Conservative Front Tracking and Level Set Algorithms

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Abstract

Hyperbolic conservation laws are foundational for many branches of continuum physics. Discontinuities in the solutions of these partial differential equations are widely recognized as a primary difficulty for numerical simulation, especially for thermal and shear discontinuities and fluid-fluid internal boundaries. We propose numerical algorithms which will (a) track these discontinuities as sharp internal boundaries, (b) fully conserve the conserved quantities at a discrete level, even at the discontinuities, and (c) display one order of numerical accuracy higher globally (at the discontinuity) than algorithms in common use. A significant improvement in simulation capabilities is anticipated through use of the proposed algorithms.

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1 Introduction

Hyperbolic conservation laws are foundational for many branches of continuum physics. Discontinuities in the solutions of these partial differential equations are widely recognized as a primary difficulty for numerical simulation. Commonly used numerical algorithms are convergent at some power of the mesh spacing Δx, but only for smooth solutions. At solution discontinuities the local truncation errors are typically $\mathcal{O}(1)$, *e.g.* not convergent. For nonlinear shock waves, this situation is mitigated by the fact that errors flow into the discontinuity (which functions as a 'black hole' in this regard), and the size of the error region does not grow. For linear type discontinuities, such as thermal or fluid material boundaries, the discontinuities spread, and often occupy 5 to 10 mesh cells as the simulation evolves into late time. The ability to solve accurately many practical problems is hampered by these facts.

Front tracking was proposed as a (partial) cure to these problems [10, 8, 6]. The method has recently been extended to three dimensions, and given a robust and simple interface description [2, 4, 3]. In this method, a sharp numerical boundary is maintained within the computation, to prevent the artificial mixing of fluids across a fluid interface. The communication of information across the interface is accomplished by use of analytic solutions of idealized jump discontinuities (Riemann problems) and by ghost cells, to maintain data extrapolated across the interface. The ghost cells are needed by the finite difference operators approximating the differential equation. The ghost cell extrapolation method was introduced in 1981 by Glimm, Marchesin and McBryan [6] for front tracking. This method, and a closely related ghost cell level set method [1] proposed in 1999 are only partial solutions to the problem of simulation of fluid interfaces. Both lack conservation in the cells cut by the interface and both have only conventional accuracy with $\mathcal{O}(1)$ local truncation errors at the discontinuities. Thus neither is a correct solution of the interface problem.

The purpose of the paper is to propose a tracking/level set algorithm which is conservative even at discontinuities and which improves by one order of accuracy over conventional algorithms.

2 Numerical Algorithms

2.1 Conservation Laws in Integral Form

A conservation law is a partial differential equation of the form

$$\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{u}) = 0 \quad , \tag{1}$$

so called because $\int u dx$ changes in time only due to net influx at the boundaries. Consider a cell with volume V with a bounding surface S part or all of which may be moving in time. Assume that in a small time interval Δt we have the increments of both the conserved quantity $u \to u + \Delta u$ and the volume $V \to V + \Delta V$. We expand

$$\int_{V+\Delta V} (u + \Delta u) dV - \int_V u dV = \int_V \Delta u dV + \int_{\Delta V} u dV + \int_{\Delta V} \Delta u dV \quad . \tag{2}$$

For the right hand side of (2), the last term is a higher order differential and can be neglected as $\Delta t \to 0$. The second term contributes

$$\int_{\Delta V} u dV = \oint_S u v_n dS \Delta t \quad . \tag{3}$$

where v_n is the component of the velocity in the direction of the outward normal to S. Dividing both sides of (2) by Δt and taking the limit of $\Delta t \to 0$, we have

$$\frac{\partial}{\partial t} \int_V u dV = \int_V \frac{\partial u}{\partial t} dV + \oint_S u v_n dS \tag{4}$$

Substitution of the conservation law (1) allows evaluation of the first term on the right side of (4). For this purpose we let $F_n(u)$ denote the component of $\mathbf{F}(u)$ in the direction of the outward normal to S. Therefore, we have the space integral form of the conservation law for a cell with moving boundary as

$$\frac{\partial}{\partial t} \int_V u dV + \oint_S (F_n(u) - u v_n) dS = 0 \quad . \tag{5}$$

For a fixed cell such as a rectangular cell in an Eulerian grid, (5) degenerates to the conventional integral form of the conservation law

$$\frac{\partial}{\partial t} \int_{V_F} u dV + \oint_S F_n(u) dS = 0 \quad . \tag{6}$$

Eq. 6 has been the foundation of many finite difference and finite volume schemes. When tracking a moving interface, it is (5) that is fundamental.

2.2 Ghost-Cell Extrapolation Tracking Methods

Active tracking of physical discontinuities have proven important in the computation of many physical problems. The 1981 front tracking paper [6] pioneered the use of ghost-cells for the separation of fluid components across a tracked interface. The state at the center of a ghost-cell is extrapolated from the state of the Riemann solution on the same side of the interface as the cell to be solved. The ghost-cell method was also used in 1999 by Fedkiw et al [1] with the ghost cell state assigned through entropy extrapolation from the states on the same side as the solution cell.

The main advantage of either of these ghost cell algorithms is that the computation needs only finite difference operations on regular cells (aside from issues of front propagation). As we will see, the main disadvantages of ghost cell methods are (a) loss of conservation and (b) only conventional order of accuracy. Conservative algorithms overcome these two disadvantages but give up the advantage of regular cell finite difference operations.

In one space dimension, assume a uniform partition (just for simplicity of notation) over the computational interval. Let x_i denote the cell center of the i-th cell, t_n denote the n-th time level, Δx denote the cell size, and $\Delta t = t_{n+1} - t_n$. Consider a second order finite difference scheme for (1),

$$U_j^{n+1} = U_j^n - \lambda \left(F_{j+1/2}^n - F_{j-1/2}^n \right), \tag{7}$$

where $F_{j+1/2}^n = F(U_{j-1}^n, U_j^n, U_{j+1}^n, U_{j+2}^n)$, U_j^n approximates $\Delta x^{-1} \int_{x_{j-1/2}}^{x_{j+1/2}} u(x, t_n) dx$, the average of the conserved quantity over the cell $[x_{j-1/2}, x_{j+1/2}]$, and $\lambda = \Delta t / \Delta x$. If an interface (tracked either by the front tracking or the level set methods) is found between cell centers x_j and x_{j+1}, the ghost-cell method will solve for U_j^{n+1} and U_{j+1}^{n+1} through the scheme

$$U_j^{n+1} = U_j^n - \lambda \left(F_{j+1/2}^{n,L} - F_{j-1/2}^n \right) \tag{8}$$

$$U_{j+1}^{n+1} = U_j^n - \lambda \left(F_{j+3/2}^n - F_{j+1/2}^{n,R} \right) \tag{9}$$

where $F_{j+1/2}^{n,L} = F(U_{j-1}^n, U_j^n, \overline{u_{j+1}^{n,L}}, \overline{u_{j+2}^{n,L}})$ and $F_{j+1/2}^{n,R} = F(\overline{u_{j-1}^{n,R}}, \overline{u_j^{n,R}}, U_{j+1}^n, U_{j+2}^n)$. Here $\overline{u_{j-1}^{n,R}}, \overline{u_j^{n,R}}, \overline{u_{j+1}^{n,L}}$, and $\overline{u_{j+2}^{n,L}}$ are the ghost states assigned by Riemann solution (front tracking) or entropy extrapolation (level set). Since in general, $F_{j+1/2}^{n,L} \neq F_{j+1/2}^{n,R}$, such extrapolation methods are not conservative.

To illustrate the failure of conservation we consider explicitly the simplest case, of a first order centered scheme, the Lax-Friedrichs scheme for Burgers' equation. In this case u is a scalar and $F(u) = \frac{1}{2}u^2$. To recover the Lax-Friedrichs scheme, notice that the numerical flux may be written as

$$F_{j+1/2}^n = -\frac{1}{2\lambda}(U_{j+1}^n - U_j^n) + \frac{1}{4}[(U_{j+1}^n)^2 + (U_j^n)^2].$$

If the interface lies between nodes j and $j+1$, the ghost cell extrapolation scheme is found by setting

$$F_{j+1/2}^{n,L} = -\frac{1}{2\lambda}(\overline{u_{j+1}^{n,L}} - U_j^n) + \frac{1}{4}[(\overline{u_{j+1}^{n,L}})^2 + (U_j^n)^2]$$

and

$$F^{n,R}_{j+1/2} = -\frac{1}{2\lambda}(U^n_{j+1} - \overline{u^{n,R}_j}) + \frac{1}{4}[(U^n_{j+1})^2 + (\overline{u^{n,R}_j})^2],$$

according to the above formulas. Since ghost cell extrapolation typically satisfies $U^n_j \neq \overline{u^{n,R}_j}$ and $U^n_{j+1} \neq \overline{u^{n,L}_{j+1}}$, and since the left and right nonidentities generally fail to be equal by different amounts, the left and right fluxes are not equal even in the most elementary possible case, and the ghost cell methods are not conservative.

To obtain a conservative method, we replace $F^{n,L}_{j+1/2}$ and $F^{n,R}_{j+1/2}$ by the dynamic flux as in (5), for which Rankine-Hugoniot conditions guarantee equally of left and right values.

2.3 Conservative Front Tracking

The front tracking method propagates the interface by solving the Riemann problem at the interface. Using the extrapolated states from the left and right sides of the front, the Riemann solution consists of several constant states separated by waves: shock, rarefaction and contact discontinuity. The Riemann solution contains the speed s and the constant states u_L, u_R on each side of a wave. They must satisfy the Rankine-Hugoniot condition

$$f(u_L) - su_L = f(u_R) - su_R \quad . \tag{10}$$

In the present context, the primary tracked wave in the Riemann solution is the contact discontinuity.

Consider the one dimensional case and assume that the position σ^n of a tracked wave is between the two cell centers x_j and x_{j+1} at the time step t_n. Then, at the time step t_{n+1} there are two possibilities: (1) the interface position σ^{n+1} is still between x_j and x_{j+1}; (2) the interface has crossed one cell center, for example, the new interface position is between cell centers x_{j+1} and x_{j+2}. For the first case, let us introduce the notation $\overline{\Delta x}^n_j = \sigma^n - x_{j-1/2}$ and $\overline{\Delta x}^n_{j+1} = x_{j+3/2} - \sigma^n$. For $i \neq j, j+1$, let $\overline{\Delta x}^n_i \equiv \Delta x$. Also let $\overline{\lambda}^n_j = \Delta t / \overline{\Delta x}^n_j$. We can update the new interior states at j and $j+1$ respectively, through the following schemes

$$U^{n+1}_j = (\overline{\Delta x}^n_j / \overline{\Delta x}^{n+1}_j) U^n_j - \overline{\lambda}^{n+1}_j \left(F^{n,L}_I - F^n_{j-1/2} \right) \tag{11}$$

$$U^{n+1}_{j+1} = (\overline{\Delta x}^n_{j+1} / \overline{\Delta x}^{n+1}_{j+1}) U^n_{j+1} - \overline{\lambda}^{n+1}_{j+1} \left(F^n_{j+3/2} - F^{n,R}_I) \right) \tag{12}$$

where U^n_j, U^n_{j+1}, U^{n+1}_j and U^{n+1}_{j+1} are integrated over irregular cells of minimum size $\Delta x/2$ defined by the interface location. For example

$$U^n_j = (\overline{\Delta x}^n_j)^{-1} \int_{x_{j-1/2}}^{\sigma^n} u(x, n\Delta t) dx \quad . \tag{13}$$

The interface flux F_I^n is defined as

$$F_I^{n,L} = f(u_L^n) - s^n u_L^n = f(u_R^n) - s^n u_R^n = F_I^{n,R} \quad . \tag{14}$$

The second case is handled by similar formulas [5]. For the second case, small space cells may arise and to prevent this from occurring, the irregular space time cell containing the moving interface is split into two pieces, each of which is merged with a (regular) neighbor for the purpose of the finite difference algorithm.

The conservative property follows directly from (14). The improved convergence properties of this scheme result from a locally second order accurate reconstruction of the speed s^n and the states u_L^n and u_R^n at the midpoint between the (σ^n, t_n) and (σ^{n+1}, t_{n+1}) on the moving interface. These quantities must satisfy (14) as an identity. The extension to higher dimensions is developed in [5], where numerical examples in one dimension are also given.

Theorem 1. The above algorithm defines a finite difference scheme which is conservative at tracked fronts as well as in the interior, and which has L_∞ second order local truncation errors near a tracked interface in 1D and first order L_∞ local truncation errors near a smooth tracked interface in higher dimensions. Thus the algorithm is formally third order accurate in L_1 in 1D and second order accurate in L_1 in higher dimensions.

Proof. The conservativeness of this method is easily seen through the summation

$$\sum_{j=1}^{N} \overline{\Delta x}_i^{n+1} U_j^{n+1} = \sum_{j=1}^{N} \overline{\Delta x}_i^{n} U_j^{n} - \Delta t (F_{RB}^n - F_{LB}^n). \tag{15}$$

Here, N is the total number of cells, F_{LB}^n and F_{RB}^n are the flux at the left and right boundaries, respectively. The cancelation of the flux terms near the tracked interface is due to Rankine-Hugoniot condition $F_I^{n,L} = F_I^{n,R}$. For the proof of order of local truncation error, see [5]. The extension to multi-dimensions requires space time finite volume differencing, one version of which is proposed in [5]. As in the 1D algorithm, merging of selected adjacent cells is needed to assure a lower bound on the CFL time step restriction.

2.4 Conservative Level-Set Tracking

The first use of the level set method in fluid simulation [9, 7] was only a graphical tool to follow the motion of the interface through the evolution of a level set function $\psi(\mathbf{x})$ by solving

$$\frac{\partial \psi}{\partial t} + \mathbf{v} \cdot \nabla \psi = 0 \quad , \tag{16}$$

where the $\mathbf{v}$ is the flow velocity in space. This use of the level function can be replaced by other physical quantities such as the fluid density. In order to fully exploit the level set method, Fedkiw *et al.* applied a ghost-cell extrapolation method similar to that of the front tracking method [6]. The primary difference between these two ghost cell algorithms lies in the constant extrapolation of the Riemann solution states *vs.* entropy extrapolation of the states from one side for the assignment of ghost-cell states. As we have shown in Section 2.3, neither extrapolation is conservative.

In the calculation of interface speed, the major difference between [9, 7] and front tracking is that the front tracking method first solves a Riemann problem whose solution gives both the interface speed and the left and right states, while the interface speed in [9, 7] is given by the evolution of the level function through two successive time steps. Consider a one-dimensional case. The exact interface velocity in a time step Δt must be calculated through the interpolated interface positions σ^n and σ^{n+1}:

$$s = \frac{\sigma^{n+1} - \sigma^n}{\Delta t} \quad . \tag{17}$$

In order to match the Rankine-Hugoniot condition at the interface, we must construct the left and right states u_l and u_R to satisfy

$$s(u_L - u_R) = F(u_L) - F(u_R) \quad . \tag{18}$$

For a nonlinear wave such as a shock, this is a complex problem since the shock speed is local and does not equal the flow velocity on either side of the interface. However, for a contact interface, this Riemann problem is simplified, as the propagation speed for the contact discontinuity equals the continuous normal component of the fluid velocity on both sides of the interface. Also, the pressure must be continuous across the contact interface. As a result, the densities, arbitrary on both sides, are the only remaining variables available which can be chosen to satisfy the jump condition.

We can therefore construct the left and right states in the following way. First, the velocity is given by (17):

$$u_L = u_R = s, \tag{19}$$

while the pressure at the interface is interpolated from a stencil which consists of states at cell centers on both sides of the interface.

$$p_L = p_R = \lim_{x \to \sigma \pm 0} p(x,t) \quad . \tag{20}$$

The left and the right densities are extrapolated from stencils from the left and right sides respectively and are not equal to each other, as suggested by the formulas

$$\rho_L = \lim_{x \to \sigma - 0} \rho(x,t) \qquad \rho_R = \lim_{x \to \sigma + 0} \rho(x,t) \quad . \tag{21}$$

Method	N	L_1 error	L_1 order	$\Sigma U_i \Delta x_i$
Un-tracked	30	6.83e-2	-	1.732
	60	3.49e-2	0.969	1.733
	120	1.63e-2	1.10	1.733
	240	8.24e-3	0.984	1.733
Conservatively tracked	30	2.17e-2	-	1.732
	60	7.07e-3	1.62	1.733
	120	2.11e-3	1.74	1.733
	240	6.04e-4	1.80	1.733

Table 1: Comparative error analysis for the test problem (22) for Burgers' equation.

Conservative finite differencing with no mass diffusion across an interface requires use of irregular cells near the interface. In other words, state averages over regular cells cut by an interface are not sufficient, and must be supplemented by sufficient information to allow determination of the state average over each of the pieces into which the cell is divided by the interface. This aspect of conservative differencing is shared by both the front tracking and the level set algorithms we propose here. Thus we complete the numerical scheme following that of the front tracking method (11), (12). Extension to higher dimensions is through space time finite volume methods as with Front Tracking.

3 Numerical Examples

We compute the Burgers' equation $\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}(\frac{1}{2}u^2) = 0$ on $[0,6] \times [0,T]$, with initial conditions

$$u(x,0) = \begin{cases} 0.2 * (x-1)^2 + 0.2 \quad , & x \in [1,3] \quad , \\ 0.2 \quad , & \text{elsewhere} \quad . \end{cases} \tag{22}$$

In Table 1 we present the numerical results at $T = 3.2$ using the untracked MUSCL scheme and conservatively (shock) tracked scheme with a MUSCL interior solver. Fig. 1 displaces the comparative numerical results obtained with $N = 30$, $T = 3.2$ and CFL number equal to 0.4. Here L_1 error indicates the L_1 norm of $u - \tilde{U}$ at time T, where u is the exact solution and $\tilde{U}$ is the 2nd order approximate solution reconstructed from the piecewise constant numerical solution U at time T, which is supposed to be an approximation of the cell average of the the exact solution.

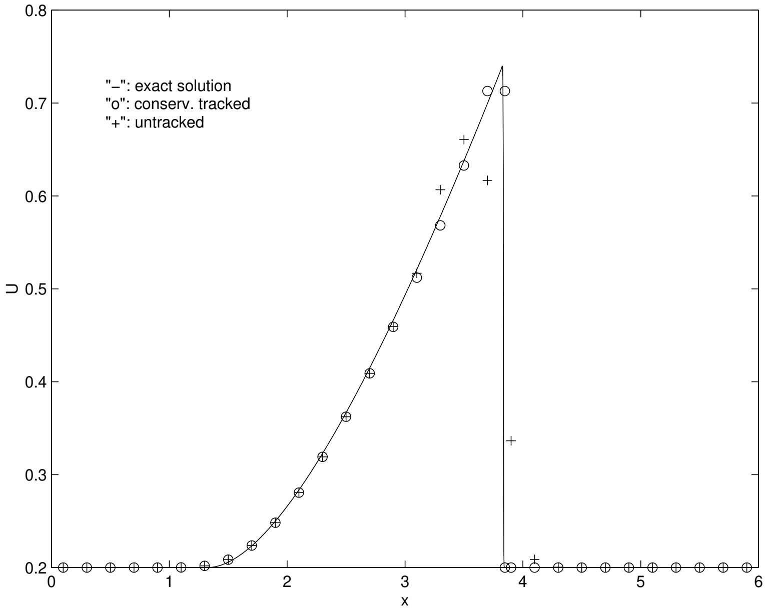

Figure 1: Comparative numerical results for Burgers' equation

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