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

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# Abstract

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# Contents

# Chapter 1

# Introduction

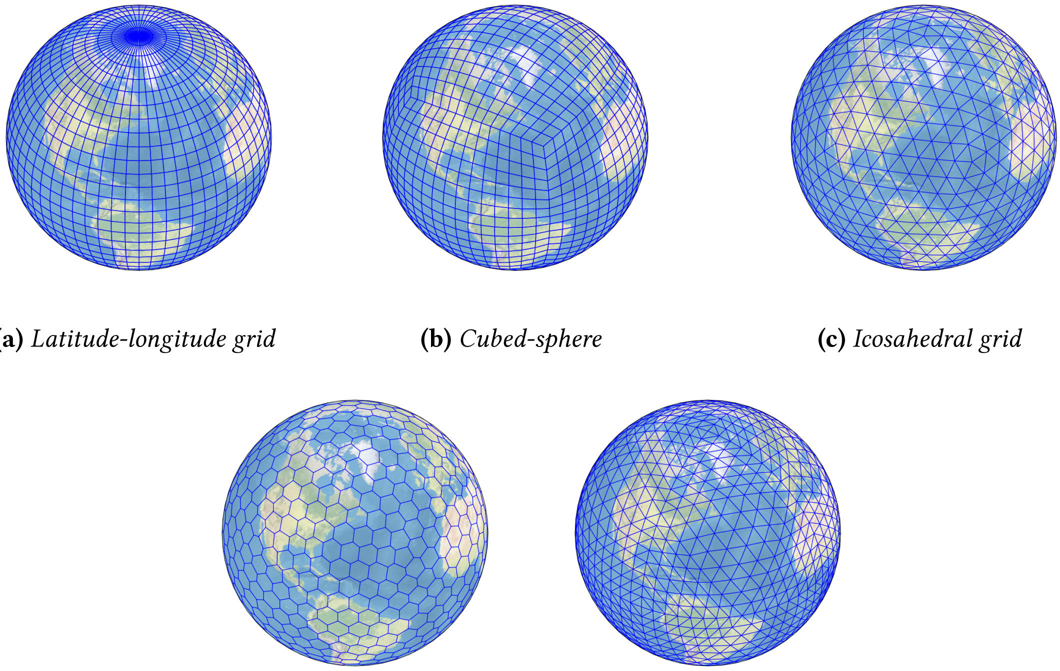
## 1.1 Background

Weather and climate predictions are recognized as a good for mankind, due to the information they yield for diverse activities. For instance, short-range forecasts are useful for public use, while medium-range forecasts are helpful for industrial activities and agriculture. Seasonal forecasts (one up to three months) are important to energy planning and agriculture. At last, longer-range forecasts (one century, for instance) are useful for climate change projections that are important for government planning.

The first global Numerical Weather Prediction models emerged in the 1960s with applications to weather, seasonal and climate forecasts. All these applications are essentially based on the same set of Partial Differential Equations (PDEs) but with distinct time scales (Williamson, 2007). These PDEs are defined on the sphere and model the evolution of the atmospheric fluid given the initial conditions. One important component of global models is the dynamical core, which is responsible for solving the PDEs that governs the atmosphere dynamics on grid-scale. The development of numerical methods for dynamical cores has been an active research area since the 1960s.

Global models use the sphere as the computational domain and therefore they require a discretization of the sphere. The first global models used the latitude-longitude grid (Figure 1.1a), which is very suitable for finite-differences schemes. The major drawback of the latitude-longitude grid is the clustering of points at the poles, known as the "pole problem", which leads to extremely small time steps for explicit-in-time schemes due to the Courant-Friedrichs-Lewy (CFL) condition, making these schemes computationally very expensive.

The most successful method adopted in global atmospheric dynamical cores that overcomes the CFL restriction is the Semi-Implicit Semi-Lagrangian (SI-SL) scheme (Randall et al., 2018), which emerged in the 1980s and consists of the Lagrangian advection scheme applied at each time-step and the solution of fast gravity waves implicitly, allowing very large time steps despite the pole problem. The SI-SL approach combined with finite differences is still used nowadays, for instance in the UKMetOffice global model ENDGame (Benacchio & Wood, 2016; Wood et al., 2014). The expensive part of the SI-SL approach is to solve an elliptic equation at each time step, that comes from the semi-implicit discretization, which requires global data communication, being inefficient to run in massive parallel supercomputers. Besides that, Semi-Lagrangian schemes are inherently non-conservatives for mass, which is critical for climate forecasts (Williamson, 2007).



**(a)** *Latitude-longitude grid* **(b)** *Cubed-sphere* **(c)** *Icosahedral grid*

**(d)** *Pentagonal/Hexagonal grid* **(e)** *Octahedral grid*

**Figure 1.1:** *Examples of spherical grids: latitude-longitude grid (a) and grids based on Platonic solids (b)-(d).*

The emergence of the Fast Fourier Transform (FFT) in the 1960s with the work from Cooley and Tukey (1965) allowed the computation of discrete Fourier transforms with $N \log(N)$ complexity. The viability of the usage of FFTs for solving atmospheric flows was shown by Orszag (1970), using the barotropic vorticity equation on the sphere, and by Eliasen et al. (1970), using the primitive equations. The spectral transform method expresses latitude-longitude grid values, that represent some scalar field, using truncated spherical harmonics expansions, which consists of Fourier expansions in latitude circles and Legendre functions expansions in longitude circles. The coefficients in the spectral expansions are known as spectral coefficients and are usually thought to live in the so-called spectral space. Given the grid values, the spectral coefficients are obtained by performing a FFT followed by a Legendre Transform (LT). Conversely, given the spectral coefficients, the grid values are obtained by performing an inverse LT followed by an inverse FFT. The main idea of the spectral method is to apply the spectral transform, in order to go the spectral space, and evaluate spatial derivatives in the spectral space, which consists of multiplying the spectral coefficients by constants. Then, the method performs the inverse spectral transform in order to get back to grid space, and the nonlinear terms are treated on the grid space (Krishnamurti et al., 2006).

The spectral transform makes the use of SI-SL methods computationally cheap, since the solution to elliptic problems becomes easy, once the spherical harmonics are eigenfunctions of the Laplacian operator on the sphere. Therefore, the spectral transform method gets faster when combined with the SI-SL approach due to the larger times-steps allowed in this case. Due to these enhancements, the spectral transform dominated global atmospheric modeling (Randall et al., 2018) since the 1980s. Indeed, the spectral method is still used in many current operational Weather Forecasting models such as the Integrated Forecast System (IFS) from European Centre for Medium-Range Weather Forecasts (ECMWF), Global Forecast System (GFS) from National Centers for Environmental Prediction (NCEP) and the Brazilian Global Atmospheric Model (BAM) (Figueroa et al., 2016) from Center for Weather Forecasting and Climate Research [Centro de Previsão de Tempo e Estudos Climáticos (CPTEC)].

With the beginning of the multicore era in the 1990s, the global atmospheric models started to move towards parallel efficiency aiming to run at very high resolutions. Even though the spectral transform expansions have a global data dependency, some parallelization is feasible among all the computations of FFTs, LTs and their inverses (Barros et al., 1995). However, the parallelization of the spectral method requires data transpositions in order to compute FFTs and LTs in parallel. These transpositions demand a lot of global communication using, for instance, the Message Passing Interface (MPI) (Zheng & Marguinaud, 2018). Indeed, the spectral transform becomes the most expensive component of global spectral models when the resolution is increased due to the amount of MPI communications (Müller et al., 2019).

The adiabatic and frictionless continuous equations that govern the atmospheric flow have conserved quantities. Among them, some of the most important are mass, total energy, angular momentum and potential vorticity (Thuburn, 2011). As we pointed out, Semi-Lagrangian schemes lack mass conservation. Nevertheless, these schemes have been employed in dynamical cores for better computational performance. However, dynamical cores should have discrete analogous of the continuous conserved quantities, especially concerning for longer simulation runs.

Aiming for better performance in massively parallel computers and conservation properties, new dynamical cores have been developed since the beginning of the 2000s. Novel spherical grids have been proposed, in order to avoid the pole problem. A popular choice are grids based on Platonic solids (Staniforth & Thuburn, 2012). The construction of these grids relies on a Platonic circumscribed on the sphere and the projection of its faces onto the sphere, which leads to quasi-uniform and more isotropic spherical grids. Some examples of spherical grids based on Platonic solids employed in the new generation of dynamical cores are the cubed-sphere (Figure 1.1b), icosahedral grid (Figure 1.1c), the pentagonal/hexagonal or Voronoi grid (Figure 1.1d) and octahedral grid (Figure 1.1e), which are based on the cube, icosahedron, dodecahedron and octahedron, respectively (Ullrich et al., 2017).

Building a highly parallelizable numerical scheme with mimetic properties in a quasi-uniform grid is far from being a trivial task. A popular mimetic method, known as TRiSK, was proposed in the literature by Thuburn et al. (2009) and Ringler et al. (2010) using finite difference and finite volume schemes. This scheme is designed for general orthogonal grids, such as the Voronoi and icosahedral grids, and ensures mass and total energy conservation. This method has been employed in the dynamical core of the Model for Prediction Across Scales (MPAS) from National Center for Atmospheric Research (NCAR) (Skamarock et al., 2012), which intended to work on general Voronoi grids, including locally refined Voronoi grids. However, the TRiSK scheme is a low-order scheme and suffers from grid imprinting, *i.e.*, geometric properties of the grid, such as cell alignment, interfere with the method accuracy (Peixoto, 2016; Peixoto & Barros, 2013; Weller, 2012). Furthermore, in locally refined Voronoi grids, the scheme may become unstable due to ill-aligned cells and numerical dissipation is needed (Santos & Peixoto, 2021), breaking the total energy conservation of the method.

# Chapter 2

# One-dimensional finite-volume methods

## 2.1 One-dimensional system of conservation laws in integral form

In this section, we are going to present the derivation of one-dimensional system of conservation laws in the integral form. The derivation presented here follows LeVeque (1990) and LeVeque (2002) closely and will be useful to fix some notation. Let us assume that $x$ and $t$ represent the spatial and time coordinate, respectively. Given $[x_1, x_2] \subset \mathbb{R}$, $x_1 \leq x_2$, and a time interval $[t_1, t_2] \subset ]0, +\infty[$, $t_1 \leq t_2$, our aim is to describe how $m$ state variable densities given by functions $q_1, \cdots, q_m : \mathbb{R} \times [0, +\infty[ \to \mathbb{R}$ evolve within time in the considered time interval, assuming that we have neither sinks nor sources for the mass of each state variable and also assuming that the mass flow rate is known for all the state variables.

To set the problem in more mathematical terms, let us denote by $q : \mathbb{R} \times [0, +\infty[ \to \mathbb{R}^m$, $q = q(x, t)$, the vector of state variables, *i.e.*, $q_k = q_k$ for $k = 1, \cdots, m$. The mass of $q$ in $[x_1, x_2]$ at time $t$ is defined by:

$$M_{[x_1,x_2]}(t) := \int_{x_1}^{x_2} q(x, t)\, dx \in \mathbb{R}^m. \tag{2.1}$$

Thus, the mass in $[x_1, x_2]$ of the $k$-th state variable $q_k$ is equal to $(M_{[x_1,x_2]}(t))_k$, $\forall k = 1, \cdots, m$. We are going to assume the following physical constraints concerning the total mass of each state variable:

1. No mass is created;
2. No mass is destroyed.

Also, let us assume that the mass flow rate in a point $x$ and at a time $t > 0$ is given by $f(q(x, t))$, where $f : \mathbb{R}^m \to \mathbb{R}^m$ is a continuously differentiable ($C^1$) function. This function $f$ is known as flux function. With the physical constraints that we imposed, the following equation must hold for the mass:

$$\frac{d}{dt}\left(\int_{x_1}^{x_2} q(x,t)\,dx\right) = f(q(x_1,t)) - f(q(x_2,t)). \tag{2.2}$$

Equation (2.2) is known as a conservation law written in integral form and tell us how the mass $M_{[x_1,x_2]}(t)$ varies with time. Another integral form of the conservation law may be obtained integrating Equation (2.2) with respect to time in $[t_1, t_2]$ leading to:

$$\int_{x_1}^{x_2} q(x,t_2)\,dx = \int_{x_1}^{x_2} q(x,t_1)\,dx + \int_{t_1}^{t_2} f(q(x_1,t))\,dt - \int_{t_1}^{t_2} f(q(x_2,t))\,dt. \tag{2.3}$$

Assuming that $q$ is a $C^1$ function, we may write:

$$\int_{t_1}^{t_2} \frac{\partial}{\partial t} q(x,t)\,dt = q(x,t_2) - q(x,t_1), \tag{2.4}$$

and

$$\int_{x_1}^{x_2} \frac{\partial}{\partial x} f(q(x,t))\,dx = f(q(x_2,t)) - f(q(x_1,t)). \tag{2.5}$$

Replacing Equations (2.4) and (2.5) in (2.3) we get the differential form of the conservation law:

$$\int_{t_1}^{t_2}\int_{x_1}^{x_2} \left(\frac{\partial}{\partial t} q(x,t) + \frac{\partial}{\partial x} f(q(x,t))\right) dx\,dt = 0. \tag{2.6}$$

Since Equation (2.6) must hold for all $x_1, x_2, t_1$ and $t_2$ such that $[x_1, x_2] \times [t_1, t_2] \subset \mathbb{R}\times]0, +\infty[$, we obtain the differential form of the conservation law:

$$\frac{\partial}{\partial t} q(x,t) + \frac{\partial}{\partial x} f(q(x,t)) = 0, \quad \forall (x,t) \in \mathbb{R}\times]0,+\infty[. \tag{2.7}$$

We shall assume that the eigenvalues of the Jacobian matrix of the flux function $Df(q)$ are all real and that $Df(q)$ is a diagonalizable matrix, $\forall q \in \mathbb{R}^m$, so that Equation (2.7) is a hyperbolic partial differential equation (LeVeque, 1990). As we will specify latter, some initial condition will also be supposed to be known as well.

Many physical relevant equations may be written as Equation (2.7). Some examples are the Euler equations for gas dynamics, obtained when $m = 3$, and the one-dimensional shallow-water equations, obtained $m = 2$. Another relevant equations are the Burgers equation, which is obtained when $m = 1$ and $f(q) = q^2$. The Burgers equation is well known for developing shocks, even for smooth initial conditions and is a simple prototype to study shock formation. At last, the linear advection equation is another interesting example, which is obtained when $m = 1$ and $f(q(x,t)) = u(x,t)q(x,t)$, where $u(x,t)$ is a given velocity. Strictly speaking, the linear advection is not in the form given by Equation (2.7) since $f$ depends on $q$ but also on $(x,t)$. But, one may check that Equation (2.7) is still hyperbolic in this case. The linear advection equation will play a key role in this work due to its importance to development of atmospheric dynamical cores.

We say that $q$ is a strong or classical solution to the conservation law (2.7) if it is $C^1$ and satisfies the Equation (2.7). Applying the steps from Equation (2.3) to Equation (2.7) in a reverse order, one may check that if $q$ is a strong solution, then it satisfies the integral form (2.3) for all $x_1, x_2, t_1$ and $t_2$ such that $[x_1, x_2] \times [t_1, t_2] \subset \mathbb{R}\times]0, +\infty[$. Therefore, Equations (2.3) and (2.7) are equivalent when $q$ is $C^1$. However, the problem (2.3) can be formulated to functions that are not $C^1$ and have discontinuities. More generally speaking, we say that $q \in L^\infty(D, \mathbb{R}^m)$ [1] if it satisfies the Equation (2.3) for all $x_1, x_2, t_1$ and $t_2$ such that $[x_1, x_2]\times[t_1, t_2] \subset \mathbb{R}\times]0, +\infty[$. It can be shown that this notion of weak solution is equivalent to requiring that (LeVeque, 1990):

$$\int_{-\infty}^{+\infty}\int_{0}^{+\infty}\left(\frac{\partial}{\partial t}\phi(x,t)q(x,t) + \frac{\partial}{\partial x}\phi(x,t)f(q(x,t))\right)dt\,dx = \int_{-\infty}^{+\infty}\phi(x,0)q(x,0)\,dx, \tag{2.8}$$

$\forall\phi \in C_0^1(\mathbb{R}\times[0, +\infty[)$ where $C_0^1(\mathbb{R}\times[0, +\infty[)$ denotes the set of all continuously differentiable functions with compact support in $\mathbb{R} \times [0, +\infty[$. This formulation of weak solution is more common employed on the construction of Discontinuous Galerkin methods (Nair et al., 2011).

In order to develop finite-volume methods for system of conservation laws, it is useful to define the vector of average values of the state variable vector $q$ in the interval $[x_1, x_2]$ at a time $t$ by:

$$Q(t) = \frac{1}{\Delta x}\int_{x_1}^{x_2} q(x,t)\,dx \in \mathbb{R}^m, \tag{2.9}$$

where $\Delta x = x_2 - x_1$. The Equation (2.2) may be rewritten in terms of $Q$ as:

$$\frac{d}{dt}Q(t) = \frac{1}{\Delta x}(f(q(x_1,t)) - f(q(x_2,t))), \tag{2.10}$$

and so is Equation (2.3):

$$Q(t_2) = Q(t_1) + \frac{1}{\Delta x}\left(\int_{t_1}^{t_2} f(q(x_1,t))\,dt - \int_{t_1}^{t_2} f(q(x_2,t))\,dt\right). \tag{2.11}$$

To move towards finite volume schemes, we will restrict our attention to a conservation law in a bounded domain of the form $D = [a, b] \times [0, T]$, $a < b$, $T > 0$. However, we must impose some boundary condition. One possible way and that we will adopted in text are the periodic boundary conditions:

$$q(a,t) = q(b,t), \quad \forall t \in [0, T]. \tag{2.12}$$

Also, we assume that an initial condition $q_0(x) = q(x, 0)$, $q_0 \in L^\infty([a, b], \mathbb{R}^m)$, is given. Thus, we have specified a Cauchy problem. We notice that Equations (2.10) and (2.11) hold for all $x_1, x_2, t_1$ and $t_2$ such that $[x_1, x_2] \times [t_1, t_2] \subset D$. So, let us discretize the domain $D$ and write Equations (2.10) and (2.11) in terms of this discretization. Given a positive integer $N_T$, we define the time step $\Delta t = \frac{T}{N_T}$, $t_n = n\Delta t$, for $n = 0, 1, \cdots, N_T$. For the spatial discretization,

[1] $L^\infty(D, \mathbb{R}^m) = \{q : D \to \mathbb{R}^m$ such that $q$ is bounded.$\}$

we consider an uniformly spaced partition of $[a,b]$ given by:

$$[a,b] = \bigcup_{i=1}^{N} X_i, \text{ where } X_i = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}] \text{ and } a = x_{\frac{1}{2}} < x_{\frac{3}{2}} < \cdots < x_{N-\frac{1}{2}} < x_{N+\frac{1}{2}} = b. \quad (2.13)$$

Each interval $X_i$ is referred to as control volume. We shall use the notations $\Delta x = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}$ and $x_i = \frac{1}{2}(x_{i+\frac{1}{2}} + x_{i-\frac{1}{2}})$, $\forall i = 1, \cdots, N$, to define the control volume length and midpoint, respectively. We also denote by $Q_i(t) \in \mathbb{R}^m$ as the vector of average values of state variable vector at time $t$ in the control volume $X_i$, $\forall i = 1, \cdots, N$. Replacing $t_1, t_2, x_1$ and $x_2$ by $t_n, t_{n+1}, x_{i-\frac{1}{2}}$ and $x_{i+\frac{1}{2}}$, respectively, in Equation (2.10), we get:

$$\frac{d}{dt} Q_i(t) = \frac{1}{\Delta x}(f(q(x_{\frac{i-1}{2}}, t)) - f(q(x_{\frac{i+1}{2}}, t))), \quad \forall i = 1, \cdots, N. \quad (2.14)$$

Similarly, Equation (2.11) becomes:

$$Q_i(t_{n+1}) = Q_i(t_n) + \frac{1}{\Delta x}\left( \int_{t_n}^{t_{n+1}} f(q(x_{i-\frac{1}{2}}, t))\, dt - \int_{t_n}^{t_{n+1}} f(q(x_{i+\frac{1}{2}}, t))\, dt \right), \quad \forall i = 1, \cdots, N, \quad \forall n = 1, \cdots, N_T. \quad (2.15)$$

In order to use a more compact notation, it is helpful to use the following centered difference notation:

$$\delta_x g(x_i, t) = g(x_{i+\frac{1}{2}}, t) - g(x_{i-\frac{1}{2}}, t), \quad (2.16)$$

for an arbitrary vector valued function $g$. Using this notation, Equations (2.14) and (2.15) lead to:

$$\frac{d}{dt} Q_i(t) = -\frac{1}{\Delta x} \delta_x f(q(x_i, t)) \quad \forall i = 1, \cdots, N, \quad (2.17)$$

and

$$Q_i(t_{n+1}) = Q_i(t_n) - \frac{\Delta t}{\Delta x} \delta_x \left( \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} f(q(x_i, t))\, dt \right), \quad \forall i = 1, \cdots, N, \quad \forall n = 1, \cdots, N_T, \quad (2.18)$$

respectively. It is worth pointing out that we have made no approximation in Equations (2.17) and (2.18). Indeed, if $q$ satisfies Equation (2.2), $\forall [x_1, x_2] \subset [a,b]$ and $\forall t \in [0,T]$, then Equation (2.17) is just Equation (2.2) evaluated in the control volumes and written in terms of the average values $Q$. Similarly, if $q$ satisfies Equation (2.3), $\forall [x_1, x_2] \times [t_1, t_2] \subset D$, then Equation (2.18) is just Equation (2.3) evaluated in the control volumes, at the time instants $t_n$, and written in terms of the average values $Q$.

Notice that in Equation (2.18) we divided and multiplied by $\Delta t$, so that we can interpret $\frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} f(q(x_i, t))\, dt$ as a mean-time average flux. This interpretation is very handy for the derivation of finite-volume schemes.

The formulations given by Equations (2.17) and (2.18) are the cornerstone of the development of finite volume methods for conservation laws. On the right-hand side of Equation (2.17), the flux function $f$ may be discretized leading to an ordinary differential equation (ODE) that might be solved using classical ODE integrators. These methods are known as semi-discrete methods (LeVeque, 2002), since only the spatial coordinate is discretized. In this work we shall restrict our attention to methods based on Equation (2.18).

## 2.2 The finite-volume approach

We summarize the problem of the system of conservation laws in the integral form discussed in Section 2.1 in Problem 2.1.

**Problem 2.1.** *Given $D = [a,b] \times [0,T]$, a $C^1$ flux function $f : \mathbb{R}^m \to \mathbb{R}^m$, $m \geq 1$, we would like to find the weak solution $q \in L^\infty(D, \mathbb{R}^m)$ of the system of conservation laws in the integral form:*

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

*$\forall [x_1,x_2] \times [t_1,t_2] \subset D$, given the initial condition $q(x,0) = q_0(x)$, $\forall x \in [a,b]$, and assuming periodic boundary conditions, i.e., $q(a,t) = q(b,t)$, $\forall t \in [0,T]$.*

We point out that, for Problem 2.1, the total mass in $[a,b]$ satisfies:

$$M_{[a,b]}(t) = M_{[a,b]}(0), \quad \forall t \in [0,T]. \tag{2.19}$$

This is the conservation of total mass propriety and is highly desirable for any numerical scheme that intends to give a robust approximation of the system of conservation laws solution.

In Section 2.1 we introduced a version of Problem 2.1 considering a discretization of the domain $D$. This idea is summarized in Problem 2.2.

**Problem 2.2.** *Assume the framework of Problem 2.1. We consider positive integers $N$ and $N_T$, a spatial discretization of [a,b] given by $X_i = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$, $\forall i = 1, \cdots, N$, $a = x_{\frac{1}{2}} < x_{\frac{3}{2}} < \cdots < x_{N-\frac{1}{2}} < x_{N+\frac{1}{2}} = b$, $\Delta x = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}$, a time discretization $t_n = n\Delta t$, $\Delta t = \frac{T}{N_T}$, $\forall n = 1, \cdots, N_T$. Since we are in the framework of Problem 2.1, it follows that:*

$$Q_i(t_{n+1}) = Q_i(t_n) - \frac{\Delta t}{\Delta x}\delta_x\left(\frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} f(q(x_i,t))\,dt\right), \quad \forall i = 1, \cdots, N, \quad \forall n = 1, \cdots, N_T,$$

*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 $Q_i(t_n)$, $\forall i = 1, \cdots, N$, $\forall n = 1, \cdots, N_T$, given the initial values $Q_i(0)$, $\forall i = 1, \cdots N$. In other words, we would like to find the average values of $q$ in each control volume $X_i$ at the considered time instants.*

Finally, we define the one-dimensional (1D) finite-volume (FV) scheme problem as follows in Problem 2.3. We use the notation $q_i^n = q(x_i, t_n)$ to represent the values of $q$ in the discrete domain $D$.

**Problem 2.3** (1D-FV scheme)**.** *Assume the framework defined in Problem 2.2. The finite-*

*volume approach of Problem 2.2 consists of a finding a scheme of the form:*

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x}(F_{i+\frac{1}{2}}^n - F_{i-\frac{1}{2}}^n), \quad \forall i = 1, \cdots, N, \quad \forall n = 1, \cdots, N_T,$$

*where $Q_i^n \in \mathbb{R}^m$ is intended to be an approximation of $Q_i(t_n)$ in some sense. We define by $Q_i^0 = Q_i(0)$ or $Q_i^0 = q_i^0$. The term $F_{i+\frac{1}{2}}^n$ approximates $\frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} f(q(x_{i+\frac{1}{2}}, t))\,dt$ and the term $F_{i-\frac{1}{2}}^n$ approximates $\frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} f(q(x_{i-\frac{1}{2}}, t))\,dt$, or, in other words, they estimate the time-averaged fluxes at the control volume $X_i$ boundaries.*

(Colella & Woodward, 1984) (Carpenter et al., 1990) (Van Leer, 1977) (Lin et al., 1994) (Lin & Rood, 1996)

## 2.3 The piecewise-parabolic method

Let us consider a function $q \in L^\infty([a,b],\mathbb{R})$, a discretization of $[a,b]$ as in Problem 2.2 and assume that we are given the average values $Q_i = \frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} q(x)\,dx$ on each control volume $X_i$, $\forall i = 1, \cdots, N$. Throughout this subsection, it will be useful to make use of the indicator function of each control volume $X_i$ defined by:

$$\chi_i(x) = \begin{cases} 1 & \text{if } x \in X_i \\ 0 & \text{otherwise} \end{cases} \tag{2.20}$$

Our task is to find a piecewise-parabolic (PP) function:

$$q_{PP}(x) = \sum_{i=1}^{N} \chi_i(x) q_i(x), \tag{2.21}$$

where $q_i \in \mathcal{P}_2$ [2] is such that:

1. $\frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} q_i(x)\,dx = Q_i$, that is, $q_i$ preserves the mass on each control volume $X_i$;
2. No new extreme is generated, that is, $Q_{i-1} \leq q_i(x) \leq Q_{i+1}$, $\forall x \in X_i$.

### 2.3.1 Reconstruction

We shall assume that each $q_i$ may be expressed as:

$$q_i(x) = q_{L,i} + z_i(x)(\Delta q_i + q_{6,i}(1 - z_i(x))), \quad \text{where } z_i(x) = \frac{x - x_{i-\frac{1}{2}}}{\Delta x}, \quad x \in X_i, \tag{2.22}$$

where the values $q_{L,i}$, $\Delta q_i$ and $q_{6,i}$ will be specified latter. Note that each $z_i$ is just a normalization function that maps $X_i$ onto $[0,1]$. Under this assumption, it is easy to see that

[2] $\mathcal{P}_n$ stands for the space of real polynomials of degree $\leq$ n.

$\lim_{x\to x^+_{i-\frac{1}{2}}} q_i(x) = q_{L,i}$. If we define $q_{R,i} = \lim_{x\to x^-_{i+\frac{1}{2}}} q_i(x)$, then we have:

$$\Delta q_i = q_{R,i} - q_{L,i}. \tag{2.23}$$

The average value of $q_i$ is given by:

$$\frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} q_i(x)\,dx = \frac{(q_{L,i}+q_{R,i})}{2} + \frac{q_{6,i}}{6} \tag{2.24}$$

Under the hypothesis of mass conservation, we have:

$$q_{6,i} = 6\left(Q_i - \frac{(q_{L,i}+q_{R,i})}{2}\right). \tag{2.25}$$

Therefore, we have found the parameters $\Delta q_i$ and $q_{6,i}$ as functions of the parameters $q_{L,i}$ and $q_{R,i}$, such that the polynomial $p_i$ from (2.21) guarantees mass conservation. To completely determine the polynomial $p_i$, we need to set the values $q_{L,i}$ and $q_{R,i}$, which, as we have seen, represent the limits of $q_i$ when $x$ tends to the left and right boundaries of $X_i$, respectively. Hence, it is natural to seek for $q_{L,i}$ as an approximation of $q(x_{i-\frac{1}{2}})$ and $q_{R,i}$ as an approximation of $q(x_{i+\frac{1}{2}})$. So, let us describe a way to approximate $q(x_{i+\frac{1}{2}})$, and denote its estimation by $q_{i+\frac{1}{2}}$ $\forall i = 0, 1, \cdots, N$. We introduce the following function:

$$Q(x) = \int_a^x q(\xi)\,d\xi, \tag{2.26}$$

and we notice that:

$$Q(x_{i+1}) = \Delta x \sum_{k=1}^{i} Q_k \text{ and } Q'(x) = q(x). \tag{2.27}$$

Therefore $Q'(x_{i+\frac{1}{2}}) = q(x_{i+\frac{1}{2}})$, $\forall i = 0, 1, \cdots, N$. We introduce a quartic polynomial $Q_{i4} \in \mathcal{P}_4$ that interpolates the data $\left(x_{i+k+\frac{1}{2}}, Q(x_{i+k+\frac{1}{2}})\right)_{k=-2,-1,0,1,2}$. Then, we define $q_{i+\frac{1}{2}} = \frac{d}{dx}Q_{i4}(x_{i+k+\frac{1}{2}})$. An explicit expression for $q_{i+\frac{1}{2}}$ is given by (Colella & Woodward, 1984):

$$q_{i+\frac{1}{2}} = \frac{1}{2}\left(Q_{i+1} + Q_i\right) - \frac{1}{6}\left(\delta Q_{i+1} - \delta Q_i\right), \tag{2.28}$$

where $\delta Q_i$ is the average slope in the $i$-th control-volume:

$$\delta Q_i = \frac{1}{2}\left(Q_{i+1} - Q_{i-1}\right). \tag{2.29}$$

We notice that Formula (2.29) may be rewritten more explicitly as:

$$q_{i+\frac{1}{2}} = \frac{7}{12}\left(Q_{i+1} + Q_i\right) - \frac{1}{12}\left(Q_{i+2} + Q_{i-1}\right). \tag{2.30}$$

The Formula (2.30) is fourth-order accurate if $q$ is at least $C^4$ (Colella & Woodward, 1984).

Indeed, we prove this in Proposition 2.1 by noticing that this Formula may be thought as a finite-difference scheme.

**Proposition 2.1.** *Given $h > 0$, let $q \in C^4([-2h, 2h])$. Then, the following identity holds:*

$$q(0) = \frac{7}{12}\left(\frac{1}{h}\int_0^h q(x)\,dx + \frac{1}{h}\int_{-h}^0 q(x)\,dx\right) - \frac{1}{12}\left(\frac{1}{h}\int_h^{2h} q(x)\,dx + \frac{1}{h}\int_{-2h}^{-h} q(x)\,dx\right) + Ch^4, \tag{2.31}$$

*where $C$ is a constant that depends only on $q$ and $h$.*

*Proof.* We define $F(z) = \int_0^z q(x)\,dx$ for $z \in [-2h, 2h]$. It follows that:

$$\begin{aligned}
\int_0^h q(x)\,dx &= F(h),\\
\int_{-h}^0 q(x)\,dx = -\int_0^{-h} q(x)\,dx &= F(-h),\\
\int_h^{2h} q(x)\,dx = \int_0^{2h} q(x)\,dx - \int_0^h q(x)\,dx &= F(2h) - F(h),\\
\int_{-h}^{-2h} q(x)\,dx = \int_{-2h}^0 q(x)\,dx - \int_{-h}^0 q(x)\,dx &= -F(-2h) + F(-h),
\end{aligned}$$

which yields:

$$\begin{aligned}
\int_0^h q(x)\,dx + \int_{-h}^0 q(x)\,dx &= F(h) - F(-h),\\
\int_h^{2h} q(x)\,dx + \int_{-2h}^{-h} q(x)\,dx &= F(2h) - F(-2h) - (F(h) - F(-h)).
\end{aligned}$$

Using these identities, Equation (2.31) may be rewritten as:

$$q(0) = \frac{4}{3}\left(\frac{F(h) - F(-h)}{2h}\right) - \frac{1}{3}\left(\frac{F(2h) - F(-2h)}{4h}\right) + Ch^4, \tag{2.32}$$

which consists of finite-difference approximations. Thus, Equation (2.31) follows from Lemma A.1 with:

$$C = \frac{1}{240}\left(q^{(4)}(\theta_h) + q^{(4)}(\theta_{-h})\right) - \frac{1}{45}\left(q^{(4)}(\theta_{2h}) + q^{(4)}(\theta_{-2h})\right), \tag{2.33}$$

where $\theta_h \in [0, h], \theta_{-h} \in [-h, 0], \theta_{2h} \in [0, 2h], \theta_{-2h} \in [-2h, 0]$, which concludes the proof.

### 2.3.2 Flux

# Chapter 3

# Two-dimensional finite-volume methods

## 3.1 Two-dimensional system of conservation laws in integral form

Let us consider $C^1$ flux functions $f : \mathbb{R}^m \to \mathbb{R}^m$ and $g : \mathbb{R}^m \to \mathbb{R}^m$ in $x$ and $y$ direction, respectively. A two-dimensional system of conservation laws in the differential form in a domain $\Omega = [a, b] \times [c, d] \subset \mathbb{R}^2$ associated to the fluxes $f$ and $g$ is given by:

$$\frac{\partial}{\partial t} q(x, y, t) + \frac{\partial}{\partial x} f(q(x, y, t)) + \frac{\partial}{\partial y} g(q(x, y, t)) = 0, \quad \forall (x, y, t) \in \Omega^{\circ} \times ]0, +\infty[.[1] \tag{3.1}$$

The solution $q$ is interpreted as the vector of state variable densities. A classical or strong solution to this system of conservation laws is a $C^1$ function $q$ satisfying Equation (3.1). As we did in Section 2.1, our goal is to deduce an integral form of Equation (3.1). To do so, let us consider $[x_1, x_2] \times [y_1, y_2] \subset \Omega^{\circ}$ and $[t_1, t_2] \subset [0, +\infty[$. Integrating Equation (3.1) over $[x_1, x_2] \times [y_1, y_2]$ yields:

$$\begin{aligned} \frac{d}{dt}\left( \int_{x_1}^{x_2} \int_{y_1}^{y_2} q(x, y, t)\, dx\, dy \right) = &- \int_{y_1}^{y_2} \Big( f(q(x_2, y, t)) - f(q(x_1, y, t)) \Big)\, dy \\ &- \int_{x_1}^{x_2} \Big( g(q(x, y_2, t)) - g(q(x, y_1, t)) \Big)\, dx. \end{aligned} \tag{3.2}$$

Integrating Equation (3.2) over the time interval $[t_1, t_2]$, we have:

[1] $\Omega^{\circ}$ denotes the interior of $\Omega$. Namely, $\Omega^{\circ} = ]a, b[ \times ]c, d[$.

$$\int_{x_1}^{x_2}\int_{y_1}^{y_2} q(x,y,t_{n+1})\,dx\,dy = \int_{x_1}^{x_2}\int_{y_1}^{y_2} q(x,y,t_n)\,dx\,dy \\ - \int_{t_1}^{t_2}\int_{y_1}^{y_2}\Big(f(q(x_2,y,t)) - f(q(x_1,y,t))\Big)\,dy\,dt \\ - \int_{t_1}^{t_2}\int_{x_1}^{x_2}\Big(g(q(x,y_2,t)) - g(q(x,y_1,t))\Big)\,dx\,dt. \tag{3.3}$$

Equation (3.3) is the integral form of Equation (3.1). We say that $q \in L^\infty(\Omega \times [0,+\infty[, \mathbb{R}^m)$ is a weak solution to the system of conservation laws (3.1) if $q$ satisfies the integral form (3.3), $\forall [x_1,x_2]\times[y_1,y_2] \subset \Omega^o$ and $\forall [t_1,t_2] \subset [0,+\infty[$. Similarly to Section 2.1, these problems are equivalent when $q$ is a $C^1$ function.

We consider an initial condition $q_0 \in L^\infty(\Omega)$, $q(x,y,0) = q_0(x,y)$, $\forall (x,y) \in \Omega$. Boundary conditions will be assumed bi-periodic. At last, the matrix $\alpha Df(q) + \beta Dg(q)$ is assumed to have real eigenvalues and be diagonalizable $\forall q \in \mathbb{R}^m, \forall \alpha,\beta \in \mathbb{R}$ (LeVeque, 1990), so that we have a hyperbolic conservation law. Therefore, we are again dealing with a Cauchy problem.

To move in the direction of a discrete version of Equation (3.3), let us discretize the domain $D = \Omega \times [0,T]$ following the notations of Section 2.1. Given a positive integer $N_T$, we define the time step $\Delta t = \frac{T}{N_T}$, $t_n = n\Delta t$, for $n = 0,1,\cdots,N_T$. The spatial discretization is constructed through an uniformly spaced partition of $\Omega$ given by:

$$[a,b] = \bigcup_{i=1}^{N} X_i, \text{ where } X_i = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}] \text{ and } a = x_{\frac{1}{2}} < x_{\frac{3}{2}} < \cdots < x_{N-\frac{1}{2}} < x_{N+\frac{1}{2}} = b, \tag{3.4}$$

$$[c,d] = \bigcup_{j=1}^{M} Y_j, \text{ where } Y_j = [y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}}] \text{ and } c = y_{\frac{1}{2}} < y_{\frac{3}{2}} < \cdots < y_{M-\frac{1}{2}} < y_{M+\frac{1}{2}} = d, \tag{3.5}$$

$$\Omega = \bigcup_{i=1}^{N}\bigcup_{j=1}^{M} \Omega_{ij}, \text{ where } \Omega_{ij} = X_i \times Y_j. \tag{3.6}$$

The regions $\Omega_{ij}$ are known as control volumes. Similarly to Chapter 2 we employ the notations $\Delta x = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}$, $\Delta y = y_{j+\frac{1}{2}} - y_{j-\frac{1}{2}}$ and $x_i = \frac{1}{2}(x_{i+\frac{1}{2}} + x_{i-\frac{1}{2}})$ $y_j = \frac{1}{2}(y_{j+\frac{1}{2}} + y_{j-\frac{1}{2}})$, $\forall i = 1,\cdots,N, \forall j = 1,\cdots,M$, to define the control volume lengths and midpoints, respectively. Finally, we denote by $Q_{ij}(t) \in \mathbb{R}^m$ as the vector of average values of state variable vector at time $t$ in the control volume $\Omega_{ij}$, that is:

$$Q_{ij}(t) = \frac{1}{\Delta x \Delta y}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}}\int_{y_{j-\frac{1}{2}}}^{y_{j-\frac{1}{2}}} q(x,t)\,dx \in \mathbb{R}^m. \tag{3.7}$$

Substituting $t_1, t_2, x_1, x_2, y_1$ and $y_2$ by $t_n, t_{n+1}, x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}, y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}}$, respectively, in Equation (3.3), we obtain:

$$Q_{ij}(t_{n+1}) = Q_{ij}(t_n) - \frac{\Delta t}{\Delta x \Delta y}\delta_x\left(\frac{1}{\Delta t}\int_{t_1}^{t_2}\int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} f(q(x_i, y, t))\,dy\,dt\right) - \frac{\Delta t}{\Delta x \Delta y}\delta_y\left(\frac{1}{\Delta t}\int_{t_1}^{t_2}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} g(q(x, y_j, t))\,dx\,dt\right), \tag{3.8}$$

where we are using the centered finite-difference notation:

$$\delta_x h(x_i, y, t) = h(x_{i+\frac{1}{2}}, y, t) - h(x_{i-\frac{1}{2}}, y, t), \tag{3.9}$$

$$\delta_y h(x, y_j, t) = h(x, y_{j+\frac{1}{2}}, t) - h(x, y_{j-\frac{1}{2}}, t), \tag{3.10}$$

for any function $h$. The Equation (3.8) is useful to motivate two-dimensional finite-volume schemes, as we shall see in the next section.

## 3.2 The finite-volume approach

This Section is basically an extension to two dimensions of the concepts presented in Section 2.2. The problem of two-dimensional system of conservation laws in the integral form presented Section 3.1 is written in a concise way in Problem 3.1.

**Problem 3.1.** *Given $\Omega = [a, b] \times [c, d]$, $D = \Omega \times [0, T]$, $C^1$ flux functions $f, g : \mathbb{R}^m \to \mathbb{R}^m$, $m \geq 1$, we would like to find the weak solution $q \in L^\infty(D, \mathbb{R}^m)$ of the two-dimensional system of conservation laws in the integral form:*

$$\int_{x_1}^{x_2}\int_{y_1}^{y_2} q(x, y, t)\,dx\,dy = \int_{x_1}^{x_2}\int_{y_1}^{y_2} q(x, y, t)\,dx\,dy - \int_{t_1}^{t_2}\int_{y_1}^{y_2}\Big(f(q(x_2, y, t)) - f(q(x_1, y, t))\Big)\,dy\,dt - \int_{t_1}^{t_2}\int_{x_1}^{x_2}\Big(g(q(x, y_2, t)) - g(q(x, y_1, t))\Big)\,dx\,dt.$$

*$\forall [x_1, x_2] \times [y_1, y_2] \times [t_1, t_2] \subset D$, given the initial condition $q(x, y, 0) = q_0(x, y), \forall (x, y) \in \Omega$, and assuming bi-periodic boundary conditions, i.e., $q(a, y, t) = q(b, y, t)$, $\forall t \in [0, T]$, $\forall y \in [c, d]$, and $q(x, c, t) = q(x, d, t)$, $\forall t \in [0, T]$, $\forall x \in [a, b]$.*

For Problem 3.1, the total mass in $\Omega$ is defined by:

$$M_\Omega(t) = \int_\Omega q(x, y, t)\,dx\,dy \in \mathbb{R}^m, \quad \forall t \in [0, T], \tag{3.11}$$

and is conserved within time:

$$M_\Omega(t) = M_\Omega(0), \quad \forall t \in [0, T]. \tag{3.12}$$

Section 3.1 introduced a version of Problem 3.1 considering a discretization of the domain $D$. This version is also summarized in Problem 3.2.

**Problem 3.2.** *Assume the framework of Problem 3.1. We consider positive integers $N$ and $N_T$, a spatial discretization of [a,b] given by $X_i = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$, $\forall i = 1, \cdots, N$, $a = x_{\frac{1}{2}} < x_{\frac{3}{2}} < \cdots < x_{N-\frac{1}{2}} < x_{N+\frac{1}{2}} = b$, $\Delta x = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}$, $Y_j = [y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}}]$, $\forall j = 1, \cdots, M$, $c = y_{\frac{1}{2}} < y_{\frac{3}{2}} < \cdots < y_{M-\frac{1}{2}} < y_{M+\frac{1}{2}} = d$, $\Delta y = y_{j+\frac{1}{2}} - y_{j-\frac{1}{2}}$, $\Omega_{ij} = X_i \times Y_j$, a time discretization $t_n = n\Delta t$, $\Delta t = \frac{T}{N_T}$, $\forall n = 1, \cdots, N_T$. Since we are in the framework of Problem 3.2, it follows that:*

$$
\begin{aligned}
Q_{ij}(t_{n+1}) = Q_{ij}(t_n) &- \frac{\Delta t}{\Delta x \Delta y}\delta_x\left(\frac{1}{\Delta t}\int_{t_1}^{t_2}\int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} f(q(x_i, y, t))\,dy\,dt\right) \\
&- \frac{\Delta t}{\Delta x \Delta y}\delta_y\left(\frac{1}{\Delta t}\int_{t_1}^{t_2}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} g(q(x, y_j, t))\,dx\,dt\right),
\end{aligned}
$$

*where $Q_{ij}(t) = \frac{1}{\Delta x \Delta y}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}}\int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} q(x, y, t)\,dx\,dy$.*

*Our problem now consists of finding the values $Q_{ij}(t_n)$, $\forall i = 1, \cdots, N$, $\forall j = 1, \cdots, M$, $\forall n = 1, \cdots, N_T$, given the initial values $Q_{ij}(0)$, $\forall i = 1, \cdots N$, $\forall j = 1, \cdots, M$. In other words, we would like to find the average values of $q$ in each control volume $\Omega_{ij}$ at the considered time instants.*

Finally, we define the one-dimensional (2D) finite-volume (FV) scheme problem as follows in Problem 3.3. We use the notation $q_{ij}^n = q(x_i, y_j, t_n)$ to represent the values of $q$ in the discrete domain $D$.

**Problem 3.3** (2D-FV scheme)**.** *Assume the framework defined in Problem 3.2. The finite-volume approach of Problem 3.1 consists of a finding a scheme of the form:*

$$
\begin{gathered}
Q_{ij}^{n+1} = Q_{ij}^n - \frac{\Delta t}{\Delta x \Delta y}(F_{i+\frac{1}{2},j}^n - F_{i-\frac{1}{2},j}^n) - \frac{\Delta t}{\Delta x \Delta y}(G_{i,j+\frac{1}{2}}^n - G_{i,j-\frac{1}{2}}^n), \\
\forall i = 1, \cdots, N, \quad \forall j = 1, \cdots, M, \quad \forall n = 1, \cdots, N_T,
\end{gathered}
$$

*where $Q_{ij}^n \in \mathbb{R}^m$ is intended to be an approximation of $Q_{ij}(t_n)$ in some sense. We define by $Q_{ij}^0 = Q_{ij}(0)$ or $Q_{ij}^0 = q_{i,j}^0$.*

*The term $F_{i+\frac{1}{2},j}^n$ approximates $\frac{1}{\Delta t}\int_{t_n}^{t_{n+1}}\int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} f(q(x_{i+\frac{1}{2}}, y, t))\,dy\,dt$, $F_{i-\frac{1}{2},j}^n$ approximates $\frac{1}{\Delta t}\int_{t_n}^{t_{n+1}}\int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} f(q(x_{i-\frac{1}{2}}, y, t))\,dy\,dt$, $G_{i,j+\frac{1}{2}}^n$ approximates $\frac{1}{\Delta t}\int_{t_n}^{t_{n+1}}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} g(q(x, y_{j+\frac{1}{2}}, t))\,dx\,dt$, $G_{i,j-\frac{1}{2}}^n$ approximates $\frac{1}{\Delta t}\int_{t_n}^{t_{n+1}}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} g(q(x, y_{j-\frac{1}{2}}, t))\,dx\,dt$, or, in other words, they estimate the time-averaged fluxes at the control volume $\Omega_{ij}$ boundaries.*

## 3.3 Dimension splitting

(Lin & Rood, 1997) (Lin, 2004) (Putman, 2007) (Putman & Lin, 2007)

# Chapter 4

# Cubed-sphere grids

(Sadourny, 1972) (Ronchi et al., 1996) (Rančić et al., 1996) (Taylor et al., 1997) (Nair et al., 2005) (Lauritzen et al., 2011)

To be written!

## 4.1 To be written

# Chapter 5

# Cubed-sphere finite-volume methods

To be written!

## 5.1 To be written

# Appendix A

# Finite-difference estimatives

**Lemma A.1.** *Given $h > 0$, $x_0 \in \mathbb{R}$, let $F \in C^5([x_0 - 2h, x_0 + 2h])$. Then, the following identity holds:*

$$F'(x_0) = \frac{4}{3}\left(\frac{F(x_0+h) - F(x_0-h)}{2h}\right) - \frac{1}{3}\left(\frac{F(x_0+2h) - F(x_0-2h)}{4h}\right) + Ch^4, \qquad \text{(A.1)}$$

*where $C$ is a constant that depends only on $F$ and $h$.*

*Proof.* Given $\delta \in ]0, 2h]$, then $x_0 + \delta \in ]x_0, x_0 + 2h]$ and $x_0 - \delta \in ]x_0 - 2h, x_0]$. Then, we get using the Taylor expansion of $F$:

$$F(x_0+\delta) = F(x_0) + F'(x_0)\delta + F^{(2)}(0)\frac{\delta^2}{2} + F^{(3)}(x_0)\frac{\delta^3}{3!} + F^{(4)}(x_0)\frac{\delta^3}{4!} + F^{(5)}(\theta_\delta)\frac{\delta^5}{5!} \quad \theta_\delta \in [x_0, x_0+\delta],$$
$$F(x_0-\delta) = F(x_0) - F'(x_0)\delta + F^{(2)}(0)\frac{\delta^2}{2} - F^{(3)}(x_0)\frac{\delta^3}{3!} + F^{(4)}(x_0)\frac{\delta^4}{4!} - F^{(5)}(\theta_{-\delta})\frac{\delta^5}{5!}, \quad \theta_{-\delta} \in [x_0-\delta, x_0].$$

Thus:

$$\frac{F(x_0+\delta) - F(x_0-\delta)}{2\delta} = F'(x_0) + F^{(3)}(x_0)\frac{\delta^2}{3!} + \left(F^{(5)}(\theta_\delta) + F^5(\theta_{-\delta})\right)\frac{\delta^4}{2 \cdot 5!}, \qquad \text{(A.2)}$$

Applying Equation (A.2) for $\delta = h$ and $\delta = 2h$, we get, respectively:

$$\frac{F(x_0+h) - F(x_0-h)}{2h} = F'(x_0) + F^{(3)}(x_0)\frac{h^2}{3!} + \left(F^{(5)}(\theta_h) + F^{5)}(\theta_{-h})\right)\frac{h^4}{2 \cdot 5!}, \quad \theta_h \in [x_0, x_0+h], \quad \theta_{-h} \in [x_0-h, x_0], \qquad \text{(A.3)}$$

and

$$\frac{F(x_0+2h) - F(x_0-2h)}{4h} = F'(x_0) + F^{(3)}(x_0)\frac{4h^2}{3!} + \left(F^{(5)}(\theta_{2h}) + F^{(5)}(\theta_{-2h})\right)\frac{16h^4}{2 \cdot 5!}, \qquad \text{(A.4)}$$
$$\theta_{2h} \in [x_0, x_0+2h], \quad \theta_{-2h} \in [x_0-2h, x_0].$$

Using Equations (A.3) and (A.4), we obtain:

$$\frac{4}{3}\left(\frac{F(h)-F(-h)}{2h}\right) = \frac{4}{3}F'(x_0) + F^{(3)}(x_0)\frac{4h^2}{3\cdot 3!} + \left(F^{(5)}(\theta_h) + F^{(5)}(\theta_{-h})\right)\frac{h^4}{2\cdot 5!}, \tag{A.5}$$

$$\frac{1}{3}\left(\frac{F(2h)-F(-2h)}{4h}\right) = \frac{1}{3}F'(x_0) + F^{(3)}(x_0)\frac{4h^2}{3\cdot 3!} + \left(F^{(5)}(\theta_{2h}) + F^{(5)}(\theta_{-2h})\right)\frac{16h^4}{3\cdot 2\cdot 5!} \tag{A.6}$$

Subtracting Equation (A.6) from Equation (A.5) we get the desired Equation (A.1) with

$$C = \frac{1}{240}\left(F^{(5)}(\theta_h) + F^{(5)}(\theta_{-h})\right) - \frac{1}{45}\left(F^{(5)}(\theta_{2h}) + F^{(5)}(\theta_{-2h})\right), \tag{A.7}$$

where $\theta_h \in [x_0, x_0 + h], \theta_{-h} \in [x_0 - h, x_0]$, $\theta_{2h} \in [x_0, x_0 + 2h], \theta_{-2h} \in [x_0 - 2h, x_0]$, which concludes the proof.

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