Gas dynamics and Heat and Mass Transfer

Numerical Solution of the Convection–Diffusion Equations

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Contents

1 Convection–diffusion equations

In this section we derive the continuity equation and the general convection–diffusion equation. To begin, we present and prove Reynolds Transport Theorem, which is a generalization of Leibniz integral rule. Next we deduce the aforementioned equations using this theorem.

1.1 Notation and assumption

First of all, we shall introduce some notation that will be exhaustively used in the project.

- Let Ω be a subset of $\mathbb{R}^n$. The subsets $\partial\Omega$ and $\overline{\Omega}$ of $\mathbb{R}^n$ will denote the boundary and the closure of Ω, respectively.
- Let $x \in \mathbb{R}^n$ and $R > 0$. We will denote by $B(x,R) = \{y \in \mathbb{R}^n \mid \|x-y\| < R\}$ the open ball centered at x of radius R. The set $\overline{B(x,R)} = \{y \in \mathbb{R}^n \mid \|x-y\| \leq R\}$ is the closure $B(x,R)$.
- Let $U \subset \mathbb{R}^n$ be an open set. We will denote by $\mathcal{C}^k(U,\mathbb{R}^m)$ the set of k times continously differentiable functions $f\colon U \to \mathbb{R}^m$. If the codomain is clear from the context, we will use $\mathcal{C}^k(U)$. The set of continuous functions $f\colon U \to \mathbb{R}^m$ will be denoted $\mathcal{C}(U,\mathbb{R}^m)$ or $\mathcal{C}(U)$ when the codomain is clear.
- The velocity of a fluid will be the vector field $\mathbf{v} = \mathbf{v}(x,t)$. When working in $\mathbb{R}^2$ it will be written as $\mathbf{v} = u\mathbf{i} + v\mathbf{j}$.

Hereinafter, if $\mathcal{V} \subset \mathbb{R}^n$ is a control volume, we will assume it satisfies the following:

(i) $\mathcal{V}$ is an open set of $\mathbb{R}^n$, i.e. for all $x \in \mathcal{V}$ there exists $R > 0$ such that $B(x,R) \subset \mathcal{V}$.

(ii) $\mathcal{V}$ is bounded, that is to say, there exist $x_0 \in \mathbb{R}^n$ and $R > 0$ such that $\mathcal{V} \subset B(x_0,R)$.

(iii) $\mathcal{V}$ is a $\mathcal{C}^1$–domain. This implies that for every point $x \in \partial\mathcal{V}$ there exists a system of coordinates $(y_1,\ldots,y_{n-1},y_n) \equiv (\mathbf{y}',y_n)$ with origin at x, a ball $B(x,R)$ and a function φ defined in an open subset $\mathcal{N} \subset \mathbb{R}^{n-1}$ containing $\mathbf{y}' = \mathbf{0}'$, such that [1]:
   (a) $\varphi(\mathbf{0}') = 0$ and $\varphi \in \mathcal{C}^1(\mathcal{N},\mathbb{R})$ (φ is a $\mathcal{C}^1$ function from $\mathcal{N}$ to $\mathbb{R}$),
   (b) $\partial\mathcal{V} \cap B(x,R) = \{(\mathbf{y}',y_n) \mid y_n = \varphi(\mathbf{y}'),\ \mathbf{y}' \in \mathcal{N}\}$,
   (c) $\mathcal{V} \cap B(x,R) = \{(\mathbf{y}',y_n) \mid y_n > \varphi(\mathbf{y}'),\ \mathbf{y}' \in \mathcal{N}\}$.

Condition (i) will be useful to cast an integral equation into a differential equation. Condition (ii) prevents the integral of a continuous function defined on $\overline{\mathcal{V}}$ from becoming infinite. Moreover, an unbounded control volume, that is to say, a subset of $\mathbb{R}^n$ that extends indefinitely, makes no physical sense. Condition (iii), which is more technical, will allow us to apply vector calculus theorems.

Finally, we shall assume that all physical magnitudes, such as the velocity field $\mathbf{v}$, the density ρ or the temperature T are differentiable functions on their domains of definition as many times as necessary.

1.2 Reynolds Transport Theorem

Before stating and proving Reynolds Transport Theorem, we tackle the simpler Leibniz integral rule. To gain some physical intuition on it, suppose we have a very thin tube along the x–axis containing a fluid in motion. In this context we may assume that the fluid only moves along the tube direction. Let $f = f(x,t)$ be a magnitude of the fluid, for instance, the velocity u, the temperature T or the

concentration of some chemical species Y. So as to study how this magnitude variates on a portion of fluid, we consider a control volume $U(t) = [a(t), b(t)]$ that depends upon time. This situation is picture in figure 1.1. The total ammount of magnitude f in the control volume at time t, which we will denote by $\mathcal{F}(t)$, is given by

$$\mathcal{F}(t) = \int_{a(t)}^{b(t)} f(x,t)\,\mathrm{d}x \tag{1.1}$$

and its rate of variation

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(t) = \frac{\mathrm{d}}{\mathrm{d}t}\int_{a(t)}^{b(t)} f(x,t)\,\mathrm{d}x \tag{1.2}$$

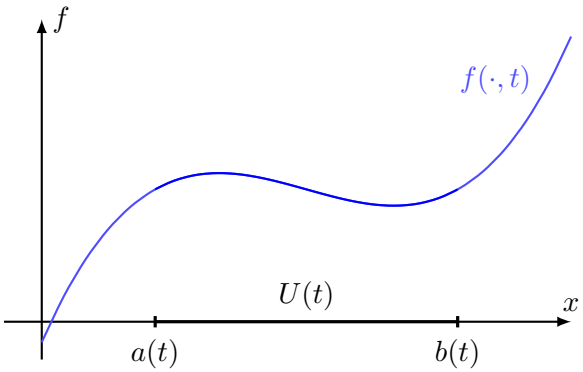

Figure 1.1. Control volume and magnitude f at time t.

Computing the derivative in equation (1.2) can be difficult depending on the case. Here is where Leibniz integral rule comes into play:

Theorem 1.1 (Leibniz integral rule)**.** Let $U \subset \mathbb{R}$ be a closed bounded interval and let $I = [t_1, t_2]$ be the time interval. Let $a, b\colon I \to U$ be differentiable functions with continuous derivative. Let $f\colon U \times I \to \mathbb{R}$, $(x,t) \mapsto f(x,t)$ be a differentiable function such that $\frac{\partial f}{\partial t}$ is also continuous. Then for all $t \in (t_1, t_2)$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{a(t)}^{b(t)} f(x,t)\,\mathrm{d}x = \int_{a(t)}^{b(t)} \frac{\partial f}{\partial t}\,\mathrm{d}x + f(b(t),t)b'(t) - f(a(t),t)a'(t) \tag{1.3}$$

Proof. See [2]. □

Consider the more general case where we have a fluid in n–dimensional space $\mathbb{R}^n$ and magnitude $f = f(x,t)$ defined on a control volume $\mathcal{V}(t) \subset \mathbb{R}^n$. The total ammount of f on $\mathcal{V}$ at time t and its variation are given by similar formulas,

$$\mathcal{F}(t) = \int_{\mathcal{V}(t)} f(x,t)\,\mathrm{d}x\,, \quad \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(t) = \frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}(t)} f(x,t)\,\mathrm{d}x \tag{1.4}$$

however now computing the derivative might be impracticable. In this case we have Reynolds Transport Theorem:

Theorem 1.2 (Reynolds Transport Theorem [3])**.** Let $U \subset \mathbb{R}^n$ be a compact set (i.e. U is closed and bounded) and let $\mathcal{V}(t)$ be a control volume depending on time such that $\mathcal{V} \subset U$ for all $t \in I = [0, T]$ with $T > 0$. Let $\mathcal{S}(t) = \partial\mathcal{V}(t)$ be the boundary of $\mathcal{V}(t)$ and let $F \in \mathcal{C}^1(U \times I, \mathbb{R})$ be a scalar field.

Then for all $t \in I$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}(t)} F(x,t)\,\mathrm{d}x = \int_{\mathcal{V}(t)} \frac{\partial F}{\partial t}(x,t)\,\mathrm{d}x + \int_{\mathcal{S}(t)} F(x,t)\mathbf{b}\cdot\mathbf{n}\,\mathrm{d}S \tag{1.5}$$

where $\mathbf{b}\colon \mathcal{S}(t) \to \mathbb{R}^n$ is the local velocity of the control surface.

Proof. The moving control volume $\mathcal{V}(t)$ can be seen as the image of an initial region $\mathcal{V}(0)$ by a family of $\mathcal{C}^1$ maps $\xi\colon U \times I \subset \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$, that is to say, $\mathcal{V}(t) = \xi(\mathcal{V}(0), t)$ for all $t \in I$. Furthermore, by fixing one time t, the mapping $\xi(\cdot, t)\colon \mathcal{V}(0) \to \mathcal{V}(t)$ can be assumed to be a diffeomorphism. Since F is continuous, we can apply the Change of Variables Theorem taking $x = \xi(x_0, t)$,

$$\int_{\mathcal{V}(t)} F(x,t)\,\mathrm{d}x = \int_{\mathcal{V}(0)} F(\xi(x_0,t),t)\left|\det\left(\frac{\partial \xi}{\partial x_0}(x_0,t)\right)\right|\mathrm{d}x_0$$

where the determinant of the jacobian matrix $\det\left(\frac{\partial \xi}{\partial x_0}(x_0,t)\right)$ can be assumed to be positive for small enough T, hence the absolute value is dropped. Applying differentiation under the integral sign (Theorem A.1) with respect to t yields

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}(t)} F(x,t)\,\mathrm{d}x &= \int_{\mathcal{V}(0)} \frac{\partial}{\partial t}\left\{F(\xi(x_0,t),t)\ \det\left(\frac{\partial \xi}{\partial x_0}(x_0,t)\right)\right\}\mathrm{d}x_0 \\ &= \int_{\mathcal{V}(0)} \frac{\partial}{\partial t}\left\{F(\xi(x_0,t),t)\right\}\det\left(\frac{\partial \xi}{\partial x_0}(x_0,t)\right)\mathrm{d}x_0 + \int_{\mathcal{V}(0)} F(\xi(x_0,t),t)\,\frac{\partial}{\partial t}\left\{\det\left(\frac{\partial \xi}{\partial x_0}(x_0,t)\right)\right\}\mathrm{d}x_0\end{aligned}$$

On the one hand,

$$\frac{\partial}{\partial t}\left\{F(\xi(x_0,t),t)\right\}\det\left(\frac{\partial \xi}{\partial x_0}(x_0,t)\right) = \left\{\frac{\partial F}{\partial t}(\xi(x_0,t),t) + \boldsymbol{\nabla} F(\xi(x_0,t),t)\cdot\xi_t(x_0,t)\right\}\det\left(\frac{\partial \xi}{\partial x_0}(x_0,t)\right)$$

where $\xi_t = \frac{\partial \xi}{\partial t}$. On the other hand, using matrix calculus,

$$F(\xi(x_0,t),t)\,\frac{\partial}{\partial t}\left\{\det\left(\frac{\partial \xi}{\partial x_0}(x_0,t)\right)\right\} = F(\xi(x_0,t),t)\det\left(\frac{\partial \xi}{\partial x_0}(x_0,t)\right)\boldsymbol{\nabla}\cdot\xi_t(x_0,t)$$

Thereby the integral is written as

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}(t)} F(x,t)\,\mathrm{d}x &= \int_{\mathcal{V}(0)}\left\{\frac{\partial F}{\partial t} + \boldsymbol{\nabla}F\cdot\xi_t + F\boldsymbol{\nabla}\cdot\xi_t\right\}\det\left(\frac{\partial \xi}{\partial x_0}\right)\mathrm{d}x_0 \\ &= \int_{\mathcal{V}(0)}\left\{\frac{\partial F}{\partial t} + \boldsymbol{\nabla}\cdot(F\xi_t)\right\}\det\left(\frac{\partial \xi}{\partial x_0}\right)\mathrm{d}x_0\end{aligned}$$

So as to obtain an integral over $\mathcal{V}(t)$, the previous change of variables is reverted, that is, $x_0 = \xi^{-1}(x,t)$. In order not to complicate notation, let $\mathbf{b}(x,t) = \xi_t(\xi^{-1}(x,t),t)$, then

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}(t)} F(x,t)\,\mathrm{d}x = \int_{\mathcal{V}(t)}\left\{\frac{\partial F}{\partial t} + \boldsymbol{\nabla}\cdot(F\mathbf{b})\right\}(x,t)\,\mathrm{d}x$$

For a fixed $x_0 \in \mathcal{V}(0)$, $\xi(x_0,\cdot)$ is a function of time giving how x_0 moves, hence $\xi_t(x_0,t)$ is the instantaneous velocity of x_0. To end, an application of divergence theorem yields the final formula:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}(t)} F(x,t)\,\mathrm{d}x = \int_{\mathcal{V}(t)} \frac{\partial F}{\partial t}(x,t)\,\mathrm{d}x + \int_{\mathcal{S}(t)} F(x,t)\mathbf{b}\cdot\mathbf{n}\,\mathrm{d}S$$

□

1.3 Continuity equation

For the purposes of this project, where no nuclear nor relativistic effects are considered, mass is a property preserved over time. Let $\mathcal{V} \subset \mathbb{R}^n$ be a control volume, which may depend on time, and let $\rho = \rho(x,t)$ be the mass density defined over $\mathcal{V}$ for each time $t \in I$. The mass enclosed by $\mathcal{V}$ at time t is

$$m(t) = \int_{\mathcal{V}(t)} \rho(x,t)\,\mathrm{d}x = \int_{\mathcal{V}(t)} \rho\,\mathrm{d}x \tag{1.6}$$

and as a result of the mass conservation principle

$$\frac{\mathrm{d}}{\mathrm{d}t} m(t) = \frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathcal{V}(t)} \rho(x,t)\,\mathrm{d}x = 0 \tag{1.7}$$

Now applying Reynolds Transport Theorem to (1.7) setting $\mathbf{b} = \mathbf{v}$,

$$\int_{\mathcal{V}(t)} \frac{\partial \rho}{\partial t}\,\mathrm{d}x + \int_{\mathcal{S}(t)} \rho\mathbf{v}\cdot\mathbf{n}\,\mathrm{d}S = 0 \tag{1.8}$$

We apply the divergence theorem on the surface integral to transform it into a volume integral,

$$\int_{\mathcal{V}(t)} \frac{\partial \rho}{\partial t}\,\mathrm{d}x + \int_{\mathcal{V}(t)} \boldsymbol{\nabla}\cdot(\rho\mathbf{v})\,\mathrm{d}x = \int_{\mathcal{V}(t)} \left\{\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v})\right\}\mathrm{d}x = 0 \tag{1.9}$$

We claim that the integrand in equation (1.9) vanishes at every point in space and time. Indeed, assume there exists a time t_0 and a point $x_0 \in \mathcal{V}(t_0)$ such that

$$\left\{\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v})\right\}\Big|_{(x_0,t_0)} > 0 \tag{1.10}$$

Recall that we assumed the physical magnitudes are differentiable functions as many times as necessary. In particular, by fixing $t = t_0$, $(\partial_t\rho + \boldsymbol{\nabla}\cdot(\rho\mathbf{v}))(\cdot,t_0)$ is a continuous function of x. Since $\mathcal{V}(t_0)$ is open, there exists $\tilde{\delta} > 0$ such that $B(x_0,\tilde{\delta}) \subset \mathcal{V}(t_0)$. By continuity we can take $\delta > 0$, with $\delta < \tilde{\delta}$ such that for all $y \in B(x_0,\delta) \subset \mathcal{V}(t_0)$,

$$\left\{\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v})\right\}\Big|_{(y,t_0)} > 0 \tag{1.11}$$

Hence integrating on $B(x_0,\delta)$ yields

$$\int_{B(x_0,\delta)} \left\{\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v})\right\}\mathrm{d}x > 0 \tag{1.12}$$

a contradiction as it should be zero according to equation (1.9). The same contradiction is reached if we assume the existence of a point x_0 and a time t_0 where

$$\left\{\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v})\right\}\Big|_{(x_0,t_0)} < 0 \tag{1.13}$$

thereby proving our claim. Because this is true for each $x_0 \in \mathcal{V}(t_0)$ and $t_0 \in I$ is arbitrary, we obtain the continuity equation

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v}) = 0 \tag{1.14}$$

1.4 General convection–diffusion equation

Let $\mathcal{V} \subset \mathbb{R}^n$ be a control volume which may depend on time $t \in I \subset \mathbb{R}$ and let $\phi\colon \mathbb{R}^n \times I \to \mathbb{R}$, $(x,t) \mapsto \phi(x,t)$ be a magnitude of the fluid (such as the concentration of some chemical substance) per unit of mass. Then the total ammount of ϕ in $\mathcal{V}(t)$ is

$$\Phi(t) = \int_{\mathcal{V}(t)} \rho(x,t)\phi(x,t)\,\mathrm{d}x \tag{1.15}$$

and its variation over time is

$$\dot{\Phi}(t) = \frac{\mathrm{d}}{\mathrm{d}t}\Phi(t) = \frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}(t)} \rho(x,t)\phi(x,t)\,\mathrm{d}x \tag{1.16}$$

The variation of Φ is a consequence of two contributions: the flux of ϕ through the control surface $\mathcal{S}(t)$ and the generation/elimination of ϕ in $\mathcal{V}(t)$ due to source terms. Let $\mathbf{f}\colon \mathbb{R} \times \mathcal{S} \times I \to \mathbb{R}^n$, $(\phi,x,t) \mapsto \mathbf{f}(\phi,x,t)$ be the vector field which gives the flux of ϕ through $\mathcal{S}$. Then the total ammount of ϕ flowing through $\mathcal{S}(t)$ is given by

$$\mathscr{F}(t) = \int_{\mathcal{S}(t)} \mathbf{f}(\phi,x,t)\cdot\mathbf{n}\,\mathrm{d}S \tag{1.17}$$

In order to find out which sign has $\mathscr{F}(t)$, we may assume for a moment that there are no source terms. If $\mathscr{F}(t) > 0$, then ϕ is exiting $\mathcal{V}(t)$ and, as a result, $\dot{\Phi}(t) < 0$. Conversely, if $\mathscr{F}(t) < 0$, then $\dot{\Phi}(t) > 0$, therefore $\dot{\Phi}(t)$ and $F(t)$ have opposite signs. Now, let $\dot{s}_\phi\colon \to \mathbb{R}$ be te source term, which provides the ammount of ϕ generated/eliminated in $\mathcal{V}(t)$ per unit of time. Then the total ammount of ϕ generated/eliminated in $\mathcal{V}(t)$ is

$$\mathscr{S}(t) = \int_{\mathcal{V}(t)} \dot{s}_\phi(\phi,x,t)\,\mathrm{d}x \tag{1.18}$$

Assume that there is no flux of ϕ through $\mathcal{S}(t)$, that is to say, $\mathscr{F}(t) = 0$. If ϕ is generated in $\mathcal{V}(t)$, then $\mathscr{S}(t) > 0$, which implies $\dot{\phi}(t) > 0$; whereas if $\mathscr{S}(t) < 0$ then $\dot{\phi}(t) > 0$, thus $\dot{\phi}(t)$ and $\mathscr{S}(t)$ have the same sign. Introducing these terms in (1.16) leads to

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}(t)} \rho(x,t)\phi(x,t)\,\mathrm{d}x = -\int_{\mathcal{S}(t)} \mathbf{f}(\phi,x,t)\cdot\mathbf{n}\,\mathrm{d}S + \int_{\mathcal{V}(t)} \dot{s}_\phi(\phi,x,t)\,\mathrm{d}x \tag{1.19}$$

Hereinafter we shall become less formal by omitting on which variables depends each function. In order to relate the flux $\mathbf{f}$ and ϕ, we need to apply some constitutive law. Fourier's law for heat conduction and Fick's law for concentration state that $\mathbf{f}$ depends linearly on the gradient of ϕ with respect to the spatial variables [4], that is,

$$\mathbf{f} = -\Gamma_\phi \boldsymbol{\nabla}_x \phi = -\Gamma_\phi \begin{pmatrix} \dfrac{\partial\phi}{\partial x_1} & \cdots & \dfrac{\partial\phi}{\partial x_n} \end{pmatrix}^T \tag{1.20}$$

where Γ_ϕ is known as the diffusion coefficient. So as not to complicate the notation, we will write $\boldsymbol{\nabla}\phi$ in place of $\boldsymbol{\nabla}_x\phi$. Recall that $\boldsymbol{\nabla}\phi \in \mathbb{R}^n$ gives the direction of maximum growth of $\phi(\cdot,t)$ (the time is fixed because the gradient is computed with respect to x). The minus sign in (1.20) is the consequence of heat (concentration of a chemical) flowing from regions of higher to lower temperature (concentration) regions. With this in mind, equation (1.19) is rewritten as

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}(t)} \rho\phi\,\mathrm{d}x = \int_{\mathcal{S}(t)} \Gamma_\phi \boldsymbol{\nabla}\phi\cdot\mathbf{n}\,\mathrm{d}S + \int_{\mathcal{V}(t)} \dot{s}_\phi\,\mathrm{d}x \tag{1.21}$$

and applying Reynolds Transport Theorem on the left–hand side of (1.21) with $\mathbf{b} = \mathbf{v}$,

$$\int_{\mathcal{V}(t)} \frac{\partial(\rho\phi)}{\partial t}\,\mathrm{d}x + \int_{\mathcal{S}(t)} \rho\phi\mathbf{v}\cdot\mathbf{n}\,\mathrm{d}S = \int_{\mathcal{S}(t)} \Gamma_\phi \boldsymbol{\nabla}\phi\cdot\mathbf{n}\,\mathrm{d}S + \int_{\mathcal{V}(t)} \dot{s}_\phi\,\mathrm{d}x \tag{1.22}$$

To turn surface integrals into volume integrals we apply divergence theorem,

$$\int_{\mathcal{V}(t)} \frac{\partial(\rho\phi)}{\partial t}\,\mathrm{d}x + \int_{\mathcal{V}(t)} \boldsymbol{\nabla}\cdot(\rho\phi\mathbf{v})\,\mathrm{d}x = \int_{\mathcal{V}(t)} \boldsymbol{\nabla}\cdot(\Gamma_\phi\boldsymbol{\nabla}\phi)\,\mathrm{d}x + \int_{\mathcal{V}(t)} \dot{s}_\phi\,\mathrm{d}x \tag{1.23}$$

Proceeding in a similar way to the continuity equation, we assume the existence of a time t_0 and a point x_0 where

$$\left\{\frac{\partial(\rho\phi)}{\partial t}\,\mathrm{d}x + \boldsymbol{\nabla}\cdot(\rho\phi\mathbf{v})\,\mathrm{d}x - \boldsymbol{\nabla}\cdot(\Gamma_\phi\boldsymbol{\nabla}\phi)\,\mathrm{d}x - \dot{s}_\phi\,\mathrm{d}x\right\}\Big|_{(x_0,t_0)} \neq 0 \tag{1.24}$$

and we reach a contradiction, thereby obtaining the general convection diffusion equation:

$$\frac{\partial(\rho\phi)}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\phi\mathbf{v}) = \boldsymbol{\nabla}\cdot(\Gamma_\phi\boldsymbol{\nabla}\phi) + \dot{s}_\phi \tag{1.25}$$

The left–hand side of (1.25) can be expanded to find

$$\phi\left\{\frac{\partial\rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v})\right\} + \rho\frac{\partial\phi}{\partial t} + \rho\mathbf{v}\cdot\boldsymbol{\nabla}\phi = \boldsymbol{\nabla}\cdot(\Gamma_\phi\boldsymbol{\nabla}\phi) + \dot{s}_\phi \tag{1.26}$$

Since the term between keys is the continuity equation, (1.26) is simplified to

$$\rho\frac{\partial\phi}{\partial t} + \rho\mathbf{v}\cdot\boldsymbol{\nabla}\phi = \boldsymbol{\nabla}\cdot(\Gamma_\phi\boldsymbol{\nabla}\phi) + \dot{s}_\phi \tag{1.27}$$

Equations (1.25) and (1.27) are two equivalent forms of the same equation, each having its applications and benefits.

By taking ϕ to be the temperature T of the fluid or the concentration of the k–th chemical substance Y_k in the fluid, one obtains the energy conservation equation (1.28) and the k–species equation (1.29) [5]:

$$\frac{\partial(\rho T)}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v}T) = \boldsymbol{\nabla}\cdot\left(\frac{\lambda}{c_v}\boldsymbol{\nabla}T\right) + \left\{\frac{\tau\circ\boldsymbol{\nabla}\mathbf{v} - \boldsymbol{\nabla}\cdot\dot{\mathbf{q}}^R - p\boldsymbol{\nabla}\cdot\mathbf{v}}{c_v}\right\} \tag{1.28}$$

$$\frac{\partial(\rho Y_k)}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v}Y_k) = \boldsymbol{\nabla}\cdot(\rho D_{km}\boldsymbol{\nabla}Y_k) + \{\dot{\omega}_k\} \tag{1.29}$$

If ϕ is not a scalar magnitude but a vector magnitude, i.e. $\phi \equiv (\phi_1,\ldots,\phi_n)\colon \mathbb{R}^n\times I \to \mathbb{R}^n$, $(x,t)\mapsto\phi(x,t)$, the same process applied on each component function ϕ_i leads to n equations similar to (1.25) that can be gathered in the following vector equation

$$\frac{\partial(\rho\phi)}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v}\otimes\phi) = \boldsymbol{\nabla}\cdot(\mu\boldsymbol{\nabla}\phi) + \dot{s}_\phi \tag{1.30}$$

where $\mathbf{v}\otimes\phi$ is the exterior product:

$$\mathbf{v}\otimes\phi = \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix}\begin{pmatrix} \phi_1 & \cdots & \phi_n \end{pmatrix} = \begin{pmatrix} v_1\phi_1 & \cdots & v_1\phi_n \\ \vdots & \ddots & \vdots \\ v_n\phi_1 & \cdots & v_n\phi_n \end{pmatrix} \tag{1.31}$$

The previous product can also be regarded as the tensor product of two 1–covariant tensors which yields a 2–covariant tensor. Notice that, in general, this product is not commutative, that is to say, $\mathbf{v}\otimes\phi \neq \phi\otimes\mathbf{v}$.

By taking ϕ to be the velocity $\mathbf{v}$ of the fluid, the momentum conservation equation is obtained [5]:

$$\frac{\partial(\rho\mathbf{v})}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v}\otimes\mathbf{v}) = \boldsymbol{\nabla}\cdot(\mu\boldsymbol{\nabla}\mathbf{v}) + \{\boldsymbol{\nabla}\cdot(\tau - \mu\boldsymbol{\nabla}\mathbf{v}) - \boldsymbol{\nabla}p + \rho\mathbf{g}\} \tag{1.32}$$

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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 1. 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 [6].

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 [7])**.** 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 [1].

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

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

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 [8])**.** 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 [8], 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 [9])**.** 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 [9], page 38. □

C Numerical resolution of linear systems

C.1 Gauss–Seidel algorithm

C.2 LU factorization