Lessons in Applied Mathematics

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Contents

Lesson 1

The advection-diffusion equation: manipulating tensors

1.1 Einstein notation, and tensor notation

Our goal is to obtain the advection-diffusion equation using indicial notation, or Einstein notation:

$$\frac{\partial c}{\partial t} + u_i \frac{\partial c}{\partial x_i} = D \frac{\partial^2 c}{\partial x_i \partial x_i}.$$

Above, c is mass concentration, u_i are the components of the velocity in a fluid, and D is the diffusivity. Diffusivities of many kinds appear in different physical contexts. Later on, we will sophisticate things a little bit and consider directional diffusivities, so that the right-hand side of the equation above will become

$$D_{ij} \frac{\partial^2 c}{\partial x_i \partial x_j}.$$

But for now, let us keep it simple.

Einstein's or indicial notation is quite convenient to shorten expressions involving vectors and tensors (for the time being, accept the word "tensor" and consider it a creature that is like a vector, only bigger and more powerful).

For example, the expression

$$u_i \frac{\partial c}{\partial x_i}$$

is a condensed form of writing

$$u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} + w \frac{\partial c}{\partial z},$$

where we can "see" that there is a velocity vector $\boldsymbol{u} = (u, v, w)$ in the expression. In this way, there is a sum of 3 terms: how can we summarize it within a summation sign? The best way seems to be to rename the elements of $\boldsymbol{u}$, as well as the coordinate axes, in the following way:

$$\begin{aligned} u &\rightarrow u_1 & x &\rightarrow x_1 \\ v &\rightarrow u_2 & y &\rightarrow x_2 \\ w &\rightarrow u_3 & z &\rightarrow x_3 \end{aligned}$$

With that, the expresion has become

$$\sum_{i=1}^{3} u_i \frac{\partial c}{\partial x_i}.$$

The cherry on the cake is *Einstein's convention*:

> If an index appears repeated in an expression, the latter must be read as a sum with the index varying (for stuff happening in $\mathbb{R}^3$) from 1 to 3.

Let us return to our original expression,

$$\frac{\partial c}{\partial t} + u_i \frac{\partial c}{\partial x_i} = D \frac{\partial^2 c}{\partial x_i \partial x_i},$$

and now let us open it up using Einstein's convention. It becomes:

$$\frac{\partial c}{\partial t} + u_1 \frac{\partial c}{\partial x_1} + u_2 \frac{\partial c}{\partial x_2} + u_3 \frac{\partial c}{\partial x_3} = D \left(\frac{\partial^2 c}{\partial x_1 \partial x_1} + \frac{\partial^2 c}{\partial x_2 \partial x_2} + \frac{\partial^2 c}{\partial x_3 \partial x_3} \right).$$

We conclude that Einstein was a rather frugal fellow.

Since we are so close to the subject, let us remember: given the vectors

$$\boldsymbol{u} = (u, v, w),$$
$$\boldsymbol{a} = (a, b, c),$$

their dot product is

$$\boldsymbol{u} \cdot \boldsymbol{a} = ua + vb + wc.$$

Using Einstein's notation,

$$\boldsymbol{u} \cdot \boldsymbol{a} = u_1 a_1 + u_2 a_2 + u_3 a_3 = u_i a_i.$$

Now, going quickly back to the left-hand side of the advection-diffusion equation, we see the dot product between the vectors

$$(u_1, u_2, u_3) \qquad \text{and} \qquad \left(\frac{\partial c}{\partial x_1}, \frac{\partial c}{\partial x_2}, \frac{\partial c}{\partial x_3} \right).$$

The second term above is the *gradient* of the concentration c:

$$\textbf{grad}\, c = \boldsymbol{\nabla} c \equiv \left(\frac{\partial c}{\partial x_1}, \frac{\partial c}{\partial x_2}, \frac{\partial c}{\partial x_3} \right).$$

The divergence of a vector $\boldsymbol{g}$ is defined (in cartesian coordinates) as

$$\operatorname{div} \boldsymbol{g} = \boldsymbol{\nabla} \cdot \boldsymbol{g} \equiv \frac{\partial g_1}{\partial x_1} + \frac{\partial g_2}{\partial x_2} + \frac{\partial g}{\partial x_3} = \frac{\partial g_i}{\partial x_i}.$$

Note that **grad** and div can be interpreted symbolically as operations involving a "pseudo-vector"

$$\boldsymbol{\nabla} = \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3} \right).$$

In this highly metaphorical way, **grad** c is interpreted as the pseudo vector $\boldsymbol{\nabla}$ post-multiplied by the scalar c, and div $\boldsymbol{g}$ is interpreted as the dot product between the "vectors" $\boldsymbol{\nabla}$ and $\boldsymbol{g}$.

Let us now return to the advection-diffusion equation: we can immediately recognize that

$$u_i \frac{\partial c}{\partial x_i} = \boldsymbol{u} \cdot \boldsymbol{\nabla} c.$$

This means that we can rewrite our equation:

$$\frac{\partial c}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} c = D \frac{\partial^2 c}{\partial x_i \partial x_i}.$$

But now we have two different notations on the two sides of the equation, which is aesthetically unpleasant. Is there a corresponding tensor notation for the right-hand side? Yes: first note that the right-hand side is a divergence:

$$\frac{\partial^2 c}{\partial x_1 \partial x_1} + \frac{\partial^2 c}{\partial x_2 \partial x_2} + \frac{\partial^2 c}{\partial x_3 \partial x_3} = \frac{\partial}{\partial x_1}\left[\frac{\partial c}{\partial x_1}\right] + \frac{\partial}{\partial x_2}\left[\frac{\partial c}{\partial x_2}\right] + \frac{\partial}{\partial x_3}\left[\frac{\partial c}{\partial x_3}\right].$$

But now, inside the square brackets, we see the components of $\boldsymbol{\nabla} c$! Therefore, the advection-diffusion equation can be written in the form

$$\frac{\partial c}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} c = D\left(\boldsymbol{\nabla} \cdot \boldsymbol{\nabla} c\right).$$

This last expression is so common that it has received a name, the *Laplacian*:

$$\nabla^2 c \equiv \boldsymbol{\nabla} \cdot \boldsymbol{\nabla} c = \frac{\partial^2 c}{\partial x_i \partial x_i},$$

and now is a good time for a break ■

1.2 Material balances: conservation of mass

Where does the advection-diffusion equation come from? How is it obtained? It comes from a "global" mass balance for the substance whose concentration is c. Here is the idea: consider a region, which we will call $\mathscr{C}$, in a fluid. The region has a volume, is "closed", and has a bounding surface that we will call $\mathscr{S}$. Now suppose that in the fluid is mixed a scalar (that we shall call "scalar A", or simply "A").

In continuum mechanics, macroscopic quantities are always defined, in a postulatory way, as quantities derived from continuous functions valid at each point in space. Consider for example the total mass of A inside of $\mathscr{C}$. We will assume that there is a continuous and differentiable function, the *density of A* (that we shall call ρ_A), whose integral gives the total mass of A:

$$M_A = \int_{\mathscr{C}} \rho_A(\boldsymbol{x}, t)\, \mathrm{d}V.$$

It is well to remember that the integral above is a *triple integral*. If you do not remember the details, look the subject up.

It would be great if the mass of A inside the *material volume* $\mathscr{C}$ remained constant. However, we cannot avoid that A enter or leave $\mathscr{C}$ due to *diffusion*.

Indeed (for example) mix some salt in distilled water, and place the solution in a small plastic bag of 200 ml (and remove all the air from the bag). Next, place the bag in a bucket with 10 l of distilled water, and open the plastic bag as fast as possible (or simply make it disappear in a split second). Instantly, $\mathscr{C}$ is given by the region occupied by the just-removed plastic bag, the recently gone bag itself defining the boundary of C, which is the border between salty and distilled water. You can now fix mentally this region and its surface $\mathscr{S}$: inevitably, the salt will diffuse across $\mathscr{S}$ and out of $\mathscr{C}$, as nature tries to establish equilibrium inside the bucket as a whole.

This is a good example. It reminds us that there exists "distilled water": there is a pure substance B, the *solvent*, and another pure substance A, the *solute*. B has its own density and mass:

$$M_B = \int_{\mathscr{C}} \rho_B(\boldsymbol{x}, t)\,\mathrm{d}V.$$

Note that B will also undergo diffusion: distilled water will diffuse into $\mathscr{C}$ in our example. The total mass of the solution, on the other hand, *will not* undergo diffusion! The total mass in our binary system is

$$M = M_A + M_B.$$

The total density is

$$\rho = \rho_A + \rho_B.$$

In the postulatory approach of continuum mechanics, the total mass within $\mathscr{C}$ is

$$M = \int_{\mathscr{C}} \rho(\boldsymbol{x}, t)\,\mathrm{d}V.$$

The conservation law for M is simpler, because there is no diffusion involved; it is

$$\frac{\mathrm{d}M}{\mathrm{d}t} = 0.$$

This simple form is good news. Alas, there are still complications. The main problem is that usually $\mathscr{C}$ is moving. Fluids move in general, and the velocity field will *advect* $\mathscr{C}$ as each particle within it and on its boundary moves with the velocity at its point. In continuum mechanics, $\mathscr{C}$ is a *material region*, or *material volume*, or, more simply, a *body*. But now we need to find how to calculate the rate of change of different physical macroscopic quantities present in $\mathscr{C}$, such as its internal energy, its mass, its momentum, etc.. For example, for mass the problem is

$$\begin{aligned} 0 &= \frac{\mathrm{d}M}{\mathrm{d}t}, \\ M(t) &= \int_{\mathscr{C}(t)} \rho(\boldsymbol{x}, t)\,\mathrm{d}V. \end{aligned}$$

But, as we know, $\mathscr{C} = \mathscr{C}(t)$: we need to calculate the derivative of an integral whose domain is itself a function of t. The solution is called the Leibniz rule in 1 dimension. In 3 dimensions, it is known in the fluid mechanics community as the Reynolds Transport Theorem. The 1D version is

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{a(t)}^{b(t)} f(x, t)\,\mathrm{d}x = \int_{a(t)}^{b(t)} \frac{\partial f(x, t)}{\partial t}\,\mathrm{d}x + f(b, t)\frac{\mathrm{d}b}{\mathrm{d}t} - f(a, t)\frac{\mathrm{d}a}{\mathrm{d}t}.$$

The 3D version, the Reynolds Transport Theorem, will come next. But first, some notation. Fluid dynamicists have their own symbol for $\mathrm{d}/\mathrm{d}t$ when the derivative is calculated "following the flow". Remember that $\mathscr{C}$ is begin *advected* by the flow field, and this necessitates a vector function, defined at each point in space and instant in time, that is (most of the time) continuous and differentiable as many times as needed: the velocity $\boldsymbol{u}(\boldsymbol{x}, t)$.

For the Leibniz rule, the velocity field is one-dimensional, $u = \mathrm{d}x/\mathrm{d}t$. The boundary is just the two end points $a(t)$ and $b(t)$, with velocities $\mathrm{d}a/\mathrm{d}t$ and $\mathrm{d}b/\mathrm{d}t$.

Fluid dynamicists emphasize this point by writing the total derivatives with an uppercase D, and call the resulting derivative the *material derivative*. The fluid mechanics version of the Leibniz rule, therefore, is

$$\frac{\mathrm{D}}{\mathrm{D}t}\int_{a(t)}^{b(t)} f(x,t)\,\mathrm{d}x = \int_{a(t)}^{b(t)} \frac{\partial f(x,t)}{\partial t}\,\mathrm{d}x + f(b,t)\frac{\mathrm{D}b}{\mathrm{D}t} - f(a,t)\frac{\mathrm{D}a}{\mathrm{D}t}.$$

With notation fully defined, here is the Reynolds transport theorem:

$$\frac{\mathrm{D}}{\mathrm{D}t}\int_{\mathscr{C}} f\,\mathrm{d}V = \int_{\mathscr{C}} \frac{\partial f}{\partial t}\,\mathrm{d}V + \oint_{\mathscr{S}} (\boldsymbol{n}\cdot[f\boldsymbol{u}])\,\mathrm{d}A.$$

Above, f is any scalar function of space and time $f(\boldsymbol{x},t)$, and $\boldsymbol{u}$ is shorthand for $\boldsymbol{u}(\boldsymbol{x},t)$. The vector $\boldsymbol{n}$ is the unit vector pointing outwards at each point of the surface $\mathscr{S}$ of the body $\mathscr{C}$. The second integral on the right-hand side is an integral over a closed surface, and therefore we used the symbol $\oint$.

Application of the Reynolds Transport Theorem for total density ρ, together with the principle of mass conservation, leads to our first conservation law in a mathematically useful form:

$$\begin{aligned} 0 &= \frac{\mathrm{D}}{\mathrm{D}t}\int_{\mathscr{C}} \rho\,\mathrm{d}V, \\ \frac{\mathrm{D}}{\mathrm{D}t}\int_{\mathscr{C}} \rho\,\mathrm{d}V &= \int_{\mathscr{C}} \frac{\partial \rho}{\partial t}\,\mathrm{d}V + \oint_{\mathscr{S}} (\boldsymbol{n}\cdot[\rho\boldsymbol{u}])\,\mathrm{d}A \;\Rightarrow \\ 0 &= \int_{\mathscr{C}} \frac{\partial \rho}{\partial t}\,\mathrm{d}V + \oint_{\mathscr{S}} (\boldsymbol{n}\cdot[\rho\boldsymbol{u}])\,\mathrm{d}A. \end{aligned}$$

The last equation above is the law of conservation of total mass in a fluid whose density is $\rho(\boldsymbol{x},t)$, and whose velocity field is $\boldsymbol{u}(\boldsymbol{x},t)$. In indicial notation, it reads

$$0 = \int_{\mathscr{C}} \frac{\partial \rho}{\partial t}\,\mathrm{d}V + \oint_{\mathscr{S}} n_i(\rho u_i)\,\mathrm{d}A.$$

The two integrals above are different: one is a triple (volume) integral, and the other is a double (surface) integral. Moreover, although already very useful, the equation is a global or macroscopic balance. It is usefull for bulk estimates in finite regions of the space. Typical applications involve simplifying hypotheses on the variation of ρ and $\boldsymbol{u}$ in space and time, so that the integrals can be calculated, and useful relations obtained among a small number of physical quantities involved in the problem. For a lot of very good examples of this *control-volume* approach for integral balances, the book by Fox et al. (2006) is an excellent source.

But one can obtain much more. We can derive an equation valid at each *point* in space-time, that represents a *local* balance of mass. For this, all that is needed is the beautiful theorem attributed to Gauss (but for the whole story, see Katz (1979)): Gauss's theorem or the Divergence theorem. Let $\boldsymbol{v}(\boldsymbol{x})$ be a vector field with enough smoothness to be continuous, differentiable, etc., as needed. The theorem reads

$$\oint_{\mathscr{S}} (\boldsymbol{n}\cdot\boldsymbol{v})\,\mathrm{d}A = \int_{\mathscr{C}} (\boldsymbol{\nabla}\cdot\boldsymbol{v})\,\mathrm{d}V.$$

In indicial notation,

$$\oint_{\mathscr{S}} n_i v_i\,\mathrm{d}A = \int_{\mathscr{C}} \frac{\partial v_i}{\partial x_i}\,\mathrm{d}V.$$

Back to the integral mass balance, the second (surface) integral can be converted into a volume integral by means of the divergence theorem:

$$\oint_{\mathscr{S}} n_i(\rho u_i)\,\mathrm{d}A = \int_{\mathscr{C}} \frac{\partial(\rho u_i)}{\partial x_i}\,\mathrm{d}V.$$

The equation for mass conservation then becomes

$$0 = \int_{\mathscr{C}} \frac{\partial \rho}{\partial t}\,\mathrm{d}V + \int_{\mathscr{C}} \frac{\partial(\rho u_i)}{\partial x_i}\,\mathrm{d}V,$$

$$0 = \int_{\mathscr{C}} \left[\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} \right] \mathrm{d}V.$$

It is very tempting to assert that the term within square brackets is null. Of course, if it is, the integral equation holds true, but that is not enough. What we need is that the last equation above *imply* that the term within brackets is zero. But this is indeed the case, for the following reason: $\mathscr{C}$ is arbitrary. The integral mass balance is valid for any material volume $\mathscr{C}$. In other words, we can choose literally *any* $\mathscr{C}$ for the balance. The mass balance equation is universal, and holds for any of these $\mathscr{C}$s. The only way to garantee this, of course, is if the term within brackets is always equal to zero, and that leads us, finally, to our local or differential mass conservation law:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = 0,$$

and now is a good point to end our lesson ■

Lesson 2

Diffusion and tensors, continued

2.1 The advection-diffusion equation (finally)

All the essential elements of the beautiful machinery that retrieves mathematical expressions for each of the conservation laws available from Physics are already in place. Its application will lead to all of these laws in convenient global and local forms. It is not our job to derive all of them: this is not a fluid mechanics course (although I am guilty of a fluid-mechanical bias), but an applied math course. We do not hesitate to wander a little further in fluid mechanics land (or should it be sea?), however.

All of the remaining laws will need an extra ingredient: a constitutive relation. We will only venture into diffusion. What is diffusion? How do you express it mathematically?

Going back to our salt water imaginary experiment, salt mass is slowly moving from regions of high salt concentration to regions of pristine distilled water. At each point, there is a *mass flux of salt*. It is a vector, and we will call it $\boldsymbol{j}$. How is it defined? So that it will give the total mass of salt crossing a surface (in the presence of a *zero* velocity field!) during a certain amount of time Δt. Now if $\mathscr{S}$ is a surface, the total mass of salt crossing it during an interval of time Δt (starting from 0 for the sake of simplicity) will be

$$M_A = \left| \int_{t=0}^{\Delta t} \int_{\mathscr{S}} (\boldsymbol{n} \cdot \boldsymbol{j}) \, \mathrm{d}A \, \mathrm{d}t \right| .$$

Pay attention to the *zero velocity field*: diffusion is something that occurs "on top" of the mean flow. Better still for our purposes: it happens relative to the moving (with the mean flow) body $\mathscr{C}$.

What does it mean in terms of a body $\mathscr{C}$ that contains a scalar A? That, instantly, it is gaining or losing mass at the rate

$$\frac{\mathrm{D}M_A}{\mathrm{D}t} = - \oint_{\mathscr{S}} (\boldsymbol{n} \cdot \boldsymbol{j}) \, \mathrm{d}A.$$

The minus sign is due to the convention that $\boldsymbol{n}$ points outwards of the bounding surface $\mathscr{S}$: think about it!

Before we move on, we need a few more things. First, we need the definition of mass concentration of A. That is simple: we define c to be

$$c \equiv \frac{\rho_A}{\rho} \Rightarrow \rho_A = c\rho.$$

Next, who is $\boldsymbol{j}$? How do we evaluate it? This turns out to be an empirical law (not directly derived from Physics, but consistent with physical constraints; in some simplified settings we can actually derive these laws from first principles, usually with the help of some statistics), that we will call a *constitutive relation*.

For $\boldsymbol{j}$ this is the celebrated *Fick's law*:

$$\boldsymbol{j} = -\rho D \boldsymbol{\nabla} c = -\rho D \frac{\partial c}{\partial x_i} \boldsymbol{e}_i.$$

We know ρ: it is the total mass density. c is the mass concentration just introduced, and D is an empirical constant called the *molecular diffusivity of A in B*. The gradient is there for a reason: the steeper the concentration differences, the greater the flux will be; makes sense. The minus sign also makes a lot of sense, because mass of A will flow "down the gradient", *i.e.*, it will flow from regions where A is more concentrated to regions where it is less concentrated.

The new element above are the *basis vectors* $\boldsymbol{e}_1$, $\boldsymbol{e}_2$, $\boldsymbol{e}_3$. Remember your basic Analytic Geometry stuff: if $\boldsymbol{v}$ is a vector, you can decompose it into three unit vectors along mutually perpendicular axes as

$$\boldsymbol{v} = u\boldsymbol{i} + v\boldsymbol{j} + w\boldsymbol{k}.$$

I am terribly sorry for having changed the meaning of $\boldsymbol{j}$ in the middle of the argument: it is now the unit vector along the y-axis. But you get the point, and this is how you learned it. We can quickly get rid of this inconsistency by rewriting

$$\boldsymbol{v} = u_1\boldsymbol{e}_1 + u_2\boldsymbol{e}_2 + u_3\boldsymbol{e}_3 = u_i\boldsymbol{e}_i.$$

The $\boldsymbol{e}_i$'s are the *basis* vectors, in our case three mutually perpendicular unit vectors pointing alone the 3 coordinate axes x_1, x_2 and x_3.

The mass flux vector $\boldsymbol{j}$ (restored to its principal meaning in this lecture) is, according to Fick's law,

$$\boldsymbol{j} = -\rho D \left[\frac{\partial c}{\partial x_1}\boldsymbol{e}_1 + \frac{\partial c}{\partial x_2}\boldsymbol{e}_2 + \frac{\partial c}{\partial x_3}\boldsymbol{e}_3 \right].$$

With the help of Fick's law, we calculate the rate of change of mass of A inside a body $\mathscr{C}$ as

$$\frac{\mathrm{D}M_A}{\mathrm{D}t} = \oint_{\mathscr{S}} (\boldsymbol{n} \cdot [\rho D \boldsymbol{\nabla} c]) \, \mathrm{d}A.$$

This is the conservation law for the mass of A. But we also have Reynolds' Transport Theorem, which reads, in this case,

$$\frac{\mathrm{D}M_A}{\mathrm{D}t} = \frac{\mathrm{D}}{\mathrm{D}t} \int_{\mathscr{C}} \rho_A \, \mathrm{d}V = \int_{\mathscr{C}} \frac{\partial \rho_A}{\partial t} \, \mathrm{d}V + \oint_{\mathscr{S}} (\boldsymbol{n} \cdot [\rho_A \boldsymbol{u}]) \, \mathrm{d}A.$$

We can combine the two above into

$$\oint_{\mathscr{S}} (\boldsymbol{n} \cdot [\rho D \boldsymbol{\nabla} c]) \, \mathrm{d}A = \int_{\mathscr{C}} \frac{\partial \rho_A}{\partial t} \, \mathrm{d}V + \oint_{\mathscr{S}} (\boldsymbol{n} \cdot [\rho_A \boldsymbol{u}]) \, \mathrm{d}A.$$

Indicial (that is: Einstein's) notation is always better to manipulate:

$$\oint_{\mathscr{S}} \left(n_i \rho D \frac{\partial c}{\partial x_i} \right) \mathrm{d}A = \int_{\mathscr{C}} \frac{\partial \rho_A}{\partial t} \, \mathrm{d}V + \oint_{\mathscr{S}} (n_i \rho_A u_i) \, \mathrm{d}A.$$

We know the "drill": the two area integrals can be converted to volume integrals by means of the Divergence Theorem, as follows:

$$\oint_{\mathscr{S}} \left(n_i \rho D \frac{\partial c}{\partial x_i} \right) \mathrm{d}A, = \int_{\mathscr{V}} \frac{\partial}{\partial x_i} \left(\rho D \frac{\partial c}{\partial x_i} \right) \mathrm{d}V,$$

$$\oint_{\mathscr{S}} (n_i \rho_A u_i) \, \mathrm{d}A = \int_{\mathscr{C}} \frac{\partial}{\partial x_i} (\rho_A u_i) \, \mathrm{d}V = \int_{\mathscr{C}} \frac{\partial}{\partial x_i} (\rho c u_i) \, \mathrm{d}V.$$

Putting everything together, we have

$$\int_{\mathscr{C}} \frac{\partial}{\partial x_i} \left(\rho D \frac{\partial c}{\partial x_i} \right) \mathrm{d}V = \int_{\mathscr{C}} \frac{\partial (\rho c)}{\partial t} \mathrm{d}V + \int_{\mathscr{C}} \frac{\partial}{\partial x_i} (\rho c u_i) \, \mathrm{d}V,$$

or

$$\int_{\mathscr{C}} \left[\frac{\partial (\rho c)}{\partial t} + \frac{\partial}{\partial x_i} (\rho c u_i) - \frac{\partial}{\partial x_i} \left(\rho D \frac{\partial c}{\partial x_i} \right) \right] \mathrm{d}V = 0$$

For exactly the same argument used previously for (total) mass conservation, the bracket is zero; without ado,

$$\frac{\partial (\rho c)}{\partial t} + \frac{\partial}{\partial x_i} (\rho c u_i) = \frac{\partial}{\partial x_i} \left(\rho D \frac{\partial c}{\partial x_i} \right).$$

I would like to suggest that you always try to use the equation above: it is in what we call *conservative* form. This is particularly important in numerical implementations, because in this form it is easier to enforce mass conservation. There is no room for elaboration here, but it turns out that many numerical schemes fail to some extent to preserve mass. Beware.

Analytically, however, it is possible to simplify the equation further. For the better or worse, this is what most texts do. Let's show how. The left-hand side is simplified with the mass conservation equation as follows:

$$\begin{aligned}
\frac{\partial (\rho c)}{\partial t} + \frac{\partial}{\partial x_i} (\rho c u_i) &= c \frac{\partial \rho}{\partial t} + \rho u_i \frac{\partial c}{\partial t} + \rho u_i \frac{\partial c}{\partial x_i} + c \frac{\partial (\rho u_i)}{\partial x_i} \\
&= c \underbrace{\left[\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} \right]}_{\equiv 0} + \rho \left[\frac{\partial c}{\partial t} + u_i \frac{\partial c}{\partial x_i} \right] \\
&= \rho \left[\frac{\partial c}{\partial t} + u_i \frac{\partial c}{\partial x_i} \right].
\end{aligned}$$

The right-hand side is approximated as

$$\frac{\partial}{\partial x_i} \left(\rho D \frac{\partial c}{\partial x_i} \right) \approx \rho D \frac{\partial}{\partial x_i} \left(\frac{\partial c}{\partial x_i} \right) = \rho D \frac{\partial^2 c}{\partial x_i \partial x_i}.$$

This approximation is quite common (usually without any justification!) in transport phenomena and fluid mechanics applications. It says that ρD (not each one of them separately!) is approximately constant in space. Clearly, it gives rise to the appearance of the Laplacian. We will use it as unashamedly as many others, but we will at least have told you that this is a little cheating to get better-looking, simpler, mathematical expressions.

Let's put everything together, and keep an equal sign (instead of $\approx$) for the sake of cleanliness:

$$\rho \left[\frac{\partial c}{\partial t} + u_i \frac{\partial c}{\partial x_i} \right] = \rho D \frac{\partial^2 c}{\partial x_i \partial x_i};$$

$$\frac{\partial c}{\partial t} + u_i \frac{\partial c}{\partial x_i} = D \frac{\partial^2 c}{\partial x_i \partial x_i}.$$

This is the equation with which we started the first lesson, and it was the lesson's goal to show you the mathematical details of its derivation ■

2.2 More sophisticated ideas and tensors

Now diffusion as we presented here is a *mathematical model* of something that occurs in nature. The first thing that was called this way was probably what we now call *molecular diffusion*, and this is how we derived it so far. It has to do with molecules, or ions, moving in a medium and generating transport of mass that is different from that stricly related to the *mean* flow.

In time, other "diffusions" became a matter of convenience, probably because most of the math was already in place! In groundwater and soil problems, often it is convenient to model things with analogies with Fick's law, and so it is in turbulence. Often, in these cases we must re-interpret the physical meaning of c, $\boldsymbol{u}$, etc.. For example, these variables will often represent *averages* of the turbulent flow.

In particular, sometimes diffusion proceeds with different speeds on different directions. This is not going to happen in an *isotropic* medium, but often turbulent flows are anisotropic, or soils are layered and therefore diffusion in them is different along different directions. What is a sensible generalization of Ficks's law that allows for these effects?

The answer is: we need to "upgrade" D to something that still operates on $\boldsymbol{\nabla} c$, and that still produces the mass flux vector $\boldsymbol{j}$, but now this "D" must be able to produce different effects over different directions. This means, essentially, that its effects, say, on $\partial c/\partial x$ and on $\partial c/\partial y$ need to be allowed to be different. One thing that does this is a matrix product. In fact, look at

$$[\boldsymbol{j}] = [\boldsymbol{D}][\boldsymbol{\nabla} c].$$

The brackets indicate matrices. For example,

$$[\boldsymbol{j}] = \begin{bmatrix} j_1 \\ j_2 \\ j_3 \end{bmatrix}; \qquad [\boldsymbol{\nabla} c] = \begin{bmatrix} \frac{\partial c}{\partial x_1} \\ \frac{\partial c}{\partial x_2} \\ \frac{\partial c}{\partial x_3} \end{bmatrix}.$$

What about $[\boldsymbol{D}]$? From what you know about matrix multiplication, for the matrix product proposed to work we must have a 3×3 matrix for D. Indeed,

$$[\boldsymbol{D}] = \begin{bmatrix} D_{11} & D_{12} & D_{13} \\ D_{21} & D_{22} & D_{23} \\ D_{31} & D_{32} & D_{33} \end{bmatrix}$$

The only problem is that matrices tie us down to particular coordinate systems, and we want to write our laws as generally as possible. For example, to represent the vector $\boldsymbol{j}$ we say

$$\boldsymbol{j} = j_i \boldsymbol{e}_i.$$

The advantage is that the $\boldsymbol{e}_i$ in the expression above represent any cartesian system, and we can produce as many such systems as we please by rigid-body rotations of the coordinate axes. On the other hand,

$$\begin{bmatrix} j_1 \\ j_2 \\ j_3 \end{bmatrix}$$

represents $\boldsymbol{j}$ in one particular coordinate system.

Now, we need to pull the same trick, to write D as generally as possible, and not tie it down to one particular basis. This is how we do it:

$$\boldsymbol{D} = D_{ij}\boldsymbol{e}_i\boldsymbol{e}_j.$$

What emerges is a new object, *second-order tensor* $\boldsymbol{D}$. It is written in boldface just like the vectors, and like the vectors it must be represented in a basis. The basis for those objects are the groups of nine "basis vectors" $\boldsymbol{e}_i\boldsymbol{e}_j$, but to distinguish them from the ordinary basis vectors we will call them "basis tensors".

Differently from vectors, you cannot see them, but you *can* operate with them. Let's rederive the diffusion equation with directional diffusivity. The only thing that needs to be changed is the expression for the time rate of change of the mass of A, which we rewrite as follows. First, as you might be guessing, our generalized Fick's law is

$$\boldsymbol{j} = \boldsymbol{D} \cdot \boldsymbol{\nabla} c.$$

The product above is a kind of generalized dot product. It occurs between a second-order tensor $\boldsymbol{D}$ and a first-order tensor $\boldsymbol{\nabla} c$. It is really easy to evaluate, and it will mimic matrix multiplication. Here is how we do it (have faith!)

$$\begin{aligned}
\boldsymbol{j} &= D_{ij}\boldsymbol{e}_i\boldsymbol{e}_j \cdot \frac{\partial c}{\partial x_k}\boldsymbol{e}_k \\
&= D_{ij}\frac{\partial c}{\partial x_k}\boldsymbol{e}_i \underbrace{(\boldsymbol{e}_j \cdot \boldsymbol{e}_k)}_{\delta_{jk}} \\
&= D_{ij}\delta_{jk}\frac{\partial c}{\partial x_k}\boldsymbol{e}_i \\
&= D_{ij}\frac{\partial c}{\partial x_j}\boldsymbol{e}_i.
\end{aligned}$$

We have discovered Kronecker's delta:

$$\delta_{jk} = \begin{cases} 1, & j = k, \\ 0, & j \neq k. \end{cases}$$

To practice, let's unfold j_1 above:

$$j_1 = \left[D_{11}\frac{\partial c}{\partial x_1} + D_{12}\frac{\partial c}{\partial x_2} + D_{13}\frac{\partial c}{\partial x_3}\right]\boldsymbol{e}_1.$$

You can do the same for the other components.

One of the beautiful things of this scheme is that it becomes a snap to calculate the gradient of a vector, and the divergence of a tensor! Remember, the gradient was previously defined to operate on a scalar field, and the divergence was previously defined to operate on a vector field.

First, let us re-calculate the "standard" gradient and divergence, but with a new trick, which is to use $\boldsymbol{\nabla}$ "directly". If c is a scalar field, we can produce the gradient with

$$\begin{aligned}
\boldsymbol{\nabla} c &= \boldsymbol{e}_i\frac{\partial}{\partial x_i}c \\
&= \boldsymbol{e}_i\frac{\partial c}{\partial x_i} \\
&= \frac{\partial c}{\partial x_i}\boldsymbol{e}_i.
\end{aligned}$$

This trick was already mentioned when we talked about interpreting $\boldsymbol{\nabla}$ as a "pseudo-vector", but now its status has improved! Likewise, for the divergence,

$$\begin{aligned}\boldsymbol{\nabla}\cdot\boldsymbol{v} &= \boldsymbol{e}_i\frac{\partial}{\partial x_i}\cdot v_j\boldsymbol{e}_j\\ &= \frac{\partial v_j}{\partial x_i}(\boldsymbol{e}_i\cdot\boldsymbol{e}_j)\\ &= \delta_{ij}\frac{\partial v_j}{\partial x_i}\\ &= \frac{\partial v_i}{\partial x_i}.\end{aligned}$$

Let's do the same with higher-order operands. Consider for example the velocity field $\boldsymbol{u}(\boldsymbol{x},t)$ in a flow. It has a gradient, and it is obtained as follows.

$$\begin{aligned}\boldsymbol{\nabla}\boldsymbol{u} &= \boldsymbol{e}_i\frac{\partial}{\partial x_i}u_j\boldsymbol{e}_j\\ &= \frac{\partial u_j}{\partial x_i}\boldsymbol{e}_i\boldsymbol{e}_j,\end{aligned}$$

and that's it! Here is the divergence of a tensor $\boldsymbol{T} = T_{ij}\boldsymbol{e}_i\boldsymbol{e}_j$:

$$\begin{aligned}\boldsymbol{\nabla}\cdot\boldsymbol{T} &= \boldsymbol{e}_i\frac{\partial}{\partial x_i}\cdot T_{jk}\boldsymbol{e}_j\boldsymbol{e}_k\\ &= \frac{\partial T_{jk}}{\partial x_i}(\boldsymbol{e}_i\cdot\boldsymbol{e}_j)\boldsymbol{e}_k\\ &= \delta_{ij}\frac{\partial T_{jk}}{\partial x_i}\boldsymbol{e}_k\\ &= \frac{\partial T_{jk}}{\partial x_j}\boldsymbol{e}_k.\end{aligned}$$

This all makes perfect sense. The gradient raises the order of the operand. The gradient of a first-order tensor is a second-order tensor. The divergence of a second-order tensor is a first-order tensor.

With this in place, our generalized ("directional") Fick's law will be as follows:

$$\begin{aligned}\frac{\mathrm{D}M_A}{\mathrm{D}t} &= \oint_{\mathscr{S}}(\boldsymbol{n}\cdot\rho\boldsymbol{D}\cdot\boldsymbol{\nabla}c)\;\mathrm{d}A\\ &= \oint_{\mathscr{S}}\left([n_i\boldsymbol{e}_i]\cdot\left[\rho D_{jk}\boldsymbol{e}_j\boldsymbol{e}_k\cdot\boldsymbol{e}_l\frac{\partial}{\partial x_l}c\right]\right)\mathrm{d}A\\ &= \oint_{\mathscr{S}}\left([n_i\boldsymbol{e}_i]\cdot\left[\rho D_{jk}\boldsymbol{e}_j(\boldsymbol{e}_k\cdot\boldsymbol{e}_l)\frac{\partial c}{\partial x_l}\right]\right)\mathrm{d}A\\ &= \oint_{\mathscr{S}}\left([n_i\boldsymbol{e}_i]\cdot\left[\rho D_{jk}\frac{\partial c}{\partial x_k}\boldsymbol{e}_j\right]\right)\mathrm{d}A.\end{aligned}$$

This last expression is ready for the divergence theorem:

$$\begin{aligned}\frac{\mathrm{D}M_A}{\mathrm{D}t} &= \int_{\mathscr{C}}\boldsymbol{e}_i\frac{\partial}{\partial x_i}\cdot\left[\rho D_{jk}\frac{\partial c}{\partial x_k}\boldsymbol{e}_j\right]\mathrm{d}V\\ &= \int_{\mathscr{C}}(\boldsymbol{e}_i\cdot\boldsymbol{e}_j)\frac{\partial}{\partial x_i}\left[\rho D_{jk}\frac{\partial c}{\partial x_k}\boldsymbol{e}_j\right]\mathrm{d}V\\ &= \int_{\mathscr{C}}\delta_{ij}\frac{\partial}{\partial x_i}\left[\rho D_{jk}\frac{\partial c}{\partial x_k}\right]\mathrm{d}V\\ &= \int_{\mathscr{C}}\frac{\partial}{\partial x_j}\left[\rho D_{jk}\frac{\partial c}{\partial x_k}\right]\mathrm{d}V.\end{aligned}$$

The rest is the same, so we can put

$$\frac{\partial(\rho c)}{\partial t} + \frac{\partial}{\partial x_i}(\rho c u_i) = \frac{\partial}{\partial x_j}\left[\rho D_{jk}\frac{\partial c}{\partial x_k}\right],$$

which is in conservative form. I will leave it for you to simplify it further with the equation of conservation of total mass, and with the assumption that the ρD_{jk} are constant in space.

Lesson 3

Similarity transforms for diffusion problems

3.1 A classical problem: the Boltzmann transform

The Boltzmann transform is often useful in diffusion problems. The classic one is the problem of a mixture with initially zero concentration of a solute A which is instantly changed to a value c_0 at $z = 0$ (The analogous problem in fluid mechanics is known as Stokes first problem, or Rayleigh problem). The governing equation is

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial z^2};$$

and the initial and boundary conditons are

$$\begin{aligned} c(z, 0) &= 0, \\ c(0, t) &= c_0, \\ c(\infty, t) &= 0. \end{aligned}$$

First, let us look at the problem from the point of view of dimensional analysis. There are 5 variables involved: z, t and the molecular diffusivity D with kinematic dimensions L and T, and $c(z, t)$ and c_0, whose dimensions are those of concentration, C. The dimensional matrix is

	z	t	D	$c(z,t)$	c_0
C	0	0	0	1	1
L	1	0	2	0	0
T	0	1	−1	0	0

whose rank is 3:

```
(%i1) A : matrix([0, 0, 0, 1, 1],[1, 0, 2, 0, 0],[0, 1, -1, 0, 0]) ;
                              [ 0  0   0   1  1 ]
                              [                 ]
(%o1)                         [ 1  0   2   0  0 ]
                              [                 ]
                              [ 0  1  - 1  0  0 ]
(%i2) rank(A);
(%o2)                                3
```

Therefore, from the Pi Theorem we have $s = 5 - 3 = 2$ dimensionless groups. The first one is trivial:

$$\Pi_1 = \frac{c(z, t)}{c_0};$$

For the other one,

$$
\begin{aligned}
\Pi_2 &= z t^a D^b; \\
[\![\Pi_2]\!] &= \mathsf{L}\mathsf{T}^a \left[\mathsf{L}^2\mathsf{T}^{-1}\right]^b, \\
1 &= \mathsf{L}^{1+2b}\mathsf{T}^{a-b},
\end{aligned}
$$

whence $a = b = -1/2$ and

$$
\Pi_2 = \frac{z}{\sqrt{4Dt}}.
$$

The numerical (dimensionless) factor 4 is immaterial; it has been introduced to conform to most solutions found in the literature.

With only two dimensionless groups, the solution must be of the form

$$
\Pi_1 = \phi\left(\Pi_2\right),
$$

or

$$
\frac{c(z,t)}{c_0} = \phi\left(\frac{z}{\sqrt{4Dt}}\right). \tag{$\star$}
$$

This in turn strongly suggests that the PDE with which we started the problem can in fact be reduced to an ODE in ϕ. The variable

$$
\xi = \frac{z}{\sqrt{4Dt}} = \frac{z}{\sqrt{4D}} t^{-1/2}
$$

is a *similarity* variable, and the solution to the problem is said to be *self-similar*.

But there is another way that leads to ξ and ϕ, and which does not proceed, *at first sight*, along the ideas of dimensional analysis. It is a more abstract idea, that consists in looking for *symmetries* in the original problem. The aproach is as follows: is there a change of variables

$$
\begin{aligned}
Z &= \alpha z, \\
T &= \beta t, \\
C(Z,T) &= \gamma c(z,t),
\end{aligned}
$$

under which the original PDE remains *invariant*? In other words, can we make such a change of variables and arrive at a new PDE with the same *form*, namely

$$
\frac{\partial C}{\partial T} = D' \frac{\partial^2 C}{\partial Z^2} \; ?
$$

Above, of course, we require that D' be a constant. But

$$
\begin{aligned}
\frac{\partial c}{\partial t} &= \frac{\partial (C/\gamma)}{\partial (T/\beta)} = \frac{\beta}{\gamma}\frac{\partial C}{\partial T}; \\
\frac{\partial^2 c}{\partial z^2} &= \frac{\partial^2 (C/\gamma)}{\partial (Z/\alpha)^2} = \frac{\alpha^2}{\gamma}\frac{\partial^2 C}{\partial Z^2},
\end{aligned}
$$

so that the PDE in C, Z, T is

$$
\begin{aligned}
\frac{\beta}{\gamma}\frac{\partial C}{\partial T} &= D\frac{\alpha^2}{\gamma}\frac{\partial^2 C}{\partial Z^2}, \\
\frac{\partial C}{\partial T} &= D\alpha^2\beta^{-1}\frac{\partial^2 C}{\partial Z^2}.
\end{aligned}
$$

By the same token, the only non-zero boundary condition becomes

$$c(0,t) = \frac{C}{\gamma}\left(0, \frac{T}{\beta}\right) = c_0$$

Therefore, for the EDP to be invariant under the transformations, we must satisfy two requirements:

$$\begin{aligned} D\alpha^2\beta^{-1} &= \text{const} = \frac{1}{4}, \\ \gamma c_0 &= \text{const} = 1. \end{aligned}$$

The constants above can have any values, and we just picked two (1/4 and 1) that are particularly convenient to simplify the upcoming calculations.

The problem in C, Z and T is a *little bit* simpler:

$$\begin{aligned} \frac{\partial C}{\partial T} &= \frac{1}{4}\frac{\partial^2 C}{\partial Z^2}, \\ C(Z,0) &= 0, \\ C(0,T) &= 1, \\ C(\infty,T) &= 0. \end{aligned}$$

Note also that there is a lot of freedom to choose α and β as long as $D\alpha^2\beta^{-1} = 1/4$ is satisfied.

At this point, we still haven't determined particular values for α and β (but we have for $\gamma = 1/c_0$, so that we have

$$c(z,t) = c_0 C(\alpha z, \beta t). \tag{$\star\star$}$$

What we are going to do next is *strange*, but perfectly ok (think about it): For each t we are going to pick a different β, and hence a different α as well. Because we are using different β's, we will also end up with different (in fact, infinite) corresponding solutions $C(Z,T)$. Proceeding, for each t, pick

$$\beta = \frac{1}{t} \Rightarrow D\alpha^2 = \frac{1}{4t} \Rightarrow \alpha = \frac{1}{\sqrt{4Dt}},$$

so that

$$c(z,t) = c_0 C\left(\frac{z}{\sqrt{4Dt}}, 1\right).$$

Note that this is the same as what we obtained with ($\star$) before! Just write

$$\begin{aligned} \xi &= \frac{z}{\sqrt{4Dt}}, \\ \frac{c(z,t)}{c_0} &= C(\xi, 1) \equiv \phi(\xi). \end{aligned}$$

A note of caution: the new function $C(\xi,1) = \phi(\xi)$ is obviously a function of one variable only (the similarity variable ξ), and the diffusion equation in ξ is not invariant under stretching through α, β and γ as the diffision equation in $c(z,t)$ is. The reason is obvious: we did not use a constant β to arrive at $\phi(\xi)$! But we kept β a generic constant all the way up to ($\star\star$). Only after that equation did we pick $\beta = 1/t$, which is clever, even perversely clever, but otherwise does not break any rule of algebra or calculus.

3.2 The diffusion equation in $\phi(\xi)$

The equation in $\phi(\xi)$ is best found from the original diffusion equation. The PDE in C, Z and T has played its role, which essentially was to show that a solution in $\phi(\xi)$ exists. The two numerically equal boundary conditions $c(z,0) = c(\infty,t) = 0$ because they will lead to a *single boundary condition* in ϕ at $\xi = \infty$. Proceeding, the change of variables from z, t to ξ requires the systematic use of the chain rule:

$$\begin{aligned}
\frac{\partial c}{\partial t} &= \frac{\mathrm{d}\phi}{\mathrm{d}\xi}\frac{\partial \xi}{\partial t} \\
&= -\frac{1}{2}\frac{z}{\sqrt{4D}}t^{-3/2}\frac{\mathrm{d}\phi}{\mathrm{d}\xi} \\
&= -\frac{1}{2}\frac{z}{\sqrt{4Dt}}t^{-1}\frac{\mathrm{d}\phi}{\mathrm{d}\xi} \\
&= -\frac{1}{2t}\xi\frac{\mathrm{d}\phi}{\mathrm{d}\xi}.
\end{aligned}$$

For the derivatives with respect to z,

$$\begin{aligned}
\frac{\partial c}{\partial z} &= c_0\frac{\mathrm{d}\phi}{\mathrm{d}\xi}\frac{\partial \xi}{\partial z} \\
&= \frac{c_0}{\sqrt{4Dt}}\frac{\mathrm{d}\phi}{\mathrm{d}\xi}; \\
\frac{\partial^2 c}{\partial z^2} &= c_0\frac{\mathrm{d}}{\mathrm{d}\xi}\left[\frac{\mathrm{d}\phi}{\mathrm{d}\xi}\frac{\partial \xi}{\partial z}\right]\frac{\partial \xi}{\partial z} \\
&= c_0\frac{\mathrm{d}}{\mathrm{d}\xi}\left[\frac{1}{\sqrt{4Dt}}\frac{\mathrm{d}\phi}{\mathrm{d}\xi}\right]\frac{1}{\sqrt{4Dt}} \\
&= \frac{c_0}{4Dt}\frac{\mathrm{d}^2\phi}{\mathrm{d}\xi^2}
\end{aligned}$$

Substituting back in the original diffusion equation,

$$\begin{aligned}
\frac{\partial c}{\partial t} &= D\frac{\partial^2 c}{\partial z^2}, \\
-\frac{c_0}{2t}\xi\frac{\mathrm{d}\phi}{\mathrm{d}\xi} &= \frac{c_0 D}{4Dt}\frac{\mathrm{d}^2 c}{\mathrm{d}\xi^2}, \\
\frac{\mathrm{d}^2\phi}{\mathrm{d}\xi^2} + 2\xi\frac{\mathrm{d}\phi}{\mathrm{d}\xi} &= 0.
\end{aligned}$$

The two boundary conditions in ϕ are

$$\begin{aligned}
\phi(0) &= 1, \\
\phi(\infty) &= 0.
\end{aligned}$$

It is not to difficult to solve this ODE using *reduction of order*:

$$
\begin{aligned}
g &\equiv \frac{\mathrm{d}\phi}{\mathrm{d}\xi};\\
\frac{\mathrm{d}g}{\mathrm{d}\xi} + 2\xi g &= 0;\\
\frac{\mathrm{d}g}{g} &= -2\xi \mathrm{d}\xi;\\
\int_{g_0}^{g(\xi)} \frac{\mathrm{d}g'}{g'} &= -2\int_0^{\xi} \xi' \mathrm{d}\xi';\\
\ln\frac{g(\xi)}{g_0} &= -\mathrm{e}^{-\xi^2};\\
g(\xi) &= -g_0 \mathrm{e}^{-\xi^2}\\
\frac{\mathrm{d}\phi}{\mathrm{d}\xi} &= -g_0 \mathrm{e}^{-\xi^2}\\
\int_{\phi=\phi_0}^{\phi(\xi)} \mathrm{d}\phi' &= -g_0 \int_{\xi=0}^{\xi} \mathrm{e}^{-\xi'^2}\,\mathrm{d}\xi'\\
\phi(\xi) - \phi_0 &= -\frac{g_0\sqrt{\pi}}{2}\,\mathrm{erf}(\xi);\\
\phi(\xi) &= \phi_0 - \frac{g_0\sqrt{\pi}}{2}\,\mathrm{erf}(\xi).
\end{aligned}
$$

Some points are important to note here, if this is the first time you are seeing this problem.

First, we needed to use the definition of the *error function* $\mathrm{erf}(\xi)$:

$$
\mathrm{erf}(\xi) \equiv \frac{2}{\sqrt{\pi}} \int_0^{\xi} \mathrm{e}^{-u^2}\,\mathrm{d}u.
$$

The error function needs to be introduced because the corresponding integral cannot be obtained in terms of elementary transcedental functions (sen, cos, tg, …, exp, ln), polynomials, or rational functions of the former. This is a deep result, that was originally proved (apparently for a restricted class of functions) by Liouville (Liouville, 1833a,b,c); see also Conrad (2005). Most scientific computer languages have an erf function available in some library. The $\mathrm{erf}(\xi)$ function is *odd*, with

$$
\begin{aligned}
\mathrm{erf}(0) &= 0,\\
\mathrm{erf}(\infty) &= 1.
\end{aligned}
$$

Two, we need to calculate g_0. Note that the boundary condition

$$
\phi_0 = \frac{c(0,t)}{c_0}
$$

is built-in in the integration of the ODE. But

$$
\begin{aligned}
\phi(\infty) = 0 = \phi_0 - \frac{g_0\sqrt{\pi}}{2} &\Rightarrow\\
\frac{g_0\sqrt{\pi}}{2} = \phi_0 &\Rightarrow\\
\phi(\xi) = \phi_0\,[1 - \mathrm{erf}(\xi)] &\ \blacksquare
\end{aligned}
$$

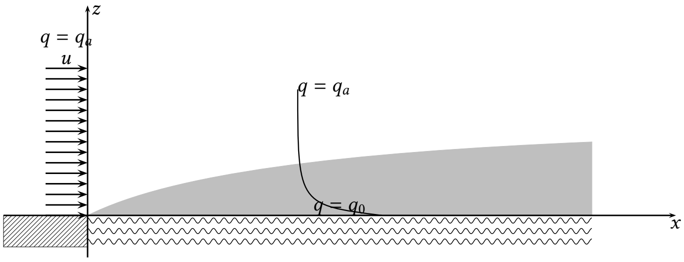

Figure 3.1: "O problema de Sutton"

3.3 Sutton's problem

Considere agora uma equação diferencial totalmente diferente:

$$u\frac{\partial q}{\partial x} = D\frac{\partial^2 q}{\partial z^2}$$

Naturalmente, trata-se de uma versão simplificada (e estacionária: note a ausência da derivada parcial em relação ao tempo) da equação geral de difusão-advecção. Nós vamos utilizá-la para resolver o problema esboçado na figura 3.1, que ficou conhecido na literatura como "O problema de Sutton".

Nesse problema, ar seco sopra sobre um lago, sobre o qual se forma uma camada-limite interna de ar úmido, à medida que o vento (representado por um perfil uniforme em x e em z de velocidade u advecta ar sobre o lago.

É importante notar que a física é totalmente diferente daquela que usamos para deduzir a equação de advecção-difusão no capítulo **??**! Aqui, q é a umidade específica *média*; u é a velocidade do vento *média*; e D é a difusividade turbulenta de vapor d'água na vertical.

Vamos especificar as condições de contorno deste problema:

$$\begin{aligned} q(0,z) &= q_a, \\ q(x,0) &= q_0, \\ q(x,\infty) &= q_a. \end{aligned}$$

Olhando para a figura e considerando a física do problema você consegue explicá-las?

Observe também que $q(0,z) = q(x,\infty)$ sugere fortemente, mais uma vez, a transformação de Boltzmann. Sejamos claros: desejamos reaproveitar a solução que já obtivemos no início deste capítulo! Para tanto, seria muito bom se $q(0,z) = 0$. Mas isso não é um grande problema. Primeiramente, faça

$$\mathcal{X} = \frac{q - q_a}{q_0 - q_a};$$

esta é uma transformação linear na variável q, e portanto segue-se imediatamente que vale

$$u\frac{\partial \mathcal{X}}{\partial x} = D\frac{\partial^2 \mathcal{X}}{\partial z^2}.$$

Na variável $\mathcal{X}$, as condições de contorno são

$$
\begin{aligned}
\mathcal{X}(0,z) &= 0,\\
\mathcal{X}(x,0) &= 1,\\
\mathcal{X}(x,\infty) &= 0.
\end{aligned}
$$

De fato, tentemos

$$
\xi = \frac{z}{\sqrt{4Dx/u}}.
$$

Esta variável é adimensional:

$$
[\![\xi]\!] = \frac{\mathsf{L}}{(\mathsf{L}^2\,\mathsf{T}^{-1}\mathsf{L}\mathsf{T}\,\mathsf{L}^{-1})^{1/2}} = 1.
$$

Nosso procedimento agora repete o do início do capítulo, "com x no lugar de t":

$$
\begin{aligned}
\frac{\partial \mathcal{X}}{\partial x} &= \frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi}\frac{\partial \xi}{\partial x}\\
&= -\frac{1}{2}\frac{z}{\sqrt{4D/u}}x^{-3/2}\frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi}\\
&= -\frac{1}{2}\frac{z}{\sqrt{4Dx/u}}x^{-1}\frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi}\\
&= -\frac{1}{2x}\xi\frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi}.
\end{aligned}
$$

Para as derivadas em z,

$$
\begin{aligned}
\frac{\partial \mathcal{X}}{\partial z} &= \frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi}\frac{\partial \xi}{\partial z}\\
&= \frac{1}{\sqrt{4Dx/u}}\frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi};\\
\frac{\partial^2 \mathcal{X}}{\partial z^2} &= \frac{\mathrm{d}}{\mathrm{d}\xi}\left[\frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi}\frac{\partial \xi}{\partial z}\right]\frac{\partial \xi}{\partial z}\\
&= \frac{\mathrm{d}}{\mathrm{d}\xi}\left[\frac{1}{\sqrt{4Dx/u}}\frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi}\right]\frac{1}{\sqrt{4Dx/u}}\\
&= \frac{1}{4Dx/u}\frac{\mathrm{d}^2\mathcal{X}}{\mathrm{d}\xi^2}
\end{aligned}
$$

Substituímos agora em

$$
\begin{aligned}
u\frac{\partial \mathcal{X}}{\partial x} &= D\frac{\partial^2 \mathcal{X}}{\partial z^2},\\
-u\frac{1}{2x}\xi\frac{\mathrm{d}c}{\mathrm{d}\xi} &= \frac{D}{4Dx/u}\frac{\mathrm{d}^2\mathcal{X}}{\mathrm{d}\xi^2},\\
\frac{\mathrm{d}^2\mathcal{X}}{\mathrm{d}\xi^2} + 2\xi\frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi} &= 0.
\end{aligned}
$$

As duas condições de contorno em ϕ serão:

$$
\begin{aligned}
\mathcal{X}(0) &= 1,\\
\mathcal{X}(\infty) &= 0.
\end{aligned}
$$

O problema que temos em mãos é exatamente o mesmo de antes, de forma que já temos a solução!

$$\mathcal{X}(\xi) = 1 - \operatorname{erf}(\xi) \blacksquare$$

Considere agora a seguinte mudança *aparentemente* simples na nossa EDP. Vamos trocar u constante por uma função de z.

Considere a seguinte variação do "problema de Sutton":

$$u\frac{\partial \mathcal{X}}{\partial x} = \frac{\partial}{\partial z}\left[D\frac{\partial \mathcal{X}}{\partial z}\right]; \qquad \mathcal{X}(0,z) = 0,\ \mathcal{X}(x,0) = 1,\ \mathcal{X}(x,\infty) = 0.$$

Suponha agora que u e D variam com z segundo

$$\begin{aligned} u(z) &= az^m, \\ D(z) &= bz^n. \end{aligned}$$

Nós vamos supor que vale uma forma bem forte da *analogia de Reynolds* (Reynolds, 1900; Dias, 2013):

$$\begin{aligned} E/\rho &= -D\frac{\partial q}{\partial z}, \\ \tau/\rho &= +D\frac{\partial u}{\partial z} = Dmaz^{m-1} = mabz^{n+m-1}. \end{aligned}$$

Aqui, E é o fluxo de massa turbulento de vapor d'água, e τ é o fluxo de quantidade de movimento turbulento. Uma idéia importante em mecânica dos fluidos é que τ não depende de z em uma região próxima da superfície, denominda "sub-camada dinâmica". Se τ não depende de z, então, devemos ter

$$n + m = 1.$$

Além disso, az^m e bz^n não deixam claras as *dimensões*! Podemos contornar esse problema usando um outro conceito clássico em mecânica dos fluidos e turbulência: o conceito de *rugosidade* da superfície. Escrevamos então as equações em termos da velocidade de atrito u_* e dessa rugosidade:

$$\begin{aligned} \tau/\rho &\equiv u_*^2, \\ \frac{u}{u_*} &= c\left(\frac{z}{z_0}\right)^m. \end{aligned}$$

Note também que teremos

$$\tau/\rho = u_*^2 = mab.$$

Agora, é possível obter D em função de u_*, z_0, c e m da seguinte forma:

$$\begin{aligned} u(z) &= az^m = cu_*\left(\frac{z}{z_0}\right)^m, \\ D(z) &= bz^n = du_*z_0\left(\frac{z}{z_0}\right)^{1-m}. \end{aligned}$$

As equações acima foram escritas de forma a explicitar as *dimensões físicas* corretas de u e de D. Nelas, c e d (ao contrário de a e de b) são coeficientes adimensionais. Em seguida,

$$\begin{aligned} mab &= u_*^2, \\ m\left(cu_*z_0^{-m}\right)\left(du_*z_0^{m}\right) &= u_*^2, \\ d &= \frac{1}{mc}. \end{aligned}$$

Desse modo, a expressão para a difusividade turbulenta será

$$D = \frac{u_*}{mc} z_0^m z^{1-m}.$$

Reforcemos nosso ponto: nas equações acima, m e c são adimensionais; $[\![u_*]\!] = [\![u]\!] = \mathsf{L}\mathsf{T}^{-1}$; $[\![x]\!] = [\![z]\!] = [\![z_0]\!] = \mathsf{L}$ e $[\![D]\!] = \mathsf{L}^2\mathsf{T}^{-1}$. Usando a variável de similaridade

$$\xi = \frac{mc^2}{(2m+1)^2} \left(\frac{z}{z_0}\right)^{2m} \frac{z}{x},$$

vamos obter uma equação diferencial *ordinária* na variável independente ξ, e as condições de contorno que ela deve atender. Trata-se de um exercício de aplicação sistemática da regra da cadeia:

$$\begin{aligned}
\xi &= \left[\frac{mc^2}{(2m+1)^2} z_0^{-2m}\right] z^{2m+1} x^{-1};\\
\frac{\partial \xi}{\partial x} &= -\left[\frac{mc^2}{(2m+1)^2} z_0^{-2m}\right] z^{2m+1} x^{-2};\\
\frac{\partial \xi}{\partial z} &= (2m+1)\left[\frac{mc^2}{(2m+1)^2} z_0^{-2m}\right] x^{-1} z^{2m} = \left[\frac{mc^2}{(2m+1)} z_0^{-2m}\right] x^{-1} z^{2m}.
\end{aligned}$$

Agora,

$$\begin{aligned}
u\frac{\partial \mathcal{X}}{\partial x} &= u \frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi} \frac{\partial \xi}{\partial x}\\
&= -u \left[\frac{mc^2}{(2m+1)^2} z_0^{-2m}\right] z^{2m+1} x^{-2} \frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi}\\
&= -cu_* \left(\frac{z}{z_0}\right)^m \left[\frac{mc^2}{(2m+1)^2} z_0^{-2m}\right] z^{2m+1} x^{-2} \frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi}\\
&= -\frac{mc^3}{(2m+1)^2} u_* z_0^{-3m} z^{3m+1} x^{-2} \frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi};\\
&= -\left[\frac{mc^3 u_* z_0^{-3m}}{(2m+1)^2}\right] z^{3m+1} x^{-2} \frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi};\\
D\frac{\partial \mathcal{X}}{\partial z} &= \frac{u_*}{mc} z_0^m z^{1-m} \frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi} \frac{\partial \xi}{\partial z}\\
&= \frac{u_*}{mc} z_0^m z^{1-m} \left[\frac{mc^2}{(2m+1)} z_0^{-2m}\right] x^{-1} z^{2m} \frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi}\\
&= \left[\frac{u_* c z_0^{-m}}{(2m+1)}\right] z^{m+1} x^{-1} \frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi};\\
\frac{\partial}{\partial z}\left[D\frac{\partial \mathcal{X}}{\partial z}\right] &= \left[\frac{u_* c z_0^{-m}}{(2m+1)}\right] \left[(m+1)x^{-1} z^m \frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi} + z^{m+1} x^{-1} \frac{\mathrm{d}^2\mathcal{X}}{\mathrm{d}\xi^2} \frac{\partial \xi}{\partial z}\right]\\
&= \left[\frac{u_* c z_0^{-m}}{(2m+1)}\right] \left[(m+1)x^{-1} z^m \frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi} + \left[\frac{mc^2}{(2m+1)} z_0^{-2m}\right] z^{3m+1} x^{-2} \frac{\mathrm{d}^2\mathcal{X}}{\mathrm{d}\xi^2}\right]\\
&= \left[\frac{u_* c z_0^{-m}}{(2m+1)}\right] (m+1)x^{-1} z^m \frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi} + \left[\frac{u_* mc^3 z_0^{-3m}}{(2m+1)^2}\right] z^{3m+1} x^{-2} \frac{\mathrm{d}^2\mathcal{X}}{\mathrm{d}\xi^2}.
\end{aligned}$$

Reunindo todos os termos na equação diferencial original:

$$
\begin{aligned}
-u\frac{\partial \mathcal{X}}{\partial x} + \frac{\partial}{\partial z}\left[D\frac{\partial \mathcal{X}}{\partial z}\right] &= 0;\\
\left[\frac{mc^3 u_* z_0^{-3m}}{(2m+1)^2}\right] z^{3m+1}x^{-2}\frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi} + \left[\frac{u_* c z_0^{-m}}{(2m+1)}\right](m+1)x^{-1}z^m\frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi} + \left[\frac{u_* mc^3 z_0^{-3m}}{(2m+1)^2}\right] z^{3m+1}x^{-2}\frac{\mathrm{d}^2\mathcal{X}}{\mathrm{d}\xi^2} &= 0;\\
(2m+1)\left[\frac{mc^2 z_0^{-2m}}{(2m+1)^2}\right] z^{2m+1}x^{-1}\frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi} + (m+1)\frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi} + (2m+1)\left[\frac{mc^2 z_0^{-2m}}{(2m+1)^2}\right] z^{2m+1}x^{-1}\frac{\mathrm{d}^2\mathcal{X}}{\mathrm{d}\xi^2} &= 0.
\end{aligned}
$$

A equação diferencial que se obtém é

$$
(2m+1)\xi\frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi} + (m+1)\frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi} + (2m+1)\xi\frac{\mathrm{d}^2\mathcal{X}}{\mathrm{d}\xi^2} = 0.
$$

As condições de contorno em $\mathcal{X}(\xi)$ são as mesmas de antes:

$$
\begin{aligned}
\mathcal{X}(0) &= 1,\\
\mathcal{X}(\infty) &= 0.
\end{aligned}
$$

Vale a pena, por simplicidade, escrever

$$
\begin{aligned}
\beta &= (2m+1),\\
\delta &= (m+1),
\end{aligned}
$$

e então reduzir a ordem:

$$
\begin{aligned}
F &= \frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi},\\
\beta\xi\frac{\mathrm{d}F}{\mathrm{d}\xi} + \beta\xi F + \delta F &= 0.
\end{aligned}
$$

Curiosamente, esta é também uma equação separável:

$$
\begin{aligned}
\beta\xi\mathrm{d}F + \beta\xi F\mathrm{d}\xi + \delta F\mathrm{d}\xi &= 0,\\
\beta\mathrm{d}F + \beta F\mathrm{d}\xi + \delta F\frac{\mathrm{d}\xi}{\xi} &= 0,\\
\beta\frac{\mathrm{d}F}{F} + \beta\mathrm{d}\xi + \delta\frac{\mathrm{d}\xi}{\xi} &= 0,\\
\frac{\mathrm{d}F}{F} &= -\left(1 + \frac{\delta}{\beta\xi}\right)\mathrm{d}\xi,
\end{aligned}
$$

Por simplicidade, vamos supor que $F > 0$, $\xi > 0$ (vai funcionar). Então,

$$
\begin{aligned}
\ln F &= -\xi + \left(-\frac{\delta}{\beta}\ln(\xi)\right) + c_1\\
&= -\xi + \ln(\xi)^{-\delta/\beta} + c_1,\\
F(\xi) &= \exp\left(c_1 - \xi + \ln(\xi)^{-\delta/\beta}\right)\\
&= k_1\mathrm{e}^{-\xi}\xi^{-\frac{\delta}{\beta}}.
\end{aligned}
$$

Uma solução já está praticamente disponível:

$$
\begin{aligned}
\frac{\mathrm{d}\mathcal{X}}{\mathrm{d}\xi} &= k_1 \mathrm{e}^{-\xi} \xi^{-\frac{\delta}{\beta}};\\
\int_\xi^\infty \mathrm{d}\mathcal{X} &= k_1 \int_\xi^\infty \mathrm{e}^{-y} y^{-\frac{\delta}{\beta}}\,\mathrm{d}y;\\
\mathcal{X}(\infty) - \mathcal{X}(\xi) &= k_1 \int_\xi^\infty \mathrm{e}^{-y} y^{-\frac{\delta}{\beta}}\,\mathrm{d}y.
\end{aligned}
$$

Com um pouco de tarimba, é possível ver a função Gama completa:

$$
\Gamma\left(1 - \frac{\delta}{\beta}\right) = \int_0^\infty \mathrm{e}^{-y} y^{-\frac{\delta}{\beta}}\,\mathrm{d}y.
$$

Além disso, existe a Gama *incompleta*, cuja definição é

$$
P(a, \xi) \equiv \frac{1}{\Gamma(a)} \int_0^\xi \mathrm{e}^{-t} t^{a-1}\,\mathrm{d}t.
$$

Temos então, em termos dessas criaturas:

$$
\begin{aligned}
\mathcal{X}(\infty) - \mathcal{X}(\xi) &= k_1 \left[\Gamma\left(1 - \frac{\delta}{\beta}\right) - \int_0^\xi \mathrm{e}^{-y} y^{-\frac{\delta}{\beta}}\,\mathrm{d}y\right]\\
&= k_1 \Gamma\left(1 - \frac{\delta}{\beta}\right)\left[1 - P\left(1 - \frac{\delta}{\beta}, \xi\right)\right]\\
-\mathcal{X}(\xi) &= k_1 \Gamma\left(1 - \frac{\delta}{\beta}\right)\left[1 - P\left(1 - \frac{\delta}{\beta}, \xi\right)\right].
\end{aligned}
$$

Mas $P(a, 0) = 0$; com $\mathcal{X}(0) = 1$ temos:

$$
\begin{aligned}
-1 &= -\mathcal{X}(0) = k_1 \Gamma\left(1 - \frac{\delta}{\beta}\right),\\
k_1 &= -\frac{1}{\Gamma\left(1 - \frac{\delta}{\beta}\right)},
\end{aligned}
$$

e

$$
\mathcal{X}(\xi) = 1 - P\left(1 - \frac{\delta}{\beta}, \xi\right) \quad \blacksquare
$$

Lesson 4

Matched asymptotics and singular perturbation

We will follow van Dyke (1964)'s Chapter 5 closely. To understand what "singular perturbation" means, the best way is to quote van Dyke directly:

> The classical warning of singular behavior is familiar from Prandtl's boundary-layer theory. A small parameter multiplies one of the highest derivatives in the differential equations. Then in a straightforward perturbation scheme that derivative is lost in the first approximation so that the order of the equations is reduced. One of more boundary conditions must be abandoned, and the approximation breaks down near where they were to be imposed.

(van Dyke, 1964, p. 78)

We also use the same example as van Dyke. Consider the boundary-value problem

$$\epsilon \frac{d^2 f}{dx^2} + \frac{df}{dx} = a, \qquad f(0) = 0, \qquad f(1) = 1. \tag{4.1}$$

How do you solve this equation *exactly*? It is rather easy, because this is a *linear* equation, with constant coefficients (but non-homogeneous).

Exercise 4.1 Study classification of ordinary differential equations. What is a linear equation? What is its order? What is a homogeneous equation? Etc..

There are two ways to solve (4.1) *exactly*; one is to attack a second-order directly, for example using the method of variation of parameters, or by guessing a particular solution and then summing the homogeneous solution (you are supposed to know about this); the other is by reduction of order, which is somewhat easier and more straightforward. Let's do the second one. Put

$$g = \frac{df}{dx};$$

then (4.1) becomes

$$\epsilon \frac{dg}{dx} + g = a.$$

My preferred way to solve the above equation *systematically* is to write $g = uv$ and proceed:

$$\begin{aligned}
\epsilon\left[u\frac{\mathrm{d}v}{\mathrm{d}x} + v\frac{\mathrm{d}u}{\mathrm{d}x}\right] + uv &= a;\\
u\left[\epsilon\frac{\mathrm{d}v}{\mathrm{d}x} + v\right] + \epsilon v\frac{\mathrm{d}u}{\mathrm{d}x} &= a.
\end{aligned}$$

Now set the term inside brackets to zero:

$$\begin{aligned}
\epsilon\frac{\mathrm{d}v}{\mathrm{d}x} + v &= 0,\\
\epsilon\frac{\mathrm{d}v}{\mathrm{d}x} &= -v\\
\frac{\mathrm{d}v}{v} &= -\frac{\mathrm{d}x}{\epsilon}\\
\int_{v_0}^{v}\frac{\mathrm{d}v'}{v'} &= -\frac{x}{\epsilon},\\
\ln\frac{v}{v_0} &= -\frac{x}{\epsilon},\\
v &= v_0\exp\left(-\frac{x}{\epsilon}\right),
\end{aligned}$$

and substitute back in the remainder of the equation:

$$\begin{aligned}
\epsilon v_0\exp\left(-\frac{x}{\epsilon}\right)\frac{\mathrm{d}u}{\mathrm{d}x} &= a,\\
\mathrm{d}u &= \frac{a}{v_0}\exp\left(\frac{x}{\epsilon}\right)\frac{\mathrm{d}x}{\epsilon},\\
u - u_0 &= \frac{a}{v_0}\int_0^x \exp\left(\frac{x'}{\epsilon}\right)\frac{\mathrm{d}x'}{\epsilon}\\
u - u_0 &= \frac{a}{v_0}\left[\exp\left(\frac{x}{\epsilon}\right) - 1\right].
\end{aligned}$$

Hence,

$$\begin{aligned}
g(x) = uv &= \left\{u_0 + \frac{a}{v_0}\left[\exp\left(\frac{x}{\epsilon}\right) - 1\right]\right\} v_0\exp\left(-\frac{x}{\epsilon}\right)\\
&= u_0 v_0\exp\left(-\frac{x}{\epsilon}\right) + a - a\exp\left(-\frac{x}{\epsilon}\right)\\
&= g_0\exp\left(-\frac{x}{\epsilon}\right) + a - a\exp\left(-\frac{x}{\epsilon}\right)\\
&= (g_0 - a)\exp\left(-\frac{x}{\epsilon}\right) + a.
\end{aligned}$$

Because the order was reduced, we still need to integrate this:

$$\begin{aligned}
\frac{\mathrm{d}f}{\mathrm{d}x} &= (g_0 - a)\exp\left(-\frac{x}{\epsilon}\right) + a\\
\mathrm{d}f &= -(g_0 - a)\epsilon\exp\left(-\frac{x}{\epsilon}\right)\left(-\frac{\mathrm{d}x}{\epsilon}\right) + a\mathrm{d}x\\
f - f_0 &= -(g_0 - a)\epsilon\int_0^x \exp\left(-\frac{x'}{\epsilon}\right)\left(-\frac{\mathrm{d}x'}{\epsilon}\right) + a\int_0^x \mathrm{d}x'\\
f &= f_0 - (g_0 - a)\epsilon\left[\exp\left(-\frac{x}{\epsilon}\right) - 1\right] + ax
\end{aligned}$$

But

$$f(0) = 0 \;\Rightarrow\; f_0 = 0.$$

and

$$\begin{aligned} f(1) = 1 \;\Rightarrow \\ (g_0 - a)\epsilon\left[1 - \exp\left(-\frac{1}{\epsilon}\right)\right] + a = 1 \\ (g_0 - a) = \frac{1-a}{\epsilon\left[1 - \exp\left(-\frac{1}{\epsilon}\right)\right]}, \end{aligned}$$

so that finally

$$f(x) = (1-a)\frac{\left[1 - \exp\left(-\frac{x}{\epsilon}\right)\right]}{\left[1 - \exp\left(-\frac{1}{\epsilon}\right)\right]} + ax. \tag{4.2}$$

This is the full solution but we can also look at the differential equation when $\epsilon = 0$; this will lead to a different, simplified ODE, whose solution will also be different; let us call it f_o (for "outer solution"):

$$\frac{\mathrm{d}f_o}{\mathrm{d}x} = a. \tag{4.3}$$

This immediately leads to

$$f_o(x) = ax + b, \tag{4.4}$$

where b is the only constant of integration. Therefore, only one of the boundary conditions in (4.1) can be satisfied. Which one? We choose to satisfy $f(1) = 1$ because, as we shall see, we will need to stretch the x coordinate to understand better the behavior of the equation close to $x = 0$. Then,

$$1 = a + b; \;\Rightarrow\; b = 1 - a,$$

and the "outer" solution is

$$f_o = (1-a) + ax. \tag{4.5}$$

Now let us see what this stretching of coordinates is all about. The idea is to change the coordinates in a way that removes the ϵ from the highest-order derivative in the EDO. The only way to do this is to incorporate ϵ into the independent variable itself. Here is how to do it: put

$$X = \frac{x}{\epsilon} \;\Rightarrow\; x = \epsilon X; \tag{4.6}$$

$$F(X) = f\left(\frac{x}{\epsilon}\right). \tag{4.7}$$

Then the chain rule gives

$$\frac{\mathrm{d}F}{\mathrm{d}X} = \frac{\mathrm{d}f}{\mathrm{d}x}\frac{\mathrm{d}x}{\mathrm{d}X} = \epsilon\frac{\mathrm{d}f}{\mathrm{d}x}, \tag{4.8}$$

$$\frac{\mathrm{d}^2F}{\mathrm{d}X^2} = \epsilon^2\frac{\mathrm{d}^2f}{\mathrm{d}x^2}. \tag{4.9}$$

Now,

$$
\begin{aligned}
\epsilon \frac{\mathrm{d}^2 f}{\mathrm{d}x^2} + \frac{\mathrm{d}f}{\mathrm{d}x} &= a, \\
\epsilon^2 \frac{\mathrm{d}^2 f}{\mathrm{d}x^2} + \epsilon \frac{\mathrm{d}f}{\mathrm{d}x} &= \epsilon a, \\
\frac{\mathrm{d}^2 F}{\mathrm{d}X^2} + \frac{\mathrm{d}F}{\mathrm{d}X} &= \epsilon a, \qquad (4.10) \\
F(0) = 0, \qquad F\left(\frac{1}{\epsilon}\right) &= 1. \qquad (4.11)
\end{aligned}
$$

If you are very very close to the boundary $x = 0$, measuring things in X zooms in the behavior of the function. But because ϵ is small, we can solve the approximate version, with zero on the right hand side. We call this the approximate "inner solution" f_i and again we resort to reduction of order:

$$
\begin{aligned}
\frac{\mathrm{d}^2 f_i}{\mathrm{d}X^2} + \frac{\mathrm{d}f_i}{\mathrm{d}X} &= 0; \\
g_i &= \frac{\mathrm{d}f_i}{\mathrm{d}X}; \\
\frac{\mathrm{d}g_i}{\mathrm{d}X} + g_i &= 0; \\
g_i(X) &= g_0 \exp(-X); \\
\frac{\mathrm{d}f_i}{\mathrm{d}X} &= g_0 \exp(-X); \\
\mathrm{d}f_i &= -g_0 \exp(-X)\mathrm{d}(-X); \\
f_i - f_0 &= -g_0 \left[\exp(-X) - 1\right]; \\
f_i(X) &= f_0 - g_0 \left[\exp(-X) - 1\right]. \qquad (4.12)
\end{aligned}
$$

There are now two constants of integration, f_0 and g_0. In the new variable, the original boundary condtions are given by (4.11), but using them for the *approximate* solution f_i will not give the right answer. Instead, we set

$$
\begin{aligned}
f_i(0) = 0, \ &\Rightarrow f_0 = 0, \qquad (4.13) \\
\lim_{X\to\infty} f_i(X) = \lim_{x\to 0} f_o(x) = (1-a) \ &\Rightarrow g_0 = (1-a), \qquad (4.14) \\
f_i(X) = (1-a)\left[1 - \exp(-X)\right]&. \qquad (4.15)
\end{aligned}
$$

(4.14) gives the *overlap* solution

$$
f_{\text{over}}(x) = (1-a); \qquad (4.16)
$$

it appears both in the inner and the outer solutions. If we sum them, it is being counted twice. A composite solution, which behaves correctly as $X \to 0$ and as $x \to 1$, is the sum of the inner with the outer minus the overlap. Therefore, a good approximate solution is

$$
\begin{aligned}
f_c(x) &= f_i(X) + f_o(x) - f_{\text{over}} \\
&= (1-a)\left[1 - \exp\left(-\frac{x}{\epsilon}\right)\right] + ax. \qquad (4.17)
\end{aligned}
$$

We compare f, f_o, f_i and f_c with $a = 0.6$ and $\epsilon = 0.1$ in figure 4.1

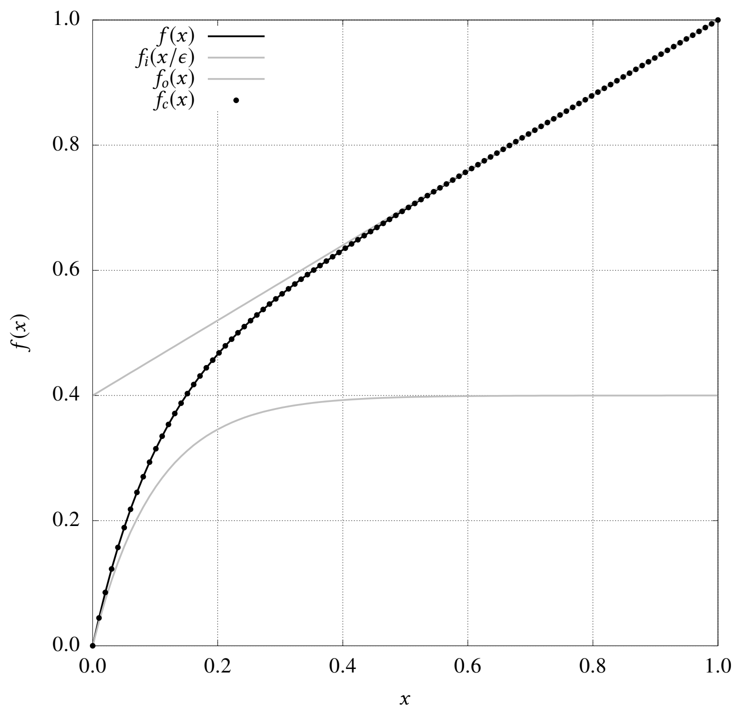

Figure 4.1: Asymptotic matching for (4.1), with $a = 0.6$ and $\epsilon = 0.1$. The composite solution is indicated by the filled circles.

Because in this case we know the analytic solution, the whole exercise may seem redundant. It is not. Having an analytical solution is an important step in testing approximate methods, because then we can obviously verify how good the approximations are. In this case, clearly, $f_c(x)$ is an excellent approximation to $f(x)$.

Moreover, although in this case the difficulty of finding the exact solution is not great, one can still note that the two approximate solutions $f_o(x)$ and $f_i(X)$ can be found more easily: f_0 comes from the solution of a (trivial) first-order EDO, whereas f_i is obtained as the solution of a second-order *homogeneous* equation.

In general, we will seek to find solutions using approximate EDOs (or EDPs) that are relatively simple to solve; and at least simpler than the full original EDOs or EDPs. The point is that in real applications the original equations may be impossible to solve (or their solution may not yet have been found), whereas the approximate ones are.

Lesson 5

The stream function and the elimination of pressure

5.1 The Navier-Stokes equations

Consider cartesian coordinates x, y, and admit that y may be the vertical direction. The acceleration of gravity vector $\boldsymbol{g}$ points downwards, so that

$$\boldsymbol{g} = -g\boldsymbol{j}, \tag{5.1}$$

where g is the magnitude of $\boldsymbol{g}$.

The two-dimensional version of the steady-state and incompressible Navier-Stokes equations is

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \tag{5.2}$$

$$u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial x} + \nu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right), \tag{5.3}$$

$$u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial y} - g + \nu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right), \tag{5.4}$$

where ρ is fluid density, u and v are the fluid velocities along x and y, p is pressure, There is a slight asymmetry due to the presence of g in (5.4). In the case of flow with constant density ρ (which we will assume here) this asymmetry can be eliminated with the introduction of the *modified pressure* p:

$$p \equiv p + \rho g y; \;\Rightarrow \tag{5.5}$$

$$-\frac{1}{\rho}\frac{\partial p}{\partial x} = -\frac{1}{\rho}\frac{\partial p}{\partial x};$$

$$-\frac{1}{\rho}\frac{\partial p}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial y} - g.$$

$$\tag{5.6}$$

Substituition in (5.3)–(5.4) yields

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \tag{5.7}$$

$$u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial x} + \nu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right), \tag{5.8}$$

$$u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial y} + \nu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right), \tag{5.9}$$

which is symmetric in (5.8)–(5.9).

Exercise 5.1 The equations above can be written in vector notation as

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = \boldsymbol{0}, \tag{5.10}$$

$$\boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} = -\boldsymbol{\nabla} p + \nu \nabla^2 \boldsymbol{u}, \tag{5.11}$$

with

$$\boldsymbol{u} = u\boldsymbol{i} + v\boldsymbol{j}. \tag{5.12}$$

Discuss every appearance of $\boldsymbol{\nabla}$ or ∇ above and their connections with the divergence, the gradient, the laplacian, and the "advective operator"

$$\boldsymbol{u} \cdot \boldsymbol{\nabla} \equiv u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y}. \tag{5.13}$$

Alternatively, one can also see $\boldsymbol{\nabla u}$ as the gradient of the vector field $\boldsymbol{u}$.

5.2 Elimination of pressure

In an incompressible flow, there is a *Poisson equation* for p. To see this, take the divergence of (5.8)–(5.9), *i.e.* $\frac{\partial}{\partial x}$(5.8) + $\frac{\partial}{\partial y}$(5.9), keeping in mind that the *order of differentiation* can be swapped:

$$\frac{\partial}{\partial x}\left[u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}\right] = -\frac{\partial}{\partial x}\frac{\partial p}{\partial x} + \frac{\partial}{\partial x}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right), \tag{5.14}$$

$$\frac{\partial}{\partial y}\left[u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y}\right] = -\frac{\partial}{\partial y}\frac{\partial p}{\partial y} + \frac{\partial}{\partial y}\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right). \tag{5.15}$$

The sum of the left-hand sides of (5.14)–(5.15) is

$$\frac{\partial u}{\partial x}\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y}\frac{\partial v}{\partial x} + u\frac{\partial}{\partial x}\underbrace{\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)}_{\equiv 0} + \frac{\partial v}{\partial x}\frac{\partial u}{\partial y} + \frac{\partial v}{\partial y}\frac{\partial v}{\partial y} + v\frac{\partial}{\partial y}\underbrace{\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)}_{\equiv 0} =$$

$$\frac{\partial u}{\partial x}\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y}\frac{\partial v}{\partial x} + \frac{\partial v}{\partial x}\frac{\partial u}{\partial y} + \frac{\partial v}{\partial y}\frac{\partial v}{\partial y}. \tag{5.16}$$

The sum of the right-hand sides of (5.14)–(5.15) is

$$-\left(\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2}\right) + \frac{\partial^2}{\partial x^2}\underbrace{\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)}_{\equiv 0} + \frac{\partial^2}{\partial y^2}\underbrace{\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)}_{\equiv 0} =$$

$$-\left(\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2}\right). \tag{5.17}$$

The final Poisson equation for the modified pressure, therefore, is

$$-\left(\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2}\right) = \frac{\partial u}{\partial x}\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y}\frac{\partial v}{\partial x} + \frac{\partial v}{\partial x}\frac{\partial u}{\partial y} + \frac{\partial v}{\partial y}\frac{\partial v}{\partial y}. \tag{5.18}$$

Exercise 5.2 Show that the vector form of (5.18) is

$$-\nabla^2 p = \boldsymbol{\nabla u} : \boldsymbol{\nabla u}. \tag{5.19}$$

Discuss the **:** operator.

The meaning of (5.18) is profound: in an incompressible flow, if you know the velocity field at every point, you can recover the pressure field by integrating (*i.e.*, by solving) (5.18). This is often used, for example, in numerical solutions of the Navier-Stokes equations.

5.3 The stream function

The stream function ψ is defined by

$$u \equiv \frac{\partial \psi}{\partial y}, \tag{5.20}$$

$$v \equiv -\frac{\partial \psi}{\partial x}. \tag{5.21}$$

For two-dimensional flows, the geometric meaning of the stream function is quite simple: ψ = const along a streamline (a streamline is a line tangential to the velocity field at every point). To see this, put

$$\psi = \text{const} \;\Rightarrow \qquad \mathrm{d}\psi = \frac{\partial \psi}{\partial x}\mathrm{d}x + \frac{\partial \psi}{\partial y}\mathrm{d}y = 0;$$

$$-v\mathrm{d}x + u\mathrm{d}y = 0;$$

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{v}{u}. \tag{5.22}$$

We can eliminate the pressure from the Navier-Stokes equations by calculating, now, $\frac{\partial}{\partial y}$(5.8) $-$ $\frac{\partial}{\partial x}$(5.9):

$$\frac{\partial}{\partial y}\left[u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}\right] = -\frac{\partial}{\partial y}\frac{\partial p}{\partial x} + \frac{\partial}{\partial y}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right), \tag{5.23}$$

$$\frac{\partial}{\partial x}\left[u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y}\right] = -\frac{\partial}{\partial x}\frac{\partial p}{\partial y} + \frac{\partial}{\partial x}\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right). \tag{5.24}$$

The difference of the left-hand sides of (5.23)–(5.24 is

$$u\frac{\partial}{\partial x}\frac{\partial u}{\partial y} + v\frac{\partial}{\partial y}\frac{\partial u}{\partial y} + \frac{\partial u}{\partial y}\underbrace{\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)}_{\equiv 0}$$

$$- u\frac{\partial}{\partial x}\frac{\partial v}{\partial x} - v\frac{\partial}{\partial y}\frac{\partial v}{\partial x} - \frac{\partial v}{\partial x}\underbrace{\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)}_{\equiv 0} =$$

$$u\frac{\partial}{\partial x}\frac{\partial^2 \psi}{\partial y^2} + v\frac{\partial}{\partial y}\frac{\partial^2 \psi}{\partial y^2} + u\frac{\partial}{\partial x}\frac{\partial^2 \psi}{\partial x^2} + v\frac{\partial}{\partial y}\frac{\partial^2 \psi}{\partial x^2} =$$

$$u\frac{\partial}{\partial x}\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2}\right) + v\frac{\partial}{\partial y}\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2}\right). \tag{5.25}$$

The difference of the right-hand sides of (5.23)–(5.24 is

$$\underbrace{-\frac{\partial^2 p}{\partial y \partial x} + \frac{\partial^2 p}{\partial x \partial y}}_{\equiv 0} + \left(\frac{\partial^2}{\partial x^2}\frac{\partial u}{\partial y} + \frac{\partial^2}{\partial y^2}\frac{\partial u}{\partial y}\right) - \left(\frac{\partial^2}{\partial x^2}\frac{\partial v}{\partial x} + \frac{\partial^2}{\partial y^2}\frac{\partial v}{\partial x}\right) =$$
$$\left(\frac{\partial^2}{\partial x^2}\frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2}{\partial y^2}\frac{\partial^2 \psi}{\partial y^2}\right) + \left(\frac{\partial^2}{\partial x^2}\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2}{\partial y^2}\frac{\partial^2 \psi}{\partial x^2}\right) =$$
$$\frac{\partial^2}{\partial x^2}\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2}\right) + \frac{\partial^2}{\partial y^2}\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2}\right). \quad (5.26)$$

Putting everything together we have an *advection-diffusion equation* for the laplacian of ψ:

$$u\frac{\partial}{\partial x}\nabla^2\psi + v\frac{\partial}{\partial y}\nabla^2\psi = \nu\nabla^4\psi, \quad (5.27)$$

where

$$\nabla^4\psi \equiv \nabla^2\left(\nabla^2\psi\right). \quad (5.28)$$

Lesson 6

The Blasius boundary-layer solution over a flat plate

6.1 Posing the problem

Consider again the Navier-Stokes equations, and flow over a flat plate, shown in figure 6.1. Experiment indicates that the horizontal velocity u varies from 0 (the no-slip condition) to u_∞ (the approaching uniform velocity field) over a small distance δ in comparison with the plate's length L. We anticipate that the boundary-layer thickness grows with x, and later we will use the notation $\delta(x)$ to indicate this, but for now just let δ be the maximum thickness at $x = L$; the important point is that

$$\frac{\delta}{L} \ll 1. \tag{6.1}$$

The problem that we want to solve is the set of Navier-Stokes equations (5.7)–(5.9) in the domain $0 \le x \le L$ and $0 \le y < \infty$, with appropriate boundary conditions:

$$u(0, y) = u_\infty, \qquad v(0, y) = 0, \tag{6.2}$$

$$u(x, 0) = 0, \qquad v(x, 0) = 0, \tag{6.3}$$

$$u(x, \infty) = u_\infty, \qquad v(x, \infty) = 0, \tag{6.4}$$

$$u(L, y) = ?, \qquad v(L, y) = ?, \tag{6.5}$$

$$p(0, y) = p_0, \qquad p(x, \infty) = p_0. \tag{6.6}$$

The presence of second partial derivatives in x and y in the Navier-Stokes equations requires that we specify the velocity field (u, v) at both ends of the plate, $x = 0$ and $x = L$. In particular, it requires a very detailed knowledge of the flow at $x = L$, which is usually not available, hence the '?' signs.

Also note that we are assigning a constant pressure upstream of the plate, and far away from it. This will lead to $P = P_0$ throughout the flow.

Outside of the boundary-layer ($y > \delta$), however, the flow is very simple: on first approximation it is just $(u, v) = (u_\infty, 0)$, although the boundary-layer induces a small vertical component, as we shall see.

6.2 Non-dimensionalization of the Navier-Stokes equations for the flow over a flat plate

The next point is to investigate if (5.7)–(5.9) can be simplified somehow, particularly in light of (6.1). This usually requires estimates of the *order of magnitude*

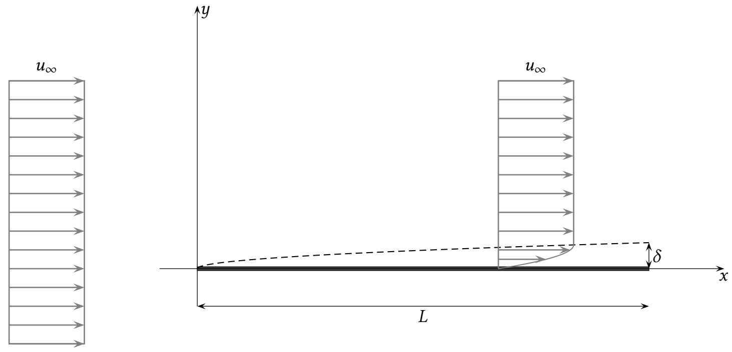

Figure 6.1: The boundary-layer over a flat plate.

of all terms, to see if some terms are so small compared to others that they can be dropped from the equation. Before doing this, we need to introduce the "big O" and "little o" notations.

Consider a function $f(\epsilon)$ whose behavior we want to analyze as $\epsilon \longrightarrow 0$. It is useful to compare $f(\epsilon)$ with a *gauge function* $\delta(\epsilon)$ whose behavior is known intuitively (van Dyke, 1964, p. 24); for example, one often uses $\delta(\epsilon) = \epsilon^m$, a power function.

Definition 6.1 We say that a function f is "of order" δ,

$$f(\epsilon) = O[\delta(\epsilon)]$$

as $\epsilon \longrightarrow 0$ if

$$\lim_{\epsilon \to 0} \frac{f(\epsilon)}{\delta(\epsilon)} = c < \infty. \tag{6.7}$$

If, moreover, c is in the vicinity of 1, $\sqrt{10^{-1}} < c < \sqrt{10}$, or $1/5 < c < 5$ (the latter being chosen by Tennekes e Lumley (1972, p. xiii)), we say that f and δ have the same *order of magnitude*, and use the notation

$$f \sim \delta.$$

On the other hand, f may decrease much faster than δ as ϵ approaches 0; then,

---

Definition 6.2 f is of higher order than δ,

$$f(\epsilon) = o[\delta(\epsilon)]$$

as $\epsilon \longrightarrow 0$ if

$$\lim_{\epsilon \to 0} \frac{f(\epsilon)}{\delta(\epsilon)} = 0. \tag{6.8}$$

Exercise 6.1 Study van Dyke (1964)'s examples in pages 24 and 25.

We now write down again the set (5.7)–(5.9)

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \tag{6.9}$$

$$u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial x} + \nu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right), \tag{6.10}$$

$$u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial y} + \nu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right). \tag{6.11}$$

To make a small parameter appear in the equations (remember chapter 4), we define the dimensionless quantities $\tilde{x}$, $\tilde{y}$, $\tilde{u}$, $\tilde{v}$ and $\tilde{p}$ via

$$x \equiv L\tilde{x}, \qquad y \equiv L\tilde{y}, \tag{6.12}$$

$$u \equiv u_\infty \tilde{u}, \qquad v \equiv u_\infty \tilde{v}, \tag{6.13}$$

$$p \equiv \rho u_\infty^2 \tilde{p}, \tag{6.14}$$

and substitute in (6.9)–(6.11). The continuity equation is

$$\frac{\partial \tilde{u}}{\partial \tilde{x}} + \frac{\partial \tilde{v}}{\partial \tilde{y}} = 0. \tag{6.15}$$

The x-momentum equation becomes

$$\begin{aligned}
\frac{u_\infty^2}{L}\left[\tilde{u}\frac{\partial \tilde{u}}{\partial \tilde{x}} + \tilde{v}\frac{\partial \tilde{u}}{\partial \tilde{y}}\right] &= -\frac{u_\infty^2}{L}\frac{\partial \tilde{p}}{\partial \tilde{x}} + \nu\frac{u_\infty}{L^2}\left(\frac{\partial^2 \tilde{u}}{\partial \tilde{x}^2} + \frac{\partial^2 \tilde{u}}{\partial \tilde{y}^2}\right),\\
\tilde{u}\frac{\partial \tilde{u}}{\partial \tilde{x}} + \tilde{v}\frac{\partial \tilde{u}}{\partial \tilde{y}} &= -\frac{\partial \tilde{p}}{\partial \tilde{x}} + \frac{\nu}{u_\infty L}\left(\frac{\partial^2 \tilde{u}}{\partial \tilde{x}^2} + \frac{\partial^2 \tilde{u}}{\partial \tilde{y}^2}\right),\\
\tilde{u}\frac{\partial \tilde{u}}{\partial \tilde{x}} + \tilde{v}\frac{\partial \tilde{u}}{\partial \tilde{y}} &= -\frac{\partial \tilde{p}}{\partial \tilde{x}} + \frac{1}{\mathrm{Re}_L}\left(\frac{\partial^2 \tilde{u}}{\partial \tilde{x}^2} + \frac{\partial^2 \tilde{u}}{\partial \tilde{y}^2}\right),
\end{aligned} \tag{6.16}$$

where the small parameter is the inverse of the Reynolds number

$$\mathrm{Re}_L = \frac{u_\infty L}{\nu}. \tag{6.17}$$

Similarly, the y-momentum equation becomes

$$\tilde{u}\frac{\partial \tilde{v}}{\partial \tilde{x}} + \tilde{v}\frac{\partial \tilde{v}}{\partial \tilde{y}} = -\frac{\partial \tilde{p}}{\partial \tilde{y}} + \frac{1}{\mathrm{Re}_L}\left(\frac{\partial^2 \tilde{v}}{\partial \tilde{x}^2} + \frac{\partial^2 \tilde{v}}{\partial \tilde{y}^2}\right). \tag{6.18}$$

6.3 An outer solution

Much as we did in chapter 4, we seek a (first-order) outer solution by solving the equations in the limit $\mathrm{Re}_L \to \infty$. Then, the second derivatives on the right-hand sides of (6.16) and (6.18) drop; moreover, the boundary-conditions at $y = 0$ can no longer be obeyed, because the higher derivatives have been lost. By the same token, either the boundary conditions at $x = 0$ or $x = L$ also have to be abandoned (we choose the latter).

Then, the approximate outer solution will be the solution of

$$\frac{\partial \tilde{u}_o}{\partial \tilde{x}} + \frac{\partial \tilde{v}_o}{\partial \tilde{y}} = 1, \tag{6.19}$$

$$\tilde{u}_o \frac{\partial \tilde{u}_o}{\partial \tilde{x}} + \tilde{v}_o \frac{\partial \tilde{u}_o}{\partial \tilde{y}} = -\frac{\partial \tilde{p}_o}{\partial x}, \tag{6.20}$$

$$\tilde{u}_o \frac{\partial \tilde{v}_o}{\partial \tilde{x}} + \tilde{v}_o \frac{\partial \tilde{v}_o}{\partial \tilde{y}} = -\frac{\partial \tilde{p}_o}{\partial y}, \tag{6.21}$$

$$\tilde{u}_o(0, \tilde{y}) = 1 \qquad \tilde{v}_o(0, \tilde{y}) = 0, \tag{6.22}$$

$$\tilde{u}_o(\tilde{x}, \infty) = 1 \qquad \tilde{v}_o(\tilde{x}, \infty) = 0, \tag{6.23}$$

$$\tilde{p}_o(0, \tilde{y}) = 1 \qquad \tilde{p}_o(\tilde{x}, \infty) = 1. \tag{6.24}$$

This is trivial, and the first-order outer solution is

$$\tilde{u}_o = 1, \tag{6.25}$$

$$\tilde{v}_o = 0, \tag{6.26}$$

$$\tilde{p}_o = 1. \tag{6.27}$$

Of course, the same non-dimensionalization can be applied to the stream function.

Exercise 6.2 Show that the non-dimensionalized form of the Navier-Stokes equations in the stream function ψ, Eq. (5.27), is

$$\tilde{u}\frac{\partial}{\partial \tilde{x}}\nabla^2\tilde{\psi} + \tilde{v}\frac{\partial}{\partial \tilde{y}}\nabla^2\tilde{\psi} = \frac{1}{\mathrm{Re}_L}\nabla^4\tilde{\psi},$$

where $\psi(x, y) = Lu_\infty\tilde{\psi}(\tilde{x}, \tilde{y})$.

In terms of $\tilde{\psi}$, the outer solution is the solution of

$$\left[\frac{\partial \tilde{\psi}_o}{\partial \tilde{x}_o} - \frac{\partial \tilde{\psi}_o}{\partial \tilde{y}}\right]\nabla^2\tilde{\psi}_o = 0, \tag{6.28}$$

$$\tilde{\psi}_o(0, \tilde{y}) = \tilde{y}, \tag{6.29}$$

$$\frac{\partial \tilde{\psi}_o}{\partial \tilde{y}}(\tilde{x}, \infty) = 1, \qquad -\frac{\partial \tilde{\psi}_o}{\partial \tilde{x}}(\tilde{x}, \infty) = 0. \tag{6.30}$$

Exercise 6.3 Show that (6.19)–(6.24) and (6.28)–(6.30) represent the same problem.

The solution is again trivial,

$$\tilde{\psi}_o(\tilde{x}, \tilde{y}) = \tilde{y}. \tag{6.31}$$

6.4 An inner solution

We now seek an inner solution that is valid close to the plate, where $\tilde{y} \ll 1$. We will stretch $\tilde{y}$ into a new variable Y,

$$Y = \frac{\tilde{y}}{\tilde{\delta}}, \tag{6.32}$$

with

$$\tilde{\delta} = \tilde{\delta}(\mathrm{Re}_L) \ll 1. \tag{6.33}$$

We want to transform the Navier-Stokes equations using this stretched variable. For the continuity equation, we must have

$$\frac{\partial \tilde{u}}{\partial \tilde{x}} + \frac{\partial\left(\frac{\tilde{v}}{\tilde{\delta}}\right)}{\partial\left(\frac{\tilde{y}}{\tilde{\delta}}\right)} = 0. \tag{6.34}$$

Note that

$$\tilde{x} \sim 1; \qquad \tilde{u} \sim 1 \qquad \text{and} \qquad \frac{\partial \tilde{u}}{\partial \tilde{x}} \sim 1; \tag{6.35}$$

therefore,

$$\frac{\tilde{v}}{\tilde{\delta}} \sim 1 \qquad \text{and} \qquad \frac{\tilde{y}}{\tilde{\delta}} \sim 1. \tag{6.36}$$

This at once establishes the order of $\tilde{v}$ in the boundary-layer: $\tilde{v} \sim \tilde{\delta}$. It also suggests the change of variables:

$$X = \tilde{x}, \qquad Y = \frac{\tilde{y}}{\tilde{\delta}}; \tag{6.37}$$

$$U(X,Y) \equiv \tilde{u}(\tilde{x}, \frac{y}{\tilde{\delta}}); \tag{6.38}$$

$$V(X,Y) \equiv \frac{1}{\tilde{\delta}}\tilde{v}(\tilde{x}, \frac{y}{\tilde{\delta}}); \tag{6.39}$$

$$P(X,Y) \equiv \tilde{p}(\tilde{x}, \frac{y}{\tilde{\delta}}). \tag{6.40}$$

With this, the continuity equation in the new variables becomes

$$\frac{\partial U}{\partial X} + \frac{\partial V}{\partial Y} = 0. \tag{6.41}$$

We now go to the y-momentum equation because, to first order, it is simpler! Of course, this can only be found on a trial-and-error basis. Anyhow, the re-scaled y-momentum equation in the stretched variable is

$$\tilde{u}\frac{\partial\left(\frac{\tilde{v}}{\tilde{\delta}}\right)}{\partial \tilde{x}} + \frac{\tilde{v}}{\tilde{\delta}}\frac{\partial\left(\frac{\tilde{v}}{\tilde{\delta}}\right)}{\partial\left(\frac{\tilde{y}}{\tilde{\delta}}\right)} = -\frac{1}{\tilde{\delta}}\frac{\partial \tilde{p}}{\partial\left(\frac{\tilde{y}}{\tilde{\delta}}\right)} + \frac{1}{\mathrm{Re}_L}\left[\frac{\partial^2\left(\frac{\tilde{v}}{\tilde{\delta}}\right)}{\partial \tilde{x}^2} + \frac{1}{\tilde{\delta}^2}\frac{\partial^2\left(\frac{\tilde{v}}{\tilde{\delta}}\right)}{\partial\left(\frac{\tilde{y}}{\tilde{\delta}}\right)^2}\right];$$

$$U\frac{\partial V}{\partial X} + V\frac{\partial V}{\partial Y} = -\frac{1}{\tilde{\delta}}\frac{\partial P}{\partial Y} + \frac{1}{\mathrm{Re}_L}\left[\frac{\partial^2 V}{\partial X^2} + \frac{1}{\tilde{\delta}^2}\frac{\partial^2 V}{\partial Y^2}\right]. \tag{6.42}$$

Note that all uppercase terms are ~ 1: $U\partial V/\partial X \sim V\partial V/\partial Y \sim \partial P/\partial Y \sim \partial^2 V/\partial X^2 \sim \partial^2 V/\partial Y^2 \sim 1$. Because $\tilde{\delta} \ll 1$, $\partial^2 V/\partial X^2 \ll (1/\tilde{\delta}^2)\partial^2 V/\partial Y^2$ and we now have the simplified equation

$$U\frac{\partial V}{\partial X} + V\frac{\partial V}{\partial Y} = -\frac{1}{\tilde{\delta}}\frac{\partial P}{\partial Y} + \frac{1}{\left[\mathrm{Re}_L\tilde{\delta}^2\right]}\frac{\partial^2 V}{\partial Y^2};$$

$$\tilde{\delta}\left[U\frac{\partial V}{\partial X} + V\frac{\partial V}{\partial Y}\right] = -\frac{\partial P}{\partial Y} + \frac{\tilde{\delta}}{\left[\mathrm{Re}_L\tilde{\delta}^2\right]}\frac{\partial^2 V}{\partial Y^2}. \tag{6.43}$$

As we will see from the x-momentum equation, $\mathrm{Re}_L\tilde{\delta}^2 \sim 1$; therefore, (6.43) involves two orders of magnitude, and effectively produces two equations, namely

$$0 = -\frac{\partial P}{\partial Y}, \tag{6.44}$$

$$U\frac{\partial V}{\partial X} + V\frac{\partial V}{\partial Y} = \frac{\partial^2 V}{\partial Y^2}. \tag{6.45}$$

It will be interesting, afterwards, to check if (6.45) obeys our solution for $V(X,Y)$, but for now it is enough to keep the *first-order* equation (6.44).

The re-scaled x-momentum equation in the stretched variable is

$$\tilde{u}\frac{\partial \tilde{u}}{\partial \tilde{x}} + \frac{\tilde{v}}{\tilde{\delta}}\frac{\partial \tilde{u}}{\partial\left(\frac{\tilde{y}}{\tilde{\delta}}\right)} = -\frac{\partial \tilde{p}}{\partial \tilde{x}} + \frac{1}{\mathrm{Re}_L}\left[\frac{\partial^2 \tilde{u}}{\partial \tilde{x}^2} + \frac{1}{\tilde{\delta}^2}\frac{\partial^2 \tilde{u}}{\partial\left(\frac{\tilde{y}}{\tilde{\delta}}\right)^2}\right];$$

$$U\frac{\partial U}{\partial X} + V\frac{\partial U}{\partial Y} = -\frac{\partial P}{\partial X} + \frac{1}{\mathrm{Re}_L}\left[\frac{\partial^2 U}{\partial X^2} + \frac{1}{\tilde{\delta}^2}\frac{\partial^2 U}{\partial Y^2}\right]. \tag{6.46}$$

There is a wealth of information to be extracted from (6.46):

1. $U\partial U/\partial X \sim V\partial U/\partial U \sim 1$; hence, the right-hand side must also be ~ 1.

2. Both second-order derivatives on the right-hand side are ~ 1; therefore, $(1/\tilde{\delta}^2)\partial^2 U/\partial Y^2 \gg \partial^2 U/\partial X^2$.

3. On account of 1. and 2., the inner equation can be approximated by

$$U\frac{\partial U}{\partial X} + V\frac{\partial U}{\partial Y} = -\frac{\partial P}{\partial X} + \frac{1}{[\mathrm{Re}_L\tilde{\delta}^2]}\frac{\partial^2 U}{\partial Y^2}. \tag{6.47}$$

4. But, since the right-hand side is ~ 1,

$$\mathrm{Re}_L\tilde{\delta}^2 \sim 1; \qquad \tilde{\delta} \sim \mathrm{Re}_L^{-1/2}. \tag{6.48}$$

Without loss of generality, we set

$$\tilde{\delta} = \mathrm{Re}_L^{-1/2}. \tag{6.49}$$

The system or inner partial differential equations that needs to be solved is (6.41) together with (6.44) and (6.46) with (6.49). We re-write them here:

$$\frac{\partial U}{\partial X} + \frac{\partial V}{\partial Y} = 0, \tag{6.50}$$

$$0 = -\frac{\partial P}{\partial Y}, \tag{6.51}$$

$$U\frac{\partial U}{\partial X} + V\frac{\partial U}{\partial Y} = -\frac{\partial P}{\partial X} + \frac{\partial^2 U}{\partial Y^2}. \tag{6.52}$$

We need boundary conditions for U and P at $X = 0$; for V at $Y = 0$; and for P and V at $Y \to \infty$. The latter 2 have to match the outer solution (6.25)–(6.27):

$$U(0,Y) = 1 \qquad V(0,Y) = 0, \tag{6.53}$$

$$U(X,0) = 0 \qquad V(X,0) = 0, \tag{6.54}$$

$$U(X,\infty) = 1 \qquad V(X,\infty) = 0, \tag{6.55}$$

$$P(0,Y) = 1 \qquad P(X,\infty) = 1. \tag{6.56}$$

It is easiest to start by solving (6.51):

$$\frac{\partial P}{\partial Y} = 0 \Rightarrow P(X,Y) = F(X),$$

where $F(X)$ is a function to be determined. But, from (6.56),

$$\lim_{Y\to\infty} F(X) = 1 \Rightarrow F(X) = 1 \Rightarrow P(X,Y) = 1.$$

This simplifies (6.50)–(6.52) even further to

$$\frac{\partial U}{\partial X} + \frac{\partial V}{\partial Y} = 0, \tag{6.57}$$

$$U\frac{\partial U}{\partial X} + V\frac{\partial U}{\partial Y} = \frac{\partial^2 U}{\partial Y^2}. \tag{6.58}$$

A solution has been obtained in terms of a stream function. By analogy with (5.20)–(5.21) let us put

$$U \equiv \frac{\partial \Psi}{\partial Y}, \tag{6.59}$$

$$V \equiv -\frac{\partial \Psi}{\partial X}. \tag{6.60}$$

Ψ and $\tilde{\psi}$ are connected:

$$\begin{aligned} V &= \frac{\tilde{v}}{\tilde{\delta}}; & X &= \tilde{x}; \\ V &= -\frac{\partial \Psi}{\partial X}; & \tilde{v} &= -\frac{\partial \tilde{\psi}}{\partial \tilde{x}}; \\ \frac{1}{\tilde{\delta}}\frac{\partial \tilde{\psi}}{\partial \tilde{x}} &= \frac{\partial \Psi}{\partial \tilde{x}} \quad \Rightarrow & \tilde{\psi} &= \tilde{\delta}\Psi. \end{aligned} \tag{6.61}$$

Substituting (6.59)–(6.60) into (6.58),

$$\frac{\partial \Psi}{\partial Y}\frac{\partial^2 \Psi}{\partial X \partial Y} - \frac{\partial \Psi}{\partial X}\frac{\partial^2 \Psi}{\partial Y^2} = \frac{\partial^3 \Psi}{\partial Y^3} \tag{6.62}$$

We need boundary equations for this equation, and they have to be translated from 6.53–6.55:

$$\Psi(0,Y) = Y, \tag{6.63}$$

$$\Psi(X,0) = 0, \qquad \frac{\partial \Psi(X,0)}{\partial Y} = 0, \tag{6.64}$$

$$\lim_{Y\to\infty} \Psi(X,Y) = \lim_{\tilde{y}\to 0} \frac{1}{\tilde{\delta}}\psi_o(\tilde{x},\tilde{y}) = \frac{\tilde{y}}{\tilde{\delta}} = Y. \tag{6.65}$$

There are 3 dimensionless variables in (6.62). Although, in principle, we look for a solution $\Psi(X,Y)$, it may be possible to rewrite the 3 variables in two groups such that a single relationship between them exists. This is usually called a *similarity transform*. If so, then it should be possible to reduce (6.62) to an ordinary differential equation. Above, note that $\Psi(0,Y) = \Psi(X,\infty)$. This is a necessary condition for a similarity transform involving X, Y and Ψ. The exact transform however has to be found: we seek a transformation of variables under which (6.58) remains invariant.

A simple method to find similarity transforms is to stretch each variable individually, and substitute back into the differential equation and its boundary conditions. Let us put

$$X' = \alpha X, \tag{6.66}$$
$$Y' = \beta Y, \tag{6.67}$$
$$\Psi' = \gamma \Psi; \tag{6.68}$$

then (6.62) becomes

$$\frac{\partial(\Psi'/\gamma)}{\partial(Y'/\beta)} \frac{\partial^2(\Psi'/\gamma)}{\partial(X'/\alpha)\partial(Y'/\beta)} - \frac{\partial(\Psi'/\gamma)}{\partial(X'/\alpha)} \frac{\partial^2(\Psi'/\gamma)}{\partial(Y'/\beta)^2} = \frac{\partial^3(\Psi'/\gamma)}{\partial(Y'/\beta)^3}$$
$$\frac{\beta^2\alpha}{\gamma^2}\left[\frac{\partial\Psi'}{\partial Y'}\frac{\partial^2\Psi'}{\partial X'\partial Y'} - \frac{\partial\Psi'}{\partial X'}\frac{\partial^2\Psi'}{\partial Y'^2}\right] = \frac{\beta^3}{\gamma}\frac{\partial^3\Psi'}{\partial Y'^3}$$

and (6.63) becomes

$$\frac{\Psi'(0,Y)}{\gamma} = \frac{Y'}{\beta}.$$

The PDE and its boundary conditions will be invariant under the transformation $(X, Y, \Psi) \to (X', Y', \Psi')$ if

$$\alpha = \beta\gamma, \tag{6.69}$$
$$\beta = \gamma. \tag{6.70}$$

The 2 equations above in 3 variables α, β and γ leave one degree of freedom; let it be α; then,

$$\gamma = \beta = \sqrt{\alpha}.$$

More interestingly still, we can view (6.66)–(6.68) as a change of variables from X, Y, Ψ to X', Y', Ψ': α does not need to be a constant! Therefore, pick (without loss of generality)

$$\alpha = \frac{1}{X}; \tag{6.71}$$

Then,

$$X' = 1, \tag{6.72}$$
$$Y' = \frac{Y}{\sqrt{X}}, \tag{6.73}$$
$$\Psi' = \frac{\Psi}{\sqrt{X}}, \tag{6.74}$$
$$\Psi' = \frac{1}{\sqrt{X}}\Psi'(1, \frac{Y}{\sqrt{X}}) \tag{6.75}$$

Lesson 7

The Boussinesq nonlinear differential equation for groundwater flow

March 14, 2016

Let us practice some of our acquired skills with an important equation. We will call it the Boussinesq equation. First of all: be careful, because there are many "Boussinesq equations" around. The one we will focus on is a model for groundwater flow. Moreover, there is a partial differential equation (which we will start with) and an ordinary differential equation. We will visit both.

We start our derivation looking at figure 7.1. The "wet" region of the soil is marked by gray, while the "dry" region is marked by light gray.

The figure shows a simple aquifer with a free surface $h(x)$ (with water below). We call this the *phreatic surface*. There is no such thing in reality, because there is no sharp boundary between "wet" and "dry" regions in real soils. The soil moisture varies smoothly from completely saturated to drier as we move up. However, if you dig a hole in the ground, you will see that a free surface appears at some depth. We therefore make the simplificaton that there is a sharp wet-dry boundary in the soil. Its position is $h(x)$.

We have delimited a material volume $\mathscr{C}$ with dashed lines in figure 7.1. We assume that the bottom (along the x axis) is impermeable. There is no mass flow across the top at all, because it has been conveniently located somewhat above the phreatic surface: even if the phreatic surface is moving up or down, it will not reach (immediately) the top dashed line that delimits this material volume. You may think that it is strange to draw a material volume a part of which has no water mass at all — and you are right, but this actually helps the analysis.

Across the closed surface of $\mathscr{C}$, therefore, there is only flow across the planes $x = a$ and $x = b$. Flow across these planes extends up to $h(a)$ and $h(b)$, respectively.

In this problem, we need to obtain an expression for the mass flux in and out of $\mathscr{C}$. The medium (the soil) is complicated! There exists in fact a maze of interconnected channels carrying water, delimited by solid soil particles. We define the soil's porosity as

$$n_d = \frac{V_p}{V_t},$$

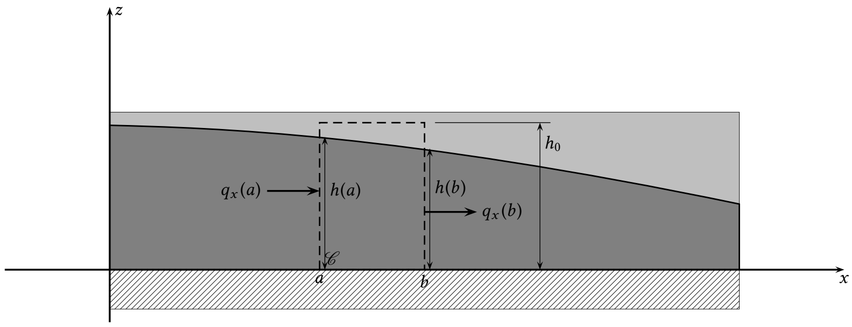

Figure 7.1: A material body mass balance for groundwater flow

where V_p is the volme of pores, and V_t is the total volume. Technically, the thing is indeed even more complicated, and we should use the *drainable* porosity. The reader is referred to Brutsaert (2005)'s book.

At any instant, the total mass of water within the material volume $\mathscr{C}$ is

$$M = \int_{\mathscr{C}} n\rho \,\mathrm{d}V,$$

where ρ is the density of water. We will be assuming that both n and ρ are constant throughout the soil.

The mass flux at any point across the plane x is given by *Darcy's Law* (once again, we need to be sketchy: look the subject up in Brutsaert (2005) and Bear (1972), for example). It reads

$$\boldsymbol{q} = -\rho k_s \boldsymbol{\nabla}\eta,$$

where k_s is the *saturated hydraulic conductivity*, and $\eta(x, z)$ is the *hydraulic head* in the soil. The physical dimensions are as follows:

$$\begin{aligned}
[\![\boldsymbol{q}]\!] &= \mathsf{ML}^{-2}\mathsf{T}^{-1},\\
[\![\rho]\!] &= \mathsf{ML}^{-3},\\
[\![k_s]\!] &= \mathsf{LT}^{-1},\\
[\![\eta]\!] &= \mathsf{L},\\
[\![\boldsymbol{\nabla}\eta]\!] &= 1.
\end{aligned}$$

You can verify that Darcy's law is dimensionally consistent (actually, it has to be, since it amounts to the definition of k_s). Notice that $\boldsymbol{q}$ is a vector, and that therefore, in the two-dimensional setting that we are working in, it has an x and a z component. We now invoke the *Dupuit-Forchheimmer hypothesis*: we assume that $\eta(x, z, t) = h(x, t)$, where $h(x, t)$ is the (already introduced) height of the phreatic surface. It follows that

$$\boldsymbol{\nabla}\eta = \frac{\partial h}{\partial x}\boldsymbol{e}_x,$$

and that, therefore, $\boldsymbol{q}$ is horizontal. Moreover, since $h(x, t)$ depends on x but not on z, the vetor q is constant along the plane x.

With $\boldsymbol{q}$ in place, the mass balance for $\mathscr{C}$ is

$$0 = \int_{\mathscr{C}} \frac{\partial (n\rho)}{\partial t}\,\mathrm{d}V + \oint_{\mathscr{S}} (\boldsymbol{n}\cdot\boldsymbol{q})\,\mathrm{d}A.$$

But if $n\rho$ = constant, its partial derivative with respect to t is zero, right? Not so fast! In our approximation, ρ *is an indicator function of the presence of water inside the material region* $\mathscr{C}$: it drops from a constant value to zero as soon as we cross the phreatic surface upwards. Give it some thought: it means that the first integral is actually the rate of change of the total mass of water inside $\mathscr{C}$, and that it can be written

$$\begin{aligned}\int_{\mathscr{C}} \frac{\partial (n\rho)}{\partial t}\,\mathrm{d}V &= \int_a^b \left[\int_{z=0}^{h_0} \frac{\partial (n_d\rho)}{\partial t}\,\mathrm{d}z\right]\mathrm{d}x\\ &= \int_a^b \left[\frac{\partial}{\partial t}\int_{z=0}^{h_0} (n_d\rho)\,\mathrm{d}z\right]\mathrm{d}x\\ &= \int_a^b (n_d\rho)\left[\frac{\partial}{\partial t}\int_{z=0}^{h(x)} \mathrm{d}z\right]\mathrm{d}x\\ &= \int_a^b (n_d\rho)\frac{\partial h(x,t)}{\partial t}\,\mathrm{d}x,\end{aligned}$$

where a unit width in the y direction is implicit. Going from the second to the third line above, we used the fact that in this model there is only water below the phreatic surface $h(x)$.

You are probably guessing, from our previous lectures, that the second integral can be handled with the Divergence Theorem, and you are right:

$$\begin{aligned}\oint_{\mathscr{S}} (\boldsymbol{n}\cdot\boldsymbol{q})\,\mathrm{d}A &= \int_a^b \int_{z'=0}^{h_0} \frac{\partial q_x}{\partial x}\,\mathrm{d}z\mathrm{d}x\\ &= \int_a^b \frac{\partial}{\partial x}\int_{z'=0}^{h_0} q_x\,\mathrm{d}z\mathrm{d}x.\end{aligned}$$

Above, notice how q_x only exists below the phreatic surface $h(x)$; therefore,

$$\begin{aligned}\oint_{\mathscr{S}} (\boldsymbol{n}\cdot\boldsymbol{q})\,\mathrm{d}A &= \int_a^b \frac{\partial}{\partial x}\int_{z=0}^{h(x)} q_x\,\mathrm{d}z\mathrm{d}x\\ &= \int_a^b \frac{\partial}{\partial x}\int_{z=0}^{h(x)} \left[-\rho k_s\frac{\partial h(x)}{\partial x}\right]\mathrm{d}z\mathrm{d}x\\ &= \int_a^b \frac{\partial}{\partial x}\left[-\rho k_s h(x)\frac{\partial h(x)}{\partial x}\right]\mathrm{d}x.\end{aligned}$$

Gathering everything,

$$0 = \int_a^b \left[\rho n\frac{\partial h}{\partial t} - \rho k_s\frac{\partial}{\partial x}\left(h\frac{\partial h}{\partial x}\right)\right]\mathrm{d}x.$$

The same argument as before (validity of the integrand for any $\mathscr{C}$, etc.) gives us Boussinesq's equation:

$$\frac{\partial h}{\partial t} = \frac{k_s}{n}\frac{\partial}{\partial x}\left[h\frac{\partial h}{\partial x}\right].$$

The equation itself is a great achievement: it was derived by Boussinesq in 1903 (Boussinesq, 1903). It can of course assume other forms, because we can

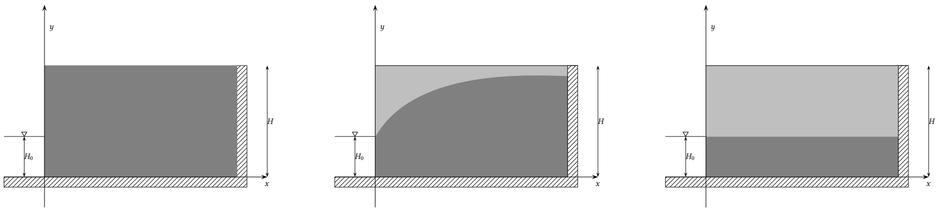

Figure 7.2: Esvaziamento de um maciço poroso

consider two-dimensional flow in the horizontal, a sloping acquifer, etc.. Again, look it up in Brutsaert (2005) if you want more details.

Following Boussinesq, we will study a *linearized* problem first. Figure 7.2 shows three stages of the draining of an aquifer. At $t = 0$, the aquifer is saturated up to height H. At an intermediate time, there is a phreatic surface, and at $t = \infty$, the phreatic surface reaches (only asymptotically) the level H_0 of the adjoining channel to which water is draining.

One way to linearize the Boussinesq equation is this: let

$$\frac{\partial h}{\partial t} \approx \frac{k_s}{n}\frac{\partial}{\partial x}\overline{h}\frac{\partial h}{\partial x} = \frac{k\overline{h}}{n}\frac{\partial^2 h}{\partial x^2}.$$

The most obvious (but not the only possible) value for para $\overline{h}$ is $(H_0 + H)/2$, but pretty much any value between H_0 and H would be a valid (initial) attempt.

Problems involving partial differential equations (PDE's) require boundary conditions. Often, we call a condition in time an *initial condition*, although technically it is a boundary condition in the time dimension. For our problem, they are:

$$\begin{aligned} h(x, 0) &= H, \\ h(0, t) &= H_0, \\ \frac{\partial h(L, t)}{\partial x} &= 0, \end{aligned}$$

and they have the following meanings:

$h(x, 0) = H \Rightarrow$ Initially the phreatic level is H in the whole domain.

$h(0, t) = H_0 \Rightarrow$ The phreatic level at $x = 0$ is H_0 for all $t > 0$.

$\dfrac{\partial h(L)}{\partial x} = 0 \Rightarrow$ Due to the impermeable boundary on the right, there is no horizontal flux of water at $x = L$.

The second condition above is *nonhomogeneous*:

$$h(0, t) \neq 0.$$

This usually spells problems, because a standard tool to solve linear PDE's analytically is to employ *Sturm-Liouville* Theory, a theory that requires homogeneous boundary conditions. At this point, therefore, it is customary to change the problem into one with homogeneous boundary conditions. For the case at hand, here is how to do it: let

$$\phi(x, t) = h(x, t) - H_0;$$

Note that H_0 is constant; we obtain

$$\frac{\partial(\phi + H_0)}{\partial t} = \alpha^2 \frac{\partial^2(\phi + H_0)}{\partial x^2} \Rightarrow \frac{\partial \phi}{\partial t} = \alpha^2 \frac{\partial^2 \phi}{\partial x^2};$$

Then, the boundary conditions in ϕ are simpler!

$$\begin{aligned}
\phi(x, 0) &= h(x, 0) - H_0 = H - H_0, \\
\phi(0, t) &= h(0, t) - H_0 = H_0 - H_0 = 0, \\
\frac{\partial \phi(L, t)}{\partial x} &= \frac{\partial(h(L, t) - H_0)}{\partial x} = \frac{\partial h(L, t)}{\partial x} = 0,
\end{aligned}$$

so that now we have homogeneous boundary conditions.

The next step is the famous method of separation of variables. It consists of assuming

$$\phi(x, t) = X(x)T(t).$$

Get

$$\begin{aligned}
\frac{\partial(XT)}{\partial t} &= \alpha^2 \frac{\partial^2(XT)}{\partial x^2} \Rightarrow \\
XT' &= \alpha^2 TX'' \Rightarrow \\
\frac{1}{\alpha^2}\frac{T'}{T} &= \frac{X''}{X} = \lambda.
\end{aligned}$$

Above, there is a function of t on the left-hand side, equal to a function of x on the right-hand side. This cannot be, unless they are both equal to the constant λ. This is the crux of the method of separation of variables. Let me tell you, right here, that this fortunate situation usually does not work in nonlinear problems.

At any rate, we have now two *ordinary differential equations* (ODE's):

$$\begin{aligned}
\frac{\mathrm{d}T}{\mathrm{d}t} - \lambda\alpha^2 T &= 0, \\
\frac{\mathrm{d}^2 X}{\mathrm{d}x^2} - \lambda X &= 0.
\end{aligned}$$

The first is a *first-order equation*, because the highest derivative is 1. The second is a *second-order equation*, because the highest derivative is two.

We will need to match the solutions $T(t)$ and $X(x)$ to the initial and boundary conditions:

$$\begin{aligned}
\phi(x, 0) &= X(x)T(0) = H - H(0), \\
\phi(0, t) &= X(0)T(t) = 0, \\
\frac{\partial \phi(L, t)}{\partial x} &= \frac{\mathrm{d}X(L)}{\mathrm{d}x} T(t) = 0.
\end{aligned}$$

Clearly, we will need to impose

$$\begin{aligned}
X(0) &= 0, \\
\frac{\mathrm{d}X(L)}{\mathrm{d}x} &= 0.
\end{aligned}$$

We can go back to the initial condition $\phi(x, 0)$ later on.

We solve the first one first:

$$\begin{aligned}
\frac{\mathrm{d}T}{\mathrm{d}t} &= \lambda\alpha^2 T, \\
\frac{\mathrm{d}T}{T} &= \lambda\alpha^2 \mathrm{d}t, \\
\int_{T_0}^{T(t)} \frac{\mathrm{d}T'}{T'} &= \int_{t=0}^{t} \lambda\alpha^2 \mathrm{d}t', \\
\ln\left(\frac{T(t)}{T_0}\right) &= \lambda\alpha^2 t, \\
T(t) &= T_0 \exp\left(\lambda\alpha^2 t\right).
\end{aligned}$$

When I am solving problems using integrals, I always try to use *definite* integrals, and to put sensible limits of integration in them. This requires understanding clearly the role of *dummy integration variables*, such as T' and t'.

The second equation is much harder. The first thing to notice is that, magically, $\exp(rx)$ is a solution! Indeed,

$$\begin{aligned}
X(x) &= \exp(rx), \\
X'(x) &= r\exp(rx), \\
X''(x) &= r^2\exp(rx).
\end{aligned}$$

If we put this back into the ODE, we get

$$\begin{aligned}
r^2\exp(rx) - \lambda\exp(rx) &= 0, \\
\left(r^2 - \lambda\right)\exp(rx) &= 0, \\
r^2 &= \lambda, \\
r &= \pm\sqrt{\lambda}.
\end{aligned}$$

What this means is that there are two functions which solve the ODE:

$$\exp(\sqrt{\lambda}x) \qquad \text{and} \qquad \exp(-\sqrt{\lambda}x).$$

Let's call the two roots r_1 and r_2. Because the ODE is linear, any *linear combination* of them will also be a solution. Indeed,

$$\begin{aligned}
X(x) &= c_1\exp(r_1x) + c_2\exp(r_2x), \\
X''(x) &= c_1r_1^2\exp(r_1x) + c_2r_2^2\exp(r_2x) \\
&= c_1\lambda\exp(r_1x) + c_2\lambda\exp(r_2x) \\
&= \lambda\left[c_1\exp(r_1x) + c_2\exp(r_2x)\right]; \\
X''(x) - \lambda X &= \lambda\left[c_1\exp(r_1x) + c_2\exp(r_2x)\right] - \lambda\left[c_1\exp(r_1x) + c_2\exp(r_2x)\right] \\
&= 0.
\end{aligned}$$

So far we have effectively solved the equation. But we must also look at the sign of λ! Notice that, if $\lambda < 0$, then r_1 and r_2 will be complex. Moreover, for $\lambda > 0$, there are more convenient forms to express the solution. Let us assume $\lambda > 0$, and that the solution $X(x) \in \mathbb{R}$. Given $c_1, c_2 \in \mathbb{R}$, it is always possible to find $a, b \in \mathbb{R}$ such that

$$\begin{aligned}
c_1 &= \frac{1}{2}(a+b), \\
c_2 &= \frac{1}{2}(a-b).
\end{aligned}$$

Replacing these into the solution, we obtain

$$
\begin{aligned}
X(x) &= \frac{1}{2}(a+b)\mathrm{e}^{+\sqrt{\lambda}x} + \frac{1}{2}(a-b)\mathrm{e}^{-\sqrt{\lambda}x} \\
&= a\frac{\mathrm{e}^{+\sqrt{\lambda}x} + \mathrm{e}^{-\sqrt{\lambda}x}}{2} + b\frac{\mathrm{e}^{+\sqrt{\lambda}x} - \mathrm{e}^{-\sqrt{\lambda}x}}{2} \\
&= a\cosh(\sqrt{\lambda}x) + b\sinh(\sqrt{\lambda}x).
\end{aligned}
$$

Let us see if $\lambda > 0$ leads to a solution that satisfies our boundary conditions:

$$
\begin{aligned}
X(x) &= a\cosh(\sqrt{\lambda}x) + b\sinh(\sqrt{\lambda}x), \\
\frac{\mathrm{d}X}{\mathrm{d}x} &= \sqrt{\lambda}\left[a\sinh(\sqrt{\lambda}x) + b\cosh(\sqrt{\lambda}x)\right].
\end{aligned}
$$

Now,

$$
\begin{aligned}
X(0) = 0 &\Rightarrow a = 0, \\
\frac{\mathrm{d}X(L)}{\mathrm{d}x} = 0 &\Rightarrow \sqrt{\lambda}b\cosh(\sqrt{\lambda}L) = 0 \Leftrightarrow b = 0.
\end{aligned}
$$

Thus, $\lambda > 0$ produces only the trivial solution

$$
X(x) \equiv 0.
$$

This is no good: it clearly cannot result in the solution $\phi(x,t)$ that we are seeking for our groundwater problem.

We must, therefore, proceed, testing the other possible signs for λ. If $\lambda = 0$,

$$
\begin{aligned}
\frac{\mathrm{d}^2X}{\mathrm{d}x^2} = 0 &\Rightarrow X(x) = ax + b \\
X(0) = 0 &\Rightarrow b = 0, \\
\frac{\mathrm{d}X(L)}{\mathrm{d}x} = 0 &\Rightarrow a = 0.
\end{aligned}
$$

Again, $\lambda = 0$ gives us only the trivial solution.

Finally, if $\lambda < 0$, we need to express the solution in a more practical form. Observe that in terms of $\exp(\cdot)$, the solution is

$$
X(x) = c_1\exp(+\sqrt{\lambda}x) + c_2\exp(-\sqrt{\lambda}x).
$$

As it is, it is a complex number, because $\lambda < 0$. The first thing we need to do is to make this as explicit as possible:

$$
\exp(+\sqrt{\lambda}x) = \exp(\mathrm{i}rx),
$$

where $r = \sqrt{|\lambda|}$. Then,

$$
X(x) = c_1\exp(\mathrm{i}rx) + c_2\exp(-\mathrm{i}rx).
$$

At this point, we must realize that in principle $X(x)$ is a complex number. This is not so good, because we are seeking a *real* $X(x)$ solution. Interestingly, we will fix this situation by letting c_1 and c_2 be complex as well.

So we want to write the solution in a purely real form. We can do this using two devices. First, we remember Euler's formula:

$$
\exp(\mathrm{i}rx) = \cos(rx) + \mathrm{i}\sin(rx).
$$

The good news is that both r and x are real, so the $\cos(\cdot)$ and $\sin(\cdot)$ functions above are the good old real versions of these trigonometric functions (there *are* complex versions, but let us not care about them for the time being). Also, $\cos(\cdot)$ is an even function:

$$\cos(-x) = \cos(x),$$

while $\sin(\cdot)$ is an odd function:

$$\sin(-x) = -\sin(x).$$

Using those facts, we rewrite the solution as

$$\begin{aligned} X(x) &= c_1 [\cos(rx) + \mathrm{i}\sin(rx)] + c_2 [\cos(rx) - \mathrm{i}\sin(rx)] \\ &= (c_1 + c_2)\cos(rx) + (c_1 - c_2)\mathrm{i}\sin(rx). \end{aligned}$$

Let us think about it again: if $X(x)$ is to be real, we need to have $c_1 + c_2$ real, and $(c_1 - c_2)\mathrm{i}$ real as well: how can we do it? Making c_1 and c_2 complex conjugates. It is actually quite simple to do this: let a and b be real, and put

$$\begin{aligned} c_1 &= \frac{1}{2}(a - b\mathrm{i}), \\ c_2 &= \frac{1}{2}(a + b\mathrm{i}). \end{aligned}$$

Let us do the algebra now:

$$\begin{aligned} X(x) &= \left[\frac{1}{2}(a - b\mathrm{i}) + \frac{1}{2}(a + b\mathrm{i})\right]\cos(rx) + \left[\frac{1}{2}(a - b\mathrm{i}) - \frac{1}{2}(a + b\mathrm{i})\right]\mathrm{i}\sin(rx) \\ &= a\cos(rx) - b(\mathrm{i}\times\mathrm{i})\sin(rx) \\ &= a\cos(rx) + b\sin(rx). \end{aligned}$$

It worked: if $\lambda < 0$, the expression above (remember: $r = \sqrt{|\lambda|}$) is the real solution. Again, we try to match this solution to the boundary conditions

$$\begin{aligned} X(x) &= a\cos(\sqrt{-\lambda}x) + b\sin(\sqrt{-\lambda}x), \\ \frac{\mathrm{d}X}{\mathrm{d}x} &= \sqrt{-\lambda}\left[-a\sin(\sqrt{-\lambda}x) + b\cos(\sqrt{-\lambda}x)\right], \\ X(0) &= 0 \;\Rightarrow\; a = 0, \\ \frac{\mathrm{d}X(L)}{\mathrm{d}x} &= 0 \;\Rightarrow\; \sqrt{-\lambda}b\cos(\sqrt{-\lambda}L) = 0 \;\blacksquare \end{aligned}$$

We don't want b to be zero: that would again give us a trivial solution. It is the cossine that must be zero:

$$\begin{aligned} \cos(r_nL) &= 0, \\ r_nL &= (n + \frac{1}{2})\pi = (2n+1)\frac{\pi}{2} \;\Rightarrow \\ r_n &= (2n+1)\frac{\pi}{2}\frac{1}{L}. \end{aligned}$$

As you can see, an n has appeared. Why? Because for any $n \geq 0$, $\cos(r_nL) = 0$. What this means is that the corresponding λ's are *eigenvalues*:

$$\begin{aligned} \sqrt{-\lambda_n} &= (2n+1)\frac{\pi}{2}\frac{1}{L}, \\ \lambda_n &= -(2n+1)^2\frac{\pi^2}{2L^2}. \end{aligned}$$

Moreover, for each n there will be a solution. They are

$$X_n(x) = b_n \sin\left((2n+1)\frac{\pi x}{2L}\right).$$

Obtaining the eigenvalues and eigenfunctions is the central part of any solution using the method of separation of variables. It is, in fact, an application of *Sturm-Liouville Theory*. In the last lecture, we applied the theory "in practice". Now you will remember that we were trying to find solutions of the form

$$\phi(x,t) = X(x)T(t).$$

Because we found infinitely many X_n's, we must change this to:

$$\phi(x,t) = \sum_{n=0}^{\infty} X_n(x)T_n(t).$$

The first thing to do is to calculate the $T_n(t)$'s. They are immediately obtained as

$$T_n(t) = T_{0n} \exp\left[-(2n+1)^2 \frac{\pi^2\alpha^2}{2L^2} t\right]$$

Observe that the boundary conditions,

$$\begin{aligned} \phi(0,t) &= 0, \\ \frac{\partial\phi(L,t)}{\partial x} &= 0, \end{aligned}$$

are already automatically obeyed. We are left to impose the initial condition:

$$\phi(x,0) = H - H_0.$$

At $t = 0$, then, we obtain:

$$\sum_{n=0}^{\infty} T_{0n} b_n \sin\left((2n+1)\frac{\pi x}{2L}\right) = [H - H_0].$$

The constants T_{0n} and b_n are not independent! We must rewrite:

$$\sum_{n=0}^{\infty} C_n \sin\left((2n+1)\frac{\pi x}{2L}\right) = [H - H_0].$$

The final step of the solution is the calculation of the C_n's. Here is how we do it:

$$\sin\left((2m+1)\frac{\pi x}{2L}\right) \sum_{n=0}^{\infty} C_n \sin\left((2n+1)\frac{\pi x}{2L}\right) = [H - H_0] \sin\left((2m+1)\frac{\pi x}{2L}\right),$$

$$\sum_{n=0}^{\infty} C_n \sin\left((2m+1)\frac{\pi x}{2L}\right) \sin\left((2n+1)\frac{\pi x}{2L}\right) = [H - H_0] \sin\left((2m+1)\frac{\pi x}{2L}\right),$$

$$\sum_{n=0}^{\infty} C_n \int_{x=0}^{L} \sin\left((2m+1)\frac{\pi x}{2L}\right) \sin\left((2n+1)\frac{\pi x}{2L}\right) \mathrm{d}x =$$

$$[H - H_0] \int_{x=0}^{L} \sin\left((2m+1)\frac{\pi x}{2L}\right) \mathrm{d}x.$$

The two integrals can be calculated really fast with the help of Maxima. If you run this script,

```
linel : 70 ;
declare([m,n], integer) ;
declare([L], noninteger) ;
assume( L > 0) ;
fm : sin( (2*m +1)*%pi*x/(2*L)) ;
fn : sin( (2*n +1)*%pi*x/(2*L)) ;
I1 : integrate(fm*fn,x,0,L);
I2 : integrate(fm*fm,x,0,L);
I3 : integrate(fm,x,0,L);
trigreduce(%);
```

you get:

```
(%i1) batch("maxints.max")
(%i2) declare([m,n],integer)
(%o2)                               done
(%i3) declare([L],noninteger)
(%o3)                               done
(%i4) assume(L > 0)
(%o4)                              [L > 0]
(%i5) fm:sin((1+2*m)*%pi*x/(2*L))
                              %pi (2 m + 1) x
(%o5)                     sin(---------------)
                                    2 L
(%i6) fn:sin((1+2*n)*%pi*x/(2*L))
                              %pi (2 n + 1) x
(%o6)                     sin(---------------)
                                    2 L
(%i7) I1:integrate(fm*fn,x,0,L)
(%o7)                                0
(%i8) I2:integrate(fm*fm,x,0,L)
                                     L
(%o8)                                -
                                     2
(%i9) I3:integrate(fm,x,0,L)
                                        2 %pi m + %pi
                                  2 cos(-------------) L
                       2 L                   2
(%o9)             ------------- - ----------------------
                  2 %pi m + %pi       2 %pi m + %pi
(%i10) trigreduce(%)
                                    2 L
(%o10)                         -------------
                               2 %pi m + %pi
```

Here is what it means:

$$m \neq n \Rightarrow \int_{x=0}^{L} \sin\left((2m+1)\frac{\pi x}{2L}\right) \sin\left((2n+1)\frac{\pi x}{2L}\right)\,\mathrm{d}x = 0,$$

$$m \neq n \Rightarrow \int_{x=0}^{L} \sin\left((2m+1)\frac{\pi x}{2L}\right) \sin\left((2n+1)\frac{\pi x}{2L}\right)\,\mathrm{d}x = \frac{L}{2},$$

$$\int_{x=0}^{L} \sin\left((2m+1)\frac{\pi x}{2L}\right)\,\mathrm{d}x = \frac{2L}{\pi(2m+1)}.$$

Only $n = m$ survives in the sum on the right-hand side. The result is

$$C_m \frac{L}{2} = [H - H_0]\,\frac{2L}{\pi(2m+1)}$$

$$C_m = [H - H_0]\,\frac{4}{\pi(2m+1)}.$$

Here is our solution:

$$h(x,t) = H_0 + \sum_{n=0}^{\infty} \frac{4\,[H - H_0]}{\pi(2n+1)} \sin\left((2n+1)\frac{\pi x}{2L}\right) \exp\left[-(2n+1)^2\frac{\pi^2\alpha^2}{2L^2}t\right].$$

Lesson 8

Misturas binárias

No início deste capítulo nós vamos seguir a essência da abordagem de Bird et al. (1960, cap. 16): ela permite entender claramente o significado de difusão molecular de uma substância em um fluido, e em nossa opinião evita totalmente confusões comuns a respeito do papel da difusão e da advecção em meios contínuos.

Além disso, nós vamos considerar, por simplicidade, apenas misturas binárias, com um soluto A dissolvido em um solvente B. A generalização para misturas com mais de 2 componentes é óbvia.

Em uma mistura binária nós postulamos a existência em cada ponto de uma densidade para cada componente, $\wp_A$ e $\wp_B$, de tal maneira que as massas totais de A e B em um volume material $\mathscr{C}$ são, respectivamente,

$$
M_A = \int_{\mathscr{C}} \rho_A \,\mathrm{d}V, \qquad M_B = \int_{\mathscr{C}} \rho_B \,\mathrm{d}V.
$$

É evidente que, em cada ponto, devemos ter

$$
\rho = \rho_A + \rho_B.
$$

Note que essa abordagem postulatória é compatível com a visão tradicional em Mecânica do Contínuo. Prosseguindo, nós também postulamos a existência de campos de velocidade para cada espécie, $\boldsymbol{U}_A$ e $\boldsymbol{U}_B$, cujas integrais em um volume material são a quantidade de movimento total de cada espécie, respectivamente $\boldsymbol{P}_A$ e $\boldsymbol{P}_B$. Por analogia com as equações acima, temos

$$
\boldsymbol{P}_A = \int_{\mathscr{C}} \rho_A \boldsymbol{u}_A \,\mathrm{d}V, \qquad \boldsymbol{P}_B = \int_{\mathscr{C}} \rho_B \boldsymbol{u}_B \,\mathrm{d}V.
$$

Agora, a quantidade de movimento total do corpo que ocupa $\mathscr{C}$ deve ser

$$
\boldsymbol{P} = \int_{\mathscr{C}} \rho\, \boldsymbol{u} \,\mathrm{d}V,
$$

onde $\boldsymbol{u}$ é a velocidade do fluido em cada ponto, de tal forma que devemos ter

$$
\rho \boldsymbol{u} = \rho_A \boldsymbol{u}_A + \rho_B \boldsymbol{u}_B.
$$

O ponto fundamental agora é perceber que é extremamente difícil, senão impossível, medir diretamente $\boldsymbol{u}_A$ e $\boldsymbol{u}_B$. Em seu lugar, é muito mais simples trabalhar unicamente com o campo de velocidade $\boldsymbol{u}$ do fluido como um todo em cada ponto. Para tanto, nós definimos o vetor fluxo difusivo de massa de A:

$$
\boldsymbol{j}_A = \rho_A \left[\boldsymbol{u}_A - \boldsymbol{u} \right].
$$

A *concentração mássica* (ou *fração de massa*) de A é

$$c_A \equiv \frac{\rho_A}{\rho},$$

e vale a lei de Fick em cada ponto:

$$\boldsymbol{j}_A = -\rho D \boldsymbol{\nabla} c,$$

onde D é a difusividade molecular de A na mistura. Relações totalmente análogas também valem para o solvente B.

Finalmente, das equações acima obtém-se:

$$\begin{aligned}\boldsymbol{j}_A + \boldsymbol{j}_B &= \rho_A [\boldsymbol{u}_A - \boldsymbol{u}] + \rho_B [\boldsymbol{u}_B - \boldsymbol{u}]\\ &= \rho_A \boldsymbol{u}_A + \rho_B \boldsymbol{u}_B - (\rho_A + \rho_B)\,\boldsymbol{u}\\ &= \rho \boldsymbol{u} - \rho \boldsymbol{u} = 0.\end{aligned}$$

Essa equação é válida em todos os pontos de um fluido, *exceto talvez em uma superfície onde haja um fluxo líquido de A para dentro da massa de fluido*. Este é um ponto muito importante, pois nosso objetivo neste capítulo é estudar com razoável detalhe o que acontece quando existe *injeção de massa* para dentro de um fluido.

Prosseguindo, o balanço integral de A é tão simples quanto

$$\begin{aligned}0 &= \frac{\partial}{\partial t}\int_{\mathscr{C}} \rho_A \, \mathrm{d}V + \oint_{\mathscr{S}} \rho_A \, (\boldsymbol{n} \cdot \boldsymbol{u}_A) \, \mathrm{d}A\\ &= \frac{\partial}{\partial t}\int_{\mathscr{C}} \rho_A \, \mathrm{d}V + \oint_{\mathscr{S}} \rho_A \, (\boldsymbol{n} \cdot [\boldsymbol{u}_A - \boldsymbol{u} + \boldsymbol{u}]) \, \mathrm{d}A;\\ -\oint_{\mathscr{S}} \rho_A \, (\boldsymbol{n} \cdot [\boldsymbol{u}_A - \boldsymbol{u}]) \, \mathrm{d}A &= \frac{\partial}{\partial t}\int_{\mathscr{C}} \rho_A \, \mathrm{d}V + \oint_{\mathscr{S}} \rho_A \, (\boldsymbol{n} \cdot \boldsymbol{u}) \, \mathrm{d}A,\\ -\oint_{\mathscr{S}} (\boldsymbol{n} \cdot \boldsymbol{j}_A) &= \frac{\partial}{\partial t}\int_{\mathscr{C}} \rho_A \, \mathrm{d}V + \oint_{\mathscr{S}} \rho_A \, (\boldsymbol{n} \cdot \boldsymbol{u}) \, \mathrm{d}A,\end{aligned}$$

onde a introdução de $\boldsymbol{j}_A$ na última linha segue-se de sua definição. Uma dedução totalmente análoga vale para B.

A aplicação dos teoremas da divergência e da localização para A e para B produz, agora, duas equações diferenciais de balanço de massa:

$$\begin{aligned}\frac{\partial \rho_A}{\partial t} + \frac{\partial \rho_A u_i}{\partial x_i} &= -\frac{\partial J_{A,i}}{\partial x_i},\\ \frac{\partial \rho_B}{\partial t} + \frac{\partial \rho_B u_i}{\partial x_i} &= -\frac{\partial J_{B,i}}{\partial x_i}.\end{aligned}$$

A soma das duas *tem* que restaurar a equação da continuidade; dada as equações

$$\begin{aligned}\rho &= \rho_A + \rho_B,\\ \rho \boldsymbol{u} &= \rho_A \boldsymbol{u}_A + \rho_B \boldsymbol{u}_B,\end{aligned}$$

segue-se necessariamente que

$$\frac{\partial j_{A,i}}{\partial x_i} + \frac{\partial j_{B,i}}{\partial x_i} \equiv 0.$$

Esta equação vale *sempre*; duas coisas podem acontecer. No caso mais geral, qualquer difusão molecular do soluto A é compensada por difusão molecular, também do solvente B, de uma certa forma, "no sentido oposto". Note entretanto que ela estipula que é a soma das *divergências* dos fluxos difusivos de massa que é nula. Uma situação particular que pode ocorrer é o caso em que $\boldsymbol{j}_A = \text{const.}$ e $\boldsymbol{j}_B = 0$; portanto é possível ocorrer fluxo difusivo apenas do soluto, desde que a sua divergência seja nula. É comum a confusão entre um fluxo e sua divergência nas equações de um meio contínuo, e este é um bom exemplo para explicitar sua diferença.

Consideremos agora uma situação em que temos um escoamento predominantemente horizontal (na direção "x") de uma mistura sobre uma placa através da qual ocorre uma injeção de um fluxo de massa de A, constante e igual a $\dot{m}_A$. Suponha também que não há fluxo de massa de B através da placa, ou seja, que $\rho_B \boldsymbol{u}_B = 0$ em $z = 0$. A conclusão a que chegamos, imediatamente, é que existe uma velocidade advectiva de A w_{A0}, normal à placa, dada por

$$\dot{m}_A = \rho_A w_{A0}$$

Isso *induz uma velocidade média vertical no escoamento em* $z = 0$, pois

$$\rho w_0 = \rho_A w_{A0} \Rightarrow w_0 = \frac{\dot{m}_A}{\rho}.$$

A existência desta velocidade média "induzida" pela injeção de massa de A é muitas vezes denominada "escoamento de Stefan".

Uma parte de $\dot{m}_A$ é de natureza difusiva:

$$\begin{aligned} j_{A0} &= \rho_A (w_{A0} - w_0) \\ &= \rho_A w_{A0} - \rho_A w_0 \Rightarrow \\ \rho_A w_{A0} &= j_{A0} + \rho_A w_0. \end{aligned}$$

Portanto,

$$\begin{aligned} \rho w_0 &= j_{A0} + \rho_A w_0, \\ (\rho - \rho_A) w_0 &= j_{A0} = -\rho D \frac{\partial c}{\partial z}, \\ (1 - c) w_0 &= -D \frac{\partial c}{\partial z}, \\ w_0 &= -\frac{D}{1 - c} \frac{\mathrm{d}c(0)}{\mathrm{d}z}. \end{aligned}$$

Compare a equação acima com a equação (3) de Browers e Chesters (1991).

Suponhamos agora que o escoamento apresenta uma concentração de A igual a c_0 em $c = 0$, e igual a c_δ em $z = \delta$. A equação de advecção-difusão de A (que já estudamos na lição **??**) será no nosso caso simplificada (supondo regime permanente e um problema bidimensional) para

$$u \frac{\partial c}{\partial x} + w \frac{\partial c}{\partial z} = D \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right).$$

Se pudermos, ainda mais, desprezar os termos advectivo e difusivo horizontais, ficaremos com

$$w \frac{\mathrm{d}c}{\mathrm{d}z} = D \frac{\mathrm{d}^2 c}{\mathrm{d}z^2}.$$

Além disso, se nossas hipóteses para o fluxo de massa vertical de A (e também o de B) valerem não somente na superfície, mas em toda a região $0 \le z \le \delta$, teremos

$$
\begin{aligned}
-\frac{D}{1-c}\left[\frac{\mathrm{d}c}{\mathrm{d}z}\right]^2 &= D\frac{\mathrm{d}^2c}{\mathrm{d}z^2},\\
-\left[\frac{\mathrm{d}c}{\mathrm{d}z}\right]^2 &= (1-c)\frac{\mathrm{d}^2c}{\mathrm{d}z^2}.
\end{aligned}
$$

Interessantemente, Browers e Chesters (1991) sequer listam a equação diferencial! É evidente que, se estivermos lendo o *paper* deles, teremos que entender (ou seja, refazer) como eles obtêm a solução deste sub-problema. Este é, agora, o nosso objetivo nesta lição.

As condições de contorno do problema serão

$$
\begin{aligned}
c(0) &= c_0,\\
c(\delta) &= c_\delta.
\end{aligned}
$$

Browers e Chesters (1991) dão a solução analítica:

$$
c(z) = 1 - (1-c_0)\exp\left[\ln\left(\frac{1-c_\delta}{1-c_0}\right)\frac{z}{\delta}\right].
$$

Não sabemos (ainda) como eles a obtiveram, mas podemos ao menos verificar se a expressão acima de fato resolve a equação diferencial. Esta é uma abordagem "de trás para frente", mas nenhuma abordagem válida, ainda que deselegante, deve ser descontada em Matemática Aplicada! Além disso, existem símbolos demais na expressão da solução, *que não afetam as derivadas em relação a* z!. Façamos portanto

$$
\begin{aligned}
c(z) &= 1-(1-c_0)\exp(kz),\\
c'(z) &= -(1-c_0)k\exp(kz),\\
c''(z) &= -(1-c_0)k^2\exp(kz).
\end{aligned}
$$

Os dois lados da equação diferencial, agora, são

$$
\begin{aligned}
-\left[\frac{\mathrm{d}c}{\mathrm{d}z}\right]^2 &= -(1-c_0)^2k^2\exp(2kz),\\
(1-c)\frac{\mathrm{d}^2c}{\mathrm{d}z^2} &= -(1-c_0)^2k^2\exp(2kz).
\end{aligned}
$$

Eles são iguais, e portanto a solução está correta. Mas como ela foi obtida? Da seguinte maneira:

$$
\begin{aligned}
f &= 1-c;\\
\frac{\mathrm{d}f}{\mathrm{d}z} &= -\frac{\mathrm{d}c}{\mathrm{d}z};\\
\frac{\mathrm{d}^2f}{\mathrm{d}z^2} &= -\frac{\mathrm{d}^2c}{\mathrm{d}z^2} \Rightarrow\\
-f\frac{\mathrm{d}^2f}{\mathrm{d}z^2} + \left[\frac{\mathrm{d}f}{\mathrm{d}z}\right]^2 &= 0.
\end{aligned}
$$

Essa equação em f é ligeiramente mais simples do que a original em c. Além disso, um pouco surpreendentemente, ela pode ser manipulada! Veja:

$$
\begin{aligned}
\frac{\mathrm{d}}{\cancel{\mathrm{d}z}}\left(\frac{\mathrm{d}f}{\mathrm{d}z}\right) &= \frac{1}{f}\frac{\mathrm{d}f}{\mathrm{d}z} \times \frac{\mathrm{d}f}{\cancel{\mathrm{d}z}};\\
\mathrm{d}\left(\frac{\mathrm{d}f}{\mathrm{d}z}\right) &= \frac{\mathrm{d}f}{f} \times \frac{\mathrm{d}f}{\mathrm{d}z};\\
\frac{\mathrm{d}\left(\frac{\mathrm{d}f}{\mathrm{d}z}\right)}{\frac{\mathrm{d}f}{\mathrm{d}z}} &= \frac{\mathrm{d}f}{f}.
\end{aligned}
$$

A integral de ambos os lados acima é o ln !

$$
\begin{aligned}
\ln\left|\frac{\mathrm{d}f}{\mathrm{d}z}\right| &= \ln|f| + \ln|k'|;\\
\ln\left|\frac{\mathrm{d}f}{\mathrm{d}z}\right| &= \ln|k'f|;\\
\frac{\mathrm{d}f}{\mathrm{d}z} &= \pm k'f;\\
\frac{\mathrm{d}f}{\mathrm{d}z} &= kf;\\
\frac{\mathrm{d}f}{f} &= k\mathrm{d}z;\\
\ln|f| &= kz + b'';\\
|f| &= \exp(b'')\exp(kz)\\
f &= \pm b'\exp(kz);\\
f &= b\exp(kz).
\end{aligned}
$$

Portanto,

$$
c = 1 - b\exp(kz).
$$

Precisamos ainda fazer com que valham as condições de contorno do problema. Elas geram o sistema de equações

$$
\begin{aligned}
c_0 &= 1 - b,\\
c_\delta &= 1 - b\exp(k\delta)
\end{aligned}
$$

Da primeira,

$$
b = 1 - c_0.
$$

Levando este resultado na segunda,

$$
\begin{aligned}
c_\delta &= 1 - (1 - c_0)\exp(k\delta);\\
c_\delta - 1 &= -(1 - c_0)\exp(k\delta);\\
(1 - c_\delta) &= (1 - c_0)\exp(k\delta);\\
\exp(k\delta) &= \frac{1 - c_\delta}{1 - c_0};\\
k\delta &= \ln\left[\frac{1 - c_\delta}{1 - c_0}\right];\\
k &= \frac{1}{\delta}\ln\left[\frac{1 - c_\delta}{1 - c_0}\right],
\end{aligned}
$$

e isso completa a solução da equação diferencial.

Lesson 9

A transformação de Boltzmann, e a equação de Boussinesq

Nem sempre as "dimensões fundamentais" de um problema são M, L e T. Considere novamente a equação de Boussinesq,

$$\frac{\partial h}{\partial t} = \frac{k_s}{n}\frac{\partial}{\partial x}\left[h\frac{\partial h}{\partial x}\right],$$

Em um aquífero semi-infino (em x), inicialmente cheio até h_0, conforme visto na figura 9.1.

O domínio espacial é $0 \le x < \infty$, e o domínio temporal é $t \ge 0$. Lembre-se de que o fluxo mássico de água através de um plano vertical é dado pela lei de Darcy,

$$q_x = -\rho k_s \frac{\partial h}{\partial x}.$$

Em princípio, as variáveis do problema (dadas pela equação diferencial parcial) e suas dimensões fundamentais são

$$\begin{aligned}
[\![x]\!] &= \mathsf{L},\\
[\![t]\!] &= \mathsf{T},\\
[\![h]\!] &= \mathsf{L},\\
[\![h_0]\!] &= \mathsf{L},\\
[\![k_s]\!] &= \mathsf{L}\,\mathsf{T}^{-1},\\
[\![n_d]\!] &= 1.
\end{aligned}$$

Uma vez que n_d é adimensioanl, há 5 variáveis dimensionais, e duas dimensões indpendentes: esperamos encontrar 3 grupos adimensionais (a rigor, entretanto, é

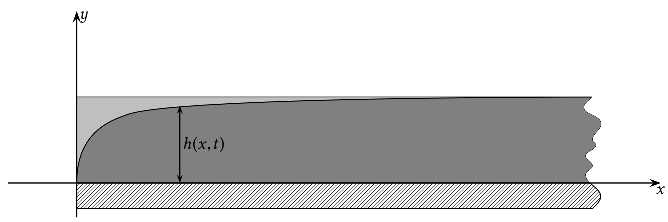

Figure 9.1: Drainage from a semi-infinite aquifer initially fully saturated.

preciso montar a matriz dimensional do problema, e calcular seu posto: veja Dias (2017)). A forma geral da solução portanto deve ser do tipo $\Pi_3 = f(\Pi_1, \Pi_2)$. Isso é razoável, já que em termos das variáveis dimensionais, estamos procurando uma função $h = h(x,t)$ de duas variáveis.

Em uma análise mais detida da física, entretanto, notamos que o vetor fluxo de massa $\boldsymbol{q}$ é horizontal. Além disso, neste particular problema as escalas horizontais são muito maiores do que as verticais. Isso sugere um conjunto diferente de dimensões fundamentais:

$$
\begin{aligned}
[\![x]\!] &= \mathsf{X},\\
[\![t]\!] &= \mathsf{T},\\
[\![h]\!] &= \mathsf{Z},\\
[\![h_0]\!] &= \mathsf{Z},\\
[\![k_s]\!] &= \mathsf{X}^2\,\mathsf{Z}^{-1}\,\mathsf{T}^{-1},\\
[\![n]\!] &= 1.
\end{aligned}
$$

Agora, estamos supondo que comprimentos horizontais possuem uma dimensão (X) distinta daquela de comprimentos verticais (Z).

Na lista acima, as dimensões de k_s foram obitdas da seguinte forma:

$$
\begin{aligned}
[\![\rho]\!] &= \mathsf{M}\,\mathsf{X}^{-1}\,\mathsf{Y}^{-1}\,\mathsf{Z}^{-1},\\
[\![q_x]\!] &= \left[\!\!\left[\rho k_s \frac{\partial h}{\partial x}\right]\!\!\right] = \mathsf{M}\,\mathsf{Y}^{-1}\,\mathsf{Z}^{-1}\,\mathsf{T}^{-1},\\
[\![k_s]\!] &= [\![q_x]\!] \left[[\![\rho]\!] \left[\!\!\left[\frac{\partial h}{\partial x}\right]\!\!\right] \right]^{-1}\\
&= \mathsf{M}\,\mathsf{Y}^{-1}\mathsf{Z}^{-1}\,\mathsf{T}^{-1}\left[\mathsf{M}\,\mathsf{X}^{-1}\,\mathsf{Y}^{-1}\,\mathsf{Z}^{-1}\,\mathsf{Z}\,\mathsf{X}^{-1}\right]^{-1} = \mathsf{X}^2\,\mathsf{Z}^{-1}\,\mathsf{T}^{-1}.
\end{aligned}
$$

Isso sugere que há apenas dois grupos adimensionais, ou seja, que a solução do problema é da forma $\Pi_1 = \phi(\Pi_2)$. Mas isso é o tipo de resultado obtido com a integração de uma *equação diferencial ordinária*! Talvez haja uma maneira de reduzir o problema a uma EDO, e de fato há.

A única maneira de adimensionalizar h é divindido-a por h_0 ($\Pi_1 = h/h_0$). Portanto, primeiro nós reescrevemos

$$
\begin{aligned}
\frac{\partial \frac{h}{h_0}}{\partial t} &= \frac{h_0 k_s}{n}\frac{\partial}{\partial x}\left[\frac{h}{h_0}\frac{\partial \frac{h}{h_0}}{\partial x}\right]\\
\frac{\partial \Pi_1}{\partial t} &= D\frac{\partial}{\partial x}\left[\Pi_1 \frac{\partial \Pi_1}{\partial x}\right]
\end{aligned}
$$

onde $D = h_0 k_s/n$.

As variáveis restantes, x, t e D, têm que formar o outro parâmetro adimensional. É trivial verificar que ele é

$$
\Pi_2 = \frac{x}{\sqrt{4Dt}}.
$$

De fato,

$$
[\![D]\!] = \mathsf{Z}\,\mathsf{X}^2\,\mathsf{Z}^{-1}\,\mathsf{T}^{-1} = \mathsf{X}^2\,\mathsf{T}^{-1}.
$$

O número adimensional 4 é introduzido apenas para simplificar a álgebra subsequente. Em seguida, será mais confortável escrever

$$
\begin{aligned}
\Phi &= \Pi_1,\\
\xi &= \Pi_2.
\end{aligned}
$$

Estamos portanto procurando a função ϕ tal que

$$\Phi = \phi(\xi).$$

Note a distinção cuidadosa entre a função ϕ e a variável dependente Φ. Algumas vezes, esse tipo de distinção carrega demasiadamente a notação, e não é de fato necessária, mas muitas outras vezes (como no nosso caso aqui), ela vale muito a pena.

Com o auxílio da regra da cadeia, temos agora

$$\begin{aligned}
\frac{\partial \Phi}{\partial t} &= \frac{\partial}{\partial t}\left[\phi\left(\frac{x}{\sqrt{4Dt}}\right)\right] \\
&= \frac{\mathrm{d}\phi}{\mathrm{d}\xi}\frac{\partial \xi}{\partial t} \\
&= -\frac{xD}{4(Dt)^{3/2}}\frac{\mathrm{d}\phi}{\mathrm{d}\xi}; \\
\frac{\partial \Phi}{\partial x} &= \frac{\mathrm{d}\phi}{\mathrm{d}\xi}\frac{\partial \xi}{\partial x} = \frac{1}{\sqrt{4Dt}}\frac{\mathrm{d}\phi}{\mathrm{d}\xi}; \\
\Phi\frac{\partial \Phi}{\partial x} &= \phi\frac{\mathrm{d}\phi}{\mathrm{d}\xi}\frac{\partial \xi}{\partial x} = \frac{1}{\sqrt{4Dt}}\phi\frac{\mathrm{d}\phi}{\mathrm{d}\xi}; \\
\frac{\partial}{\partial x}\left[\Phi\frac{\partial \Phi}{\partial x}\right] &= \frac{1}{\sqrt{4Dt}}\frac{\mathrm{d}}{\mathrm{d}\xi}\left[\phi\frac{\mathrm{d}\phi}{\mathrm{d}\xi}\right]\frac{\partial \xi}{\partial x}, \\
&= \frac{1}{4Dt}\frac{\mathrm{d}}{\mathrm{d}\xi}\left[\phi\frac{\mathrm{d}\phi}{\mathrm{d}\xi}\right].
\end{aligned}$$

Fazendo as substituições correspondentes na EDP original,

$$\begin{aligned}
-\frac{xD}{4(Dt)^{3/2}}\frac{\mathrm{d}\phi}{\mathrm{d}\xi} &= \frac{D}{4Dt}\frac{\mathrm{d}}{\mathrm{d}\xi}\left[\phi\frac{\mathrm{d}\phi}{\mathrm{d}\xi}\right] \\
-\frac{D}{4Dt}\frac{2x}{(4Dt)^{1/2}}\frac{\mathrm{d}\phi}{\mathrm{d}\xi} &= \frac{D}{4Dt}\frac{\mathrm{d}}{\mathrm{d}\xi}\left[\phi\frac{\mathrm{d}\phi}{\mathrm{d}\xi}\right] \\
-\frac{D}{4Dt}\frac{2x}{(4Dt)^{1/2}}\frac{\mathrm{d}\phi}{\mathrm{d}\xi} &= \frac{D}{4Dt}\frac{\mathrm{d}}{\mathrm{d}\xi}\left[\phi\frac{\mathrm{d}\phi}{\mathrm{d}\xi}\right] \\
\frac{\mathrm{d}}{\mathrm{d}\xi}\left[\phi\frac{\mathrm{d}\phi}{\mathrm{d}\xi}\right] + 2\xi\frac{\mathrm{d}\phi}{\mathrm{d}\xi} &= 0.
\end{aligned}$$

Essa é uma equação diferencial ordinária não-linear de ordem 2, com coeficientes não-constantes. Sua solução envolve duas condições de contorno em ϕ ou em sua derivada. As 3 condições originais eram

$$\begin{aligned}
h(x,0) &= h_0, \\
h(0,t) &= 0, \\
h(\infty,t) &= h_0.
\end{aligned}$$

Agora, elas se tornam

$$\begin{aligned}
\Phi(x,0) &= 1 & &\Rightarrow & \phi(\infty) &= 1, \\
\Phi(0,t) &= 0 & &\Rightarrow & \phi(0) &= 0, \\
\Phi(\infty,t) &= 1 & &\Rightarrow & \phi(\infty) &= 1.
\end{aligned}$$

Há portanto apenas duas condições de contorno independentes para a EDO. A coincidência dos valores de duas das condições originais é uma condição necessária para que a transformação de Boltzmann funcione.

Nós vamos resolver a EDO de Boussinesq com um método denominado *solução em série*. A ideia é relativamente simples: algumas EDO's não podem ser resolvidas analiticamente em termos de uma forma fechada simples, envolvendo funções tais como sin, cos, exp, etc.. Uma alternativa atraente é procurar uma série que represente a solução:

$$\phi(\xi) = c_0 + c_1\xi^{p_1} + c_2\xi^{p_2} + c_3\xi^{p_3} + \ldots$$

Quando os expoentes $p_1, p_2, p_3 \ldots$ são inteiros positivos nós estamos diante de uma *série de Taylor*, mas muitas vezes uma abordagem mais sofisticada, denominada *Método de Frobenius*, leva a expoentes não-inteiros (em geral racionais). No nosso caso, entretanto, nem mesmo o Método de Frobenius é aplicável, porque nossa EDO é não-linear.

Um ponto muito importante é o seguinte: o que acontece com a série em seus termos mais baixos quando $\xi \to 0$? Note que, dada a condição $\phi(0) = 0$, devemos ter $c_0 = 0$. Portanto,

$$\xi \to 0 \Rightarrow \phi(\xi) = c_1\xi^{p_1} + \text{TOA},$$

onde TOA indica "termos de ordem alta". Em seguida, nós tentaremos encontrar o valor de p_1.

Isso é possível por meio de uma *análise assintótica*. Comecemos por substituir a expressão acima na equação diferencial. Obviamente, isso *não é* a solução, mas sim uma aproximação válida apenas para ξ *muito pequeno*. Obtemos:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\xi}\left[c_1\xi^{p_1} \times c_1p_1\xi^{p_1-1}\right] + 2\xi c_1p_1\xi^{p_1-1} &\approx 0,\\
c_1^2p_1\frac{\mathrm{d}}{\mathrm{d}\xi}\left[\xi^{2p_1-1}\right] + 2c_1p_1\xi^{p_1} &\approx 0,\\
c_1^2p_1(2p_1-1)\xi^{2p_1-2} + 2c_1p_1\xi^{p_1} &\approx 0,\\
c_1(2p_1-1)\xi^{2p_1-2} + 2\xi^{p_1} &\approx 0.
\end{aligned}$$

Naturalmente, não desejamos $c_1 = 0$. O segundo termo do lado esquerdo *nunca* será nulo, mas desde que $p_1 > 0$ ele se tornará tão pequeno quando desejemos quando $\xi \to 0$, e isso é suficiente para nós.

Continuando, suponha que $p_1 < 2$; então, $2p_1 - 2 < p_1$, e isso significa que $\xi^{2p_1-2} \to 0$ *mais devagar* do que ξ^{p_1}: para ξ pequeno, *o primeiro termo será maior do que o segundo*. Nós podemos anular este primeiro termo se fizermos

$$p_1 = 1/2,$$

enquanto que devemos nos lembrar de que o segundo termo, que tende a zero mais rapidamente (ou seja, que é "menor") tem que ser deixado como está. Uma consequência interessante de fazermos $p_1 = 1/2$ é que

$$\lim_{\xi\to 0}\phi\frac{\mathrm{d}\phi}{\mathrm{d}\xi} = \text{const.}.$$

Fisicamente, o produto $\phi\mathrm{d}\phi/\mathrm{d}\xi$ é uma vazão. Isso está OK, porque deve haver uma vazão finita (fluindo através de uma área infinitamente pequena) em $x = 0$ (e consequentemente em $\xi = 0$, enquanto o aquífero se esvazia.

O grande problema da solução em série é a obtenção da constante acima, que está relacionada com c_1. De fato, temos

$$
\begin{aligned}
\phi &\sim c_1 \xi^{1/2},\\
\frac{d\phi}{d\xi} &\sim \frac{1}{2} c_1 \xi^{-1/2},\\
\psi \equiv \phi \frac{d\phi}{d\xi} &\sim \frac{1}{2} c_1^2.
\end{aligned}
$$

Todas as soluções conhecidas em série dependem criticamente do valor de ψ_0, definido como

$$2\psi_0 \equiv c_1^2.$$

Existe uma única maneira "analítica" de obter ψ_0 (Chor, 2014); todas as demais são numéricas. Alternativas numéricas podem ser encontradas em Chor et al. (2013a) assim como em Dias (2017).

Todas as alternativas numéricas significam, na prática, resolver numericamente a equação diferencial ordinária. Nesse sentido, é um pouco frustrante ter que resolver *toda* a equação numericamente para só então poder obter c_1! Isso significa que na prática qualquer solução analítica "em série" só poderá ser obtida *depois* que a solução numérica tiver sido calculada. Esquecendo um pouco isso, vamos dar aqui o valor de c_1:

$$c_1 = 1.15248832742930.$$

Considere agora uma expansão em série na forma

$$\phi(\xi) = \sum_{n=1}^{\infty} c_n \xi^{n/2}.$$

O interessante é que agora é possível obter *relações recursivas* entre os c_n's. Inicialmente, tentemos uma série bem curta:

$$\phi(\xi) = c_1 \xi^{1/2} + c_2 \xi,$$

e substituamos na equaçao diferencial para ver no que dá. Com Maxima,

```
(%i1) c[1] : 1.15248832792930 ;
(%o1)                          1.1524883279293
(%i2) fi : sum( c[n]*xi^(n/2), n, 1, 2) ;
(%o2)                   c   xi + 1.1524883279293 sqrt(xi)
                         2
(%i3) eq : expand(diff(fi*diff(fi,xi),xi) + 2*xi*diff(fi,xi)) ;
                                                   0.86436624594697 c
                                                                     2    2
(%o3)     2 c   xi + 1.1524883279293 sqrt(xi) + ------------------- + c
             2                                          sqrt(xi)          2
```

Vamos traduzir: para ξ pequeno, temos agora

$$c_1 \xi^{1/2} + 2c_2 \xi + \frac{0.86437 c_2}{\sqrt{\xi}} + c_2^2 \approx 0.$$

Porém, à medida que ξ se torna pequeno, temos agora um termo que fica cada vez maior,

$$\frac{0.86437 c_2}{\sqrt{\xi}}$$

e outro que permanece constante,

$$c_2^2.$$

Isso não é possível, a não ser, claro, que $c_2 = 0$. De posse dessa informação, tentemos o próximo termo:

$$\phi(\xi) = c_1\xi^{1/2} + c_3\xi^{3/2}.$$

Agora teremos:

```
(%i1) linel : 70 ;
(%o1)                              70
(%i2) c[1] : 1.15248832792930 ;
(%o2)                       1.1524883279293
(%i3) c[2] : 0 ;
(%o3)                              0
(%i4) fi : sum( c[n]*xi^(n/2), n, 1, 3) ;
                                3/2
(%o4)                c  xi    + 1.1524883279293 sqrt(xi)
                      3
(%i5) eq : expand(diff(fi*diff(fi,xi),xi) + 2*xi*diff(fi,xi)) ;
               3/2      2
(%o5) 3 c  xi    + 3 c  xi + 1.1524883279293 sqrt(xi)
         3            3
                                                 + 2.3049766558586 c
                                                                    3
```

Novamente, à medida em que ξ se torna pequeno, temos um termo que permanece constante,

$$2.3050c_3.$$

Não queremos isso, e fazemos $c_3 = 0$. Seguimos portanto para uma solução do tipo

$$\phi(\xi) = c_1\xi^{3/2} + c_4\xi^2.$$

Agora teremos

```
(%i1) linel : 70 ;
(%o1)                              70
(%i2) c[1] : 1.15248832792930 ;
(%o2)                       1.1524883279293
(%i3) c[2] : 0 ;
(%o3)                              0
(%i4) c[3] : 0 ;
(%o4)                              0
(%i5) fi : sum( c[n]*xi^(n/2), n, 1, 4) ;
                                2
(%o5)                 c  xi  + 1.1524883279293 sqrt(xi)
                       4
(%i6) eq : expand(diff(fi*diff(fi,xi),xi) + 2*xi*diff(fi,xi)) ;
         2   2         2
(%o6) 6 c  xi  + 4 c  xi  + 4.321831229734874 c  sqrt(xi)
         4          4                          4
                                        + 1.1524883279293 sqrt(xi)
```

Finalmente, temos algo aqui! Desprezando os termos de maior ordem (em ξ^2), nossa solução é

$$\phi(\xi) \approx [c_1 + 4.3218c_4]\,\xi^{1/2} \approx 0;$$

isso tem solução, como mostra a continuação da sessão de Maxima:

```
(%i7) coeff(%,xi,1/2) ;
(%o7)           4.321831229734874 c  + 1.1524883279293
                                   4
(%i8) solve(%,c[4]) ;
```

```

rat: replaced 1.1524883279293 by 124148713/107722317 = 1.1524883279293

rat: replaced 4.321831229734874 by 125064949/28937953 = 4.321831229734874
                                3592609621804489
(%o8)                     [c  = - ----------------]
                            4     13472286081766833
(%i9) bfloat(%);
(%o9)                   [c  = - 2.666666666666667b-1]
                          4
```

donde $c_4 = -2.6666 \times 10^{-1}$.

Uma análise cuidadosa e analítica das relações de recursão que estamos encontrando por tentativa e erro produz (Chor et al., 2013a)

$$c_n = -\frac{n+2}{4n} \sum_{k=1}^{n+3} k c_k c_{n-k+4}.$$

Os dois coeficientes nulos se repetirão após c_4 ($c_5 = c_6 = 0$), e assim por diante. Na verdade, é melhor trabalhar com a série contendo apenas coeficientes não nulos, na forma

$$\phi(\xi) = \sum_{n=0}^{\infty} a_n \xi^{\frac{3n+1}{2}},$$

que dá a relação de recorrência

$$a_{n+1} = -\frac{1}{a_0(3n+5)} \left[\frac{4(3n+1)a_n}{3n+3} + \frac{3n+5}{2} \sum_{k=1}^{n} a_k a_{n-k+1} \right].$$

O programa em Maxima a seguir calcula 50 valores de a_n, a partir de $n = 1$:

```
M : 50 ;
a[0]: 1.15248832742929 ;
fi : sum(a[n]*x^((3*n+1)/2),n,0,M) ;
eq : expand( diff(fi*diff(fi,x),x) + 2*x*diff(fi,x) ) ;
cond : [] ;
file_output_append : true ;
with_stdout("se_xi.txt",print(string(float(a[0]))));
for n : 0 thru M-1  do (
   eqqu : ev(coeff(eq,x,(3*n+1)/2),cond) ,
   this : solve(eqqu,a[n+1]),
   cond : append(cond,this),
   this : first(this),
   a[n+1] : rhs(this),
   with_stdout("se_xi.txt",print(float(a[n+1])))
);
```

A tabela a seguir (Chor et al., 2013b) dá os 11 primeiros valores:

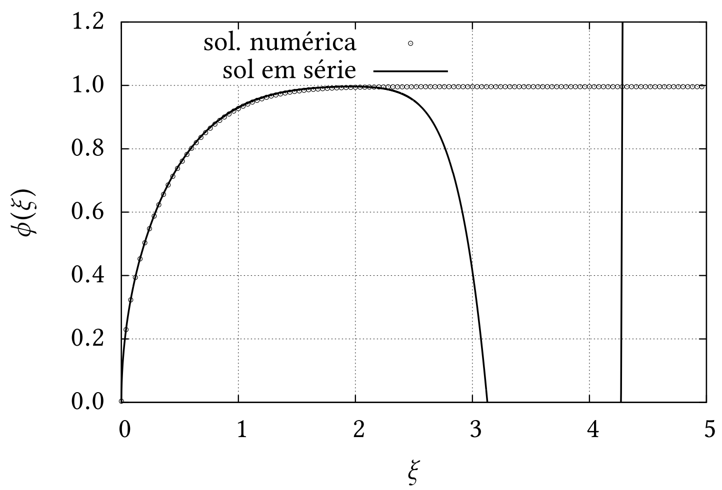

Figure 9.2: Comparação da integração numérica do problema de Boussinesq para um aquífero semi-infinito com a solução em série (11 termos).

Coeficiente	Valor
a_0	$+1{,}15248832742929 \times 10^{+0}$
a_1	$-0{,}26666666666667 \times 10^{+0}$
a_2	$+0{,}046276679827463 \times 10^{+0}$
a_3	$-6{,}4894881692528425 \times 10^{-4}$
a_4	$-9{,}4517828664332276 \times 10^{-4}$
a_5	$-2{,}5400784492116708 \times 10^{-5}$
a_6	$+3{,}5810599703874529 \times 10^{-5}$
a_7	$+3{,}8844564686017651 \times 10^{-6}$
a_8	$-1{,}4163383082670557 \times 10^{-6}$
a_9	$-3{,}2740710683167304 \times 10^{-7}$
a_{10}	$+4{,}5534502970990704 \times 10^{-8}$

Ao mesmo tempo, uma solução numérica de $\phi(\xi)$ e de $\psi(\xi)$ é mostrada na figura 9.2. É obviamente interessante compararmos uma solução numérica com a série que obtivemos. Soluções numéricas são propostas e estudadas em profundidade em Chor (2014), Chor et al. (2013a) e Chor et al. (2015). Uma solução numérica também é apresentada em Dias (2017). A figura 9.2 mostra a comparação das duas, com os 11 termos cujos coeficientes a_n estão dados na tabela acima.

O que está acontecendo? A série (linha contínua) e a solução numérica concordam muito bem até um pouco depois de $\xi = 2$. Logo depois, entretanto, a série (a rigor a soma de seus 11 primeiros termos) diverge violentamente, mergulhando para baixo e depois reaparecendo um pouco depois de $\xi = 4$ "indo para cima". O problema, analisado em detalhe em Chor (2014) e Chor et al. (2013a), é que o raio de convergência de nossa série é *finito*. O raio de convergência da série é $R = 2.3757445$ (Chor et al., 2013a).

Para valores além de (aproximadamente) 2, a série que obtivemos não pode ser aplicada. Uma alternativa de "continuar" a solução analítica para além desse ponto é obter uma *aproximação assintótica* para a solução. Fazemos isso expandindo a equação diferencial,

$$\phi\frac{\mathrm{d}^2\phi}{\mathrm{d}\xi^2} + \left[\frac{\mathrm{d}\phi}{\mathrm{d}\xi}\right]^2 + 2\xi\frac{\mathrm{d}\phi}{\mathrm{d}\xi} = 0,$$

e em seguida notando que a solução $\phi \approx 1$ após $\xi = 2$. Então, substituímos esse valor na equação acima, e encontramos uma *equação diferencial aproximada*

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}\xi^2} + \left[\frac{\mathrm{d}\phi}{\mathrm{d}\xi}\right]^2 + 2\xi\frac{\mathrm{d}\phi}{\mathrm{d}\xi} = 0.$$

Agora, temos uma equação sem ϕ, envolvendo apenas as suas derivadas de ordem 1 e 2. Isso permite imediatamente a aplicação de uma técnica denominada “redução de ordem”, e que é óbvia:

$$\begin{aligned} f(\xi) &= \frac{\mathrm{d}\phi}{\mathrm{d}\xi}, \\ \frac{\mathrm{d}f}{\mathrm{d}\xi} + f^2 + 2\xi f &= 0, \\ \frac{\mathrm{d}f}{\mathrm{d}\xi} + 2\xi f &= -f^2. \end{aligned}$$

Esta é uma equação de Bernoulli (Dias, 2017, seção 8.4), e pode ser resolvida com a transformação de variáveis:

$$\begin{aligned} g &= f^{-1}, \\ \frac{\mathrm{d}g}{\mathrm{d}\xi} &= -f^{-2}\frac{\mathrm{d}f}{\mathrm{d}\xi} \Rightarrow \\ -f^{-2}\frac{\mathrm{d}f}{\mathrm{d}\xi} - \frac{2\xi}{f} &= 1, \\ \frac{\mathrm{d}g}{\mathrm{d}\xi} - 2\xi g &= 1. \end{aligned}$$

Temos agora uma EDO *linear*, *de 1ª ordem*, que Maxima sabe resolver facilmente:

```
(%i1) edo : 'diff(g,x) - 2*x*g - 1 ;
                                       dg
(%o1)                          - 2 g x + -- - 1
                                       dx
(%i2) ode2(edo,g,x);
                              2
                             x    sqrt(%pi) erf(x)
(%o2)                  g = %e    (---------------- + %c)
                                         2
(%i3) f : 1/rhs(%);
                                          2
                                       - x
                                     %e
(%o3)                         ---------------------
                              sqrt(%pi) erf(x)
                              ---------------- + %c
                                     2
(%i4) fi : integrate(f,x);
                               sqrt(%pi) erf(x)
(%o4)                      log(---------------- + %c)
                                      2
```

Portanto,

$$\phi(\xi) = \ln\left(\frac{\sqrt{\pi}}{2}\,\mathrm{erf}(\xi) + k_1\right) + k_2$$

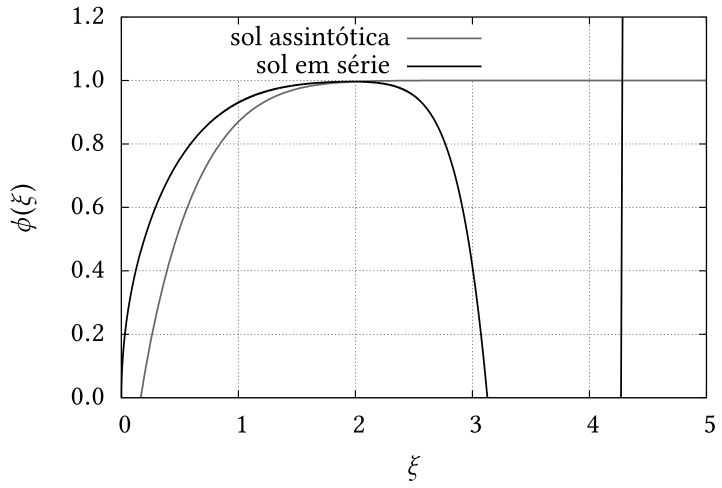

Figure 9.3: Combinação da solução em série com 11 termos com uma solução assintótica da equação de Boussinesq.

Podemos simplificar:

$$
\begin{aligned}
\phi(\xi) &= \ln\left(\frac{\sqrt{\pi}}{2}\operatorname{erf}(\xi) + \frac{\sqrt{\pi}}{2}c_1\right) + k_2,\\
\phi(\xi) &= \ln\left[\frac{\sqrt{\pi}}{2}\left(\operatorname{erf}(\xi) + c_1\right)\right] + k_2,\\
\phi(\xi) &= \ln\left[\frac{\sqrt{\pi}}{2}\right] + \ln\left(\operatorname{erf}(\xi) + c_1\right) + k_2,\\
\phi(\xi) &= \ln\left(\operatorname{erf}(\xi) + c_1\right) + c_2.
\end{aligned}
$$

Desejamos que $\phi(\infty) = 1$:

$$
1 = \ln\left(1 + c_1\right) + c_2.
$$

Uma forma elegante — e nada óbvia — de atender a essa condição é fazer

$$
\begin{aligned}
c_2 &= \ln\left(\frac{1}{1+c_1}\right) + 1,\\
\phi(\xi) &= \ln\left(\frac{\operatorname{erf}(\xi) + c_1}{1+c_1}\right) + 1.
\end{aligned}
$$

Em $\xi = 2$, a soma dos 11 primeiros termos de nossa série vale $\phi(\xi) \approx 0.993981$. Façamos

$$
\begin{aligned}
0.993981 &= \ln\left(\frac{\operatorname{erf}(2) + c_1}{1+c_1}\right) + 1 \Rightarrow\\
c1 &= 2.909725086888533 \times 10^{-1}.
\end{aligned}
$$

Plotemos agora a série juntamente com a nossa aproximação assintótica, na figura 9.3. Note como o "casamento" de ambas é bastante satisfatório: podemos portanto utilizar na prática nossa série (com 11 termos, por exemplo) até $\xi = 2$, e a aproximação assintótica, com o valor de c_1 obtido acima, a partir desse ponto.

Lesson 10

Um problema parabólico não-linear

10.1 A equação de Boussinesq não-linear

A equação de Boussinesq para águas subterrâneas, adimensionalizada, tem a forma

$$\frac{\partial \eta}{\partial t} = \frac{\partial}{\partial x}\left(\eta \frac{\partial \eta}{\partial x}\right).$$

As condições de contorno que utilizaremos são

$$\begin{aligned} \eta(0,t) &= 0, \qquad t \geq 0, \\ \frac{\partial \eta}{\partial x}(1,t) &= 0, \qquad t \geq 0. \end{aligned}$$

A condição inicial que utilizaremos é *incompleta*, e envolve apenas um ponto do perfil inicial:

$$\eta(1,0) = 1;$$

em um problema linear tradicional, a condição correspondente seria

$$\eta(x,0) = f(x).$$

Conforme veremos, o problema tem solução analítica possível apenas para uma particular forma para $f(x)$: as soluções que obteremos serão *auto-similares*. O que isso significa, e porque as soluções analíticas desse problema não-linear são apenas possíveis para particulares formas funcionais de $f(x)$ ficará claro na sequência.

Tentaremos o método de separação de variáveis (que raramente funciona em problemas não-lineares — mais vai funcionar neste caso!)

$$\eta = X(x)T(t)$$

e substituímos na equação original, que nos dá

$$\begin{aligned} X\frac{\mathrm{d}T}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}x}\left(XTT\frac{\mathrm{d}X}{\mathrm{d}x}\right) \\ X\frac{\mathrm{d}T}{\mathrm{d}t} &= T^2\frac{\mathrm{d}}{\mathrm{d}x}\left(X\frac{\mathrm{d}X}{\mathrm{d}x}\right) \\ \frac{1}{T^2}\frac{\mathrm{d}T}{\mathrm{d}t} &= \frac{1}{X}\frac{\mathrm{d}}{\mathrm{d}x}\left(X\frac{\mathrm{d}X}{\mathrm{d}x}\right) = c_1. \end{aligned}$$

Num ambiente tradicional, procuraríamos agora o problema de Sturm-Liouville; no entanto, nenhuma das duas equações diferenciais que nós podemos obter a partir do método de separação de variáveis produz um problema de Sturm-Liouville! Estamos perdidos, e a Teoria de Sturm-Liouville não nos guiará para a solução. Precisaremos ser mais “empíricos”, e ir tateando no rumo da solução. A equação ordinária em T é

$$
\begin{aligned}
\frac{\mathrm{d}T}{T^2} &= c_1 \mathrm{d}t,\\
-\frac{1}{T} - c_2 &= c_1 T\\
-\frac{1}{T} &= c_2 + c_1 T\\
-T &= \frac{1}{c_2 + c_1 T}\\
&= \frac{1}{c_2 + c_1 T} \times \frac{c_2}{c_2}\\
&= \frac{1}{c_2}\frac{1}{c_2 + c_1 t} \times \frac{1}{\frac{1}{c_2}}\\
&= \frac{1}{c_2}\frac{1}{1 + \frac{c_1}{c_2}t} \equiv \frac{1}{c_2}\frac{1}{(1 + at)}.
\end{aligned}
$$

Nesse ponto, nós “descobrimos” um tipo de solução que tem a forma

$$
\eta = \frac{X/c_2}{-(1 + at)}.
$$

É claro que é conveniente mudarmos um pouco a forma da solução; sem perda de generalidade, fazemos

$$
-F(x) \equiv \frac{X(x)}{c_2} \Rightarrow \eta(x,t) = \frac{F(x)}{1 + at}.
$$

Essa é a forma na qual procuraremos, a partir de agora, uma solução. Note também que, uma vez que a equação de Boussinesq que estamos tentando resolver é não linear, não há a possibilidade de somar (infinitos) termos de uma série: ou resolvemos o problema com uma única $F(x)$, ou nada feito! Portanto, a solução apontada acima é uma solução *auto-similar*: a forma da superfície freática, $F(x)$, uma vez atingida, não muda mais!

É nesse sentido que a solução que estamos obtendo não é suficientemente “geral”: na verdade, nós estamos encontrando a solução de um problema após a superfície freática ter evoluído, desde uma forma inicial arbitrária $f(x)$, para a forma auto-similar $F(x)$ que se manterá até o fim do problema.

Prosseguindo,

$$
\begin{aligned}
\frac{1}{X}\frac{\mathrm{d}}{\mathrm{d}x}\left(X\frac{\mathrm{d}X}{\mathrm{d}x}\right) &= c_1,\\
\frac{1}{\frac{-X}{c_2}}\frac{\mathrm{d}}{\mathrm{d}x}\left(\left(\frac{-X}{c_2}\right)\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{-X}{c_2}\right)\right) &= -\left(\frac{c_1}{c_2}\right) = -a,\\
\frac{1}{F}\frac{\mathrm{d}}{\mathrm{d}x}\left(F\frac{\mathrm{d}F}{\mathrm{d}x}\right) &= -a.
\end{aligned}
$$

Com a ajuda de

$$F\frac{\mathrm{d}F}{\mathrm{d}x} = \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{F^2}{2}\right),$$

ficamos com

$$\begin{aligned}\frac{1}{F}\frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{F^2}{2}\right)\right] &= -a\\ \frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{F^2}{2}\right)\right] &= -aF.\end{aligned}$$

A substituição que se segue é à primeira vista um pouco estranha, mas válida!

$$\begin{aligned}p &= \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{F^2}{2}\right),\\ \frac{\mathrm{d}p}{\mathrm{d}x} &= -aF,\\ \mathrm{d}x &= \frac{\mathrm{d}(F^2/2)}{p}.\end{aligned}$$

A idéia é eliminar x (!), do que resulta

$$\begin{aligned}\frac{\mathrm{d}p}{\frac{\mathrm{d}(F^2/2)}{p}} &= -aF,\\ p\mathrm{d}p &= -aF(F\mathrm{d}F),\\ \frac{p^2}{2} &= -a\frac{F^3}{3} + c_3.\end{aligned}$$

Podemos agora reintroduzir a dependência em x; ao mesmo tempo, mudamos as variáveis de integração de x para ξ, e de F para y:

$$\begin{aligned}\left[\frac{\mathrm{d}F^2/2}{\mathrm{d}x}\right]^2 &= -\frac{2a}{3}F^3 + 2c_3,\\ \frac{\mathrm{d}}{\mathrm{d}\xi}\left(\frac{y^2}{2}\right) &= \left(2c_3 - \frac{2a}{3}y^3\right)^{1/2},\\ \frac{y\mathrm{d}y}{\left(2c_3 - \frac{2a}{3}y^3\right)^{1/2}} &= d\xi.\end{aligned}$$

Agora, integramos para recuperar os símbolos x e F:

$$\begin{aligned}\int_0^F \frac{y\mathrm{d}y}{\left(2c_3 - \frac{2a}{3}y^3\right)^{1/2}} &= \int_0^x d\xi\\ \int_0^{F(x)} \frac{y\mathrm{d}y}{\left(2c_3 - \frac{2a}{3}y^3\right)^{1/2}} &= x.\end{aligned}$$

Observe que o que é calculável é o lado *esquerdo*: portanto, é mais natural pensar em (quer dizer: calcular) $x(F)$ do que $F(x)$!

As integrais acima dão conta das condições de contorno, mas ainda precisamos impor nossa "condição inicial" $\partial\eta(1,t)/\partial x = 0$, que se traduz em

$$\frac{\mathrm{d}F(1)}{\mathrm{d}x} = 0.$$

Mas como não "temos" $F(x)$, e sim $x(F)$, nós vamos precisar da regra de Leibniz:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{a(t)}^{b(t)} f(x,t)\,\mathrm{d}x = \int_a^b \frac{\partial f}{\partial t}\,\mathrm{d}x + f(b,t)\frac{\mathrm{d}b}{\mathrm{d}t} - f(a,t)\frac{\mathrm{d}a}{\mathrm{d}t}.$$

Para não interrompermos a narrativa interessante de obter a solução de uma E.D.P. não-linear, será melhor se aceitarmos a validade da regra de Leibniz por enquanto. Depois que tivermos resolvido o problema, voltaremos a ela, e a deduziremos. Seguindo,

$$\begin{aligned} 1 &= \frac{F}{\left(2c_3 - \frac{2a}{3}F^3\right)^{1/2}}\frac{\mathrm{d}F}{\mathrm{d}x}, \\ \frac{\mathrm{d}F}{\mathrm{d}x} &= \frac{\left(2c_3 - \frac{2a}{3}F^3\right)}{F}. \end{aligned}$$

Porém,

$$\begin{aligned} F(1) &= 1, \\ \frac{\mathrm{d}F(1)}{\mathrm{d}x} &= 0, \end{aligned}$$

donde

$$2c_3 - \frac{2a}{3} = 0 \Rightarrow c_3 = \frac{a}{3};$$

donde nós retornamos para

$$\begin{aligned} x &= \int_0^{F(x)} \frac{y\mathrm{d}y}{\left(2c_3 - \frac{2a}{3}y^3\right)^{1/2}}, \\ x &= \left(\frac{3}{2a}\right)^{1/2}\int_0^{F(x)} \frac{y\,\mathrm{d}y}{(1-y^3)^{1/2}}. \end{aligned}$$

É claro que falta obter o valor de a; usando uma das condições de contorno,

$$\begin{aligned} \eta(1,0) &= 1, \\ F(1) &= 1, \\ 1 &= \left(\frac{3}{2a}\right)^{1/2}\int_0^1 y(1-y^3)^{-1/2}\,\mathrm{d}y. \end{aligned}$$

O valor de a fica assim implicitamente determinado. Em termos de funções da Física Matemática, entretanto, é conveniente avançar um pouco mais, e utilizar a *função Beta*. Ela é definida por

$$B(p,q) = \int_0^1 u^{p-1}(1-u)^{q-1}\,du.$$

A função Beta é convenientemente tabelada (ou programada!) em diversas referências.

A comparação entre as duas últimas equações acima sugere imediatamente $u = y^3$; então,

$$
\begin{aligned}
y &= u^{1/3},\\
\mathrm{d}y &= \frac{1}{3}u^{-2/3}\,\mathrm{d}u,\\
1 &= \left(\frac{1}{6a}\right)^{1/2}\int_0^1 u^{-1/3}(1-u)^{-1/2}\,\mathrm{d}u\\
1 &= \left(\frac{1}{6a}\right)^{1/2} B(2/3,1/2),\\
a &= [B(2/3,1/2)]^2/6.
\end{aligned}
$$

Retornemos agora para o cálculo de $x(F)$:

$$
\begin{aligned}
x &= \left(\frac{3}{2a}\right)^{1/2}\int_0^{F(x)} y(1-y^3)^{1/2}\,\mathrm{d}y\\
&= \left(\frac{3\times 6}{2[B(2/3,1/2)]^2}\right)^{1/2}\int_0^{F(x)} y(1-y^3)^{1/2}\,\mathrm{d}y\\
&= \frac{3}{B(2/3,1/2)}\int_0^{F(x)} y(1-y^3)^{1/2}\,\mathrm{d}y\\
&= \frac{1}{B(2/3,1/2)}\int_0^{F^3(x)} u^{-1/3}(1-u)^{-1/2}\,\mathrm{d}u.
\end{aligned}
$$

A equação acima é uma função Beta incompleta $I_{F^3}(2/3,1/2)$ (veja Press et al., 1992, seção 6.4). Portanto,

$$
x = I_{F^3}(2/3,1/2)\ \blacksquare
$$

10.2 A regra de Leibniz

A regra de Leibniz é

$$
\frac{\mathrm{d}}{\mathrm{d}t}\int_{a(t)}^{b(t)} f(x,t)\,\mathrm{d}x = f(b,t)\frac{\mathrm{d}b}{\mathrm{d}t} - f(a,t)\frac{\mathrm{d}a}{\mathrm{d}t} + \int_{a(t)}^{b(t)} \frac{\partial f(x,t)}{\partial t}\,\mathrm{d}x.
$$

Uma demonstração particularmente interessante da regra de Leibniz é baseada em uma abordagem *lagrangeana* do significado da integral do lado esquerdo da equação acima. A idéia é interpretar que $a(t)$ e $b(t)$ são as posições de partículas materiais que, em $t = 0$, delimitam o intervalo $[\alpha,\beta]$ (veja a figura 10.1).

Agora, cada ponto desse intervalo também é uma partícula que descreve um movimento unidimensional do tipo

$$
x = X(\xi,t),
$$

onde ξ é a posição da partícula em $t = 0$. Observe que ξ é um marcador que define qual é a partícula, entre α e β, cujo movimento está sendo descrito (veja a linha tracejada na figura 10.1). Em particular,

$$
\begin{aligned}
a(t) &= X(\alpha,t), \qquad & \frac{\mathrm{d}a}{\mathrm{d}t} &= \frac{\partial X(\alpha,t)}{\partial t},\\
b(t) &= X(\beta,t), \qquad & \frac{\mathrm{d}b}{\mathrm{d}t} &= \frac{\partial X(\beta,t)}{\partial t}
\end{aligned}
$$

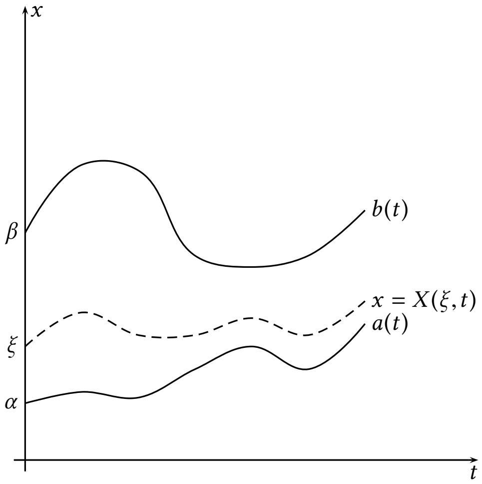

Figure 10.1: Uma dedução lagrangeana da regra de Leibniz.

(veja a figura 10.1). A derivada total de $x = X(\xi, t)$ é

$$\mathrm{d}x = \frac{\partial X}{\partial \xi}\mathrm{d}\xi + \frac{\partial X}{\partial t}\mathrm{d}t. \tag{10.1}$$

Para cada valor fixo de t, mudamos a variável de x para ξ, de modo que a integral do lado esquerdo da equação da regra de Leibniz torna-se

$$\int_\alpha^\beta f\left(X(\xi, t), t\right) \frac{\partial X}{\partial \xi}\, \mathrm{d}\xi.$$

O integrando dessa expressão é uma função apenas de t, e os limites de integração, α e β, não dependem de t. Dessa forma, é possível agora fazer

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\int_\alpha^\beta f\left(X(\xi, t), t\right) \frac{\partial X}{\partial \xi}\, \mathrm{d}\xi &= \int_\alpha^\beta \frac{\partial}{\partial t}\left[f\left(X(\xi, t), t\right) \frac{\partial X}{\partial \xi}\right] \mathrm{d}\xi \\
&= \int_\alpha^\beta \left[\frac{\partial}{\partial t}\left(f\left(X(\xi, t), t\right)\right) \frac{\partial X}{\partial \xi} + f \frac{\partial^2 X}{\partial t \partial \xi}\right] \mathrm{d}\xi \\
&= \int_\alpha^\beta \left[\frac{\partial}{\partial t}\left(f\left(X(\xi, t), t\right)\right) \frac{\partial X}{\partial \xi} + f \frac{\partial}{\partial \xi}\frac{\partial X}{\partial t}\right] \mathrm{d}\xi.
\end{aligned}$$

Este é um ponto que requer cuidado! Observe:

$$\frac{\partial}{\partial t}\left(f\left(X(\xi, t), t\right)\right) = \frac{\partial f}{\partial x}\frac{\partial X}{\partial t} + \frac{\partial f}{\partial t};$$

portanto,

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\int_{a(t)}^{b(t)} f(x, t)\, \mathrm{d}t &= \int_\alpha^\beta \left[\left(\frac{\partial f}{\partial x}\frac{\partial X}{\partial t} + \frac{\partial f}{\partial t}\right) \frac{\partial X}{\partial \xi} + f \frac{\partial}{\partial \xi}\frac{\partial X}{\partial t}\right] \mathrm{d}\xi \\
&= \int_\alpha^\beta \left[\left(\frac{\partial f}{\partial x}\frac{\partial X}{\partial t} + \frac{\partial f}{\partial t}\right) \frac{\partial X}{\partial \xi} + f \frac{\partial}{\partial x}\left(\frac{\partial X}{\partial t}\right) \frac{\partial X}{\partial \xi}\right] \mathrm{d}\xi.
\end{aligned}$$

Note o surgimento de $\partial X/\partial t$: é conveniente dar-lhe um nome:

$$u(x,t) = u(X(\xi,t),t) \equiv \frac{\partial X(\xi,t)}{\partial t}.$$

É evidente que u indica a velocidade de cada partícula. Agora, nós *voltamos* de uma integral em ξ para uma integral em x:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\int_{a(t)}^{b(t)} f(x,t)\,\mathrm{d}t &= \int_\alpha^\beta \left[u\frac{\partial f}{\partial x} + \frac{\partial f}{\partial t} + f\frac{\partial u}{\partial x}\right]\frac{\partial X}{\partial \xi}\,\mathrm{d}\xi \\
&= \int_\alpha^\beta \left[\frac{\partial f}{\partial t} + \frac{\partial (uf)}{\partial x}\right]\frac{\partial X}{\partial \xi}\,\mathrm{d}\xi \\
&= \int_{a(t)}^{b(t)} \left[\frac{\partial f}{\partial t} + \frac{\partial (uf)}{\partial x}\right]\mathrm{d}x \\
&= u(x,t)f(x,t)\Big|_{a(t)}^{b(t)} + \int_{a(t)}^{b(t)} \frac{\partial f(x,t)}{\partial t}\,\mathrm{d}x.
\end{aligned}$$

Finalmente, em vista de nossas definições para $u(t)$, $a(t)$ e $b(t)$,

$$\begin{aligned}
u(a(t),t) &= \frac{\partial X(\alpha,t)}{\partial t} = \frac{\mathrm{d}a}{\mathrm{d}t}, \\
u(b(t),t) &= \frac{\partial X(\beta,t)}{\partial t} = \frac{\mathrm{d}b}{\mathrm{d}t};
\end{aligned}$$

Com isso, nó obtemos, finalmente, a regra de Leibniz:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{a(t)}^{b(t)} f(x,t)\,\mathrm{d}t = f(b,t)\frac{\mathrm{d}b}{\mathrm{d}t} - f(a,t)\frac{\mathrm{d}a}{\mathrm{d}t} + \int_{a(t)}^{b(t)} \frac{\partial f(x,t)}{\partial t}\,\mathrm{d}x \;\blacksquare$$

A dedução acima nada mais é do que a versão unidimensional do *teorema do transporte de Reynolds* (Kundu, 1990, cap. 4): esse último desempenha um papel fundamental em Mecânica dos Fluidos.

A regra de Leibniz é extremamente útil! Por exemplo, em Finnigan (2006), encontramos o seguinte trecho:

> Generalizing the time averaging operator in Eq. (1) to a moving average filter, we define,
>
> $$\overline{\phi(t)}^P = \frac{1}{2P}\int_{t-P}^{t+P} \phi(t')\,\mathrm{d}t'$$
>
> ... and it's straightforward to show that
>
> $$\frac{\partial\, \overline{c}^P}{\partial t} = \overline{\frac{\partial c}{\partial t}}^P \ldots$$

A prova depende da regra de Leibniz: primeiramente,

$$\begin{aligned}
\overline{\frac{\partial c}{\partial t}} &= \frac{1}{2P}\int_{-P}^{P} \frac{\partial c}{\partial \tau}\,\mathrm{d}\tau \\
&= \frac{1}{2P}\left[c(P) - c(-P)\right],
\end{aligned}$$

onde nós omitimos o sobrescrito P por simplicidade. Do outro lado da igualdade nós precisamos da regra de Leibniz:

$$
\begin{aligned}
\frac{\partial \overline{c}}{\partial t} &= \frac{\partial}{\partial t}\frac{1}{2P}\int_{t-P}^{t+P} c(\tau)\,\mathrm{d}\tau \\
&= \frac{1}{2P}\frac{\partial}{\partial t}\int_{t-P}^{t+P} c(\tau)\,\mathrm{d}\tau \\
&= \frac{1}{2P}\left[c(t+P)\frac{\mathrm{d}(t+P)}{\mathrm{d}t} - c(t-P)\frac{\mathrm{d}(t-P)}{\mathrm{d}t}\right] + \frac{1}{2P}\int_{t-P}^{t+P} \underbrace{\frac{\partial c(\tau)}{\partial t}}_{\equiv 0}\,\mathrm{d}\tau \\
&= \frac{1}{2P}\left[c(P) - c(-P)\right] \quad \blacksquare
\end{aligned}
$$

Lesson 11

A Transformada de Fourier

A transformada de Fourier é uma das ferramentas mais poderosas de Matemática Aplicada. Ela é usada para decompor uma função de acordo não com o seu comportamento local ("$f(x)$"), mas com o comportamento sobre um conjunto de escalas ("$\widehat{f}(k)$"), onde k é um número de onda (uma frequência angular). À medida que nos acostumarmos com o cálculo de transformadas de Fourier, e com suas propriedades, nós poderemos começar a "entender" o par $f(x) \leftrightarrow \widehat{f}(k)$ como duas faces de uma mesma moeda, ou seja: como uma única *entidade*, que nós usualmente identificamos no domínio do espaço-tempo ($f(x)$), mas que possui uma existência igualmente "real" e válida no domínio da frequência ($\widehat{f}(k)$).

11.1 Definição e o teorema da inversão

A transformada de Fourier será definida neste texto como

$$\mathscr{F}\{f(x)\}(k) = \widehat{f}(k) \equiv \frac{1}{2\pi}\int_{-\infty}^{+\infty} f(x)\mathrm{e}^{-\mathrm{i}kx}\mathrm{d}x. \tag{11.1}$$

O resultado mais importante de toda a teoria, sem dúvida, é o

---

Teorema 11.1 (Teorema da inversão) Se $\widehat{f}(k)$ é definida por (11.1), então

$$f(x) = \int_{-\infty}^{+\infty} \widehat{f}(k)\mathrm{e}^{\mathrm{i}kx}\,\mathrm{d}k. \tag{11.2}$$

11.2 O cálculo de algumas transformadas

Esta é uma seção de "mãos à obra", com alguns cálculos de transformadas de Fourier resolvidos.

Calcule $\widehat{f}(k)$ para

$$f(x) = \mathrm{e}^{-\left(\frac{x}{a}\right)^2}.$$

A fração no argumento é para nos lembrarmos de que em geral, em aplicações, é preciso levar em consideração as dimensões físicas. Assim, se x é uma distância ao longo de uma reta,

$$[\![x]\!] = [\![a]\!] = \mathsf{L}.$$

O cálculo padrão é

$$\begin{aligned}\widehat{f}(k) &= \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{e}^{-\left(\frac{x}{a}\right)^2}\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x\\ &= \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{e}^{-\left[\left(\frac{x}{a}\right)^2+\mathrm{i}kx\right]}\,\mathrm{d}x.\end{aligned}$$

Aqui, o “truque” padrão é “completar o quadrado”. Observe como x aparece com as potências 2 e 1 acima; a idéia é encontrar um binômio de x e uma constante que resulte em um quadrado perfeito. A técnica é sistemática:

$$
\begin{aligned}
(\alpha+\beta)^2 &= \alpha^2 + 2\alpha\beta + \beta^2,\\
\alpha &= \frac{x}{a},\\
2\alpha\beta &= \mathrm{i}kx,
\end{aligned}
$$

donde

$$
\begin{aligned}
\beta &= \frac{\mathrm{i}kx}{2\alpha} = \frac{\mathrm{i}kxa}{2x} = \frac{\mathrm{i}ka}{2},\\
\beta^2 &= -\frac{k^2a^2}{4}.
\end{aligned}
$$

Agora,

$$
\begin{aligned}
\left(\frac{x}{a}\right)^2 + \mathrm{i}kx &= \left(\frac{x}{a}\right)^2 + \mathrm{i}kx - \frac{k^2a^2}{4} + \frac{k^2a^2}{4}\\
&= \left(\frac{x}{a} + \frac{\mathrm{i}ka}{2}\right)^2 + \frac{k^2a^2}{4}
\end{aligned}
$$

A transformada desejada é

$$
\begin{aligned}
\widehat{f}(k) &= \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{e}^{-\left(\frac{x}{a}+\frac{\mathrm{i}ka}{2}\right)^2 - \frac{k^2a^2}{4}}\,\mathrm{d}x\\
&= \frac{1}{2\pi}\mathrm{e}^{-\frac{k^2a^2}{4}}\int_{-\infty}^{+\infty} \mathrm{e}^{-\left(\frac{x}{a}+\frac{\mathrm{i}ka}{2}\right)^2}\,\mathrm{d}x.
\end{aligned}
$$

Essa não é uma integral elementar, e precisa ser calculada com um certo cuidado. Faça

$$
z = \xi + \mathrm{i}\eta = \frac{x}{a} + \frac{\mathrm{i}ka}{2}, \qquad \mathrm{d}z = \mathrm{d}x/a,
$$

e reescreva

$$
\widehat{f}(k) = \frac{1}{2\pi} a \mathrm{e}^{-\frac{k^2a^2}{4}} \int_{-\infty+\frac{\mathrm{i}ka}{2}}^{+\infty+\frac{\mathrm{i}ka}{2}} \mathrm{e}^{-z^2}\,\mathrm{d}z.
$$

Essa é uma integral de *linha* no plano complexo; em primeiro lugar, note que neste exemplo a parte real de z não é x, mas sim $\xi = x/a$; a parte imaginária é η, e o caminho de integração é a reta $\eta = ka/2$.

Em seguida, note que $g(z) = \mathrm{e}^{-z^2}$ é uma função *analítica* em todo o plano $\xi\times\eta$, e portanto pelo Teorema de Cauchy qualquer integral em um contorno fechado de $g(z)$ é nula. Em seguida, considere o contorno mostrado na figura 11.1.

Pelo Teorema de Cauchy, então,

$$
\int_{ABCD} g(z)\,\mathrm{d}z = 0.
$$

O trecho CD produz uma integral puramente real, e bem conhecida no lim $L \to \infty$:

$$
\lim_{L\to\infty}\int_{CD} g(z)\,dz = \lim_{L\to\infty}\int_{+L}^{-L} \mathrm{e}^{-x^2}\,\mathrm{d}x = -\sqrt{\pi}.
$$

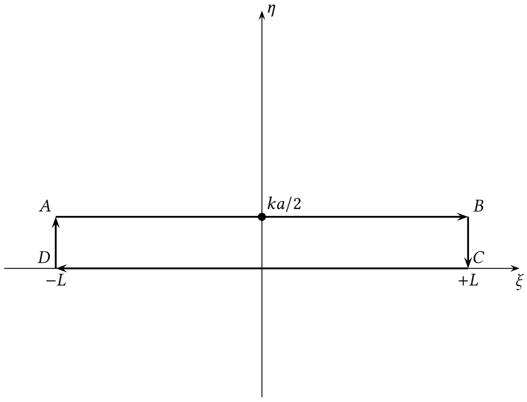

Figure 11.1: O contorno de integração de $g(z) = e^{-z^2}$.

A esperança aqui é que $\left|\int_{BC,DA}\right| \to 0$ quando $L \to \infty$, de tal maneira que a integral que precisamos calcular, $\int_{AB} g(z)\,dz$, seja dada em função da integral conhecida $\int_{CD} g(z)\,dz$.

A verificação não é muito difícil:

$$\begin{aligned}
\left|\int_{BC} g(z)\,dz\right| &\le \int_{BC} |g(z)\,dz| \\
&= \int_{\eta=0}^{ka/2} \left|e^{-z^2}\right| dz \\
&= \int_{\eta=0}^{ka/2} \left|e^{-(L+i\eta)^2}\right| d\eta \\
&= \int_{\eta=0}^{ka/2} \left|e^{-(L^2+i2L\eta-\eta^2)}\right| d\eta \\
&= e^{-L^2} \int_{\eta=0}^{ka/2} \left|e^{-i2L\eta}\right| \left|e^{-\eta^2}\right| d\eta \\
&= e^{-L^2} \int_{\eta=0}^{ka/2} e^{-\eta^2}\,d\eta \;\to 0 \text{ quando } L \to \infty.
\end{aligned}$$

Por um procedimento similar,

$$\lim_{L\to\infty} \left|\int_{DA} f(z)\,dz\right| = 0.$$

Consequentemente,

$$\int_{-\infty+ika/2}^{+\infty+ika/2} g(z)\,dz + \int_{+\infty}^{-\infty} e^{-x^2}\,dx = 0,$$

$$\int_{-\infty+ika/2}^{+\infty+ika/2} g(z)\,dz = -\int_{+\infty}^{-\infty} e^{-x^2}\,dx = +\sqrt{\pi}.$$

A transformada de Fourier desejada pode agora ser calculada, finalmente:

$$\widehat{f}(k) = \frac{\sqrt{\pi}}{2\pi} a e^{-\frac{k^2a^2}{4}} = \frac{1}{2\sqrt{\pi}} a e^{-\frac{k^2a^2}{4}}.$$

Se

$$f(x) = \frac{1}{1 + \left(\frac{x}{a}\right)^2} = \frac{a^2}{x^2 + a^2},$$

obtenha $\widehat{f}(k)$.

$$\begin{aligned}
\widehat{f}(k) &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{a^2}{x^2 + a^2} \mathrm{e}^{-\mathrm{i}kx}\, \mathrm{d}x \\
&= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{a^2}{x^2 + a^2} \left[\cos(kx) - \mathrm{i}\,\mathrm{sen}(kx)\right] \mathrm{d}x \\
&= \frac{a}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{1 + \left(\frac{x}{a}\right)^2} \cos\left(ka\frac{x}{a}\right) \mathrm{d}\left(\frac{x}{a}\right),
\end{aligned}$$

pois o integrando envolvendo sen$(\cdot)$ é uma função ímpar e a integral correspondente se anula.

Fazendo $\xi = x/a$,

$$\widehat{f}(k) = \frac{2a}{2\pi} \int_{\xi=0}^{\infty} \frac{\cos(ka\xi)}{1 + \xi^2}\, \mathrm{d}\xi = \frac{a}{2}\mathrm{e}^{-|ka|} \;\blacksquare$$

Se

$$\widehat{g}(k) = \begin{cases} \frac{1}{2\pi}, & |k| < k_0, \\ 0, & |k| > k_0, \end{cases}$$

calcule $g(x)$.

$$\begin{aligned}
g(x) &= \frac{1}{2\pi} \int_{-k_0}^{+k_0} \mathrm{e}^{+\mathrm{i}kx}\, \mathrm{d}k \\
&= \frac{1}{2\pi \mathrm{i}x} \int_{-k_0}^{+k_0} \mathrm{e}^{+\mathrm{i}kx}\, \mathrm{d}(\mathrm{i}kx) \\
&= \frac{1}{2\pi \mathrm{i}x} \left[\mathrm{e}^{+\mathrm{i}k_0x} - \mathrm{e}^{-\mathrm{i}k_0x}\right] \\
&= \frac{1}{\pi x}\,\mathrm{sen}(k_0x) \;\blacksquare
\end{aligned}$$

Calcule a transformada de Fourier de

$$f(x) = \begin{cases} 0, & |x| > 1; \\ x + 1, & -1 \le x \le 0; \\ 1 - x, & 0 < x \le 1. \end{cases}$$

Note que f é par.

$$\begin{aligned}
\mathscr{F}\{f(x)\} &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} f(x)\mathrm{e}^{-\mathrm{i}kx}\, \mathrm{d}x \\
&= \frac{1}{2\pi} \int_{-\infty}^{+\infty} f(x)\left[\cos(kx) - \mathrm{i}\,\mathrm{sen}(kx)\right] \mathrm{d}x \\
&= \frac{1}{2\pi} \int_{-\infty}^{+\infty} f(x)\cos(kx)\, \mathrm{d}x \\
&= \frac{1}{\pi} \int_{0}^{1} f(x)\cos(kx)\, \mathrm{d}x = \frac{1 - \cos k}{k^2} \;\blacksquare
\end{aligned}$$

11.3 Linearidade; a transformada das derivadas

A transformada de Fourier é *linear*: se $f(x)$ e $g(x)$ são duas funções transformáveis, então

$$
\begin{aligned}
\mathscr{F}\{\alpha f(x)+\beta g(x)\} &= \frac{1}{2\pi}\int_{-\infty}^{+\infty}[\alpha f(x)+\beta g(x)]\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x \\
&= \frac{\alpha}{2\pi}\int_{-\infty}^{+\infty} f(x)\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x + \frac{\beta}{2\pi}\int_{-\infty}^{+\infty} g(x)\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x \\
&= \alpha\widehat{f}(k)+\beta\widehat{g}(k). \qquad (11.3)
\end{aligned}
$$

Suponha que $f(x)$ e $\widehat{f}(k)$ possuam um comportamento muito bom no infinito, de tal maneira que

$$\lim_{x\to\pm\infty} f(x) = 0, \qquad (11.4)$$

$$\lim_{k\to\pm\infty} \widehat{f}(k) = 0. \qquad (11.5)$$

Intuitivamente, essas condições são necessárias para a existência "clássica" das integrais (11.1) e (11.2). Por outro lado, o tratamento de transformadas de Fourier utilizando distribuições (Richards e Youn, 1990; Saichev e Woyczyński, 1997) mostra que nós poderemos tomar liberdades consideráveis com transformadas de Fourier e ainda assim obter resultados corretos. Mas vamos aos poucos. Calculemos a transformada de Fourier da derivada de $f(x)$, integrando por partes:

$$
\begin{aligned}
\mathscr{F}\left\{\frac{\mathrm{d}f}{\mathrm{d}x}\right\} &= \frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{e}^{-\mathrm{i}kx}\frac{\mathrm{d}f}{\mathrm{d}x}\,\mathrm{d}x \\
&= \frac{1}{2\pi}\left[\mathrm{e}^{-\mathrm{i}kx}f(x) + (\mathrm{i}k)\int_{-\infty}^{+\infty} f(x)\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x\right]_{-\infty}^{+\infty};
\end{aligned}
$$

usando (11.4),

$$
\begin{aligned}
\mathscr{F}\left\{\frac{\mathrm{d}f}{\mathrm{d}x}\right\} &= \frac{\mathrm{i}k}{2\pi}\int_{-\infty}^{+\infty} f(x)\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x \\
&= \mathrm{i}k\widehat{f}(k). \qquad (11.6)
\end{aligned}
$$

E é claro que isso pode ser estendido para a n-ésima derivada:

$$\mathscr{F}\left\{\frac{\mathrm{d}^n f}{\mathrm{d}x^n}\right\} = (\mathrm{i}k)^n\widehat{f}(k). \qquad (11.7)$$

Juntas, a propriedade de linearidade (11.3) e a fórmula para as derivadas (11.7) vão permitir transformar equações diferenciais em algébricas. Esse é um dos grandes poderes da transformada de Fourier.

Uma relação oposta a (11.7) é ocasionalmente útil:

$$
\begin{aligned}
\mathscr{F}^{-1}\left\{\frac{\mathrm{d}\widehat{f}}{\mathrm{d}k}\right\} &= \int_{-\infty}^{+\infty}\mathrm{e}^{+\mathrm{i}kx}\frac{\mathrm{d}\widehat{f}}{\mathrm{d}k}\,\mathrm{d}k \\
&= \left[\mathrm{e}^{+\mathrm{i}kx}\widehat{f}(k) - (\mathrm{i}x)\int_{-\infty}^{+\infty}\widehat{f}(k)\mathrm{e}^{+\mathrm{i}kx}\,\mathrm{d}k\right]_{-\infty}^{+\infty};
\end{aligned}
$$

usando (11.5),

$$
\begin{aligned}
\mathscr{F}^{-1}\left\{\frac{\mathrm{d}\widehat{f}}{\mathrm{d}k}\right\} &= -(\mathrm{i}x)\int_{-\infty}^{+\infty}\widehat{f}(k)\mathrm{e}^{+\mathrm{i}kx}\,\mathrm{d}k \\
&= -\mathrm{i}xf(x). \qquad (11.8)
\end{aligned}
$$

Novamente, isso pode ser estendido para a n-ésima derivada:

$$
\mathscr{F}^{-1}\left\{\frac{\mathrm{d}^n\widehat{f}}{\mathrm{d}k^n}\right\} = (-\mathrm{i}x)^n f(x). \qquad (11.9)
$$

11.4 Um grande problema

Utilizando a transformada de Fourier, resolva

$$
\begin{aligned}
\frac{\partial c}{\partial t} &= D\frac{\partial^2 c}{\partial x^2}, \qquad -\infty < x < +\infty, \\
c(x,0) &= \frac{M}{A}\delta(x).
\end{aligned}
$$

Nas equações acima, M representa uma massa de soluto injetada instantaneamente em $x = 0$; A possui dimensão de área, para fazer com que c possua dimensão de concentração volumétrica (ML^{-3}).

A transformada de Fourier da equação diferencial é

$$
\frac{\mathrm{d}\widehat{c}}{\mathrm{d}t} = (\mathrm{i}k)^2 D\widehat{c}
$$

Note que usamos uma derivada ordinária em relação ao tempo, pois embora $\widehat{c}$ seja função de k e t, não há derivadas de $\widehat{c}$ em relação ao número de onda k. A EDO acima é de fácil solução:

$$
\widehat{c}(k,t) = \widehat{c}_0\mathrm{e}^{-Dk^2t}.
$$

Agora,

$$
\widehat{c}_0 = \frac{M}{2\pi A}\int_{-\infty}^{+\infty}\delta(x)\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x = \frac{M}{2\pi A},
$$

donde

$$
\widehat{c}(k,t) = \frac{M}{2\pi A}\mathrm{e}^{-Dk^2t}.
$$

Agora, do nosso primeiro exemplo de cálculo de transformadas de Fourier, sabemos que

$$
\begin{aligned}
\frac{2\sqrt{\pi}}{a}\mathrm{e}^{-\left(\frac{x}{a}\right)^2} &\leftrightarrow \mathrm{e}^{-\frac{k^2a^2}{4}}, \\
\frac{1}{a\sqrt{\pi}}\mathrm{e}^{-\left(\frac{x}{a}\right)^2} &\leftrightarrow \frac{1}{2\pi}\mathrm{e}^{-\frac{k^2a^2}{4}}.
\end{aligned}
$$

Logo,

$$
\begin{aligned}
Dt &= \frac{a^2}{4}, \\
a^2 &= 4Dt, \\
a &= 2\sqrt{Dt}, \\
c(x,t) &= \frac{M}{A\sqrt{4\pi Dt}}\mathrm{e}^{-\frac{x^2}{4Dt}} \quad \blacksquare
\end{aligned}
$$

11.5 O Teorema da convolução

A convolução entre as funções $f(x)$ e $g(x)$ (no sentido da transformada de Fourier; não confundir com a operação de convolução associada à transformada de Laplace) é

$$[f * g](x) \equiv \int_{\xi=-\infty}^{+\infty} f(x-\xi)g(\xi)\,\mathrm{d}\xi. \tag{11.10}$$

Teorema 11.2 (Teorema da convolução).

$$\mathscr{F}\{f * g\} = 2\pi \widehat{f}(k)\widehat{g}(k). \tag{11.11}$$

A transformada de Fourier da convolução é

$$\mathscr{F}\left[f * g\right](k) = \frac{1}{2\pi}\int_{x=-\infty}^{+\infty} \mathrm{e}^{-\mathrm{i}kx} \int_{y=-\infty}^{+\infty} f(x-y)g(y)\,\mathrm{d}y\,\mathrm{d}x \tag{11.12}$$

Faça

$$\begin{aligned} \xi &= x - y & & & x &= \xi + \eta \\ \eta &= y & &\Rightarrow & y &= \eta \end{aligned} \tag{11.13}$$

Nesses casos, sempre comece calculando o jacobiano! O jacobiano da transformação de variáveis é

$$\left|\frac{\partial(x,y)}{\partial(\xi,\eta)}\right| = \begin{vmatrix} \dfrac{\partial x}{\partial \xi} & \dfrac{\partial y}{\partial \xi} \\ \dfrac{\partial x}{\partial \eta} & \dfrac{\partial y}{\partial \eta} \end{vmatrix} = \begin{vmatrix} 1 & 0 \\ 1 & 1 \end{vmatrix} = 1. \tag{11.14}$$

Continuando,

$$\begin{aligned} \mathscr{F}\left[f * g\right](k) &= \frac{1}{2\pi}\int_{\xi=-\infty}^{+\infty}\int_{\eta=-\infty}^{+\infty} \mathrm{e}^{-\mathrm{i}k\xi}\mathrm{e}^{-\mathrm{i}k\eta} f(\xi)g(\eta) \left|\frac{\partial(x,y)}{\partial(\xi,\eta)}\right| \mathrm{d}\eta\ \mathrm{d}\xi \\ &= 2\pi\left[\frac{1}{2\pi}\int_{\xi=-\infty}^{+\infty} f(\xi)\mathrm{e}^{-\mathrm{i}k\xi}\,\mathrm{d}\xi\right]\left[\frac{1}{2\pi}\int_{\eta=-\infty}^{+\infty} g(\eta)\mathrm{e}^{-\mathrm{i}k\eta}\,\mathrm{d}\eta\right] \\ &= 2\pi\widehat{f}(k)\widehat{g}(k) \ \blacksquare \end{aligned}$$

O Teorema da convolução possui uma versão "inversa":

Teorema 11.3 (Teorema da convolução, versão inversa):

$$\mathscr{F}^{-1}\left\{\widehat{f}(k) * \widehat{g}(k)\right\} = f(x)g(x). \tag{11.15}$$

Um dos aspectos mais interessantes da operação de convolução é o seu uso na definição e uso de filtros. Tecnicamente, a filtragem de uma função ϕ com um filtro G é dada pela operação

$$\widetilde{\phi}(x) = \int_{-\infty}^{+\infty} G(x-\xi)\phi(\xi)\,\mathrm{d}\xi = G(x) * \phi(x). \tag{11.16}$$

Em (11.16), nós vamos supor que

$$G(\pm\infty) = 0. \tag{11.17}$$

Um fato importantíssimo é que a operação de filtragem comuta com a derivada em relação a x:

$$\begin{aligned}
\frac{\mathrm{d}\widetilde{\phi}}{\mathrm{d}x} &= \frac{\mathrm{d}}{\mathrm{d}x}\int_{-\infty}^{+\infty} G(x-\xi)\phi(\xi)\,\mathrm{d}\xi = \frac{\mathrm{d}}{\mathrm{d}x}\left[G(x) * \phi(x)\right]\\
&= \int_{-\infty}^{+\infty} \frac{\mathrm{d}G(x-\xi)}{\mathrm{d}x}\phi(\xi)\mathrm{d}\xi = \int_{-\infty}^{+\infty}\left[-\frac{\mathrm{d}G(x-\xi)}{\mathrm{d}\xi}\right]\phi(\xi)\mathrm{d}\xi\\
&= -G(x-\xi)\phi(\xi)\Big|_{\xi=-\infty}^{+\infty} + \int_{-\infty}^{+\infty} G(x-\xi)\frac{\mathrm{d}\phi(\xi)}{\mathrm{d}\xi}\,\mathrm{d}\xi
\end{aligned}$$

Em virtude de (11.17),

$$\frac{\mathrm{d}\widetilde{\phi}}{\mathrm{d}x} = G(x) * \frac{\mathrm{d}\phi}{\mathrm{d}x} = \widetilde{\frac{\mathrm{d}\phi}{\mathrm{d}x}}. \tag{11.18}$$

É trivial mostrar que

$$\frac{\mathrm{d}^n\widetilde{\phi}}{\mathrm{d}x^n} = G(x) * \frac{\mathrm{d}^n\phi}{\mathrm{d}x^n} = \widetilde{\frac{\mathrm{d}^n\phi}{\mathrm{d}x^n}}\ \blacksquare \tag{11.19}$$

Uma aplicação particularmente poderosa de filtragem é a utilização de soluções envolvendo a delta de Dirac para gerar soluções mais gerais. Por exemplo, considere o problema

$$\frac{\partial\widetilde{\phi}}{\partial t} = D\frac{\partial^2\widetilde{\phi}}{\partial x^2}, \qquad \widetilde{\phi}(x,0) = f(x), \qquad -\infty < x < +\infty.$$

Sabemos que

$$\phi(x,t) = \frac{1}{\sqrt{4\pi Dt}}\mathrm{e}^{-\frac{x^2}{4Dt}}.$$

é solução de

$$\begin{aligned}
\frac{\partial\phi}{\partial t} &= D\frac{\partial^2\phi}{\partial x^2},\\
\phi(x,0) &= \delta(x).
\end{aligned}$$

Aplicamos agora a convolução com $f(x)$ a todas as linhas acima:

$$\begin{aligned}
\frac{\partial\phi}{\partial t} * f(x) &= D\frac{\partial^2\phi}{\partial x^2} * f(x),\\
\frac{\partial\widetilde{\phi}}{\partial t} &= D\frac{\partial^2\widetilde{\phi}}{\partial x^2},\\
\widetilde{\phi}(x,0) &= \phi(x,0) * f(x) = \delta(x) * f(x) = f(x).
\end{aligned}$$

Mas esse é exatamente o problema que desejamos resolver. Logo,

$$\widetilde{\phi}(x,t) = \phi(x,t) * f(x) = \int_{\xi=-\infty}^{+\infty} \frac{1}{\sqrt{4\pi Dt}}\mathrm{e}^{-\frac{(x-\xi)^2}{4Dt}} f(\xi)\,\mathrm{d}\xi\ \blacksquare$$

11.6 O Teorema de Parseval

O Teorema de Parseval é a contrapartida da igualdade de Parseval para séries de Fourier.

Teorema 11.4 (Teorema de Parseval). Se $f(x)$ e $g(x)$ são duas funções reais da variável real x,

$$\int_{-\infty}^{+\infty} f(x)g(x)\,\mathrm{d}x = 2\pi \int_{-\infty}^{+\infty} \widehat{f}(-k)\widehat{g}(k)\,\mathrm{d}k.$$

A prova parte de

$$\widehat{f}(-k) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} f(x)\mathrm{e}^{\mathrm{i}kx}\,\mathrm{d}x, \qquad \widehat{g}(k) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} f(x)\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x.$$

Então,

$$\begin{aligned}\int_{-\infty}^{+\infty} \widehat{f}(-k)\widehat{g}(k)\,\mathrm{d}k &= \int_{k=-\infty}^{+\infty} \widehat{g}(k)\frac{1}{2\pi}\int_{x=-\infty}^{+\infty} f(x)\mathrm{e}^{\mathrm{i}kx}\,\mathrm{d}x\,\mathrm{d}k\\ &= \frac{1}{2\pi}\int_{x=-\infty}^{+\infty} f(x)\int_{k=-\infty}^{+\infty} \widehat{g}(k)\mathrm{e}^{\mathrm{i}kx}\,\mathrm{d}k\,\mathrm{d}x\\ &= \frac{1}{2\pi}\int_{x=-\infty}^{+\infty} f(x)g(x)\,\mathrm{d}x \ \blacksquare\end{aligned}$$

11.7 A fórmula da inversa da transformada de Laplace

Considere a identidade

$$F(t) = \int_{-\infty}^{+\infty} \widehat{F}(\omega)\mathrm{e}^{\mathrm{i}\omega t}\mathrm{d}\omega = \int_{-\infty}^{+\infty}\left[\frac{1}{2\pi}\int_{t=-\infty}^{+\infty} F(t)\mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{d}t\right]\mathrm{e}^{+\mathrm{i}\omega t}\,\mathrm{d}\omega. \tag{11.20}$$

Suponha agora

$$F(t) = \begin{cases}0, & t < 0,\\ \mathrm{e}^{-\gamma t}f(t), & t \geq 0.\end{cases}$$

Suponha também que $f(t)$ seja "de ordem exponencial": $f(t) < K\mathrm{e}^{ct}$, para $\gamma > c$; então,

$$\mathrm{e}^{-\gamma t}f(t) < K\mathrm{e}^{(c-\gamma)t} = K\mathrm{e}^{-(\gamma-c)t} \to 0$$

quando $t \to \infty$.

Agora, de (11.20),

$$\mathrm{e}^{-\gamma t}f(t) = \frac{1}{2\pi}\int_{\omega=-\infty}^{+\infty}\left[\int_{t=0}^{\infty}\mathrm{e}^{-\gamma t}f(t)\mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{d}t\right]\mathrm{e}^{+\mathrm{i}\omega t}\,\mathrm{d}\omega,$$

$$f(t) = \frac{1}{2\pi}\int_{\omega=-\infty}^{+\infty}\left[\int_{t=0}^{\infty} f(t)\mathrm{e}^{-\underbrace{(\gamma+\mathrm{i}\omega)}_{=s}t}\,\mathrm{d}t\right]\mathrm{e}^{+\underbrace{(\gamma+\mathrm{i}\omega)}_{=s}t}\,\mathrm{d}\omega.$$

Fazendo $s = \gamma + \mathrm{i}\omega$ e notando que ω está variando para γ constante, $\mathrm{d}s = \mathrm{i}\mathrm{d}\omega \Rightarrow$

$$f(t) = \frac{1}{2\pi\mathrm{i}}\int_{s=\gamma-\mathrm{i}\infty}^{\gamma+\mathrm{i}\infty}\mathrm{e}^{st}\left[\int_{t=0}^{\infty} f(t)\mathrm{e}^{-st}\,\mathrm{d}t\right]\mathrm{d}s,$$

e isso define a fórmula de inversão:

$$\overline{f}(s) \equiv \int_0^\infty f(t)\mathrm{e}^{-st}\,\mathrm{d}t, \tag{11.21}$$

$$f(t) = \frac{1}{2\pi\mathrm{i}} \int_{s=\gamma-\mathrm{i}\infty}^{s=\gamma+\mathrm{i}\infty} \mathrm{e}^{+st}\overline{f}(s)\,\mathrm{d}s. \tag{11.22}$$

Todas as singularidades de $\overline{f}(s)$ devem estar à esquerda da reta $z = \gamma$.

Lesson 12

Difusão turbulenta

Em um escoamento turbulento, nem sempre está claro o que queremos dizer com uma "partícula". Em particular, existe uma grande de riquezas em escoamentos turbulentos "plenamente desenvolvidos", e uma forma de lidar com essa multitude de escalas é definir algumas grandemente diferentes. A escala integral é definida matematicamente em termos da função de autocorrelação $\varrho(x)$ (em geral da velocidade longitudinal):

$$\ell = \int_0^\infty \varrho(x)\,\mathrm{d}x.$$

A microescala de Taylor λ é definida em termos da curvatura de $\varrho(x)$ na origem:

$$-\frac{2}{\lambda} \equiv \left.\frac{\mathrm{d}^2\rho}{\mathrm{d}x^2}\right|_{x=0}.$$

Finalmente temos a microescala de Kolmogorov:

$$\eta = (\nu^3/\epsilon)^{1/4}.$$

As partículas clássicas de Mecânica dos Fluidos têm que ser de tamanho η (ou menores): elas só "veem" difusão molecular, e campos suaves a seu redor. Já "partículas" de tamanho λ ou ℓ veem difusão turbulenta, e um mundo consideravelmente mais "agitado" em seu redor.

Introduzimos aqui, agora, o conceito de "difusividade turbulenta". Se F é o fluxo turbulento de um escalar cuja concentração é c, a difusividade turbulenta K desse escalar em um ponto do escoamento é *definida* via

$$F \equiv -\overline{\rho} K \frac{\mathrm{d}\overline{c}}{\mathrm{d}z}.$$

As barras sobre as variáveis indicam médias de Reynolds (1895). Em geral a difusividade turbulenta é *modelada* utilizando-se ideias dimensionais simples, tais como

$$K = c\sigma_w \ell,$$

onde σ_w é uma escala de velocidade (por exemplo, neste caso estamos pensando no desvio-padrão da velocidade vertical), e c é uma constante adimensional. O fluxo turbulento, ele próprio, é em geral definido em termos de covariâncias com a velocidade vertical, como em

$$F = \overline{\rho}\,\overline{w'c'}.$$

Prosseguimos agora para a Teoria de Difusão Turbulenta de Taylor. Fazemos isso acompanhando uma partícula (no sentido de Kolmogorov!) *lagrangeanamente*:

$$Z(t) = Z(0) + \int_0^t W(\tau)\,\mathrm{d}\tau.$$

Sem perda de generalidade, suponhamos $Z(0) \equiv 0$ (sempre), e

$$\overline{Z(t)} = 0.$$

Nossas médias agora devem ser consideradas também de um ponto de vista lagrangeano, como médias sobre um grande número de partículas. Se $Z_i(t)$ é a posição da i-ésima partícula e estamos lançando um número N muito grande delas,

$$\overline{Z(t)} = \frac{1}{N}\sum_{i=1}^{N} Z_i(t).$$

Consideremos agora o desvio quadrático médio de $Z(t)$ em relação à origem. Claramente, isso é uma medida de quanto o conjunto de partículas irá se "dispersar" em torno da origem. Interessam-nos as quantidades

$$\overline{Z^2(t)}, \qquad \frac{\mathrm{d}}{\mathrm{d}t}\left[\overline{Z^2(t)}\right].$$

Prosseguindo,

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\overline{Z^2(t)}\right] = 2\overline{Z(t)\frac{\mathrm{d}Z}{\mathrm{d}t}}.$$

Mas

$$W(t) = \frac{\mathrm{d}Z}{\mathrm{d}t};$$
$$Z(t) = \int_{t'=0}^{t} W(t')\,\mathrm{d}t'.$$

Segue-se que

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left[\overline{Z^2(t)}\right] &= 2\overline{Z(t)W(t)}\\ &= 2\overline{\left[\int_{t'=0}^{t} W(t')\,\mathrm{d}t'\right]W(t)}\\ &= 2\int_0^t \overline{W(t')W(t)}\,\mathrm{d}t'.\end{aligned}$$

Agora, se $W(t)$ for um processo estocástico *estacionário*,

$$\begin{aligned}\overline{W(t')W(t)} &= \overline{W(0)W(t-t')} \Rightarrow\\ \frac{\mathrm{d}}{\mathrm{d}t}\left[\overline{Z^2(t)}\right] &= 2\int_0^t \overline{W(0)W(t-t')\,\mathrm{d}t'}.\end{aligned}$$

Para prosseguirmos precisaremos agora introduzir a *função de autocorrelação lagrangeana*:

$$\varrho_L(\tau) \equiv \frac{1}{\overline{W^2}}\overline{W(t)W(t+\tau)},$$

em que estaremos supondo que $\overline{W^2}$, ao contrário de $\overline{Z^2(t)}$, não depende de t (que é a mesma hipótese de estacionariedade de $W(t)$ que fizéramos antes.

Com isso, temos agora:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\overline{Z^2(t)}\right] = 2\overline{W^2}\int_0^t \varrho_L(\tau)\,\mathrm{d}\tau;$$
$$\overline{Z^2(t)} = 2\overline{W^2}\int_0^t \int_0^{t'} \varrho_L(\tau)\,\mathrm{d}\tau\mathrm{d}t'.$$

Prosseguimos, integrando por partes:

$$f(t') \equiv \int_0^{t'} \varrho_L(\tau)\,\mathrm{d}\tau;$$
$$\int_0^t f(t')\,\mathrm{d}t' = t'f(t')\Big|_0^t - \int_0^t t'\varrho_L(t')\,\mathrm{d}t'; \Rightarrow$$
$$\begin{aligned}\overline{Z^2(t)} &= 2\overline{W^2}\left[t\int_0^t \varrho_L(\tau)\,\mathrm{d}\tau - \int_0^t t'\varrho_L(t')\,\mathrm{d}t'\right]\\ &= 2\overline{W^2}\left[t\int_0^t \varrho_L(\tau)\,\mathrm{d}\tau - \int_0^t \tau\varrho_L(\tau)\,\mathrm{d}\tau\right]\\ &= 2\overline{W^2}t\int_0^t \left(1-\frac{\tau}{t}\right)\varrho_L(\tau)\,\mathrm{d}\tau.\end{aligned}$$

Prosseguimos agora com uma *análise assintótica*. Para valores pequenos de t:

$$0 \le \tau \le t \Rightarrow \varrho_L(\tau) \approx 1 \Rightarrow$$
$$\int_0^t \left(1-\frac{\tau}{t}\right)\mathrm{d}\tau = \frac{t}{2},$$

donde:

$$t \text{ pequeno:} \qquad \overline{Z^2(t)} \approx \overline{W^2}t^2.$$

Por outro lado, considere a definição da *escala integral lagrangeana*:

$$\mathscr{T}_L \equiv \int_0^\infty \varrho_L(\tau)\,\mathrm{d}\tau.$$

Consideraremos que t é "grande" quando $t \gg \mathscr{T}_L$. Desejamos provar que

$$\lim_{t\to\infty}\int_0^t \frac{\tau}{t}\varrho_L(\tau)\,\mathrm{d}\tau = 0.$$

Também vamos precisar, a rigor, do *Teorema Ergódico*: se $W(t)$, além de ser um processo estacionário, for ergódico, então teremos que

$$\lim_{\tau\to\infty}\varrho_L(\tau) = 0.$$

2016-05-08T13:39:25 A dedução a seguir está totalmente errada. Para corrigi-la, precisaremos de:

(Zwillinger, 1992, II.16, p. 65)

(Comparison test for convergence) Let $f(x)$ and $g(x)$ be continuous for $a \le x \le b$ with $0 \le |f(x)| \le g(x)$. If $\int_a^b g(x)\,\mathrm{d}x$ converges, then $\int_a^b f(x)\,\mathrm{d}x$ converges, and

$$0 \le \left|\int_a^b f(x)\,\mathrm{d}x\right| \le \int_a^b g(x)\,\mathrm{d}x.$$

Na linguagem de ϵ's e δ's, o limite acima significa o seguinte: dado qualquer $\delta > 0$ (tão pequeno quanto desejarmos), é sempre possível achar um t_δ tal que

$$\tau > t_\delta \Rightarrow |\varrho(\tau)| \le \delta.$$

Agora, dado um valor t qualquer ("arbitrariamente grande"), escolhemos

$$\delta = \frac{\mathscr{T}^2}{t^2}.$$

Em seguida, dividimos a nossa integral em

$$\begin{aligned} I_1 &= \int_0^{t_\delta} \left|\frac{\tau}{t}\varrho(\tau)\right| \mathrm{d}\tau, \\ I_2 &= \int_{t_\delta}^{t} \left|\frac{\tau}{t}\varrho(\tau)\right| \mathrm{d}\tau. \end{aligned}$$

Sabemos agora que

$$\begin{aligned} \left|\int_0^t \frac{\tau}{t}\varrho_L(\tau)\,\mathrm{d}\tau\right| &\le \int_0^t \left|\frac{\tau}{t}\varrho(\tau)\right| \mathrm{d}\tau \\ &\le I_1 + I_2. \end{aligned}$$

Mas:

$$\begin{aligned} I_1 &\le \int_0^{t_\delta} \frac{\tau}{t}|\varrho(\tau)|\,\mathrm{d}\tau \\ &\le \int_0^{t_\delta} \frac{\tau}{t}\,\mathrm{d}\tau \\ &\le \int_0^{t_\delta} \frac{t_\delta}{t}\,\mathrm{d}\tau = \frac{t_\delta^2}{t} \to 0 \text{ quando } t \to \infty. \end{aligned}$$

Por outro lado,

$$\begin{aligned} I_2 &\le \int_{t_\delta}^{t} \frac{\tau}{t}|\varrho(\tau)|\,\mathrm{d}\tau \\ &\le \int_{t_\delta}^{t} \frac{\tau}{t}\delta\,\mathrm{d}\tau \\ &= \frac{\delta}{t}\int_{t_\delta}^{t} \tau\,\mathrm{d}\tau = \frac{\delta}{2t}\left[t^2 - t_\delta^2\right] \\ &= \frac{\mathscr{T}^2}{2t}\left[1 - \frac{t_\delta^2}{t^2}\right] \to 0 \text{ quando } t \to \infty. \end{aligned}$$

Consequentemente, quando $t \gg \mathscr{T}$, podemos usar

$$\lim_{t\to\infty} \int_0^t \left(1 - \frac{\tau}{t}\right)\varrho_L(\tau)\,\mathrm{d}\tau = \int_0^\infty \varrho_L(\tau)\,\mathrm{d}\tau = \mathscr{T}_L;$$

então,

$$\overline{Z^2(t)} \approx 2\overline{W^2}t\mathscr{T}_L \blacksquare$$

Em resumo, nossos resultados são:

$$\begin{aligned} Z^{\mathrm{rms}} &= W^{\mathrm{rms}}t, && t \ll \mathscr{T}_L; \\ Z^{\mathrm{rms}} &= W^{\mathrm{rms}}\sqrt{2\mathscr{T}_L t}, && t \ll \mathscr{T}_L. \end{aligned}$$

Agora nós mudamos nosso foco para o caminho de partículas lagrangenas. Cada partícula tem uma função temporal de posição do tipo

$$\boldsymbol{x} = \boldsymbol{X}(\boldsymbol{\xi}, t).$$

Nesta equação, ξ é a posição da partícula em $t = 0$. Em outras palavras,

$$\boldsymbol{\xi} = \boldsymbol{X}(\boldsymbol{\xi}, 0).$$

Portanto, em $t = 0$ $\boldsymbol{X}$ é a identidade. Agora, na ausência de difusão, a equação de transporte de um escalar cuja concentração é c é

$$\frac{\mathrm{D}c}{\mathrm{D}t} = \frac{\partial c}{\partial t} + u_i \frac{\partial c}{\partial x_i} = 0.$$

A solução dessa equação é

$$c(\boldsymbol{X}(\boldsymbol{\xi}, t), t) = c(\boldsymbol{\xi}, 0).$$

Neste ponto, precisamos introduzir a função densidade de probabilidade $P(\boldsymbol{x}, t|\boldsymbol{\xi})$. Ela dá a densidade de probabilidade de que a partícula, partindo de $\boldsymbol{\xi}$ em $t = 0$, alcance $\boldsymbol{x}$ no instante t. O valor esperado da concentração em $(\boldsymbol{x}, t)$ será então, simplesmente,

$$\overline{c}(\boldsymbol{x}, t) = \int_{\boldsymbol{\xi} \in \mathbb{R}^3} c(\boldsymbol{\xi}, 0) P(\boldsymbol{x}, t|\boldsymbol{\xi}) \mathrm{d}^3\boldsymbol{\xi}.$$

Em particular, se toda a massa M do escalar estiver concentrada em $\boldsymbol{\xi} = 0$,

$$\begin{aligned} c(\boldsymbol{\xi}, 0) &= M\delta(\boldsymbol{\xi}); \\ \overline{c}(\boldsymbol{x}, t) &= \int_{\boldsymbol{\xi} \in \mathbb{R}^3} M\delta(\boldsymbol{\xi}) P(\boldsymbol{x}, t|\boldsymbol{\xi}) \mathrm{d}^3\boldsymbol{\xi} \\ &= MP(\boldsymbol{x}, t|0). \end{aligned}$$

Em uma dimensão, devemos nos lembrar de que

$$Z(t) = \int_{t'=0}^{t} W(t')\,\mathrm{d}t'.$$

Nós interpretaremos a expressão acima utilizando o Teorema Central do Limite, de forma muito pouco rigorosa. Nós vamos considerar que $Z(t)$ é uma variável aleatória produzida pela "soma" de um grande número de variáveis $W(t')$. Pelo Teorema Central do Limite, $Z(t)$ deve ter distribuição normal. Mas nós já sabemos que o valor esperado de $Z(t)$ é zero, e que seu desvio-padrão é Z^{rms}. Para tempos "grandes", faremos

$$Z^{\mathrm{rms}} = \sigma_Z = \sigma_w \sqrt{2\mathscr{T}_L t}.$$

Admitindo em seguida que Z seja uma variável aleatória gaussiana, obteremos, imediatamente,

$$\overline{c}(z, t) = \frac{M}{\sqrt{2\pi}\sigma_Z} \exp\left[-\frac{z^2}{2\sigma_Z^2}\right].$$

Esse resultado pode ser facilmente generalizado para 3 dimensões:

$$\overline{c}(x, y, z, t) = \frac{M}{(2\pi)^{3/2}\sigma_X\sigma_Y\sigma_Z} \exp\left[-\frac{x^2}{2\sigma_X^2}\right] \exp\left[-\frac{y^2}{2\sigma_Y^2}\right] \exp\left[-\frac{z^2}{2\sigma_Z^2}\right].$$

Por outro lado, no nosso capítulo passado (sobre a Transformada de Fourier), nós encontramos a solução do problema difusivo

$$\frac{\partial \overline{c}}{\partial t} = K_{zz}\frac{\partial^2 \overline{c}}{\partial z^2}; \qquad c(z,0) = M\delta(z); \qquad \lim_{z\to\pm\infty} = 0;$$

ela é

$$\overline{c}(z,t) = \frac{M}{\sqrt{4K_{zz}\pi t}}\exp\left[-\frac{z^2}{4K_{zz}t}\right]$$

Constatamos, com grande satisfação, que as soluções lagrangeana e euleriana do problema têm a mesma forma! Isso nos permite escrever uma expressão para a difusividade turbulenta K_{zz}. Para que os resultados sejam iguais,

$$\begin{aligned} 2\sigma_Z^2 &= 4K_{zz}t, \\ 4\overline{W^2}\mathscr{T}_L t &= 4K_{zz}t \\ K_{zz} &= \overline{W^2}\mathscr{T}_L \ \blacksquare \end{aligned}$$

Na sequência, nós vamos "construir" uma série de soluções de problemas de dispersão baseadas na técnica que apresentamos. Nossa primeira adaptação será considerar o problema *permanente*

$$\overline{u}\frac{\partial \overline{c}}{\partial x} = K_{zz}\frac{\partial^2 \overline{c}}{\partial z^2}.$$

Formalmente, esta é uma equação de difusão similar à anterior, porém com t substituído por $x/\overline{u}$. Nossa condição inicial, entretanto, precisa ser especificada agora em $x = 0$. Ela será (Kumar e Sharan, 2010, eq. (2.5))

$$\overline{c}(x=0,z) = \frac{q}{\overline{u}}\delta(z).$$

Nós podemos encontrar uma primeira solução para uma injeção contínua de massa de poluente q ($[\![q]\!] = \mathsf{M}_p\mathsf{T}^{-1}$) por meio de substituição simples:

$$\overline{c}(x,z) = \frac{q}{\overline{u}\sqrt{4\pi K_{zz}(x/\overline{u})}}\exp\left[-\overline{u}\frac{z^2}{4K_{zz}x}\right].$$

Esta é uma expressão muito mais "útil" em estudos de dispersão, que em geral são feitos para períodos de cerca de 1 h em condições "permanentes". A sua generalização mais ou menos óbvia para incluir o eixo dos y's é

$$\overline{c}(x,z) = \frac{q}{4\pi x\sqrt{K_{yy}K_{zz}}}\exp\left[-\frac{\overline{u}}{4x}\left(\frac{y^2}{K_{yy}} + \frac{z^2}{K_{zz}}\right)\right].$$

Difusão longitudinal: considere agora

$$\begin{aligned} \frac{\partial \overline{c}}{\partial t} + \overline{u}\frac{\partial \overline{c}}{\partial x} &= K_{xx}\frac{\partial^2 \overline{c}}{\partial x^2}, \\ \overline{c}(x,0) &= \frac{M}{A}\delta(x). \end{aligned}$$

Podemos tentar "adivinhar a solução" argumentando que, se $\overline{u}$ for constante, no sistema de coordenadas $x' \times t$ com

$$x' = x - \overline{u}t$$

nós voltamos para a equação de difusão pura

$$\frac{\partial \overline{\chi}}{\partial t} = K_{xx}\frac{\partial^2 \overline{\chi}}{\partial x'^2}.$$

Vamos tentar ganhar algum insight. Sejam

$$\begin{aligned}
x &= x' + ut,\\
\chi(x',t) &= c(\underbrace{x'+ut}_{x},t),\\
\frac{\partial \chi(x',t)}{\partial t} &= \frac{\partial c}{\partial t} + \frac{\partial c}{\partial x}\frac{\partial x}{\partial t},\\
\frac{\partial \chi(x',t)}{\partial t} &= \frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x};\\
\frac{\partial^2 \chi}{\partial x'^2} &= K_{zz}\frac{\partial^2 c}{\partial x^2}.
\end{aligned}$$

Portanto, de fato teremos

$$\begin{aligned}
\frac{\partial \overline{\chi}}{\partial t} &= K_{xx}\frac{\partial^2 \overline{\chi}}{\partial x'^2},\\
\overline{\chi}(x',0) = \overline{c}(x,0) &= \frac{M}{A}\delta(x')
\end{aligned}$$

A solução é a conhecida

$$\begin{aligned}
\overline{\chi}(x',t) &= \frac{M}{A\sqrt{4K_{xx}\pi t}}\exp\left[-\frac{(x')^2}{4K_{xx}t}\right];\\
\overline{c}(x,t) &= \frac{M}{A\sqrt{4K_{xx}\pi t}}\exp\left[-\frac{(x-\overline{u}t)^2}{4K_{xx}t}\right].
\end{aligned}$$

Finalmente, para a equação

$$\begin{aligned}
\frac{\partial \overline{c}}{\partial t} + \overline{u}\frac{\partial \overline{c}}{\partial x} &= K_{xx}\frac{\partial^2 \overline{c}}{\partial x^2} + K_{zz}\frac{\partial^2 \overline{c}}{\partial z^2},\\
\overline{c}(x,z,0) &= \frac{M}{L_y}\delta x\delta z
\end{aligned}$$

poderemos "adivinhar" a solução

$$\overline{c}(x,z,t) = \frac{M}{L_y\sqrt{4\pi K_{xx}t}\sqrt{4\pi K_{zz}t}}\exp\left[\frac{(x-\overline{u}t)^2}{4K_{xx}t} + \frac{z^2}{4K_{zz}t}\right]?$$

Aparentemente não, e ela está errada.

Lesson 13

Um problema parabólico cilíndrico

Considere um anel cilíndrico com altura h, raio r, e espessura Δr "cravado" (virtualmente) no solo. A equação de balanço de massa para este volume de controle é

$$\frac{\partial}{\partial t}\int_V \rho\, dV + \oint_S \rho(\boldsymbol{n}\cdot\boldsymbol{u})\, dS = 0. \tag{13.1}$$

A massa de água dentro do anel é

$$\int_V \rho\, dV = f\rho\,(2\pi r\Delta r h), \tag{13.2}$$

onde ρ é a massa específica da água (aqui suposta constante), e f é a porosidade do solo.

Suponha por simplicidade que o fluxo médio $\boldsymbol{u}$ é horizontal e perfeitamente radial, sendo dado pela lei de Darcy na forma

$$u_r = -k\frac{\partial h}{\partial r}. \tag{13.3}$$

A integral de superfície será então

$$\oint_S \rho(\boldsymbol{n}\cdot\boldsymbol{u})\, dS = 2\pi\rho\left\{\left[-shk\frac{\partial h}{\partial s}\right]_{s=r+\Delta r} + \left[shk\frac{\partial h}{\partial s}\right]_{s=r}\right\} \tag{13.4}$$

Donde

$$\begin{aligned}\frac{\partial}{\partial t}(2\pi f\rho r h) &= \frac{\left[(r+\Delta r)h(h+\Delta r)k\frac{\partial h(r+\Delta r)}{\partial r} - rh(r)k\frac{\partial h(r)}{\partial r}\right]}{\Delta r}\\ \frac{\partial h}{\partial t} &= \frac{\partial}{\partial r}\left[rh\frac{k}{f}\frac{\partial h}{\partial r}\right]\end{aligned} \tag{13.5}$$

Esta é a equação de Boussinesq, não-linear, para escoamento em solo. A linearização óbvia aqui é fazer $h = \overline{h}$ no termo intermediário do lado direito, obtendo-se

$$\frac{\partial h}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[\frac{\overline{h}k}{f}r\frac{\partial h}{\partial r}\right] \tag{13.6}$$

A partir deste ponto fazemos $\alpha^2 = \overline{h}k/f$, e nos concentramos na solução de um problema linear. O problema que escolhemos é manter um cilindro de raio b e altura H de solo inicialmente seco, rodeado por solo uniformemente saturado até a altura H. O problema se torna

$$\frac{\partial h}{\partial t} = \alpha^2 \frac{1}{r}\frac{\partial}{\partial r}\left[r\frac{\partial h}{\partial r}\right]$$

com

$$\begin{aligned} h(r,0) &= 0, \qquad 0 \le r \le b,\\ h(b,t) &= H,\\ \frac{\partial h(0,t)}{\partial r} &= 0. \end{aligned}$$

Uma das condições de contorno (em $r = 0$) é homogênea (derivada nula), mas a outra (em $r = b$) não. Isso entretanto pode ser facilmente remediado, fazendo

$$h(r,t) = H + u(r,t),$$

o que produz

$$\frac{\partial u}{\partial t} = \alpha^2 \frac{1}{r}\frac{\partial}{\partial r}\left[r\frac{\partial u}{\partial r}\right]$$

e

$$u(r,0) = -H, \qquad 0 \le r \le b, \tag{13.7}$$

$$u(b,t) = 0, \tag{13.8}$$

$$\frac{\partial u(0,t)}{\partial r} = 0. \tag{13.9}$$

Substituindo

$$u(r,t) = RT$$

na equação diferencial,

$$\begin{aligned} \frac{\partial RT}{\partial t} &= \alpha^2 \frac{1}{r}\frac{\partial}{\partial r}\left[r\frac{\partial RT}{\partial r}\right]\\ RT' &= \frac{\alpha^2}{r}\frac{\partial rTR'}{\partial r}\\ RT' &= \frac{\alpha^2 T}{r}\frac{\mathrm{d}}{\mathrm{d}r}\left[r\frac{\mathrm{d}R}{\mathrm{d}r}\right]\\ \frac{1}{\alpha^2}\frac{T'}{T} &= \frac{1}{rR}\frac{\mathrm{d}}{\mathrm{d}r}\left[r\frac{\mathrm{d}R}{\mathrm{d}r}\right] = -\lambda. \end{aligned}$$

O sinal de menos em λ é arbitrário. Seria possível atacar diretamente o problema de Sturm-Liouville em R; resolvendo em vez disso para T, entretanto, obtemos

$$T(t) = T_0 e^{-\lambda\alpha^2 t}.$$

Usar $\lambda < 0$ produz uma solução que explode quando $t \to \infty$, o que não é físico; usar $\lambda = 0$ produz uma solução independente de t, o que também não é. Portanto, usaremos $\lambda > 0$. O problema de Sturm-Liouville em R será

$$\frac{\mathrm{d}}{\mathrm{d}r}\left[r\frac{\mathrm{d}R}{\mathrm{d}r}\right] + \lambda r R = 0,$$

com condições de contorno homogêneas padrão:

$$\frac{\partial R(0)}{\partial r} = 0,$$
$$R(b) = 0.$$

é evidente que, na forma padrão da equação de Sturm-Liouville, temos $p(r) = r$, $q(r) = 0$ e $w(r) = r$. Expandindo,

$$\frac{\mathrm{d}^2 R}{\mathrm{d}r^2} + \frac{1}{r}\frac{\mathrm{d}R}{\mathrm{d}r} + \lambda R = 0$$

que deve ser comparada à equação geral de Bessel de ordem μ:

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + \frac{1}{x}\frac{\mathrm{d}y}{\mathrm{d}x} + \left(1 - \frac{\mu^2}{x^2}\right) y = 0$$

Fazemos portanto $\lambda = k^2$, e dividimos a equação em R por k^2:

$$\frac{\mathrm{d}^2 R}{\mathrm{d}(kr)^2} + \frac{1}{(kr)}\frac{\mathrm{d}R}{\mathrm{d}(kr)} + R = 0,$$

que está, agora, na forma de uma equação diferencial de Bessel de ordem zero.

A solução geral é da forma

$$R(r) = AJ_0(kr) + BY_0(kr),$$

e deve atender às condições de contorno homogêneas. Vamos nos recordar das formas de $J_0(kr)$, e $Y_0(kr)$.

A figura 13.1 mostra as funções J_0 e Y_0. $Y_0(kr)$ possui uma singularidade logaritmica, e não pode atender à condição de derivada nula em $r = 0$, a não ser que $B = 0$. E quanto à derivada de J_0 em $r = 0$? Uma rápida consulta a Abramowitz e Stegun (1972) (equação 9.1.10) fornece a série

$$J_0(x) = \sum_{k=0}^{\infty} \frac{(-x^2/4)^k}{(k!)^2}.$$

Os expoentes de x são todos pares; $J_0(x)$ é uma função *par*, e $J_0'(0) = 0$. Portanto, $J_0(kr)$ atende à condição de contorno em $r = 0$. A condição de contorno homogênea em $r = b$ requer

$$J_0(kb) = 0;$$

Os autovalores $\lambda_n = k_n^2$ serão os *zeros* da função de Bessel de primeiro tipo, e ordem zero. Os 20 primeiros autovalores são dados por (Abramowitz e Stegun, 1972, Tabela 9.5, 1ª coluna) e reproduzidos na tabela 13.1

Com os autovalores em mãos, nós prosseguimos para obter a solução em série do problema. Ela será

$$h(r,t) = H + \sum_{n=1}^{\infty} A_n e^{-k_n^2 \alpha^2 t} J_0(k_n r)$$

Em particular, como os $k_n b$ são os zeros de $J_0(x)$,

$$h(b,t) = H + \sum_{n=1}^{\infty} A_n e^{-k_n^2 \alpha^2 t} \underbrace{J_0(k_n b)}_{=0} = 0.$$

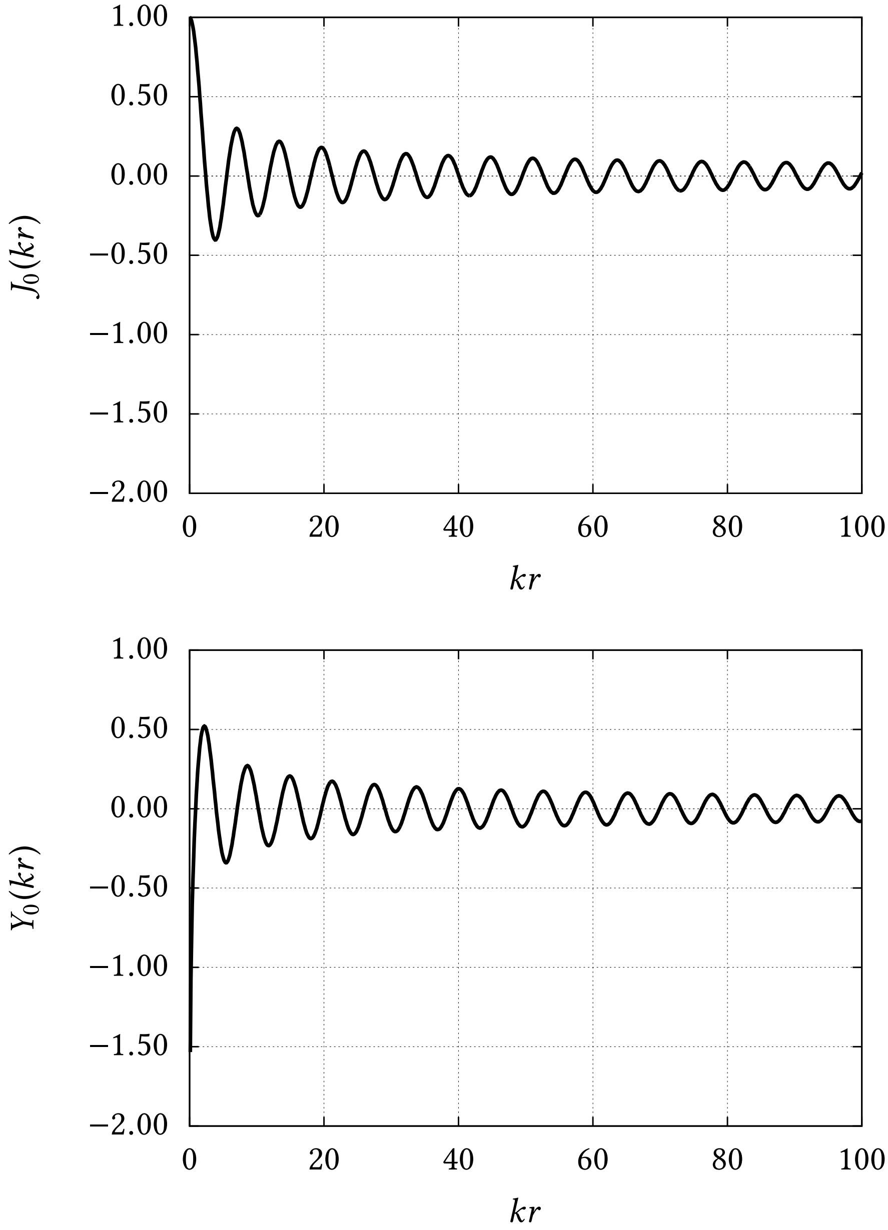

Figure 13.1: Funções de Bessel de ordem 0

Table 13.1: 20 primeiros zeros de $J_0(x)$.

n	$k_n b$	n	$k_n b$
1	2,4048255577	11	33,7758202136
2	5,5200781103	12	36,9170983537
3	8,6537279129	13	40,0584257646
4	11,7915344391	14	43,1997917132
5	14,9309177086	15	46,3411883717
6	18,0710639679	16	49,4826098974
7	21,2116366299	17	52,6240518411
8	24,3524715308	18	55,7655107550
9	27,4934791320	19	58,9069839261
10	30,6346064684	20	62,0484691902

Finalmente, precisamos calcular os coeficientes A_n, o que fazemos impondo a condição inicial do problema:

$$
\begin{aligned}
h(r,0) = H + \sum_{n=1}^{\infty} A_n J_0(k_n r) &= 0 \\
\sum_{n=1}^{\infty} A_n J_0(k_n r) &= -H \\
\sum_{n=1}^{\infty} A_n \int_{r=0}^{b} r J_0(k_n r) J_0(k_m r)\, dr &= -H \int_{r=0}^{b} r J_0(k_m r)\, dr \\
A_m \int_{r=0}^{b} r J_0^2(k_m r)\, dr &= -H \int_{r=0}^{b} r J_0(k_m r)\, dr.
\end{aligned}
$$

A última linha foi obtida, como de costume, invocando a ortogonalidade das autofunções do problema de Sturm-Liouville.

Para calcular as duas integrais restantes, são necessários dois resultados padrão da teoria de funções de Bessel. O primeiro é (Jeffrey, 2003, 17.13.1.1-4)

$$
\int_0^1 x J_n^2(ax)\, \mathrm{d}x = \frac{1}{2} J_{n+1}^2(a), \;\; J_n(a) = 0.
$$

Fazendo $r = xb$, $\mathrm{d}r = b\mathrm{d}x$, (e impondo $k_m = a/b$ na segunda linha abaixo):

$$
\begin{aligned}
\int_{r=0}^{b} \frac{r}{b} J_n^2\left(a\frac{r}{b}\right) \frac{dr}{b} &= \frac{1}{2} J_{n+1}^2(a) \\
\int_{r=0}^{b} r J_n^2(k_m r)\, dr &= \frac{b^2}{2} J_{n+1}^2(k_m b).
\end{aligned}
$$

Já para a integral do lado direito, nós aplicamos diretamente a fórmula (Jeffrey, 2003, 17.12.1.1-1)

$$
\begin{aligned}
\int x J_0(ax)\, \mathrm{d}x &= \frac{x}{a} J_1(ax) \;\; \Rightarrow \\
\int_0^b r J_0(k_m r)\, dr &= \frac{b}{k_m} J_1(k_m b),
\end{aligned}
$$

donde

$$\begin{aligned}
A_m \frac{b^2}{2} J_1^2(k_m b) &= -H \frac{b}{k_m} J_1(k_m b), \\
A_m &= -\frac{2H}{k_m b} \frac{1}{J_1(k_m b)}, \\
h(r,t) &= H - \frac{2H}{b} \sum_{n=1}^{\infty} e^{-k_n^2 \alpha^2 t} \frac{J_0(k_n r)}{k_n J_1(k_n b)} \blacksquare
\end{aligned}$$

Lesson 14

Introdução ao método das características

Considere a equação diferencial parcial de ordem 1

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0, \tag{14.1}$$

$$u(x,0) = g(x) \tag{14.2}$$

com c = constante. Suponha que $t = T(s)$, $x = X(s)$, e aplique a fórmula da derivada total; com $u = U(s)$, temos:

$$\frac{\mathrm{d}U}{\mathrm{d}s} = \frac{\partial u}{\partial t}\frac{\mathrm{d}T}{\mathrm{d}s} + \frac{\partial u}{\partial x}\frac{\mathrm{d}X}{\mathrm{d}s}. \tag{14.3}$$

Comparando (14.1) com (14.3):

$$\frac{\mathrm{d}T}{\mathrm{d}s} = 1, \tag{14.4}$$

$$\frac{\mathrm{d}X}{\mathrm{d}s} = c, \tag{14.5}$$

$$\frac{\mathrm{d}U}{\mathrm{d}s} = 0, \tag{14.6}$$

com

$$U(s=0) = u(X(0), T(0)) = g(X(0)). \tag{14.7}$$

A integração de (14.4)– (14.6) produz

$$T(s) = s + T(0); \tag{14.8}$$

$$X(s) = cs + X(0); \tag{14.9}$$

$$U(s) = \text{cte} = U(0) = g(X(0)). \tag{14.10}$$

Na figura 14.1, note que é razoável fazer $T(0) = 0$, ou seja: impor que as origens de t e de s coincidam. Mas agora a máquina do cálculo diferencial e integral entra em ação, e nós nos tornamos apenas mecânicos!

$$\begin{aligned} u(x,t) &= U(s) \\ &= g(X(0)) \\ &= g(X(s) - cs) \\ &= g(x - ct). \end{aligned} \tag{14.11}$$

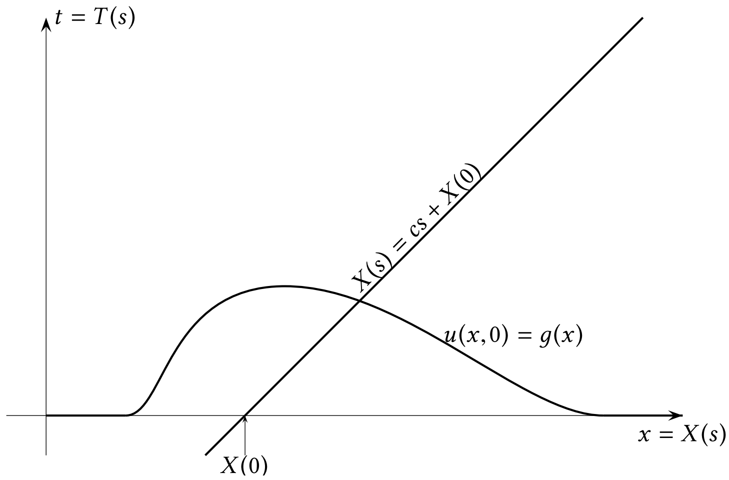

Figure 14.1: O método das características para a propagação de uma onda com celeridade constante c.

A solução é uma *equação de onda*: a forma da condição original, $g(x)$, simplesmente se translada ao longo do tempo: veja a figura 14.1.

Resolva

$$\frac{\partial u}{\partial t} + t\frac{\partial u}{\partial x} = xt, \qquad u(x,0) = g(x)$$

com o método das características.

Faça $u = U(s)$, $x = X(s)$ e $t = T(s)$ e escreva a derivada total:

$$\frac{\mathrm{d}U}{\mathrm{d}s} = \frac{\partial u}{\partial t}\frac{\mathrm{d}T}{\mathrm{d}s} + \frac{\partial u}{\partial x}\frac{\mathrm{d}X}{\mathrm{d}s};$$

Comparando,

$$\begin{aligned}
\frac{\mathrm{d}U}{\mathrm{d}s} &= X(s)T(s),\\
\frac{\mathrm{d}T}{\mathrm{d}s} &= 1,\\
\frac{\mathrm{d}X}{\mathrm{d}s} &= T(s).
\end{aligned}$$

Resolvendo o sistema acoplado,

$$\begin{aligned}
T(s) &= s = t;\\
\frac{\mathrm{d}X}{\mathrm{d}s} &= s,\\
X(s) &= \frac{1}{2}s^2 + X(0),\\
\frac{\mathrm{d}U}{\mathrm{d}s} &= \left[\frac{1}{2}s^2 + X(0)\right]s,\\
&= \frac{1}{2}s^3 + X(0)s;\\
U(s) &= \frac{1}{8}s^4 + \frac{X(0)}{2}s^2 + U(0).
\end{aligned}$$

Mas:

$$\begin{aligned}
U(0) &= U(X(0),0) = g(X(0));\\
U(s) &= \frac{1}{8}s^4 + \frac{X(0)}{2}s^2 + g(X(0)).
\end{aligned}$$

Basta agora escrever:

$$
\begin{aligned}
X(0) &= X(s) - \frac{1}{2}s^2,\\
U(s) &= \frac{1}{8}s^4 + \frac{(X(s)-(1/2)s^2)}{2}s^2 + g\left(X(s)-(1/2)s^2\right);\\
u(x,t) &= t^4/8 + (xt^2/2) - (t^4/4) + g(x-t^2/2) \blacksquare
\end{aligned}
$$

Resolva
$$
\frac{\partial u}{\partial x} + x^2\frac{\partial u}{\partial y} = -yu \qquad u(0,y) = f(y),
$$
com o método das características.

Faça $u = U(s)$, $y = Y(s)$ e $x = X(s)$, e escreva a derivada total:

$$
\frac{\mathrm{d}U}{\mathrm{d}s} = \frac{\partial u}{\partial x}\frac{\mathrm{d}X}{\mathrm{d}s} + \frac{\partial u}{\partial y}\frac{\mathrm{d}Y}{\mathrm{d}s};
$$

comparando,

$$
\begin{aligned}
\frac{\mathrm{d}U}{\mathrm{d}s} &= -Y(s)U(s),\\
\frac{\mathrm{d}X}{\mathrm{d}s} &= 1,\\
\frac{\mathrm{d}Y}{\mathrm{d}s} &= X(s)^2.
\end{aligned}
$$

Resolvendo agora o sistema acoplado, impondo $X(0) = 0$,

$$
\begin{aligned}
X(s) &= s;\\
\frac{\mathrm{d}Y}{\mathrm{d}s} &= s^2,\\
Y(s) &= \frac{1}{3}s^3 + Y(0);\\
\frac{\mathrm{d}U}{\mathrm{d}s} &= -\left[\frac{1}{3}s^3 + Y(0)\right]U(s),\\
\frac{\mathrm{d}U}{U} &= -\left[\frac{1}{3}s^3 + Y(0)\right]\mathrm{d}s,\\
\ln\frac{U(s)}{U(0)} &= -\left[\frac{1}{12}s^4 + Y(0)s\right].
\end{aligned}
$$

A condição inicial $U(0)$ é obtida “mecanicamente”:

$$
U(0) = u(0, Y(0)) = f(Y(0)) = f(y - x^3/3),
$$

onde nós já substituímos $x = X(s) = s$. Utilizando $Y(0)$ mais uma vez:

$$
\begin{aligned}
u(x,y) &= f(y-x^3/3)\exp\left[-\frac{1}{12}x^4 - (y-x^3/3)x\right]\\
&= f(y-x^3/3)\exp\left[-yx + \frac{1}{4}x^4\right] \blacksquare
\end{aligned}
$$

A “condição inicial” do método das características *não precisa ser em* $t = 0$. Considere o seguinte problema:

Seja

$$t\frac{\partial u}{\partial t} + x\frac{\partial u}{\partial x} = xt$$

com $u = 1$ na curva $\Gamma : x + t = 1$. Mostre que a solução é $U(s) = 1 + \frac{X_0 T_0}{2}\left[e^{2s} - 1\right]$ sobre cada curva característica dada por $X(s) = X_0 e^s,\ T(s) = T_0 e^s,\ X_0 + T_0 = 1$.

Suponha $X = X(s)$, $T = T(s)$ partindo de um ponto qualquer da curva $X_0 + T_0 = 1$ em uma direção transversal à mesma. Sobre a curva característica, $U = U(s)$, e comparamos:

$$\begin{aligned} t\frac{\partial u}{\partial t} + x\frac{\partial u}{\partial x} &= xt, \\ \frac{\mathrm{d}T}{\mathrm{d}s}\frac{\partial u}{\partial t} + \frac{\mathrm{d}X}{\mathrm{d}s}\frac{\partial u}{\partial x} &= \frac{\mathrm{d}U}{\mathrm{d}s}. \end{aligned}$$

Obtemos:

$$\begin{aligned} \frac{\mathrm{d}X}{\mathrm{d}s} &= X \Rightarrow X(s) = X_0 e^s, \\ \frac{\mathrm{d}T}{\mathrm{d}s} &= T \Rightarrow T(s) = T_0 e^s, \\ \frac{\mathrm{d}U}{\mathrm{d}s} &= XT = X_0 T_0 e^{2s} \Rightarrow U(s) - U_0 = X_0 T_0 \left[e^{2s}/2 - 1/2\right]; \\ U(0) = 1 &\Rightarrow U_0 = 1; \\ U(s) &= 1 + X_0 T_0 \left[e^{2s}/2 - 1/2\right], \end{aligned}$$

com $X_0 + T_0 = 1$ ■

Considere agora, novamente,

$$\frac{\partial u}{\partial t} + c(x,t)\frac{\partial u}{\partial x} = f(x,t)u \tag{14.12}$$

onde $c(x,t)$ e $f(x,t)$ são funções não especificadas de x e de t.

Faça $u = U(s)$, $x = X(s)$, $t = T(s)$; então,

$$\frac{\mathrm{d}U}{\mathrm{d}s} = \frac{\partial u}{\partial t}\frac{\mathrm{d}T}{\mathrm{d}s} + \frac{\partial u}{\partial x}\frac{\mathrm{d}X}{\mathrm{d}s}.$$

Comparando,

$$\begin{aligned} \frac{\mathrm{d}U}{\mathrm{d}s} &= f(X(s), T(s))U(s), \\ \frac{\mathrm{d}T}{\mathrm{d}s} &= 1, \\ \frac{\mathrm{d}X}{\mathrm{d}s} &= c(X(s), T(s)). \end{aligned}$$

Como sempre, $t = T(s) = s$; substituindo em X, temos a equação de uma *linha característica* no plano xt:

$$\frac{\mathrm{d}X}{\mathrm{d}t} = c(X, t),$$

cuja solução é da forma

$$X(t) = X(0) + \int_{\tau=0}^{t} c(X(\tau), \tau)\mathrm{d}\tau.$$

Note que essa última equação ainda é *implícita* em $X(t)$, mas isso não importa! O importante aqui é que podemos obter *em princípio* uma *família* de curvas em função do parâmetro $X(0)$.

A forma de (14.12) é o mais importante aqui (sem "conhecermos" $c(x,t)$, é impossível "resolver" completamente o problema): na próxima seção, nós vamos nos inspirar em (14.12) para generalizar o método das características para situações em que $\boldsymbol{u}(x,t)$ é um vetor, e aplicar essa generalização para classificar equações diferenciais parciais.

Utilizando o método das características, resolva

$$\frac{\partial u}{\partial t} - \beta k \frac{\partial u}{\partial k} - \beta u + \nu k^2 u = 0, \qquad u(k,0) = f(k)$$

para $u(k,t)$.

Suponha $u = U(s)$, $t = T(s)$, $k = K(s)$:

$$\frac{\mathrm{d}U}{\mathrm{d}s} = \frac{\partial u}{\partial t}\frac{\mathrm{d}T}{\mathrm{d}s} + \frac{\partial u}{\partial k}\frac{\mathrm{d}K}{\mathrm{d}s},$$

donde

$$\begin{aligned}
\frac{\mathrm{d}T}{\mathrm{d}s} &= 1,\\
\frac{\mathrm{d}K}{\mathrm{d}s} &= -\beta K,\\
\frac{\mathrm{d}U}{\mathrm{d}s} &= \beta U - \nu K^2 U.
\end{aligned}$$

Encontre: $T = s$ (sem perda de generalidade, a constante de integração $T(0) = 0$), $K(s) = \xi \mathrm{e}^{-\beta s}$. Agora, $K^2(s) = \xi^2 \mathrm{e}^{-2\beta s}$, e

$$\frac{\mathrm{d}U}{\mathrm{d}s} = \beta U - \nu \xi^2 \mathrm{e}^{-2\beta s} U.$$

Esta entretanto é uma equação *separável*:

$$\begin{aligned}
\frac{\mathrm{d}U}{U} &= \beta \mathrm{d}s - \nu \xi^2 \mathrm{e}^{2\beta s}\,\mathrm{d}s\\
\int_{u(\xi,0)}^{u(\xi,t)} \frac{\mathrm{d}U}{U} &= \int_0^t \beta \mathrm{d}s - \nu \xi^2 \mathrm{e}^{2\beta s}\,\mathrm{d}s\\
\ln \frac{u(\xi,t)}{f(\xi)} &= \beta t - \frac{\nu \xi^2}{2\beta}\left[1 - \mathrm{e}^{-2\alpha t}\right]\\
u(k,t) &= f(k) \exp\left[\beta t - \frac{\nu k^2 \mathrm{e}^{2\beta t}}{2\beta}\left(1 - \mathrm{e}^{-2\beta t}\right)\right]\\
u(k,t) &= f(k) \exp\left[\beta t - \frac{\nu k^2}{2\beta}\left(\mathrm{e}^{2\beta t} - 1\right)\right] \ \blacksquare
\end{aligned}$$

Resolva a equação diferencial

$$\frac{\partial \psi}{\partial \kappa} + \alpha \kappa^{-5/3} \frac{\partial \psi}{\partial \tau} = -\left[\frac{5}{3}\kappa^{-1} + 2\alpha \kappa^{1/3}\right]\psi; \qquad \psi(\kappa,0) = f(\kappa)$$

(onde α é uma constante, e $f(\kappa)$ é uma condição inicial conhecida), transformando o lado esquerdo na derivada total $d\psi/d\kappa$, identificando as linhas características, e integrando.

Este é obviamente um problema para ser resolvido pelo método das características; compare:

$$
\begin{aligned}
-\left[\frac{5}{3}\kappa^{-1}+2\alpha\kappa^{1/3}\right]\psi &= \frac{\partial\psi}{\partial\kappa}+\alpha\kappa^{-5/3}\frac{\partial\psi}{\partial\tau},\\
\frac{\mathrm{d}\psi}{\mathrm{d}\kappa} &= \frac{\partial\psi}{\partial\kappa}+\frac{\mathrm{d}\tau}{\mathrm{d}\kappa}\frac{\partial\psi}{\partial\tau}.
\end{aligned}
$$

A equação característica é

$$
\begin{aligned}
\frac{\mathrm{d}\tau}{\mathrm{d}\kappa} &= \alpha\kappa^{-5/3},\\
d\tau &= \alpha\kappa^{-5/3}\,d\kappa,\\
\int_0^\tau dt &= \alpha\int_\chi^\kappa k^{-5/3}\,dk.
\end{aligned}
$$

Note que na notação utilizada χ é a configuração de κ em $\tau = 0$; integrando:

$$
\begin{aligned}
\tau &= \frac{3\alpha}{2}\left[\chi^{-2/3}-\kappa^{-2/3}\right],\\
\frac{2\tau}{3\alpha} &= \chi^{-2/3}-\kappa^{-2/3},\\
\chi^{-2/3} &= \frac{2\tau}{3\alpha}+\kappa^{-2/3},\\
\chi(\kappa,\tau) &= \left[\frac{2\tau}{3\alpha}+\kappa^{-2/3}\right]^{-3/2}.
\end{aligned}
$$

De fato: $\tau = 0 \Rightarrow \chi = \kappa$. Agora integramos em κ:

$$
\begin{aligned}
\frac{\mathrm{d}\psi}{\mathrm{d}\kappa} &= -\left[\frac{5}{3}\kappa^{-1}+2\alpha\kappa^{1/3}\right]\psi,\\
\frac{d\psi}{\psi} &= -\left[\frac{5}{3}\kappa^{-1}+2\alpha\kappa^{1/3}\right]d\kappa,\\
\int_{f(\chi)}^{\psi(\kappa,\tau)}\frac{du}{u} &= -\int_\chi^\kappa\left[\frac{5}{3}k^{-1}+2\alpha k^{1/3}\right]dk,\\
\ln\frac{\psi(\kappa,\tau)}{f(\chi)} &= -\frac{5}{3}\int_\chi^\kappa\frac{dk}{k}-2\int_\chi^\kappa k^{1/3}\,dk,\\
\ln\frac{\psi(\kappa,\tau)}{f(\chi)} &= -\frac{5}{3}\ln\frac{\kappa}{\chi}-\frac{3}{2}\left[\kappa^{4/3}-\chi^{4/3}\right],\\
\psi(\kappa,\tau) &= f(\chi)\left(\frac{\kappa}{\chi}\right)^{-5/3}\exp\left[-\frac{3}{2}\left(\kappa^{4/3}-\chi^{4/3}\right)\right] \blacksquare
\end{aligned}
$$

Resolva o problema de valor inicial

$$
3x\frac{\partial u}{\partial x}+3\frac{\partial u}{\partial y} = xy, \qquad u(x,0) = \mathrm{e}^{-x^2}.
$$

O método das características se impõe. Se

$$
\begin{aligned}
x &= X(s),\\
y &= Y(s),
\end{aligned}
$$

são as equações paramétricas de uma curva no $\mathbb{R}^2$,

$$u = u(x, y) = u(X(s), Y(s)) = U(s),$$

isto é: $u = U(s)$ é uma *nova* função de s. Escrevemos agora lado a lado a equação diferencial parcial original e a derivada total de U:

$$\begin{aligned} xy &= 3x\frac{\partial u}{\partial x} + 3\frac{\partial u}{\partial y}, \\ \frac{\mathrm{d}U}{\mathrm{d}s} &= \frac{\partial u}{\partial X}\frac{\mathrm{d}X}{\mathrm{d}s} + \frac{\partial u}{\partial Y}\frac{\mathrm{d}Y}{\mathrm{d}s}. \end{aligned}$$

Deste par, obtemos 3 equações ordinárias:

$$\begin{aligned} \frac{\mathrm{d}X}{\mathrm{d}s} &= 3X(s), & X(0) &= \xi, \\ \frac{\mathrm{d}Y}{\mathrm{d}s} &= 3, & Y(0) &= 0, \\ \frac{\mathrm{d}U}{\mathrm{d}s} &= X(s)Y(s), & U(0) &= u(\xi, 0) = \mathrm{e}^{-\xi^2}. \end{aligned}$$

Que merecem ser integradas:

$$\begin{aligned} \frac{dX}{X} &= 3ds, \\ \ln\frac{X}{\xi} &= 3s, \\ X &= \xi\mathrm{e}^{3s}; \\ Y &= 3s; \\ \frac{\mathrm{d}U}{\mathrm{d}s} &= \xi\mathrm{e}^{3s}3s, \\ U(s) - U(0) &= 3\xi\int_0^s z\mathrm{e}^{3z}\,dz \\ &= \frac{((3s-1)\mathrm{e}^{3s}+1)\xi}{3}. \end{aligned}$$

Recuperamos agora as variáveis originais:

$$\begin{aligned} s &= y/3, \\ \xi &= x/\mathrm{e}^{3s} = x/\mathrm{e}^{y}; \\ u(x, y) = U(s) &= U(0) + \frac{((3s-1)\mathrm{e}^{3s}+1)\xi}{3} \\ &= \mathrm{e}^{-\xi^2} + \frac{((3s-1)\mathrm{e}^{3s}+1)\xi}{3} \\ &= \mathrm{e}^{-(x/\mathrm{e}^{y})^2} + \frac{((y-1)\mathrm{e}^{y}+1)\,\frac{x}{\mathrm{e}^{y}}}{3} \ \blacksquare \end{aligned}$$

Obtenha $\phi(x, t)$ pelo método das características:

$$\frac{\partial\phi}{\partial t} + \mathrm{e}^{-t}\frac{\partial\phi}{\partial x} = x, \qquad \phi(x, 0) = f(x).$$

Faça $\phi(x,t) = F(s)$ sobre $x = X(s)$ e $t = T(s)$:

$$\begin{aligned}
\phi(X(s),T(s)) &= F(s);\\
\frac{dF}{ds} &= \frac{\partial\phi}{\partial t}\frac{dT}{ds} + \frac{\partial\phi}{\partial x}\frac{dX}{ds};\\
\frac{dT}{ds} &= 1 \Rightarrow T(s) = \underbrace{T(0)}_{\equiv 0} + s,\\
\frac{dX}{ds} &= e^{-t} = e^{-s},\\
\int_{X(0)}^{X(s)} d\xi &= \int_0^s e^{-\tau}\, d\tau,\\
X(s) - X(0) &= 1 - e^{-s} \Rightarrow X(0) = X(s) - 1 + e^{-s}.
\end{aligned}$$

Mas

$$\begin{aligned}
\frac{\partial\phi}{\partial t} + e^{-t}\frac{\partial\phi}{\partial x} &= x,\\
\frac{dF}{ds} &= X(0) + 1 - e^{-s},\\
F(s) - F(0) &= \int_{\tau=0}^{s} \left[X(0) + 1 - e^{-tau}\right] d\tau\\
F(s) &= F(0) + (X(0)+1)s + (e^{-s} - 1)\\
F(0) &= f(X(0)) = f(x - 1 + e^{-t});\\
\phi(x,t) &= F(s) = f(x - 1 + e^{-t}) + (x - 1 + e^{-t} + 1)t + (e^{-t} - 1)\\
\phi(x,t) &= f(x - 1 + e^{-t}) + (x + e^{-t})t + (e^{-t} - 1) \blacksquare
\end{aligned}$$

14.1 O método das características e a classificação de Equações Diferenciais Parciais

Suponha agora que $\boldsymbol{u}(x,t) \in \mathbb{R}^2$; a generalização de (14.12) para duas dimensões é

$$\frac{\partial\boldsymbol{u}}{\partial t} + \boldsymbol{C}(x,t)\cdot\frac{\partial\boldsymbol{u}}{\partial x} = \boldsymbol{F}(x,y)\cdot\boldsymbol{u}, \tag{14.13}$$

onde $\boldsymbol{C}$ e $\boldsymbol{F}$ são tensores, representados por matrizes 2×2 em uma base particular. Supondo como antes que $x = X(s)$, $t = T(s)$, a derivada total de $\boldsymbol{u}$ em relação a s é

$$\frac{d\boldsymbol{u}}{ds} = \frac{\partial\boldsymbol{u}}{\partial t}\frac{dT}{ds} + \frac{\partial\boldsymbol{u}}{\partial x}\frac{dX}{ds}.$$

A comparação com (14.13) sugere

$$\begin{aligned}
\frac{dT}{ds} &= 1,\\
\frac{dX}{ds} &= \boldsymbol{C}(X(s),T(s)).
\end{aligned}$$

A segunda equação acima, entretanto, é absurda: o lado esquerdo é um escalar, e o lado direito é um tensor. É preciso lidar com cada uma das funções incógnitas de $\boldsymbol{u}$ separadamente.

Suponha agora que C possua dois autovetores LI, associados a dois autovalores λ_1 e λ_2. Nesse caso, podemos escrever (14.13) na base dos autovetores como

$$\frac{\partial}{\partial t}\begin{bmatrix}u_1\\u_2\end{bmatrix} + \begin{bmatrix}\lambda_1 & 0\\ 0 & \lambda_2\end{bmatrix}\begin{bmatrix}\frac{\partial u_1}{\partial x}\\ \frac{\partial u_2}{\partial x}\end{bmatrix} = \begin{bmatrix}f_{11} & f_{12}\\ f_{21} & f_{22}\end{bmatrix}\begin{bmatrix}u_1\\u_2\end{bmatrix},$$

ou

$$\frac{\partial u_1}{\partial t} + \lambda_1 \frac{\partial u_1}{\partial x} = f_{11}u_1 + f_{12}u_2, \tag{14.14}$$

$$\frac{\partial u_2}{\partial t} + \lambda_2 \frac{\partial u_2}{\partial x} = f_{21}u_1 + f_{22}u_2. \tag{14.15}$$

Essa é uma situação muito mais próxima do método das características unidimensional que apresentamos na seção anterior. Por exemplo, podemos fazer $t = T_1(s)$, $x = X_1(s)$, $u_1 = U_1(s)$, e obter

$$\frac{\mathrm{d}U_1}{\mathrm{d}s} = \frac{\partial u_1}{\partial t}\frac{\mathrm{d}T}{\mathrm{d}s} + \frac{\partial u_1}{\partial x}\frac{\mathrm{d}X_1}{\mathrm{d}s}.$$

A comparação com (14.14) produz

$$\frac{\mathrm{d}T_1}{\mathrm{d}s} = 1,$$

$$\frac{\mathrm{d}X_1}{\mathrm{d}s} = \lambda_1.$$

É evidente que o mesmo pode ser feito para (14.15). Isso nos dará duas curvas parametrizadas em s: $(x,t) = (X_1(s), T_1(s))$ e $(x,t) = (X_2(s), T_2(s))$. Essas são as curvas características do sistema (14.13).

A conexão com equações diferenciais parciais de ordem *dois* se segue. Considere uma equação diferencial parcial de ordem 2, linear, do tipo

$$A\phi_{xx} + 2B\phi_{xy} + C\phi_{yy} = F. \tag{14.16}$$

Nós vamos permitir que A, B, C sejam funções genéricas de x, y, e que o termo F seja ainda mais geral. Por exemplo, F poderá conter inclusive derivadas de ordem 1 de ϕ. O plano é reescrever (14.16) na forma

$$\frac{\partial \boldsymbol{u}}{\partial x} + \boldsymbol{C}\cdot\frac{\partial \boldsymbol{u}}{\partial y} = \boldsymbol{F}.$$

Isso pode ser feito com

$$u = \phi_x \qquad \text{e} \qquad v = \phi_y$$

donde se seguem duas equações acopladas:

$$\begin{aligned} Au_x + 2Bu_y + Cv_y &= F,\\ v_x &= u_y; \end{aligned}$$

melhor ainda,

$$\begin{aligned} u_x + \frac{2B}{A}u_y + \frac{C}{A}v_y &= \frac{F}{A},\\ v_x - u_y &= 0. \end{aligned}$$

Agora temos a forma “correta”:

$$\frac{\partial}{\partial x}\begin{bmatrix} u \\ v \end{bmatrix} + \begin{bmatrix} 2B/A & C/A \\ -1 & 0 \end{bmatrix}\frac{\partial}{\partial y}\begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} F/A \\ 0 \end{bmatrix}.$$

A matriz da equação acima possui os autovalores

$$\lambda_{1,2} = \frac{B}{A} \pm \frac{\sqrt{B^2 - AC}}{A}.$$

Dependendo dos autovalores que nós encontrarmos, nós classificaremos a EDP (14.16) como se segue:

$$\Delta = B^2 - AC \begin{cases} < 0 & \text{Elítica,} \\ = 0 & \text{Parabólica,} \\ > 0 & \text{Hiperbólica.} \end{cases}$$

Vejamos, a seguir, alguns exemplos de interesse prático em Engenharia.

Classifique e analise a equação da difusão,

$$\frac{\partial \phi}{\partial t} = \alpha^2 \frac{\partial^2 \phi}{\partial x^2}.$$

Fazendo $x = x$, $t = y$ em (14.16), temos $A = \alpha^2$, $B = 0$ e $C = 0$. Consequentemente, $B^2 - AC = 0$, e a EDP é parabólica. Existe apenas um autovalor, $\lambda = 0$.

Classifique e analise a equação da onda,

$$\frac{\partial^2 \phi}{\partial t^2} = c^2 \frac{\partial^2 \phi}{\partial x^2}.$$

Agora, $A = c^2$, $B = 0$ e $C = -1$; $B^2 - AC = c^2 >$, e a EDP é hiperbólica.

Classifique e analise a equação de Laplace,

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0.$$

Com $A = 1$, $B = 0$ e $C = 1$, $B^2 - AC = 1$, e a equação é elítica.

Classifique e analise a equação de difusão-advecção,

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} - D\frac{\partial^2 \phi}{\partial x^2} = 0.$$

Com $A = -D$, $B = 0$ e $C = 0$, $B^2 - AC = 0$, e a equação é parabólica.

Exercícios Propostos

Mostre que

$$\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left[h\frac{\partial h}{\partial x}\right]$$

é uma EDP parabólica.

$$\begin{aligned} \frac{\partial h}{\partial t} &= h\frac{\partial^2 h}{\partial x^2} + \frac{\partial h}{\partial x}\frac{\partial h}{\partial x}, \\ h\frac{\partial^2 h}{\partial x^2} &= \frac{\partial h}{\partial t} - \frac{\partial h}{\partial x}\frac{\partial h}{\partial x}, \\ B^2 - AC &= 0 - h \times 0 = 0 \blacksquare \end{aligned}$$

Appendix A

Generalized homogeneous functions

We use some help from Hankey e Stanley (1972):

Definition A.1 A function $f(x_1, x_2)$ is a generalized homogeneous function (GHF) if there exist two numbers a_1, a_2 such that for all $\lambda > 0$,

$$f(\lambda^{a_1} x_1, \lambda^{a_2} x_2) = \lambda^{a_f} f(x_1, x_2).$$

a_f is the *scaling power* of f.

Hankey e Stanley (1972) show (trivially, almost) that a GHF is either *scale-invariant*,

$$f(\lambda^{a_1} x_1, \lambda^{a_2} x_2) = f(x_1, x_2),$$

or else one can choose a_1 and a_2 such that

$$f(\lambda^{a_1} x_1, \lambda^{a_2} x_2) = \lambda f(x_1, x_2).$$

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