Vector Calculus and Partial Differential Equations

ChE 132A handout

(Adapted from Graham and Rawlings (2022).)

1 Let's talk . . . Coordinate Systems!

We start with a question that might seem almost too obvious to ask: why do we use different coordinate systems in science and engineering? After all, the physical answer cannot depend on which coordinate system we choose to solve a problem. Yet as we will see, the choice of coordinates can determine whether a problem is easy or nearly impossible to solve. We start in 2-d for easy visualization.

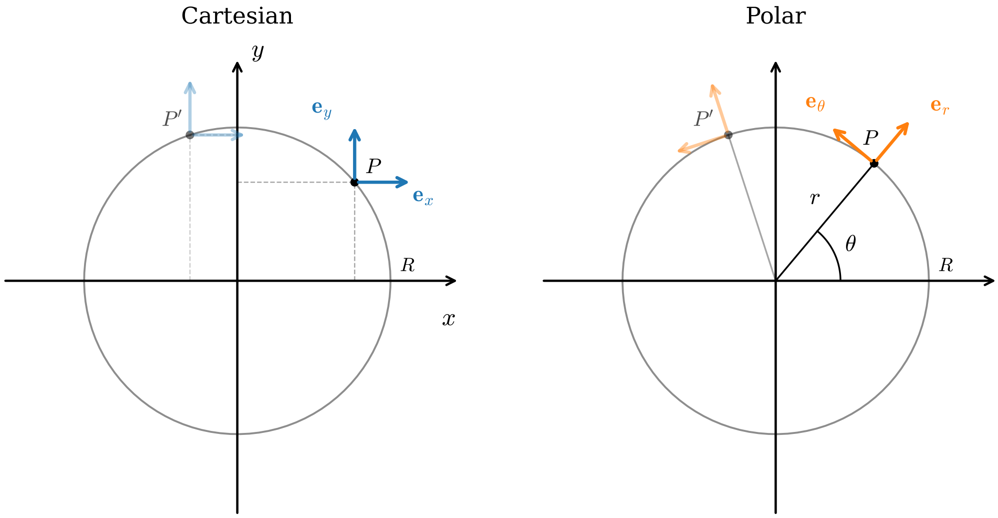

Figure 1: Cartesian (left) and polar (right) coordinate systems. In Cartesian coordinates $\boldsymbol{e}_x$ and $\boldsymbol{e}_y$ point the same way at every point in the plane — the faded vectors at P are identical to those at the origin. In polar coordinates $\boldsymbol{e}_r$ and $\boldsymbol{e}_\theta$ rotate with position: the faded vectors at P' point in completely different directions from those at P, even though both points lie on the same circle. Note also that both systems use orthonormal unit vectors.

In Cartesian coordinates every point in the plane is specified by (x, y), and the position vector is

$$\boldsymbol{x} = x\boldsymbol{e}_x + y\boldsymbol{e}_y$$

The unit vectors $\boldsymbol{e}_x$ and $\boldsymbol{e}_y$ are fixed directions. No matter where you look in the plane, they always point the same way.

In polar coordinates every point is specified by (r, θ), and the position vector is simply

$$\boldsymbol{x} = r\boldsymbol{e}_r$$

Notice that $\boldsymbol{e}_\theta$ does not appear in the position vector at all. Yet if we move along a circle by increasing θ while holding r fixed, $\boldsymbol{x}$ changes *because* $\boldsymbol{e}_r$ *rotates with* θ. Two points at the same r but different θ have unit vectors pointing in completely different directions, as Figure 1 shows. There is a lot happening in the polar unit vectors that simply does not happen in the Cartesian ones. To capture this feature, we should really say that $\boldsymbol{e}_r = \boldsymbol{e}_r(\theta)$ and $\boldsymbol{e}_\theta = \boldsymbol{e}_\theta(\theta)$, i.e., both unit vectors depend on the angle θ, but neither one depends on the radius, r.[1]

Area Integrals: Why Coordinate Choice Matters

Consider a disk of radius R. Suppose we have a temperature or concentration defined inside it and want to compute the mean value over the disk. Before we can integrate, we need the area element dA.

Cartesian coordinates. The area element is $dA = dx\,dy$. By symmetry we can integrate over the first quadrant and multiply by four

$$A = 4\int_0^R \int_0^{\sqrt{R^2-y^2}} dx\,dy = 4\int_0^R \sqrt{R^2-y^2}\,dy$$

Here we run straight into trouble. The standard way to evaluate this integral is to transform the variable of integration by substituting $y = R\sin\theta$ — but that is essentially changing to polar coordinates. Staying in Cartesian coordinates, we cannot even perform this integral (analytically) and compute the area of a circle.

Polar coordinates. Consider the small patch swept out by moving from r to $r + dr$ and from θ to $\theta + d\theta$. The radial side has length dr; the circumferential arc has length $r\,d\theta$. So the area element is

$$dA = r\,d\theta\,dr$$

and the calculation is elementary:

$$A = \int_0^{2\pi}\int_0^R r\,dr\,d\theta = \int_0^{2\pi} \frac{R^2}{2}\,d\theta = \pi R^2$$

The flip side. Now let the body be a rectangle with sides of length a and b. In Cartesian coordinates the integral is easy and gives $A = ab$. Try setting up the limits in polar coordinates: the sides of the rectangle are lines of constant x or y, which become $r\cos\theta = \text{const}$ and $r\sin\theta = \text{const}$ in polar form, and the integration in closed form is possible without changing the variable of integration, but the limits of integration are a mess. (See Exercise 1 for the steps.)

The lesson: *the coordinate system should match as closely as possible the geometry of the problem.* Circular and cylindrical geometries call for polar or cylindrical coordinates; rectangular geometries call for Cartesian coordinates.

The ∇ Operator

If we must use different coordinate systems for different problems, we need to re-express every physical law in each one — or find a smarter approach. After careful thought, physicists developed a single vector differential operator ∇ (read *del* or *nabla*) that encodes the physical laws in a *coordinate free* manner that we can then

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[1] And in Cartesian coordinates neither $\boldsymbol{e}_x$ nor $\boldsymbol{e}_y$ depend on either x or y. They are truly constant. Let's be sure that we're all on the same page here, because this is the most significant difference between Cartesian and polar coordinates.

specialize to any coordinate system. You have already seen it in your math courses. In Cartesian coordinates it is

$$\nabla = \boldsymbol{e}_x \frac{\partial}{\partial x} + \boldsymbol{e}_y \frac{\partial}{\partial y}$$

Applied to a scalar function $\phi(x, y)$, it gives the *gradient*

$$\nabla\phi = \boldsymbol{e}_x \frac{\partial \phi}{\partial x} + \boldsymbol{e}_y \frac{\partial \phi}{\partial y}$$

a vector that points in the direction of steepest increase of ϕ and tells us how rapidly ϕ changes as we move in any given direction.

The key property of ∇ is this: a small displacement $d\boldsymbol{x} = dx\, \boldsymbol{e}_x + dy\, \boldsymbol{e}_y$ from $\boldsymbol{x}$ changes ϕ by

$$d\phi = \nabla\phi \cdot d\boldsymbol{x} \tag{1}$$

Substituting both expressions and using orthonormality ($\boldsymbol{e}_x \cdot \boldsymbol{e}_x = \boldsymbol{e}_y \cdot \boldsymbol{e}_y = 1,\ \boldsymbol{e}_x \cdot \boldsymbol{e}_y = 0$)

$$d\phi = \nabla\phi \cdot d\boldsymbol{x} = \left(\boldsymbol{e}_x \frac{\partial \phi}{\partial x} + \boldsymbol{e}_y \frac{\partial \phi}{\partial y}\right) \cdot \left(dx\, \boldsymbol{e}_x + dy\, \boldsymbol{e}_y\right) = \frac{\partial \phi}{\partial x}\, dx + \frac{\partial \phi}{\partial y}\, dy$$

which is exactly the multivariable chain rule

$$d\phi = \frac{\partial \phi}{\partial x}\, dx + \frac{\partial \phi}{\partial y}\, dy$$

This dot-product relation (1) is the *defining property* of ∇: it is the unique operator such that $d\phi = \nabla\phi \cdot d\boldsymbol{x}$ holds for every scalar ϕ and every infinitesimal change in position.

The operator ∇ can also be applied twice, as $\nabla \cdot \nabla$, to form the scalar-valued *Laplacian* denoted ∇^2. In Cartesian coordinates the unit vectors are constant, so the derivation is direct

$$\begin{aligned}
\nabla^2\phi &= \nabla \cdot \nabla\phi = \left(\boldsymbol{e}_x \frac{\partial}{\partial x} + \boldsymbol{e}_y \frac{\partial}{\partial y}\right) \cdot \left(\boldsymbol{e}_x \frac{\partial \phi}{\partial x} + \boldsymbol{e}_y \frac{\partial \phi}{\partial y}\right) \\
\nabla^2\phi &= \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2}
\end{aligned}$$

The cross terms $\boldsymbol{e}_x \cdot \boldsymbol{e}_y$ vanish by orthogonality, and the constant unit vectors produce no extra terms. In polar coordinates the unit vectors depend on θ, so the Laplacian picks up additional terms — as Example 1.1 shows.

Most textbooks derive ∇ in polar coordinates by starting from the Cartesian form and substituting $x = r\cos\theta$, $y = r\sin\theta$. That is correct, but it makes Cartesian coordinates look like the “primary” system from which all others descend. There is nothing special or primary about Cartesian coordinates. Instead, we use the defining property (1) directly — no mention of (x, y) is required.

Example 1.1 (Gradient and Laplacian in polar (cylindrical) coordinates)**.**

(a) Without referring to Cartesian coordinates at all, derive a formula for ∇ in polar coordinates (Figure 2) such that $d\phi = \nabla\phi \cdot d\boldsymbol{x}$ for any scalar function ϕ.

(b) Using this formula for ∇, derive the Laplacian ∇^2 in polar coordinates.

Solution.

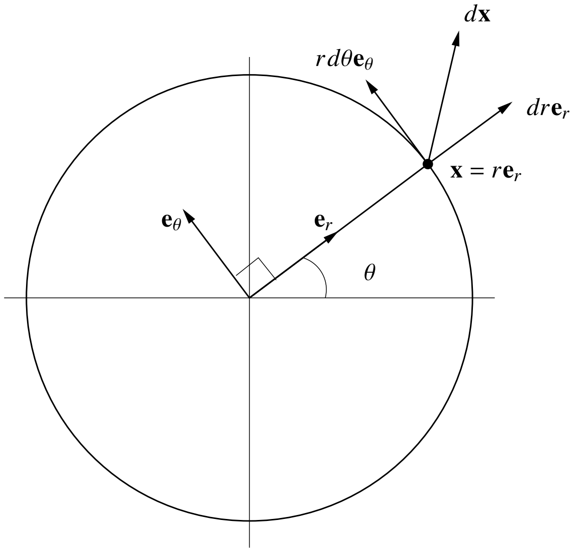

Figure 2: Polar coordinates (r, θ) with unit vectors $\boldsymbol{e}_r$, $\boldsymbol{e}_\theta$, and the position differential $d\boldsymbol{x} = dr\,\boldsymbol{e}_r + r\,d\theta\,\boldsymbol{e}_\theta$.

(a) As shown in Figure 2, the position differential is $d\boldsymbol{x} = dr\,\boldsymbol{e}_r + r\,d\theta\,\boldsymbol{e}_\theta$. The total differential of $\phi(r, \theta)$ is

$$d\phi = \frac{\partial \phi}{\partial r}\,dr + \frac{\partial \phi}{\partial \theta}\,d\theta$$

We express $\nabla\phi = \boldsymbol{e}_r a_1 + \boldsymbol{e}_\theta a_2$ with *unknowns* a_1 and a_2. Then using $d\phi = \nabla\phi \cdot d\boldsymbol{x}$ we have

$$d\phi = \frac{\partial \phi}{\partial r}\,dr + \frac{\partial \phi}{\partial \theta}\,d\theta = (\boldsymbol{e}_r a_1 + \boldsymbol{e}_\theta a_2) \cdot (dr\,\boldsymbol{e}_r + r\,d\theta\,\boldsymbol{e}_\theta) = a_1\,dr + a_2\,r\,d\theta$$

Subtracting the two expressions for $d\phi$ gives

$$0 = (\frac{\partial \phi}{\partial r} - a_1)dr + (\frac{\partial \phi}{\partial \theta} - a_2\,r)d\phi$$

and we conclude $a_1 = \partial\phi/\partial r$ and $a_2 = (1/r)\partial\phi/\partial\theta$, giving

$$\nabla\phi = \boldsymbol{e}_r\frac{\partial \phi}{\partial r} + \boldsymbol{e}_\theta\frac{1}{r}\frac{\partial \phi}{\partial \theta}, \qquad \nabla = \boldsymbol{e}_r\frac{\partial}{\partial r} + \boldsymbol{e}_\theta\frac{1}{r}\frac{\partial}{\partial \theta} \tag{2}$$

(b) The derivatives of the polar unit vectors are (see Exercise 2)

$$\frac{\partial \boldsymbol{e}_r}{\partial r} = \mathbf{0}, \quad \frac{\partial \boldsymbol{e}_\theta}{\partial r} = \mathbf{0}, \quad \frac{\partial \boldsymbol{e}_r}{\partial \theta} = \boldsymbol{e}_\theta, \quad \frac{\partial \boldsymbol{e}_\theta}{\partial \theta} = -\boldsymbol{e}_r \tag{3}$$

Apply $\nabla^2\phi = \nabla \cdot (\nabla\phi)$ using (2). Expanding by the product rule and noting that $\partial\boldsymbol{e}_r/\partial r = \partial\boldsymbol{e}_\theta/\partial r = \mathbf{0}$

$$\begin{aligned}\nabla^2\phi = {} & \boldsymbol{e}_r \cdot \left(\boldsymbol{e}_r\frac{\partial^2 \phi}{\partial r^2} + \boldsymbol{e}_\theta\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial \phi}{\partial \theta}\right)\right) \\ & + \frac{1}{r}\,\boldsymbol{e}_\theta \cdot \left(\frac{\partial \boldsymbol{e}_r}{\partial \theta}\frac{\partial \phi}{\partial r} + \boldsymbol{e}_r\frac{\partial^2 \phi}{\partial r\,\partial \theta} + \frac{\partial \boldsymbol{e}_\theta}{\partial \theta}\frac{1}{r}\frac{\partial \phi}{\partial \theta} + \boldsymbol{e}_\theta\frac{1}{r}\frac{\partial^2 \phi}{\partial \theta^2}\right)\end{aligned}$$

Substitute $\partial\boldsymbol{e}_r/\partial\theta = \boldsymbol{e}_\theta$, $\partial\boldsymbol{e}_\theta/\partial\theta = -\boldsymbol{e}_r$. Then dot with $\boldsymbol{e}_r$ (top line) and $\boldsymbol{e}_\theta$ (bottom line). Cross dot products $\boldsymbol{e}_r \cdot \boldsymbol{e}_\theta = 0$ kill three of the four bottom terms; $\boldsymbol{e}_r \cdot \boldsymbol{e}_r = \boldsymbol{e}_\theta \cdot \boldsymbol{e}_\theta = 1$ for the survivors

$$\nabla^2\phi = \frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r}\left(\frac{\partial \phi}{\partial r} + \frac{1}{r}\frac{\partial^2 \phi}{\partial \theta^2}\right)$$

$$
\begin{aligned}
\nabla^2 &= \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} \\
&= \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}
\end{aligned} \tag{4}
$$

□

Table 1 collects the gradient and Laplacian in the three most common coordinate systems; see Exercise 4 for the spherical case. The angles θ and ϕ for spherical coordinates follow the convention shown in Figure 3.

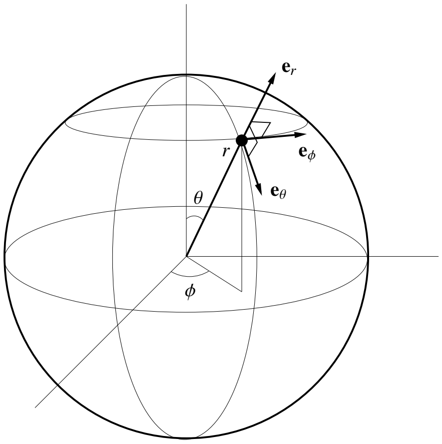

Figure 3: Orthonormal unit vectors $\boldsymbol{e}_r, \boldsymbol{e}_\theta, \boldsymbol{e}_\phi$ in spherical coordinates (r, θ, ϕ).

Table 1: Gradient and Laplacian operators in Cartesian, cylindrical, and spherical coordinates.

Cartesian	$\nabla = \boldsymbol{e}_x\frac{\partial}{\partial x} + \boldsymbol{e}_y\frac{\partial}{\partial y} + \boldsymbol{e}_z\frac{\partial}{\partial z}$	$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$
Cylindrical	$\nabla = \boldsymbol{e}_r\frac{\partial}{\partial r} + \boldsymbol{e}_\theta\frac{1}{r}\frac{\partial}{\partial \theta} + \boldsymbol{e}_z\frac{\partial}{\partial z}$	$\nabla^2 = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} + \frac{\partial^2}{\partial z^2}$
Spherical	$\nabla = \boldsymbol{e}_r\frac{\partial}{\partial r} + \boldsymbol{e}_\theta\frac{1}{r}\frac{\partial}{\partial \theta} + \boldsymbol{e}_\phi\frac{1}{r\sin\theta}\frac{\partial}{\partial \phi}$	$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial \phi^2}$

2 The Divergence Theorem

The divergence theorem relates the integral of the divergence of a vector field $\boldsymbol{v}(\boldsymbol{x})$ over a volume V to the flux of $\boldsymbol{v}$ through its bounding surface S:

$$
\int_V \nabla \cdot \boldsymbol{v}\, d\Omega = \int_S \boldsymbol{n} \cdot \boldsymbol{v}\, d\sigma \tag{5}
$$

where $\boldsymbol{n}$ is the outward unit normal to S. This result is central to the derivation of partial differential equations from conservation laws.

Derivation for a Rectangle

We establish (5) first for the rectangle $V = [0, a] \times [0, b]$ shown in the left panel of Figure 4. Label the four sides S_1 (bottom), S_2 (right), S_3 (top), and S_4 (left), with outward unit normals $\boldsymbol{n}_1 = -\boldsymbol{e}_y$, $\boldsymbol{n}_2 = \boldsymbol{e}_x$, $\boldsymbol{n}_3 = \boldsymbol{e}_y$, $\boldsymbol{n}_4 = -\boldsymbol{e}_x$.

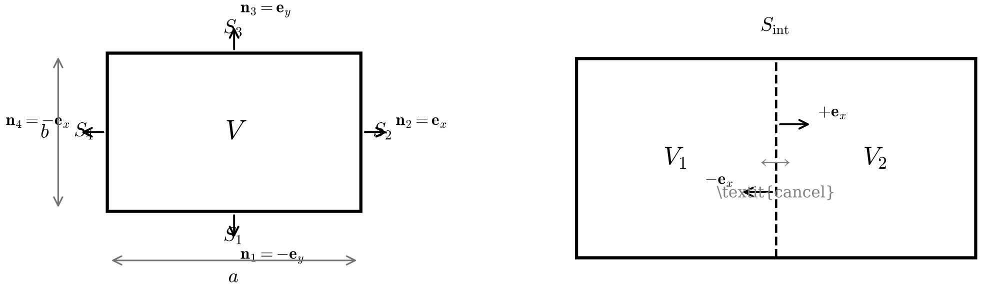

Figure 4: Left: rectangle V with sides S_1–S_4 and outward unit normals. Right: two rectangles V_1, V_2 sharing edge S_{int}; the opposing normals on the shared edge cancel.

The volume integral on the left of (5) is

$$\int_V \nabla \cdot \boldsymbol{v} \, d\Omega = \int_0^b \int_0^a \left[\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} \right] dx \, dy$$

We split this into two double integrals and use a *different* integration order for each term — the key step that makes the calculation work:

$$\int_V \nabla \cdot \boldsymbol{v} \, d\Omega = \underbrace{\int_0^b \int_0^a \frac{\partial v_x}{\partial x} \, dx \, dy}_{I_x} + \underbrace{\int_0^a \int_0^b \frac{\partial v_y}{\partial y} \, dy \, dx}_{I_y}$$

The inner integrations follow directly from the fundamental theorem of calculus:

$$I_x = \int_0^b \big[v_x(a, y) - v_x(0, y) \big] \, dy$$
$$I_y = \int_0^a \big[v_y(x, b) - v_y(x, 0) \big] \, dx$$

Now we identify each piece with the flux through one side of the rectangle. On S_2 ($x = a$): $\boldsymbol{n}_2 \cdot \boldsymbol{v} = +v_x(a, y)$; on S_4 ($x = 0$): $\boldsymbol{n}_4 \cdot \boldsymbol{v} = -v_x(0, y)$. On S_3 ($y = b$): $\boldsymbol{n}_3 \cdot \boldsymbol{v} = +v_y(x, b)$; on S_1 ($y = 0$): $\boldsymbol{n}_1 \cdot \boldsymbol{v} = -v_y(x, 0)$. Therefore

$$\int_V \nabla \cdot \boldsymbol{v} \, d\Omega = \int_{S_1} \boldsymbol{n}_1 \cdot \boldsymbol{v} \, d\sigma + \int_{S_2} \boldsymbol{n}_2 \cdot \boldsymbol{v} \, d\sigma + \int_{S_3} \boldsymbol{n}_3 \cdot \boldsymbol{v} \, d\sigma + \int_{S_4} \boldsymbol{n}_4 \cdot \boldsymbol{v} \, d\sigma = \int_S \boldsymbol{n} \cdot \boldsymbol{v} \, d\sigma$$

and the divergence theorem is established for a rectangle.

Joining Two Rectangles

Now consider two rectangles V_1 and V_2 sharing a common edge S_{int}, as shown in the right panel of Figure 4. Applying the divergence theorem to each rectangle separately and adding:

$$\int_{V_1} \nabla \cdot \boldsymbol{v}\, d\Omega + \int_{V_2} \nabla \cdot \boldsymbol{v}\, d\Omega = \int_{S_1^{\text{out}}} \boldsymbol{n} \cdot \boldsymbol{v}\, d\sigma + \int_{S_{\text{int}}} \boldsymbol{n}_1 \cdot \boldsymbol{v}\, d\sigma + \int_{S_2^{\text{out}}} \boldsymbol{n} \cdot \boldsymbol{v}\, d\sigma + \int_{S_{\text{int}}} \boldsymbol{n}_2 \cdot \boldsymbol{v}\, d\sigma$$

On the shared edge, V_1 sees outward normal $+\boldsymbol{e}_x$ while V_2 sees $-\boldsymbol{e}_x$, so $\boldsymbol{n}_1 = -\boldsymbol{n}_2$ and the two interior integrals cancel exactly:

$$\int_{S_{\text{int}}} \boldsymbol{n}_1 \cdot \boldsymbol{v}\, d\sigma + \int_{S_{\text{int}}} \boldsymbol{n}_2 \cdot \boldsymbol{v}\, d\sigma = \int_{S_{\text{int}}} (\boldsymbol{n}_1 + \boldsymbol{n}_2) \cdot \boldsymbol{v}\, d\sigma = 0$$

We are left with only the outer boundary $S = S_1^{\text{out}} \cup S_2^{\text{out}}$:

$$\int_{V_1 \cup V_2} \nabla \cdot \boldsymbol{v}\, d\Omega = \int_S \boldsymbol{n} \cdot \boldsymbol{v}\, d\sigma$$

The same cancellation argument applies when any number of rectangles are joined: all shared interior edges cancel and only the outer boundary survives. By a limiting argument this extends to regions with curved boundaries.

Derivation for a Circle

We confirm the divergence theorem directly for a disk V of radius R. In polar coordinates the divergence is (Exercise 3)

$$\nabla \cdot \boldsymbol{v} = \frac{1}{r}\frac{\partial (r v_r)}{\partial r} + \frac{1}{r}\frac{\partial v_\theta}{\partial \theta}$$

and the area element is $d\Omega = r\, dr\, d\theta$, so

$$\int_V \nabla \cdot \boldsymbol{v}\, d\Omega = \int_0^{2\pi} \int_0^R \left[\frac{1}{r}\frac{\partial (r v_r)}{\partial r} + \frac{1}{r}\frac{\partial v_\theta}{\partial \theta} \right] r\, dr\, d\theta$$

Splitting and using different integration orders for the two terms, just as in the rectangle derivation:

$$\int_V \nabla \cdot \boldsymbol{v}\, d\Omega = \int_0^{2\pi} \underbrace{\int_0^R \frac{\partial (r v_r)}{\partial r}\, dr}_{\left[r v_r\right]_0^R = R v_r(R,\theta)} \, d\theta \;+\; \int_0^R \underbrace{\int_0^{2\pi} \frac{\partial v_\theta}{\partial \theta}\, d\theta}_{v_\theta(r,2\pi) - v_\theta(r,0) = 0} \, dr$$

The second integral vanishes because v_θ is 2π-periodic in θ. Therefore

$$\int_V \nabla \cdot \boldsymbol{v}\, d\Omega = \int_0^{2\pi} R\, v_r(R,\theta)\, d\theta$$

On the circle $r = R$ the outward unit normal is $\boldsymbol{n} = \boldsymbol{e}_r$, so $\boldsymbol{n} \cdot \boldsymbol{v} = v_r(R,\theta)$, and the arc-length element is $d\sigma = R\, d\theta$. Therefore

$$\int_S \boldsymbol{n} \cdot \boldsymbol{v}\, d\sigma = \int_0^{2\pi} v_r(R,\theta)\, R\, d\theta$$

The two sides are equal, confirming (5).

3 Conservation Laws

A chemical species A with molar concentration c_A (moles per unit volume) and flux $\boldsymbol{N}_A$ (moles per unit area per unit time) satisfies the integral conservation law

$$\frac{d}{dt}\int_V c_A\,dV = -\int_S \boldsymbol{n}\cdot\boldsymbol{N}_A\,dS + \int_V R_A\,dV \tag{6}$$

where V is a fixed control volume with boundary S, and R_A is the volumetric rate of production of A. Applying the divergence theorem to the surface integral and using $\frac{d}{dt}\int_V c_A\,dV = \int_V \frac{\partial c_A}{\partial t}\,dV$ (since V is fixed)

$$\int_V \frac{\partial c_A}{\partial t}\,dV = -\int_V \nabla\cdot\boldsymbol{N}_A\,dV + \int_V R_A\,dV$$

Since all three terms are integrals over the same arbitrary volume V, the integrand must vanish pointwise:

$$\frac{\partial c_A}{\partial t} = -\nabla\cdot\boldsymbol{N}_A + R_A \tag{7}$$

This is the pointwise conservation law for A.

For dilute species transported by convection with fluid velocity $\boldsymbol{v}$ and by molecular diffusion with diffusivity D_A, a common model for the flux is

$$\boldsymbol{N}_A = c_A\boldsymbol{v} - D_A\nabla c_A \tag{8}$$

Substituting this into (7) gives

$$\frac{\partial c_A}{\partial t} = -\nabla\cdot(c_A\boldsymbol{v}) + D_A\nabla^2 c_A + R_A \tag{9}$$

This partial differential equation governs the spatial and temporal distribution of species A. The relative importance of convection and diffusion is measured by the Péclet number $\mathrm{Pe} = UL/D_A$, where U and L are characteristic velocity and length scales.

The same conservation framework applies to any transported quantity. Exercise 8 shows that an energy balance with Fourier's law $\boldsymbol{q} = -k\nabla T$ yields the heat equation

$$\rho\hat{C}_P\frac{\partial T}{\partial t} = k\nabla^2 T + \dot{q}$$

identical in form to (9) with $\boldsymbol{v} = \boldsymbol{0}$ and thermal diffusivity $\alpha = k/(\rho\hat{C}_P)$. For a Newtonian fluid the analogous momentum balance gives the Navier-Stokes equation

$$\rho\left(\frac{\partial\boldsymbol{v}}{\partial t} + \boldsymbol{v}\cdot\nabla\boldsymbol{v}\right) = -\nabla p + \mu\nabla^2\boldsymbol{v} + \rho\boldsymbol{g}$$

This is a vector PDE — one equation for each velocity component — and structurally richer than the scalar species or energy equations because of the nonlinear convection term $\boldsymbol{v}\cdot\nabla\boldsymbol{v}$. In the exercises below both the energy and momentum equations appear with $\boldsymbol{v} = \boldsymbol{0}$, reducing each to a pure diffusion equation with diffusivity $\alpha = k/(\rho\hat{C}_P)$ for heat and $\nu = \mu/\rho$ for momentum.

4 Examples

The three worked examples below illustrate the main analytical approaches for the heat equation on bounded and unbounded domains.

4.1 Laplace transforms, finite domain: diffusion-reaction in a membrane

A membrane of thickness L is initially free of solute A. At $\tau = 0$ the concentration at $z = 0$ is raised to c_{A0} while the far face $z = 1$ is held at zero; a first-order reaction with rate constant K consumes A throughout. After nondimensionalising with $c = c_A/c_{A0}$, $z = x/L$, $\tau = D_A t/L^2$, and Thiele modulus $k = KL^2/D_A$, the model is

$$\frac{\partial c}{\partial \tau} = \frac{\partial^2 c}{\partial z^2} - kc, \qquad c(0,\tau) = 1, \quad c(1,\tau) = 0, \quad c(z,0) = 0 \tag{10}$$

Step 1 — Laplace transform. With $c(z,0) = 0$ the transform converts (10) to the ODE

$$\frac{d^2\bar{c}}{dz^2} = (s+k)\bar{c}, \qquad \bar{c}(0,s) = \frac{1}{s}, \quad \bar{c}(1,s) = 0$$

Writing the general solution centred at $z = 1$: $\bar{c} = A\cosh(\sqrt{s+k}(1-z)) + B\sinh(\sqrt{s+k}(1-z))$. The condition $\bar{c}(1,s) = 0$ gives $A = 0$, and $\bar{c}(0,s) = 1/s$ then fixes $B = 1/(s\sinh\sqrt{s+k})$:

$$\bar{c}(z,s) = \frac{\sinh\big(\sqrt{s+k}\,(1-z)\big)}{s\ \sinh\sqrt{s+k}} \tag{11}$$

Step 2 — Steady state (final-value theorem).

$$c_s(z) = \lim_{s\to 0} s\bar{c}(z,s) = \frac{\sinh\big(\sqrt{k}(1-z)\big)}{\sinh\sqrt{k}}$$

For $k \to 0$ this approaches $1 - z$, the pure-diffusion linear profile.

Step 3 — Inversion via the Heaviside expansion. The denominator of (11) is $q(s) = s\sinh\sqrt{s+k}$, with simple zeros at $s = 0$ and at

$$s_n = -(k + n^2\pi^2), \quad n = 1, 2, \ldots$$

(since $\sinh(n\pi i) = i\sin(n\pi) = 0$). At $s = s_n$ we have $\sqrt{s_n + k} = n\pi i$, so using $\sinh(n\pi i(1-z)) = i\sin(n\pi(1-z)) = i(-1)^{n+1}\sin(n\pi z)$ and

$$q'(s_n) = \sinh(n\pi i) + \frac{s_n\cosh(n\pi i)}{2n\pi i} = -\frac{(k+n^2\pi^2)(-1)^n}{2n\pi i}$$

the residue at s_n is

$$\frac{p(s_n)}{q'(s_n)} = \frac{i(-1)^{n+1}\sin(n\pi z)}{-(k+n^2\pi^2)(-1)^n/(2n\pi i)} = -\frac{2n\pi\ \sin(n\pi z)}{k+n^2\pi^2}$$

Summing the residues at $s = 0$ (steady state) and all $s_n < 0$ (transient):

$$c(z,\tau) = \underbrace{\frac{\sinh\big(\sqrt{k}(1-z)\big)}{\sinh\sqrt{k}}}_{c_s(z)} - 2\sum_{n=1}^{\infty}\frac{n\pi}{k+n^2\pi^2}\ \sin(n\pi z)\, e^{-(k+n^2\pi^2)\tau} \tag{12}$$

The poles at $s = 0$ produced the steady state automatically; the poles at $s_n < 0$ produced the exponentially decaying transient modes. The next example shows that the eigenfunction method requires this decomposition to be set up by hand.

4.2 Eigenfunctions, finite domain: startup of plane Couette flow

A fluid at rest between two parallel plates at $\eta = 0$ (fixed) and $\eta = 1$ (moving at speed U_0) is released at $\tau = 0$. With $\hat{u} = u/U_0$ and $\tau = \nu t/L^2$, the dimensionless velocity satisfies

$$\frac{\partial \hat{u}}{\partial \tau} = \frac{\partial^2 \hat{u}}{\partial \eta^2}, \qquad \hat{u}(0,\tau) = 0, \quad \hat{u}(1,\tau) = 1, \qquad \hat{u}(\eta,0) = 0 \tag{13}$$

The BC $\hat{u}(1,\tau) = 1$ is inhomogeneous. A pure sine series $\sum a_n(\tau)\sin(n\pi\eta)$ satisfies $\hat{u}(0) = \hat{u}(1) = 0$ and therefore cannot represent the moving-plate condition — the method must be modified.

Steady-state decomposition. Write $\hat{u} = \hat{u}_s(\eta) + w(\eta,\tau)$, where $\hat{u}_s$ satisfies the steady problem: $\hat{u}_s'' = 0$, $\hat{u}_s(0) = 0$, $\hat{u}_s(1) = 1$. The solution is $\hat{u}_s = \eta$. Substituting, the transient w satisfies

$$\frac{\partial w}{\partial \tau} = \frac{\partial^2 w}{\partial \eta^2}, \quad w(0,\tau) = 0, \quad w(1,\tau) = 0, \quad w(\eta,0) = -\eta$$

Both BCs are now homogeneous, and the sine basis applies:

$$w(\eta,\tau) = \sum_{n=1}^{\infty} a_n\, e^{-n^2\pi^2\tau}\sin(n\pi\eta)$$

The initial condition gives $a_n = 2\int_0^1(-\eta)\sin(n\pi\eta)\,\mathrm{d}\eta$. Integration by parts with $u = \eta$, $dv = \sin(n\pi\eta)\,\mathrm{d}\eta$:

$$\int_0^1 \eta\sin(n\pi\eta)\,\mathrm{d}\eta = \Big[-\frac{\eta\cos(n\pi\eta)}{n\pi}\Big]_0^1 + \frac{1}{n\pi}\int_0^1\cos(n\pi\eta)\,\mathrm{d}\eta = \frac{(-1)^{n+1}}{n\pi}$$

so $a_n = 2(-1)^n/(n\pi)$ and the complete solution is

$$\hat{u}(\eta,\tau) = \eta + \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{(-1)^n}{n}\,e^{-n^2\pi^2\tau}\sin(n\pi\eta) \tag{14}$$

Figure 5 shows the approach to steady state.

4.3 Semi-infinite domain: two methods

A half-space $\xi > 0$ initially at rest receives a step change in surface temperature at $\tau = 0$:

$$\frac{\partial T}{\partial \tau} = \frac{\partial^2 T}{\partial \xi^2}, \quad T(0,\tau) = 1, \quad T \to 0\ (\xi \to \infty), \quad T(\xi,0) = 0 \tag{15}$$

There is no finite length scale, so the eigenfunction method on a finite interval does not apply. We show two independent methods that both give $T = \operatorname{erfc}(\xi/2\sqrt{\tau})$.

Method I: Laplace transform. Transforming (15) in τ (with $T(\xi,0) = 0$) gives $d^2\bar{T}/d\xi^2 = s\bar{T}$. The solution decaying as $\xi \to \infty$ is $\bar{T} = Ae^{-\xi\sqrt{s}}$; the surface condition $\bar{T}(0,s) = 1/s$ fixes $A = 1/s$:

$$\bar{T}(\xi,s) = \frac{e^{-\xi\sqrt{s}}}{s}$$

The first entry in the Laplace table (Exercise 7) gives directly

$$T(\xi,\tau) = \operatorname{erfc}\left(\frac{\xi}{2\sqrt{\tau}}\right) \tag{16}$$

Figure 6 shows $T(\xi,\tau)$ for several values of τ.

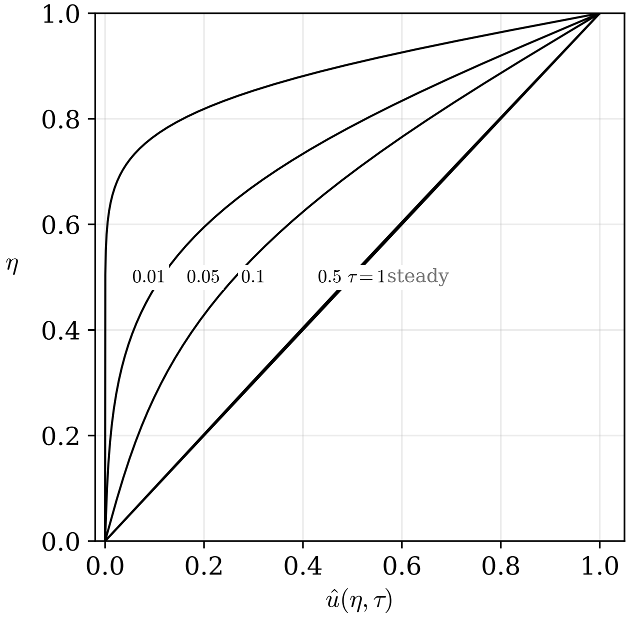

Figure 5: Startup of plane Couette flow (14). Velocity profiles $\hat{u}(\eta, \tau)$ for $\tau = 0.01, 0.05, 0.1, 0.5, 1.0$ (left to right) approach the steady linear profile $\hat{u}_s = \eta$ (dashed).

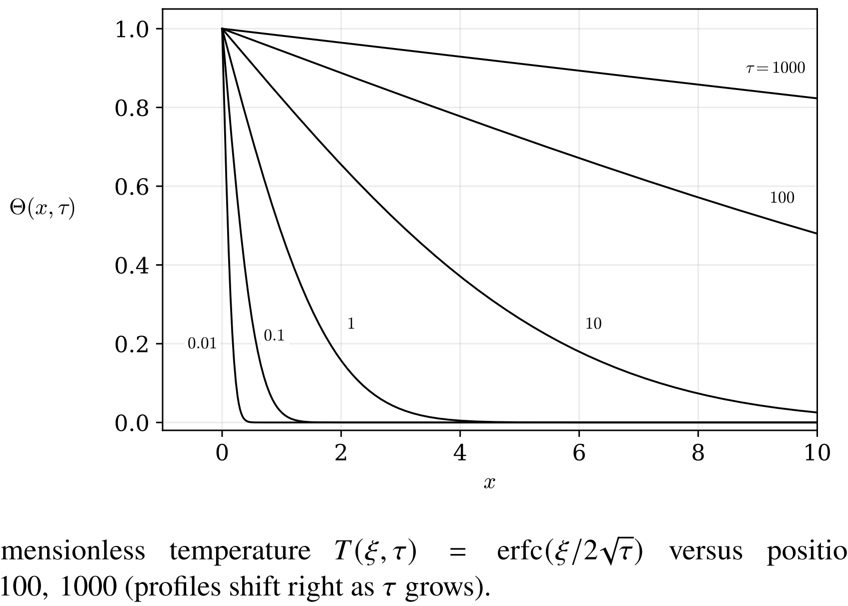

Figure 6: Dimensionless temperature $T(\xi, \tau) = \mathrm{erfc}(\xi/2\sqrt{\tau})$ versus position ξ for $\tau =$ 0.01, 0.1, 1, 10, 100, 1000 (profiles shift right as τ grows).

Method II: Similarity (combination of) variables. The PDE and all data in (15) are invariant under the rescaling $(\xi, \tau) \to (\lambda\xi, \lambda^2\tau)$ for any $\lambda > 0$. Because the problem has this scale symmetry, its solution can depend on ξ and τ only through the dimensionless combination $\eta = \xi/(2\sqrt{\tau})$. Writing $T = f(\eta)$ and applying the chain rule:

$$\frac{\partial T}{\partial \tau} = f'(\eta) \cdot \left(-\frac{\xi}{4\tau^{3/2}}\right) = -\frac{\eta}{2\tau} f', \qquad \frac{\partial^2 T}{\partial \xi^2} = f''(\eta) \cdot \frac{1}{4\tau}$$

Multiplying through by 4τ, the PDE reduces to the ODE

$$f'' + 2\eta f' = 0, \qquad f(0) = 1, \quad f(\infty) = 0 \tag{17}$$

Setting $g = f'$: the equation $g' + 2\eta g = 0$ integrates to $g = Ce^{-\eta^2}$. Integrating again with the lower limit chosen to satisfy $f(\infty) = 0$:

$$f(\eta) = C \int_{\eta}^{\infty} e^{-t^2}\, \mathrm{d}t$$

The condition $f(0) = 1$ with $\int_0^\infty e^{-t^2}\, \mathrm{d}t = \sqrt{\pi}/2$ gives $C = 2/\sqrt{\pi}$, so

$$T(\xi, \tau) = \frac{2}{\sqrt{\pi}} \int_{\xi/(2\sqrt{\tau})}^{\infty} e^{-t^2}\, \mathrm{d}t = \operatorname{erfc}\left(\frac{\xi}{2\sqrt{\tau}}\right)$$

confirming (16).

Exercises

Exercise 1 (Computing area of a rectangle in polar coordinates).

Consider the rectangle with sides of length a and b depicted in Figure 7. Compute its area using polar coordinates. Can you perform the required integrals without transforming the variables of integration back to Cartesian coordinates?

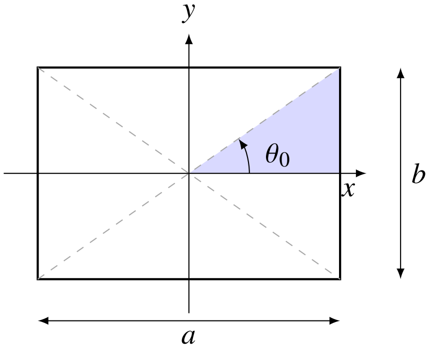

Figure 7: Rectangle of sides a and b centered at the origin. The coordinate axes and the two diagonals (dashed) partition it into eight congruent right triangles; the shaded triangle has area $ab/8$.

Hint: by symmetry the area of the shaded triangle in Figure 7 is $1/8$ of the total, so that is the only integral you need to compute.

Exercise 2 (Derivatives of unit vectors in polar (cylindrical) coordinates).

Taken from (Graham and Rawlings, 2022, Exercise 3.2).

By taking limits in polar coordinates, derive the formulas for the derivatives of the unit vectors $\boldsymbol{e}_r$ and $\boldsymbol{e}_\theta$

$$\frac{\partial \boldsymbol{e}_r}{\partial r} = \mathbf{0}, \quad \frac{\partial \boldsymbol{e}_\theta}{\partial r} = \mathbf{0}, \quad \frac{\partial \boldsymbol{e}_r}{\partial \theta} = \boldsymbol{e}_\theta, \quad \frac{\partial \boldsymbol{e}_\theta}{\partial \theta} = -\boldsymbol{e}_r$$

Do not refer to Cartesian coordinates in your derivation.

Exercise 3 (Divergence of the flux in polar coordinates).

Taken from (Graham and Rawlings, 2022, Exercise 3.3).

Derive an expression for the divergence of an arbitrary vector $\boldsymbol{q}$ in polar coordinates without using Cartesian coordinates

$$\nabla \cdot \boldsymbol{q} = \frac{1}{r}\frac{\partial}{\partial r}(r q_r) + \frac{1}{r}\frac{\partial q_\theta}{\partial \theta}$$

Hint: write $\boldsymbol{q} = q_r \boldsymbol{e}_r + q_\theta \boldsymbol{e}_\theta$ and apply ∇ from equation (2).

Exercise 4 (Gradient and Laplacian in spherical coordinates).

Taken from (Graham and Rawlings, 2022, Exercise 3.4).

Repeat Example 1.1 for spherical coordinates (r, θ, ϕ) shown in Figure 3. Do not refer to Cartesian coordinates. The answers are given in Table 1.

Exercise 5 (The error function and some useful integrals).

Taken from (Graham and Rawlings, 2022, Exercise 3.17).

The error function is defined by

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2}\, \mathrm{d}t, \qquad z > 0$$

with the standard result $\int_0^\infty e^{-t^2}\, \mathrm{d}t = \sqrt{\pi}/2$. The complementary error function is

$$\operatorname{erfc}(z) = 1 - \operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_z^\infty e^{-t^2}\, \mathrm{d}t, \qquad z > 0$$

(a) Sketch $\operatorname{erf}(x)$ and $\operatorname{erfc}(x)$.

(b) Consider the function

$$f(x) = \int_0^\infty e^{-t^2} \cos(2tx)\ \mathrm{d}t$$

Differentiate $f(x)$ and then integrate by parts to show that f satisfies

$$\frac{df}{dx} + 2x\, f(x) = 0$$

What is the initial condition for this ODE?

(c) Solve the ODE and show that

$$f(x) = \frac{\sqrt{\pi}}{2}\, e^{-x^2}$$

(d) Let $t = au$ and $x = b/(2a)$ and show that

$$\frac{\sqrt{\pi}}{2a} \exp\left(-\frac{b^2}{4a^2}\right) = \int_0^\infty e^{-a^2u^2} \cos(bu)\ \mathrm{d}u$$

(e) Integrate the equation in (d) with respect to b on $[0, \beta]$, change the order of integration, and show that

$$\frac{\pi}{2} \operatorname{erf}\left(\frac{\beta}{2a}\right) = \int_0^\infty e^{-a^2u^2} \frac{\sin(\beta u)}{u}\ \mathrm{d}u$$

Exercise 6 (Other useful integrals).

Taken from (Graham and Rawlings, 2022, Exercise 3.18).

Differentiate the following function with respect to x and thereby derive the indefinite integral (Abramowitz and Stegun, 1965, p. 304)

$$\frac{\sqrt{\pi}}{4a}\left[e^{2ab} \operatorname{erf}\bigl(ax + b/x\bigr) + e^{-2ab} \operatorname{erf}\bigl(ax - b/x\bigr)\right]$$

$$\int e^{-a^2x^2-b^2/x^2}\,\mathrm{d}x = \frac{\sqrt{\pi}}{4a}\left[e^{2ab}\operatorname{erf}\big(ax+b/x\big)+e^{-2ab}\operatorname{erf}\big(ax-b/x\big)\right]+\text{const},\qquad a\neq 0$$

Use this indefinite integral to derive the definite integral

$$\int_0^x e^{-a^2x'^2-b^2/x'^2}\,\mathrm{d}x' = \frac{\sqrt{\pi}}{4a}\left[e^{-2ab}\operatorname{erfc}\big(b/x-ax\big)-e^{2ab}\operatorname{erfc}\big(b/x+ax\big)\right],\qquad a\neq 0,\ b\geq 0 \tag{3.98}$$

From this result show that

$$\int_0^\infty e^{-x^2-b^2/x^2}\,\mathrm{d}x = \frac{\sqrt{\pi}}{2}\,e^{-2b},\qquad b\geq 0 \tag{18}$$

This integral arises in transport problems in semi-infinite domains.

Exercise 7 (Some useful Laplace transforms).

Taken from (Graham and Rawlings, 2022, Exercise 3.19).

The following Laplace transform pairs are useful for solving transient heat-conduction and diffusion problems

$\bar{f}(s)$	$f(t)$
$\dfrac{e^{-k\sqrt{s}}}{s},\quad k>0$	$\operatorname{erfc}\left(\dfrac{k}{2\sqrt{t}}\right)$
$e^{-k\sqrt{s}},\quad k>0$	$\dfrac{k}{2\sqrt{\pi t^3}}\,e^{-k^2/(4t)}$
$\dfrac{e^{-k\sqrt{s}}}{\sqrt{s}},\quad k>0$	$\dfrac{1}{\sqrt{\pi t}}\,e^{-k^2/(4t)}$

(a) Establish the first entry by taking the Laplace transform of $f(t)=\operatorname{erfc}\big(k/(2\sqrt{t})\big)$. Use the definition of the Laplace transform, switch the order of integration, and use the result (18) from Exercise 6.

(b) Establish the second entry by differentiating the first $f(t)$ with respect to t.

(c) Establish the third entry by differentiating the second $\bar{f}(s)$ with respect to s.

Exercise 8 (Conservation of energy and the heat equation).

A solid with density ρ, heat capacity $\hat{C}_P$, and thermal conductivity k has a volumetric heat-generation rate $\dot{q}$ (W/m^3). There is no fluid motion. The integral energy balance for a fixed control volume V with boundary S is

$$\frac{d}{dt}\int_V \rho\hat{C}_P T\,dV = -\int_S \boldsymbol{n}\cdot\boldsymbol{q}\,dS + \int_V \dot{q}\,dV$$

where $\boldsymbol{q}$ is the heat flux vector.

(a) Fourier's law states $\boldsymbol{q}=-k\nabla T$. Apply the divergence theorem to the surface integral and derive the pointwise energy equation

$$\rho\hat{C}_P\frac{\partial T}{\partial t} = k\nabla^2 T + \dot{q}$$

(b) Compare with (9) (setting $\boldsymbol{v} = \mathbf{0}$). Identify the roles played by D_A, c_A, and R_A in the energy context, and define the thermal diffusivity α.

(c) For unidirectional flow of an incompressible Newtonian fluid with kinematic viscosity ν, the streamwise momentum equation reduces to $\partial u/\partial t = \nu\, \partial^2 u/\partial y^2$. What plays the role of α here?

Exercise 9 (Flux heating of a semi-infinite slab).

A semi-infinite solid ($x > 0$), density ρ, heat capacity $\hat{C}_P$, conductivity k, and thermal diffusivity $\alpha = k/(\rho\hat{C}_P)$, is initially at zero temperature. At $t = 0$ a constant heat flux q_0 is applied at the surface $x = 0$. The energy equation and conditions are

$$\rho\hat{C}_P \frac{\partial T}{\partial t} = k\frac{\partial^2 T}{\partial x^2}, \qquad -k\frac{\partial T}{\partial x}\bigg|_{x=0} = q_0, \quad T(x, 0) = 0, \quad T \to 0\ (x \to \infty)$$

(a) Define $\Theta = kT/q_0$ and $\tau = \alpha t$. Show that Θ satisfies

$$\frac{\partial \Theta}{\partial \tau} = \frac{\partial^2 \Theta}{\partial x^2}, \qquad -\frac{\partial \Theta}{\partial x}\bigg|_{x=0} = 1, \quad \Theta(x, 0) = 0, \quad \Theta \to 0\ (x \to \infty)$$

Note that there is no natural length scale in this problem.

(b) Take the Laplace transform of the scaled PDE (in τ) and show that the transform satisfies $d^2\bar{\Theta}/dx^2 = s\bar{\Theta}$ with $-d\bar{\Theta}/dx|_{x=0} = 1/s$. Find the solution

$$\bar{\Theta}(x, s) = \frac{e^{-x\sqrt{s}}}{s^{3/2}}$$

Observe that $-\partial\bar{\Theta}/\partial x = e^{-x\sqrt{s}}/s$, which inverts (Exercise 7) to $-\partial\Theta/\partial x = \operatorname{erfc}(x/2\sqrt{\tau})$. Integrate from x to ∞ (using $\Theta \to 0$) to obtain

$$\Theta(x, \tau) = \int_x^\infty \operatorname{erfc}\!\left(\frac{u}{2\sqrt{\tau}}\right) \mathrm{d}u$$

(c) Evaluate the integral in (b) by integration by parts to show

$$\Theta(x, \tau) = 2\sqrt{\frac{\tau}{\pi}}\, e^{-x^2/(4\tau)} - x\operatorname{erfc}\!\left(\frac{x}{2\sqrt{\tau}}\right)$$

(d) Verify that your solution satisfies the PDE and boundary conditions. Check in particular that $-\partial\Theta/\partial x|_{x=0} = 1$ and that $\Theta(0, \tau) = 2\sqrt{\tau/\pi}$ grows as $\sqrt{\tau}$, as expected for a surface heated by a constant flux.

Exercise 10 (Transient heat conduction in a slab).

A solid rod of length L, density ρ, heat capacity $\hat{C}_P$, and thermal conductivity k is initially at temperature $T_0(x)$. At $t = 0$ both ends are clamped to a fixed reference temperature, taken as 0 for convenience. The temperature $T(x, t)$ satisfies

$$\rho\hat{C}_P \frac{\partial T}{\partial t} = k\,\frac{\partial^2 T}{\partial x^2}, \qquad T(0, t) = T(L, t) = 0, \qquad T(x, 0) = T_0(x)$$

(a) Nondimensionalize with $\xi = x/L$ and $\tau = \alpha t/L^2$, where $\alpha = k/(\rho \hat{C}_P)$, to obtain

$$\frac{\partial T}{\partial \tau} = \frac{\partial^2 T}{\partial \xi^2}, \qquad T(0,\tau) = T(1,\tau) = 0, \qquad T(\xi,0) = T_0(L\xi)$$

(b) Use separation of variables $T(\xi,\tau) = \varphi(\xi)\psi(\tau)$ to show that φ satisfies the eigenvalue problem

$$\varphi'' + \lambda\,\varphi = 0, \qquad \varphi(0) = \varphi(1) = 0$$

whose eigenpairs are $\lambda_n = (n\pi)^2$, $\varphi_n(\xi) = \sin(n\pi\xi)$ for $n = 1, 2, \ldots$, and that ψ satisfies $\psi_n' = -\lambda_n \psi_n$ with solution $\psi_n(\tau) = e^{-n^2\pi^2\tau}$.

(c) Conclude that the general solution is

$$T(\xi,\tau) = \sum_{n=1}^{\infty} a_n\, e^{-n^2\pi^2\tau}\, \sin(n\pi\xi), \qquad a_n = 2\int_0^1 T_0(L\xi)\, \sin(n\pi\xi)\, \mathrm{d}\xi$$

(d) Specialize to the uniform initial temperature $T_0(x) = T_c$ and show that

$$T(\xi,\tau) = \frac{4T_c}{\pi} \sum_{n\,\text{odd}}^{\infty} \frac{1}{n}\, e^{-n^2\pi^2\tau}\, \sin(n\pi\xi)$$

Estimate the time required for the rod to lose 90% of its initial thermal energy. Plot $T(\xi,\tau)/T_c$ as a function of ξ on $[0,1]$ for $\tau = 0.005, 0.02, 0.05, 0.1, 0.2, 0.5$.

(e) (Laplace check.) Take the Laplace transform (in τ) of the general solution in (c) and show that the resulting $\bar{T}(\xi,s)$ satisfies the ODE

$$\frac{d^2\bar{T}}{d\xi^2} - s\bar{T} = -T_0(L\xi)$$

with $\bar{T}(0,s) = \bar{T}(1,s) = 0$. Explain why this confirms that the eigenfunction series is correct.

Exercise 11 (Startup of plane Couette flow).

A Newtonian fluid of kinematic viscosity ν fills the gap between two parallel plates at $y = 0$ and $y = L$. The plates are at rest until time $t = 0$, when the upper plate is set in motion at constant velocity U_0 (the lower plate remains stationary). The streamwise velocity $u(y,t)$ satisfies the momentum equation for a unidirectional flow,

$$\frac{\partial u}{\partial t} = \nu\,\frac{\partial^2 u}{\partial y^2}, \qquad u(0,t) = 0, \quad u(L,t) = U_0, \qquad u(y,0) = 0$$

The boundary condition at $y = L$ is inhomogeneous, so the sine basis cannot be applied directly. We follow the same superposition trick used in the Fourier-analysis handout (the nonhomogeneous-BC heat-equation example): split the solution into a steady particular solution that absorbs the inhomogeneous BC and a transient correction that satisfies homogeneous BCs.

(a) Nondimensionalize with $\eta = y/L$, $\tau = \nu t/L^2$, and $\hat{u} = u/U_0$ to obtain

$$\hat{u}_\tau = \hat{u}_{\eta\eta}, \qquad \hat{u}(0,\tau) = 0, \quad \hat{u}(1,\tau) = 1, \qquad \hat{u}(\eta,0) = 0$$

(b) Find the steady-state solution $\hat{u}_p(\eta)$ satisfying $\hat{u}_p'' = 0$, $\hat{u}_p(0) = 0$, $\hat{u}_p(1) = 1$.

(c) Write $\hat{u}(\eta,\tau) = \hat{u}_p(\eta) + w(\eta,\tau)$ and show that the transient w satisfies the heat equation with *homogeneous* Dirichlet BCs and initial condition $w(\eta,0) = -\hat{u}_p(\eta)$.

(d) Use the result of Exercise 10 to write $w(\eta,\tau)$ as a sine series and then assemble the full solution

$$\hat{u}(\eta,\tau) = \eta + \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{(-1)^n}{n}\, e^{-n^2\pi^2\tau}\,\sin(n\pi\eta)$$

Plot $\hat{u}(\eta,\tau)$ for $\tau = 0.01, 0.05, 0.1, 0.5, 1$ and verify that at large τ it approaches the linear Couette profile.

Exercise 12 (Transient cooling of an infinite cylinder).

A long cylindrical rod of radius R, initially at uniform temperature T_0, is suddenly immersed in a stirred bath that holds its surface at a fixed temperature T_∞. Axial heat conduction is negligible, so the temperature depends only on the radial coordinate r and time t. The energy balance in cylindrical coordinates is

$$\rho\hat{C}_P\,\frac{\partial T}{\partial t} = \frac{k}{r}\,\frac{\partial}{\partial r}\left(r\,\frac{\partial T}{\partial r}\right)$$

with $T(R,t) = T_\infty$, T bounded at $r = 0$, and $T(r,0) = T_0$.

(a) Nondimensionalize with $\xi = r/R$, $\tau = \alpha t/R^2$ (where $\alpha = k/(\rho\hat{C}_P)$), and $\Theta = (T - T_\infty)/(T_0 - T_\infty)$ to obtain

$$\frac{\partial\Theta}{\partial\tau} = \frac{1}{\xi}\,\frac{\partial}{\partial\xi}\left(\xi\,\frac{\partial\Theta}{\partial\xi}\right), \qquad \Theta(1,\tau) = 0, \qquad \Theta(\xi,0) = 1$$

with Θ bounded at $\xi = 0$.

(b) Separate variables, $\Theta(\xi,\tau) = R(\xi)\psi(\tau)$, and show that R satisfies the cylindrical eigenvalue problem

$$\frac{1}{\xi}(\xi R')' + \lambda\,R = 0, \qquad R(1) = 0, \quad R \text{ bounded at } \xi = 0$$

whose eigenfunctions are $R_n(\xi) = J_0(\sqrt{\lambda_n}\,\xi)$ with the $\sqrt{\lambda_n}$ the positive zeros of J_0, and that $\psi_n(\tau) = e^{-\lambda_n\tau}$.

(c) Use the Fourier–Bessel expansion of the constant initial condition,

$$1 = \sum_{n=1}^{\infty} a_n\,J_0\left(\sqrt{\lambda_n}\,\xi\right)$$

with the inner product $\langle f,g\rangle_\xi = \int_0^1 f g\,\xi\,\mathrm{d}\xi$ to determine the a_n. You may use the identity

$$\int_0^1 J_0\left(\sqrt{\lambda_n}\,\xi\right)\,\xi\,\mathrm{d}\xi = \frac{J_1(\sqrt{\lambda_n})}{\sqrt{\lambda_n}}$$

along with the Fourier–Bessel orthogonality relation $\langle R_m, R_n\rangle_\xi = \frac{1}{2}J_1(\sqrt{\lambda_n})^2\,\delta_{mn}$.

(d) Combine the results to write the full solution and identify the dimensional thermal-equilibration timescale. Plot $\Theta(\xi,\tau)$ as a function of ξ on $[0,1]$ for $\tau = 0.02, 0.05, 0.1, 0.2, 0.5$.

Exercise 13 (Steady heat conduction in a cylinder with internal generation).

Consider the cylindrical analog of the steady-state heat-equation example of the Fourier-analysis handout: a cylindrical rod of radius 1 with internal volumetric heat source $f(r)$, wall held at $T(1) = 0$, T bounded at $r = 0$. The steady energy balance is

$$\frac{1}{r}\frac{d}{dr}\left(r\,\frac{dT}{dr}\right) = -f(r)$$

We solve it by Fourier–Bessel expansion, using the basis $u_n(r) = J_0\big(\sqrt{\lambda_n}\,r\big)$ from Exercise 12.

(a) Expand both T and f in the Fourier–Bessel basis,

$$T(r) = \sum_{n=1}^{\infty} a_n\,u_n(r), \qquad f(r) = \sum_{n=1}^{\infty} b_n\,u_n(r)$$

Substitute into the ODE, use the eigenvalue relation $Lu_n = -\lambda_n u_n$ where $L = \frac{1}{r}\frac{d}{dr}(r\,\frac{d}{dr})$, and conclude that

$$a_n = \frac{b_n}{\lambda_n}$$

The structural similarity to the slab result $a_n = b_n/(n^2\pi^2)$ from the Fourier-analysis handout is the point of this exercise.

(b) Specialize to a uniform heat source $f(r) = 1$, giving $b_n = 2/(\sqrt{\lambda_n}\,J_1(\sqrt{\lambda_n}))$ from Exercise 12, and write out the resulting series for $T(r)$.

(c) Verify the answer against the closed-form result obtained by direct integration of the ODE, $T(r) = (1 - r^2)/4$. Compute the partial sums $T_N(r)$ for $N = 1, 5, 20$ and confirm convergence to $(1 - r^2)/4$.

Exercise 14 (Steady temperature in a sphere with angular boundary data).

A solid sphere of radius 1 is held at the prescribed surface temperature $T(1, \theta) = g(\theta)$, where θ is the polar angle measured from the north pole. The interior temperature is axisymmetric and satisfies Laplace's equation $\nabla^2 T = 0$, which in spherical coordinates with no ϕ-dependence is

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\,\frac{\partial T}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\,\frac{\partial T}{\partial \theta}\right) = 0$$

with T bounded at $r = 0$ and regular at $\theta = 0, \pi$.

(a) Separate variables, $T(r, \theta) = R(r)\Theta(\theta)$, and show that the angular factor satisfies

$$\frac{1}{\sin\theta}\big(\sin\theta\,\Theta'\big)' + \mu\,\Theta = 0$$

while the radial factor satisfies the Cauchy–Euler equation $(r^2 R')' = \mu R$.

(b) Substitute $x = \cos\theta$ and show that the angular equation becomes Legendre's equation,

$$\big((1 - x^2)\Theta'\big)' + \mu\,\Theta = 0$$

Regularity at $x = \pm 1$ (i.e., at $\theta = 0, \pi$) forces $\mu = n(n + 1)$ for $n = 0, 1, 2, \ldots$, with eigenfunctions $\Theta_n(x) = P_n(x)$ (Legendre polynomials).

(c) Solve $(r^2 R_n')' = n(n+1)R_n$ by trying $R_n = r^p$, finding $p = n$ or $p = -(n+1)$. Boundedness at $r = 0$ forces $R_n \propto r^n$. Conclude that the general solution is

$$T(r,\theta) = \sum_{n=0}^{\infty} a_n\, r^n\, P_n(\cos\theta)$$

with coefficients determined by the boundary condition at $r = 1$

$$a_n = \frac{2n+1}{2} \int_{-1}^{1} g\left(\cos^{-1} x\right) P_n(x)\ \mathrm{d}x$$

(d) Specialize to $g(\theta) = \cos^2\theta$. Use $P_0(x) = 1$ and $P_2(x) = (3x^2 - 1)/2$ to verify the decomposition $x^2 = \frac{1}{3}P_0(x) + \frac{2}{3}P_2(x)$ and conclude that

$$T(r,\theta) = \frac{1}{3} + \frac{r^2}{3}\left(3\cos^2\theta - 1\right)$$

Verify that T satisfies Laplace's equation and matches the boundary condition at $r = 1$.

Exercise 15 (Slab cooling from a parabolic initial profile).

Return to the slab geometry of Exercise 10: the dimensionless heat equation on $[0,1]$ with zero Dirichlet conditions

$$\frac{\partial T}{\partial \tau} = \frac{\partial^2 T}{\partial \xi^2}, \qquad T(0,\tau) = T(1,\tau) = 0$$

but now with the *parabolic* initial temperature

$$T(\xi,0) = 4\xi(1-\xi)$$

which has a maximum of 1 at $\xi = \frac{1}{2}$ and satisfies the zero BCs exactly.

(a) Use the eigenfunction series from Exercise 10(c) to write the solution. Compute the Fourier sine coefficients $a_n = 2\int_0^1 4\xi(1-\xi)\sin(n\pi\xi)\ \mathrm{d}\xi$ and show that

$$a_n = \begin{cases} \dfrac{32}{n^3\pi^3}, & n \text{ odd} \\ 0, & n \text{ even} \end{cases}$$

so that

$$T(\xi,\tau) = \frac{32}{\pi^3} \sum_{n \text{ odd}}^{\infty} \frac{1}{n^3}\, e^{-n^2\pi^2\tau}\ \sin(n\pi\xi)$$

(b) Compare the convergence of this series with the series for the uniform IC in Exercise 10(d) (coefficients $\sim 1/n^3$ vs. $\sim 1/n$). Why does the smoother initial condition produce faster convergence?

(c) Plot $T(\xi,\tau)$ for $\tau = 0, 0.005, 0.02, 0.05, 0.1, 0.2$ and compare with the uniform-IC result of Exercise 10(d). Your plot should look like Figure 8.

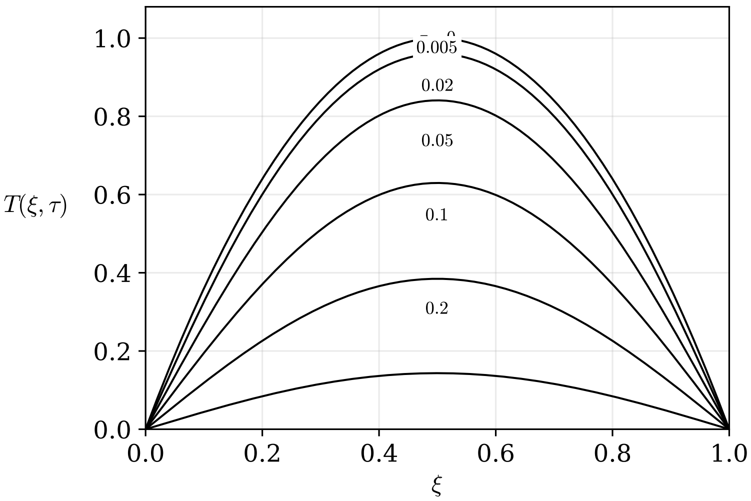

Figure 8: Dimensionless temperature $T(\xi, \tau)$ vs ξ for $\tau = 0, 0.005, 0.02, 0.05, 0.1, 0.2$ (top to bottom at the centre). The $\tau = 0$ curve is the parabolic IC $4\xi(1 - \xi)$; subsequent profiles decay smoothly to zero.

References

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