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Semi-Lagrangian advection–propagation (SLAP) scheme for three-dimensional interface tracking

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ABSTRACT

A fully three-dimensional semi-Lagrangian scheme is developed for computing the evolution of advected self-propagating surfaces (e.g., premixed flames) governed by a level-set advection–propagation equation. The scheme provides third-order spatial accuracy and shape preservation. Example numerical simulations of three-dimensional front propagation are presented to illustrate the capability of the scheme of capturing cusp formation and associated surface-area annihilation as well as the formation and consumption of detached closed-surface pockets behind fronts propagating in highly vortical flow.

1. Introduction

Markstein and Squire [1] introduced the advection–propagation equation below to describe the propagation of a flame surface through an arbitrary unsteady flow field. This equation governs the evolution of a scalar field $G(\mathbf{x},t)$, describing the motion of any one of its isoscalar surfaces which propagates normal to itself locally while being advected by the flow field $\mathbf{U}(\mathbf{x},t)$

$$\frac{\partial G}{\partial t}+(\mathbf{U}-S_N\mathbf{n})\cdot\nabla G=0. \tag{1}$$

The propagation velocity is $-S_N\mathbf{n}$, where $\mathbf{n}(\mathbf{x},t)\equiv\nabla G/|\nabla G|$ is the local surface normal vector. Thus, the isoscalar surface propagates intrinsically at the speed S_N down the gradient of the scalar field. This is in analogy with the transport of heat by molecular diffusion, which occurs down the gradient of the temperature field. The works of Markstein and Squire [1], Markstein [2] and Williams [3] employed the advection–propagation equation in analytical studies of flame-front stability. Kerstein et al. [4] subsequently used the formulation to investigate attributes of arbitrary-interface propagation in Navier–Stokes turbulence. Osher and Sethian [5] developed the first stable numerical methods for the solution of Eq. (1), also known as the level-set equation, for front propagation in quiescent flow.

In the present work, both S_N and the flow-field velocity $\mathbf{U}$ are measured in units of the known constant planar-surface speed S_L (*e.g.*, the laminar-flame speed); G and the spatial variables ($\mathbf{x}$) are measured in units of a constant length scale l characterizing order-unity variations of the advection field, and time is measured in units of l/S_L. In general, S_N depends locally on properties of the flow field (e.g., the rate of flow-field strain normal to the isoscalar surface) and isoscalar surface geometry

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(*e.g.*, the surface curvature) [1–3,5–7]. However, in the present work the case $S_N = 1$ is considered for simplicity, without a loss of generality of the proposed numerical scheme.

Numerical schemes developed for the accurate solution of Eq. (1) should be shape preserving in the sense that no new local maxima or minima of the scalar field should be created. In other words, although the volume of space between two given isoscalar surfaces will in general vary in time, the range of G over this volume should remain constant. This shape-preservation property is a consequence of the simple fact that the value of G must by definition remain constant along the path of motion of its level set, as determined by its local velocity $\mathbf{v} \equiv \mathbf{U} - S_N\mathbf{n}$ according to Eq. (1). Since $\mathbf{v}$ is not generally solenoidal even when the advection flow-field $\mathbf{U}$ is incompressible (due to the presence of the surface-propagation term), except possibly for the simplest case of planar-surface propagation, G is not generally conserved. A conserved scalar ϕ_{CS}, the integral of which (over the volume of space between two given isoscalar surfaces) remains constant, is governed by the following conservation law

$$\frac{\partial \phi_{CS}}{\partial t} + \nabla \cdot (\phi_{CS}\mathbf{v}) = 0. \tag{2}$$

It can be shown by use of the Reynolds-transport and divergence theorems that any non-propagating scalar field exclusively advected by a solenoidal velocity field is conserved. If the advection flow is compressible, on the other hand, it can be shown in a similar manner that the product of any non-propagating scalar field ψ with the density of the flow ρ is conserved (again assuming no diffusion, production or consumption of the scalar field). In this case, one has $\phi_{CS} = \rho\psi$ and

$$\frac{\partial(\rho\psi)}{\partial t} + \nabla \cdot (\rho\psi\mathbf{U}) = 0, \quad \frac{\partial \psi}{\partial t} + \mathbf{U} \cdot \nabla\psi = 0; \tag{3}$$

the second, advection form of the two relations resulting from mass continuity. An accurate numerical scheme designed to predict the evolution of ψ should be therefore both conservative with regard to $\rho\psi$ and shape-preserving with regard to ψ. Note that the continuity equation, obtained from the first relation in Eq. (3) by setting $\psi = 1$, is not in general shape preserving (except for the trivial case of incompressible flow) because the source term $-\rho\nabla \cdot U$ can cause new maxima or minima in ρ to develop in the flow [8]. Schemes based on Eulerian, control-volume analyses are inherently conservative and have traditionally been popular for solving conservation laws such as Eq. (2) and the first relation of Eq. (3) [8–15]. Semi-Lagrangian schemes which are not inherently conservative but may offer greater computational efficiency over traditional Eulerian methods through the use of larger time steps [16,17] have been attractive for solving advection laws such as the second relation of Eq. (3). Recently, multidimensional schemes which are both conservative and shape-preserving and allow unrestricted time steps have been developed using both Eulerian [13,18,19] and semi-Lagrangian [20,21] formulations. Strain [22] provides an excellent introduction of semi-Lagrangian methods for moving interfaces using time steps unconstrained by numerical-stability issues, including many two-dimensional examples. Ultimately, however, the time step may be limited in many practical simulations by the effect of existing temporal gradients of S_N and $\mathbf{U}$ on the accuracy of isoscalar-surface-element trajectory approximations.

In the present work, we employ a nonconservative shape-preserving semi-Lagrangian scheme for the solution of Eq. (1), consistent with the nonconservative nature of the advection–propagation equation. The scheme is based on a multidimensional formulation which allows for CFL numbers as large as 1. In the following section the formulation of the numerical scheme is presented, followed by examples, discussion and a conclusion in subsequent sections.

2. Formulation

The semi-Lagrangian formulation employed herein for solution of Eq. (1) is derived using upwind transient interpolation modeling (TIM), as described by Leonard et al. [10,14]. Accordingly, the scalar field G at each grid point $\mathbf{x}_{ijk} \equiv (x_i, y_j, z_k)$ is updated at each new time step using the following Lagrangian transport law

$$\left.\begin{aligned} &G(\mathbf{x}_{ijk}, t_n + \Delta t) = G\left(\mathbf{x}^L_{ijk}(t_n), t_n\right), \\ &\mathbf{x}^L_{ijk}(t_n) \equiv \mathbf{x}_{ijk} - \mathbf{v}_{ave}\Delta t, \\ &\mathbf{v}_{ave} = \tfrac{1}{\Delta t}\int_{t_n}^{t_n+\Delta t} \mathbf{v}\left(\mathbf{x}^L_{ijk}(t), t\right) dt. \end{aligned}\right\} \tag{4}$$

Here $\mathbf{x}^L_{ijk}(t)$ is the location at time t of an element of the isoscalar surface on its path from its original location $\mathbf{x}^L_{ijk}(t_n)$ at t_n to its final location $\mathbf{x}_{ijk}$ at $t_n + \Delta t$. In this sense the path defined by $\mathbf{x}^L_{ijk}(t)$ for $t_n \leqslant t \leqslant t_n + \Delta t$ is peculiar to $\mathbf{x}_{ijk}$, being associated with a different surface element at each time step. Since the set of surface elements tracked are not fixed but are redefined at each time step, the transport scheme is characterized as semi-Lagrangian. The value of $\mathbf{x}^L_{ijk}(t_n)$ is specified implicitly by the last two relations of Eq. (4) and is obtained most accurately by iteration if large time steps associated with motion of surface elements over multiple grid cells are to be considered. In the present formulation, we will derive an explicit relation for $\mathbf{x}^L_{ijk}(t_n)$ but prevent surface elements from completely traversing more than one grid cell during a given time step to preserve accuracy. Consequently, the local CFL number based on the magnitude of the surface-element velocity $\mathbf{v} \equiv \mathbf{U} - S_N\mathbf{n}$ and the grid spacing Δx will be limited to a value of no greater than 1.