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ARBITRARY HIGH ORDER SCHEMES FOR THE SOLUTION OF THE LINEAR ADVECTION EQUATION

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Abstract. In this work an arbitrary high order formulation for solving the linear advection equation with constant coefficients is presented. The conservative formulation is explicit, one step, and provides information at the sub-mesh scale. High order accuracy in space and time is achieved by means of polynomial representation of the states in each cell and conservative functional approximation of the exact solution of the advection equation. Altough high order methods are widely used when high precision of the numerical results is required, in this work we study the use of high order methods to compute faster than first order methods when low or middle precision of the numerical results is required. Numerical results for one-dimensional problems using schemes up to order of accuracy 5 are presented.

Keywords: Linear advection, high-order schemes, CFA, computational efficiency, Legendre polynomials.

§1. Introduction

The study of mixing in fluid flows is a complex problem involving different phenomena that can be faced under different degrees of approximation. For many hydraulic and environmental applications it is widely assumed that the fate of a tracer concentration can be modeled by means of the differential tracer mass conservation equation. This contains information on the mechanism of advection by the average flow velocity as well as molecular diffusion and turbulence mixing. The latter are often formulated as general diffusion or dispersion terms in the equation [6]. Using the mass conservation equation for the fluid flow it can be simplified to get the most widely used non-conservative form known as the convection-dispersion equation.

It is possible to solve numerically the advection-diffusion equation by discretizing the complete equation or by solving separately the advection and the diffusion. In this work, letting aside the technique that could be applied to the diffusive part, we are concerned with an efficient and accurate treatment of the convective part.

Finite volume methods rely on an integral formulation of the conservation law. The evolution of the cell averaged value of the conserved variable is evaluated through an estimation of the fluxes at the cell edges. Godunov's method, for instance, evaluates the flux using the exact solution of the Riemann problem at the edge [3]. Several approximate Riemann solvers have been proposed in order to generate efficient schemes [5], [4]. High order finite volume methods use also high order spatial reconstrucions at the grid cells in order to improve the evaluation of the numerical fluxes and Taylor time series or Runge-Kutta time integrations.

The limiting procedure to avoid oscillations follows the same criteria than in finite differences. A well known second order finite volume method is the MUSCL-Hancock scheme [10]. Ben-Artzi [1] and Toro [8] proposed methods based on the solution of the generalized Riemann plobem (piecewise polynomial), up to second order [1] and arbitrary high order (ADER) [8] [7] [9] in space and time. The ADER formulation offers the main advantage of requiring a single time step, however, it is associated to the necessity of following the steps of high order reconstruction, high order limitation, flux estimation and finally the storage of a single cell averaged value. This is a disadvantage common to all finite volume methods.

Dumbser [2] introduced the ADER methodolgy in the discontinuos Galerkin finite element framework. The variable is represented at every cell as a linear combination of basis functions leading to high order discretization avoiding the reconstruction step. Time accuracy is achieved in a single step thanks to the ADER formulation that transforms time derivatives into space derivatives. The finite element formulation projects the conservation law on every basis function in the time-space domain and evaluates the resulting integrals by means of quadrature formulae, allowing the resolution in both structured and unstructured grids.

This work presents a high order discretization technique analogous to the finite element methodology, based on Legendre polynomials. High order in space is achieved thanks to the polynomial representation within each cell avoiding the reconstruction step. High order in time is achieved in a single step by a conservative functional approximation (CFA technique) of the exact solution of the conservation law and a direct evaluation of the resulting integrals that does not require quadrature formulae. The resulting scheme is efficient in the sense that it requires a minimum number of mathematical operations. The scheme of order N to solve the linear advection equation in D dimensions requires $2DN^{2D}$ multiplications and additions per cell to calculate the evolution of the variable in a time step.

§2. Spatial discretization and sub-grid information

The numerical schemes considered in this work start from the basis that the information stored in a cell is a functional approximation, of a certain order of accuracy, of the spatial distribution of the variable within that cell. The numerical scheme is built to calculate the system evolution by providing an approximation of the new spatial distribution of the variable, at every cell, in the next time step.

The spatial representation of the variables at every grid cell is based on the mathematical concept of Hilbert space, an infinite-dimensional function space, defined over a spatial domain. The particular basis functions used in the present work are Legendre polynomials $P_n(x)$, defined in the spatial domain $x \in [-1, 1]$. Their orthogonality is given by the property:

$$\langle P_m, P_n \rangle = \int_{-1}^{1} P_m(x) P_n(x)\, dx = \frac{2}{2n-1} \delta_{m,n} \tag{1}$$

with the norm

$$\|P_n\| = \sqrt{\langle P_n, P_n \rangle} = \sqrt{\frac{2}{2n-1}}. \tag{2}$$

One useful property of the Legendre polynomials in the context of the present work is

that, for $n > 1$ they do not have net area:

$$\int_{-1}^{1} P_n(x)\,dx = \int_{-1}^{1} P_n(x)P_1(x)\,dx = \langle P_n, P_1\rangle = 2\,\delta_{n,1}. \tag{3}$$

An approximation of order of accuracy N of a square-integrable function $g(x)$ in the interval $x \in [-1, 1]$ can be obtained as linear combination of the N first Legendre polynomials:

$$\bar{g}(x) = \sum_{n=1}^{N} g_n P_n(x) \approx g(x), \tag{4}$$

with the coefficients

$$g_n = \frac{2n-1}{2}\,\langle g, P_n\rangle. \tag{5}$$

It is important to note that the mentioned approximation is conservative. To prove this property, fundamental to the conservative character of the numerical scheme, equation (4) is integrated using (5) and (3):

$$\int_{-1}^{1} \bar{g}(x)\,dx = \sum_{n=1}^{N} g_n \int_{-1}^{1} P_n(x)\,dx = \sum_{n=1}^{N} g_n\langle P_n, P_1\rangle = 2g_1 = \int_{-1}^{1} g(x)\,dx. \tag{6}$$

Due to the restrictions on the domain where the Hilbert space is defined, it is necessary, to move from a global to a local coordinate system within each cell, that is adapted to the domain of orthogonality of the basis functions. For that purpose x' will be used to denote the global coordinate and x to denote the local, cell adapted, coordinate.

To summarize, for the scheme of order of accuracy N, the state of the system at time t will be represented by means of the storage of N numbers at every grid cell ${}^{n}q_i^t$ representing the spatial distribution of the variable as linear combination of the Legendre polynomials

$$q_i(x,t) = \sum_{n=1}^{N} {}^{n}q_i^t P_n(x). \tag{7}$$

2.1. Time evolution

The form to build a numerical scheme able to solve the time evolution of a given spatial distribution based on the Legendre polynomial representation is next presented. The linear advection equation in one dimension for a function $q(x', t)$ is

$$\partial_t q(x', t) + \lambda \partial_x q(x', t) = 0, \tag{8}$$

with λ constant and positive. Instead of seeking an approximation of the individual terms in the equation, the existing exact solution is used as the basis of the advective method, that can be expressed in local coordinate

$$q(x, t + \Delta t) = q(x - 2c, t), \tag{9}$$

where c is the CFL number

$$c = \frac{|\lambda|\Delta t}{\Delta x'}. \tag{10}$$

Hence, starting from the known initial conditions, already expressed in local coordinates (7), we are interested in an expression for the solution at time $t = t + \Delta t$.

To achieve that, the pure transport formulated by (9) of the initial condition (7) is performed leading to the exact solution in cell i:

$$\widetilde{q}_i(x, t + \Delta t) = \begin{cases} q_{i-1}(x + 2 - 2c, t) & \text{if } -1 < x < 2c - 1, \\ q_i(x - 2c, t) & \text{if } 2c - 1 < x < 1. \end{cases} \tag{11}$$

Finally a conservative functional approximation of (11) is performed in order to reach the updated set of coefficients in the grid cell:

$$q_i(x, t + \Delta t) = \sum_{n=1}^{N} {}^n q_i^{t+\Delta t} P_n(x), \tag{12}$$

with the coefficients

$${}^n q_i^{t+\Delta t} = \frac{2n - 1}{2} \int_{-1}^{1} \widetilde{q}_i(x, t + \Delta t) P_n(x)\, dx. \tag{13}$$

2.2. Updating scheme

The exact calculation of the integrals present in the definition of the coefficients (13) leads to the following updating numerical scheme of order accuracy N:

$${}^n q_i^{t+\Delta t} = \sum_{j=1}^{N} {}^j q_{i-1}^t L_{n,j}(c) + \sum_{j=1}^{N} {}^j q_i^t R_{n,j}(c), \tag{14}$$

where c is the CFL number (10) used to evaluate the left matrix L:

$$L(c) = T(c, 1 - c) \tag{15}$$

and the right matrix R:

$$R(c) = T(1 - c, -c). \tag{16}$$

Both L and R matrix are written in terms of a translation matrix T:

$$T_{i,j}(a, b) = a \frac{2j - 1}{2} \sum_{n=1}^{min(i,j)} \frac{2}{2n - 1} A_{i,n}(a, b) A_{j,n}(a, -b), \tag{17}$$

where A is a matrix with the property

$$P_i(ax + b) = \sum_{n=1}^{N} A_{i,n}(a, b) P_n(x). \tag{18}$$

To illustrate the procedure, the expression of the auxiliary matrix A up to third order of accuracy is next provided:

$$A(a,b) = \begin{pmatrix} 1 & 0 & 0 \\ b & a & 0 \\ d & 3ab & a^2 \end{pmatrix}, \quad d = \frac{a^2 + 3b^2 - 1}{2}, \tag{19}$$

and the corresponding T matrix

$$T(a,b) = a\begin{pmatrix} 1 & -3b & 5d \\ b & a^2 - 3b^2 & 5\left(bd - a^2 b\right) \\ d & 3\left(a^2 b - bd\right) & a^4 - 15a^2b^2 + 5d^2 \end{pmatrix}, \quad d = \frac{a^2 + 3b^2 - 1}{2}. \tag{20}$$

The numerical scheme (14) is conditionally stable provided that $c \leq 1$ for all orders of accuracy. This is dictated by the advection rule assumed (11) that only holds for $c \leq 1$. The scheme is exact when $c = 1$ in the sense that it transports exactly the polynomial distribution within every grid cell.

It is worth noting that in a simulation with fixed Δt and Δx, matrices L and R are constant. The scheme of order of accuracy N requires in this case $2N^2$ multiplications and additions per cell and time step. Taking in to account that the maximum time step allowed is independent of the order of accuracy, the total computational cost grows with the order of accuracy at a rate N^2.

§3. Numerical tests

3.1. Test 1

A Gaussian initial distribution is used as first test case to quantify the actual order of accuracy of the different approximations:

$$q(x', 0) = e^{-(x'-1)^2/0.05}. \tag{21}$$

A domain $x' \in [0, 2]$ is considered and periodical boundary conditions assumed. The advection velocity is chosen $\lambda = 1$ and a simulation time of $t = 20$ is performed so that the Gaussian distribution crosses 10 times the computational domain. The exact solution is the initial distribution at the same location. Using $c = 0.95$, simulations with different cell size Δx have been performed and their error has been evaluated using the L_1 norm as follows:

$$L_1 = \frac{1}{2M} \sum_{i=1}^{M} \int_{-1}^{1} |q_i(x) - q_{Exact}(x)| \, dx, \tag{22}$$

where M represent the cell number and the integrals in (22) are numerically computed.

The L_1 error norm corresponding to numerical schemes of orders of accuracy 2, 3, 4 and 5 versus the grid spacing is represented in logarithmic scale in Figure 1. In all the cases, the results have been fit to a straight line and the slope found is indicated in the figure.

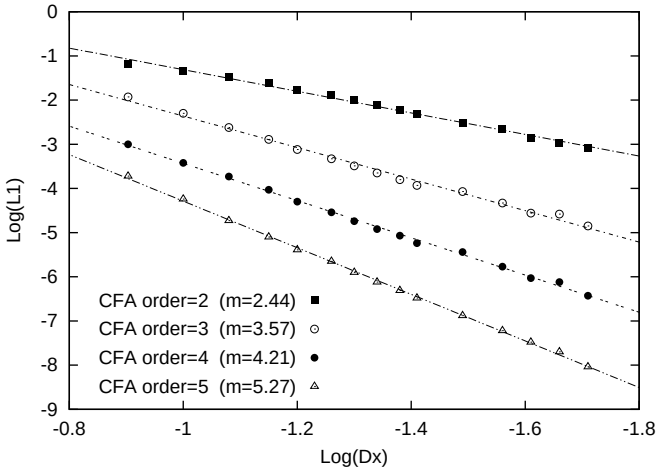

Figure 1: Error convergence of the CFA methods of order of accuracy 2, 3, 4 and 5 in the numerical test 1.

3.2. Test 2

The same initial distribution (21) and the same domain $x' \in [0, 2]$ are considered with the focus on the computational efficiency of the different schemes. We are interested in comparing the computational time required by the different schemes to achieve a target computational accuracy. The error of the schemes is quantified using the L_1 norm (22). Figure 2 displays the shape of the numerical solutions corresponding to values of $\log(L_1) = -1$ and $\log(L_1) = -2$ compared to the exact solution in order to state the acceptable size of this error in practical applications.

Two sets of computations, corresponding to a simulation time of $t = 20$ and $t = 200$, have been made and are plotted in Figures 3 a) and 3 b) respectively. These figures are a representation of the L_1 errors produced by the CFA schemes of orders of accuracy 1, 2, 3, 4 and 5 as a function of the computational time used, in logarithmic scale. In general, given a desired maximum error there is a scheme of a certain order of accuracy able to provide the solution at the lowest cost. Also, the figures show that if, when starting by a first order approach the numerical error is excessive, refining the grid is never the best option to reduce the error. This tendency continues and indicates that, for longer simulations (either in larger domains) higher order approximations gain in relative efficiency.

§4. Conclusions

A new approximation well suited for high order advection simulation has been presented. The scheme is explicit and based on a single updating step. Piecewise polynomial spatial discretization using Legendre polynomials provides the required spatial accuracy and the subgrid information. The updating scheme is built from the functional approximation of the

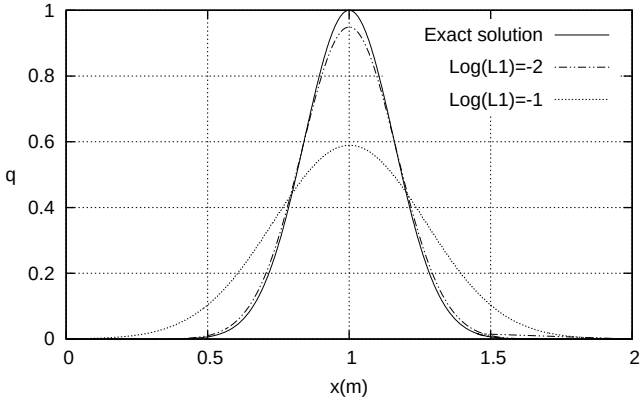

Figure 2: Shape of the numerical solutions corresponding to values of $\log(L_1) = -1$ and $\log(L_1) = -2$ compared to the exact solution in order to visualize the size of the L_1 error in Test case 2.

exact solution of the advection equation and a direct evaluation of the resulting integrals.

The numerical details have been provided and the schemes have been validated using a set of numerical experiments. Some of the test cases have been oriented to the convergence analysis of the schemes of different order of accuracy with an special interest in the computational efficiency of the different options. The results from the schemes from 1^{st} to 5^{th} order of accuracy have been presented showing that, in general, given a desired maximum error, there is a scheme of a certain order of accuracy able to provide the solution at the lowest cost. It is also worth remarking that if when starting by a first order approach the numerical error is excessive, refining the grid is never the best option to reduce the error. It is also true that for longer simulations (either in larger domains) higher order approximations gain in relative efficiency.

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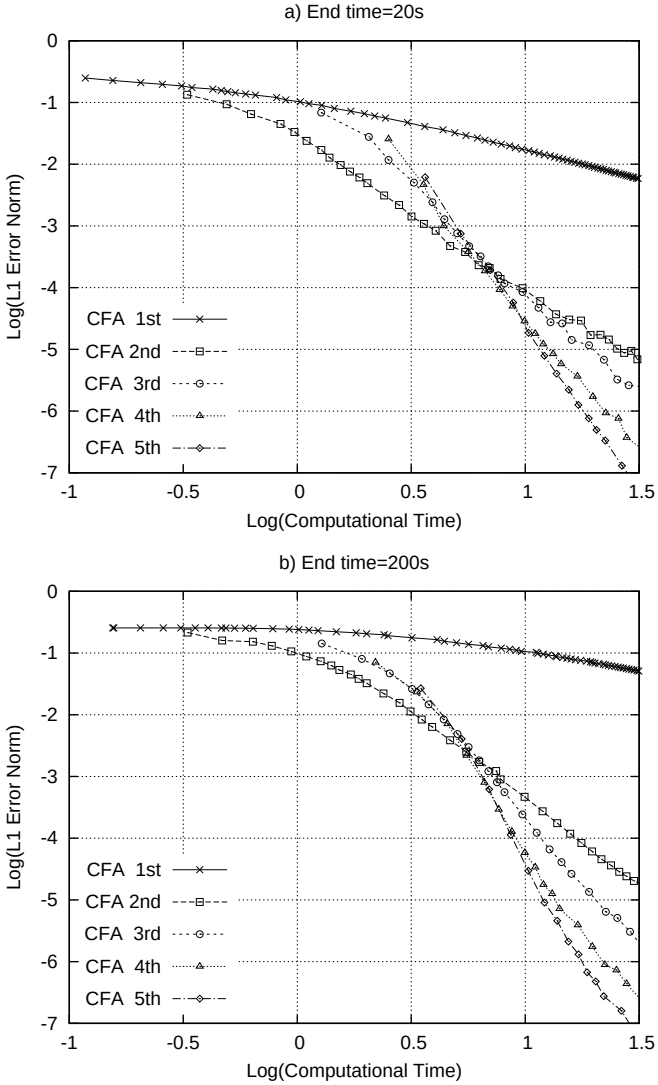

Figure 3: L_1 error norm produced by the CFA schemes of orders of accuracy 1, 2, 3, 4 and 5 as a function of the computational time used in numerical Test 2.

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