution $u(x,t)$ in (10) as the **convolution** of the initial function $u(x,0)$ with the fundamental solution. Three important properties are immediate:

1. ***If $u(x,0) \ge 0$ for all x then $u(x,t) \ge 0$ for all x and t.*** Nothing in formula (10) will be negative.

2. ***The solution is infinitely smooth.*** The Fourier transform $\widehat{u}_0(k)$ in (5) is multiplied by e^{-k^2t}. In (10), we can take all the x and t derivatives we want.

3. ***The scaling matches x^2 with t.*** A diffusion constant d in the equation $u_t = du_{xx}$ will lead to the same solution with t replaced by dt, when we write the equation as $\partial u/\partial(dt) = \partial^2 u/\partial x^2$. The fundamental solution has $e^{-x^2/4dt}$ and its Fourier transform has e^{-dk^2t}.

Example 2 Suppose the initial temperature is a step function $u(x,0) = 0$. Then for negative x and $u(x,0) = 1$ for positive x. The discontinuity is smoothed out immediately, as heat flows to the left. The integral in formula (10) is zero up to the jump:

$$u(x,t) = \frac{1}{\sqrt{4\pi t}} \int_0^\infty e^{-(x-s)^2/4t}\, ds\,. \tag{11}$$

No luck with this integral! We can find the area under a complete bell-shaped curve (or half the curve) but there is no elementary formula for the area under a piece of the curve. No elementary function has the derivative e^{-x^2}. That is unfortunate, since those integrals give *cumulative probabilities* and statisticians need them all the time. So they have been normalized into the **error function** and tabulated to high accuracy:

Error function
$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-s^2}\, ds\,. \tag{12}$$

The integral from $-x$ to 0 is also $\operatorname{erf}(x)$. The normalization by $2/\sqrt{\pi}$ gives $\operatorname{erf}(\infty) = 1$.

We can produce this error function from the heat equation integral (11) by setting $S = (s-x)/\sqrt{4t}$. Then $s = 0$ changes to $S = -x/\sqrt{4t}$ as the lower limit on the integral, and $dS = ds/\sqrt{4t}$. Split into an integral from 0 to ∞, and from $-x/\sqrt{4t}$ to 0:

$$u(x,t) = \frac{\sqrt{4t}}{\sqrt{4\pi t}} \int_{-x/\sqrt{4t}}^\infty e^{-S^2}\, dS = \frac{1}{2}\left(1 + \operatorname{erf}\left(\frac{x}{\sqrt{4t}}\right)\right). \tag{13}$$

Good idea to check that this gives $u = \frac{1}{2}$ at $x = 0$ (where the error function is zero). This is the only temperature we know exactly, by symmetry between left and right.

Explicit Finite Differences

The simplest finite differences are *forward* for $\partial u/\partial t$ and *centered* for $\partial^2 u/\partial x^2$:

Explicit method $\displaystyle \frac{\boldsymbol{\Delta_t U}}{\boldsymbol{\Delta t}} = \frac{\boldsymbol{\Delta_x^2 U}}{\boldsymbol{(\Delta x)^2}}$
$$\frac{U_{j,n+1} - U_{j,n}}{\Delta t} = \frac{U_{j+1,n} - 2U_{j,n} + U_{j-1,n}}{(\Delta x)^2}. \tag{14}$$

Each new value $U_{j,n+1}$ is given explicitly by $U_{j,n} + R(U_{j+1,n} - 2U_{j,n} + U_{j,n-1})$. The crucial ratio for the heat equation $u_t = u_{xx}$ is now $\boldsymbol{R = \Delta t/(\Delta x)^2}$.

We substitute $U_{j,n} = G^n\, e^{ikj\Delta x}$ to find the growth factor $G = G(k, \Delta t, \Delta x)$:

One-step growth factor
$$G = 1 + R(e^{ik\Delta x} - 2 + e^{-ik\Delta x}) = \mathbf{1 + 2}\boldsymbol{R}\mathbf{(\cos}\, \boldsymbol{k\Delta x} \mathbf{- 1)}\,. \quad (15)$$

G is real, just as the exact one-step factor $e^{-k^2\Delta t}$ is real. Stability requires $|G| \le 1$. Again the most dangerous case is when the cosine equals -1 at $k\Delta x = \pi$:

Stability condition
$$|G| = |1 - 4R| \le 1 \text{ which requires } \boldsymbol{R = \frac{\Delta t}{(\Delta x)^2} \le \frac{1}{2}}\,. \quad (16)$$

In many cases we accept that small time step Δt and use this simple method. The accuracy from forward Δ_t and centered Δ_x^2 is $|U - u| = O(\Delta t + (\Delta x)^2)$. Those two error terms are comparable when R is fixed.

We could improve this one-step method to a **multistep method**. The "**method of lines**" calls an ODE solver for the system of differential equations (continuous in time, discrete in space). There is one equation for every meshpoint $x = jh$:

Method of Lines
$$\boldsymbol{\frac{dU}{dt} = \frac{\Delta_x^2 U}{(\Delta x)^2}} \qquad \frac{dU_j}{dt} = \frac{U_{j+1} - 2U_j + U_{j-1}}{(\Delta x)^2}\,. \quad (17)$$

This is a **stiff system**, because its matrix $-K$ (second difference matrix) has a large condition number: $\lambda_{\max}(K)/\lambda_{\min}(K) \approx N^2$. We could choose a stiff solver like `ode15s` in MATLAB.

Implicit Finite Differences

A fully implicit method for $u_t = u_{xx}$ computes $\Delta_x^2 U$ at the new time $(n+1)\Delta t$:

Implicit
$$\boldsymbol{\frac{\Delta_t U_n}{\Delta t} = \frac{\Delta_x^2 U_{n+1}}{(\Delta x)^2}} \qquad \frac{U_{j,n+1} - U_{j,n}}{\Delta t} = \frac{U_{j+1,n+1} - 2U_{j,n+1} + U_{j-1,n+1}}{(\Delta x)^2}\,. \quad (18)$$

The accuracy is still first-order in time and second-order in space. But stability no longer depends on the ratio $R = \Delta t/(\Delta x)^2$. We have *unconditional* stability, with a growth factor $0 < G \le 1$ for all k. Substituting $U_{j,n} = G^n e^{ijk\Delta x}$ into (18) and then canceling those terms from both sides leaves an extra G on the right side:

$$G = 1 + RG(e^{ik\Delta x} - 2 + e^{-ik\Delta x}) \quad \text{leads to} \quad G = \frac{1}{1 + 2R(1 - \cos k\Delta x)}\,. \quad (19)$$

The denominator is at least 1, which ensures that $0 < G \le 1$. The time step is controlled by accuracy, because stability is no longer a problem.

There is a simple way to improve to second-order accuracy. *Center everything at step* $n + \frac{1}{2}$. Average an explicit $\Delta_x^2 U_n$ with an implicit $\Delta_x^2 U_{n+1}$. This produces the famous ***Crank-Nicolson method*** (like the trapezoidal rule):

Crank-Nicolson $$\frac{U_{j,n+1} - U_{j,n}}{\Delta t} = \frac{1}{2(\Delta x)^2}(\Delta_x^2 U_{j,n} + \Delta_x^2 U_{j,n+1})\,. \qquad (20)$$

Now the growth factor G, by substituting $U_{j,n} = G^n e^{ijk\Delta x}$ into (20), solves

$$\frac{G-1}{\Delta t} = \frac{G+1}{2(\Delta x)^2}\,(2\cos k\Delta x - 2)\,. \qquad (21)$$

Separate out the part involving G, write R for $\Delta t/(\Delta x)^2$, and cancel the 2's:

Unconditional stability $$G = \frac{1 + R(\cos k\Delta x - 1)}{1 - R(\cos k\Delta x - 1)} \quad \text{has} \quad \boldsymbol{|G| \le 1\,.} \qquad (22)$$

The numerator is smaller than the denominator, since $\cos k\Delta x \le 1$. We do notice that $\cos k\Delta x = 1$ whenever $k\Delta x$ is a multiple of 2π. Then $G = 1$ at those frequencies, so Crank-Nicolson does not give the strict decay of the fully implicit method. We could weight the implicit $\Delta_x^2 U_{n+1}$ by $a > \frac{1}{2}$ and the explicit $\Delta_x^2 U_n$ by $1 - a < \frac{1}{2}$, to give a whole range of unconditionally stable methods (Problem ____).

Numerical example

Finite Intervals with Boundary Conditions

We introduced the heat equation on the whole line $-\infty < x < \infty$. But a physical problem will be on a **finite interval** like $0 \le x \le 1$. We are back to Fourier series (not Fourier integrals) for the solution $u(x,t)$. And second differences bring back the great matrices K, T, B, C that depend on the boundary conditions:

Absorbing boundary at $x = 0$: The temperature is held at $\boldsymbol{u(0,t) = 0}$.

Insulated boundary: No heat flows through the left boundary if $\boldsymbol{u_x(0,t) = 0}$.

If both boundaries are held at zero temperature, the solution will approach $u(x,t) = 0$ everywhere as t increases. If both boundaries are insulated as in a freezer, the solution will approach $u(x,t) =$ *constant*. No heat can escape, and it is evenly distributed as $t \to \infty$. This case still has the conservation law $\int_0^1 u(x,t)\,dx =$ constant.

Example 3 (Fourier series solution) We know that e^{ikx} is multiplied by $e^{-k^2 t}$ to give a solution of the heat equation. Then $u = e^{-k^2 t}\sin kx$ is another solution (combining $+k$ with $-k$). With zero boundary conditions $u(0,t) = u(1,t) = 0$, the only allowed frequencies are $k = n\pi$ (then $\sin n\pi x = 0$ at both ends $x = 0$ and $x = 1$). The complete solution is a combination of these exponential solutions with $k = n\pi$:

Complete solution $$u(x,t) = \sum_{n=1}^{\infty} b_n \, e^{-n^2\pi^2 t} \sin n\pi x \, . \tag{23}$$

The Fourier sine coefficients b_n are chosen to match $u(x,0) = \sum b_n \sin n\pi x$ at $t = 0$.

You can expect cosines to appear for insulated boundaries, where the slope (not the temperature) is zero. This gives exact solutions to compare with finite difference solutions. For finite differences, *absorbing boundary conditions produce the matrix* K (not B or C). The choice between explicit and implicit decides whether we have second differences $-KU$ at time level n or level $n+1$:

Explicit method $$U_{n+1} - U_n = -RKU_n \tag{24}$$

Fully implicit $$U_{n+1} - U_n = -RKU_{n+1} \tag{25}$$

Crank-Nicolson $$U_{n+1} - U_n = -\tfrac{1}{2}RK(U_n + U_{n+1})\, . \tag{26}$$

The explicit stability condition is again $R \le \frac{1}{2}$ (Problem ____). Both implicit methods are unconditionally stable (in theory). The reality test is to try them in practice.

An insulated boundary at $x = 0$ changes K to T. Two insulated boundaries produce B. Periodic conditions will produce C. The fact that B and C are singular no longer stops the computations. In the fully implicit method $(I + RB)U_{n+1} = U_n$, the extra identity matrix makes $I + RB$ invertible.

The **two-dimensional heat equation** describes the temperature distribution in a plate. For a square plate with absorbing boundary conditions, the difference matrix K changes to $\boldsymbol{K}$**2D**. The bandwidth jumps from 1 (triangular matrix) to N (when meshpoints are ordered a row at a time). Each time step of the implicit method now requires a serious computation. So implicit methods pay an increased price for stability, to avoid the explicit restriction $\Delta t \le \frac{1}{4}(\Delta x)^2 + \frac{1}{4}(\Delta y)^2$.

Convection-Diffusion

Put a chemical into flowing water. It diffuses while it is carried along by the flow. A diffusion term $d\,u_{xx}$ appears together with a convection term $c\,u_x$. This is the simplest model for one of the most important differential equations in engineering:

Convection-diffusion equation $$\frac{\partial u}{\partial t} = c\frac{\partial u}{\partial x} + d\frac{\partial^2 u}{\partial x^2}\, . \tag{27}$$

On the whole line $-\infty < x < \infty$, the flow and the diffusion don't interact. If the velocity is c, convection just carries along the diffusing solution to $h_t = d\,h_{xx}$:

Diffusing traveling wave $$\boldsymbol{u(x,t) = h(x+ct,t)\, .} \tag{28}$$

Substituting into equation (27) confirms that this is the solution (correct at $t = 0$):

$$\textbf{Chain rule} \qquad \frac{\partial u}{\partial t} = c\,\frac{\partial h}{\partial x} + \frac{\partial h}{\partial t} = c\,\frac{\partial h}{\partial x} + d\,\frac{\partial^2 h}{\partial x^2} = c\,\frac{\partial u}{\partial x} + d\,\frac{\partial^2 u}{\partial x^2}\,. \qquad (29)$$

Exponentials also show this separation of convection e^{ikct} from diffusion e^{-dk^2t}:

$$\textbf{Starting from } \boldsymbol{e^{ikx}} \qquad \boldsymbol{u(x,t) = e^{-dk^2t}\, e^{ik(x\,+\,ct)}}\,. \qquad (30)$$

Convection-diffusion is a terrific model problem, and the constants c and d clearly have different units. We take this small step into *dimensional analysis*:

$$\text{Convection coefficient } c\text{:} \quad \frac{\textbf{distance}}{\textbf{time}} \qquad \text{Diffusion coefficient } d\text{:} \quad \frac{\textbf{(distance)}^{\mathbf{2}}}{\textbf{time}} \qquad (31)$$

Suppose L is a typical length scale in the problem. ***The Peclet number*** $\boldsymbol{Pe = cL/d}$ is dimensionless. It measures the relative importance of convection and diffusion. This Peclet number for the linear equation (27) corresponds to the *Reynolds number* for the nonlinear Navier-Stokes equations (Section).

In the difference equation, the ratios $r = c\Delta t/\Delta x$ and $2R = 2d\Delta t/(\Delta x)^2$ are also dimensionless. That is why the stability conditions $r \le 1$ and $2R \le 1$ were natural for the wave and heat equations. The new problem combines convection and diffusion, and the ***cell Peclet number*** $\boldsymbol{P}$ uses $\Delta x/2$ as the length scale in place of L:

$$\textbf{Cell Peclet Number} \qquad P = \frac{r}{2R} = \frac{c\,\Delta x}{2d}\,. \qquad (32)$$

We still don't have agreement on the best finite difference approximation! Here are three natural candidates (you may have an opinion after you try them):

1. Forward in time, centered convection, centered diffusion

2. Forward in time, upwind convection, centered diffusion

3. Explicit convection (*centered or upwind*)**, with implicit diffusion.**

Each method will show the effects of r and R and P (we can replace $r/2$ by RP):

$$\textbf{1. Centered explicit} \qquad \frac{U_{j,n+1} - U_{j,n}}{\Delta t} = c\,\frac{U_{j+1,n} - U_{j-1,n}}{2\Delta x} + d\,\frac{\Delta_x^2 U_{j,n}}{(\Delta x)^2}\,. \qquad (33)$$

Every new value $U_{j,n+1}$ is a combination of three known values at time n:

$$U_{j,n+1} = (\mathbf{1} - \mathbf{2}\boldsymbol{R})U_{j,n} + (\boldsymbol{R} + \boldsymbol{RP})U_{j+1,n} + (\boldsymbol{R} - \boldsymbol{RP})U_{j-1,n}\,. \qquad (34)$$

Those three coefficients add to 1, and $U =$ constant certainly solves equation (33). ***If all three coefficients are positive, the method is surely stable.*** More than that, *oscillations cannot appear*. Positivity of the middle coefficient requires $R \le \frac{1}{2}$, as usual for diffusion. Positivity of the other coefficients requires $|\boldsymbol{P}| \leq \mathbf{1}$. Of course P will be small when Δx is small (so we have convergence as $\Delta x \to 0$). In avoiding oscillations, the actual cell size Δx is crucial to the quality of U.

Figure 5.12 was created by Strikwerda [59] and Persson to show the oscillations for $P > 1$ and the smooth approximations for $P < 1$. Notice how the initial hat function is smoothed and spread and shrunk by diffusion. Problem ____ finds the exact solution, which is moved along by convection. Strictly speaking, even the oscillations might pass the stability test $|G| \leq 1$ (Problem ____). But they are unacceptable.

Figure 5.12: Convection-diffusion with and without numerical oscillations: $R =$ ____, $r =$ ____ and ____.

2. Upwind convection

$$\frac{U_{j,n+1} - U_{j,n}}{\Delta t} = c\,\frac{U_{j+1,n} - U_{j,n}}{\Delta x} + d\,\frac{\Delta_x^2 U_{j,n}}{(\Delta x)^2}. \tag{35}$$

The accuracy in space has dropped to first order. But the oscillations are eliminated whenever $r + 2R \leq 1$. That condition ensures three positive coefficients when (35) is solved for the new value $U_{j,n+1}$:

$$U_{j,n+1} = (\boldsymbol{RP} + \boldsymbol{R})U_{j+1,n} + (\mathbf{1} - \boldsymbol{RP} - \mathbf{2}\boldsymbol{R})U_{j,n} + \boldsymbol{R}U_{j-1,n}\,. \tag{36}$$

Arguments are still going, comparing the centered method 1 and the upwind method 2. The difference between the two convection terms, **upwind minus centered**, is actually a diffusion term hidden in (35)!

Extra diffusion

$$\frac{U_{j+1} - U_j}{\Delta x} - \frac{U_{j+1} - U_{j-1}}{2\Delta x} = \left(\frac{\Delta x}{2}\right) \frac{U_{j+1} - 2U_j + U_{j-1}}{(\Delta x)^2}\,. \tag{37}$$

So the upwind method has this extra numerical diffusion or "***artificial viscosity***" to kill oscillations. It is a non-physical damping. If the upwind approximation were included in Figure 5.12, it would be *distinctly below* the exact solution. Nobody is perfect.

3. Implicit diffusion

$$\frac{U_{j,n+1} - U_{j,n}}{\Delta t} = c\,\frac{U_{j+1,n} - U_{j,n}}{\Delta x} + d\,\frac{\Delta_x^2 U_{j,\boldsymbol{n+1}}}{(\Delta x)^2}\,. \tag{38}$$

MORE TO DO

Problem Set 5.4

1 Solve the heat equation starting from a combination $u(x, 0) = \delta(x+1) - 2\delta(x) + \delta(x-1)$ of three delta functions. What is the total heat $\int u(x,t)\,dx$ at time t? Draw a graph of $u(x, 1)$ by hand or by MATLAB.

2 Integrating the answer to Problem 1 gives another solution to the heat equation:

$$\text{Show that} \quad w(x,t) = \int_0^x u(X,t)\,dX \quad \text{solves} \quad w_t = w_{xx}\,.$$

Graph the initial function $w(x, 0)$ and sketch the solution $w(x, 1)$.

3 Integrating once more solves the heat equation $h_t = h_{xx}$ starting from $h(x,0) = \int w(X,0)\,dX = \textit{hat function}$. Draw the graph of $h(x,0)$. Figure 5.12 shows the graph of $h(x,t)$, shifted along by convection to $h(x+ct,t)$.

4 In convection-diffusion, compare the condition $R \le \frac{1}{2}, P \le 1$ (for positive coefficients in the centered method) with $r + 2R \le 1$ (for the upwind method). For which c and d is the upwind condition less restrictive, in avoiding oscillations?

5 The eigenvalues of the n by n second difference matrix K are $\lambda_k = 2 - 2\cos\frac{k\pi}{n+1}$. The eigenvectors y_k in Section 1.5 are discrete samples of $\sin k\pi x$. Write the general solutions to the fully explicit and fully implicit equations (14) and (18) after N steps, as combinations of those discrete sines y_k times powers of λ_k.

6 Another exact integral involving $e^{-x^2/4t}$ is

$$\int_0^\infty x\,e^{-x^2/4t}\,dx = \left[-2t\,e^{-x^2/4t}\right]_0^\infty = 2t\,.$$

From (17), show that the temperature is $u = \sqrt{t}$ at the center point $x = 0$ starting from a ramp $u(x,0) = \max(0,x)$.

7 A ramp is the integral of a step function. So the solution of $u_t = u_{xx}$ starting from a ramp (Problem 6) is the integral of the solution starting from a step function (Example 2 in the text). Then $\sqrt{t}$ must be the total amount of heat that has crossed from $x > 0$ to $x < 0$ in Example 2 by time t. Explain each of those three sentences.