Gas dynamics and Heat and Mass Transfer

Numerical Solution of the Convection–Diffusion Equations

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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

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

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

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

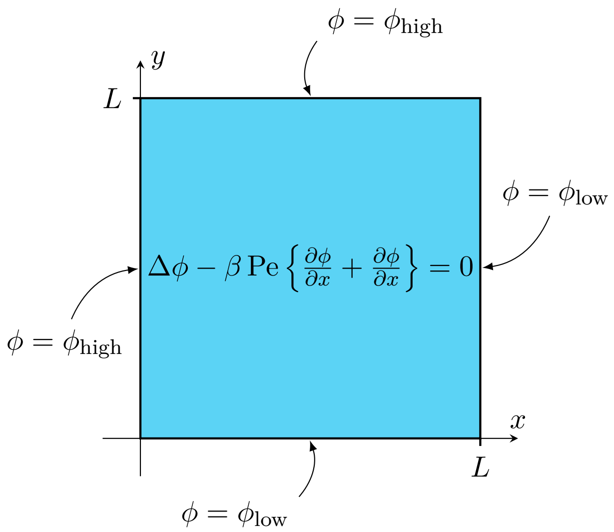


Figure 1.1. Cauchy problem for the diagonal flow case.

1.2 Analytical solution

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

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

Note that the factor β in the PDE from problem (1.4) is a constant determined by the geometry, whereas Peclet's number depends on the fluid and on the velocity field. Since no more factors intervene on the PDE, this tells us that the behaviour of the solution will depend greatly on Peclet's number.

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

Whenever $\text{Pe} \to +\infty$, 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,

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

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:

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

The solution to (1.9) exists and is unique due to theorem B.5, and is given by

$$h(s) = (x_0 + s, y_0 + s) = (x_0, y_0) + s(1, 1) \quad (1.10)$$

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

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

or in implicit form by the equation

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

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 $c \in [-L, L]$.

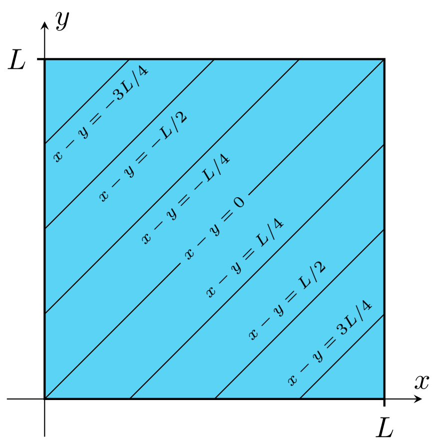


Figure 1.2. Some characteristics of problem (1.6).

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

$$\tilde{g}(x,y) = \begin{cases} \phi_{\text{low}} & \text{if } (x,y) \in D_1 \\ \phi_{\text{high}} & \text{if } (x,y) \in D_2 \end{cases} \tag{1.14}$$

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

Hereafter we consider problem (1.4) with $0 < \mathrm{Pe} < +\infty$ with $\phi_{\mathrm{low}} < \phi_{\mathrm{high}}$. A classical solution to (1.4) is a function $\phi \in \mathcal{C}^2(\Omega) \cap \mathcal{C}(\overline{\Omega})$, i.e. a twice differentiable function with continuity which is continuous up to the boundary as well, that satisfies the PDE and the boundary conditions. The function g giving the boundary conditions is not continuous at $(0,0)$ nor at (L,L) unless $\phi_{\mathrm{low}} = \phi_{\mathrm{high}}$. Therefore problem (1.4) cannot have a classical solution. Nonetheless it might have a solution in the weak sense.

Before studying the theorem that deals with the existence of a weak

Definition 1.4. contenidos...

1.2.4 Expected nature of the solution

1.3 Numerical solution

In this section we present the numerical solution of problem (1.4) for several Péclet numbers. The width and height of the domain are $L = 1$ m and the velocity of the flow is $u = 1$ m/s. The density is kept constant at $\rho = 1000$ kg/m^3, therefore Péclet's number is varied by chaging the diffusion coefficient Γ. The boundary conditions are $\phi_{\text{low}} = 0$ and $\phi_{\text{high}} = 1$. A uniform mesh of $N = 200$ nodes has been used to discretize the domain, with a tolerance of 10^{-12} as a stop criterion for the Gauss–Seidel algorithm. The Upwind–Difference Scheme (UDS) has been chosen to compute the convective properties.

Figure 1.3 shows the solution to the diagonal case problem for $\text{Pe} = 1$. Transport and diffusion have a similar strength as can be seen in the central zone of the domain Ω. There is clearly a transport phenomena carrying the fluid from the lower left corner to the upper right corner of Ω, but there is also mixing due to the diffusion process. Note that the solution is not continuous at the lower left and upper right corners because of the sudden jump from ϕ_{low} to ϕ_{high}. The zone around the upper left corner does not seem affected by the diffusion process as it is far from the boundary where $\phi = \phi_{\text{low}}$. The same applies to the zone close to the lower right corner.

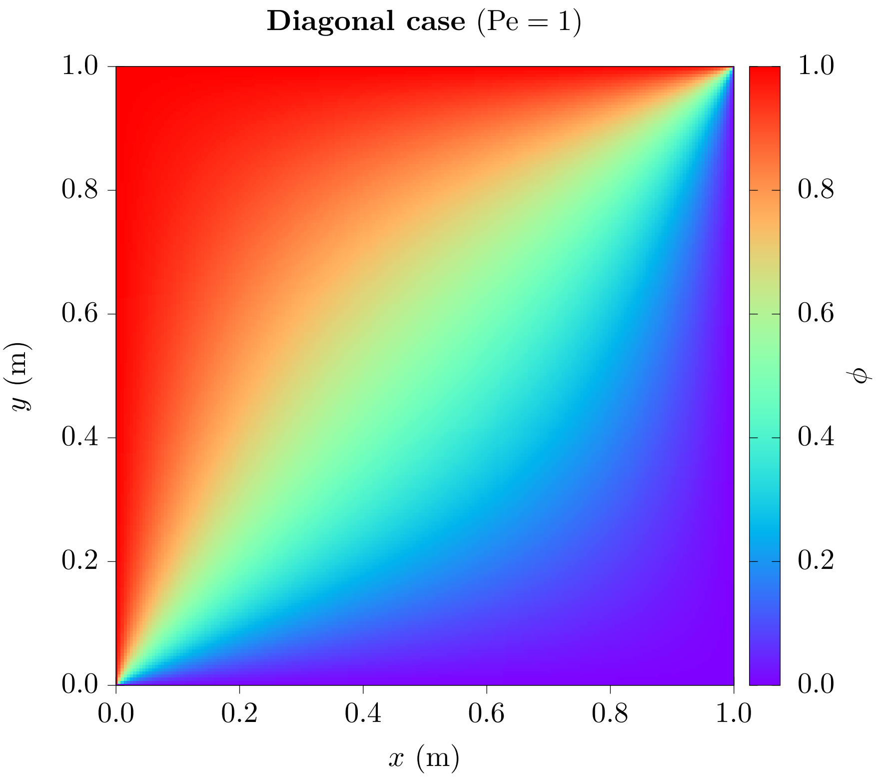
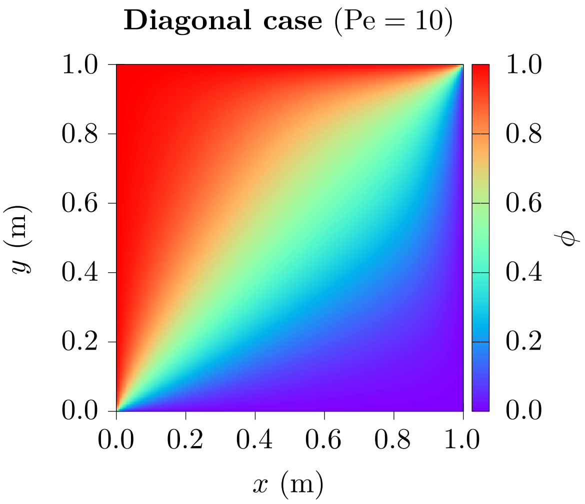
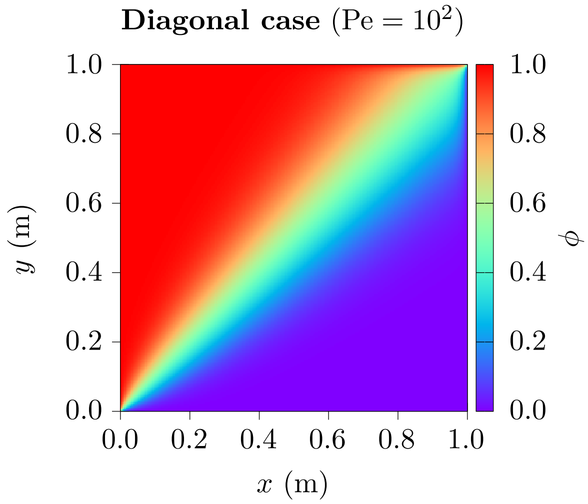


Figure 1.3. Numerical solution to the diagonal case for $\text{Pe} = 1$.

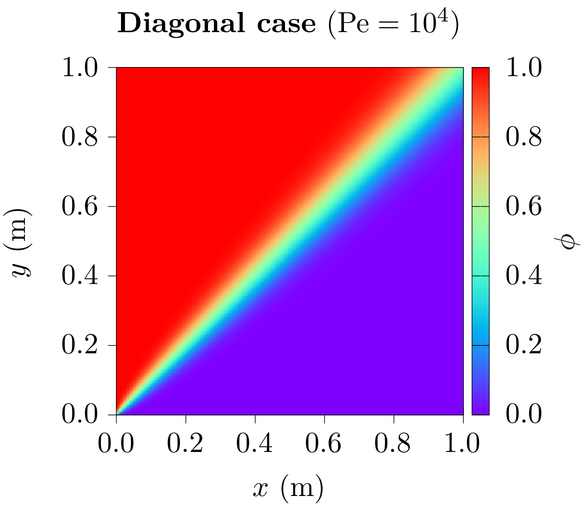
Figures (1.4a) to (1.4c) show the diagonal case solution for $\mathrm{Pe} = 10,\ 10^2,\ 10^4$ and 10^9. The solution for $\mathrm{Pe} = 10$ (figure 1.4a) has a similar appearance to the solution for $\mathrm{Pe} = 1$ (figure 1.3). As Péclet's number grows, the transport process takes over the diffusion process. Therefore the diffusion zone, which is centered in the diagonal along the fluid flow, tends to shrink. This change in the behaviour of the solution can be observed by comparing the cases for $\mathrm{Pe} = 10$ (figure 1.4a) and $\mathrm{Pe} = 10^2$ (figure 1.4b). For $\mathrm{Pe} = 10^4$ the diffusion zone becomes even narrower. Beyond $\mathrm{Pe} = 10^4$ there are no obvious changes in the solution, as can be checked by looking at the case for $\mathrm{Pe} = 10^9$ (figure 1.4d).



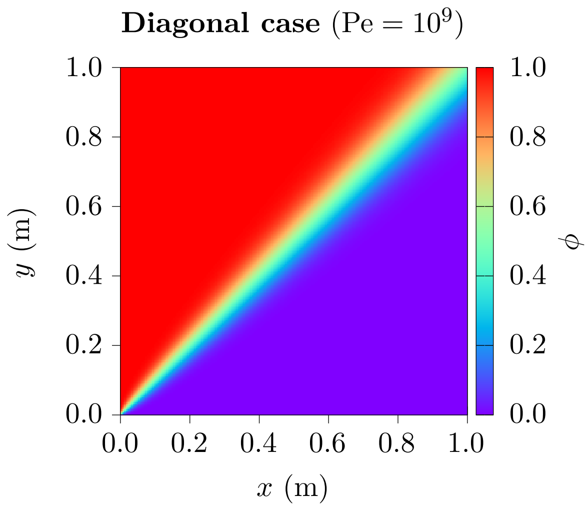
(a) Numerical solution to the diagonal case for $\mathrm{Pe} = 10$.



(b) Numerical solution to the diagonal case for $\mathrm{Pe} = 10^2$.



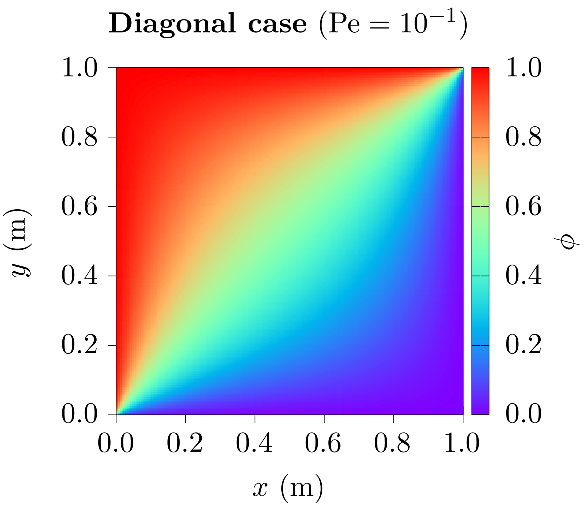
(c) Numerical solution to the diagonal case for $\mathrm{Pe} = 10^3$.



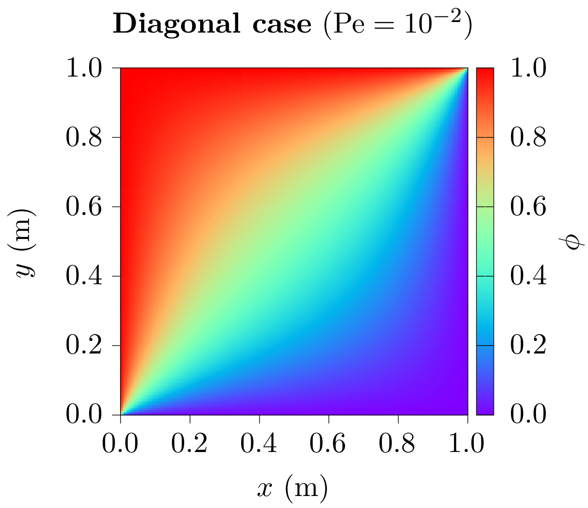
(d) Numerical solution to the diagonal case for $\mathrm{Pe} = 1^{9}0$.

Figure 1.4. Numerical solution to the diagonal case for $\mathrm{Pe} = 10,\ 10^2, 10^4$ and 10^9.

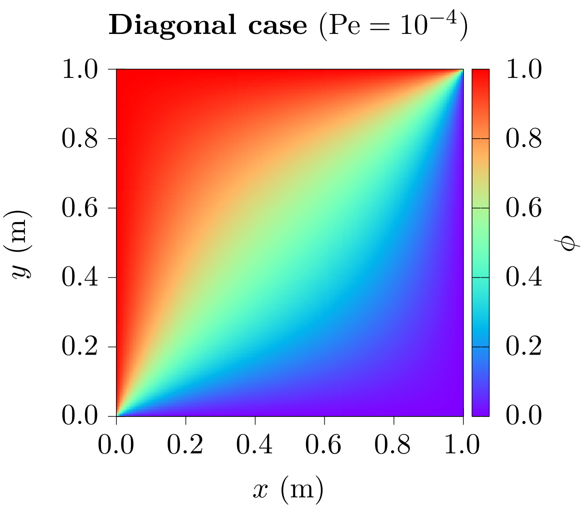
Figures 1.5a to 1.5d show the diagonal case solution to $\mathrm{Pe} = 10^{-1}$, 10^{-2}, 10^{-4} and 10^{-9}. As it can be observed, all the solutions have a similar appearance to that for $\mathrm{Pe} = 1$ (figure 1.3), whence it can be deduced that reducing Péclet's number has not obvious effect.



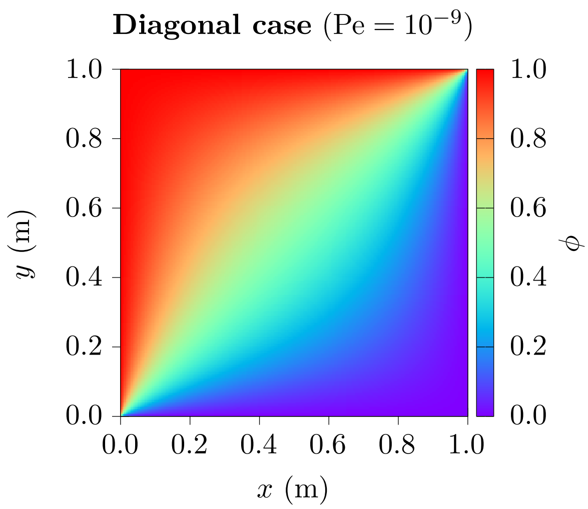
(a) Numerical solution to the diagonal case for $\mathrm{Pe} = 10^{-1}$.



(b) Numerical solution to the diagonal case for $\mathrm{Pe} = 10^{-2}$.



(c) Numerical solution to the diagonal case for $\mathrm{Pe} = 10^{-4}$.



(d) Numerical solution to the diagonal case for $\mathrm{Pe} = 10^{-9}$.

Figure 1.5. Numerical solution to the diagonal case for $\mathrm{Pe} = 10^{-1}$, 10^{-2}, 10^{-4} and 10^{-9}.

2 Smith–Hutton case

2.1 Statement

This section deals with the steady state version of the problem proposed by Smith and Hutton (1982) described in [1]. The problem takes place in the domain $\Omega = (-L, L) \times (0, L) \subset \mathbb{R}^2$ where $L > 0$ is a constant length. Both density and diffusion coefficient are assumed to be constant and known values. In Ω the steady state version of the general convection–diffusion equation with no source term is considered, that is,

$$\frac{\rho}{\Gamma}\mathbf{v} \cdot \boldsymbol{\nabla}\phi = \Delta\phi \tag{2.1}$$

On the boundary of Ω the following conditions are prescribed:

- $\phi = 1 + \tanh(10(2x + 1))$ on $C_1 = [-L, 0] \times \{0\}$ (inlet flow).
- $\phi = 1 - \tanh(10)$ on $C_2 = (\{-L\} \times (0, L)) \cup ([-L, L] \times \{L\}) \cup (\{L\} \times [0, L))$.
- $\dfrac{\partial\phi}{\partial y} = 0$ on $C_3 = (0, L) \times \{0\}$ (outlet flow).

Notice that the curves C_1, C_2, C_3 give a partition of $\partial\Omega$. To encode the first two boundary conditions in a compact manner, we define the function $g\colon C_1 \cup C_2 \to \mathbb{R}$ by

$$g(x, y) = \begin{cases} 1 + \tanh(10(2x + 1)) & \text{if } (x, y) \in C_1 \\ 1 - \tanh(10) & \text{if } (x, y) \in C_2 \end{cases} \tag{2.2}$$

The velocity field is given by $u = 2y(1 - x^2)$ and $v = -2x(1 - y^2)$. The Cauchy problem resulting from the PDE (2.1) and the boundary conditions is given by (2.3) and is summarized in figure 2.1.

$$\begin{cases} \Delta\phi - \dfrac{\rho}{\Gamma}\mathbf{v} \cdot \boldsymbol{\nabla}\phi = 0 & \text{in } \Omega \\ \phi = g & \text{on } C_1 \cup C_2 \\ \dfrac{\partial\phi}{\partial y} = 0 & \text{on } C_3 \end{cases} \tag{2.3}$$

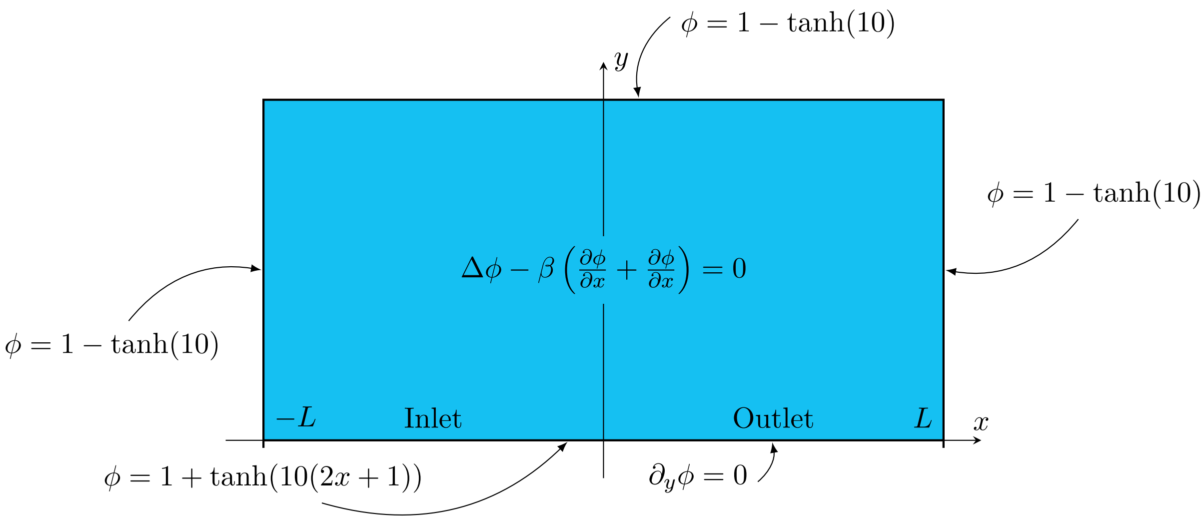


Figure 2.1. Cauchy problem for the diagonal flow case.

2.2 Velocity field

The velocity field for the Smith-Hutton case, given by $\mathbf{v} = 2y(1-x^2)\mathbf{i} - 2x(1-y^2)\mathbf{j}$ and verifies the incompressibility condition since $\boldsymbol{\nabla} \cdot \mathbf{v} = 0$.

The only points where $\mathbf{v}$ vanishes are $(0,0)$, $(-1,1)$, $(1,1)$, $(-1,-1)$ and $(1,-1)$. If $L < 1$, then only $(0,0)$ belongs to $\overline{\Omega}$. If $L > 1$, the first three points belong to $\overline{\Omega}$.

Henceforth we will assume $L = 1$. The stream function associated to $\mathbf{v}$ is $\psi(x,y) = -(1-x^2)(1-y^2)$. Recall that the streamlines are defined to be the curves $C \subset \Omega$ tangent to the vector field $\mathbf{v}$ at each point. Let $h\colon I \subset \mathbb{R} \to \Omega$, $t \mapsto h(t) = (x(t), y(t))$ be the parametrization of a streamline. Then it satisfies the following system of ODEs:

$$\begin{cases} \dot{x}(t) = 2y(1-x^2) \\ \dot{y}(t) = -2x(1-y^2) \end{cases} \tag{2.4}$$

Since at each point in Ω there is a unique velocity vector, each point is contained in a single streamline. In order to find the streamlines, we can specify an initial condition $(x_0, y_0) \in \Omega$ and then pose an initial value problem with the system (2.4). The streamlines must fill Ω since $\mathbf{v}$ is defined everywhere, hence $(x_0, y_0) \in \Omega$ is arbitrary. However, we may become less formal and take $x_0 \in (-L, 0)$ and $y_0 = 0$. With this in mind, the resulting initial value problem for the streamlines is the following:

$$\begin{cases} \dot{x}(t) = 2y(1-x^2) & x(0) = x_0 \\ \dot{y}(t) = -2x(1-y^2) & y(0) = 0 \end{cases} \tag{2.5}$$

Finding a solution to (2.5) might be difficult as the system is non–linear. Nonetheless, even more important than finding an explicit formula that solves the initial value problem is proving the existence and uniqueness of solution. To do so, we define the following vector field:

$$f\colon \Omega \subset \mathbb{R}^2 \longrightarrow \mathbb{R}^2 \tag{2.6}$$

$$(x,y) \longmapsto f(x,y) = \begin{pmatrix} 2y(1-x^2) \\ -2x(1-y^2) \end{pmatrix} \tag{2.7}$$

Then the problem (2.5) is rewritten as:

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = f(x,y) \qquad \begin{pmatrix} x(0) \\ y(0) \end{pmatrix} = \begin{pmatrix} x_0 \\ 0 \end{pmatrix} \tag{2.8}$$

The ODE (2.8) is autonomous since f does not depend upon time. Let $U \subset \mathbb{R}^2$ be an open bounded convex subset containing $\Omega \cup ([-L, L] \times \{0\})$ (for instance, the ball $B(\mathbf{0}, 3)$). The vector field f is actually defined on all $\mathbb{R}^2$ and is a $\mathcal{C}^\infty(\mathbb{R}^2, \mathbb{R}^2)$ map and, in particular, is a $\mathcal{C}^1(\overline{U}, \mathbb{R}^2)$ map. By theorem B.4, f is Lipschitz on $\overline{U}$. By the Picard–Lindelöf theorem (Theorem B.5), the solution of (2.5) exists and is unique.

Once we have proven that a solution to (2.5) exists and is unique, we aim to find the solution for several $x_0 \in (-L, 0)$. As we have previously mentioned, we cannot expect to find an analytical solution since the ODE is non–linear. Nevertheless we may apply a numerical method, such as the Runge–Kutta 4 algorithm to sort out the problem. This is precisely what has been done to produce figure 2.2. In it, the norm of the vector field $\mathbf{v}$ is shown, along with the streamlines for several x_0 values.

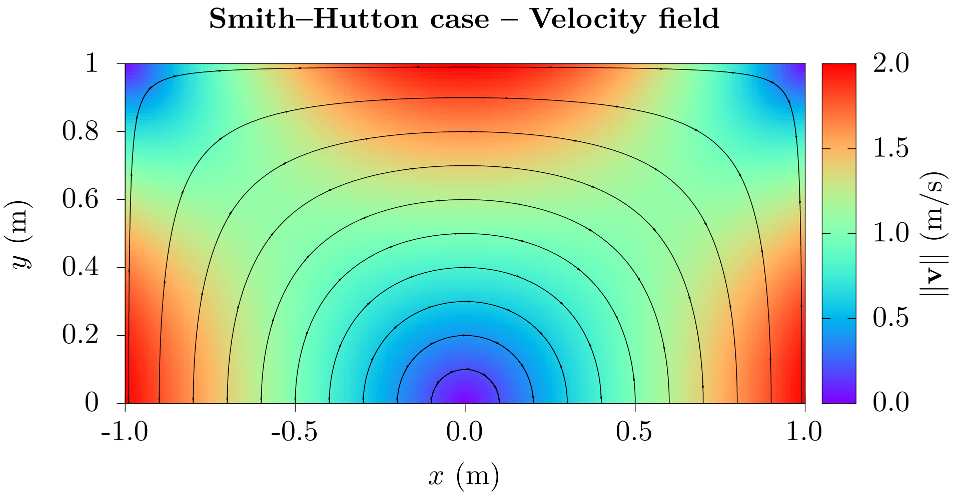


Figure 2.2. Norm of the Smith–Hutton velocity field and streamlines for x_0 = 0.10, 0.20, 0.30, 0.40, 0.50, 0.60, 0.70, 0.80, 0.90 and 0.99 m. The vectors tangent to the streamlines are normalized and then scaled down by a factor of $\sqrt{2}/50$.

2.3 Analytical solution

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

2.3.2 General problem

2.4 Numerical solution

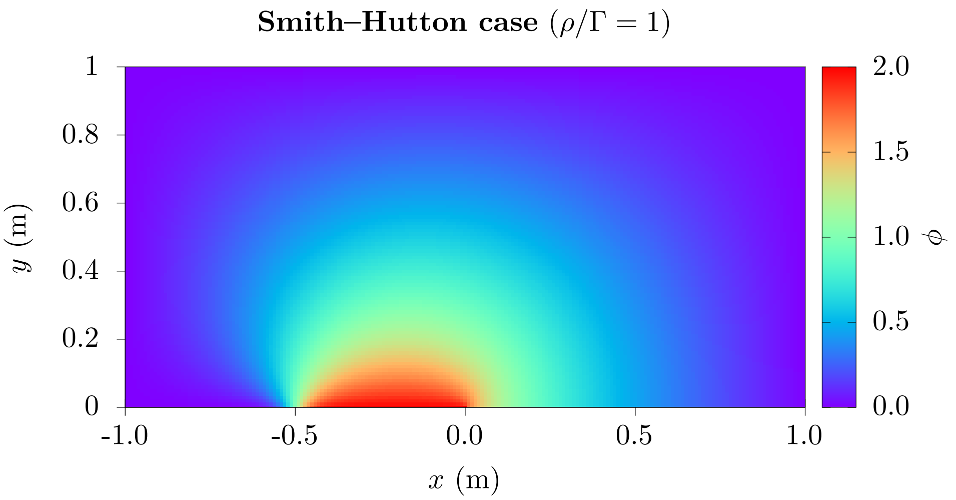


Figure 2.3

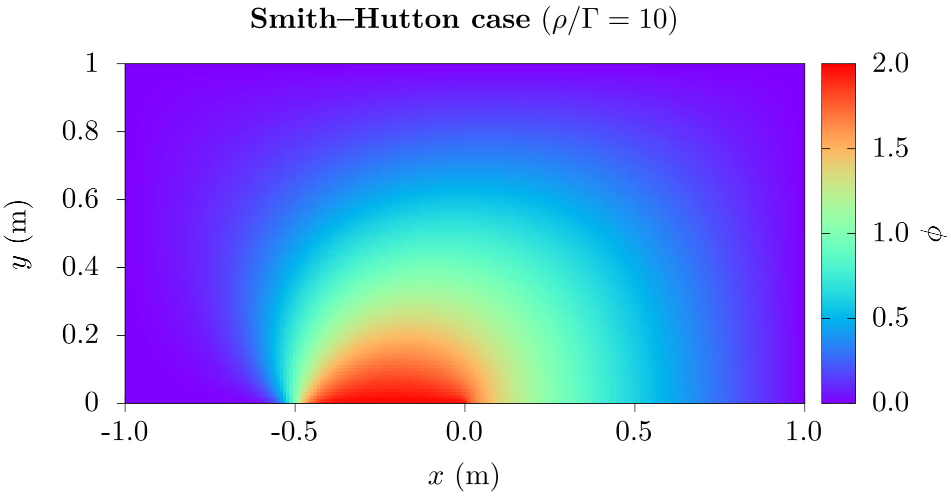


Figure 2.4

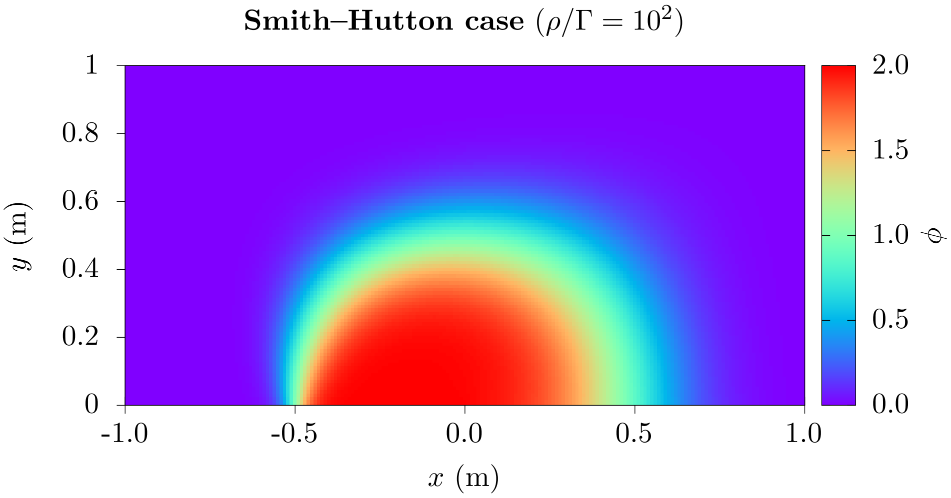


Figure 2.5

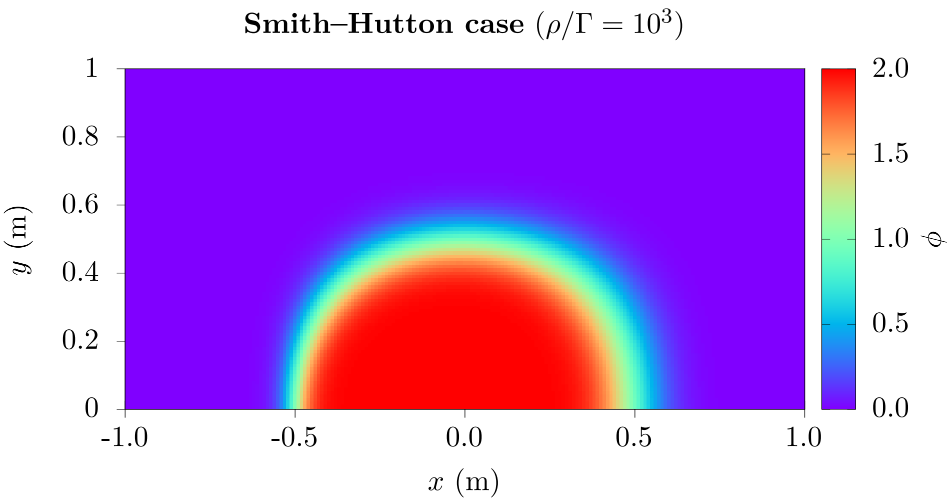


Figure 2.6

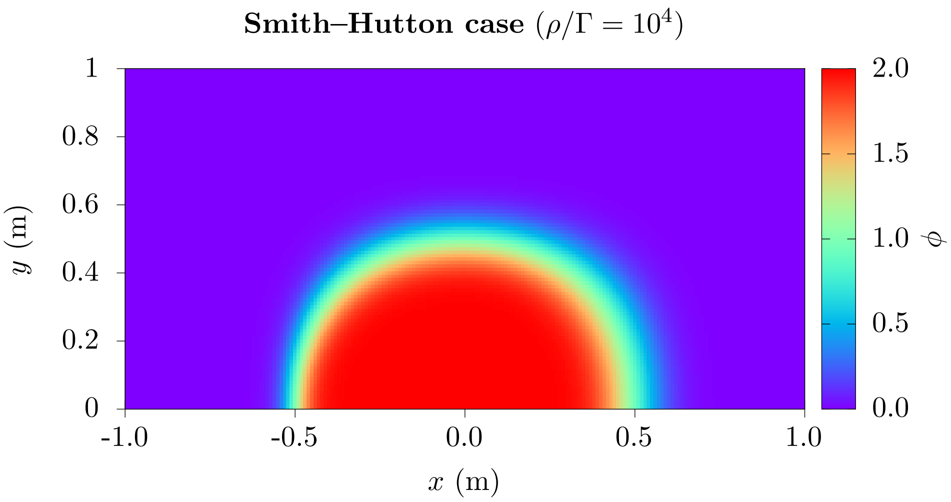


Figure 2.7

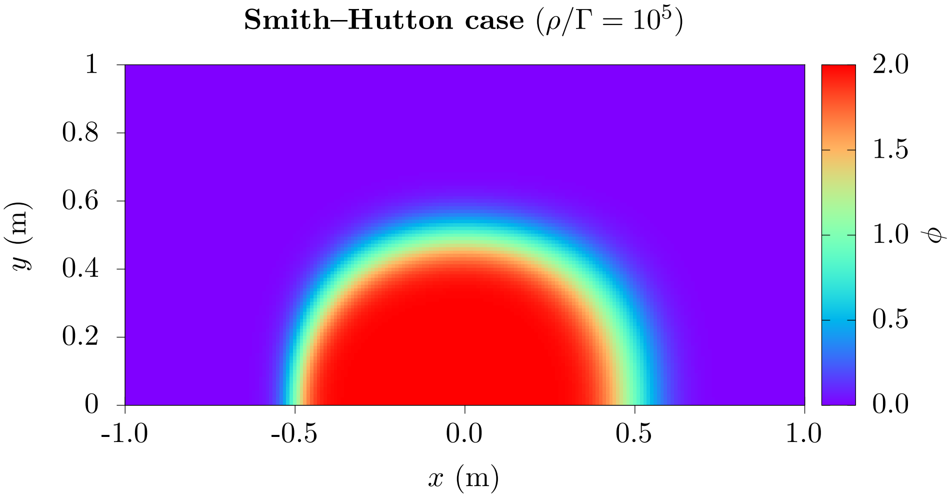


Figure 2.8

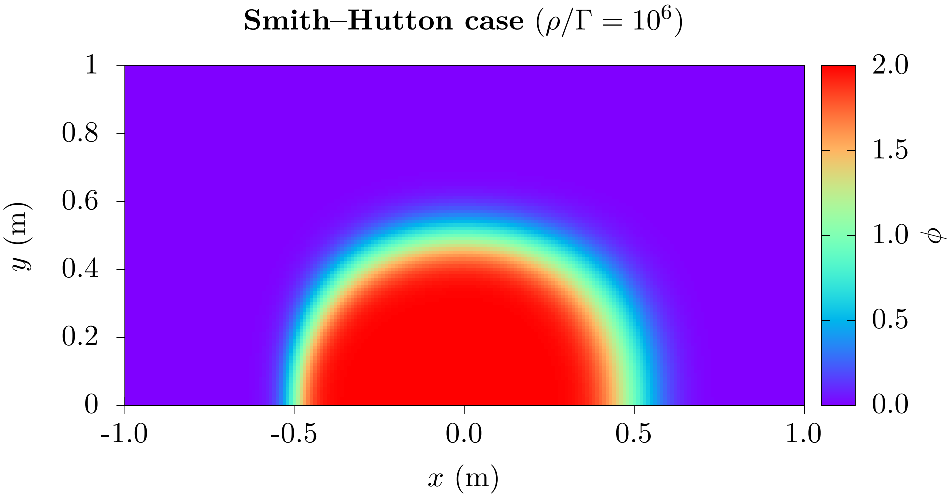


Figure 2.9

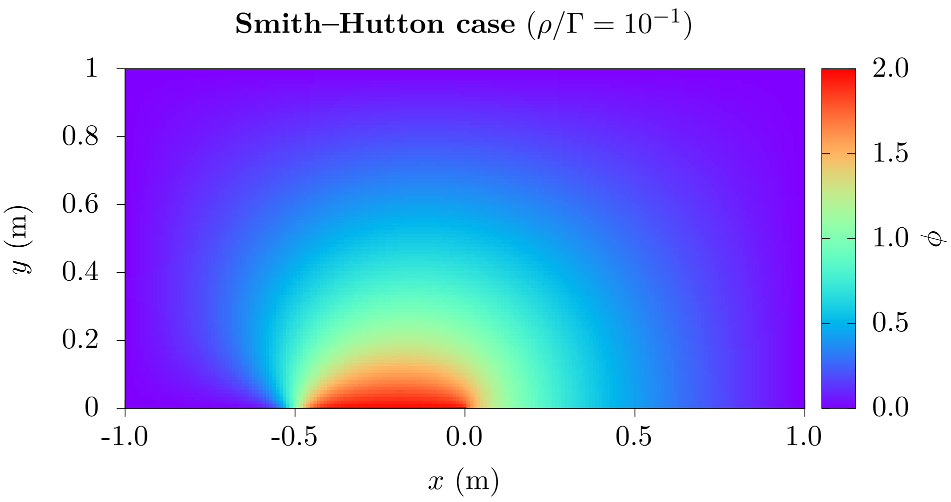


Figure 2.10

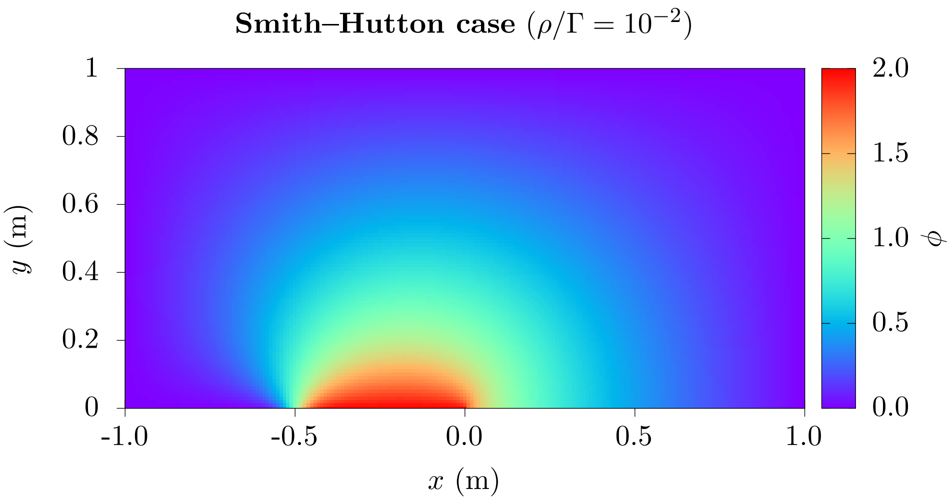


Figure 2.11

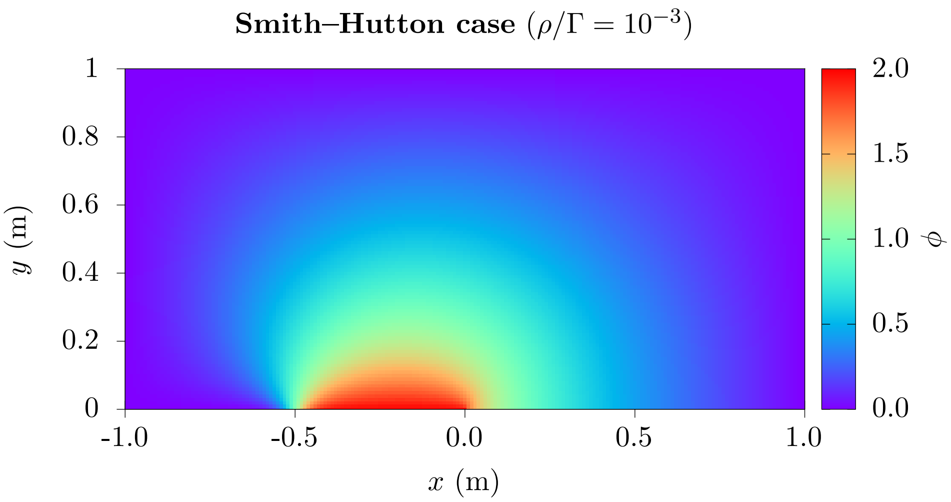


Figure 2.12

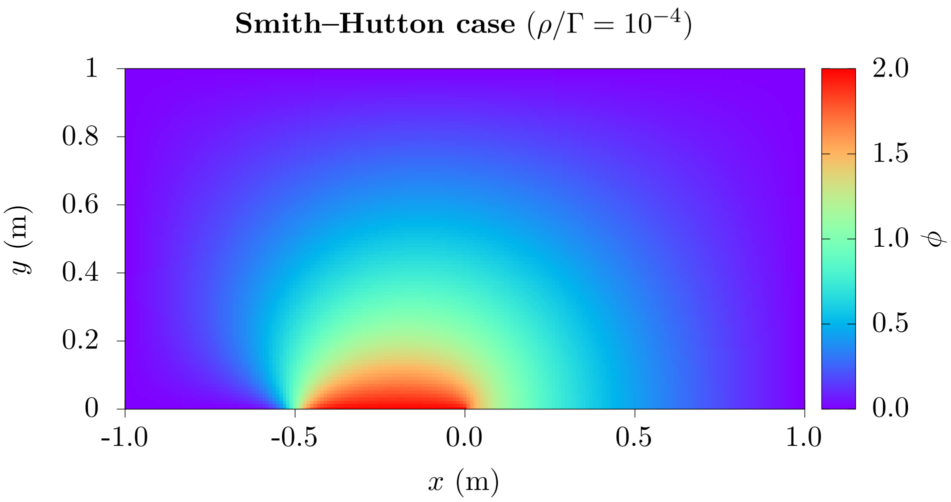


Figure 2.13

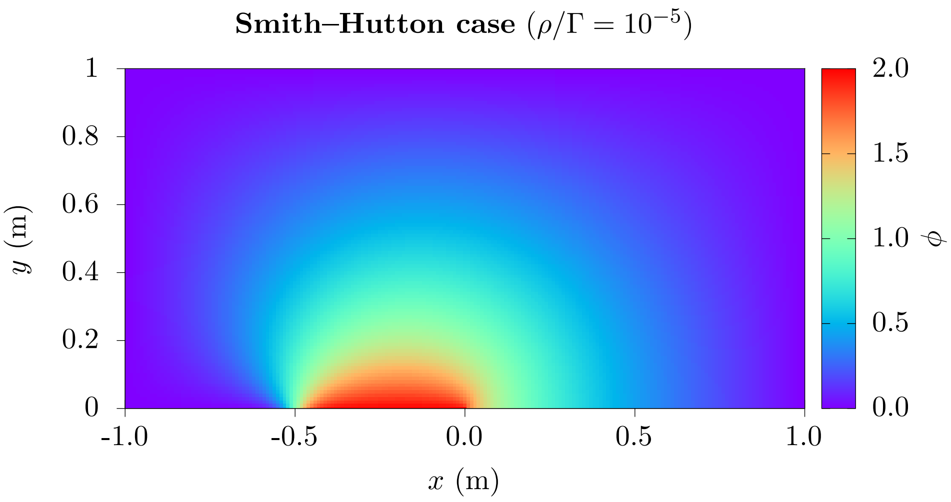


Figure 2.14

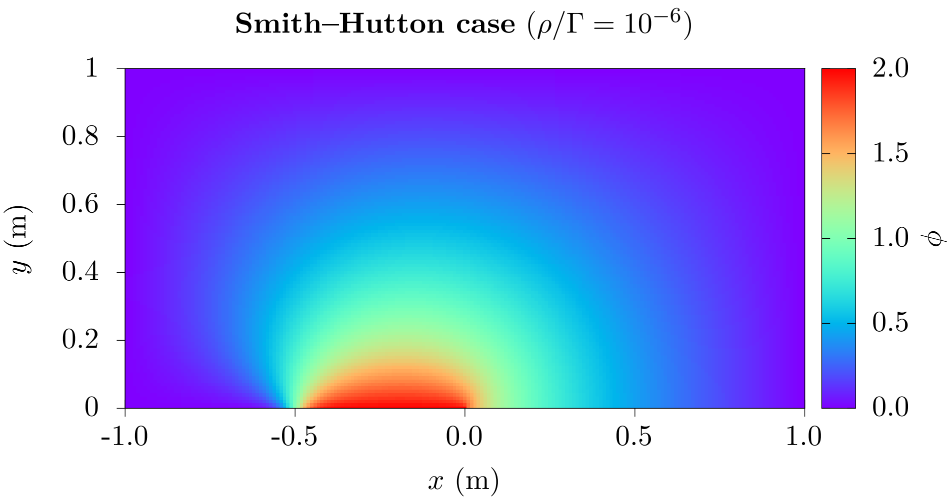


Figure 2.15

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[2] Walter Rudin. *Real and Complex Analysis*. 3rd ed. McGraw–Hill, 1987.

[3] Lawrence C. Evans. *Partial Differential Equations*. 1st ed. Vol. 19. American Mathematical Society, 1998. Chap. E, p. 649.

[4] Sandro Salsa. *Partial Differential Equations in Action*. 1st ed. Springer, 2009. Chap. 1, pp. 1–12.

[5] Gerald Teschl. *Ordinary Differential Equations and Dynamical Systems*. PUV, 2008. Chap. 3, pp. 59–99.

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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 [2].

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 $\left|\dfrac{\partial f}{\partial t}(\mathbf{x}, t)\right| \le g(\mathbf{x})$ 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 $1 \le m \le 3$, $\mathcal{A}$ 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 [3]). 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 Ordinary Differential Equations

In this section we present the Picard–Lindelöf theorem which aids on proving the existence and uniqueness of solution to initial value problems involving ordinary differential equations (ODEs) initial value problems. We begin with the definition of a Lipschitz function:

Definition B.1. A function $f\colon \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$ is said to be Lipschitz or Lipschitz continuous if there exists a constant L such that

$$\|f(\mathbf{x}) - f(\mathbf{y})\| \leq L\|\mathbf{x} - \mathbf{y}\| \tag{B.1}$$

for every $\mathbf{x}, \mathbf{y} \in \Omega$. The constant L is called the Lipschitz constant of f [4].

It can be easily proven that every Lipschitz function on Ω is also a continuous function in the usual sense on Ω. The converse is not true in general, and depends on the properties of Ω. The Lipschitz continuity is actually a very restrictive condition, since it imposes that the function can grow at most as a linear function.

Definition B.2. Let $(E, \|\cdot\|_E)$ and $(F, \|\cdot\|_F)$ be two finite dimensional normed vector spaces and let $A\colon E \to F$ be a linear mapping between them. The norm of A is defined to be

$$\|A\| \coloneqq \sup \left\{ \|Ax\|_F \mid x \in E,\ \|x\|_E \leq 1 \right\} \tag{B.2}$$

It is a well known fact that $\|A\|$ is finite. In some cases, proving that a function is Lipschitz continuous is a laborious task. In these situations we have the following theorems:

Theorem B.3 (Corollary of the mean value theorem [5]). Let $\Omega \subset \mathbb{R}^n$ an open set and let $f\colon \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$ a differentiable function on Ω. Let $\mathbf{x}, \mathbf{y} \in \Omega$ such that the segment $\overline{\mathbf{xy}} = \{\lambda\mathbf{x} + (1-\lambda)\mathbf{y} \mid \lambda \in [0,1]\}$ is contained in Ω. Then the following inequality holds:

$$\|f(\mathbf{x}) - f(\mathbf{y})\| \leq \sup_{\mathbf{z} \in \overline{\mathbf{xy}}} \|Df(\mathbf{z})\| \|\mathbf{x} - \mathbf{y}\| \tag{B.3}$$

Proof. See [5], page 78. □

Theorem B.4. Let $\Omega \subset \mathbb{R}^n$ a compact convex set and let $f \equiv (f_1, \ldots, f_m)\colon \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$ a $\mathcal{C}^1(\Omega)$ function. Then f is Lipschitz in Ω.

Proof. The differential of Df, given by

$$Df = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{pmatrix} \tag{B.4}$$

is a linear mapping $Df \colon \mathbb{R}^n \to \mathbb{R}^m$. Since f is $\mathcal{C}^1(\Omega)$ function, the partial derivatives $\frac{\partial f_1}{\partial x_1}, \ldots, \frac{\partial f_m}{\partial x_n}$ are continuous functions on Ω. Moreover, the norm of the differential depends continuously on the partial derivatives $\frac{\partial f_1}{\partial x_1}, \ldots, \frac{\partial f_m}{\partial x_n}$ and on $\mathbf{z}$. As a consequence, $\|Df\|$ is a continuous function on Ω. By Weierstrass theorem, $\|Df\|$ reaches a maximum M on Ω. Applying theorem B.3 we have

$$\|f(\mathbf{x}) - f(\mathbf{y})\| \leq \sup_{\mathbf{z} \in \overline{\mathbf{xy}}} \|Df(\mathbf{z})\| \|\mathbf{x} - \mathbf{y}\| \leq M \|\mathbf{x} - \mathbf{y}\| \tag{B.5}$$

for all $\mathbf{x}, \mathbf{y} \in \Omega$, hence f is Lipschitz on $\overline{\Omega}$. □

Finally we can state the Picard–Lindelöf theorem. Let U be an open subset of $\mathbb{R}^{n+1}$ and let $f \in C(U, \mathbb{R})$, $(t_0, \mathbf{x_0}) \in U$. Consider the following IVP:

$$\begin{cases} \dot{\mathbf{x}}(t) = f(t, \mathbf{x}) \\ \mathbf{x}(t_0) = \mathbf{x_0} \end{cases} \tag{B.6}$$

The Picard–Lindelöf theorem gives us the existence and uniqueness of solution for (B.6).

Theorem B.5 (Picard–Lindelöf [6])**.** Suppose $f \in \mathcal{C}(U, \mathbb{R}^n)$, where U is an open subset of $\mathbb{R}^{n+1}$, and $(t_0, \mathbf{x_0}) \in U$. If f is locally Lipschitz continuous in the second argument, uniformly with respect to the first, then there exists a unique local solution $vbx(t) \in \mathcal{C}^1(I)$ of the initial value problem (B.6), where I is some interval around t_0.

More specifically, if $V = [t_0, t_0 + T] \times \overline{B(\mathbf{x_0}, \delta)} \subset U$ and M denotes the maximum of $|f|$ on V, then the solution exists at least for $t \in [t_0, t_0 + T_0]$ and remains in $\overline{B(\mathbf{x_0}, \delta)}$ where $T_0 = \min \left\{ T, \frac{\delta}{M} \right\}$. The analogous result holds for the interval $[t_0 - T, t_0]$.

Proof. See [6], page 38. □

C Numerical resolution of linear systems

C.1 Gauss–Seidel algorithm

C.2 LU factorization