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

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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**. Exame de Qualificação (Doutorado). Instituto de Matemática e Estatística, Universidade de São Paulo, São Paulo, 2022.

Elemento obrigatório, constituído de uma sequência de frases concisas e objetivas, em forma de texto. Deve apresentar os objetivos, métodos empregados, resultados e conclusões. O resumo deve ser redigido em parágrafo único, conter no máximo 500 palavras e ser seguido dos termos representativos do conteúdo do trabalho (palavras-chave). Deve ser precedido da referência do documento. Texto texto. Texto texto.

Palavras-chave: Palavra-chave1. Palavra-chave2. Palavra-chave3.

Abstract

Luan da Fonseca Santos. **Analysis and development of finite volume methods for the new generation of cubed sphere dynamical cores for the atmosphere**. Qualifying Exam (Doctorate). Institute of Mathematics and Statistics, University of São Paulo, São Paulo, 2022.

Elemento obrigatório, elaborado com as mesmas características do resumo em língua portuguesa. De acordo com o Regimento da Pós-Graduação da USP (Artigo 99), deve ser redigido em inglês para fins de divulgação. É uma boa ideia usar o sítio www.grammarly.com na preparação de textos em inglês. Text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text. Text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text text.

Keywords: Keyword1. Keyword2. Keyword3.

Contents

Introduction

To be written!

Chapter 1

One-dimensional finite-volume methods

1.1 One-dimensional conservation laws in integral form

In this section, we are going to present the derivation of one-dimensional 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 variables given by functions $q_1, \cdots, q_m : \mathbb{R} \times [0, +\infty[\longrightarrow \mathbb{R}$ evolve within time in the considered time interval, assuming that we have neither sinks nor sources for the mass of each state variable and that the mass flow rate is known for all the state variables.

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

$$\mathbf{M}_{[x_1,x_2]}(t) := \int_{x_1}^{x_2} \mathbf{q}(x, t)\, dx \in \mathbb{R}^m. \tag{1.1}$$

Thus, the total mass in $[x_1, x_2]$ of the k-th state variable q_k is equal to $(\mathbf{M}_{[x_1,x_2]}(t))_k$, $\forall k = 1, \cdots, m$. 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 $\mathbf{f}(\mathbf{q}(x, t))$, where $\mathbf{f} : \mathbb{R}^m \longrightarrow \mathbb{R}^m$ is a continuously differentiable ($\mathcal{C}^1$) function. This function $\mathbf{f}$ is known as flux function. With the physical constraints that we imposed, the following equation must hold for the mass:

$$\frac{d}{dt}\left(\int_{x_1}^{x_2} \mathbf{q}(x,t)\,dx\right) = \mathbf{f}(\mathbf{q}(x_1,t)) - \mathbf{f}(\mathbf{q}(x_2,t)). \tag{1.2}$$

Equation (1.2) is known as a conservation law written in integral form and tell us how the total mass $\mathbf{M}_{[x_1,x_2]}(t)$ varies with time. Another integral form of the conservation law may be obtained integrating Equation (1.2) with respect to time in $[t_1, t_2]$ leading to:

$$\int_{x_1}^{x_2} \mathbf{q}(x,t_2)\,dx = \int_{x_1}^{x_2} \mathbf{q}(x,t_1)\,dx + \int_{t_1}^{t_2} \mathbf{f}(\mathbf{q}(x_1,t))\,dt - \int_{t_1}^{t_2} \mathbf{f}(\mathbf{q}(x_2,t))\,dt. \tag{1.3}$$

Assuming that $\mathbf{q}$ is a C^1 function, we may write:

$$\int_{t_1}^{t_2} \frac{\partial}{\partial t}\mathbf{q}(x,t)\,dt = \mathbf{q}(x,t_2) - \mathbf{q}(x,t_1), \tag{1.4}$$

and

$$\int_{x_1}^{x_2} \frac{\partial}{\partial x}\mathbf{f}(\mathbf{q}(x,t))\,dx = \mathbf{f}(\mathbf{q}(x_2,t)) - \mathbf{f}(\mathbf{q}(x_1,t)). \tag{1.5}$$

Replacing Equations (1.4) and (1.5) in (1.3) we get the differential form of the conservation law:

$$\int_{t_1}^{t_2}\int_{x_1}^{x_2} \left(\frac{\partial}{\partial t}\mathbf{q}(x,t) + \frac{\partial}{\partial x}\mathbf{f}(\mathbf{q}(x,t))\right) dx\,dt = 0. \tag{1.6}$$

Since Equation (1.6) 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:

$$\frac{\partial}{\partial t}\mathbf{q}(x,t) + \frac{\partial}{\partial x}\mathbf{f}(\mathbf{q}(x,t)) = 0, \quad \forall (x,t) \in \mathbb{R}\times]0,+\infty[. \tag{1.7}$$

Hyperbolic and eigenvalues. Initial conditions.

Many physical relevant equations may be written as Equation (1.7). 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 $f(q) = q^2$, and the linear advection equation, 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 (1.7) since f depends on q but also on (x,t). But, one may check that Equation (1.7) 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 $\mathbf{q}$ is a strong or classical solution to the conservation law (1.7) if it is C^1 and satisfies the Equation (1.7). Applying the steps from Equation (1.3) to Equation (1.7) in a reverse order, one may check that if $\mathbf{q}$ is a strong solution, then it satisfies the integral form (1.3) 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 (1.3) and (1.7) are equivalent when $\mathbf{q}$ is C^1. However, the problem (1.3) can be formulated functions that are not C^1 and have discontinuities. More generally speaking, we say that $\mathbf{q} \in L^\infty(\Omega, \mathbb{R}^m)$ [1] if it satisfies the Equation (1.3) 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):

$$\int_{-\infty}^{+\infty} \int_{0}^{+\infty} \left(\frac{\partial}{\partial t}\phi(x,t)\mathbf{q}(x,t) + \frac{\partial}{\partial x}\phi(x,t)\mathbf{f}(\mathbf{q}(x,t)) \right) dt\, dx = \int_{-\infty}^{+\infty} \phi(x,0)\mathbf{q}(x,0)\, dx, \tag{1.8}$$

$\forall \phi \in C_0^1(\mathbb{R} \times [0, +\infty[)$ 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 Discontinous Galerkin methods (Nair *et al.*, 2011).

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

$$\mathbf{Q}(t) = \frac{1}{\Delta x} \int_{x_1}^{x_2} \mathbf{q}(x,t)\, dx \in \mathbb{R}^m, \tag{1.9}$$

where $\Delta x = x_2 - x_1$. The Equation (1.2) may be rewritten in terms of $\mathbf{Q}$ as:

$$\frac{d}{dt}\mathbf{Q}(t) = \frac{1}{\Delta x}(\mathbf{f}(\mathbf{q}(x_1,t)) - \mathbf{f}(\mathbf{q}(x_2,t))), \tag{1.10}$$

and so is Equation (1.3):

$$\mathbf{Q}(t_2) = \mathbf{Q}(t_1) + \frac{1}{\Delta x}\left(\int_{t_1}^{t_2} \mathbf{f}(\mathbf{q}(x_1,t))\, dt - \int_{t_1}^{t_2} \mathbf{f}(\mathbf{q}(x_2,t))\, dt \right). \tag{1.11}$$

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

$$\mathbf{q}(a,t) = \mathbf{q}(b,t), \quad \forall t \in [0, T]. \tag{1.12}$$

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 (1.10) and (1.11) hold for all x_1, x_2, t_1 and t_2 such that $[x_1, x_2] \times [t_1, t_2] \subset \Omega$. So, let us discretize the domain Ω and write Equations (1.10) and (1.11) 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, we consider a partition of $[a, b]$ given by:

$$[a, b] = \bigcup_{i=1}^{N} X_i, \text{ where } X_i = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}] \text{ and } a = x_{\frac{1}{2}} < x_{\frac{3}{2}} < \cdots < x_{N-\frac{1}{2}} < x_{N+\frac{1}{2}} = b. \tag{1.13}$$

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

Each interval X_i is refered to as control volume. We shall use the notations $|X_i| = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}$ 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 $\mathbf{Q}_i(t) \in \mathbb{R}^m$ 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 1.10, we get:

$$\frac{d}{dt}\mathbf{Q}_i(t) = \frac{1}{|X_i|}(\mathbf{f}(\mathbf{q}(x_{\frac{i-1}{2}}, t)) - \mathbf{f}(\mathbf{q}(x_{\frac{i+1}{2}}, t))), \quad \forall i = 1, \cdots, N. \tag{1.14}$$

Similarly, Equation (1.11) becomes:

$$\mathbf{Q}_i(t_{n+1}) = \mathbf{Q}_i(t_n) + \frac{1}{|X_i|}\left(\int_{t_n}^{t_{n+1}} \mathbf{f}(\mathbf{q}(x_{i-\frac{1}{2}}, t))\, dt - \int_{t_n}^{t_{n+1}} \mathbf{f}(\mathbf{q}(x_{i+\frac{1}{2}}, t))\, dt \right), \\ \forall i = 1, \cdots, N, \quad \forall n = 1, \cdots, N_T. \tag{1.15}$$

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

$$\delta_x \mathbf{g}(x_i, t) = \mathbf{g}(x_{i+\frac{1}{2}}, t) - \mathbf{g}(x_{i-\frac{1}{2}}, t), \tag{1.16}$$

for an arbitrary vector valued function $\mathbf{g}$. Using this notation, Equations (1.14) and (1.15) lead to:

$$\frac{d}{dt}\mathbf{Q}_i(t) = \frac{1}{|X_i|}\delta_x \mathbf{f}(\mathbf{q}(x_i, t)) \quad \forall i = 1, \cdots, N, \tag{1.17}$$

and

$$\mathbf{Q}_i(t_{n+1}) = \mathbf{Q}_i(t_n) - \frac{\Delta t}{|X_i|}\delta_x \left(\frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} \mathbf{f}(\mathbf{q}(x_i, t))\, dt \right), \quad \forall i = 1, \cdots, N, \quad \forall n = 1, \cdots, N_T, \tag{1.18}$$

respectively. It is worth pointing out that we have made no approximation in Equations (1.17) and (1.18). Indeed, if $\mathbf{q}$ satisfies Equation (1.2), $\forall [x_1, x_2] \subset [a, b]$ and $\forall t \in [0, T]$, then Equation (1.17) is just Equation (1.2) evaluated in the control volumes and written in terms of the average values $\mathbf{Q}$. Similarly, if $\mathbf{q}$ satisfies Equation (1.3), $\forall [x_1, x_2] \times [t_1, t_2] \subset \Omega$, then Equation (1.18) is just Equation (1.3) evaluated in the control volumes, in the time instants t_n, and written in terms of the average values $\mathbf{Q}$.

Notice that in Equation (1.18) we divided and multiplied by Δt, so that we can interpret $\frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} \mathbf{f}(\mathbf{q}(x_i, t))\, dt$ as a mean-time average flux. This interpretation is very handy for the derivation of finite-volume schemes.

The formulations given by Equations (1.17) and (1.18) are the cornerstone of the development of finite volume methods for conservation laws. On the right-hand side of Equation (1.14), the flux function $\mathbf{f}$ may be discretized leading to an ordinary differential equation (ODE) that might be solved using classical ODE integrators (LeVeque, 2002). These methods are known as semi-discrete methods, since only the spatial coordinate is discretized. In this work we shall restrict our attention to methods based on Equation (1.18).

1.2 The finite-volume approach

We summarize the problem of the conservation law in the integral form discussed in Section 1.1 in Problem 1.

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

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

$\forall [x_1, x_2] \times [t_1, t_2] \subset \Omega$, given the initial condition $\mathbf{q}(x, 0) = \mathbf{q}_0(x)$, $\forall x \in [a, b]$, and assuming periodic boundary conditions, i.e., $\mathbf{q}(a, t) = \mathbf{q}(b, t)$, $\forall t \in [0, T]$.

We point out that, for Problem 1, the total mass in $[a, b]$ satisfies:

$$\mathbf{M}_{[a,b]}(t) = \mathbf{M}_{[a,b]}(0), \quad \forall t \in [0, T]. \tag{1.19}$$

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

In Section 1.1 we introduced a version of Problem 1 considering a discretization of the domain Ω. This idea is summarized in Problem 2.

Problem 2: *Assume the framework of Problem 1. We consider positive integers N and N_T, a spatial discretization of [a,b] given by $X_i = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$, $\forall i = 1, \cdots, N$, $a = x_{\frac{1}{2}} < x_{\frac{3}{2}} < \cdots < x_{N-\frac{1}{2}} < x_{N+\frac{1}{2}} = b$, 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 1, it follows that:*

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

where $\mathbf{Q}_i(t) = \frac{1}{|X_i|}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \mathbf{q}(x, t)\, dx$.

Our problem now consists of finding the values $\mathbf{Q}_i(t_n)$, $\forall i = 1, \cdots, N$, $\forall n = 1, \cdots, N_T$, given the initial values $\mathbf{Q}_i(0)$, $\forall i = 1, \cdots N$. In other words, we would like to find the average values of $\mathbf{q}$ 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 3.

Problem 3 (1D FV scheme): *Assume the framework defined in Problem 2. The finite-volume approach of Problem 2 consists of a finding a scheme of the form:*

$$\mathbf{Q}_i^{n+1} = \mathbf{Q}_i^n - \frac{\Delta t}{|X_i|}(\mathbf{F}_{i+\frac{1}{2}}^n - \mathbf{F}_{i-\frac{1}{2}}^n), \quad \forall i = 1, \cdots, N, \quad \forall n = 1, \cdots, N_T,$$

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

1.3 The piecewise parabolic method

Chapter 2

Two-dimensional finite-volume method

2.1 Two-dimensional consevartion laws in integral form

2.2 Dimension splitting

Chapter 3

Cubed-sphere grids

3.1 Equiangular

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