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ON THE NUMERICAL METHODS FOR DISCONTINUITIES AND INTERFACES

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ABSTRACT. Discontinuous solutions or interfaces are common in nature, for examples, shock waves or material interfaces. However, their numerical computation is difficult by the feature of discontinuities. In this paper, we summarize the numerical approaches for discontinuities and interfaces appearing mostly in the system of hyperbolic conservation laws, and explain various numerical methods for them. We explain two numerical approaches to handle discontinuities in the solution: shock capturing and shock tracking, and illustrate their underlying algorithms and mathematical problems. The front tracking method is explained in details and the level set method is outlined briefly. The several applications of front tracking are illustrated, and the research issues in this field are discussed.

1. Introduction

Discontinuities or interfaces are common phenomena in physics and other applications. The boundary between an ice and water, when an ice melts, is one of examples of interfaces, and the seismic waves in earthquake is an example of propagating discontinuities. However, the appearance of discontinuities causes difficulties in their numerical computations because the differential operator does not hold near discontinuities. A finite difference discretization behaves well in smooth regions, but it can behave terribly near discontinuities. The solutions are oscillatory near discontinuities if higher order schemes are used, or can smear the sharp resolution of discontinuities if lower order schemes are used. The solution of numerical

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methods even could converge to the physically irrelevant solution which is not meaningful at all.

An enormous amount of efforts has been made in this field to handle these difficulties, and special numerical methods have been developed. The purpose of this paper is to summarize the approaches to handle these difficulties, and review recent numerical methods for them. We explain their underlying algorithms and mathematical problems. Especially, we concentrate on the front tracking method which the author had participated its development for several years and has been applied extensively to various applications. The governing system of equations is concentrated on the system of hyperbolic conservation laws since the formation of discontinuities is the most significant and common feature of solutions of hyperbolic conservation laws.

The paper consists as follows. In Sec. 2, we introduce the system of hyperbolic conservation laws and explain two main approaches for its numerical solutions. In Sec. 3, we explain basic concepts and convergence theories for general numerical methods for the system of conservation laws. Shock capturing methods are described in Sec. 4. The approximate Riemann solver is explained and BCT method are illustrated as an example of this approaches. In Sec. 5, as a representative of shock tracking methods, the front tracking method is described in detail and its various applications are illustrated. The code structure and mathematical issues of underlying algorithm is also provided. In Sec. 6, a level set method is outlined as an interface tracking method for the completeness of description. We conclude this paper in Sec. 7.

2. Shock capturing and shock tracking

We consider the numerical solution of the nonlinear system of hyperbolic conservation laws which is a specific type of partial differential equations having such a form:

$$U_t + F(U)_x = 0, \tag{2.1}$$

$$U(x,0) = U_0(x). \tag{2.2}$$

Here $U(x,t) \in \mathbf{R}^m$ is an m-dimensional vector of conserved quantities, $F : \mathbf{R}^m \to \mathbf{R}^m$ is a smooth function called the *flux function*, and U_0 is the initial data. x could be a multi-dimensional vector for the space.

Equation (2.1)–(2.2) arises in the modeling of physical processes through conservation principles, and it describes many important physical phenomena. Examples include gas dynamics, combustion theory, shallow water theory, elasto-plasticity, magneto-hydrodynamics, and petroleum reservoir engineering.

The fundamental feature of solutions of Eqs. (2.1)–(2.2) is the formation of discontinuities within finite time even for smooth initial data. This phenomenon is caused by the nonlinearity of the flux function; it leads to mathematical and numerical difficulties because derivatives are not defined at discontinuities. The general methodology to overcome these difficulties is the expansion of the solution space through the weak formulation, however, weak solutions are not unique in general. Therefore, we must have some criterion to choose the physically relevant solution from among the many possible weak solutions and the solution which satisfies a certain criterion is called *entropy solutions*. These all features of hyperbolic conservation laws cause the difficulties in the design of computation methods for it.

When we devise a numerical method for solutions having discontinuities, there are two requirements on it. One is the convergence to the correct physical solution, *i.e.*, entropy solution, and the other is obtaining the sharp resolution of discontinuities. A finite difference discretization behaves well in smooth regions, but it can behave terribly near discontinuities. In order to assure the convergence to the correct solution, a typical remedy for poor behavior near discontinuities is adding a small amount of numerical diffusion. This is the *shock capturing* method. However, numerical diffusion spoils the sharp resolution of discontinuities.

An alternative for overcoming poor behavior near discontinuities is to combine a standard finite difference method in the smooth region with some specialized procedure for tracking the location and structure of discontinuities. This method uses analytic information such as jump conditions, to propagate tracked discontinuities, which are perfectly sharp. This is the *shock tracking* or *front tracking* method. Front tracking has proved very useful for many applications (*e.g.*, gas dynamics [7, 5, 18, 23, 26, 29], petroleum reservoir simulation [12, 20, 21], elasto-plastic deformation [15]). However, the implementation of front tracking can be very complicated, especially for three dimensional flow.

The shock capturing method, by contrast, tries to produce sharp approximations to discontinuous solutions automatically by means of high

order approximations in smooth regions. A significant advantage is that shock capturing requires less knowledge of the wave structures, hence its implementation is simple. This method finds the physically correct solution by adding the sufficient amount of numerical diffusion near discontinuities while keeping higher order accuracy in smooth regions. A great deal of progress has been made in the design of shock capturing schemes, and a variety of such schemes are available today. However, shock capturing can not handle shock waves that are sensitive to numerical diffusion, like deflagration waves in combustion, and transitional shock waves. For more discussion of this issue, refer Ref. [30, 32].

In fact, tracking or capturing is not an either or choice. A front tracking code can use a capturing methods in the flow regions away from the tracked waves. Depending on the features of the problem, such a hybrid methods can give more accurate answers.

3. Basic concepts and convergence theories

We discretize the (x, t) plane by choosing a mesh width $h = \Delta x$ and a time step $k = \Delta t$, and define discrete mesh points (x_i, t_n) by

$$x_i = i\Delta x, \quad i = \ldots, -1, 0, 1, \ldots \tag{3.1}$$

$$t_n = n\Delta t, \quad n = 0, 1, \ldots . \tag{3.2}$$

Intermediate points $x_{i+1/2}$ are defined such as

$$x_{i+1/2} = \left(i + \frac{1}{2}\right)\Delta x. \tag{3.3}$$

For simplicity we take a uniform mesh. The finite difference methods produce approximations $U_i^n \in \mathbf{R}^m$ to the true solution $u(x_i, t_n)$ at the discrete mesh points. It is also convenient to define a piecewise constant mesh function $U(x, t)$ for all x and t from the discrete values U_i^n as assigning the value U_i^n in the grid cell, *i.e.*,

$$U(x, t) = U_i^n \quad \text{for}(x, t) \in [x_{i-1/2}, x_{i+1/2}) \times [t_n, t_{n+1}). \tag{3.4}$$

In the following it is assumed that the mesh width Δx and time step Δt are related by

$$\frac{\Delta t}{\Delta x} = \tau, \tag{3.5}$$

with $\tau > 0$ a given constant. Hence, the choice of Δt defines a unique mesh.

Concerning numerical methods for hyperbolic conservation laws, there is a very simple and natural requirement we can impose to guarantee that approximate solutions converge to a weak solution. This requirement is that the method be in *conservation form.*

DEFINITION 3.1. Consider a $(2k+1)$ - point finite difference method for the conservation law. This method is said to be *conservative* if it can be written as

$$U_i^{n+1} = U_i^n - \frac{k}{h}(F_{i+1/2} - F_{i-1/2}), \tag{3.6}$$

where F is a continuous function of $2k$ states:

$$F_{i+1/2} = F(U_{i-k+1}^n, \ldots, U_{i+k}^n). \tag{3.7}$$

The function F is called the *numerical flux.*

It can be shown that for consistency of a conservative method, it is sufficient to require the numerical flux function F to be Lipschitz continuous and to satisfy

$$F(u, \ldots, u) = f(u) \tag{3.8}$$

where f is the true flux of the original conservation law.

Lax and Wendroff [34] proved that if a conservative and consistent scheme converges to some function $u(x,t)$ as the grid is refined through some sequence, then this function will in fact be a weak solution of the conservation law. However, since there can be more than one weak solution, different sequences might converge to different weak solutions dependent on the convergent sequence. We need a numerical admissibility criterion to insure that the limit function u is the physically correct weak solution of the conservation law. However, the most criteria used for mathematical theories are hard to apply to discrete solutions since a discrete approximation defined only at grid points is discontinuous everywhere in some sense. The widely used approach to overcome this problem is to define a function called an *entropy function* $\eta(U)$ for which an additional conservation law holds for smooth solutions that becomes an inequality for discontinuous as similar as a physical entropy. This function is assumed to be convex and to satisfy a conservation law of the form

$$\eta(u)_t + \psi(u)_x = 0 \tag{3.9}$$

for some *entropy flux* $\psi(u)$. Combining this entropy function with the notion that the physically relevant solution is the stable limit of vanishing viscosity weak solutions, we can easily derive the admissibility condition in terms of the entropy function $\eta(u)$ and corresponding entropy fluxes $\psi(u)$ [35].

DEFINITION 3.2. The function $u(x,t)$ is the *entropy stable solution* of a system of conservation laws if, for all convex entropy functions η and corresponding entropy fluxes ψ, the inequality

$$\eta(u)_t + \psi(u)_x \leq 0 \tag{3.10}$$

is satisfied in the weak sense (for all non-negative test functions).

This formulation is very useful in analyzing numerical methods. The discrete form of this is given as

$$\eta(U_i^{n+1}) \leq \eta(U_i^n) - \frac{k}{h}[\Psi(U^n; i) - \Psi(U^n; i-1)], \tag{3.11}$$

where Ψ is some numerical entropy flux function that must be consistent with ψ in the same manner that we require F to be consistent with f.

DEFINITION 3.3. A conservative numerical method is called an *entropy stable method* if, for all convex entropy functions η and corresponding entropy flux ϕ, the inequality Eq. (3.11) is satisfied.

The following theorem is the extension of the theorem of Lax and Wendroff and is proved in Ref. [34].

THEOREM 3.4. *Suppose that a conservative method is consistent with the conservation law and is entropy stable. Let $U_l(x,t)$ denote the numerical approximation on the l-th grid indexed by $l = 1, 2, \ldots$, with mesh parameters $k_l, h_l \to 0$ as $l \to \infty$. If U_l converge to u as $l \to \infty$ in the sense of bounded, L_1 convergence, then the limit u is an entropy stable solution of conservation law.*

The Lax and Wendroff theorem and its extension does not guarantee the convergence of the method; only says that if a sequence of approximations converges, then the limit is a weak solution. To guarantee convergence, we need some form of stability condition. Such stability has been developed for scalar conservation laws; examples include a monotonicity preserving or total variation diminishing (**TVD**) conditions. However, for general systems of conservation laws with arbitrary initial data, no

numerical method has been proved to be stable or convergent, except in some special cases. Therefore we restrict attention to convergence results in the scalar case.

For a given function $u(x,t)$, the total variation $TV(u)$ at time t is defined by

$$\begin{aligned} TV(u) &= \limsup_{\epsilon\to 0} \frac{1}{\epsilon}\int_{-\infty}^{\infty} |u(x+\epsilon,t)-u(x,t)|\,dx \\ &\quad + \limsup_{\epsilon\to 0} \frac{1}{\epsilon}\int_{-\infty}^{\infty} |u(x,t+\epsilon)-u(x,t)|\,dx. \end{aligned} \tag{3.12}$$

When u is discretized by some numerical method, the analogous definition at time t_n is

$$TV(U(\cdot,t_n)) = \sum_{i=-\infty}^{+\infty} |U_{i+1}^n - U_i^n|. \tag{3.13}$$

DEFINITION 3.5. The numerical method is total variation diminishing (TVD) if

$$TV(U(\cdot,t_{n+1})) \le TV(U(\cdot,t_n)), \tag{3.14}$$

for all grid functions $U(\cdot,t_n)$.

THEOREM 3.6. *Let T be a given constant and suppose that U is generated by a numerical method. Suppose that this numerical method is entropy stable, and suppose that for each initial data $u_0 = u(x,0)$, there exist k_0 and $R > 0$ such that*

$$TV(U(\cdot,t_n)) \le R \quad \forall n,k \text{ with } k < k_0 \text{ and } nk \le T. \tag{3.15}$$

Then the method is convergent for $k \to 0$ in the sense of bounded, L_1 convergence and its limit is the unique entropy stable solution.

The proof of this theorem can be found in the Ref. [35]. Thus, if TVD method is used, then the inequalities

$$TV((U(\cdot,t_n)) \le TV(U(\cdot,0)) \le TV(u_0) \tag{3.16}$$

guarantee that the TVD method is convergent.

DEFINITION 3.7. The numerical method is called *monotonicity preserving* if the following statement holds: whenever u_0 is monotone (either nonincreasing or nondecreasing), then $U(\cdot,t_n)$ is also monotone for all $t > 0$.

DEFINITION 3.8. The numerical method is called *monotone* if the following implication holds:

$$V(x,t_n) \geq U(x,t_n)\ \forall x \Rightarrow V(x,t_{n+1}) \geq U(x,t_{n+1})\ \forall x. \tag{3.17}$$

DEFINITION 3.9. The numerical method is called L_1-*contracting* if the following statement holds;

$$\|U(\cdot,t_{n+1}) - V(\cdot,t_{n+1})\|_1 \leq \|U(\cdot,t_n) - V(\cdot,t_n)\|_1. \tag{3.18}$$

Here, $\|\cdot\|_1$ denotes the L_1 norm in the space variable.

If the numerical method is monotone, then it is L_1 contracting. A numerical method which is L_1 contracting, is always TVD. Furthermore, a numerical method that is TVD is always monotonicity preserving [10, 35].

THEOREM 3.10. *If the numerical method is monotone, then the method is convergent in the sense of bounded L_1 convergence and its limit is the unique entropy stable solution.*

Although this monotonicity requirement always lead to convergence to the entropy stable solution, this method is at most first-order accurate:

THEOREM 3.11. *A monotone numerical method is consistent of at most order one.*

The proofs of above two theorems can be found in Ref. [28]. A three-point stencil TVD method is also at most first-order accurate. However, five-point stencil TVD methods are possible to be second-order accurate in smooth regions as a second-order upgraded versions of three-point stencil method through limiters. For example, van Leer's MUSCL scheme [51], Harten's ULTIMATE scheme [27]. The most common analytic tool for the proof of convergence for them is the compensated compactness arguments which are based on H^{-1} compact entropy production. The good reference for the weak convergence and compensated compactness would be a book by Evans [14], and refer DiPerna's paper [44] to see the application of this theory to the system of hyperbolic conservation laws.

Although Goodman and LeVeque proved that any method that is TVD in two space dimension is at most first order accurate [24], many multi-dimensional methods, such as operator splitting methods, finite volume methods, the wave propagation method, *etc*, have been designed with their own advantages. The main design strategy of them is to achieve the

second-order accurate in smooth regions but reduce the spurious oscillation near discontinuities. The proofs of convergence to entropy satisfying solutions are mostly missing yet in most multi-dimensional schemes. The compensated compactness frame works well to prove their convergence in one-dimensional schemes, and the concept of measure valued solutions is using to prove the convergence of finite volume methods in the multi-dimensional case. The results of multi-dimensional case are mostly for a scalar case and still many problems are open for multi-dimensional systems.

4. Shock capturing methods

In this section, we will restrict the scope of our discussion to one important class of shock capturing methods for hyperbolic conservation laws: Godunov-type methods. In a Godunov-type method, the numerical solution $U(x, t_n)$ is considered to be a piecewise constant function $\tilde{u}^n(x, t_n)$ with the value U_i^n in each mesh cell $(x_{i-1/2}, x_{i+1/2})$ at time level t_n. The cell interface at $x_{i+1/2}$ separates two constant states, U_i and U_{i+1}. Therefore the initial-value problem is a Riemann problem the solution of which gives informations about the local wave interaction. The evolution of the solution in a cell to the next time step is carried out by solving Riemann problems at the two cell interfaces and averaging the solution at time t_{n+1}:

$$U_i^{n+1} = \frac{1}{h} \int_{x_{i-1/2}}^{x_{i-1/2}} \tilde{u}^n(x, t_{n+1}) dx. \tag{4.1}$$

In order for adjacent Riemann problems not to interfere, the inequality

$$\Delta t \, |\lambda|_{max} < \frac{1}{2} \Delta x \tag{4.2}$$

must hold, where $|\lambda|_{max} = \max(|\lambda_1|, \ldots, |\lambda_m|)$, this is a CFL condition [48, 33]. However, the exact solution of a Riemann problem is hard to obtain and computationally expensive. Instead approximate Riemann solvers are often used.

There are also two important assumptions underlying Godunov type methods equipped with approximate Riemann solvers. First, the system must be strictly hyperbolic, so that the linearized coefficient matrix possesses a complete set of eigenvectors. Second, each mode of wave propagation must be either genuinely nonlinear or linearly degenerate. Since the

systems and waves we are considering do not satisfy these assumptions, standard Riemann solvers cannot be directly applied. Efforts to overcome this restriction and extend methods to general systems have been made by Bell, Colella and Trangenstein [3]. The basis of these approaches is to add sufficient dissipation that an entropy satisfying solution is obtained. We find that as a result, they cannot handle the waves we are considering which are sensitive to the numerical regularization. In next sections, we describe approximate Riemann solvers and the method of Bell, Colella and Trangenstein (BCT) as an example of the Godunov-type method extended to higher order accuracy and general systems of conservation laws.

4.1. Approximate Riemann solvers

As mentioned earlier, approximate Riemann solvers are preferred, even when exact Riemann solutions are known, because of computational efficiency. Also, in a Godunov method, since the exact solution is later averaged over each grid cell, it seems appropriate the use of an less expensive approximate Riemann solution. An approximate Riemann solver can be viewed simply as giving a new form of numerical flux in Eq. (3.6).

The most commonly used approximate Riemann solvers are Roe's method [50] and Osher's method [43]; the latter is used in the BCT method as we describe in next section. Therefore here we examine a Roe's approximate Riemann solver.

The idea of Roe's method is to approximate the original nonlinear system by a constant coefficient linear system with flux $\hat{A}(U_L, U_R)\bar{U}(x,t)$ at each cell. Then Roe suggested that the matrix $\hat{A}$ should satisfy following conditions:

(i) If $U_L, U_R \to \bar{U}$ with some point $\bar{U}$ between U_L and U_R, then $\hat{A}(U_L, U_R) \to A(\bar{U})$.
(ii) $\hat{A}(U_L, U_R)(U_R - U_L) = F(U_R) - F(U_L)$.
(iii) $\hat{A}(U_L, U_R)$ is diagonalizable with real eigenvalues.

Given such a matrix $\hat{A}$, the numerical flux function is given as

$$\begin{aligned} F_{i+1/2} &= f(U_{i+1}) - \sum_{\lambda_p>0} \lambda_p \alpha_p \hat{r}_p \\ &= f(U_i) + \sum_{\lambda_p<0} \lambda_p \alpha_p \hat{r}_p, \end{aligned} \tag{4.3}$$

where $U_{i+1} - U_i = \sum_p \alpha_p \hat{r}_p$ and $\hat{r}_p$ is the p-th eigenvector of $\hat{A}(\bar{U})$.

Generally, however, it is not easy to derive a suitable $\hat{A}$ matrix for a system of conservation laws. In Ref. [50], Roe found such a matrix for the Euler equations.

4.2. BCT method

One problem to be addressed is eigenvector deficiency. The BCT method is an extension of Godunov type of methods to handle the case of eigenvector deficiency which often appears in several applications such as magnetohydrodynamics, three-phase flow through porous media, and combustion. The BCT method has a procedure to detect points where the solution exhibits local linear degeneracy or non-strictly hyperbolicity. At these points, the Godunov method is modified, by adding sufficient dissipation so that the scheme is stable. At all other points, a variation of the standard Godunov method is used, with the Engquist-Osher type of an approximate Riemann solver [13, 43].

The detection algorithm is based on an inequality that estimates the possibility that two wave speeds coincide in the vicinity. Let us call U_L and U_R the states in neighboring cells. The jump from U_L to U_R is decomposed into m jumps corresponding to each of the wave modes:

$$U_R - U_L = \sum_{k=1}^{m} \bar{\alpha}_k \bar{r}_k, \tag{4.4}$$

where, $\bar{U} = 1/2(U_L + U_R)$ and $\bar{r}_k := r_k(\bar{U})$ is the k-th eigenvector of $F'(\bar{U})$. Then the inequality is given as

$$|\lambda_i - \lambda_j| < 0.1 \sum_{k=1}^{m} \bar{\alpha}_k |\kappa_{ik} - \kappa_{jk}|, \tag{4.5}$$

where κ_{ik}, called the structure coefficients, are defined to be

$$\kappa_{ik} \equiv \lambda_i' \cdot \bar{r}_k. \tag{4.6}$$

If this inequality is satisfied, then λ_i and λ_j are assumed to be involved in an eigenvector deficiency.

When there is no eigenvector deficiency, the numerical flux in Eq. (3.6) is given as

(4.7)
$$F(U_L, U_R) = F(U_L) + \sum_{k=1}^{m} [\int_0^{\bar{\alpha}_k} \min(\lambda_k(\alpha), 0)\, d\alpha] \cdot \bar{r}_k \quad \text{when } \bar{\sigma} \geq 0,$$

where $\bar{\sigma}$ is the mean speed defined as

(4.8)
$$\bar{\sigma} = \frac{(F(U_L) - F(U_R)) \cdot (U_L - U_R)}{\|U_L - U_R\|^2}.$$

If $\bar{\sigma}$ is less than 0, then an analogous formula based on U_R instead of U_L is used:

(4.9)
$$F(U_L, U_R) = F(U_R) - \sum_{k=1}^{m} [\int_0^{\bar{\alpha}_k} \max(\lambda_k(\alpha), 0)\, d\alpha] \cdot \bar{r}_k \quad \text{when } \bar{\sigma} < 0.$$

In contrast, when eigenvector deficiency is detected at U_L and U_R, say i-th and j-th families, the calculation of the flux is divided into two cases, depending on the sign of the maximum and minimum eigenvalues involved in eigenvector deficiency. Let

(4.10)
$$\lambda_{ij}^{\min} = \min(\lambda_i^L, \lambda_j^L, \lambda_i^R, \lambda_j^R),$$

(4.11)
$$\lambda_{ij}^{\max} = \max(\lambda_i^L, \lambda_j^L, \lambda_i^r, \lambda_j^R).$$

When $\lambda_{ij}^{\min}$ and $\lambda_{ij}^{\max}$ have the same sign, set

(4.12)
$$\bar{r}_{ij} = \frac{\bar{\alpha}_i \bar{r}_i + \bar{\alpha}_j \bar{r}_j}{\bar{\alpha}_{ij}},$$

where $\bar{\alpha}_{ij} = \|\bar{\alpha}_i \bar{r}_i + \bar{\alpha}_j \bar{r}_j\|$, and define the numerical flux by

$$F(U_L, U_R) = F(U_L) + \sum_{k \neq i,j} \int_0^{\bar{\alpha}} \min(\bar{\lambda}_k(\alpha), 0)\, d\alpha \cdot \bar{r}_k$$

(4.13)
$$+ \int_0^{\bar{\alpha}_{ij}} \min(\bar{\lambda}_{ij}(\alpha), 0)\, d\alpha \cdot \bar{r}_{ij}.$$

where $\bar{\lambda}_{ij}$ is a linear function such that

(4.14)
$$\bar{\lambda}_{ij}(0) = \max(\lambda_i^L, \lambda_j^L)$$

and

$$\bar{\lambda}_{ij}(\bar{\alpha}_{ij}) = \min(\lambda_i^R, \lambda_j^R). \tag{4.15}$$

This choice of $\bar{\lambda}$ assumes the maximally compressive wave and makes the scheme to incorporates a judicious amount of additional dissipation in this formalism. Otherwise, when $\lambda_{ij}^{\min}$ and $\lambda_{ij}^{\max}$ have opposite signs, the deficiency is assumed to be associated with a transonic wave, the integral correction term is replaced by a dissipative term such as

$$F(U_L, U_R) = F(U_L) + \Sigma_{k \neq i,j} \left[\int_0^{\bar{\alpha}_k} \min(\lambda_k(\alpha), 0)\, d\alpha \cdot \bar{r}_k \right] - \frac{1}{2} \nu \bar{\alpha}_{ij} \bar{r}_{ij}, \tag{4.16}$$

where $\nu = \max(|\lambda_i^L, |\lambda_i^L|, |\lambda_j^R|, |\lambda_j^R|)$. The higher order extension could be accomplished through the slope limiter method as same as in the paper by Colella [8].

5. Front tracking methods

Front tracking method is an adaptive computational method in which a lower dimensional moving grid is fitted to and follows the dynamical evolution of distinguished waves in a fluid flow. The method takes advantage of known analytic solutions for idealized discontinuities. Numerous approaches to front tracking have been taken since Richtmyer and Morton first proposed the method [49]. One of the important issues among these approaches is to keep the conservation principle on each side of fluids. Chern and Colella [6] and recently LeVeque and Shyue [36, 37] have proposed tracking methods coupled with conservative finite volume method and the propagation of fronts using Rankine-Hugoniot condition of the front. The Stony Brook group, led by Glimm, has developed a very extensive set of tools for shock and interface tracking in one, two, and three space dimensions and successfully applied to a wide variety of problems [38, 45, 5, 7, 17, 16, 26]. The code structure and underlying ideas are very effective and useful, therefore, it would be worthwhile to briefly discuss ideas behind the Stony Brook front tracking method in this section.

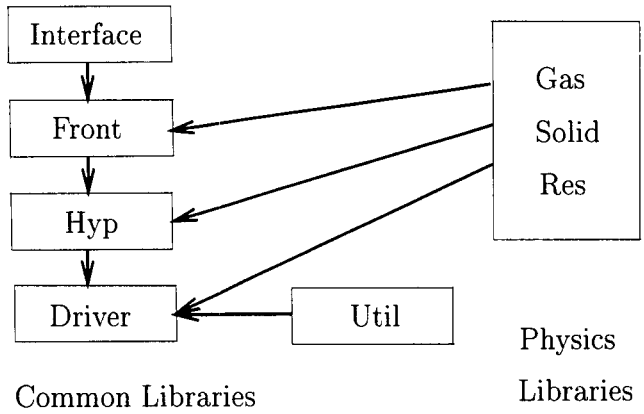

FIGURE 1. Basic structure of front tracking code

5.1. Basic structure

Front tracking is composed of two basic sets of libraries: a physics-independent set of libraries, which manipulates the geometry of fronts and performs the high-level operations; and a set of physics-dependent libraries, which handles all operations specific to a given application. Currently, the Stony Brook code handles three classes of physics: gas dynamics, porous media flow, and elasto-plastic solid mechanics.

In front tracking, the most basic physics-independent data structures are the *interface* and the *front*. The interface contains data structures and routines for manipulating the geometry and topology of the tracked waves. In contrast, the front contains the routine for the propagation of tracked waves.

The interface data structure consists of recursive data structures such as points, bonds, curves, nodes, triangles, and surfaces (see Fig. 2), and its routines perform elementary operations, including creating, deleting, copying, printing, and reading these objects. The linear pieces of a curve are called bonds, and the start and end points of a curve are called nodes. In general, several curves may start or end at a common node. Surfaces are discretized in terms of triangles, and they are bounded by and meet

along curves. Other routines are provided to join or split curves, check for intersections, and compute the topological component containing a given point. For more complete description of this data structure, see Ref. [22, 4, 16].

The front library is a collection of subroutines that support states and boundary conditions; it manages the data and geometries for the dynamical propagation of tracked waves. The front library includes the interface data structure to represent the geometries of fronts and has values for state variables at each points of fronts. Fronts are points in one dimension, curves and nodes in two dimension, and surface and curves in three dimension. All physics dependent operations are confined to a few subroutines that are accessed through pointers to functions, which are set in a physics library.

The other physics independent libraries are called *hyp*, *driver* and *util*. The hyp library contains subroutines for solving hyperbolic equation by usual finite difference schemes. The util and driver have subroutines that format the input and output, allocate storage, and perform debugging. access physics-dependent operations through pointers to functions defined in a physics library.

5.2. Propagation of the front

The propagation of the solution to the next time step is divided into two main parts: the propagation of the tracked wave structures (front propagation) and the updating of the values of the states at locations away from the tracked interface (interior propagation).

The propagation of a front involves the motion of points on the front and the evolution of the states on the front. Here we concentrate on the front propagation algorithm for the two dimensional case, in which fronts are curves. For each curve the operator is split into two sweeps over its points, the *normal* and *tangential sweeps*.

During the normal sweep, a Riemann problem is solved at each point; the left and right states in this Riemann problem come from the states on the two sides of the curve. A second-order approximation to this Riemann solution can be attained by drawing characteristic curves from the front into the interior of the domain. This also provides coupling from the interior to the front. The solutions to this Riemann problem gives the velocity of the wave and a pair of states values at the advanced points of the curve at next time step. The information corresponding to the

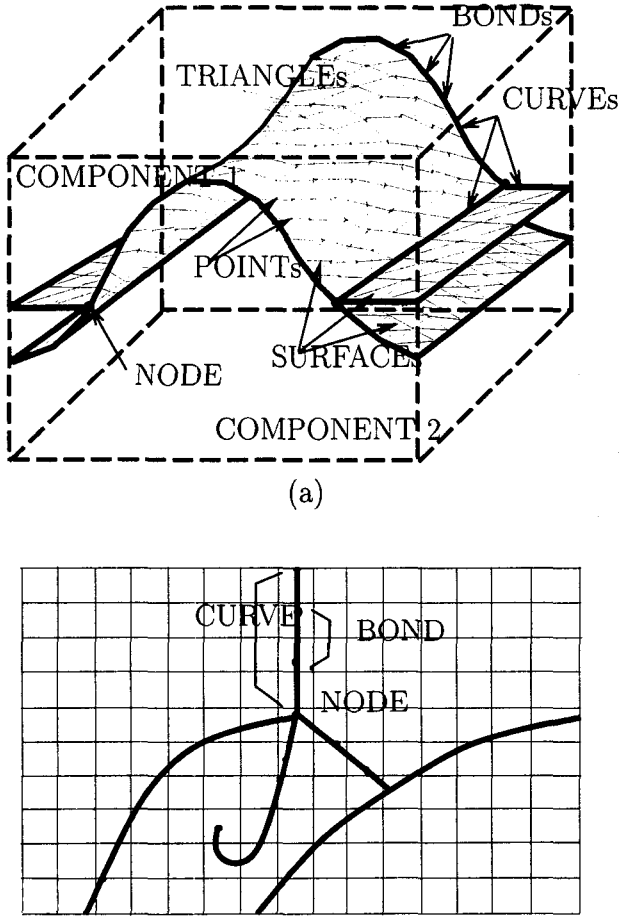

FIGURE 2. These figures show the recursive data structures of interface used in front tracking code: (a) in three dimensions, (b) in two dimensions. The figure (a) is adapted from Ref. [37].

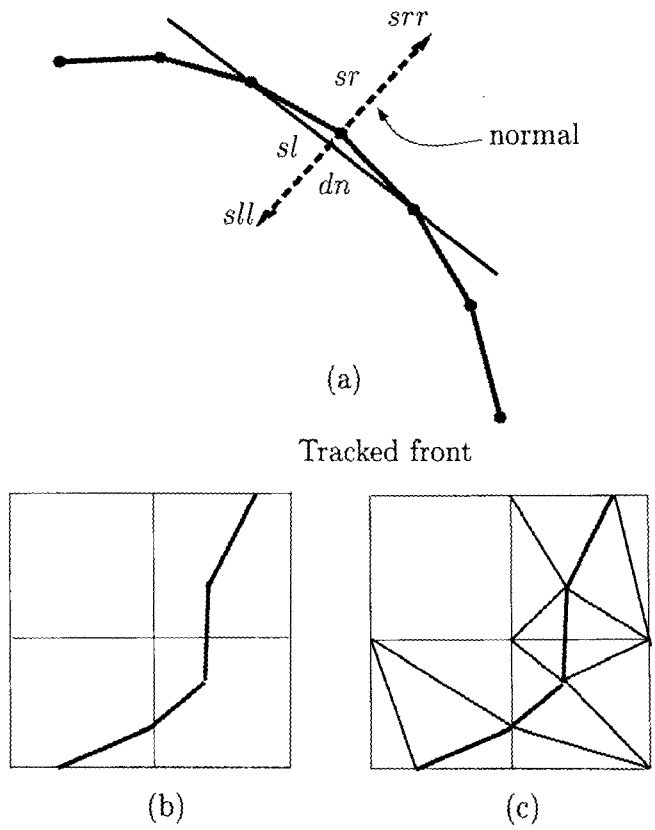

FIGURE 3. Figure (a) shows the normal and tangential sweep over the front, and (b),(c) show the interpolation of interior states in a cell crossed by the front.

tangential component is included in the solution at the front by using an one-dimensional finite difference sweep along each of the curves. (See Fig. 3.)

This approach works away from nodes where the discontinuity curves meet, because at such intersection points the geometry does not in general allow an operator splitting into normal and tangential directions. In a neighborhood of a node the curves are approximated by straight lines.

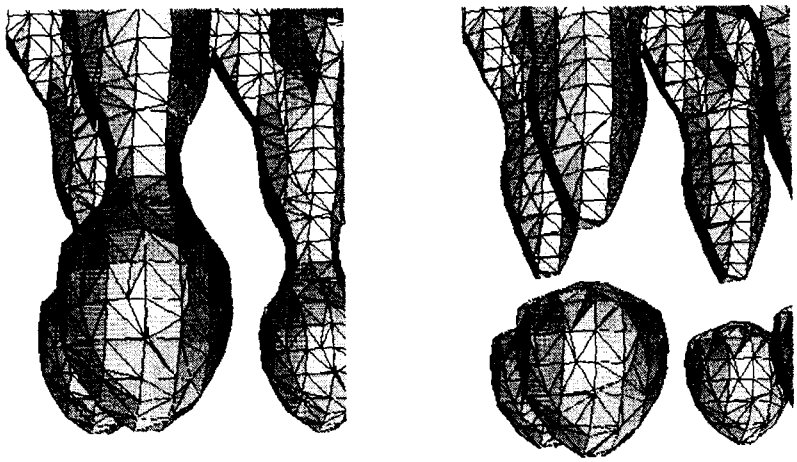

FIGURE 4. Pinch-off of the tracked front in the simulation of Rayleigh-Taylor in three dimensions.

Thus the evolution of nodes are determined as the solution of a two-dimensional Riemann problem. Each type of node requires a specialized propagation algorithm depending on the geometry of curves near a node. In the case of gas dynamics, various node types have been classified [18, 1, 2] and their propagation algorithms have been implemented by using shock polar analysis [9, 25].

The normal and tangential sweeps are carried out, and after propagating the nodes, algorithms are applied to redistribute and untangle curves. This prevents pile-ups, thinning and self-intersections of the front. This completes the propagation of the front.

After the propagation of fronts, the next step is to compute the solution in the interior. Each grid block has a list containing component and bond information; this permits finding components and nearest interface points efficiently. For grid cells crossed by the front are triangulated making it possible to interpolate as (c) in Fig. 3. Then all interior grid points are updated by using common shock capturing schemes, it completes the propagation of solutions to the next time step. For more details of implementation, refer Ref. [4, 26], and for the history and summary of front tracking methods, refer Ref. [31].

5.3. Applications of front tracking method

The front tracking method has been applied to various problems which contain important singularities, or jump discontinuities such as shock waves and material interfaces. Here we introduce some of applications of front tracking, especially the results of Stony Brook's front tracking code which the author has worked for several years.

The first application to show is the problem of fluid mixing caused from the fluid instability known as Rayleigh-Taylor (RT) or Richtmeyer-Meshkov (RM) instability. These instabilities are originated from the acceleration of the fluid interface separating fluids of different densities. Since the fluid interface is very sensitive to the numerical diffusions which most numerical methods adopt, the computation results of other methods do not match with experimental results well. However, front tracking methods have shown that the computation of mixing rates agrees well with laboratory experiments [29]. These results lies in the absence of numerical diffusion at the interface of front tracking method since the physical diffusion at a molecular level is not an important factor in these instabilities. Fig. 4 and Fig. 5, which are computed by colleagues of the author (Dr. Xiao Lin Li and Dr. Mary Jane Graham) and adopted under their allowance, show the simulation results of RM and RT instabilities respectively.

The next example is an etching and deposition simulation appearing in the manufacture of semiconductor chip. These processes are modeled as the evolution of level surface $S(X,t)$ which satisfies a Hamilton-Jacobi equation:

$$S_t + H(S_x) = 0, \tag{5.1}$$

where H is a Hamiltonian function. H has the form

$$H(P) = c(P/\|P\|)\|P\|, \tag{5.2}$$

where $P = S_x$ and c is a function called the etching or deposition efficiency which is different by the property of the incoming beam. This example shows that front tracking method is not restricted to the form of hyperbolic conservation laws. Any type of equations can be applied when they contain discontinuous curve or surface if their propagation algorithms are provided. In the case of a Hamilton-Jacobi equation, the propagation algorithm for the level surface S has been analyzed through the concept of viscosity solutions [11], and the cusp, corners, and nodes

FIGURE 5. The simulation of Richtmeyer-Meshkov (RM) instability in the cylindrical coordinate. The dense black line represents a tracked interface and it conserves the symmetries of the mushroom shape of growing interfaces.

are handled by solving Riemann problems and the approximation of its characteristic equation. Refer [19] for details. The figure Fig. 6, simulated by Dr. Dechun Tan, shows some of results of the etching and deposition simulation.

The third application to show is the elasto-plastic material simulation. When two materials impact, its simulation is difficult because the phenomena is highly nonlinear: it could lead to material fracture and failure. It also involves material boundaries and complicated wave patterns with discontinuous solution features. The fully conservative Eulerian formulation was proposed by Plohr and Sharp [46, 47] and its numerical computation in multi-dimension is currently under development. Here we omit in details, but present a computational result of the impact simulation using front tracking of material interfaces. The full description of its numerical algorithm and Riemann solution is in preparation [40, 39] and will be published soon.

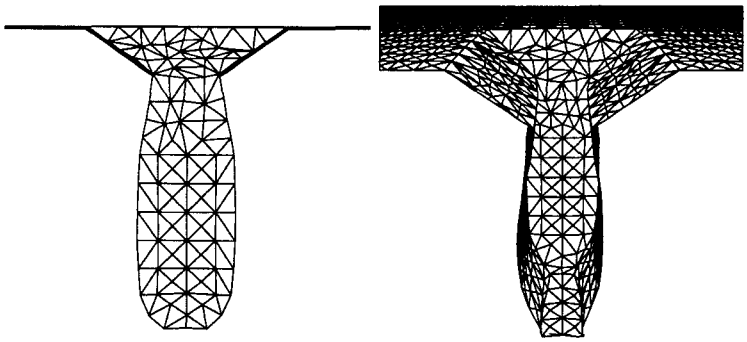

FIGURE 6. Etching and deposition simulation. 3D images of the void formation simulation at $t = 0.11$. From left to right: end view, cut by the plane $y = 0$, and a corner, respectively.

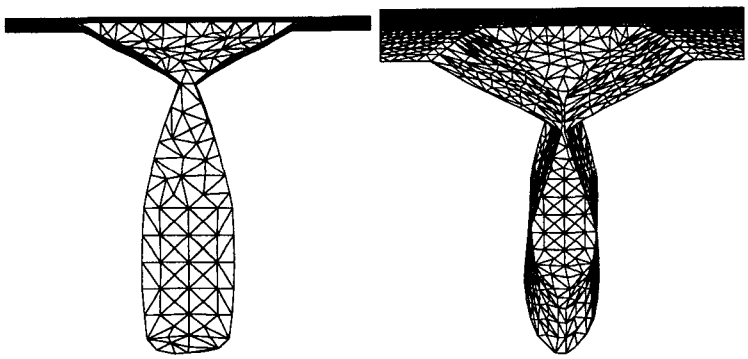

FIGURE 7. The same simulation at time $t = 0.22$. The surface has just intersected itself near the top of the trench.

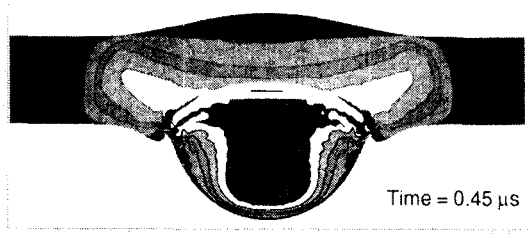

FIGURE 8. The picture shows the penetration of a tantalum projectile impacting normally on a tantalum target. The contour is drawn in the pressure plane, and the material interface is tracked by the front tracking method.

6. The level set method

In 1987, S. Osher and J. A. Sethian devised a numerical method called *the level set method* to capture the moving fronts appearing in solutions [42]. The moving front is represented by an auxiliary function $\phi(x,t)$ which is Lipschitz continuous and called a level set function since $\phi(x,t) = 0$ represents the boundary of the moving front. A level set function ϕ satisfies

$$\phi_t + \bar{u} \cdot \nabla\phi = 0, \tag{6.1}$$

where $\bar{u}$ is the average velocity of the moving front. When $\hat{n}$ is the normal vector of the moving front, generally $\bar{u} \cdot \hat{n}$ is a function of the geometry of the moving front, therefore it leads to the Hamilton-Jacobi equation such as

$$\phi_t + |\nabla\phi| H(\nabla\phi, \phi) = 0. \tag{6.2}$$

For example, H could be a function of the curvature κ of the front which is given as $\kappa = \nabla \cdot \left(\frac{\nabla\phi}{|\nabla\phi|}\right)$. Any numerical method for the Hamilton-Jacobi equation can be used to solve this equation, and the motion of front is represented as a zero level set function. This method has been applied in several applications which contain moving fronts like rising air bubbles or falling water drops [41].

Both front tracking and the level set method are methods to handle the same kind of problems which contain moving fronts or interfaces. The main difference of two methods is that front tracking can adopts the analytical information on the motion of fronts, on the other hand, the level set method is purely numerical. The other difference is that front tracking handles topological changes of fronts and the interaction of fronts artificially using the computational geometry algorithms, however, the level set method can handle the topological changes of fronts by just solving Eq. (6.2) numerically. The easy handling of topological changes of the front is a major advantage of the level set method, but the level set method can not handle the interactions of several fronts. Since front tracking could apply analytical solutions of moving fronts whenever they are available, its computational results of the problems which are sensitive to numerical diffusion should be accurate than those of the level set method. In fact, unphysical pressure waves are noticed at an accelerated fluid interface when the level set method is used. However, the level set method is faster and simpler to implement than the front tracking method. Therefore both methods have their own advantages and could be used dependent on the properties of problems and analytical information on the problems.

7. Conclusion

Many problems are still open both in theories and numerics on the system of hyperbolic conservation laws. Regarding numerical methods, the design of higher order accurate multi-dimensional scheme is a challenging project. Although Goodman and LeVeque proved that any method that is TVD in two space dimension is at most first order accurate [24], many multi-dimensional methods, such as operator splitting methods, finite volume method, wave propagation method, *etc.* have been designed with their own advantages. However, their convergence results to entropy satisfying solutions are mostly missing yet. The compensated compactness frame or measure valued solutions works well to prove their convergence in one-dimensional schemes, however, the results of multi-dimensional cases are mostly for a scalar case and the problems of multi-dimensional systems are still open.

The approach for treating discontinuities or interfaces separately is preferred recently in the problems having complex moving interfaces. The front tracking method combined with advanced shock capturing schemes could generate the best results when analytic solutions are available. Obtaining analytic solutions is a good mathematical problem as itself, for example, solving a one or two-dimensional Riemann problems. These all of problems are waiting for the attacks of many mathematicians.

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