

Chapter 3

Basic partial differential equation models

This chapter extends the scaling technique to well-known partial differential equation (PDE) models for waves, diffusion, and transport. We start out with the simplest 1D models of the PDEs and then progress with additional terms, different types of boundary and initial conditions, and generalizations to 2D and 3D.

3.1 The wave equation

A standard, linear, one-dimensional wave equation problem in a homogeneous medium may be written as

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}, \quad x \in (0, L), \quad t \in (0, T], \quad (3.1)$$

where c is the constant wave velocity of the medium. With a briefer notation, where subscripts indicate derivatives, the PDE (3.1) can be written $u_{tt} = c^2 u_{xx}$. This subscript notation will occasionally be used later.

For any number of dimensions in heterogeneous media we have the generalization

$$\frac{\partial^2 u}{\partial t^2} = \nabla \cdot (c^2 \nabla u) + f, \quad x, y, z \in \Omega, \quad t \in (0, T], \quad (3.2)$$

where f represents a forcing.

3.1.1 Homogeneous Dirichlet conditions in 1D

Let us first start with (3.1), homogeneous Dirichlet conditions in space, and no initial velocity u_t :

$$u(x, 0) = I(x), \quad x \in [0, L], \quad (3.3)$$

$$\frac{\partial}{\partial t} u(x, 0) = 0, \quad x \in [0, L], \quad (3.4)$$

$$u(0, t) = 0, \quad t \in (0, T], \quad (3.5)$$

$$u(L, t) = 0, \quad t \in (0, T]. \quad (3.6)$$

The independent variables are x and t , while u is the dependent variable. The rest of the parameters, c , L , T , and $I(x)$, are given data.

We start with introducing dimensionless versions of the independent and dependent variables:

$$\bar{x} = \frac{x}{x_c}, \quad \bar{t} = \frac{t}{t_c}, \quad \bar{u} = \frac{u}{u_c}.$$

Inserting the $x = x_c \bar{x}$, etc., in (3.1) and (3.3)-(3.6) gives

$$\begin{aligned} \frac{\partial^2 \bar{u}}{\partial \bar{t}^2} &= \frac{t_c^2 c^2}{x_c^2} \frac{\partial^2 \bar{u}}{\partial x^2}, & \bar{x} &\in (0, L/x_c), \quad \bar{t} \in (0, T/t_c], \\ \bar{u}(\bar{x}, 0) &= \frac{I(x_c \bar{x})}{u_c}, & \bar{x} &\in [0, L/x_c], \\ \frac{\partial}{\partial \bar{t}} \bar{u}(\bar{x}, 0) &= 0, & \bar{x} &\in [0, L/x_c], \\ \bar{u}(0, \bar{t}) &= 0, & \bar{t} &\in (0, T/t_c], \\ \bar{u}(L/x_c, \bar{t}) &= 0, & \bar{t} &\in (0, T/t_c]. \end{aligned}$$

The key question is how to define the scales. A natural choice is $x_c = L$ since this makes $\bar{x} \in [0, 1]$. For the spatial scale and the problem governed by (3.1) we have some analytical insight that can help. The solution behaves like

$$u(x, t) = f_R(x - ct) + f_L(x + ct), \quad (3.7)$$

i.e., a right- and left-going wave with velocity c . The initial conditions constrain the choices of f_R and f_L to $f_L + f_R = I$ and $-cf'_L + cf'_R = 0$. The solution is $f_R = f_L = \frac{1}{2}I$, and consequently

$$u(x, t) = \frac{1}{2}I(x - ct) + \frac{1}{2}I(x + ct),$$

which tells that the initial condition splits in two, half of it moves to the left and half to the right. This means in particular that we can choose $u_c = \max_x |I(x)|$ and get $|\bar{u}| \leq 1$, which is a goal. It must be added that boundary conditions may result in reflected waves, and the solution is then more complicated than indicated in the formula above.

Regarding the time scale, we may look at the two terms in the scaled PDE and argue that if $|u|$ and its derivatives are to be of order unity, then the size of the second-order derivatives should be the same, and t_c can be chosen to make the coefficient $t_c^2 c^2 / x_c^2$ unity, i.e., $t_c = L/c$. Another reasoning may set t_c as the time it takes the wave to travel through the domain $[0, L]$. Since the wave has constant speed c , $t_c = L/c$.

With the described choices of scales, we end up with the dimensionless initial-boundary value problem

$$\frac{\partial^2 \bar{u}}{\partial \bar{t}^2} = \frac{\partial^2 \bar{u}}{\partial \bar{x}^2}, \quad \bar{x} \in (0, 1), \bar{t} \in (0, \bar{T}], \quad (3.8)$$

$$\bar{u}(\bar{x}, 0) = \frac{I(\bar{x}L)}{\max_{x \in (0, L)} |I(x)|}, \quad \bar{x} \in [0, 1], \quad (3.9)$$

$$\frac{\partial}{\partial \bar{t}} \bar{u}(\bar{x}, 0) = 0, \quad \bar{x} \in [0, 1], \quad (3.10)$$

$$\bar{u}(0, \bar{t}) = 0, \quad \bar{t} \in (0, \bar{T}], \quad (3.11)$$

$$\bar{u}(1, \bar{t}) = 0, \quad \bar{t} \in (0, \bar{T}]. \quad (3.12)$$

Here, $\bar{T} = Tc/L$.

The striking feature of (3.8)-(3.12) is that there are *no physical parameters* involved! Everything we need to specify is the shape of the initial condition and then scale it such that it is less than or equal to 1.

The physical solution with dimension is recovered from $\bar{u}(\bar{x}, \bar{t})$ through

$$u(x, t) = \max_{x \in (0, L)} I(x) \bar{u}(\bar{x}L, \bar{t}L/c) \quad (3.13)$$

3.1.2 Implementation of the scaled wave equation

How do we implement (3.8)-(3.12)? As for the simpler mathematical models, we suggest to implement the model with dimensions and observe how to set parameters to obtain the scaled model. In the present case, one must choose $L = 1$, $c = 1$, and scale I by its maximum value. That's all!

Several implementations of 1D wave equation models with different degree of mathematical and software complexity come along with these notes. The simplest version is `wave1D_u0.py` that implements (3.1) and (3.3)-(3.6). This is the code to be used in the following. It is described in Section 2.3 in [7].

Waves on a string. As an example, we may let the original initial-boundary value problem (3.1)-(3.6) model vibrations of a string on a string instrument (e.g., a guitar). With u as the displacement of the string, the boundary conditions $u = 0$ at the ends are relevant, as well as the zero velocity condition $\partial u / \partial t = 0$ at $t = 0$. The initial condition $I(x)$ typically has a triangular shape

for a picked guitar string. The physical problem needs parameters for the amplitude of $I(x)$, the length L of the string, and the value of c for the string. Only the latter is challenging as it involves relating c to the pitch (i.e., time frequency) of the string. In the scaled problem, we can forget about all this. We simply set $L = 1$, $c = 1$, and let $I(x)$ have a peak of unity at $x = x_0 \in (0, 1)$:

$$\frac{I(x)}{\max_x I(x)} = \begin{cases} x/x_0, & x < x_0, \\ (1-x)/(1-x_0), & \text{otherwise} \end{cases}$$

The dimensionless coordinate of the peak, x_0 , is the only dimensionless parameter in the problem. For fixed x_0 , one single simulation will capture all possible solutions with such an initial triangular shape.

Detecting an already computed case. The file `wave1D_u0_scaled.py` has functionality for detecting whether a simulation corresponds to a previously run scaled case, and if so, the solution is retrieved from file. The implementation technique makes use of `joblib`, but is more complicated than shown previously in these notes since some of the arguments to the function that computes the solution are functions, and one must recognized if the function has been used as argument before or not. There is documentation in the `wave1D_u0_scaled.py` file explaining how this is done.

3.1.3 Time-dependent Dirichlet condition

A generalization of (3.1)-(3.6) is to allow for a time-dependent Dirichlet condition at one end, say $u(0, t) = U_L(t)$. At the other end we may still have $u = 0$. This new condition at $x = 0$ may model a specified wave that enters the domain. For example, if we feed in a monochromatic wave $A \sin(k(x - ct))$ from the left end, $U_L(t) = A \sin(kct)$. This forcing of the wave motion has its own amplitude and time scale that could affect the choice of u_c and t_c .

The main difference from the previous initial-boundary value problem is the condition at $x = 0$, which now reads

$$\bar{u}(0, \bar{t}) = \frac{U_L(\bar{t}t_c)}{u_c}$$

in scaled form.

Scaling. Regarding the characteristic time scale, it is natural to base this scale on the wave propagation velocity, together with the length scale, and not on the time scale of $U_L(t)$, because the time scale of U_L basically determines whether short or long waves are fed in at the boundary. All waves, long or short, propagate with the same velocity c . We therefore continue to use $t_c = L/c$.

The solution u will have one wave contribution from the initial condition I and one from the feeding of waves at $x = 0$. This gives us three choices of u_c :

$\max_x |I| + \max_t |U_L|$, $\max_x |I|$, or $\max_t |U_L|$. The first seems relevant if the size of I and U_L are about the same, but then we can choose either $\max_x |I|$ or $\max_t |U_L|$ as characteristic size of u since a factor of 2 is not important. If I is much less than U_L , $u_c = \max_t |u_L|$ is relevant, while $u_c = \max_x |I|$ is the choice when I has much bigger impact than U_L on u .

With $u_c = \max_t |U_L(t)|$, we get the scaled problem

$$\frac{\partial^2 \bar{u}}{\partial \bar{t}^2} = \frac{\partial^2 \bar{u}}{\partial \bar{x}^2}, \quad \bar{x} \in (0, 1), \bar{t} \in (0, \bar{T}], \quad (3.14)$$

$$\bar{u}(\bar{x}, 0) = \frac{I(x_c \bar{x})}{\max_t |U_L(t)|}, \quad \bar{x} \in [0, 1], \quad (3.15)$$

$$\frac{\partial}{\partial \bar{t}} \bar{u}(\bar{x}, 0) = 0, \quad \bar{x} \in [0, 1], \quad (3.16)$$

$$\bar{u}(0, \bar{t}) = \frac{U_L(\bar{t} t_c)}{\max_t |U_L(t)|}, \quad \bar{t} \in (0, \bar{T}], \quad (3.17)$$

$$\bar{u}(1, \bar{t}) = 0, \quad \bar{t} \in (0, \bar{T}]. \quad (3.18)$$

Also this problem is free of physical parameters like c and L . The input is completely specified by the shape of $I(x)$ and $U_L(t)$.

Software. Software for the original problem with dimensions can be reused for (3.14)-(3.18) by setting $L = 1$, $c = 1$, and scaling $U_L(t)$ and $I(x)$ by $\max_t |U_L(t)|$.

Specific case. As an example, consider

$$U_L(t) = a \sin(\omega t) \text{ for } 0 \leq t \leq 2 \frac{\omega}{2\pi}, \text{ else } 0,$$

$$I(x) = A e^{-(x-L/2)^2/\sigma^2}.$$

That is, we start with a Gaussian peak-shaped wave in the center of the domain and feed in a sinusoidal wave at the left end for two periods. The solution will be the sum of three waves: two parts from the initial condition, plus the wave fed in from the left.

Since $\max_t |U_L| = a$ we get

$$\bar{u}(\bar{x}, 0) = \frac{A}{a} e^{-(L/\sigma)^2 (\bar{x} - \frac{1}{2})^2}, \quad (3.19)$$

$$\bar{u}(0, \bar{t}) = \sin(\bar{t} \omega L/c). \quad (3.20)$$

Here, U_L models an incoming wave $a \sin(k(x-ct))$, with k specified. The result is incoming waves of length $\lambda = 2\pi/k$. Since $\omega = kc$, $\bar{u}(0, \bar{t}) = \sin(kL\bar{t}) = \sin(2\pi\bar{t}L/\lambda)$. (This formula demonstrates the previous assertion that the time scale of U_L , i.e., $1/\omega$, determines the wave length $1/\omega = \lambda/(2\pi)$ in space.) We

realize from the formulas (3.19) and (3.20) that there are three key dimensionless parameters related to these specific choices of initial and boundary conditions:

$$\alpha = \frac{A}{a}, \quad \beta = \frac{L}{\sigma}, \quad \gamma = kL = 2\pi \frac{L}{\lambda}.$$

With α , β , and γ we can write the dimensionless initial and boundary conditions as

$$\begin{aligned} \bar{u}(\bar{x}, 0) &= \alpha e^{-\beta^2(\bar{x}-\frac{1}{2})^2}, \\ \bar{u}(0, \bar{t}) &= \sin(\gamma \bar{t}). \end{aligned}$$

The dimensionless parameters have the following interpretations:

- α : ratio of initial condition amplitude and amplitude of incoming wave at $x = 0$
- β : ratio of length of domain and width of initial condition
- γ : ratio of length of domain and wave length of incoming wave

Again, these dimensionless parameters tell a lot about the interplay of the physical effects in the problem. And only some ratios count!

We can simulate two special cases:

1. $\alpha = 10$ (large) where the incoming wave is small and the solution is dominated by the two waves arising from $I(x)$,
2. $\alpha = 0.1$ (small) where the incoming waves dominate and the solution has the initial condition just as a small perturbation of the wave shape.

We may choose a peak-shaped initial condition: $\beta = 10$, and also a relatively short incoming wave compared to the domain size: $\gamma = 6\pi$ (i.e., wave length of incoming wave is $L/6$). A function `simulate_Gaussian_and_incoming_wave` in the file `session.py` applies the general unscaled solver in `wave1D_dn.py` for solving the wave equation with constant c , and any time-dependent function or $\partial u / \partial x = 0$ at the end points. This solver is trivially adapted to the present case. Figures 3.1 and 3.2 shows snapshots of how $\bar{u}(\bar{x}, \bar{t})$ evolves due to a large/small initial condition and small/large incoming wave at the left boundary.

Movie 1: $\alpha = 10$. https://github.com/hplgit/scaling-book/raw/master/doc/pub/book/html/mov-scaling/gaussian_plus_incoming/alpha10.mp4

Movie 2: $\alpha = 0.1$. https://github.com/hplgit/scaling-book/raw/master/doc/pub/book/html/mov-scaling/gaussian_plus_incoming/alpha01.mp4

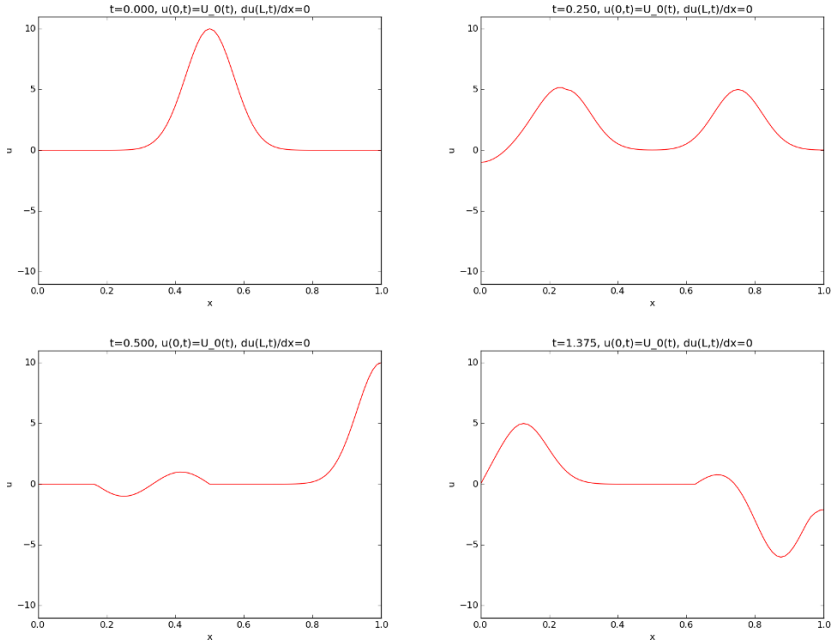


Fig. 3.1 Snapshots of solution with large initial condition and small incoming wave ($\alpha = 10$).

3.1.4 Velocity initial condition

Now we change the initial condition from $u = I$ and $\partial u / \partial t = 0$ to

$$u(x, 0) = 0, \tag{3.21}$$

$$\frac{\partial}{\partial t} u(x, 0) = V(x). \tag{3.22}$$

Impact problems are often of this kind. The scaled version of $u_t(x, 0) = V(x)$ becomes

$$\frac{\partial}{\partial \bar{t}} \bar{u}(\bar{x}, 0) = \frac{t_c}{u_c} V(\bar{x}x_c).$$

Analytical insight. From (3.7) we now get $f_L + f_R = 0$ and $cf'_L - cf'_R = V$. Introducing $W(x)$ such that $W'(x) = V(x)$, a solution is $f_L = \frac{1}{2}W/c$ and $-f_R = \frac{1}{2}W/c$. We can express this solution through the formula

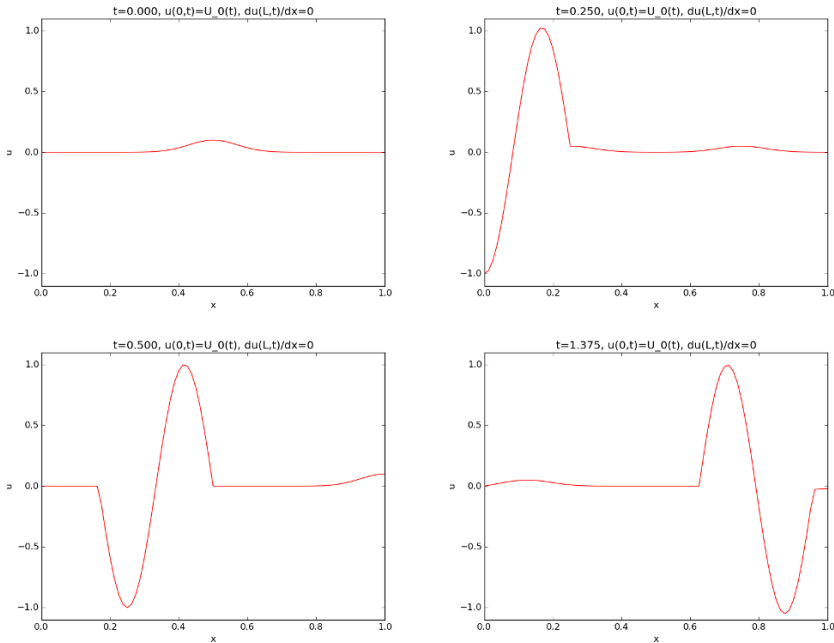


Fig. 3.2 Snapshots of solution with small initial condition and large incoming wave ($\alpha = 0.1$).

$$u(x,t) = \frac{1}{2c} \int_{x-ct}^{x+ct} V(\xi) d\xi = \frac{1}{2c} (W(x+ct) - W(x-ct)). \quad (3.23)$$

Scaling. Since V is the time-derivative of u , the characteristic size of V , call it V_c , is typically u_c/t_c . If we, as usual, base t_c on the wave speed, $t_c = L/c$, we get $u_c = V_c L/c$. Looking at the solution (3.23), we see that u_c has size $\text{mean}(V)L/(2c)$, where $\text{mean}(V)$ is the mean value of V ($W \sim \text{mean}(V)L$). This result suggests $V_c = \text{mean}(V)$ and $u_c = \text{mean}(V)L/(2c)$. One may argue that the factor 2 is not important, but if we want $|\bar{u}| \in [0, 1]$ it is convenient to keep it.

The scaled initial condition becomes

$$\frac{\partial}{\partial t} \bar{u}(\bar{x}, 0) = \frac{t_c}{u_c} V(\bar{x}x_c) = \frac{V(\bar{x}x_c)}{\frac{1}{2} \text{mean}(V)}.$$

Nonzero initial shape. Suppose we change the initial condition $u(x, 0) = 0$ to $u(x, 0) = I(x)$. The scaled version of this condition with the above u_c based on V becomes

$$\bar{u}(\bar{x}, 0) = \frac{2cI(\bar{x}x_c)}{L \text{mean}(V)}. \quad (3.24)$$

Check that dimensionless numbers are dimensionless!

Is a dimensionless number really dimensionless? It is easy to make errors when scaling equations, so checking that such fractions are dimensionless is wise. The dimension of I is the same as u , here taken to be displacement: $[L]$. Since V is $\partial u/\partial t$, its dimension is $[LT^{-1}]$. The dimensions of c and L are $[LT^{-1}]$ and $[L]$. The dimension of the right-hand side of (3.24) is then

$$\frac{[LT^{-1}][L]}{[L][LT^{-1}]} = 1,$$

demonstrating that the fraction is indeed dimensionless.

One may introduce a dimensionless initial shape, $\bar{I}(\bar{x}) = I(\bar{x}L)/\max_x |I|$. Then

$$\bar{u}(\bar{x}, 0) = \alpha \bar{I}(\bar{x}),$$

where α the dimensionless number

$$\alpha = \frac{2c \max_x |I(x)|}{L \text{ mean}(V)}.$$

If V is much larger than I , one expects that the influence of I is small. However, it takes time for the initial velocity V to influence the wave motion, so the speed of the waves c and the length of the domain L also play a role. This is reflected in α , which is the important parameter. Again, the scaling and the resulting dimensionless parameter(s) teach us much about the interaction of the various physical effects.

3.1.5 Variable wave velocity and forcing

The next generalization regards wave propagation in a non-homogeneous medium where the wave velocity c depends on the spatial position: $c = c(x)$. To simplify the notation we introduce $\lambda(x) = c^2(x)$. We introduce homogeneous Neumann conditions at $x = 0$ and $x = L$. In addition, we add a force term $f(x, t)$ to the PDE, modeling wave generation in the interior of the domain. For example, a moving slide at the bottom of a fjord will generate surface waves and is modeled by such an $f(x, t)$ term (provided the length of the waves is much larger than the depth so that a simple wave equation like (3.25) applies). The initial-boundary value problem can be then expressed as

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x} \left(\lambda(x) \frac{\partial u}{\partial x} \right) + f(x, t), \quad x \in (0, L), \quad t \in (0, T], \quad (3.25)$$

$$u(x, 0) = I(x), \quad x \in [0, L], \quad (3.26)$$

$$\frac{\partial}{\partial t} u(x, 0) = 0, \quad x \in [0, L], \quad (3.27)$$

$$\frac{\partial}{\partial x} u(0, t) = 0, \quad t \in (0, T], \quad (3.28)$$

$$\frac{\partial}{\partial x} u(L, t) = 0, \quad t \in (0, T]. \quad (3.29)$$

Non-dimensionalization. We make the coefficient λ non-dimensional by

$$\bar{\lambda}(\bar{x}) = \frac{\lambda(\bar{x}x_c)}{\lambda_c}, \quad (3.30)$$

where one normally chooses the characteristic size of λ , λ_c , to be the maximum value such that $|\lambda| \leq 1$:

$$\lambda_c = \max_{x \in (0, L)} \lambda(x).$$

Similarly, f has a scaled version

$$\bar{f}(\bar{x}, \bar{t}) = \frac{f(\bar{x}x_c, \bar{t}t_c)}{f_c},$$

where normally we choose

$$f_c = \max_{x, t} |f(x, t)|.$$

Inserting dependent and independent variables expressed by their non-dimensional counterparts yields

$$\frac{\partial^2 \bar{u}}{\partial \bar{t}^2} = \frac{t_c^2 \lambda_c}{L^2} \frac{\partial}{\partial \bar{x}} \left(\bar{\lambda}(\bar{x}) \frac{\partial \bar{u}}{\partial \bar{x}} \right) + \frac{t_c^2 f_c}{u_c} \bar{f}(\bar{x}, \bar{t}), \quad \bar{x} \in (0, 1), \quad \bar{t} \in (0, \bar{T}],$$

$$\bar{u}(\bar{x}, 0) = \frac{I(x)}{u_c}, \quad \bar{x} \in [0, 1],$$

$$\frac{\partial}{\partial \bar{t}} \bar{u}(\bar{x}, 0) = 0, \quad \bar{x} \in [0, 1],$$

$$\frac{\partial}{\partial \bar{x}} \bar{u}(0, \bar{t}) = 0, \quad \bar{t} \in (0, \bar{T}],$$

$$\frac{\partial}{\partial \bar{x}} \bar{u}(1, \bar{t}) = 0, \quad \bar{t} \in (0, \bar{T}],$$

with $\bar{T} = Tc/L$.

Choosing the time scale. The time scale is, as before, chosen as $t_c = L/\sqrt{\lambda_c}$. Note that the previous (constant) wave velocity c now corresponds to $\sqrt{\lambda(x)}$. Therefore, $\sqrt{\lambda_c}$ is a characteristic wave velocity.

One could wonder if the time scale of the force term, $f(x, t)$, should influence t_c , but as we reasoned for the boundary condition $u(0, t) = U_L(t)$, we let the characteristic time be governed by the signal speed in the medium, i.e., by $\sqrt{\lambda_c}$ here and not by the time scale of the excitation f , which dictates the length of the generated waves and not their propagation speed.

Choosing the spatial scale. We may choose u_c as $\max_x |I(x)|$, as before, or we may fit u_c such that the coefficient in the source term is unity, i.e., all terms balance each other. This latter idea leads to

$$u_c = \frac{L^2 f_c}{\lambda_c}$$

and a PDE without parameters,

$$\frac{\partial^2 \bar{u}}{\partial \bar{t}^2} = \frac{\partial}{\partial \bar{x}} \left(\bar{\lambda}(\bar{x}) \frac{\partial \bar{u}}{\partial \bar{x}} \right) + \bar{f}(\bar{x}, \bar{t}).$$

The initial condition $u(x, 0) = I(x)$ becomes in dimensionless form

$$\bar{u}(\bar{x}, 0) = u_c^{-1} \max_x |I(x)| \bar{I}(\bar{x}) = \beta^{-1} \bar{I}(\bar{x}),$$

where

$$\beta = \frac{L^2 \max_{x,t} |f(x, t)|}{\lambda_c \max_x |I(x)|}.$$

In the case $u_c = \max_x |I(x)|$, $\bar{u}(\bar{x}, 0) = \bar{I}(\bar{x})$ and the β parameter appears in the PDE instead:

$$\frac{\partial^2 \bar{u}}{\partial \bar{t}^2} = \frac{\partial}{\partial \bar{x}} \left(\bar{\lambda}(\bar{x}) \frac{\partial \bar{u}}{\partial \bar{x}} \right) + \beta \bar{f}(\bar{x}, \bar{t}).$$

With $V = 0$, and $u = 0$ or $u_x = 0$ on the boundaries $x = 0, L$, this scaling normally gives $|\bar{u}| \leq 1$, since initially $|I| \leq 1$, and no boundary condition can increase the amplitude. However, the forcing, \bar{f} , may inherit spatial and temporal scales of its own that may complicate the matter. The forcing may, for instance, be some disturbance moving with a velocity close to the propagation velocity of the free waves. This will have an effect akin to the resonance for the vibration problem discussed in section 2.2.2 and the waves produced by the forcing may be much larger than indicated by β . On the other hand, the forcing may also consist of alternating positive and negative parts (retrogressive slides constitute an example). These may interfere to reduce the wave generation by an order of magnitude.

Scaling the velocity initial condition. The initial condition $u_t(x, 0) = V(x)$ has its dimensionless variant as

$$\bar{V}(\bar{x}) = \frac{t_c}{u_c} \frac{V(L\bar{x})}{\max_x |V(x)|},$$

which becomes

$$\frac{\partial \bar{u}}{\partial \bar{t}}(\bar{x}, 0) = \frac{L}{\sqrt{\lambda_c}} \frac{\max_x |V(x)|}{\max_x |I(x)|} \bar{V}(\bar{x}), \text{ if } u_c = \max_x |I(x)|,$$

or

$$\frac{\partial \bar{u}}{\partial \bar{t}}(\bar{x}, 0) = \frac{\sqrt{\lambda_c}}{L} \frac{\max_x |V(x)|}{\max_{x,t} |f(x,t)|} \bar{V}(\bar{x}), \text{ if } u_c = t_c^2 f_c = \frac{L^2}{\lambda_c} \max_{x,t} |f(x,t)|.$$

Introducing the dimensionless number α (cf. Section 3.1.4),

$$\alpha^{-1} = \frac{\sqrt{\lambda_c}}{L} \frac{\max_x |V(x)|}{\max_{x,t} |f(x,t)|},$$

we can write

$$\frac{\partial \bar{u}}{\partial \bar{t}}(\bar{x}, 0) = \begin{cases} \alpha^{-1} \bar{V}(\bar{x}), & u_c = \max_x |I| \\ \alpha^{-1} \beta^{-1} \bar{V}(\bar{x}), & u_c = t_c^2 f_c \end{cases}$$

3.1.6 Damped wave equation

A linear damping term $b \partial u / \partial t$ is often added to the wave equation to model energy dissipation and amplitude reduction. Our PDE then reads

$$\frac{\partial^2 u}{\partial t^2} + b \frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left(\lambda(x) \frac{\partial u}{\partial x} \right) + f(x, t). \quad (3.31)$$

The scaled equation becomes

$$\frac{\partial^2 \bar{u}}{\partial \bar{t}^2} + \frac{t_c}{b} \frac{\partial \bar{u}}{\partial \bar{t}} = \frac{t_c^2 \lambda_c}{L^2} \frac{\partial}{\partial \bar{x}} \left(\bar{\lambda}(\bar{x}) \frac{\partial \bar{u}}{\partial \bar{x}} \right) + \frac{t_c^2 f_c}{u_c} \bar{f}(\bar{x}, \bar{t}).$$

The damping term is usually much smaller than the two other terms involving \bar{u} . The time scale is therefore chosen as in the undamped case, $t_c = L/\sqrt{\lambda_c}$. As in Section 3.1.5, we have two choices of u_c : $u_c = \max_x |I|$ or $u_c = t_c^2 f_c$. The former choice of u_c gives a PDE with two dimensionless numbers,

$$\frac{\partial^2 \bar{u}}{\partial \bar{t}^2} + \gamma \frac{\partial \bar{u}}{\partial \bar{t}} = \frac{\partial}{\partial \bar{x}} \left(\bar{\lambda}(\bar{x}) \frac{\partial \bar{u}}{\partial \bar{x}} \right) + \beta \bar{f}(\bar{x}, \bar{t}), \quad (3.32)$$

where

$$\gamma = \frac{bL}{\sqrt{\lambda_c}},$$

measures the size of the damping, and β is as given in Section 3.1.5. With $u_c = t_c^2 f_c$ we get a PDE where only γ enters,

$$\frac{\partial^2 \bar{u}}{\partial \bar{t}^2} + \gamma \frac{\partial \bar{u}}{\partial \bar{t}} = \frac{\partial}{\partial \bar{x}} \left(\bar{\lambda}(\bar{x}) \frac{\partial \bar{u}}{\partial \bar{x}} \right) + \bar{f}(\bar{x}, \bar{t}). \quad (3.33)$$

The scaled initial conditions are as in Section 3.1.5, so in this latter case β appears in the initial condition for u .

To summarize, the effects of V , f , and damping are reflected in the dimensionless numbers α , β , and γ , respectively.

3.1.7 A three-dimensional wave equation problem

To demonstrate how the scaling extends to in three spatial dimensions, we consider

$$\frac{\partial^2 \bar{u}}{\partial \bar{t}^2} = \frac{\partial}{\partial \bar{x}} \left(\lambda \frac{\partial u}{\partial \bar{x}} \right) + \frac{\partial}{\partial \bar{y}} \left(\lambda \frac{\partial u}{\partial \bar{y}} \right) + \frac{\partial}{\partial \bar{z}} \left(\lambda \frac{\partial u}{\partial \bar{z}} \right). \quad (3.34)$$

Introducing

$$\bar{x} = \frac{x}{x_c}, \quad \bar{y} = \frac{y}{y_c}, \quad \bar{z} = \frac{z}{z_c}, \quad \bar{t} = \frac{t}{t_c}, \quad \bar{u} = \frac{u}{u_c},$$

and scaling λ as $\bar{\lambda} = \lambda(\bar{x}x_c, \bar{y}y_c, \bar{z}z_c)/\lambda_c$, we get

$$\frac{\partial^2 \bar{u}}{\partial \bar{t}^2} = \frac{t_c^2 \lambda_c}{x_c^2} \frac{\partial}{\partial \bar{x}} \left(\bar{\lambda} \frac{\partial \bar{u}}{\partial \bar{x}} \right) + \frac{t_c^2 \lambda_c}{y_c^2} \frac{\partial}{\partial \bar{y}} \left(\bar{\lambda} \frac{\partial \bar{u}}{\partial \bar{y}} \right) + \frac{t_c^2 \lambda_c}{z_c^2} \frac{\partial}{\partial \bar{z}} \left(\bar{\lambda} \frac{\partial \bar{u}}{\partial \bar{z}} \right).$$

Often, we will set $x_c = y_c = z_c = L$ where L is some characteristic size of the domain. As before, $t_c = L/\sqrt{\lambda_c}$, and these choices lead to a dimensionless wave equation without physical parameters:

$$\frac{\partial^2 \bar{u}}{\partial \bar{t}^2} = \frac{\partial}{\partial \bar{x}} \left(\bar{\lambda} \frac{\partial \bar{u}}{\partial \bar{x}} \right) + \frac{\partial}{\partial \bar{y}} \left(\bar{\lambda} \frac{\partial \bar{u}}{\partial \bar{y}} \right) + \frac{\partial}{\partial \bar{z}} \left(\bar{\lambda} \frac{\partial \bar{u}}{\partial \bar{z}} \right). \quad (3.35)$$

The initial conditions remain the same as in the previous one-dimensional examples.

3.2 The diffusion equation

The diffusion equation in a one-dimensional homogeneous medium reads

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}, \quad x \in (0, L), \quad t \in (0, T], \quad (3.36)$$

where α is the diffusion coefficient. The multi-dimensional generalization to a heterogeneous medium and a source term takes the form

$$\frac{\partial u}{\partial t} = \nabla \cdot (\alpha \nabla u) + f, \quad x, y, z \in \Omega, \quad t \in (0, T]. \quad (3.37)$$

We first look at scaling of the PDE itself, and thereafter we discuss some types of boundary conditions and how to scale the complete initial-boundary value problem.

3.2.1 Homogeneous 1D diffusion equation

Choosing the time scale. To make (3.36) dimensionless, we introduce, as usual, dimensionless dependent and independent variables:

$$\bar{x} = \frac{x}{x_c}, \quad \bar{t} = \frac{t}{t_c}, \quad \bar{u} = \frac{u}{u_c}.$$

Inserting the dimensionless quantities in the one-dimensional PDE (3.36) results in

$$\frac{\partial \bar{u}}{\partial \bar{t}} = \frac{t_c \alpha}{L^2} \frac{\partial^2 \bar{u}}{\partial \bar{x}^2}, \quad \bar{x} \in (0, 1), \quad \bar{t} \in (0, \bar{T} = T/t_c].$$

Arguing, as for the wave equation, that the scaling should result in

$$\frac{\partial \bar{u}}{\partial \bar{t}} \text{ and } \frac{\partial^2 \bar{u}}{\partial \bar{x}^2}$$

of the same size (about unity), implies $t_c \alpha / L^2 = 1$ and therefore $t_c = L^2 / \alpha$.

Analytical insight. The best way to obtain the scales inherent in a problem is to obtain an exact analytic solution, as we have done in many of the ODE examples in this booklet. However, as a rule this is not possible. Still, often highly simplified analytic solutions can be found for parts of the problem, or for some closely related problem. Such solutions may provide crucial guidance to the nature of the complete solution and to the appropriate scaling of the full problem. We will employ such solutions now to learn about scales in diffusion problems.

One can show that $u = Ae^{-pt} \sin(kx)$ is a solution of (3.36) if $p = \alpha k^2$, for any k . This is the typical solution arising from separation of variables and reflects the dynamics of the space and time in the PDE. Exponential decay in time is a characteristic feature of diffusion processes, and the e-folding time can then be taken as a time scale. This means $t_c = 1/p \sim k^{-2}$. Since k

is related to the spatial wave length λ through $k = 2\pi/\lambda$, it means that t_c depends strongly on the wave length of the sine term $\sin(kx)$. In particular, short waves (as found in noisy signals) with large k decay very rapidly. For the overall solution we are interested in how the longest meaningful wave decays and use that time scale for t_c . The longest wave typically has half a wave length over the domain $[0, L]$: $u = Ae^{-pt} \sin(\pi x/L)$ ($k = \pi/L$), provided $u(0, t) = u(L, t) = 0$ (with $u_x(L, t) = 0$, the longest wave is $L/4$, but we look at the case with the wave length $L/2$). Then $t_c = L^2/\alpha\pi^{-2}$, but the factor π^{-2} is not important and we simply choose $t_c = L^2/\alpha$, which equals the time scale we arrived at above. We may say that t_c is the time it takes for the diffusion to significantly change the solution in the entire domain.

Another fundamental solution of the diffusion equation is the diffusion of a Gaussian function: $u(x, t) = K(4\pi\alpha t)^{-1/2} \exp(-x^2/(4\alpha t))$, for some constant K with the same dimension as u . For the diffusion to be significant at a distance $x = L$, we may demand the exponential factor to have a value of $e^{-1} \approx 0.37$, which implies $t = L^2/(4\alpha)$, but the factor 4 is not of importance, so again, a relevant time scale is $t_c = L^2/\alpha$.

Choosing other scales. The scale u_c is chosen according to the initial condition: $u_c = \max_{x \in (0, L)} |I(x)|$. For a diffusion equation $u_t = \alpha u_{xx}$ with $u = 0$ at the boundaries $x = 0, L$, the solution is bounded by the initial condition $I(x)$. Therefore, the listed choice of u_c implies that $|u| \leq 1$. (The solution $u = Ae^{-pt} \sin(kx)$ is such an example if $k = n\pi/L$ for integer n such that $u = 0$ for $x = 0$ and $x = L$.)

The resulting dimensionless PDE becomes

$$\frac{\partial \bar{u}}{\partial \bar{t}} = \frac{\partial^2 \bar{u}}{\partial \bar{x}^2}, \quad \bar{x} \in (0, 1), \quad \bar{t} \in (0, \bar{T}], \quad (3.38)$$

with initial condition

$$\bar{u}(\bar{x}, 0) = \bar{I}(\bar{x}) = \frac{I(x_c \bar{x})}{\max_x |I(x)|}.$$

Notice that (3.38) is without physical parameters, but there may be parameters in $I(x)$.

3.2.2 Generalized diffusion PDE

Turning the attention to (3.37), we introduce the dimensionless diffusion coefficient

$$\bar{\alpha}(\bar{x}, \bar{y}, \bar{z}) = \alpha_c^{-1} \alpha(x_c \bar{x}, y_c \bar{y}, z_c \bar{z}),$$

typically with

$$\alpha_c = \max_{x,y,z} \alpha(x, y, z).$$

The length scales are

$$\bar{x} = \frac{x}{x_c}, \quad \bar{y} = \frac{y}{y_c}, \quad \bar{z} = \frac{z}{z_c}.$$

We scale f in a similar fashion:

$$\bar{f}(\bar{x}, \bar{y}, \bar{z}, \bar{t}) = f_c^{-1} f(\bar{x}x_c, \bar{y}y_c, \bar{z}z_c, \bar{t}t_c),$$

with

$$f_c = \max_{x,y,z,t} |f(x, y, z, t)|.$$

Also assuming that $x_c = y_c = z_c = L$, and $u_c = \max_{x,y,z} (I(x, y, z))$, we end up with the scaled PDE

$$\frac{\partial \bar{u}}{\partial \bar{t}} = \bar{\nabla} \cdot (\bar{\alpha} \bar{\nabla} \bar{u}) + \beta \bar{f}, \quad \bar{x}, \bar{y}, \bar{z} \in \bar{\Omega}, \quad \bar{t} \in (0, \bar{T}]. \quad (3.39)$$

Here, $\bar{\nabla}$ means differentiation with respect to dimensionless coordinates \bar{x} , \bar{y} , and \bar{z} . The dimensionless parameter β takes the form

$$\beta = \frac{t_c f_c}{u_c} = \frac{L^2 \max_{x,y,z,t} |f(x, y, z, t)|}{\alpha \max_{x,y,z} |I(x, y, z)|}.$$

The scaled initial condition is $\bar{u} = \bar{I}$ as in the 1D case.

An alternative choice of u_c is to make the coefficient $t_c f_c / u_c$ in the source term unity. The scaled PDE now becomes

$$\frac{\partial \bar{u}}{\partial \bar{t}} = \bar{\nabla} \cdot (\bar{\alpha} \bar{\nabla} \bar{u}) + f, \quad (3.40)$$

but the initial condition features the β parameter:

$$\bar{u}(\bar{x}, \bar{y}, \bar{z}, 0) = \frac{I}{t_c f_c} = \beta^{-1} \bar{I}(\bar{x}, \bar{y}, \bar{z}).$$

The β parameter can be interpreted as the ratio of the source term and the terms with u :

$$\beta = \frac{f_c}{u_c/t_c} \sim \frac{|f|}{|u_t|}, \quad \beta = \frac{f_c}{u_c/t_c} = \frac{f_c}{L^2/t_c u_c/L^2} \sim \frac{|f_c|}{|\alpha \nabla^2 u|}.$$

We may check that β is really non-dimensional. From the PDE, f must have the same dimensions as $\partial u / \partial t$, i.e., $[\Theta T^{-1}]$. The dimension of α is more intricate, but from the term αu_{xx} we know that u_{xx} has dimensions $[\Theta L^{-2}]$, and then α must have dimension $[L^2 T^{-1}]$ to match the target $[\Theta T^{-1}]$. In the expression for β we get $[L^2 \Theta T^{-1} (L^2 T^{-1} \Theta)^{-1}]$, which equals 1 as it should.

3.2.3 Jump boundary condition

A classical one-dimensional heat conduction problem goes as follows. An insulated rod at some constant temperature U_0 is suddenly heated from one end ($x = 0$), modeled as a constant Dirichlet condition $u(0, t) = U_1 \neq U_0$ at that end. That is, the boundary temperature jumps from U_0 to U_1 at $t = 0$. All the other surfaces of the rod are insulated such that a one-dimensional model is appropriate, but we must explicitly demand $u_x(L, t) = 0$ to incorporate the insulation condition in the one-dimensional model at the end of the domain $x = L$. Heat cannot escape, and since we supply heat at $x = 0$, all of the material will eventually be warmed up to the temperature U_1 : $u \rightarrow U_1$ as $t \rightarrow \infty$.

The initial-boundary value problem reads

$$\rho c \frac{\partial u}{\partial t} = k \frac{\partial^2 u}{\partial x^2}, \quad x \in (0, L), \quad t \in (0, T], \quad (3.41)$$

$$u(x, 0) = U_0, \quad x \in [0, L], \quad (3.42)$$

$$u(0, t) = U_1, \quad t \in (0, T], \quad (3.43)$$

$$\frac{\partial}{\partial x} u(L, t) = 0, \quad t \in (0, T]. \quad (3.44)$$

The PDE (3.41) arises from the energy equation in solids and involves three physical parameters: the density ρ , the specific heat capacity parameter c , and the heat conduction coefficient (from Fourier's law). Dividing by ρc and introducing $\alpha = k/(\rho c)$ brings (3.41) on the standard form (3.36). We just use the α parameter in the following.

The natural dimensionless temperature for this problem is

$$\bar{u} = \frac{u - U_0}{U_1 - U_0},$$

since this choice makes $\bar{u} \in [0, 1]$. The reason is that u is bounded by the initial and boundary conditions (in the absence of a source term in the PDE), and we have $\bar{u}(\bar{x}, 0) = 0$, $\bar{u}(\bar{x}, \infty) = 1$, and $\bar{u}(0, \bar{t}) = 1$.

The choice of t_c is as in the previous cases. We arrive at the dimensionless initial-boundary value problem

$$\frac{\partial \bar{u}}{\partial \bar{t}} = \frac{\partial^2 \bar{u}}{\partial \bar{x}^2}, \quad \bar{x} \in (0, 1), \quad \bar{t} \in (0, \bar{T}], \quad (3.45)$$

$$\bar{u}(\bar{x}, 0) = 0, \quad \bar{x} \in [0, 1], \quad (3.46)$$

$$\bar{u}(0, \bar{t}) = 1, \quad \bar{t} \in (0, \bar{T}], \quad (3.47)$$

$$\frac{\partial}{\partial \bar{x}} \bar{u}(1, \bar{t}) = 0, \quad \bar{t} \in (0, \bar{T}]. \quad (3.48)$$

The striking feature is that there are no physical parameters left in this problem. One simulation can be carried out for $\bar{u}(\bar{x}, \bar{t})$, see Figure 3.3, and the temperature in a rod of any material and any constant initial and boundary temperature can be retrieved by

$$u(x, t) = U_0 + (U_1 - U_0)\bar{u}(x/L, t\alpha/L^2).$$

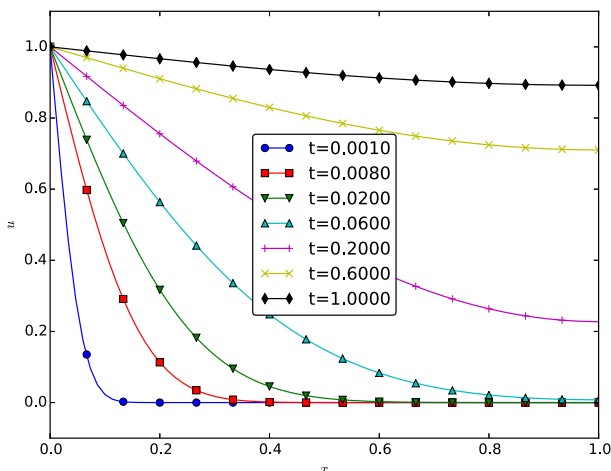


Fig. 3.3 Scaled temperature in an isolated rod suddenly heated from the end.

3.2.4 Oscillating Dirichlet condition

Now we address a heat equation problem where the temperature is oscillating on the boundary $x = 0$:

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}, \quad x \in (0, L), \quad t \in (0, T], \quad (3.49)$$

$$u(x, 0) = U_0, \quad x \in [0, L], \quad (3.50)$$

$$u(0, t) = U_0 + A \sin(\omega t), \quad t \in (0, T], \quad (3.51)$$

$$\frac{\partial}{\partial x} u(L, t) = 0, \quad t \in (0, T]. \quad (3.52)$$

One important physical application is temperature oscillations in the ground, either day and night variations at a short temporal and spatial scale, or seasonal variations in the Earth's crust. An important modeling assumption is (3.52), which means that the boundary $x = L$ is placed sufficiently far from $x = 0$ such that the solution is much damped and basically constant so $u_x = 0$ is a reasonable condition.

Scaling issues. Since the boundary temperature is oscillating around the initial condition, we expect $u \in [U_0 - A, U_0 + A]$. The dimensionless temperature is therefore taken as

$$\bar{u} = \frac{u - U_0}{A},$$

such that $\bar{u} \in [-1, 1]$.

What is an appropriate time scale? There will be two time scales involved, the oscillations $\sin(\omega t)$ with period $P = 2\pi/\omega$ at the boundary and the “speed of diffusion”, or more specifically the “speed of heat conduction” in the present context, where $t_c = x_c^2/\alpha$ is the appropriate scale, x_c being the length scale. Choosing the right length scale is not obvious. As we shall see, the standard choice $x_c = L$ is not a good candidate, but to understand why, we need to examine the solution, either through simulations or through a closed-form formula. We are so lucky in this relatively simple pedagogical problem that one can find an exact solution of a related problem.

Exact solution. As usual, investigating the exact solution of the model problem can illuminate the involved scales. For this particular initial-boundary value problem the exact solution as $t \rightarrow \infty$ (such that the initial condition $u(x, 0) = U_0$ is forgotten) and $L \rightarrow \infty$ (such that (3.52) is certainly valid) can be shown to be

$$u(x, t) = U_0 - Ae^{-bx} \sin(bx - \omega t), \quad b = \sqrt{\frac{\omega}{2\alpha}}. \quad (3.53)$$

This solution is of the form $e^{-bx}g(x - ct)$, i.e., a damped wave that moves to the right with velocity c and a damped amplitude e^{-bx} . This is perhaps more easily seen if we make a rewrite

$$u(x, t) = U_0 - Ae^{-bx} \sin(b(x - ct)), \quad c = \omega/b = \sqrt{2\alpha\omega}, \quad b = \sqrt{\frac{\omega}{2\alpha}}.$$

Time and length scales. The boundary oscillations lead to the time scale $t_c = 1/\omega$. The speed of the wave suggests another time scale: the time it takes to propagate through the domain, which is L/c , and hence $t_c = L/c = L/\sqrt{2\alpha\omega}$.

One can argue that L is not the appropriate length scale, because u is damped by e^{-bx} . So, for $x > 4/b$, u is close to zero. We may instead use

$1/b$ as length scale, which is the e-folding distance of the damping factor, and base t_c on the time it takes a signal to propagate one length scale, $t_c^{-1} = bc = \omega$. Similarly, the time scale based on the “speed of diffusion” changes to $t_c^{-1} = b^2\alpha = \frac{1}{2}\omega$ if we employ $1/b$ as length scale.

To summarize, we have three candidates for the time scale: $t_c = L^2/\alpha$ (diffusion through the entire domain), $t_c = 2/\omega$ (diffusion through a distance $1/b$ where u is significantly different from zero), and $t_c = 1/\omega$ (wave movement over a distance $1/b$).

Let us look at the dimensionless exact solution to see if it can help with the choice of scales. We introduce the dimensionless parameters

$$\beta = bx_c = x_c\sqrt{\frac{\omega}{2\alpha}}, \quad \gamma = \omega t_c.$$

The scaled solution becomes

$$\bar{u}(\bar{x}, \bar{t}; \beta, \gamma) = e^{-\beta\bar{x}} \sin(\gamma\bar{t} - \beta\bar{x}).$$

The three choices of γ , implied by the three choices of t_c , are

$$\gamma = \begin{cases} 1, & t_c = 1/\omega, \\ 2, & t_c = 2/\omega, \\ 2\beta^2, & t_c = L^2/\alpha, \quad x_c = L \end{cases} \quad (3.54)$$

The former two choices leave only β as parameter in \bar{u} , and with $x_c = 1/b$ as length scale, β becomes unity, and there are no parameters in the dimensionless solution:

$$\bar{u}(\bar{x}, \bar{t}) = e^{-\bar{x}} \sin(\bar{t} - \bar{x}). \quad (3.55)$$

Therefore, $x_c = 1/b$ and $t_c = 1/\omega$ (or $t_c = 2/\omega$, but the factor 2 is of no importance) are the most appropriate scales.

To further argue why (3.55) demonstrates that these scales are preferred, think of ω as large. Then the wave is damped over a short distance and there will be a thin boundary layer of temperature oscillations near $x = 0$ and little changes in u in the rest of the domain. The scaling (3.55) resolves this problem by using $1/b \sim \omega^{-1/2}$ as length scale, because then the boundary layer thickness is independent of ω . The length of the domain can be chosen as, e.g., $4/b$ such that $\bar{u} \approx 0$ at the end $x = L$. The length scale $1/b$ helps us to zoom in on the part of u where significant changes take place.

In the other limit, ω small, b becomes small, and the wave is hardly damped in the domain $[0, L]$ unless L is large enough. The imposed boundary condition on $x = L$ in fact requires u to be approximately constant so its derivative vanishes, and this property can only be obtained if L is large enough to ensure that the wave becomes significantly damped. Therefore, the length scale is dictated by b , not L , and L should be adapted to b , typically $L \geq 4/b$ if $e^{-4} \approx 0.018$ is considered enough damping to consider $\bar{u} \approx 0$ for the boundary

condition. This means that $x \in [0, 4/b]$ and then $\bar{x} \in [0, 4]$. Increasing the spatial domain to $[0, 6]$ implies a damping $e^{-6} \approx 0.0025$, if more accuracy is desired in the boundary condition.

The scaled problem. Based on the discussion of scales above, we arrive at the following scaled initial-boundary value problem:

$$\frac{\partial \bar{u}}{\partial \bar{t}} = \frac{1}{2} \frac{\partial^2 \bar{u}}{\partial \bar{x}^2}, \quad \bar{x} \in (0, 4), \quad \bar{t} \in (0, \bar{T}], \quad (3.56)$$

$$\bar{u}(\bar{x}, 0) = 0, \quad \bar{x} \in [0, 1], \quad (3.57)$$

$$\bar{u}(0, \bar{t}) = \sin(\bar{t}), \quad \bar{t} \in (0, \bar{T}], \quad (3.58)$$

$$\frac{\partial}{\partial \bar{x}} \bar{u}(\bar{L}, \bar{t}) = 0, \quad \bar{t} \in (0, \bar{T}]. \quad (3.59)$$

The coefficient in front of the second-derivative is $\frac{1}{2}$ because

$$\frac{t_c \alpha}{1/b^2} = \frac{b^2 \alpha}{\omega} = \frac{1}{2}.$$

We may, of course, choose $t_c = 2/\omega$ and get rid of the $\frac{1}{2}$ factor, if desired, but then it turns up in (3.58) instead, as $\sin(2\bar{t})$.

The boundary condition at $\bar{x} = \bar{L}$ is only an approximation and relies on sufficient damping of \bar{u} to consider it constant ($\partial/\partial \bar{x} = 0$) in space. We could, therefore, assign the condition $\bar{u} = 0$ instead at $\bar{x} = \bar{L}$.

Simulations. The file `session.py` contains a function `solver_diffusion_FE` for solving a diffusion equation in one dimension. This function can be used to solve the system (3.56)-(3.59), see `diffusion_oscillatory_BC`.

Movie 3: Diffusion wave. https://github.com/hplgit/scaling-book/raw/master/doc/pub/book/html/mov-scaling/diffusion_osc_BC/movie.mp4

3.3 Reaction-diffusion equations

3.3.1 Fisher's equation

Fisher's equation is essentially the logistic equation at each point for population dynamics (see Section 2.1.9) combined with spatial movement through ordinary diffusion:

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} + \rho u(1 - u/M). \quad (3.60)$$

This PDE is also known as the KPP equation after Kolmogorov, Petrovsky, and Piskunov (who introduced the equation independently of Fisher).

Setting

$$\bar{x} = \frac{x}{x_c}, \quad \bar{t} = \frac{t}{t_c}, \quad \bar{u} = \frac{u}{u_c},$$

results in

$$\frac{\partial \bar{u}}{\partial \bar{t}} = \frac{t_c \alpha}{x_c^2} \frac{\partial^2 \bar{u}}{\partial \bar{x}^2} + t_c \varrho \bar{u} (1 - u_c \bar{u} / M).$$

Balance of all terms. If all terms are equally important, the scales can be determined from demanding the coefficients to be unity. Reasoning as for the logistic ODE in Section 2.1.9, we may choose $t_c = 1/\varrho$. Then the coefficient in the diffusion term dictates the length scale $x_c = \sqrt{t_c \alpha}$. A natural scale for u is M , since M is the upper limit of u in the model (cf. the logistic term). Summarizing,

$$u_c = M, \quad t_c = \frac{1}{\varrho}, \quad x_c = \sqrt{\frac{\alpha}{\varrho}},$$

and the scaled PDE becomes

$$\frac{\partial \bar{u}}{\partial \bar{t}} = \frac{\partial^2 \bar{u}}{\partial \bar{x}^2} + \bar{u}(1 - \bar{u}). \quad (3.61)$$

With this scaling, the length scale $x_c = \sqrt{\alpha/\varrho}$ is not related to the domain size, so the scale is particularly relevant for infinite domains.

An open question is whether the time scale should be based on the diffusion process rather than the initial exponential growth in the logistic term. The diffusion time scale means $t_c = x_c^2/\alpha$, but demanding the logistic term then to have a unit coefficient forces $x_c^2 \varrho/\alpha = 1$, which implies $x_c = \sqrt{\alpha/\varrho}$ and $t_c = 1/\varrho$. That is, equal balance of the three terms gives a unique choice of the time and length scale.

Fixed length scale. Assume now that we fix the length scale to be L , either the domain size or some other naturally given length. With $x_c = L$, $t_c = \varrho^{-1}$, $u_c = M$, we get

$$\frac{\partial \bar{u}}{\partial \bar{t}} = \beta \frac{\partial^2 \bar{u}}{\partial \bar{x}^2} + \bar{u}(1 - \bar{u}), \quad (3.62)$$

where β is a dimensionless number

$$\beta = \frac{\alpha}{\varrho L^2} = \frac{\varrho^{-1}}{L^2/\alpha}.$$

The last equality demonstrates that β measures the ratio of the time scale for exponential growth in the beginning of the logistic process and the time scale of diffusion L^2/α (i.e., the time it takes to transport a signal by diffusion through the domain). For small β we can neglect the diffusion and spatial

movements, and the PDE is essentially a logistic ODE at each point, while for large β , diffusion dominates, and t_c should in that case be based on the diffusion time scale L^2/α . This leads to the scaled PDE

$$\frac{\partial \bar{u}}{\partial \bar{t}} = \frac{\partial^2 \bar{u}}{\partial \bar{x}^2} + \beta^{-1} \bar{u}(1 - \bar{u}), \quad (3.63)$$

showing that a large β encourages omission of the logistic term, because the point-wise growth takes place over long time intervals while diffusion is rapid. The effect of diffusion is then more prominent and it suffices to solve $\bar{u}_{\bar{t}} = \bar{u}_{\bar{x}\bar{x}}$. The observant reader will in this latter case notice that $u_c = M$ is an irrelevant scale for u , since logistic growth with its limit is not of importance, so we implicitly assume that another scale u_c has been used, but that scale cancels anyway in the simplified PDE $\bar{u}_{\bar{t}} = \bar{u}_{\bar{x}\bar{x}}$.

3.3.2 Nonlinear reaction-diffusion PDE

A general, nonlinear reaction-diffusion equation in 1D looks like

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} + f(u). \quad (3.64)$$

By scaling the nonlinear reaction term $f(u)$ as $f_c \bar{f}(u_c \bar{u})$, where f_c is a characteristic size of $f(u)$, typically the maximum value, one gets a non-dimensional PDE like

$$\frac{\partial \bar{u}}{\partial \bar{t}} = \frac{t_c \alpha}{x_c^2} \frac{\partial^2 \bar{u}}{\partial \bar{x}^2} + \frac{t_c f_c}{u_c} \bar{f}(u_c \bar{u}).$$

The characteristic size of u can often be derived from boundary or initial conditions, so we first assume that u_c is given. This fact uniquely determines the space and time scales by demanding that all three terms are equally important and of unit size:

$$t_c = \frac{u_c}{f_c}, \quad x_c = \sqrt{\frac{\alpha u_c}{f_c}}.$$

The corresponding PDE reads

$$\frac{\partial \bar{u}}{\partial \bar{t}} = \frac{\partial^2 \bar{u}}{\partial \bar{x}^2} + \bar{f}(u_c \bar{u}). \quad (3.65)$$

If x_c is based on some known length scale L , balance of all three terms can be used to determine u_c and t_c :

$$t_c = \frac{L^2}{\alpha}, \quad u_c = \frac{L^2 f_c}{\alpha}.$$

This scaling only works if f is nonlinear, otherwise u_c cancels and there is no freedom to constrain this scale.

With given L and u_c , there are two choices of t_c since it can be based on the diffusion or the reaction time scales. With the reaction scale, $t_c = u_c/f_c$, one arrives at the PDE

$$\frac{\partial \bar{u}}{\partial \bar{t}} = \beta \frac{\partial^2 \bar{u}}{\partial \bar{x}^2} + \bar{f}(u_c \bar{u}), \quad (3.66)$$

where

$$\beta = \frac{\alpha u_c}{L^2 f_c} = \frac{u_c/f_c}{L^2/\alpha}$$

is a dimensionless number reflecting the ratio of the reaction time scale and the diffusion time scale. On the contrary, with the diffusion time scale, $t_c = L^2/\alpha$, the scaled PDE becomes

$$\frac{\partial \bar{u}}{\partial \bar{t}} = \frac{\partial^2 \bar{u}}{\partial \bar{x}^2} + \beta^{-1} \bar{f}(u_c \bar{u}). \quad (3.67)$$

The size of β in an application will determine which of the scalings that is most appropriate.

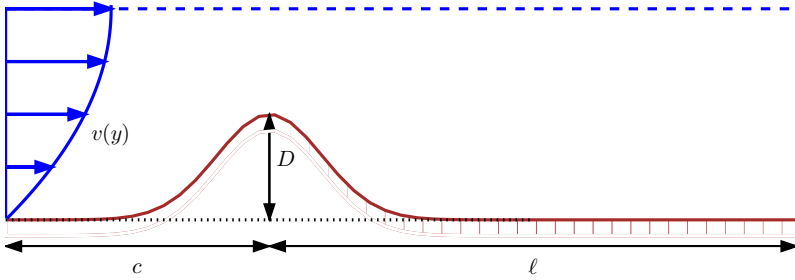
3.4 The convection-diffusion equation

3.4.1 Convection-diffusion without a force term

We now add a convection term $\mathbf{v} \cdot \nabla u$ to the diffusion equation to obtain the well-known convection-diffusion equation:

$$\frac{\partial u}{\partial t} + \mathbf{v} \cdot \nabla u = \alpha \nabla^2 u, \quad x, y, z \in \Omega, \quad t \in (0, T]. \quad (3.68)$$

The velocity field \mathbf{v} is prescribed, and its characteristic size V is normally clear from the problem description. In the sketch below, we have some given flow over a bump, and u may be the concentration of some substance in the fluid. Here, V is typically $\max_y v(y)$. The characteristic length L could be the entire domain, $L = c + \ell$, or the height of the bump, $L = D$. (The latter is the important length scale for the flow.)



Inserting

$$\bar{x} = \frac{x}{x_c}, \quad \bar{y} = \frac{y}{y_c}, \quad \bar{z} = \frac{z}{z_c}, \quad \bar{t} = \frac{t}{t_c}, \quad \bar{\mathbf{v}} = \frac{\mathbf{v}}{V}, \quad \bar{u} = \frac{u}{u_c}$$

in (3.68) yields

$$\frac{u_c}{t_c} \frac{\partial \bar{u}}{\partial \bar{t}} + \frac{u_c V}{L} \bar{\mathbf{v}} \cdot \bar{\nabla} \bar{u} = \frac{\alpha u_c}{L^2} \bar{\nabla}^2 \bar{u}, \quad \bar{x}, \bar{y}, \bar{z} \in \Omega, \quad \bar{t} \in (0, \bar{T}].$$

For u_c we simply introduce the symbol U , which we may estimate from an initial condition. It is not critical here, since it vanishes from the scaled equation anyway, as long as there is no source term present. With some velocity measure V and length measure L , it is tempting to just let $t_c = L/V$. This is the characteristic time it takes to transport a signal by convection through the domain. The alternative is to use the diffusion length scale $t_c = L^2/\alpha$. A common physical scenario in convection-diffusion problems is that the convection term $\mathbf{v} \cdot \nabla u$ dominates over the diffusion term $\alpha \nabla^2 u$. Therefore, the time scale for convection (L/V) is most appropriate of the two. Only when the diffusion term is very much larger than the convection term (corresponding to very small Peclet numbers, see below) $t_c = L^2/\alpha$ is the right time scale.

The non-dimensional form of the PDE with $t_c = L/V$ becomes

$$\frac{\partial \bar{u}}{\partial \bar{t}} + \bar{\mathbf{v}} \cdot \bar{\nabla} \bar{u} = \text{Pe}^{-1} \bar{\nabla}^2 \bar{u}, \quad \bar{x}, \bar{y}, \bar{z} \in \Omega, \quad \bar{t} \in (0, \bar{T}], \quad (3.69)$$

where Pe is the *Peclet number*,

$$\text{Pe} = \frac{LV}{\alpha}.$$

Estimating the size of the convection term $\mathbf{v} \cdot \nabla u$ as VU/L and the diffusion term $\alpha \nabla^2 u$ as $\alpha U/L^2$, we see that the Peclet number measures the ratio of the convection and the diffusion terms:

$$\text{Pe} = \frac{\text{convection}}{\text{diffusion}} = \frac{VU/L}{\alpha U/L^2} = \frac{LV}{\alpha}.$$

In case we use the diffusion time scale $t_c = L^2/\alpha$, we get the non-dimensional PDE

$$\frac{\partial \bar{u}}{\partial \bar{t}} + \text{Pe} \bar{\mathbf{v}} \cdot \bar{\nabla} \bar{u} = \bar{\nabla}^2 \bar{u}, \quad \bar{x}, \bar{y}, \bar{z} \in \Omega, \quad \bar{t} \in (0, \bar{T}]. \quad (3.70)$$

Discussion of scales and balance of terms in the PDE

We see that (3.69) and (3.70) are not equal, and they are based on two different time scales. For moderate Peclet numbers around 1, all terms have the same size in (3.69), i.e., a size around unity. For large Peclet numbers, (3.69) expresses a balance between the time derivative term and the convection term, both of size unity, and then there is a very small $\text{Pe}^{-1} \bar{\nabla}^2 \bar{u}$ term because Pe is large and $\bar{\nabla}^2 \bar{u}$ should be of size unity. That the convection term dominates over the diffusion term is consistent with the time scale $t_c = L/V$ based on convection transport. In this case, we can neglect the diffusion term as Pe goes to infinity and work with a pure convection (or advection) equation

$$\frac{\partial \bar{u}}{\partial \bar{t}} + \bar{\mathbf{v}} \cdot \bar{\nabla} \bar{u} = 0.$$

For small Peclet numbers, $\text{Pe}^{-1} \bar{\nabla}^2 \bar{u}$ becomes very large and can only be balanced by two terms that are supposed to be unity of size. The time-derivative and/or the convection term must be much larger than unity, but that means we use suboptimal scales, since right scales imply that $\partial \bar{u} / \partial \bar{t}$ and $\bar{\mathbf{v}} \cdot \bar{\nabla} \bar{u}$ are of order unity. Switching to a time scale based on diffusion as the dominating physical effect gives (3.70). For very small Peclet numbers this equation tells that the time-derivative balances the diffusion. The convection term $\bar{\mathbf{v}} \cdot \bar{\nabla} \bar{u}$ is around unity in size, but multiplied by a very small coefficient Pe, so this term is negligible in the PDE. An approximate PDE for small Peclet numbers is therefore

$$\frac{\partial \bar{u}}{\partial \bar{t}} = \bar{\nabla}^2 \bar{u}.$$

Scaling can, with the above type of reasoning, be used to neglect terms from a differential equation under precise mathematical conditions.

3.4.2 Stationary PDE

Suppose the problem is stationary and that there is no need for any time scale. How is this type of convection-diffusion problem scaled? We get

$$\frac{VU}{L} \bar{\mathbf{v}} \cdot \bar{\nabla} \bar{u} = \frac{\alpha U}{L^2} \bar{\nabla}^2 \bar{u},$$

or

$$\bar{\mathbf{v}} \cdot \bar{\nabla} \bar{u} = \text{Pe}^{-1} \bar{\nabla}^2 \bar{u}. \quad (3.71)$$

This scaling only “works” for moderate Peclet numbers. For very small or very large Pe , either the convection term $\bar{\mathbf{v}} \cdot \bar{\nabla} \bar{u}$ or the diffusion term $\bar{\nabla}^2 \bar{u}$ must deviate significantly from unity.

Consider the following 1D example to illustrate the point: $\mathbf{v} = v\mathbf{i}$, $v > 0$ constant, a domain $[0, L]$, with boundary conditions $u(0) = 0$ and $u(L) = U_L$. (The vector \mathbf{i} is a unit vector in x direction.) The problem with dimensions is now

$$vu' = \alpha u'', \quad u(0) = 0, \quad u(L) = U_L.$$

Scaling results in

$$\frac{d\bar{u}}{d\bar{x}} = \text{Pe}^{-1} \frac{d^2\bar{u}}{d\bar{x}^2}, \quad \bar{x} \in (0, 1), \quad \bar{u}(0) = 0, \quad \bar{u}(1) = 1,$$

if we choose $U = U_L$. The solution of the scaled problem is

$$\bar{u}(\bar{x}) = \frac{1 - e^{-\bar{x}\text{Pe}}}{1 - e^{-\text{Pe}}}.$$

Figure 3.4 indicates how \bar{u} depends on Pe : small Pe values give approximately a straight line while large Pe values lead to a *boundary layer* close to $x = 1$, where the solution changes very rapidly.

We realize that for large Pe ,

$$\max_{\bar{x}} \frac{d\bar{u}}{d\bar{x}} \approx \text{Pe}, \quad \max_{\bar{x}} \frac{d^2\bar{u}}{d\bar{x}^2} \approx \text{Pe}^2,$$

which are consistent results with the PDE, since the double derivative term is multiplied by Pe^{-1} . For small Pe ,

$$\max_{\bar{x}} \frac{d\bar{u}}{d\bar{x}} \approx 1, \quad \max_{\bar{x}} \frac{d^2\bar{u}}{d\bar{x}^2} \approx 0,$$

which is also consistent with the PDE, since an almost vanishing second-order derivative is multiplied by a very large coefficient Pe^{-1} . However, we have a problem with very large derivatives of \bar{u} when Pe is large.

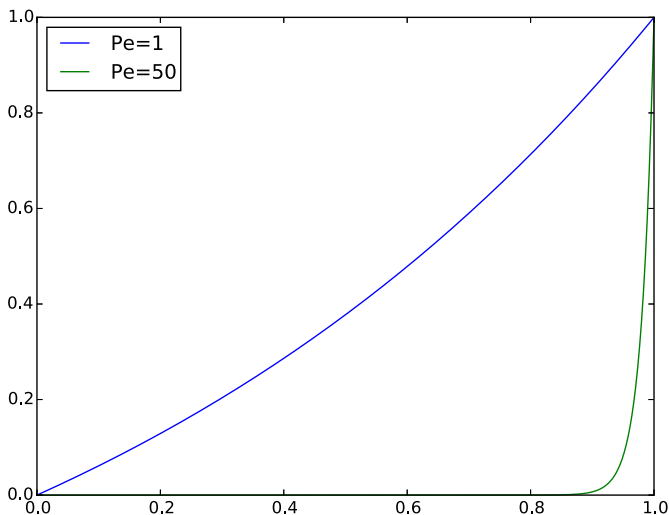


Fig. 3.4 Solution of scaled problem for 1D convection-diffusion.

To arrive at a proper scaling for large Peclet numbers, we need to remove the Pe coefficient from the differential equation. There are only two scales at our disposal: u_c and x_c for u and x , respectively. The natural value for u_c is the boundary value U_L at $x = L$. The scaling of $Vu_x = \alpha u_{xx}$ then results in

$$\frac{d\bar{u}}{d\bar{x}} = \frac{\alpha}{Vx_c} \frac{d^2\bar{u}}{d\bar{x}^2}, \quad \bar{x} \in (0, \bar{L}), \quad \bar{u}(0) = 0, \quad \bar{u}(\bar{L}) = 1,$$

where $\bar{L} = L/x_c$. Choosing the coefficient $\alpha/(Vx_c)$ to be unity results in the scale $x_c = \alpha/V$, and \bar{L} becomes Pe. The final, scaled boundary-value problem is now

$$\frac{d\bar{u}}{d\bar{x}} = \frac{d^2\bar{u}}{d\bar{x}^2}, \quad \bar{x} \in (0, \text{Pe}), \quad \bar{u}(0) = 0, \quad \bar{u}(\text{Pe}) = 1,$$

with solution

$$\bar{u}(\bar{x}) = \frac{1 - e^{-\bar{x}}}{1 - e^{-\text{Pe}}}.$$

Figure 3.5 displays \bar{u} for some Peclet numbers, and we see that the shape of the graphs are the same with this scaling. For large Peclet numbers we realize that \bar{u} and its derivatives are around unity ($1 - e^{-\text{Pe}} \approx -e^{-\text{Pe}}$), but for small Peclet numbers $d\bar{u}/d\bar{x} \sim \text{Pe}^{-1}$.

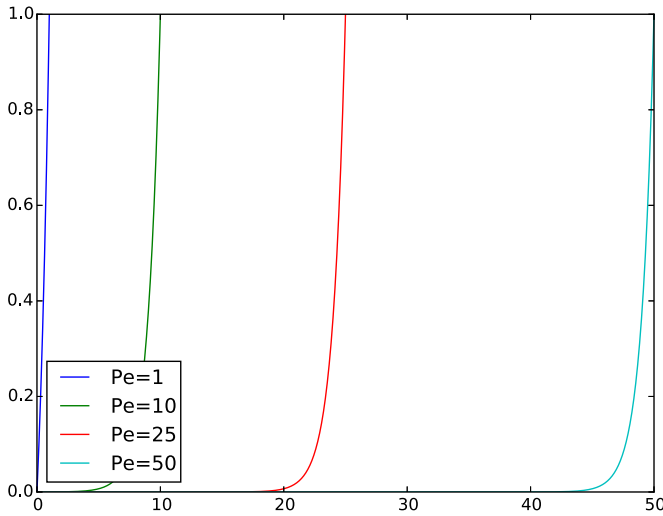


Fig. 3.5 Solution of scaled problem where the length scale depends on the Peclet number.

The conclusion is that for small Peclet numbers, $x_c = L$ is an appropriate length scale. The scaled equation $Pe \bar{u}' = \bar{u}''$ indicates that $\bar{u}'' \approx 0$, and the solution is close to a straight line. For large Pe values, $x_c = \alpha/V$ is an appropriate length scale, and the scaled equation $\bar{u}' = \bar{u}''$ expresses that the terms \bar{u}' and \bar{u}'' are equal and of size around unity.

3.4.3 Convection-diffusion with a source term

Let us add a force term $f(\mathbf{x}, t)$ to the convection-diffusion equation:

$$\frac{\partial u}{\partial t} + \mathbf{v} \cdot \nabla u = \alpha \nabla^2 u + f. \quad (3.72)$$

The scaled version reads

$$\frac{\partial \bar{u}}{\partial \bar{t}} + \frac{t_c V}{L} \bar{\mathbf{v}} \cdot \bar{\nabla} \bar{u} = \frac{t_c \alpha}{L^2} \bar{\nabla}^2 \bar{u} + \frac{t_c f_c}{u_c} \bar{f}.$$

We can base t_c on convective transport: $t_c = L/V$. Now, u_c could be chosen to make the coefficient in the source term unity: $u_c = t_c f_c = L f_c / V$. This leaves us with

$$\frac{\partial \bar{u}}{\partial t} + \bar{\mathbf{v}} \cdot \bar{\nabla} \bar{u} = \text{Pe}^{-1} \bar{\nabla}^2 \bar{u} + \bar{f}.$$

In the diffusion limit, we base t_c on the diffusion time scale: $t_c = L^2/\alpha$, and the coefficient of the source term set to unity determines u_c according to

$$\frac{L^2 f_c}{\alpha u_c} = 1 \quad \Rightarrow \quad u_c = \frac{L^2 f_c}{\alpha}.$$

The corresponding PDE reads

$$\frac{\partial \bar{u}}{\partial t} + \text{Pe} \bar{\mathbf{v}} \cdot \bar{\nabla} \bar{u} = \bar{\nabla}^2 \bar{u} + \bar{f},$$

so for small Peclet numbers, which we have, the convective term can be neglected and we get a pure diffusion equation with a source term.

What if the problem is stationary? Then there is no time scale and we get

$$\frac{V u_c}{L} \bar{\mathbf{v}} \cdot \bar{\nabla} \bar{u} = \frac{u_c \alpha}{L^2} \bar{\nabla}^2 \bar{u} + f_c \bar{f},$$

or

$$\bar{\mathbf{v}} \cdot \bar{\nabla} \bar{u} = \text{Pe}^{-1} \bar{\nabla}^2 \bar{u} + \frac{f_c L}{V u_c} \bar{f}.$$

Again, choosing u_c such that the source term coefficient is unity leads to $u_c = f_c L/V$. Alternatively, u_c can be based on the initial condition, with similar results as found in the sections on the wave and diffusion PDEs.

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