Analysis and development of finite volume methods for the new generation of cubed sphere dynamical cores for the atmosphere

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Education is what remains after one has forgotten everything he learned in school.

— Albert Einstein

Acknowledgements

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Resumo

Luan da Fonseca Santos. **Análise e desenvolvimento de métodos de volumes finitos para modelos da nova geração da dinâmica atmosférica baseados na esfera cubada**. Tese (Doutorado). Instituto de Matemática e Estatística, Universidade de São Paulo, São Paulo, 2023.

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Palavras-chave: Núcleo dinâmico da atmosfera, esfera cubada, volumes finitos, dimension splitting, ponto de partida, corretor de massa.

Abstract

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Keywords: Dynamical core, cubed-sphere, finite-volume, dimension splitting, departure point, mass fixer.

Contents

Chapter 1

Introduction

1.1 Background

Chapter 2

One-dimensional finite-volume methods

The aim of this chapter is to provide a detailed description of one-dimensional (1D) finite-volume (FV) schemes within a Semi-Lagrangian (SL) framework, specifically applied to the 1D advection equation. These schemes are also known as flux-form Semi-Lagrangian schemes, and they allow for time steps beyond the Courant-Friedrichs-Lewy (CFL) condition while preserving the total mass. FV-SL schemes have been explored in the literature since the work of LeVeque (1985), which extended the finite-volume schemes from Godunov (1959) to accommodate larger time steps. This approach has been further investigated in the literature (c.f, e.g. . Leonard et al. (1996) and Lin and Rood (1996)). We are going to focus on the linear advection equation because in FV3, the horizontal dynamics are solved by using flux advection operators to compute the fluid density, absolute vorticity, and the kinetic energy (L. Harris et al., 2021; L. M. Harris & Lin, 2013; Lin & Rood, 1997; Putman, 2007). The boundary conditions are assumed to be periodic for simplicity.

To introduce the FV-SL schemes, we begin by discretizing the spatial and temporal domains into uniform grids. Subsequently, the FV-SL schemes involve three steps. The first step involves computing the departure points of the spatial grid edges. The second step, known as reconstruction, utilizes the grid cell average values to determine a piecewise function within each cell. This piecewise function approximates the values of the advected quantity and ensures the preservation of its local mass within each grid cell. The third step involves updating the fluxes at the grid edges by integrating the reconstruction function over a domain that extends from the departure point of the grid edge to the grid edge itself.

The first step of FV-SL schemes can be accomplished by integrating an ordinary differential equation backward in time. The second step is performed using the Piecewise-Parabolic Method (PPM) proposed by Colella and Woodward (1984). As the name suggests, PPM employs piecewise-parabolic functions. The third and final step is computed easily, as the reconstruction functions consist of parabolas that preserve the local mass.

It is worth noting that the reconstruction function can be constructed using functions other than parabolas. In fact, PPM can be seen as an extension of the Piecewise-Linear method proposed by Van Leer (1977), which, in turn, was inspired by the Piecewise-Constant method introduced by Godunov (1959). Additionally, other schemes inspired by PPM have been proposed in the literature utilizing higher-order polynomials, such as quartic polynomials (White & Adcroft, 2008). For a comprehensive review of general piecewise-polynomial reconstruction, we recommend referring to the technical report by Engwirda and Kelley (2016), Lauritzen et al. (2011), and the references therein.

The PPM approach has become popular in the literature for gas dynamics simulations, astrophysical phenomena modeling (Woodward, 1986), and later on atmospheric simulations (Carpenter et al., 1990). Indeed, PPM has been implemented in the FV3 dynamical core on its latitude-longitude grid (Lin, 2004) and cubed-sphere (Putman & Lin, 2007) versions. Although many other shapes for the basis functions and higher-order schemes are available in the literature, L. Harris et al. (2021) points out that the PPM scheme suits the needs of FV3 well. It is a flexible method that can be modified to ensure low diffusivity or shape preservation, for example. Additionally, a finite-volume numerical method usually requires monotonicity constraints, which, according to Godunov's order barrier theorem (Wesseling, 2001), limit the order of convergence to at most 1. Therefore, a higher-order scheme needs to strike a well-balanced trade-off between increasing computational cost and potential benefits.

This chapter begins with a basic review of one-dimensional advection equation in the integral form in Section 2.1. In Section 2.2, we establish the framework for general one-dimensional finite-volume Semi-Lagrangian schemes. Section **??** presents methods for computing the departure point. The PPM reconstruction is described in Section **??**, while Subsection **??** introduces different approaches to ensure the monotonicity of parabolas. Section **??** focuses on the description and investigation of the PPM flux computation. Section **??** presents numerical results using the PPM scheme for the advection equation. Finally, Section **??** presents some concluding remarks. The application of PPM to solve two-dimensional problems will be addressed in Chapter **??**.

2.1 One-dimensional advection equation in integral form

2.1.1 Notation

Before introducing the FV-SL schemes, let us establish some notation by introducing the concepts of a Δx-grid, a Δt-temporal grid, and the $(\Delta x, \Delta t, \lambda)$-discretization, as well as the concept of grid function/winds. In this chapter, we will use the notation $\Omega = [a, b]$ to represent the interval under consideration, and ν to represent a non-negative integer indicating the number of ghost cell layers in each boundary. We also use the notations $\mathbb{R}^N_\nu := \mathbb{R}^{N+2\nu}$ and $\mathbb{R}^{N+1}_\nu := \mathbb{R}^{N+1+2\nu}$.

Definition 2.1 (Δx-grid)**.** *For a given interval Ω and a positive real number Δx such that $\Delta x = (b-a)/N$ for some positive integer N, we say that $\Omega_{\Delta x} = \{X_i\}_{i=-\nu+1}^{N+\nu}$ is a Δx-grid for Ω if*

$$X_i = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}] = [a + (i-1)\Delta x, a + i\Delta x],$$

and $\Delta x = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}$. *Each* X_i *is referred to as a control volume or cell, and* $x_{i-\frac{1}{2}}$ *and* $x_{i+\frac{1}{2}}$ *are the edges of the control volume* X_i. *The cell centroid is defined by*

$$x_i = \frac{1}{2}(x_{i+\frac{1}{2}} + x_{i-\frac{1}{2}}), \quad \forall i = -\nu + 1, \dots, N + \nu,$$

and Δx *is the cell length.*

Remark 2.1. *If* $1 \leq i \leq N$, *we refer to* i *as an interior index; otherwise,* i *is considered a ghost cell index and we say the* X_i *is a ghost cell.*

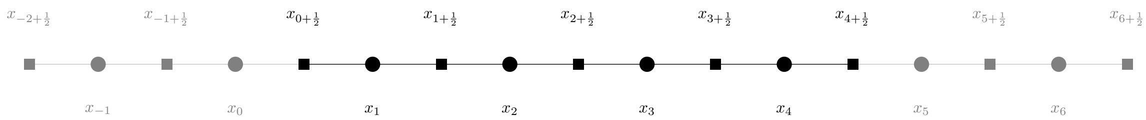

Figure 2.1: *Illustration of a* Δx*-grid with* $N = 4$ *cells in its interior (in black) and* $\nu = 2$ *ghost cell layers (in gray). The edges are denoted by squares and the cell centroids are denoted using circles.*

Definition 2.2 (Δt-temporal grid)**.** *For a given interval* $[0, T]$ *and a positive real number* Δt *such that* $\Delta t = T/N_T$ *for some positive integer* N_T, *we say that* $T_{\Delta T} = \{T_n\}_{n=0}^{N_T}$ *a* Δt*-temporal grid for* $[0, T]$ *if*

$$T_n = [t^n, t^{n+1}], \quad t^n = n\Delta t, \quad \Delta t = \frac{T}{N_T}, \quad \forall n = 0, \dots, N_T.$$

In this context, we also define $t^{n+\frac{1}{2}} = \frac{t^n + t^{n+1}}{2}$.

Definition 2.3 ($(\Delta x, \Delta t, \lambda)$-discretization)**.** *Given* $\Omega \times [0, T]$ *and positive real numbers* Δx *and* Δt, *we say that* $(\Omega_{\Delta x}, T_{\Delta t})$ *is a* $(\Delta x, \Delta t, \lambda)$*-discretization of* $\Omega \times [0, T]$ *if* $\Omega_{\Delta x}$ *is a* Δx*-grid for* Ω, $T_{\Delta t}$ *is a* Δt*-temporal grid for* $[0, T]$, *and* $\frac{\Delta t}{\Delta x} = \lambda$.

Remark 2.2. *Whenever we refer to a* Δx*-grid, a* Δt*-temporal grid, or a* $(\Delta x, \Delta t, \lambda)$*-discretization,* X_i, N, t^n, *and* N_T *are assumed to be implicitly defined.*

Next, we introduce the definitions of grid functions at cell centroids and edges.

Definition 2.4 (Δx-grid function)**.** *For a* Δx*-grid, we say that* Q *is a* Δx*-grid function if* $Q = (Q_{-\nu+1}, \dots, Q_{N+\nu}) \in \mathbb{R}^N_\nu$.

Definition 2.5 (Δx-grid wind)**.** *For a* Δx*-grid, we say that* u *is a* Δx*-grid wind if* $u = (u_{-\nu+\frac{1}{2}}, \dots, u_{N+\nu+\frac{1}{2}}) \in \mathbb{R}^{N+1}_\nu$.

The definition of a Δx-grid wind is based on the Arakawa grids (Arakawa & Lamb, 1977). Considering functions $q, u : \Omega \times [0, T] \to \mathbb{R}$ and a $(\Delta x, \Delta t, \lambda)$-discretization of $\Omega \times [0, T]$, we introduce the grid functions $q^n \in \mathbb{R}^N_\nu$ and $u^n \in \mathbb{R}^{N+1}_\nu$ where $q^n_i \approx q(x_i, t^n)$ and $u^n_{i+\frac{1}{2}} = u(x_{i+\frac{1}{2}}, t^n)$. The grid function q^n approximate the discrete values of q at cell centroids and u^n represents the values of u approximates edges, both for each time level t^n (Figure 2.2).

In this Chapter, our focus lies on periodic grid functions. We define a Δx-grid function

Q as periodic if it satisfies the following conditions:

$$Q_i = Q_{N+i}, \quad i = -\nu+1, \dots, 0,$$
$$Q_i = Q_{i-N}, \quad i = N+1, \dots, N+\nu.$$

Similarly, we define a Δx-grid wind as periodic if it meets the following requirements:

$$u_{i-\frac{1}{2}} = u_{N+i+\frac{1}{2}}, \quad i = -\nu, \dots, -1,$$
$$u_{i+\frac{1}{2}} = u_{i+\frac{1}{2}-N}, \quad i = N+1, \dots, N+\nu.$$

We use the notation $\mathbb{P}_\nu^N$ and $\mathbb{P}_\nu^{N+1}$ to represent the spaces of periodic Δx-grid functions and winds, respectively.

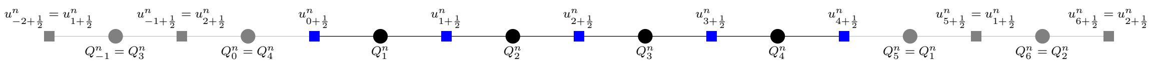

Figure 2.2: *Illustration of Δx-grid function Q (black circles) and a Δx-grid wind u (blue squares) and its ghost cell values (in gray) assuming periodicity.*

Given $Q \in \mathbb{P}_\nu^N$, we define the p-norm as

$$\|Q\|_{p,\Delta x} = \begin{cases} \left(\sum_{i=1}^N |Q_i|^p \right)^{\frac{1}{p}} & \text{if } 1 \le p < \infty, \\ \max_{i=1,\dots,N} |Q_i| & \text{otherwise}, \end{cases} \tag{2.1}$$

which is indeed a norm for periodic grid functions. Using a similar notation as in Engwirda and Kelley (2016), we define the stencil and a grid function evaluated on a stencil as follows.

Definition 2.6 (Stencil). *For a Δx-grid, and each $i = 0, \dots, N$, we define a stencil as a set of the form $S_{i+\frac{1}{2}} = \{i-r+1, \dots, i-1, i, i+1, \dots, i+s\} \subset \{-\nu+1, \dots, N+\nu\}$.*

Definition 2.7 (Grid function restricted to a stencil). *For a Δx-grid, a stencil $S_{i+\frac{1}{2}}$, and a Δx-grid function Q, we define $Q(S_{i+\frac{1}{2}}) = (Q_k)_{k \in S_{i+\frac{1}{2}}}$.*

These definitions provide the necessary notation for describing grid functions and their evaluations on stencils. To achieve a more compact notation in some situations, we introduce the centered difference notation:

$$\delta_x g(x_i, t) = g(x_{i+\frac{1}{2}}, t) - g(x_{i-\frac{1}{2}}, t), \tag{2.2}$$

for any function $g : \Omega \times [0, T] \to \mathbb{R}$. Additionally, we introduce the average value of q in the i-th control volume at time t, denoted as $Q_i(t)$, defined by:

$$Q_i(t) = \frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} q(x,t)\, dx. \tag{2.3}$$

Moreover, we define the Δx-grid function of average values as $Q(t) = (Q_i(t))_{i=-\nu+1}^{N+\nu}$. Here, $Q_i(t)$ represents the average value of q in the i-th control volume at time t.

For the consideration of periodic boundary conditions, we can define spaces of periodic functions over the interval Ω as follows:

$$\mathcal{S}_P(\Omega) = \{q : \mathbb{R} \times [0, +\infty[\to \mathbb{R} : q(x + b - a, t) = q(x, t), \quad \forall x \in \mathbb{R}, \quad t \geq 0\}.$$

Similarly, the space of k-times periodically differentiable functions $C_P^k(\Omega)$ can be defined as:

$$C_P^k(\Omega) = \mathcal{S}_P(\Omega) \cap C^k(\mathbb{R} \times [0, \infty[),$$

where $C^k(\mathbb{R} \times [0, +\infty[)$ denotes the space of functions that are k times continuously differentiable in both the spatial and temporal variables. In summary, $\mathcal{S}_P(\Omega)$ represents the space of periodic functions, and $C_P^k(\Omega)$ represents the space of k-times periodically differentiable functions over the interval Ω subject to periodic boundary conditions.

2.1.2 The 1D advection equation

In this section, we will derive the integral form of the 1D advection equation with periodic boundary conditions over the interval Ω. What is going to be presented here follows LeVeque (1990, 2002) closely. The advection equation with periodic boundary conditions in its differential form is given by:

$$\begin{cases} [\partial_t q + \partial_x(uq)](x, t) = 0, \quad \forall (x, t) \in \mathbb{R} \times]0, +\infty[, \\ q(a, t) = q(b, t), \quad \forall t \geq 0, \\ q_0(x) = q(x, 0), \quad \forall x \in \Omega. \end{cases} \tag{2.4}$$

Here, $q \in C_P^1(\Omega)$ represents the advected quantity, and $u \in C_P^1(\Omega)$ represents the velocity. We will focus on Equation (2.4) over the domain $D = \Omega \times [0, T]$, where $T > 0$ is a finite time. A strong or classical solution to the advection equation is defined as a function $q \in C_P^1(\Omega)$ and satisfies Equation (2.4). In order to deduce the integral form of Equation (2.4), we consider $[x_1, x_2] \times [t_1, t_2] \subset D$. Integrating Equation (2.5) over $[x_1, x_2]$, we obtain:

$$\frac{d}{dt} \int_{x_1}^{x_2} q(x, t)\, dx = -((uq)(x_2, t) - (uq)(x_1, t)), \tag{2.5}$$

and integrating Equation (2.5) over $[t_1, t_2]$, we get

$$\int_{x_1}^{x_2} q(x, t_2)\, dx = \int_{x_1}^{x_2} q(x, t_1) - \left(\int_{t_1}^{t_2} (uq)(x_2, t)\, dt - \int_{t_1}^{t_2} (uq)(x_1, t)\, dt \right). \tag{2.6}$$

The presented problem, Problem 2.1, aims to find a solution, called weak solution, to the advection equation in its integral form, considering the given initial condition q_0 and velocity function u.

Problem 2.1. *Given an initial condition q_0 and a velocity function u we would like to find a weak solution q of the advection equation in the integral form:*

$$\int_{x_1}^{x_2} q(x, t_2)\, dx = \int_{x_1}^{x_2} q(x, t_1)\, dx + \int_{t_1}^{t_2} (uq)(x_1, t)\, dt - \int_{t_1}^{t_2} (uq)(x_2, t)\, dt,$$

$\forall[x_1, x_2] \times [t_1, t_2] \subset \Omega \times [0, T]$, *and* $q(x, 0) = q_0(x)$, $\forall x \in \Omega$, $q(a, t) = q(b, t)$, $\forall t \in [0, T]$.

We point out that, for Problem 2.1, the total mass in Ω at time t defined by:

$$M_{[a,b]}(t) = \int_a^b q(x, t)\, dx,$$

remains constant over time, i.e.,

$$M_{[a,b]}(t) = M_{[a,b]}(0), \quad \forall t \in [0, T].$$

This conservation of total mass property is highly desirable for numerical schemes aiming to approximate general conservation law solutions accurately.

Applying the steps from Equation (2.4) to Equation (2.6) in reverse order, one can verify that if q is a weak solution and $q \in C_P^1(\Omega)$, then it satisfies Equation (2.4). Therefore, Equation (2.4) and Problem (2.1) are equivalent when $q \in C_P^1(\Omega)$. However, Problem (2.1) can be formulated for functions that are not C^1 and have discontinuities. In fact, Problem (2.1) only requires that q and uq are locally integrable.

It is worth noting that Equation (2.6) holds for all x_1, x_2, t_1, and t_2 such that $[x_1, x_2] \times [t_1, t_2] \subset D$. Therefore, let us consider a $(\Delta x, \Delta t, \lambda)$-discretization of D and rewrite Equation (2.6) in terms of this discretization. By replacing t_1, t_2, x_1, and x_2 with $t^n, t^{n+1}, x_{i-\frac{1}{2}}$, and $x_{i+\frac{1}{2}}$, respectively, in Equation (2.6), we obtain:

$$Q_i(t^{n+1}) = Q_i(t^n) - \frac{1}{\Delta x}\left(\int_{t^n}^{t^{n+1}} (uq)(x_{i+\frac{1}{2}}, t)\, dt - \int_{t^n}^{t^{n+1}} (uq)(x_{i-\frac{1}{2}}, t)\, dt \right), \qquad \forall i = 1, \ldots, N, \quad \forall n = 0, \ldots, N_T - 1. \tag{2.7}$$

To achieve a more compact notation, we use the centered difference notation and then Equation (2.7) can be rewritten as:

$$Q_i(t^{n+1}) = Q_i(t^n) - \frac{1}{\Delta x}\delta_x\left(\int_{t^n}^{t^{n+1}} (uq)(x_i, t)\, dt \right), \quad \forall i = 1, \ldots, N, \quad \forall n = 0, \ldots, N_T - 1. \tag{2.8}$$

Now we can define a discretized version of Problem 2.1 as Problem 2.2.

Problem 2.2. *Let us consider the framework of Problem 2.1 and a* $(\Delta x, \Delta t, \lambda)$*-discretization of* $\Omega \times [0, T]$*. Since we are operating within the framework of Problem 2.1, the following relationship holds:*

$$Q_i(t^{n+1}) = Q_i(t^n) - \lambda\delta_x\left(\frac{1}{\Delta t}\int_{t^n}^{t^{n+1}} (uq)(x_i, t)\, dt \right), \quad \forall i = 1, \ldots, N, \quad \forall n = 0, \ldots, N_T - 1, \tag{2.9}$$

where $Q_i(t) = \frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} q(x, t)\, dx$*. Our objective now is to determine the values* $Q_i(t^n)$, $\forall i = 1, \ldots, N$, $\forall n = 0, \ldots, N_T - 1$*, given the initial values* $Q_i(0)$, $\forall i = 1, \ldots N$*. In other words, we aim to find the average values of* q *in each control volume* X_i *at the specified time instances.*

It is important to note that no approximations have been made in problems (2.1) and

(2.2). In Equation (2.9), we divided and multiplied by Δt to interpret $\frac{1}{\Delta t}\int_{t^n}^{t^{n+1}}(uq)(x_{i\pm\frac{1}{2}}, t)\,dt$ as a time-averaged flux. This interpretation is useful for deriving finite-volume schemes.

In Problem 2.2, we need to approximate the time-averaged flux at the cell edges $x_{i\pm\frac{1}{2}}$ to derive a finite-volume scheme. This flux, in principle, requires knowledge of q over the entire interval $[t^n, t^{n+1}]$. To overcome this, we can express the temporal integral as a spatial integral at time t^n. This approach avoids the need for information about q throughout the entire interval $[t^n, t^{n+1}]$. Furthermore, this spatial integral domain is closely related to the definition of the departure point.

To introduce the definition of departure point, for each $s \in [t^n, t^{n+1}]$, we consider the following Cauchy problem backward in time:

$$\begin{cases} \partial_t x^d_{i+\frac{1}{2}}(t,s) = u(x^d_{i+\frac{1}{2}}(t,s), t), & t \in [t^n, s] \\ x^d_{i+\frac{1}{2}}(s,s) = x_{i+\frac{1}{2}}. \end{cases} \tag{2.10}$$

The point $x^d_{i+\frac{1}{2}}(t^n, s)$ is called departure point at time t^n of the point $x_{i+\frac{1}{2}}$ at time s. In Figure 2.3 we illustrate the departure point idea.

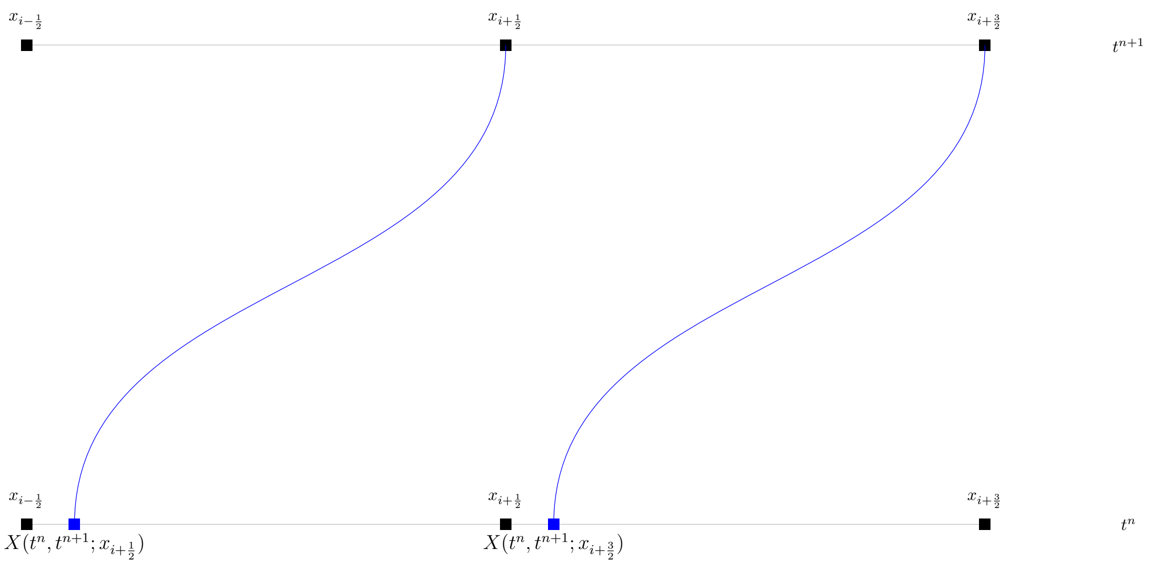

Figure 2.3: *Illustration of the departure point of the cell edges from time t^{n+1} to t^n.*

Integrating Equation (2.10) over the interval $[t, s]$, we get:

$$x^d_{i+\frac{1}{2}}(t,s) = x_{i+\frac{1}{2}} - \int_t^s u(x^d_{i+\frac{1}{2}}(\theta, s), \theta)\,d\theta. \tag{2.11}$$

In the following Proposition, we show how the time-averaged flux is related to a spatial integral over a interval depending on departure points.

Proposition 2.1. *Assume the framework of Problem 2.2. If q and u are C^1 functions, then:*

$$\int_{t^n}^{t^{n+1}} (uq)(x_{i+\frac{1}{2}}, s)\,ds = \int_{x^d_{i+\frac{1}{2}}(t^n, t^{n+1})}^{x_{i+\frac{1}{2}}} q(x, t^n)\,dx \tag{2.12}$$

Proof. Using the Leibniz rule for integration (Theorem A.2 with $f(s,\theta) = u\big(x^d_{i+\frac{1}{2}}(\theta,s)\big)$), in Equation (2.11), it follows that:

$$\begin{aligned}\partial_s x^d_{i+\frac{1}{2}}(t,s) &= -\left(u(x_{i+\frac{1}{2}},s) + \int_t^s \frac{du}{ds}\big(x^d_{i+\frac{1}{2}}(\theta,s),\theta\big)\,d\theta\right)\\ &= -u(x_{i+\frac{1}{2}},s) - \int_t^s \partial_s u\big(x^d_{i+\frac{1}{2}}(\theta,s),\theta\big)\partial_s x^d_{i+\frac{1}{2}}(\theta,s)\,d\theta.\end{aligned} \tag{2.13}$$

Taking the derivative with respect to t of Equation (2.13), we have:

$$\partial_t\partial_s x^d_{i+\frac{1}{2}}(t,s) = \partial_x u\big(x^d_{i+\frac{1}{2}}(t,s),t\big)\partial_s x^d_{i+\frac{1}{2}}(t,s). \tag{2.14}$$

Using standard ordinary differential equations techniques (ODE), we get that $x^d_{i+\frac{1}{2}}$ that solves Equations (2.13) and (2.14) is given by:

$$\partial_s x^d_{i+\frac{1}{2}}(t,s) = -\exp\left(\int_t^s \partial_x u\big(x^d_{i+\frac{1}{2}}(\theta,s),\theta\big)\,d\theta\right)u(x_{i+\frac{1}{2}},s). \tag{2.15}$$

Computing q on the trajectory give by $x^d_{i+\frac{1}{2}}(t,s)$ and taking its time derivative, we obtain:

$$\begin{aligned}\frac{d}{dt}q\big(x^d_{i+\frac{1}{2}}(t,s),t\big) &= \partial_t q\big(x^d_{i+\frac{1}{2}}(t,s),t\big) + (u\partial_x q)\big(x^d_{i+\frac{1}{2}}(t,s),t\big)\\ &= -\partial_x u\big(x^d_{i+\frac{1}{2}}(t,s),t\big)q\big(x^d_{i+\frac{1}{2}}(t,s),t\big),\end{aligned} \tag{2.16}$$

where we used that q satisfies the linear advection equation on its differential (2.4) form and that $x^d_{i+\frac{1}{2}}(t,s)$ solves Equation (2.10). Using again standard ODE techniques, we get that q that solves Equation (2.16) is given by:

$$q\big(x^d_{i+\frac{1}{2}}(t,s),t\big) = \exp\left(-\int_t^s \partial_x u\big(x^d_{i+\frac{1}{2}}(\theta,s),\theta\big)\,d\theta\right)q(x_{i+\frac{1}{2}},s). \tag{2.17}$$

Notice that if u does not depend on x, then q is constant along the trajectory $x^d_{i+\frac{1}{2}}(t,s)$.

Let us consider the mapping $s \in [t^n, t^{n+1}] \to x^d_{i+\frac{1}{2}}(t^n,s)$. Integrating q over all departure points at time t^n from $x_{i+\frac{1}{2}}$ at time s, we have

$$\int_{x^d_{i+\frac{1}{2}}(t^n,t^n)=x_{i+\frac{1}{2}}}^{x^d_{i+\frac{1}{2}}(t^n,t^{n+1})} q(x,t^n)\,dx = \int_{t^n}^{t^{n+1}} q\big(x^d_{i+\frac{1}{2}}(t^n,s),t^n\big)\partial_s x^d_{i+\frac{1}{2}}(t^n,s)\,ds, \tag{2.18}$$

where we are just using the variable change integration formula. Then, it follows from Equations (2.15) and (2.17) with $t = t^n$ that:

$$\int_{x_{i+\frac{1}{2}}}^{x^d_{i+\frac{1}{2}}(t^n,t^{n+1})} q(x,t^n)\,dx = -\int_{t^n}^{t^{n+1}} (uq)(x_{i+\frac{1}{2}},s)\,ds, \tag{2.19}$$

which is the desired formula. □

With the aid of Proposition 2.1, we can rewrite Problem 2.2 in terms of the departure point, avoiding the need for knowledge about q over the entire interval $[t^n, t^{n+1}]$. This is described in Problem 2.3:

Problem 2.3. *Assume the framework of Problem 2.1 and a $(\Delta x, \Delta t, \lambda)$-discretization of $\Omega \times [0, T]$. Since we are in the framework of Problem 2.1, it follows that:*

$$Q_i(t^{n+1}) = Q_i(t^n) - \lambda\left(\frac{1}{\Delta t}\int_{X(t^n,t^{n+1};x_{i+\frac{1}{2}})}^{x_{i+\frac{1}{2}}} q(x,t^n)\,dx - \frac{1}{\Delta t}\int_{x^d_{i-\frac{1}{2}}(t^n,t^{n+1})}^{x_{i-\frac{1}{2}}} q(x,t^n)\,dx\right), \quad \forall i = 1,\dots,N, \quad \forall n = 0,\dots,N_T - 1, \tag{2.20}$$

where $Q_i(t) = \frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} q(x,t)\,dx$. Our problem now consists of finding the values $Q_i(t^n)$, $\forall i = 1,\dots,N$, $\forall n = 0,\dots,N_T - 1$, given the initial values $Q_i(0)$, $\forall i = 1,\dots N$. In other words, we would like to find the average values of q in each control volume X_i at the considered time instants.

At each time step t^n, we compute the values of $Q_i(t^{n+1})$ based on $Q_i(t^n)$ and the integrals of $q(x,t^n)$ over specific intervals. These intervals are defined by the departure points $X(t^n, t^{n+1}; x_{i+\frac{1}{2}})$ and $X(t^n, t^{n+1}; x_{i-\frac{1}{2}})$. To perform the computations, we need to determine the departure points from the edges of all control volumes and calculate the required integrals. This idea serves as the motivation for defining finite-volume Semi-Lagrangian schemes. These schemes involve estimating the departure points and reconstructing the function q at time t^n using its average values $Q_i(t^n)$, which enables us to compute the necessary integrals.

2.2 The finite-volume Semi-Lagrangian approach

Finally, we define the 1D FV-SL scheme problem as follows in Problem 2.3.

Problem 2.4 (1D FV-SL scheme)**.** *Assume the framework defined in Problem 2.3. The finite-volume Semi-Lagrangian approach of Problem 2.3 consists of finding a scheme of the form:*

$$Q_i^{n+1} = Q_i^n - \lambda(F^n_{i+\frac{1}{2}} - F^n_{i-\frac{1}{2}}), \quad \forall i = 1,\dots,N, \quad \forall n = 0,\dots,N_T - 1, \tag{2.21}$$

where $Q^n \in \mathbb{P}_\nu^N$ is intended to be an approximation of $Q(t^n) \in \mathbb{P}_\nu^N$ in some sense. We define $Q_i^0 = Q_i(0)$ or $Q_i^0 = q_i^0$. The terms $F^n_{i\pm\frac{1}{2}}$ are known as numerical flux and are given by

$$F^n_{i\pm\frac{1}{2}} = \frac{1}{\Delta t}\int_{\tilde{x}^n_{i\pm\frac{1}{2}}}^{x_{i\pm\frac{1}{2}}} \tilde{q}(x; Q^n)\,dx, \tag{2.22}$$

where $\tilde{x}^n_{i\pm\frac{1}{2}}$ is an estimate of the departure point $x^d_{i-\frac{1}{2}}(t^n, t^{n+1})$, and $\tilde{q}$ is a reconstruction function for q built with the values Q^n. Thus, $F^n_{i\pm\frac{1}{2}}$ approximates $\frac{1}{\Delta t}\int_{x^d_{i\pm\frac{1}{2}}(t^n,t^{n+1})}^{x_{i\pm\frac{1}{2}}} q(x,t^n)\,dx$.

For a 1D FV-SL the discrete total mass at the time-step n is given by

$$M^n = \Delta x \sum_{i=1}^{N} Q_i^n. \tag{2.23}$$

Therefore, the discrete total mass is constant for a 1D-FV scheme, which follows from a straightforward computation:

$$M^{n+1} = \Delta x \sum_{i=1}^{N} Q_i^{n+1} = M^n - \Delta t \sum_{i=1}^{N} (F^n_{i+\frac{1}{2}} - F^n_{i-\frac{1}{2}}) = M^n - \Delta t (F^n_{N+\frac{1}{2}} - F^n_{\frac{1}{2}}) = M^n,$$

where we are using that $F^n_{N+\frac{1}{2}} = F^n_{\frac{1}{2}}$, since we are assuming periodic boundary conditions.

We would like to highlight an important relationship between the average values of q and its values at the cell centroids. In Problem 2.4, we mentioned that the initial condition can be represented as q_i^0 instead of $Q_i(0)$. Moreover, when analyzing the convergence of a FV-SL scheme, it is useful to compare Q_i^n with q_i^n since computing $Q_i(t^n)$ requires evaluating an analytical integral, which can be challenging in certain cases. In Proposition 2.2, we provide a simple proof that q_i^n approximates $Q_i(t^n)$ with second-order error when q is twice continuously differentiable.

Proposition 2.2. *If $q \in C^2_P(\Omega)$, then $Q_i(t^n) - q_i^n = C_1 \Delta x^2$, where $C_1 = \frac{1}{24}\frac{\partial^2 q}{\partial x^2}(\eta, t^n)$, $\eta \in X_i$.*

Proof. Just apply Theorem A.4 for the function $q(x, t^n)$. □

Hence, 1D FV-SL schemes may be conceptualized as schemes that update the centroid values. The Problem of the convergence of 1D FV-SL schemes is addressed in Section A.3. Now we are going to address the problem of the departure point estimation and the reconstruction problem.

Appendix A

Numerical Analysis

A.1 Lagrange interpolation

Given real numbers, called nodes, $x_0 < x_1 < \ldots < x_m$, we define the k-th Lagrange polynomial by

$$L_k(x) = \prod_{j=0, j\neq k}^{m} \frac{x - x_j}{x_k - x_j}.$$

They satisfy $L_k(x_j) = \delta_{kj}$, where δ_{kj} is the Kronecker delta. Given a function f defined at the nodes x_j, its interpolating polynomial of degree m is given by:

$$P_m(x) = \sum_{k=0}^{m} f(x_k) L_k(x).$$

Indeed, this polynomial interpolates f since $P_m(x_j) = f(x_j)$. It is well known that P_m always exists and is unique. Besides that, we have the following error formula for Lagrange interpolation.

Theorem A.1. *Let $f \in C^{m+1}(\mathbb{R})$. Then, then there is ξ in the smallest interval containing $x_0, \ldots, x_m, x$ such that:*

$$f(x) - P_m(x) = \omega(x) \frac{f^{(m+1)}(\xi)}{(m+1)!}, \tag{A.1}$$

where $\omega(x) = (x - x_0)(x - x_1) \ldots (x - x_m)$.

Proof. See Stoer and Bulirsch (2002, Theorem 2.1.4.1. on p. 49). □

A.2 Numerical integration

Theorem A.2 (Leibniz integral rule)**.** *If f…*

$$\frac{d}{dx} \int_a^x f(x,t)\, dt = f\big(x, x\big) + \int_a^x \partial_x f(x,t)\, dt$$

Proof. See Courant and John (1999, p. 143). □

The following mean value theorem for integrals is a very useful tool when working with numerical integration errors.

Theorem A.3 (Mean value theorem for integrals)**.** *If $f \in C([a,b])$, and g is a integrable function in $[a,b]$ whose sign does not change in $[a,b]$, then there exists $c \in]a,b[$ such that*

$$\int_a^b f(x)g(x)\,dx = f(c)\int_a^b g(x)\,dx.$$

Proof. See Courant and John (1999, p. 143). □

A.2.1 Midpoint rule

When considering finite-volume schemes, it is useful to compare the average value on a control volume of a function with its value at the control volume centroid. In the following theorems, for the one and two dimensional cases, respectively, we show that the value of a function at the centroid of a control volume given a second-order approximation to its average value on the control volume.

Theorem A.4. *If $f \in C^2([x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}])$, then*

$$\frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} f(x)\,dx - f(x_i) = C_1\Delta x^2, \tag{A.2}$$

where C_1 is a constant that depends only on f, and $x_i = \frac{x_{i+\frac{1}{2}}+x_{i-\frac{1}{2}}}{2}$, $\Delta x = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}$.

Proof. From Taylor's expansion, it follows that, for $x \in [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$, we have:

$$f(x) = f(x_i) + f(x_i)(x - x_i) + f''(\xi)\frac{(x-x_i)^2}{2}, \tag{A.3}$$

for some ξ between x and x_i. Therefore:

$$\begin{aligned}\frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} f(x)\,dx - f(x_i) &= \frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \left(f'(x_i)(x-x_i) + f''(\xi)\frac{(x-x_i)^2}{2}\right)dx \\ &= \frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} f''(\xi)\frac{(x-x_i)^2}{2}\,dx.\end{aligned}$$

Using the mean value theorem for integrals (see Theorem A.3), we have:

$$\frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} f(x)\,dx - f(x_i) = f''(\eta_i)\frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \frac{(x-x_i)^2}{2}\,dx = f''(\eta_i)\frac{\Delta x^2}{24}$$

for some $\eta_i \in [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$, from which the proposition follows with

$$C_1 = \frac{1}{24} f''(\eta_i). \tag{A.4}$$

□

Theorem A.5. *If $f \in C^2([x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}] \times [y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}}])$, then*

$$\frac{1}{\Delta x \Delta y} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} f(x,y)\, dx\, dy - f(x_i, y_j) = C \Delta x^2, \tag{A.5}$$

where C_1 is a constants that depends only on f, where we assume $x_i = \frac{x_{i+\frac{1}{2}} + x_{i-\frac{1}{2}}}{2}$, $y_i = \frac{y_{j+\frac{1}{2}} + y_{j-\frac{1}{2}}}{2}$, $\Delta x = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}$, $\Delta y = y_{j+\frac{1}{2}} - y_{j-\frac{1}{2}}$ and $\Delta x = \Delta y$.

Proof. Applying Theorem A.4 in the y direction, we have

$$\int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} f(x,y)\, dy = \Delta y f(x, y_j) + \frac{\Delta y^3}{24} \partial_y^2 f(x, \eta_j),$$

for $\eta_j \in [y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}}]$. Hence:

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} f(x,y)\, dx\, dy = \Delta y \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} f(x, y_j)\, dx + \frac{\Delta y^3}{24} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \partial_y^2 f(x, \eta_j)\, dx.$$

Applying Theorem A.4 in the x direction for $y = y_j$, we get

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} f(x, y_j)\, dx = \Delta x f(x_i, y_j) + \frac{\Delta x^3}{24} \partial_x^2 f(\xi_i, y_j)\, dx,$$

for $\xi_i \in [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$. From this, we obtain

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} f(x,y)\, dx\, dy = \Delta x \Delta y f(x_i, y_j) + \frac{\Delta x^3}{24} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \partial_x^2 f(\xi_i, y_j)\, dx + \frac{\Delta y^3}{24} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \partial_y^2 f(x, \eta_j)\, dx.$$

Using Theorem A.3, we obtain the desired formula:

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} f(x,y)\, dx\, dy = \Delta x \Delta y f(x_i, y_j) + \frac{\Delta x^2}{24} \Delta x \Delta y \partial_x^2 f(\nu_i, y_j) + \frac{\Delta y^2}{24} \Delta x \Delta y \partial_y^2 f(\theta_i, \eta_j),$$

where $\nu_i, \theta_i \in [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$, recalling that $\Delta x = \Delta y$. □

Corollary A.1. *If $f \in C^2([a,b] \times [c,d])$, and $[a,b] \times [c,d]$ is written as the union of the uniformed-spaces control volumes $[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}] \times [y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}}]$, $i, j = 1, \ldots, N$, with lengths*

$\Delta x = \Delta y$, we have

$$\int_a^b \int_c^d f(x,y)\,dx\,dy - \sum_{i,j=1}^{N} f(x_i,y_j)\Delta x \Delta y = C_1 \Delta x^2, \tag{A.6}$$

where C_1 depends only on f.

Proof. Using Theorem A.5, we have:

$$\begin{aligned}\frac{1}{\Delta x \Delta y}\int_a^b \int_c^d f(x,y)\,dx\,dy &= \frac{1}{\Delta x \Delta y}\sum_{i,j=1}^{N}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}}\int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} f(x,y)\,dx\,dy \\ &= \sum_{i,j=1}^{N} f(x_i,y_j) + \frac{\Delta x^2}{24}\sum_{i,j=1}^{N}\left(\partial_x^2 f(v_i,y_j) + \partial_y^2 f(v_i,y_j)\right).\end{aligned}$$

We notice that

$$\Delta x \Delta y \sum_{i,j=1}^{N}\left(\partial_x^2 f(v_i,y_j) + \partial_y^2 f(v_i,y_j)\right) = \frac{(b-a)(d-c)}{N^2}\sum_{i,j=1}^{N}\left(\partial_x^2 f(v_i,y_j) + \partial_y^2 f(v_i,y_j)\right)$$

and we also point that from the inequality

$$\min\left(\partial_x^2 f + \partial_y^2 f\right)(x,y) \le \frac{1}{N^2}\sum_{i,j=1}^{N}\left(\partial_x^2 f(v_i,y_j) + \partial_y^2 f(v_i,y_j)\right) \le \max\left(\partial_x^2 f + \partial_y^2 f\right)(x,y),$$

and with the aid of the intermediate value theorem, we have

$$\frac{1}{N^2}\sum_{i,j=1}^{N}\left(\partial_x^2 f(v_i,y_j) + \partial_y^2 f(v_i,y_j)\right) = \left(\partial_x^2 f + \partial_y^2 f\right)(\overline{x},\overline{y})$$

for some $(\overline{x},\overline{y}) \in [a,b]\times[c,d]$ from which the claim follows. □

A.2.2 Multi-step schemes

Let us consider the following problem: given a function $f \in C^{m+1}([0,T])$, a discretization of $[0,T]$ given by $t^n = n\Delta t$, $\Delta t = \frac{T}{N_T}$, for some $N_T \in \mathbb{N}$, we wish to estimate $\int_{t^n}^{t^{n+1}} f(t)\,dt$ using the values $f(t_{n-k})$, for $k = 0,\cdots,m$. This kind of problem arises, for instance, when we are interested in computing departure points as in Equation 2.11. We can estimate the desired integral by computing the interpolating polynomial of $f(t_{n-k})$, for $k = 0,\cdots,m$ and then integrating this polynomial. This approach is exactly what is used in multi-step Adams-Bashforth methods. On the next theorem, we give an expression the error of this approach.

Theorem A.6. *If $f \in C^{m+1}([0,T])$, $t^n = n\Delta t$, $n = 0,\cdots,N_T$, $\Delta t = \frac{T}{N_T}$ for some $N_T \in \mathbb{N}$, then:*

$$\int_{t^n}^{t^{n+1}} f(t)\,dt = \Delta t \sum_{k=0}^{m}\left(\int_0^1 L_k(s)\,ds\right) f(t_{n-k}) + \frac{(\Delta t)^{k+1}}{(m+1)!} f^{(m+1)}(\eta)\int_0^1 \omega(s)\,ds, \tag{A.7}$$

where $w(s) = s(s+1)\cdots(s+m)$, $\eta \in [t^{n-m}, t^n]$.

Proof. We introduce auxiliary functions $\theta(s) = s\Delta t + t_n$, $s \in [-m, 1]$ and $g(s) = f(\theta(s))$. It is clear that $f(t_{n-k}) = g(-k)$, for $k = -1, 0, \cdots, m$. Hence, we can write:

$$\int_{t^n}^{t^{n+1}} f(t)\,dt = \Delta t \int_0^1 f(\theta(s))\,ds = \Delta t \int_0^1 g(s)\,ds. \tag{A.8}$$

Defining the nodes $s_k = -k$ for $k = 0, \cdots, m$, it follows from Theorem A.1 that the interpolating polynomial P_m of $g(s_k)$ satisfies:

$$g(s) - P_m(s) = \omega(s)\frac{g^{(m+1)}(\xi)}{(m+1)!}, \tag{A.9}$$

where $\xi \in [-m, 1]$. Substituting Equation (A.9) in Equation (A.8), we obtain

$$\int_{t^n}^{t^{n+1}} f(t)\,dt = \Delta t \sum_{k=0}^{m} \left(\int_0^1 L_k(s)\,ds \right) g(-k) + \frac{\Delta t}{(m+1)!} \int_0^1 g^{(m+1)}(\xi)\omega(s)\,ds. \tag{A.10}$$

Since $w(s)$ does not change its sign in $[0, 1]$ it follows from Theorem A.3 that:

$$\int_{t^n}^{t^{n+1}} f(t)\,dt = \Delta t \sum_{k=0}^{m} \left(\int_0^1 L_k(s)\,ds \right) g(-k) + \frac{\Delta t}{(m+1)!} g^{(m+1)}(\bar{\xi}) \int_0^1 \omega(s)\,ds, \tag{A.11}$$

for some $\bar{\xi} \in [-m, 1]$. Notice that by the chain rule we get $g^{(m+1)}(s) = (\Delta t)^k f^{(m+1)}(\theta(s))$, therefore Equation (A.11) in terms of f reads:

$$\int_{t^n}^{t^{n+1}} f(t)\,dt = \Delta t \sum_{k=0}^{m} \left(\int_0^1 L_k(s)\,ds \right) f(t_{n-k}) + \frac{(\Delta t)^{k+1}}{(m+1)!} f^{(m+1)}(\eta) \int_0^1 \omega(s)\,ds, \tag{A.12}$$

where $\eta \in [t^{n-m}, t^n]$, which is the desired identity. □

In the following corollaries, we give the explicit formulas for Equation (A.12) for $m = 0, m = 1, m = 2$. This is achieved by computing the terms $\int_0^1 L_k(s)\,ds$ and $\int_0^1 \omega(s)\,ds$, which are trivial to be computed.

Corollary A.2. *If* $f \in C^1([0, T])$, $t^n = n\Delta t$, $n = 0, \cdots, N_T$, $\Delta t = \frac{T}{N_T}$ *for some* $N_T \in \mathbb{N}$, *then:*

$$\int_{t^n}^{t^{n+1}} f(t)\,dt = \Delta t f(t_n) + \frac{\Delta t^2}{2} f'(\bar{t}), \tag{A.13}$$

for some $\bar{t} \in [t^n, t^{n+1}]$.

Corollary A.3. *If* $f \in C^2([0, T])$, $t^n = n\Delta t$, $n = 0, \cdots, N_T$, $\Delta t = \frac{T}{N_T}$ *for some* $N_T \in \mathbb{N}$, *then:*

$$\int_{t^n}^{t^{n+1}} f(t)\,dt = \frac{\Delta t}{2}(3f(t_n) - f(t_{n-1})) + \frac{5\Delta t^3}{12} f^{(2)}(\bar{t}), \tag{A.14}$$

for some $\bar{t} \in [t^{n-1}, t^{n+1}]$.

Corollary A.4. *If* $f \in C^3([0,T])$, $t^n = n\Delta t$, $n = 0, \cdots, N_T$, $\Delta t = \frac{T}{N_T}$ *for some* $N_T \in \mathbb{N}$, *then:*

$$\int_{t^n}^{t^{n+1}} f(t)\,dt = \frac{\Delta t}{12}(23f(t_n) - 16f(t_{n-1}) + 5f(t_{n-2})) + \frac{3\Delta t^4}{8} f^{(3)}(\bar{t}), \tag{A.15}$$

for some $\bar{t} \in [t^{n-2}, t^{n+1}]$.

When using these schemes for and ODE written in its integral form, $m = 0$ gives the classical Euler method; for $m = 1$ we get the second-order Adams-Bashforth scheme and for $m = 2$ we have the third-order Adams-Bashforth scheme.

Observe that from the midpoint rule (Theorem A.4), we can write

$$\frac{1}{\Delta t}\int_{t^n}^{t^{n+1}} f(t)\,dt = f(t_{n+\frac{1}{2}}) + \frac{\Delta t^2}{2} f'(\tilde{t}), \tag{A.16}$$

where $t_{n+\frac{1}{2}} = (t_{n+1} + t_n)/2$ and $\tilde{t} \in [t^n, t^{n+1}]$. Combining this with Corollary A.3, we have the second-order extrapolation formula as follows.

Corollary A.5. *If* $f \in C^2([0,T])$, $t^n = n\Delta t$, $n = 0, \cdots, N_T$, $\Delta t = \frac{T}{N_T}$ *for some* $N_T \in \mathbb{N}$, *then:*

$$f(t_{n+\frac{1}{2}}) = \frac{3}{2} f(t_n) - \frac{1}{2} f(t_{n-1}) + O(\Delta t^2). \tag{A.17}$$

A.3 Convergence of 1D FV-SL schemes

A.3.1 Consistency and convergence

Hereafter, we are going to use the notations introduced in Section 2.1.1. To move towards the convergence of 1D-FV schemes, for Problem 2.4 we introduce the local truncation error (LTE hereafter) τ_i^n following LeVeque (2002):

$$Q_i(t^{n+1}) = Q_i(t^n) - \lambda\left(F^n_{i+\frac{1}{2}}(Q(t^n), \tilde{u}^n_{i+\frac{1}{2}}) - F^n_{i-\frac{1}{2}}(Q(t^n), \tilde{u}^n_{i-\frac{1}{2}})\right) + \Delta t \tau_i^n. \tag{A.18}$$

We the define $\tau^n \in \mathbb{P}_v^N$, which represent the LTEs at the time-step n. Notice the LTE is obtained by replacing the exact solution in Equation (2.21). Since $Q_i(t^n)$ is the exact solution of Equation (2.9), the LTE may be rewritten as

$$\begin{aligned} \tau_i^n = \frac{1}{\Delta x}\Bigg[&\left(\frac{1}{\Delta t}\int_{t^n}^{t^{n+1}} (uq)(x_{i+\frac{1}{2}}, t)\,dt - F^n_{i+\frac{1}{2}}(Q(t^n), \tilde{u}^n_{i+\frac{1}{2}})\right) + \\ &\left(\frac{1}{\Delta t}\int_{t^n}^{t^{n+1}} (uq)(x_{i-\frac{1}{2}}, t)\,dt - F^n_{i-\frac{1}{2}}(Q(t^n), \tilde{u}^n_{i-\frac{1}{2}})\right)\Bigg]. \end{aligned} \tag{A.19}$$

The LTE gives a measure of how well the 1D-FV scheme approximates the integral form of the considered conservation law. Another interpretation of the LTE is that the LTE gives the error obtained after applying the scheme for a single time-step using the exact solution. Now we can define consistency.

Definition A.1 (Consistency)**.** *Let us consider the framework of Problem 2.4. A 1D-FV scheme is said to be consistency in the p-norm if for any sequence of* $(\Delta x^{(k)}, \Delta t^{(k)}, \lambda)$*-discretizations,* $k \in \mathbb{N}$*, with* $\lim_{k\to\infty} \Delta x^{(k)} = \lim_{k\to\infty} \Delta t^{(k)} = 0$*, we have:*

$$\lim_{k\to\infty} \left[\max_{1\le n\le N_T^{(k)}} \|\tau^n\|_{p,\Delta x^{(k)}} \right] = 0,$$

and it is said to be consistent with order P in the p−norm if

$$\max_{1\le n\le N_T^{(k)}} \|\tau^n\|_{p,\Delta x^{(k)}} = O(\Delta x^P).$$

From Equation (A.19), it follows that we basically need to ensure that the numerical flux function $\mathcal{F}^n_{i+\frac{1}{2}}$ converges to the time-averaged flux at edges when $\Delta x \to 0$ in order to guarantee consistency.

At last, we define the point-wise error at time-step n by:

$$E_i^n = Q_i(t^n) - Q_i^n, \quad i = 1, \dots, N,$$

and we define the vector of errors by $E^n \in \mathbb{P}_\nu^N$ with entries E_i^n.

Definition A.2 (Convergence)**.** *Let us consider the framework of Problem 2.4. A 1D-FV scheme is said to be convergent in the p-norm if for any sequence of* $(\Delta x^{(k)}, \Delta t^{(k)}, \lambda)$*-discretizations,* $k \in \mathbb{N}$*, with* $\lim_{k\to\infty} \Delta x^{(k)} = \lim_{k\to\infty} \Delta t^{(k)} = 0$*, we have:*

$$\lim_{k\to\infty} \left[\max_{1\le n\le N_T^{(k)}} \|E^n\|_{p,\Delta x^{(k)}} \right] = 0,$$

and it is said to converge with order P in the p−norm if

$$\max_{1\le n\le N_T^{(k)}} \|E^n\|_{p,\Delta x^{(k)}} = O(\Delta x^P).$$

Subtracting Equation (2.21) from Equation (A.18) we get the following equation for the error:

$$\begin{aligned} E_i^{n+1} = E_i^n - \lambda \Bigg[&\left(F^n_{i+\frac{1}{2}}(Q(t^n), \tilde{u}^n_{i+\frac{1}{2}}) - F^n_{i+\frac{1}{2}}(Q^n, \tilde{u}^n_{i+\frac{1}{2}}) \right) \\ &- \left(F^n_{i-\frac{1}{2}}(Q(t^n), \tilde{u}^n_{i-\frac{1}{2}}) - F^n_{i-\frac{1}{2}}(Q^n, \tilde{u}^n_{i-\frac{1}{2}}) \right) \Bigg] + \tau_i^n \Delta t. \end{aligned} \tag{A.20}$$

Notice that if $q, u \in C^3$, we can rewrite Equation (A.19) as:

$$\tau_i^n = \left[\frac{1}{\Delta x \Delta t} \int_{t^n}^{t^{n+1}} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \frac{\partial (uq)}{\partial x}(x,t)\, dx\, dt - \left(\frac{F^n_{i+\frac{1}{2}}(Q(t^n), \tilde{u}^n_{i-\frac{1}{2}}) - F^n_{i-\frac{1}{2}}(Q(t^n), \tilde{u}^n_{i-\frac{1}{2}})}{\Delta x} \right) \right].$$

Using the midpoint rule for integration (Theorem A.4) and the mean value theorem for integrals (Theorem A.3), we have:

$$\begin{aligned}\tau_i^n &= \left[\frac{1}{\Delta t}\int_{t^n}^{t^{n+1}}\left(\frac{\partial(uq)}{\partial x}(x_i,t)+\frac{\Delta x^2}{24}\frac{\partial(uq)}{\partial x}(\xi,t)\right)dt-\left(\frac{F^n_{i+\frac{1}{2}}(Q(t^n),\tilde{u}^n_{i+\frac{1}{2}})-F^n_{i-\frac{1}{2}}(Q(t^n),\tilde{u}^n_{i-\frac{1}{2}})}{\Delta x}\right)\right]\\ &= \left[\frac{1}{\Delta t}\int_{t^n}^{t^{n+1}}\frac{\partial(uq)}{\partial x}(x_i,t)\,dt-\left(\frac{F^n_{i+\frac{1}{2}}(Q(t^n),\tilde{u}^n_{i+\frac{1}{2}})-F^n_{i-\frac{1}{2}}(Q(t^n),\tilde{u}^n_{i-\frac{1}{2}})}{\Delta x}\right)\right]+\frac{\Delta x^2}{24}\frac{\partial^3(uq)}{\partial x^3}(\xi,\bar{t}),\end{aligned} \tag{A.21}$$

for $\xi \in X_i$ and $\bar{t} \in [t^n, t^{n+1}]$. Therefore, if $q, u \in C^3$ the scheme is consistent, if and only if, $\frac{1}{\Delta t}\int_{t^n}^{t^{n+1}}\frac{\partial(uq)}{\partial x}(x_i,t)\,dt$ is approximated by $\frac{F^n_{i+\frac{1}{2}}(Q(t^n),\tilde{u}^n_{i+\frac{1}{2}}))-F^n_{i-\frac{1}{2}}(Q(t^n),\tilde{u}^n_{i-\frac{1}{2}})}{\Delta x}$. This shall be very useful when we consider two-dimensional schemes, where we are going to use the discrete operators to estimate the divergence of velocity fields.

A.3.2 Stability

In order to define the concept of stability, it is useful to introduce an operator representation of 1D-FV schemes. In the context of Problem 2.4, we define the operators $\mathcal{H}_{\Delta x,n} : \mathbb{P}_v^N \to \mathbb{P}_v^N$ whose i-th entry is given by:

$$[\mathcal{H}_{\Delta x,n}(Q)]_i = Q_i - \lambda\left(F^n_{i+\frac{1}{2}}(Q,\tilde{u}^n_{i+\frac{1}{2}}) - F^n_{i-\frac{1}{2}}(Q,\tilde{u}^n_{i-\frac{1}{2}})\right), \tag{A.22}$$

for $i = 1, \dots, N$, $n = 0, \dots, N_T - 1$. Notice that the dependence on n is due to the velocity that may be allowed to vary with time. As it is usual, we are assuming periodicity in the entries of Q when we apply the operator $\mathcal{H}_{\Delta x,n}$. Thus, Equation (2.21) may be rewritten in a vector form by

$$Q^{n+1} = \mathcal{H}_{\Delta x,n}(Q^n),$$

and Equation (A.18) in a vector form reads

$$Q(t^{n+1}) = \mathcal{H}_{\Delta x,n}(Q(t^n)) + \Delta t\tau^n,$$

and the error equation (A.20) is given by

$$E^{n+1} = \mathcal{H}_{\Delta x,n}(Q(t^n)) - \mathcal{H}_{\Delta x,n}(Q^n) + \Delta t\tau^n. \tag{A.23}$$

The stability theory focus on uniformly bounding the norm of $\mathcal{H}_{\Delta x,n}(Q(t^n)) - \mathcal{H}_{\Delta x,n}(Q^n)$ (LeVeque, 2002). We define stability as follows.

Definition A.3 (Stability)**.** *In the context of Problem 2.4, a 1D-FV scheme is stable in the $p-$norm if for any $(\Delta x, \Delta t, \lambda)$-discretization of $[a,b]\times[0,T]$ we have:*

$$\|\mathcal{H}_{\Delta x,n}(Q) - \mathcal{H}_{\Delta x,n}(P)\|_{p,\Delta x} \leq (1+\alpha\Delta t)\|Q-P\|_{p,\Delta x}, \tag{A.24}$$

for all $Q, P \in \mathbb{R}_v^N$ and α is a constant that does not depend neither on Δx nor on Δt.

Assuming that the scheme is stable in the $p-$norm, then it follows from Equation

(A.23) that:

$$
\begin{aligned}
\|E^{n+1}\|_{p,\Delta x} &\le \|\mathcal{H}_{\Delta x,n}(Q(t^n)) - \mathcal{H}_{\Delta x,n}(Q^n)\|_{p,\Delta x} + \Delta t \max_{n=1,\dots,N_T} \|\tau^n\|_{p,\Delta x} \\
&\le (1+\alpha\Delta t)\|E^n\|_{p,\Delta x} + \Delta t \max_{n=1,\dots,N_T} \|\tau^n\|_{p,\Delta x} \\
&\le (1+\alpha\Delta t)^n\|E^0\|_{p,\Delta x} + \Delta t \max_{n=1,\dots,N_T} \|\tau^n\|_{p,\Delta x} \sum_{k=0}^{n-1}(1+\alpha\Delta t)^k \\
&\le e^{\alpha T}(\|E^0\|_{p,\Delta x} + T \max_{n=1,\dots,N_T} \|\tau^n\|_{p,\Delta x}),
\end{aligned}
\tag{A.25}
$$

where we used $n\Delta t \le T$, $T = N\Delta t$ and the inequality $e^t > 1 + t$. When computing the initial average values using the value at the cell centroid, the initial error E^0 converges to zero provided q is twice continuously differentiable by Proposition 2.2. Therefore, it follows that if the scheme is stable and consistent then it is convergent. Furthermore, if it is stable and consistent with order P, then the convergence order is at least equal to $\min\{P, 2\}$. In the case where both the conservation law and $\mathcal{H}_{\Delta x,n}$ are linear, this result is a particular case of the Lax-Ritchmyer stability and the convergence is guaranteed by the Lax equivalence theorem (LeVeque, 2002). In this Chapter, we are interested only in the linear advection equation. However, as pointed in Section **??**, the operator $\mathcal{H}_{\Delta x,n}$ may become non-linear when monotonicity constraints are activated.

Notice that, if $\mathcal{H}_{\Delta x,n}$ is linear, then stability is equivalent to require that

$$\|\mathcal{H}_{\Delta x,n}\|_{p,\Delta x} \le 1 + \alpha\Delta t,$$

where

$$\|\mathcal{H}_{\Delta x,n}\|_{p,\Delta x} = \sup_{Q\in\mathbb{R}^{\Delta x}} \frac{\|\mathcal{H}_{\Delta x,n}(Q)\|_{p,\Delta x}}{\|Q\|_{p,\Delta x}},$$

is the operator p-norm.

For linear operators, we may use the discrete Fourier transform (Trefethen, 2000) to estimate the 2-norm of $\mathcal{H}_{\Delta x,n}$. This approach is known as Von Neumann stability analysis. We define the nodes $\theta_i = i\frac{2\pi}{N}$, $i = 1, \dots, N$, $\Delta\theta = \frac{2\pi}{N}$, $\theta = (\theta_1, \theta_2, \dots, \theta_N)$. The imaginary unit is denoted by $\imath$. We define $\mathbb{C}^N_\nu$ similarly as $\mathbb{P}^N_\nu$. The Fourier modes $e^{\imath k\theta}] \in \mathbb{C}^N_\nu$ for $k = 1, \dots, N$, have entries are given by:

$$[e^{\imath k\theta}]_i = e^{\imath k\theta_i}, \quad \text{for } i = 1, \dots, N.$$

Each k is referred to wavenumber and θ_k is called dimensionless wavenumber. The Fourier modes form an orthogonal basis of $\mathbb{C}^N_\nu$ with respect to the inner product

$$\langle Q, P\rangle = \frac{1}{N}\sum_{i=1}^{N} Q_i\overline{P_i},$$

for $P, Q \in \mathbb{C}^N_\nu$ and $\bar{z}$ denotes the complex conjugate of z. Given $Q \in \mathbb{P}^N_\nu$, we may may express it in terms of the Fourier modes

$$Q = \sum_{k=1}^{N} a_k e^{\imath k\theta},$$

where $a_k \in \mathbb{C}$. The 2-norm of Q is then given by:

$$\|Q\|_{2,\Delta x} = \sqrt{N \sum_{k=1}^{N} |a_k|^2}.$$

The idea of Von Neumann stability analysis is to apply the operator $\mathcal{H}_{\Delta x,n}$ on each Fourier mode and analyze how it modifies its amplitude. For ease of analysis, we assume that the velocity is constant, which implies that the operator $\mathcal{H}_{\Delta x,n}$ has constant coefficients and does not depend on n. For the general case, where the velocity is not constant, the stability can be ensured using the frozen coefficients method (Strikwerda, 2004, p. 59). This method boils down to performing multiple times the stability analysis with a constant velocity being equal to each one of the possible values of the velocity on the grid. If the scheme is stable for all the possible constant velocities, then stability is ensured. Since the operator is supposed to be linear with constant coefficients and we are assuming periodic boundaries conditions, we may write:

$$\mathcal{H}_{\Delta x,n}(e^{\imath k\theta}) = \rho(k)e^{\imath k\theta},$$

where the term $\rho(k)$ is called amplification factor and it is an eigenvalue of $\mathcal{H}_{\Delta x,n}$. The norm of $\mathcal{H}_{\Delta x,n}(Q)$ is bounded by:

$$\|\mathcal{H}_{\Delta x,n}(Q)\|_{2,\Delta x}^2 = N \sum_{k=1}^{N} |a_k|^2 |\rho(k)|^2 \leq \max_{k=1,\ldots,N} |\rho(k)|^2 \|Q\|_{2,\Delta x}^2.$$

Therefore:

$$\|\mathcal{H}_{\Delta x,n}\|_{2,\Delta x} \leq \max_{k=1,\ldots,N} |\rho(k)|.$$

If we show that $\max_{k=1,\ldots,N} |\rho(k)| \leq 1 + \alpha\Delta t$, with α independent of Δt, N and n, then we ensure the stability of $\mathcal{H}_{\Delta x,n}$.

A.3.3 Flux accuracy analysis

With the PPM operator, we can compute the amplification factor by applying it on each Fourier mode considering the PPM and the hybrid PPM schemes, both without monotonization. We assume a constant velocity equal to one and $N = 100$ (number of control volumes). In Figure A.1 we show the amplification factor for both PPM and hybrid PPM schemes considering different CFL numbers. We can observe that both schemes damp most of the Fourier modes for larger k, regardless of the CFL number. Besides that, the hybrid scheme is more effective when reducing the Fourier modes amplitude. We point out that both schemes are exact when the CFL number is equal to 1. From this analysis, we can conclude that the PPM and hybrid PPM schemes satisfy the Von Neumann stability criteria when the CFL restriction is respected. For an analysis of stability for larger time-steps, we refer to Lauritzen (2007).

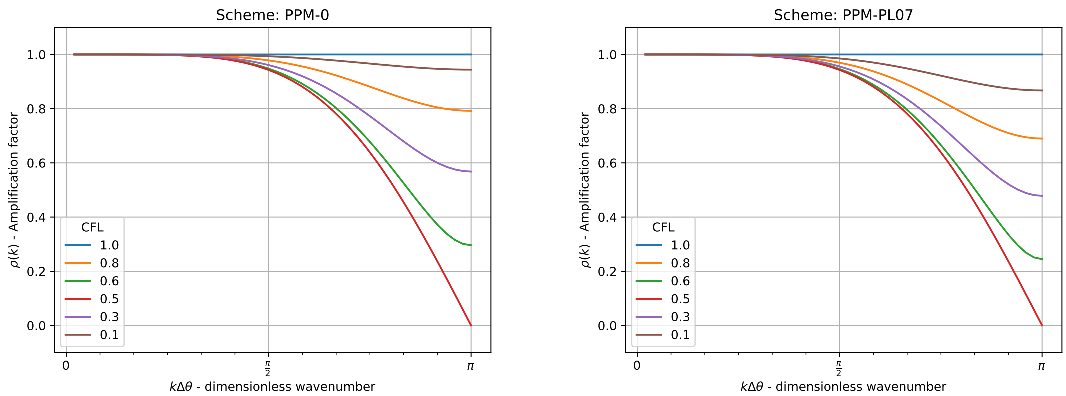

Figure A.1: *Amplification factor for the PPM (left) and hybrid PPM (right) schemes for different CFL numbers.*

A.4 Convergence, consistency and stability of 2D-FV schemes

The notions of convergence, consistency and stability for a 2D-FV schemes are straightforward from these notions for 1D-FV schemes (see Subsections A.3.1 and A.3.2). Indeed, in the context of Problem **??**, we define the operators $\mathcal{H}_{\Delta x,\Delta y,n} : \mathbb{R}^{N\times M} \to \mathbb{R}^{N\times M}$ whose (i, j) entry is given by:

$$[\mathcal{H}_{\Delta x,\Delta y,n}(Q)]_{ij} = Q_{ij} - \Delta t \mathbb{D}^n_{ij}$$

for $i = 1, \dots, N$, $j = 1, \dots, M$, $n = 0, \dots, N_T - 1$. The 2D-FV is then expressed as

$$Q^{n+1} = \mathcal{H}_{\Delta x,\Delta y,n}(Q^n).$$

The local error truncation $\tau^n \in \mathbb{R}^{N\times M}$ is given by

$$Q(t^{n+1}) = \mathcal{H}_{\Delta x,\Delta y,n}(Q(t^n)) + \Delta t \tau^n.$$

The error equation is given by

$$E^{n+1} = \mathcal{H}_{\Delta x,\Delta y,n}(Q(t^n)) - \mathcal{H}_{\Delta x,\Delta y,n}(Q^n) + \Delta t \tau^n. \tag{A.26}$$

The stability in the p-norm is defined as in the 1D case.

Definition A.4. *A 2D-FV scheme is stable in the $p-$norm if*

$$\|\mathcal{H}_{\Delta x,\Delta y,n}(Q) - \mathcal{H}_{\Delta x,\Delta y,n}(P)\|_{p,\Delta x\times\Delta y} \leq (1 + \alpha\Delta t)\|Q - P\|_{p,\Delta x\times\Delta y}, \tag{A.27}$$

for all $Q, P \in \mathbb{R}^{N\times M}$ and α is a constant that does not depend neither on Δx, Δy, Δt nor on n.

If a 2D-FV scheme is stable in the p−norm, similarly to Equation (A.25) we have:

$$\|E^{n+1}\|_{p,\Delta x\times\Delta y} \leq e^{\alpha T}(\|E^0\|_{p,\Delta x\times\Delta y} + T \max_{n=1,\ldots,N_T} \|\tau^n\|_{p,\Delta x\times\Delta y}).$$

Again, we point out that from Proposition ??, we have that the initial error E^0 shall be second-order accurate. Consistency is defined as in Definition A.1 and convergence is defined as in Definition A.2.

The Von Neumann analysis can be applied when $\mathcal{H}_{\Delta x,\Delta y,n}$ is linear, since we are considering periodic boundary conditions. The idea is the same as in the one-dimensional case, we just apply the operator $\mathcal{H}_{\Delta x,\Delta y,n}$ on the Fourier modes to obtain the amplification factor. We introduce the nodes $\theta_i = i\frac{2\pi}{N}$, $i = 1,\ldots,N$, $\Delta\theta = \frac{2\pi}{N}$, $\theta_i = (\theta_1,\theta_2,\ldots,\theta_N)$, $\phi_j = j\frac{2\pi}{M}$, $j = 1,\ldots,M$, $\Delta\phi = \frac{2\pi}{M}$, $\phi = (\phi_1,\phi_2,\ldots,\phi_M)$. For $k_1 = 1,\ldots,N$, $k_2 = 1,\ldots,M$, the two-dimensional Fourier mode $\boldsymbol{k} = (k_1,k_2)$ from $\mathbb{C}^{N\times M}$ has its (i,j) entry given by $[e^{\imath \boldsymbol{k}\theta}]_{ij} = e^{\imath k_1\theta_i}e^{\imath k_2\phi_j}$. For an analysis of stability for the dimension splitting method, we refer to Lauritzen (2007) and Lin and Rood (1996).

Notice that if $q,u,v \in C^3$, we can rewrite the LTE as:

$$\tau_{ij}^n = \left[\frac{1}{\Delta x\Delta y\Delta t}\int_{t^n}^{t^{n+1}}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}}\int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \nabla\cdot(\boldsymbol{u}q)(x,y,t)\,dy\,dx\,dt - \mathbb{D}_{ij}^n\right].$$

Using the midpoint rule for integration (Theorem A.5), the mean value theorem for integrals (Theorem A.3) and recalling the discrete divergence (Definition ??), we have:

$$\tau_{ij}^n = \frac{1}{\Delta t}\int_{t^n}^{t^{n+1}} \nabla\cdot(\boldsymbol{u}q)(x_i,y_j,t)\,dt - \mathbb{D}_{ij}^n + O(\Delta x^2) + O(\Delta y^2). \tag{A.28}$$

Therefore, in order to investigate the consistency, we may compare how well the discrete divergence approximates the divergence.

Appendix B

Code avaibility

The codes needed for this work have been built openly at GitHub. The PPM implementation for the one-dimensional advection equation used in Chapter 2 is available at https://github.com/luanfs/FV3_adv_1D

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