

# Mat1062: Computational Methods for PDE

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## 1 Ownership

These notes are built upon those of Rob Almgren who taught an analogous course in 2003. Whatever you learn of value from them is due to him. All mistakes and sources of confusion are to be blamed on me.

## 2 General classification

A partial differential equation (PDE) is an equation expressing a relationship among partial derivatives of an unknown function. If the function is  $u$  (a scalar or a vector), and it depends on variables  $x, y, \dots$  (it must depend on more than one variable to have *partial* derivatives), then the most general PDE would have the form

$$F(x, y, \dots, u, u_x, u_y, \dots, u_{xx}, u_{xy}, u_{yy}, \dots, u_{xxx}, \dots) = 0 \quad (1)$$

where the arguments include all derivatives of  $u$  up to some finite order.

In addition to the PDE (1), we need to specify a *domain*  $\Omega \subset \mathbb{R}^n$ , where  $n$  is the number of independent variables, and *boundary conditions* that  $u$  and some appropriate combination of its derivatives should satisfy on the boundary of  $\Omega$ . If one of the variables is time, then some part of the boundary conditions may be called *initial* or *terminal conditions*.

**Example:** Robert Merton (1969) considered the problem of “Lifetime portfolio selection under uncertainty.” The independent variables are  $t$ , representing time throughout an person's life, and  $w$ , representing his or her total wealth. Then the optimal investment/consumption strategy is determined

by the “utility”  $u(w, t)$  which satisfies the PDE

$$u_t - \rho u + rwu_w + \frac{1-p}{p} \frac{1}{u_w^{p/(1-p)}} - \frac{\beta^2}{2} \frac{u_w^2}{u_{ww}} = 0,$$

on the domain  $w > 0$  and  $t < T$  where  $T$  is time of death (assumed known). Terminal conditions are given at  $t = T$ . The parameters  $\rho, r$ , etc. represent various financial coefficients.<sup>1</sup>

This PDE is highly nonlinear, since the first derivative  $u_w$  appears with various exponents, and the second derivative  $u_{ww}$  appears in a denominator; in addition, the solution has singular behavior near the boundaries. There are no good numerical methods for solving such an equation; Merton obtained analytical solutions by exploiting a scaling symmetry and reducing the problem to an ODE.

## 2.1 Simple forms

Fortunately, most problems arising in physical sciences (and even in finance) do not have such horrible structures. We will therefore define a more restricted class of problems than the general (1).

A PDE is *quasilinear* if the highest derivatives appear linearly. For the simplest case of two independent variables  $x, y$  (one of which may represent time), and restricting attention to second-order PDEs (at most two derivatives), a quasilinear equation may be written

$$\begin{aligned} a(x, y, u, u_x, u_y) u_{xx} + b(x, y, u, u_x, u_y) u_{xy} + c(x, y, u, u_x, u_y) u_{yy} \\ = F(x, y, u, u_x, u_y) \end{aligned}$$

where  $a(\cdot), b(\cdot), c(\cdot), F(\cdot)$  may be arbitrary nonlinear functions.

It is *semilinear* if it is quasilinear, and the coefficient functions on the highest derivatives do not involve  $u$  or its lower derivatives:

$$a(x, y) u_{xx} + b(x, y) u_{xy} + c(x, y) u_{yy} = F(x, y, u, u_x, u_y)$$

It is *linear* if  $u$  appears only linearly:

$$a(x, y) u_{xx} + b(x, y) u_{xy} + c(x, y) u_{yy} = F(x, y).$$

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<sup>1</sup> $\rho$  is a utility discount rate,  $r$  is a riskless interest rate,  $p$  is a utility exponent, and  $\beta$  is a risk-adjusted excess return rate.

A linear equation has the property that if  $u_1$  and  $u_2$  are solutions, then  $u_1 + u_2$  is also a solution. Also, if  $\mu$  is a number then  $\mu u_1$  is also a solution.

The qualitative behavior of a PDE is determined by how its highest derivatives enter the equation. For a second-order, quasilinear equation the coefficients on the second derivatives define a quadratic form

$$G(p, q) = ap^2 + bpq + cq^2 = (p \ q) Q \begin{pmatrix} p \\ q \end{pmatrix}, \quad Q = \begin{pmatrix} a & \frac{1}{2}b \\ \frac{1}{2}b & c \end{pmatrix}$$

where  $p, q$  are only dummy variables. It is then natural to classify the equation depending on the type of the matrix  $Q$ :

- The PDE is *elliptic* if  $Q$  is positive definite or negative definite:  $G(p, q)$  has the same sign for all nonzero  $p, q$ . The paradigmatic example of a linear elliptic equation is *Poisson's equation* with  $G = I$ :

$$u_{xx} + u_{yy} = F(x, y)$$

If  $F = 0$  then it is *Laplace's equation*. Elliptic equations generally do not have a time variable, and come from equilibrium problems.

- The PDE is *hyperbolic* if  $Q$  is indefinite:  $G(p, q)$  takes opposite signs for different values of  $p, q$ . The classic example is the *wave equation*

$$u_{yy} - u_{xx} = 0.$$

In this case,  $y$  would represent time. Hyperbolic equations tend to be associated with transport phenomena.

- The PDE is *parabolic* in the in-between case that  $Q$  is semidefinite:  $G(p, q)$  is always either  $\geq 0$  or always  $\leq 0$ , but does take zero values. The classic example is the *diffusion equation*

$$u_y = u_{xx}.$$

Again,  $y$  would represent time. Note that the first-order term  $u_y$  comes from the right-hand side  $F(x, y, u, u_x, u_y)$ .

These define broad categories that we often apply qualitatively to more general problems.

A vaguer but broader classification is *time-dependent vs. stationary*:

- Time-dependent problems are conceptually similar to ODEs in lots of dimensions (infinitely many). The time derivative or derivatives are generally determined as an explicit function of the space derivatives, and the problem can be marched forward in time. In addition to the accuracy of the discrete formulation, the main issue is *stability*.
- Stationary problems must be solved across the entire domain at once. The main issue in solving them is how to solve the large systems of simultaneous equations that result from the discretization. Problems of this form often appear as parts of other problems; for example, solving an implicit discretization of a parabolic equation is equivalent to solving an elliptic problem at each step.

Here are a few more examples of PDEs. They are single equations or systems, depending on whether the unknown  $u$  has one or several components.

**Reaction-diffusion**  $u(x, t)$  is a vector representing concentration of something or another, perhaps with several components. It solves the semilinear parabolic equation

$$u_t = \Delta u + f(u)$$

where  $f(u)$  is a vector of reaction rates in terms of local concentrations, and the Laplacian operator  $\Delta = \nabla^2 = \partial_{xx} + \partial_{yy}$  (2-D) or  $\partial_{xx} + \partial_{yy} + \partial_{zz}$  (3-D).

**Incompressible fluid dynamics** The *incompressible Euler equations* for velocity  $\mathbf{u}$  and pressure  $p$  are

$$\begin{aligned} \mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u} &= -\nabla p \\ \operatorname{div} \mathbf{u} &= 0. \end{aligned}$$

In 3-D, there are four components in all:  $\mathbf{u} = (\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3)$  and  $p$ . Although this system does not fall within our classification above, we say that it is partly hyperbolic, by virtue of the transport behavior, and is partly elliptic, because of the need to solve for the pressure field (which is in equilibrium to acoustic waves). The appearance of the time derivative is deceptive: this is much more complicated system than a simple evolution problem.

The *Navier-Stokes equations* add a diffusion term:

$$\begin{aligned} \mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u} &= -\nabla p + \nu \Delta \mathbf{u} \\ \operatorname{div} \mathbf{u} &= 0, \end{aligned}$$

which makes the system parabolic as well.

**Compressible fluid dynamics** The *compressible Euler equations* are the first-order quasilinear conservation law

$$\mathbf{u}_t + \operatorname{div}(\mathbf{F}(\mathbf{u})) = \mathbf{0}, \quad (2)$$

where  $\mathbf{F}(\mathbf{u})$  is a vector-valued function of the solution vector  $\mathbf{u}$ , whose components include velocity (three components if in 3-D), pressure, density, temperature, etc. With appropriate assumptions on  $\mathbf{F}(\cdot)$ , these are hyperbolic problems even though they are first-order. As an example, in one dimension ( $\operatorname{div} = \partial_x$ ), for a scalar  $u$ , taking the simplest nonlinear function  $\mathbf{F}(u) = \frac{1}{2}u^2$  gives the *inviscid Burgers' equation*

$$u_t + u u_x = 0.$$

We can also add a diffusion term to the right-hand side of (2) obtain the *compressible Navier-Stokes equation*, which has parabolic nature as well as hyperbolic.

**Optimal glider flying** One model of the optimal strategy for a glider aircraft flying in uncertain lift constructs a value function  $u(x, z, \ell)$ , where  $u$  is expected time to reach the goal,  $x$  is distance from the goal,  $z$  is altitude, and  $\ell$  is local lift. This function solves the system of partial differential inequalities

$$\begin{aligned} u_x + H(u_z, \ell) + \frac{\ell}{\xi} u_\ell &\leq \frac{\bar{\ell}^2}{\xi} u_{\ell\ell} \\ u_z(x, \ell, z) &\geq -\frac{1}{\ell - s_{\min}}, \end{aligned}$$

where  $H(\cdot)$  is a known function incorporating the glide performance of the aircraft,  $\bar{\ell}$  is a root-mean-square lift strength, and  $\xi$  is a correlation length. Each inequality is an equality on part of the domain, and part of the problem is to find the dividing line between the two regions.

More examples can be found everywhere. I have given these just to emphasize that the classification elliptic/parabolic/hyperbolic must be interpreted qualitatively as well as quantitatively. A vast amount of theoretical

work goes into classifying the behavior of solutions to such equations; in this course we shall discuss only the simplest phenomena and methods. We shall begin with parabolic equations to illustrate consistency, convergence, and stability, continue with elliptic equations to discuss solving large linear systems, and finally consider hyperbolic equations and systems, where the conservation properties of the physical problem must be reflected in the discretization.

### 3 Parabolic equations

#### Physical derivation

Suppose  $u(x, t)$  is temperature of some medium, in one or more space dimensions. The internal energy per unit volume is some function  $H(u)$  of the temperature. Suppose  $F$  is the vector flux of energy through the material, driven primarily by thermal gradients. By conservation of energy, the total energy inside  $\Omega$  changes only due to flux in or out across the boundaries. If  $c$  is the specific heat per unit volume, then this may be written

$$\frac{d}{dt} \int_{\Omega} H(u(x, t)) \, dx = - \int_{\partial\Omega} F \cdot \hat{n} \, dA$$

where  $\hat{n}$  is the unit outward normal,  $\partial\Omega$  denotes the boundary surface of  $\Omega$ , and  $dA$  is surface area. Integrating by parts (also known as Green's formula), we may write this as

$$\int_{\Omega} c u_t \, dV = - \int_{\Omega} \operatorname{div}(F) \, dV$$

where  $c = dH/du$  is the specific heat per unit volume. Since this is true for every volume  $\Omega$ , if the integrands are continuous then they must be equal pointwise, and we obtain the differential equation

$$c u_t + \operatorname{div}(F) = 0$$

which is satisfied at every point in  $\Omega$ .

To complete the model, we must specify how  $F$  depends on  $u$ . In the conservation law (2) above, we assumed that  $F$  was a function of  $u$  itself, giving a first-order system. Now we shall let  $F$  depend on derivatives of  $u$ .

The simplest model is the linear Fourier law, in which the flux  $F$  is simply proportional to the temperature gradient  $\nabla u$ :

$$F(x, t, u, \nabla u) = -\kappa(x, t, u) \nabla u$$

where the coefficient of thermal conductivity  $\kappa$  in principle may depend on position, time, and the local density itself. We thus obtain the quasilinear parabolic equation

$$cu_t = \operatorname{div}(\kappa \nabla u).$$

If  $c$  and  $\kappa$  are constant in space and time, and independent of  $u$  itself, then this reduces to the linear equation

$$u_t = D \Delta u, \tag{3}$$

where  $D = \kappa/c$  is the *diffusivity*. The units of  $D$  are  $\text{length}^2/\text{time}$ . The same equation arises from other physical models; for example,  $u$  could be a chemical potential with a driving particle flux  $F$  which changes the particle density  $H(u)$ . In one dimension our model is

$$u_t = D u_{xx}. \tag{4}$$

We shall spend several weeks talking about numerical methods for equations (3,4). But before we begin, let us outline a few of their mathematical properties.

### Properties of the diffusion equation

For simplicity, we shall focus on the one-dimensional version (4).

**Conservation** For any fixed interval  $[a, b]$ , a smooth solution of (4) will satisfy

$$\frac{d}{dt} \int_a^b u(x, t) dx = \int_a^b D u_{xx}(x, t) dx = D u_x(x, t) \Big|_{x=a}^b. \tag{5}$$

This does not say that “stuff” is conserved in the sense that it never changes, but that we can account for the total change in an interval by looking at what crosses the endpoints. Stuff doesn’t appear or disappear from the interior because there are no sources or sinks in equation (4).

The analogue for equation (3) is as follows. Let  $\Omega \in \mathbb{R}^n$  be a bounded set with a reasonably smooth boundary. Then

$$\frac{d}{dt} \int_{\Omega} u(x, t) dx = D \int_{\Omega} \nabla \cdot \nabla u(x, t) dx = D \int_{\partial\Omega} \nabla u(x, t) \cdot \hat{n} = D \int_{\partial\Omega} \frac{\partial u}{\partial \hat{n}}(x, t)$$

where  $\hat{n}$  is the unit outward normal. And so the change in mass is equal to the total flux through the boundary of  $\Omega$ .

**Maximum principle** Suppose  $u(x, t)$  has a smooth interior local maximum, when viewed as a function of  $x$  for a fixed  $t$ . Then the second derivative  $u_{xx} \leq 0$ . Thus the time derivative  $u_t$  is also  $\leq 0$ , and the *local maximum cannot move upwards*. Similarly, at a local minimum  $u_{xx} \geq 0$  and so  $u_t \geq 0$ , and the *local minimum cannot move downwards*. If  $M$  is an upper bound at time  $t_0$  then the graph of  $u$  cannot get any higher later on

$$\max_{x \in \mathbb{R}} u(x, t_0) \leq M \implies \max_{x \in \mathbb{R}} u(x, t) \leq M, \quad \text{for } t \geq t_0.$$

Similarly, if  $m$  is a lower bound at time  $t_0$  then the graph of  $u$  cannot get any lower later on

$$m \leq \max_{x \in \mathbb{R}} u(x, t_0) \implies m \leq \max_{x \in \mathbb{R}} u(x, t), \quad \text{for } t \geq t_0.$$

Note that we are considering the heat equation on all space, allowing us to ignore what might happen at the boundary, and we are assuming that the solution is smooth.

In terms of physical problems for which  $u$  is a density it follows immediately that if the initial data is everywhere nonnegative, then the solution will never become negative at a later time.

In addition, because the diffusion equation is linear and has constant coefficients it follows that any space or time derivative of  $u$  also satisfies the diffusion equation. Therefore, since the derivatives do not get larger than their initial value, the solution only becomes smoother as it evolves in time. In fact the solution instantly becomes infinitely smooth. This justifies the invocation of derivatives above.

It will be very nice if the numerical scheme can preserve these properties. But to put this principle in perspective, let us describe an alternative source for a parabolic PDE, arising in pricing of financial derivatives.

**Black-Scholes equation** If  $V$  is the market price of a traded contract whose value depends on the price of an underlying asset  $S$ , then, under a suitable model for the dynamics of  $S$ ,  $V(S, t)$  must satisfy

$$\frac{\partial V}{\partial t} + \frac{1}{2}\sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + (r - q) S \frac{\partial V}{\partial S} - rV = 0.$$

where  $\sigma$ ,  $r$ ,  $q$  are parameters of the model for  $S$  (volatility, interest rate, and dividend yield). This equation is linear, but has nonconstant coefficients depending on the independent variable  $S$ . By changing variables to  $x = \log S$ , the coefficients become constant, and a few more simple changes reduce it to the form (4), in which  $D$  is a ratio of volatility to interest rate.

Although this equation has the mathematical form as the physical model above, the underlying reasoning is very different. Conservation of  $V$  has no particular significance, nor does decrease of energy; instead a principle called *absence of arbitrage* is central. This suggests that different numerical methods may be appropriate for the Black-Scholes equation than for physical diffusion problems.

### 3.1 Special solutions

Above we have described fundamental properties of the structure of the diffusion equation, especially as it arises in physical problems. To gain some insight into the behavior of its solutions in general, let us consider two particular explicit solutions.

#### 3.1.1 Green's function

Consider the function

$$G(x, t) = \frac{1}{\sqrt{4\pi Dt}} e^{-x^2/4Dt}. \quad (6)$$

For  $t > 0$ , no denominators vanish, so this function is perfectly well defined and has derivatives of all orders; it describes a Gaussian pulse centered at the origin, of total mass one, and of width  $\sqrt{2Dt}$ . (Because the solution is not compactly supported we cannot just take the length of the support as the width of the solution. Here, the "width" is the square root of variance  $\int x^2 G(x, t) dx$ .) You may verify that this function satisfies (4). (To find  $G$ , look for solutions with the similarity form  $u(x, t) = U(x/\sqrt{Dt})/\sqrt{Dt}$  for an

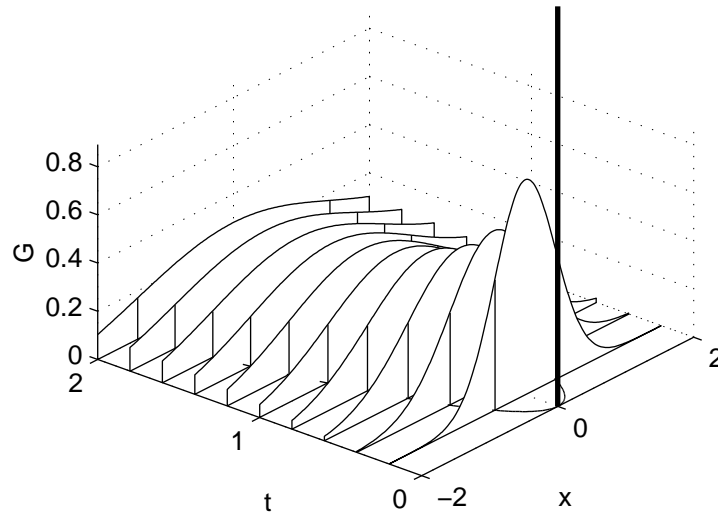


Figure 1: Green's function (6) for the diffusion equation  $u_t = \frac{1}{2}u_{xx}$ , showing a curve on which  $G$  is a fixed fraction of its height at the origin. The first few slices expand very rapidly away from  $x = 0$ , and then slow down.

unknown function  $U(\xi)$ , obtain the ODE  $2U''(\xi) + \xi U'(\xi) + U(\xi) = 0$ , find the solution  $U(\xi) = A \exp(-\xi^2/4)$ , and then choose  $A$  so mass is one.)

Note that

$$G(x, 0) := \lim_{t \searrow 0} G(x, t) = \begin{cases} 0 & \text{if } x \neq 0 \\ \infty & \text{if } x = 0 \end{cases}$$

is not a real-valued function. However, by extrapolating known properties of  $G(x, t)$  for  $t > 0$ , we may say that  $G(x, 0)$  is some sort of unit mass, centered at the origin, but of width zero—this strange object is called a *Dirac delta distribution*. Of course, no physical object can really have zero width, so you may think of this solution as an “outer asymptotics,” approximately valid on scales larger than the length scale of the initial data. I want to draw your attention to two aspects of this solution.

First, because our PDE is linear, we can solve the initial-value problem

$$u_t = Du_{xx} \quad \text{on } -\infty < x < \infty, t \geq 0. \quad \text{with } u(x, 0) = u_0(x),$$

by adding up the contributions from each part of the initial data to get the famous Green's formula:

$$u(x, t) = \int_{-\infty}^{\infty} G(x - y, t) u_0(y) dy.$$

Note that if  $u_0(x) \geq 0$  for all  $x$ , then,  $u(x, t) \geq 0$  for all  $(x, t)$  since  $G > 0$ . Furthermore, if  $u_0 \geq 0$  is continuous and if  $u_0 > 0$  *somewhere*, then  $u(x, t) > 0$  for all  $x$  and for all  $t > 0$  *no matter how small t is*. Thus initial data which is positive in a bounded set and zero elsewhere results in a solution which is instantaneously positive everywhere — the “speed of propagation” is infinite. However, for small  $t$ , the largest contributions to  $u$  at  $x$  come from values  $u_0(y)$  for  $y$  near  $x$ .

Second, in (6),  $x$  appears only in the combination  $x/\sqrt{Dt}$ . This means that if we look at the physical location of any qualitative aspect of the solution—for example, the boundaries between which half of the solution mass is contained—then we will see  $x$  scaling proportional to  $\sqrt{Dt}$ . For small  $t$ , this  $x$  will move very rapidly, but for large  $t$ , the speed of advance will be slower and slower.

### 3.1.2 Eigenfunctions

The second class of special solutions takes sinusoidal initial data  $u_0(x) = \sin kx$ , where  $k$  is any real number. You may easily verify that the solution with this initial data is

$$u(x, t) = e^{-\sigma t} \sin kx, \quad \sigma = Dk^2. \quad (7)$$

The formula  $\sigma = Dk^2$  is called the *dispersion relation*: it gives us the time dependence of wave-like solutions in terms of their spatial wave number  $k$ . For any positive value of  $D$ ,  $\sigma$  becomes very large as  $k$  increases, meaning that *high-frequency waves damp fast*. Describing this behavior in terms of wavelengths and periods rather than wave numbers and decay rates, the wavelength  $\Lambda = 2\pi/k$  and the decay time  $T = 1/\sigma$ , so  $\Lambda = 2\pi\sqrt{DT}$ . This is the same length  $\propto \sqrt{\text{time}}$  that we observed in the Green's function.

Since the PDE is linear, a general solution may be considered as a superposition of all these periodic waves, and we conclude that small-scale features of the initial data are very rapidly smoothed out.

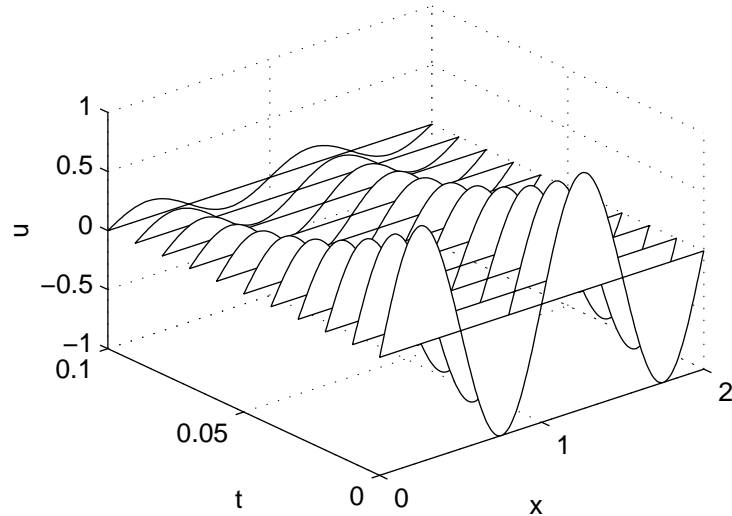


Figure 2: Periodic solutions (7) for the diffusion equation, with  $k = 2\pi$  so the spatial period is 1. The time decay constant is  $k^2/2 \approx 20$ , so the decay is extremely rapid (note the time scale of the plot). By  $t = 0.1$  the amplitude is only about  $1/7$  of its initial value.

## 4 Numerical methods for diffusion equation

Now let us construct a numerical model for the diffusion equation. We shall first talk about the pure initial value problem: find  $u(x, t)$  defined for all  $-\infty < x < \infty$  and for  $t \geq 0$ , so that  $u_t = Du_{xx}$  on this region, and so that  $u(x, 0) = u_0(x)$  where  $u_0(x)$  is given initial data. We shall discretize first in space, then in time.

### 4.1 Space discretization

Thus to begin, let us choose a *grid spacing*  $h$  and introduce grid points  $x_j = jh$ . We want to approximate the PDE's solution,  $u(x, t)$ , on  $\mathbb{R} \times [0, \infty)$  by an infinite collection of functions,  $\{U_j(t)\}$ , on  $[0, \infty)$  such that  $U_j(t)$  will be a good approximation for  $u(x_j, t)$  as  $h \rightarrow 0$ .

The  $U_j(t)$  will be solutions of an infinite collection of ODEs; the ODEs are determined by the PDE (the diffusion equation, in this case). To do

this, we need to approximate the spatial derivative  $u_{xx}(x, t)$  by a *difference formula*. We do this by computing first derivatives twice, mimicking the two first derivatives (gradient and divergence) which we used to construct the second-order PDE (4).

First, let us note that if the  $U_j(t)$  are a good approximation to the grid values of a smooth function  $u(x, t)$ , then they can be used to approximate the first  $x$ -derivative of  $u(x, t)$ :

$$u_x((j + \frac{1}{2})h, t) \approx \frac{1}{h}(u(x_{j+1}, t) - u(x_j, t)) \approx \frac{1}{h}(U_{j+1}(t) - U_j(t)).$$

This approximates the first derivative at the “half-grid point”  $j + \frac{1}{2}$ , centered between the points  $j$  and  $j + 1$  at which we evaluate  $u$  itself. Next, we take the second derivative by differencing this expression:

$$\begin{aligned} u_{xx}(x_j, t) &\approx \frac{1}{h} \left( u_x((j + \frac{1}{2})h, t) - u_x((j - \frac{1}{2})h, t) \right) \\ &\approx \frac{1}{h} \left( \frac{U_{j+1}(t) - U_j(t)}{h} - \frac{U_j(t) - U_{j-1}(t)}{h} \right) \\ &= \frac{1}{h^2} (U_{j+1}(t) - 2U_j(t) + U_{j-1}(t)). \end{aligned}$$

To confirm that this expression is a good approximation to the second derivative, let us assume that  $u(x, t)$  is a smooth function, and expand its values at  $x_{j\pm 1}$  as a local asymptotic series<sup>2</sup> in terms of its derivatives at  $x_j$ :

$$\begin{aligned} U_{j\pm 1}(t) &\approx u(x_j \pm h, t) \\ &\sim u(x_j, t) \pm hu_x(x_j, t) + \frac{1}{2}h^2u_{xx}(x_j, t) \\ &\quad \pm \frac{1}{6}h^3u_{xxx}(x_j, t) + \frac{1}{24}h^4u_{xxxx}(x_j, t) + \dots \end{aligned}$$

as  $h \rightarrow 0$ . We therefore find

$$\frac{1}{h^2}(U_{j+1}(t) - 2U_j(t) + U_{j-1}(t)) \sim u_{xx}(x_j, t) + \frac{1}{12}h^2u_{xxxx}(x_j, t) + \dots$$

as  $h \rightarrow 0$ . Since the “error” term  $u_{xxxx}$  has a coefficient proportional to  $h^2$ , the difference expression on the left is a *second-order accurate* approximation to the second derivative.

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<sup>2</sup>An *asymptotic* series expresses the local behavior of  $f(h)$  as  $h \rightarrow 0$ ; each fixed number of terms gives a more accurate approximation in that limit. This is in contrast to a *power series*, which is intended to converge as the number of terms  $\rightarrow \infty$ , for a fixed value of  $h$ . Any power series is an asymptotic series, but the latter are much more robust.

We could have written down this second-order difference formula directly, but constructing it as two first derivatives tells us the proper way to handle nonconstant coefficients. If  $c$  and  $\kappa$  are not constant, then we will see that a good approximation is

$$\frac{1}{c}(\kappa u_x)_x \Big|_{x=x_j} \approx \frac{1}{c_j} \frac{1}{h} \left( \kappa_{j+\frac{1}{2}} \frac{U_{j+1} - U_j}{h} - \kappa_{j-\frac{1}{2}} \frac{U_j - U_{j-1}}{h} \right)$$

where  $c_j$  and  $\kappa_{j\pm\frac{1}{2}}$  are approximations to  $c$  at  $x_j$  and to  $\kappa$  at  $x_{j\pm 1/2}$ . For example,  $\kappa_{j+\frac{1}{2}} = (\kappa_j + \kappa_{j+1})/2$ . A *bad* approximation would be

$$\text{BAD: } \frac{1}{c}(\kappa u_x)_x \Big|_{x=x_j} \approx \frac{\kappa_j}{c_j} \frac{1}{h^2} (U_{j+1} - 2U_j + U_{j-1}),$$

since we will see that it does not properly respect conservation.

## 4.2 Time discretization

Now that we have approximated the space derivatives, our PDE becomes a collection of ODEs for  $U_j(t)$ . Returning to the case of constant  $c$ ,  $\kappa$ , and hence  $D$ , we may write this system as

$$\begin{aligned} \frac{dU_j}{dt}(t) &= \frac{D}{h} \left( \frac{U_{j+1}(t) - U_j(t)}{h} - \frac{U_j(t) - U_{j-1}(t)}{h} \right) \\ &= \frac{D}{h^2} (U_{j+1}(t) - 2U_j(t) + U_{j-1}(t)), \end{aligned}$$

on the lattice  $j = \dots, -2, -1, 0, 1, 2, \dots$  in  $\mathbb{R}$ .

Following our approach to space discretization, we choose a *time step*  $k$ , introduce *time levels*  $t_n = nk$ , for  $n = 0, 1, \dots$ , and let  $u_j^n$  denote an approximation to the (ODE) solution  $U_j(t)$  at the time level  $t_n = nk$ . Which is, in turn, an approximation to the (PDE) solution  $u(x, t)$  at the grid point  $(x_j, t_n) = (jh, nk)$ . In short:

$$u_j^n \approx U_j(nk) \approx u(jh, nk)$$

Note that the superscript  $n$  is a *label* rather than an *exponent*.

Once we have figured out how to generate  $u_j^n$  for all  $n > 0$  from a collection of initial values  $u_j^0$  we will have gone from  $u(x, t)$  which is a function on  $\mathbb{R} \times [0, \infty)$  to a collection of numbers  $\{u_j^n\}$  which are located

on the lattice  $\{(jh, nk) \mid j \in \mathbb{Z}, n \in \mathbb{N}\}$ . The hope is that if we do our job well then as  $h \rightarrow 0$  and  $k \rightarrow 0$  these numbers will become better and better approximations of  $u(x_j, t_n)$ .

The simplest way to approximate a solution to the ODE  $y_t = f(y)$  is the *forward Euler* approximation: set  $y^{n+1} = y^n + k f(y^n)$ . That is, just assume that  $dy/dt$  is constant across the time interval from  $t_n$  to  $t_{n+1}$  even though  $y(t)$  itself is changing. Applied to this system of ODEs, we get the approximation

$$u_j^{n+1} = u_j^n + \frac{Dk}{h^2} (u_{j+1}^n - 2u_j^n + u_{j-1}^n). \quad (8)$$

Every term on the right side of this equation involves only grid values at level  $n$ , and the result is an explicit formula for grid values at level  $n + 1$ .

This formula is very easy to implement: At  $t = 0$ , set the initial grid value  $u_j^0 = u_0(jh)$ , where  $u_0(x)$  is the given initial data. Then for each  $n = 1, 2, \dots$ , evaluate all grid points  $u_j^n$  at level  $n$  by evaluating formula (8) in terms of the previous level  $n - 1$ . Once level  $n$  is done, then we have all the information we need to continue on to level  $n + 1$ ; in this way we can proceed forward as far as we like. We hope that each computed value  $u_j^n$  will be reasonably close to the corresponding value  $u(x_j, t_n)$  of the true solution  $u(x, t)$ , especially if  $h$  and  $k$  are chosen small enough; this desirable property is called *convergence*.

Before we study convergence, let us consider the properties of the PDE that we identified above, to see whether they are preserved in the discrete model (8). As a preliminary, let us note that the scheme may be written as

$$u_j^{n+1} = \lambda u_{j+1}^n + (1 - 2\lambda) u_j^n + \lambda u_{j-1}^n, \quad \lambda = \frac{Dk}{h^2}. \quad (9)$$

Note that the parameter  $\lambda$  is dimensionless; it is roughly the grid time step divided by the diffusion time on one spatial grid cell.

**Conservation** If  $a = Ah$ ,  $b = Bh$ , and  $t = nk$  for integers  $A$ ,  $B$ , and  $n$  then the analogue of  $\int_a^b u(x, t) dx$  is the sum  $S_n = \sum_{j=A}^B u_j^n h$ . The change in this quantity across one time step is

$$\begin{aligned} \frac{S_{n+1} - S_n}{k} &= \frac{D}{k} \sum_{j=A}^B (u_j^{n+1} - u_j^n) h = D \sum_{j=A}^B \left( \frac{u_{j+1}^n - u_j^n}{h} - \frac{u_j^n - u_{j-1}^n}{h} \right) \\ &= D \frac{u_{B+1}^n - u_B^n}{h} - D \frac{u_A^n - u_{A-1}^n}{h} \end{aligned}$$

(in the second sum, change  $j \mapsto j + 1$ , then the middle part all cancels). Because the two terms on the right-hand side are the discrete approximation of  $u_x$  at  $x = a$  and  $x = b$ , we see that this spatial discretization results in the discrete analogue of the conservation law (5) whatever the value of  $h$ ,  $k$ , and  $D$ . It's clear that this property is preserved even if  $c$  and  $\kappa$  are not constant, as long as the "good" discretization described above is used. (Check this!)

**Maximum principle** We first note that the local maxima decrease and local minima increase. Assume  $u_j^n > u_{j\pm 1}^n$ . Because  $\lambda > 0$  it follows that

$$u_j^{n+1} = \lambda u_{j+1}^n + (1 - 2\lambda) u_j^n + \lambda u_{j-1}^n < \lambda u_j^n + (1 - 2\lambda) u_j^n + \lambda u_j^n = u_j^n.$$

And so  $u_j^{n+1} < u_j^n$ ; the local maximum moves downwards. Similarly, if  $u_j^n < u_{j\pm 1}^n$ , then  $u_j^n < u_j^{n+1}$ ; the local minimum moves upwards.

In terms of global upper and lower bounds, this will hold for discrete model if and only if  $\lambda \leq \frac{1}{2}$ , for only then are all the weights in the expression (9) positive. Assume that  $u^nl \leq M$  for all  $j$ . Then if  $\lambda \leq 1/2$  the rule (9) yields

$$u_j^{n+1} = \lambda u_{j+1}^n + (1 - 2\lambda) u_j^n + \lambda u_{j-1}^n < \lambda M + (1 - 2\lambda) M + \lambda M = M.$$

Similarly, lower bounds will be respected. If  $\lambda > 1/2$  then you can find positive initial data that results in solutions that become negative a certain locations at certain later times, violating the maximum principle.

The condition  $\lambda \leq 1/2$  is a constraint on the size of the time step  $k$ :

$$\lambda = \frac{Dk}{h^2} \leq \frac{1}{2} \implies 2Dk \leq h^2.$$

That is, the time step must be short enough to resolve the diffusion time on one grid cell.