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An improved bounded semi-Lagrangian scheme for the turbulent transport of passive scalars

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ABSTRACT

An improved bounded semi-Lagrangian scalar transport scheme based on cubic Hermite polynomial reconstruction is proposed in this paper. Boundedness of the scalar being transported is ensured by applying derivative limiting techniques. Single sub-cell extrema are allowed to exist as they are often physical, and help minimize numerical dissipation. This treatment is distinct from enforcing strict monotonicity as done by D.L. Williamson and P.J. Rasch [5], and allows better preservation of small scale structures in turbulent simulations. The proposed bounding algorithm, although a seemingly subtle difference from strict monotonicity enforcement, is shown to result in significant performance gain in laminar cases, and in three-dimensional turbulent mixing layers. The scheme satisfies several important properties, including boundedness, low numerical diffusion, and high accuracy. Performance gain in the turbulent case is assessed by comparing scalar energy and dissipation spectra produced by several bounded and unbounded schemes. The results indicate that the proposed scheme is capable of furnishing extremely accurate results, with less severe resolution requirements than all the other bounded schemes tested. Additional simulations in homogeneous isotropic turbulence, with scalar timestep size unconstrained by the CFL number, show good agreement with spectral scheme results available in the literature. Detailed analytical examination of gain and phase error characteristics of the original cubic Hermite polynomial is also included, and points to dissipation and dispersion characteristics comparable to, or better than, those of a fifth order upwind Eulerian scheme.

1. Introduction

The need for high accuracy at small scales makes turbulent simulations extremely sensitive to numerical errors. This presents considerable challenges when conducting practical simulations of important turbulent phenomena such as weather modelling [1–3], and tracking of pollutants in the atmosphere and oceans. Turbulent transport of scalars is especially susceptible to numerical errors, and imposes stringent grid resolution requirements [4]. To alleviate the computational cost involved in turbulent scalar transport, we propose a novel bounding algorithm for cubic Hermite polynomial-based semi-Lagrangian schemes [5,6]. Numerical performance of the scheme is compared to that of several bounded and unbounded schemes, with regard to the following scheme properties

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- Boundedness
- Low numerical diffusion
- High accuracy
- Conservation

Of the four properties listed, scalar boundedness is a crucial property that must be respected when required by physical constraints. Almost all transported scalars, both passive and active, have physical bounds that must be maintained during transport. Violating boundedness in certain cases can lead to severe detrimental effects. Some examples include irreversible spurious precipitation in weather simulations [5], and the appearance of negative absolute temperature and unphysical species mass fractions (*i.e.*, outside the bounds $[0, 1]$) in reacting flows.

Due to the critical nature of scalar boundedness in such simulations, there has been significant effort in the past to construct bounded finite-volume (*e.g.*, WENO3 [7], MPWENO5 [8], OSMP7 [9], BQUICK [10]) schemes based on the Eulerian treatment [11] of the scalar transport equation. Unfortunately, these transport schemes exhibit significant numerical diffusion, which leads to a decrease in simulation accuracy. Higher order schemes coupled with a Flux Corrected Transport (FCT) algorithm [12,13] can mitigate the issue of numerical diffusion. However, the resulting increase in accuracy comes at a significant increase in computational cost, owing to the need for a larger computational stencil. The use of high order finite-volume schemes is also accompanied with increasingly restrictive stability criteria (*i.e.*, a smaller limiting Courant–Friedrichs–Lewy (CFL) number) [1], which leads to further increase in computational cost. In addition, high-order schemes give rise to larger and more frequent oscillations (Runge's phenomenon), which makes ensuring boundedness difficult. The proposed Bounded Cubic Hermite polynomial (BCH) transport scheme, which is based on the semi-Lagrangian treatment of the advection–diffusion equation [1], addresses several of these numerical issues.

As an alternative to Eulerian schemes, semi-Lagrangian (SL) schemes are known to be stable at large CFL values, but suffer from the inability to conserve mass inherently [1]. This may not be an issue of major concern in certain scenarios [5]. The ability of SL schemes to maintain stability for $\text{CFL} > 1$ makes them especially suitable for applications involving long integration times. This has led to widespread adoption of SL schemes in the atmospheric community, and a vast body of work exists in the literature [1,5,6,14–19]. An exhaustive review in this regard can be found in Ref. [1]. In addition to decreased restriction on time-step size, SL schemes can yield enhanced spatial accuracy, which makes them suitable for use in interface tracking in multiphase flows [16], and for turbulent simulations, which is the primary motivation for the current work.

As already discussed, simulations often require that the scalar being transported respects physical bounds, and the use of high-order interpolation can violate this constraint (Godunov's theorem [20]). Algorithms that restore boundedness can introduce numerical dissipation, and minimizing this is one of the main goals of the proposed BCH scheme. Most existing SL schemes that make an effort to maintain scalar boundedness are based on the use of either Lagrange polynomials [14,15] or Hermite polynomials [5,6] for interpolation. The form of the polynomial used, in addition to the bounding mechanism used, can have a measurable impact on the accuracy of the simulation [6]. This will become evident from the results presented in Section 5.

The objective of this paper is to provide a description of the BCH scheme, and to test its performance with regard to the four properties listed earlier. Performance evaluation of certain existing semi-Lagrangian schemes [6,14,15] that make an effort to maintain scalar boundedness is also included, to assess the improvement that the proposed scheme offers. A brief discussion of the basic workings of semi-Lagrangian schemes is outlined in Section 2. The formulation of the proposed bounding algorithm is presented in Section 3. Section 4 presents an in-depth analysis of gain and phase error characteristics of the original cubic Hermite polynomial, for uniform one dimensional (1D) advection of a passive scalar. Section 5 provides configuration description of the numerical tests used, which include three laminar cases and two turbulent cases. One of the turbulent test cases is used to assess numerical performance in comparison to spectral schemes, when working with large timesteps unconstrained by the CFL number. Section 5 also involves discussion of scheme performance with regard to the scheme properties listed earlier, in addition to comparison with several other commonly used Eulerian and semi-Lagrangian schemes.

2. Semi-Lagrangian schemes

This section provides a brief outline of the numerical implementation of semi-Lagrangian schemes. Readers interested in the proposed bounding algorithm may proceed directly to Section 3.

2.1. Numerical implementation

The transport of passive scalars is governed by the advection–diffusion equation

$$\frac{Dz}{Dt} = \frac{\partial z}{\partial t} + \boldsymbol{u} \cdot \nabla z = \mathcal{D}\nabla^2 z \tag{1}$$

where the transported scalar quantity is denoted by 'z', $\mathcal{D}$ is the molecular diffusivity, and the $\frac{D}{Dt}$ operator represents the material derivative. All numerical tests used in this paper assume the incompressibility condition ($\nabla \cdot \boldsymbol{u} = 0$). To solve the