Gas dynamics and Heat and Mass Transfer

Numerical Solution of the Convection–Diffusion Equations

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Contents

1 Diagonal flow case

1.1 Statement

The diagonal flow case takes places in the domain $\Omega = (0, L) \times (0, L) \subset \mathbb{R}^2$ where $L > 0$ is a constant length. In Ω the steady state general convection–diffusion equation with no source term, constant density and constant diffusion coefficient is considered. Under these hypothesis equation (**??**) is

$$\frac{\rho}{\Gamma}\mathbf{v} \cdot \boldsymbol{\nabla}\phi = \Delta\phi \tag{1.1}$$

The following Dirichlet boundary conditions are prescribed:

- $\phi = \phi_{\text{low}}$ on $C_1 = [0, L) \times \{0\} \cup \{L\} \times [0, L)$.
- $\phi = \phi_{\text{high}}$ on $C_2 = \{0\} \times (0, L] \cup (0, L] \times \{L\}$.

Notice that $C_1,\ C_2 \subset \mathbb{R}^2$ constitute a partition of the boundary of Ω. In order to encode the boundary conditions more easily, we define the function $g\colon \Omega \to \mathbb{R}$ in the following way:

$$g(x, y) = \begin{cases} \phi_{\text{low}} & \text{if } (x, y) \in C_1 \\ \phi_{\text{high}} & \text{if } (x, y) \in C_2 \end{cases} \tag{1.2}$$

The velocity field is $\mathbf{v} = v_0 \cos(\alpha)\mathbf{i} + v_0 \sin(\alpha)\mathbf{j}$ with $v_0 > 0$ constant and $\alpha = \pi/4$, whence

$$\frac{\rho}{\Gamma}\mathbf{v} \cdot \boldsymbol{\nabla}\phi = \frac{\rho v_0 \cos(\alpha)}{\Gamma}\left\{\frac{\partial\phi}{\partial x} + \frac{\partial\phi}{\partial y}\right\} = \underbrace{\frac{\cos(\alpha)}{L}}_{\beta}\underbrace{\frac{\rho v_0 L}{\Gamma}}_{\text{Pe}}\left\{\frac{\partial\phi}{\partial x} + \frac{\partial\phi}{\partial y}\right\} = \beta\,\text{Pe}\left\{\frac{\partial\phi}{\partial x} + \frac{\partial\phi}{\partial y}\right\} \tag{1.3}$$

The resulting Cauchy problem is gathered in (1.4) and summarized in figure 1.1.

$$\begin{cases} \Delta\phi - \beta\,\text{Pe}\left\{\dfrac{\partial\phi}{\partial x} + \dfrac{\partial\phi}{\partial y}\right\} = 0 & \text{in } \Omega \\ \phi = g & \text{on } \partial\Omega \end{cases} \tag{1.4}$$

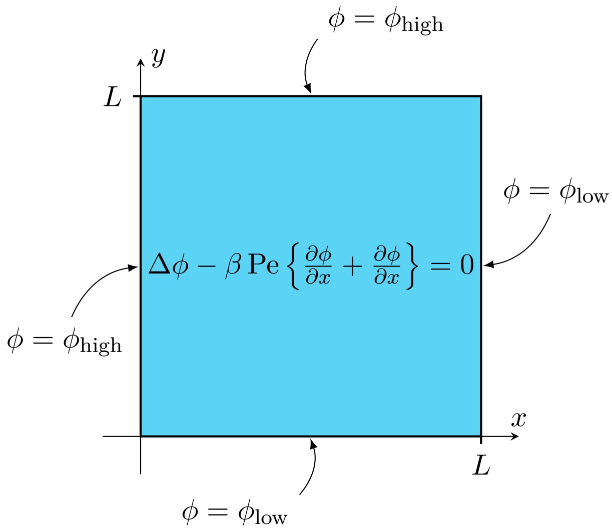


Figure 1.1. Cauchy problem for the diagonal flow case.

1.2 Analytical solution

1.2.1 Analytical solution for $\mathrm{Pe} = \infty$

As we have previously seen, Péclet's number is defined as

$$\mathrm{Pe} = \frac{\text{convection transport rate}}{\text{diffusion transport rate}} = \frac{\rho u L}{\Gamma} \tag{1.5}$$

Whenever $\mathrm{Pe} \to +\infty$, it implies $\Gamma \to 0^+$ since infinite values for the density, velocity or characteristic length make no physical sense. Therefore the difussion coefficient tends to 0, which means the Laplacian term, linked to the diffusion process, is negligible. Dividing the PDE from (1.4) by Péclet's number results in the following Cauchy problem:

$$\begin{cases} \dfrac{\partial \phi}{\partial x} + \dfrac{\partial \phi}{\partial y} = 0 & \text{in } \Omega \\ \phi = g & \text{on } \partial\Omega \end{cases} \tag{1.6}$$

The PDE (1.6) is known as the transport equation, which is a first order linear PDE. In our case it has constant coefficients, making it easier to solve analitically.

Definition 1.1. A classical solution to (1.6) is a function $\phi\colon \overline{\Omega} \to \mathbb{R}$ that satisfies:

(i) $\phi \in \mathcal{C}^1(\Omega) \cap \mathcal{C}(\overline{\Omega})$, i.e. ϕ is differentiable with continuity in Ω and continuous up to the boundary,

(ii) ϕ satisfies the PDE, and

(iii) ϕ satisfies the boundary conditions.

In order to find the solution to (1.6), we will assume ϕ is a $\mathcal{C}^1(\Omega) \cap \mathcal{C}(\overline{\Omega})$ function. Once we find the solution, we will be able to tell whether ϕ is a classical solution, or otherwise give a meaning to ϕ.

We introduce some notation that will be useful. Given m vectors $\mathbf{w}_1, \dots, \mathbf{w}_m \in \mathbb{R}^n$, the set $[\mathbf{w}_1, \dots, \mathbf{w}_m] = \{\sum_{i=1}^m \lambda_i \mathbf{w}_i \mid \lambda_1, \dots, \lambda_m \in \mathbb{R}\}$ is the vector subspace of $\mathbb{R}^n$ spanned by $\mathbf{w}_1, \dots, \mathbf{w}_m$. If $W \subset \mathbb{R}^m$ is a vector subspace, $W^\perp = \{v \in \mathbb{R}^n \mid v \cdot w = 0 \ \forall w \in W\}$ is the vector subspace orthogonal to W.

To deduce the solution to (1.6) we shall follow the method of characteristics. Using the gradient of ϕ we can write the PDE as

$$(1,1) \cdot \boldsymbol{\nabla}\phi = (1,1) \cdot \begin{pmatrix} \dfrac{\partial \phi}{\partial x} \\ \dfrac{\partial \phi}{\partial y} \end{pmatrix} = \frac{\partial \phi}{\partial x} + \frac{\partial \phi}{\partial y} = 0 \tag{1.7}$$

Recall from vector calculus that the gradient vector of ϕ gives the direction of maximum growth of ϕ at each point, whilst a non–zero vector $\mathbf{w} \in [\boldsymbol{\nabla}\phi(x,y)]^\perp$ provides the direction at (x,y) along which ϕ remains constant. Equation (1.7) tells us than ϕ is constant along the direction given by $(1,1)$. To check this, we may exploit the fact that the PDE is first–order linear and use the chain rule to rewrite (1.7). Let $I \subset \mathbb{R}$ be an open interval and let $h \equiv (h_1, h_2)\colon I \subset \mathbb{R} \to \Omega \subset \mathbb{R}^2$, $s \mapsto h(s) = (h_1(s), h_2(s))$ be a $\mathcal{C}^1$ mapping such that $h_1' = h_2' = 1$. The image of h, $C = \operatorname{Im} h = \{(x,y) \in \mathbb{R}^2 \mid x = h_1(s),\ y = h_2(s),\ s \in I\} \subset \Omega$ is a $\mathcal{C}^1$ curve in $\mathbb{R}^2$. The restriction of ϕ to C, given by $\varphi = \phi \circ h\colon \mathbb{R} \to \mathbb{R}$, is also a $\mathcal{C}^1$ function. By the chain rule,

$$\frac{\mathrm{d}}{\mathrm{d}s}\varphi(s) = \frac{\mathrm{d}}{\mathrm{d}s}\phi(h_1(s), h_2(s)) = \frac{\partial \phi}{\partial x}(h_1(s), h_2(s))\, h_1'(s) + \frac{\partial \phi}{\partial y}(h_1(s), h_2(s))\, h_2'(s) = \frac{\partial \phi}{\partial x} + \frac{\partial \phi}{\partial y} = 0 \tag{1.8}$$

which implies that ϕ is constant on $C \subset \Omega$. Now we would like to find C. By hypothesis, we have $h_1' = h_2' = 1$. Moreover, the component functions of h can be interpreted as the coordinates of a point in $\mathbb{R}^2$, that is $(h_1(s), h_2(s)) = (x, y)$. Given this information, we can pose the following Cauchy problem:

$$\begin{cases} h'(s) = (h_1'(s), h_2'(s)) = (1,1) & \text{in } I \subset \mathbb{R} \\ h(0) = (h_1(0), h_2(0)) = (x_0, y_0) \end{cases} \tag{1.9}$$

The solution to (1.9) exists and is unique due to Teorema existencia y unicidad, and is given by

$$h(s) = (x_0 + s, y_0 + s) = (x_0, y_0) + s(1,1) \tag{1.10}$$

The point $(x_0, y_0) \in \mathbb{R}^2$ is arbitrary, but it should be chosen so that it eases finding the solution to (1.6). Since part of the information of the solution is given by the boundary conditions, we may choose the point to be on the boundary. Therefore the curve along which ϕ is constant is not a single curve, but rather a family of curves given by

$$h(s; x_0, y_0) = (x_0, y_0) + s(1,1), \quad (x_0, y_0) \in \partial\Omega \tag{1.11}$$

or in implicit form by the equation

$$x - y = x_0 - y_0, \quad (x_0, y_0) \in \partial\Omega \tag{1.12}$$

These curves are named characteristic curves or simply characteristics. Some of them are represented in figure 1.2. As it can be seen, the characteristics have implicit equation $x - y = c$ with $c \in [-L, L]$.

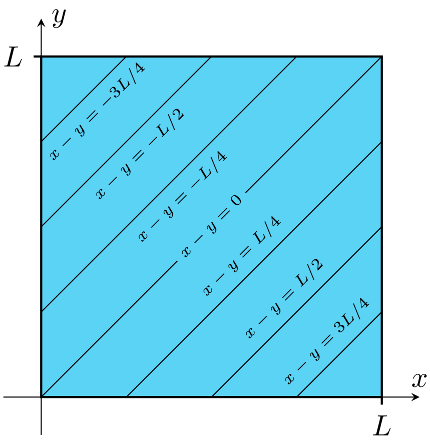


Figure 1.2. Some characteristics of problem (1.6).

Intuitively, the characteristics give the paths in $\mathbb{R}^2$ through which the information of the boundary conditions is transported. Notice that each characteristic starting on C_1 ends on C_1, and the same holds for C_2. Moreover, by definition of the Cauchy problem, ϕ is constant on C_1 and on C_2. Therefore the value of ϕ on the characteristic $x - y = c$ is the value that g takes on the part of the boundary the characteristic intersects:

$$\phi(x,y) = \begin{cases} g(x-y) = \phi_{\text{low}} & \text{if } x - y \geq 0 \\ g(y-x) = \phi_{\text{high}} & \text{if } x - y < 0 \end{cases} \quad (x,y) \in \overline{\Omega} \tag{1.13}$$

Notice that it is not necessary to prescribe boundary conditions on $(0, L] \times \{L\}$ nor on $\{L\} \times (0, L)$, since the value of the solution on those parts of the boundary is already given by the value ϕ takes on $[0, L] \times \{0\} \cup \{0\} \times (0, L]$.

Now we check our initial assumption that $\phi \in \mathcal{C}^1(\Omega) \cap \mathcal{C}(\overline{\Omega})$. If $\phi_{\text{low}} = \phi_{\text{high}}$ the solution (1.13) is constant and therefore is a solution in the classical sense.

Theorem 1.2. Assume $\phi_{\text{low}} = \phi_{\text{high}}$. Then the solution to problem (1.6) exists, is unique and is a solution in the classical sense.

Proof. We have proved the existence of a solution by giving formula (1.13). The uniqueness comes from the method of characteristics we have followed. In it we have seen that ϕ is constant on the characteristic curves and then we have found the equation of characteristics. These curves are unique due to the Theorem of Existence and Uniqueness of solutions to ODEs. Finally ϕ is a $\mathcal{C}^1(\Omega) \cap \mathcal{C}(\overline{\Omega})$ function because it is constant on $\overline{\Omega}$. □

Assume that $\phi_{\text{low}} < \phi_{\text{high}}$. Then ϕ is not continuous on the segment $\{x - y = 0\} \cap \overline{\Omega}$ whence it cannot be a differentiable function. Notice that to find the function (1.13) it was not necessary to prescribe boundary conditions on $(0, L] \times \{L\}$ nor on $\{L\} \times (0, L)$, since the value of the solution on those parts of the boundary is already given by the value ϕ takes on $[0, L] \times \{0\} \cup \{0\} \times (0, L]$. In order to give a meaning to function (1.13) we will formulate a similar problem to (1.6). Let $D_1 = [0, L] \times \{0\}$, $D_2 = \{0\} \times (0, L]$, and let $\tilde{g}\colon D_1 \cup D_2 \to \mathbb{R}$ be defined by

$$\tilde{g}(x, y) = \Big\{ \phi_{\text{low}} \quad \text{if } (x, y) \in D_1 \quad \phi_{\text{high}} \quad \text{if } (x, y) \in D_2 \tag{1.14}$$

Consider the following Cauchy problem:

$$\begin{cases} \dfrac{\partial \phi}{\partial x} + \dfrac{\partial \phi}{\partial y} = 0 & \text{in } \Omega \\ \phi = \tilde{g} & \text{on } D_1 \cup D_2 \end{cases} \tag{1.15}$$

It is essentially the same problem as (1.6) but without prescribing boundary conditions on the right and top boundaries. It can be checked that the solution to (1.15) found by following the method of characteristics is also given by (1.13). But we again encounter the problem to give a meaning to the derivatives, since (1.13) is not continuous on $\overline{\Omega}$.

Definition 1.3. A function $\psi\colon \overline{\Omega} \to \mathbb{R}$ is said a weak solution of (1.6) if

$$\int_\Omega$$

1.2.2 Analytical solution for $\mathrm{Pe} = 0$

Now we consider the problem (1.4) when $\mathrm{Pe} \to 0$. Since $\rho > 0$ and $L > 0$, the fact that Péclet's number is close to zero implies that velocity u is close to zero. In the extreme case when $u = 0$, there is no transport, therefore $\mathrm{Pe} = 0$ and problem (1.4) becomes

$$\begin{cases} \Delta \phi = 0 & \text{in } \Omega \\ \phi = g & \text{on } \partial\Omega \end{cases} \tag{1.16}$$

which is Laplace's problem in the square Ω.

1.2.3 General problem

1.2.4 Expected nature of the solution

1.3 Numerical solution

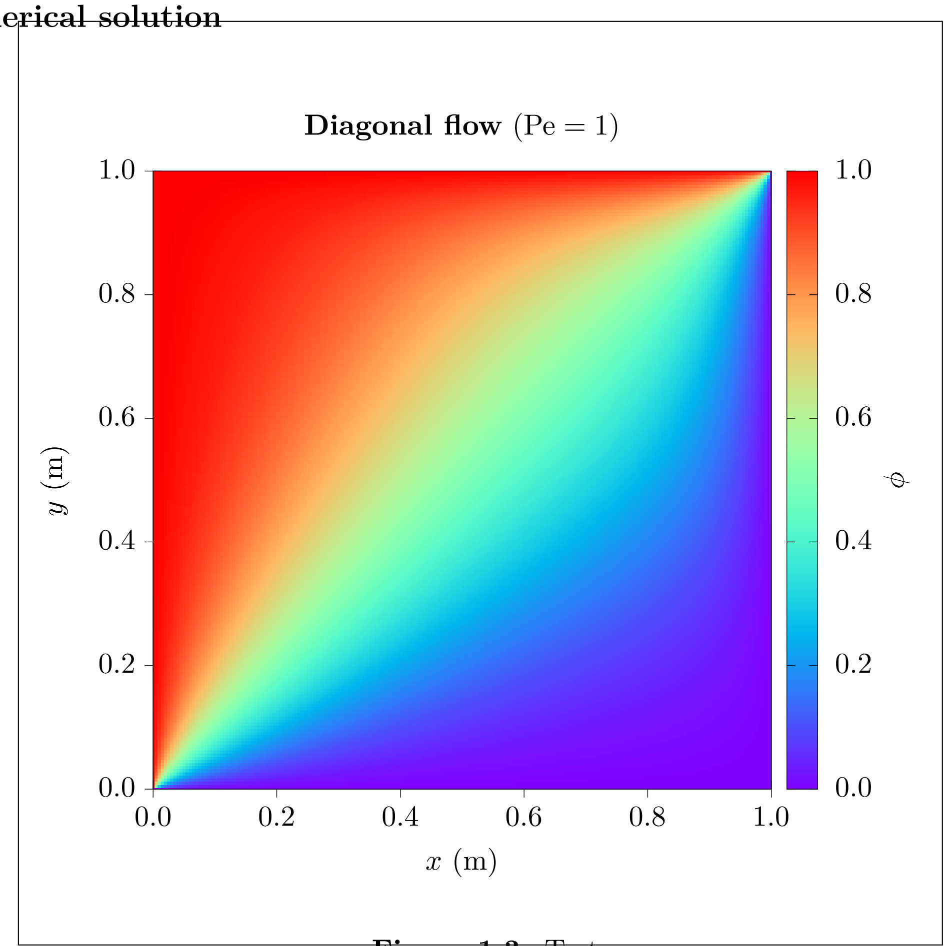
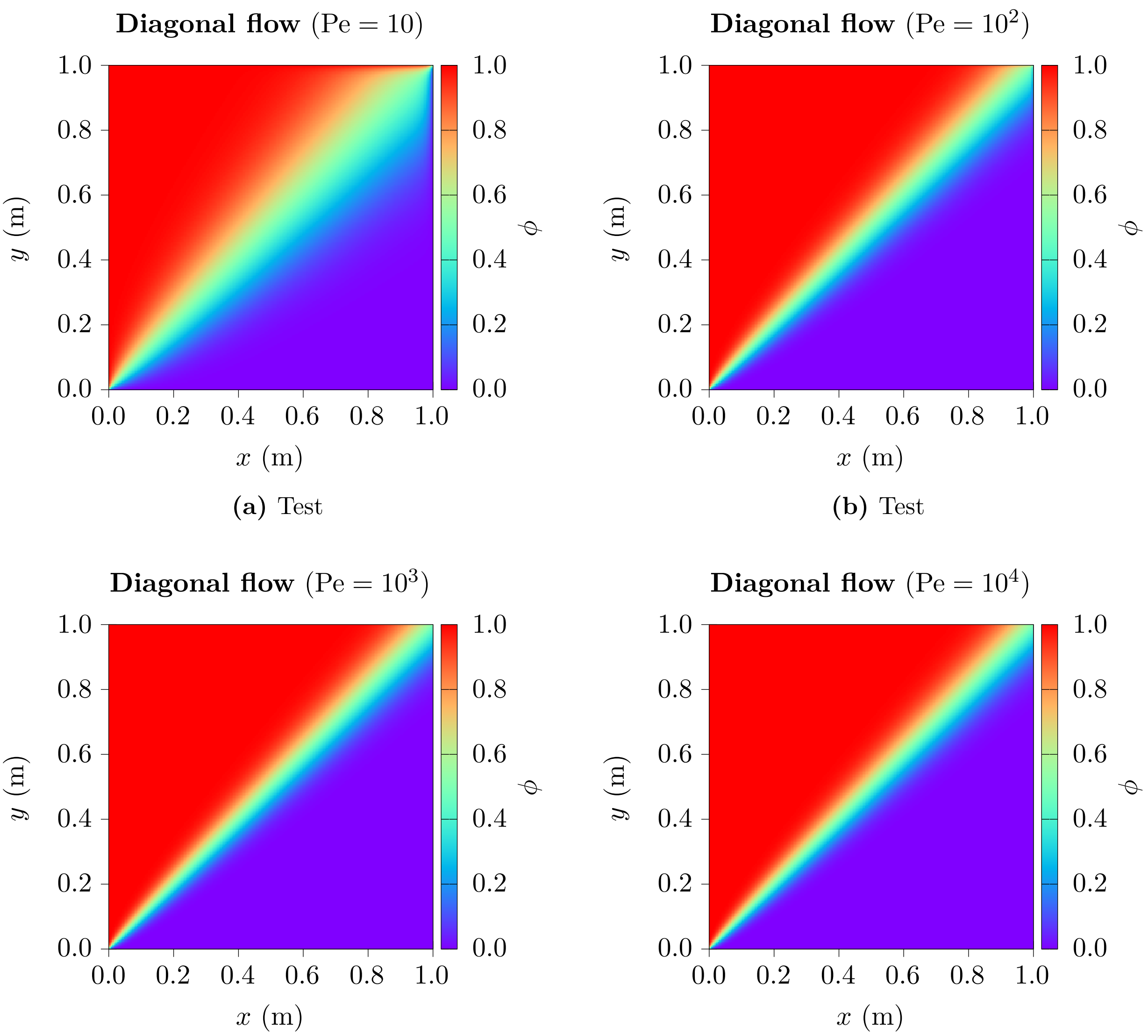


Figure 1.3. Test



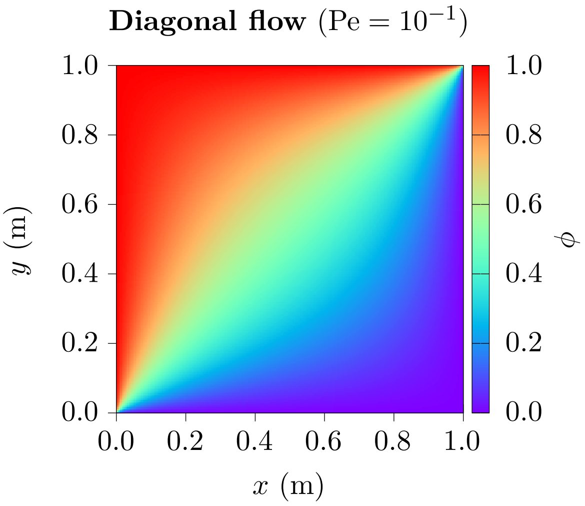
(a) Test

(b) Test

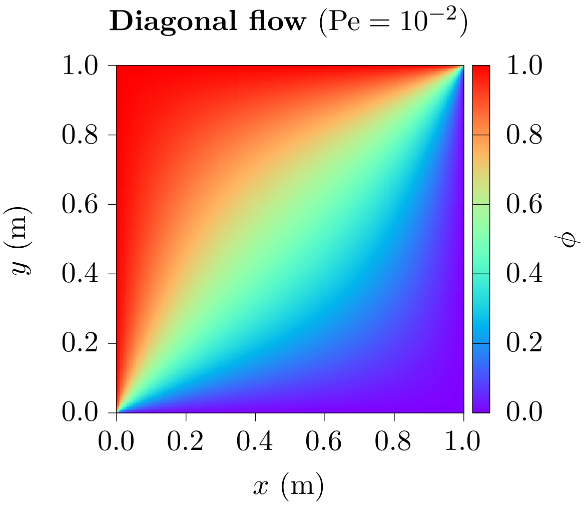
(c) Test

(d) Test

Figure 1.4. A figure with two subfigures



(a) Test



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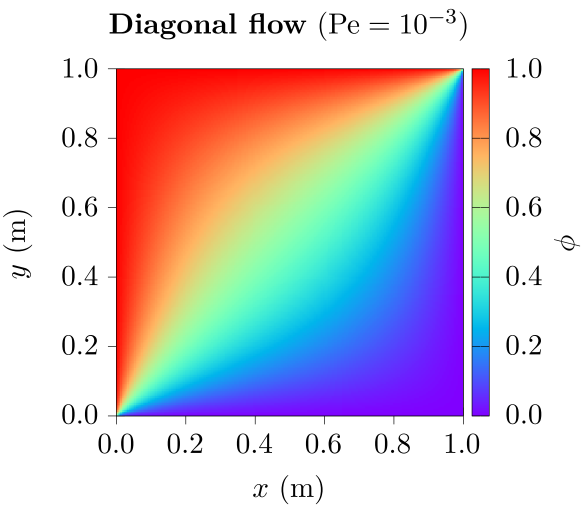

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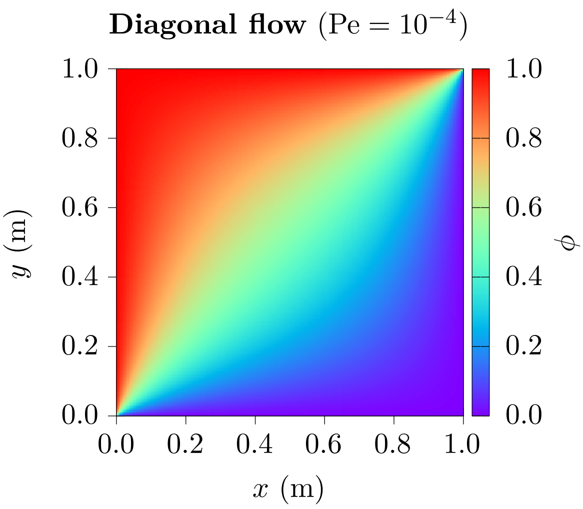

(d) Test

Figure 1.5. A figure with two subfigures

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A Some results on measure theory

In this appendix we gather two important theorems needed to justify some steps in the derivation of conservation laws in section **??**. Despite these results are basic, a previous study of real analysis is required in order to understand and prove them. A good reference for the interested reader is Real and Complex Analysis of Walter Rudin [10].

A.1 Differentiation under the integral sign

Differentiation under the integral sign allows us to compute the derivative of an integral of a function of two parameters in a simple way. It is needed, for instance, when the mass conservation law or the heat diffusion equation are derived.

Let $(X, \mathcal{A}, \mu)$ be a measure space and let $[a, b] \subset \mathbb{R}$. Hereinafter we deal with functions $f\colon X \times [a, b] \to \mathbb{R}$, where $t \in [a, b]$ is the parameter on which f depends. We assume that $f(\cdot, t)$ is a measurable function for each $t \in [a, b]$.

Theorem A.1 (Differentiation under the integral sign)**.** Let $F(t) = \int_X f(\mathbf{x}, t)\,\mathrm{d}\mu$. Assume that

(i) $f(\mathbf{x}, t_0)$ is an integrable function for some $t_0 \in [a, b]$.

(ii) $\dfrac{\partial f}{\partial t}(\mathbf{x}, t)$ is defined for all $(\mathbf{x}, t) \in X \times [a, b]$.

(iii) There exists an integral function $g\colon X \to \mathbb{R}$ such that $\left|\dfrac{\partial f}{\partial t}(\mathbf{x}, t)\right| \leq g(\mathbf{x})$ for all $(\mathbf{x}, t) \in X \times [a, b]$.

Then F is a differentiable function and

$$F'(t) = \frac{\mathrm{d}}{\mathrm{d}t}F(t) = \int_X \frac{\partial f}{\partial t}(\mathbf{x}, t)\,\mathrm{d}\mu$$

For the applications needed in this project, $X = \mathbb{R}^m$ with $1 \leq m \leq 3$, $\mathcal{A}$ is the Borel σ–algebra on $\mathbb{R}^m$ and μ is Lebesgue's measure on $\mathbb{R}^m$, which for most of the "natural" sets of $\mathcal{A}$ coincides with the usual notion of m–dimensional volume.

A.2 Lebesgue's differentiation lemma

A common way to derive a conservation law is to integrate some functions in a control volume, then apply Differentiation under the integral sign to obtain an integral equation and finally get to a differential equation using Lebesgue's differentiation lemma.

An intuitive way to understand and to motivate Lebesgue's differentiation lemma is the following. Let $f\colon \mathbb{R} \to \mathbb{R}$ be a continuous function, let $a \in \mathbb{R}$ be a fixed point and let $F(x) = \int_a^x f(y)\,\mathrm{d}y$, which is a differentiable function. Due to a corollary of the Fundamental Theorem of Calculus, we have $F'(x) = f(x)$. Using the definition of derivative,

$$F'(x) = \lim_{h\to 0} \frac{F(x+h) - F(x)}{h} = \lim_{h\to 0} \frac{1}{h}\left\{\int_a^{x+h} f(y)\,\mathrm{d}y - \int_a^{x} f(y)\,\mathrm{d}y\right\} = \lim_{h\to 0} \frac{1}{h}\int_x^{x+h} f(y)\,\mathrm{d}y = f(x)$$

Notice that the integral is divided by the length of the interval $[x, x+h]$, otherwise the limit would be zero. Lebesgue's lemma generalizes the previous equality by considering functions $f\colon \mathbb{R}^n \to \mathbb{R}$ and integrating them on open balls $B(\mathbf{x_0}, r) = \{x \in \mathbb{R}^n \mid \|\mathbf{x} - \mathbf{x_0}\| < r\}$. Furthermore, the integral is divided by the n–dimensional volume of $B(\mathbf{x_0}, r)$, which is denoted by $|B(\mathbf{x_0}, r)|$.

Theorem A.2 (Lebesgue's differentiation lemma [11]). Let $f\colon \mathbb{R}^n \to \mathbb{R}$ be a locally integrable function.

(1) Then for almost everywhere point $\mathbf{x_0} \in \mathbb{R}^n$,

$$\frac{1}{|B(\mathbf{x_0}, r)|} \int_{B(\mathbf{x_0}, r)} f(\mathbf{x})\,\mathrm{d}\mathbf{x} \to f(\mathbf{x_0}) \quad \text{as } r \to 0$$

(2) In fact, for almost everywhere point $\mathbf{x_0} \in \mathbb{R}^n$,

$$\frac{1}{|B(\mathbf{x_0}, r)|} \int_{B(\mathbf{x_0}, r)} |f(\mathbf{x}) - f(\mathbf{x_0})|\,\mathrm{d}\mathbf{x} \to 0 \quad \text{as } r \to 0$$

B Numerical resolution of linear systems

B.1 Gauss–Seidel algorithm

B.2 LU factorization