The next generation CIP as a conservative semi-Lagrangian solver for solid, liquid and gas

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Received 26 November 2001; received in revised form 13 January 2002

Abstract

We present a review of the CIP method, which is a kind of semi-Lagrangian scheme and has been extended to treat incompressible flow in the framework of compressible fluid. Since it uses primitive Euler representation, it is suitable for multi-phase analysis. The recent version of this method guarantees the exact mass conservation even in the framework of semi-Lagrangian scheme. Comprehensive review is given for the strategy of the CIP method that has a compact support and subcell resolution including front capturing algorithm with functional transformation.

Keywords: Multi-phase flow; Semi-Lagrangian; Solid; Liquid; Gas; Universal solver; CIP

1. Introduction

Recent development of simulation technology made possible the combined analysis of solid, liquid and gas. However, simultaneous treatment of materials undergoing phase state transition is still not well established. This is because the conventional combined analysis relies on the separate treatment of each phase. For example, overset grid is the easiest way to treat the structure-fluid interaction but it fails for a severely distorted structure or for melting of structure. A universal treatment of all phases by one simple algorithm is essential. In order to attack the problems mentioned above, we must first find a method to treat a sharp interface and to solve the interaction of compressible gas with incompressible liquid or solid.

Toward this goal, we take Eulerian approach based on the CIP (cubic-interpolated propagation) method (see for review, Ref. [14]) which does not need adaptive grid system and therefore removes...
the problems of grid distortion caused by structural break up and topology change. The material surface can be captured almost by one grid throughout the computation. Furthermore, the code can treat all the phases of matter from solid state through liquid and two phase state to gas without restriction on the time step from high sound speed.

Although the CIP can give accurate results keeping conservation error in quite low level, the semi-Lagrangian form cannot guarantee the exact mass conservation by itself. Recent version of the CIP-CSL [10,13] can overcome this difficulty and provide exactly conservative semi-Lagrangian scheme. Since these schemes do not use the cubic polynomial but use different orders of polynomial, we redefine the name of these CIP families as “constrained interpolation profile” and still keep the abbreviation, CIP. This means that various constraints such as the time evolution of spatial gradient, that is used in the original CIP method, or spatially integrated conservative quantities can be used to construct the profile. In this paper, we shall give a review of the CIP method and related schemes to attack these important subjects.

2. CIP method

2.1. Advection processes

Although the nature is in a continuous world, digitization process is unavoidable in order to be implemented in numerical simulations. Primary goal of numerical algorithm will be to retrieve the lost information inside the grid cell between these digitized points. Most of numerical schemes proposed before, however, did not take care of real solution inside the grid cell and resolution has been limited to the grid size. The CIP method proposed by one of the authors tries to construct a solution inside the grid cell close enough to this real solution of the given equation with some constraints [14]. A simple advection equation

\[ \frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} = 0. \]

(1)

is calculated by \( f^{n+1} = F(x - u\Delta t), g^{n+1} = dF(x - u\Delta t)/dx \) in the CIP where \( g \) stands for \( \partial f/\partial x \). If two values of \( f \) and \( g \) are given at two grid points, the profile between these points can be interpolated by cubic polynomial \( F(x) = ax^3 + bx^2 + cx + d \). Thus, the profile at \( n + 1 \) step can be obtained as

\[ f_i^{n+1} = a_i \xi^3 + b_i \xi^2 + g_i' \xi + f_i^n, \]

\[ g_i^{n+1} = 3a_i \xi^2 + 2b_i \xi + g_i^n, \]

(2)

where we define \( \xi = -u\Delta t \). The coefficients of polynomial \( a, b \) are given by continuity requirement [14].

It would be interesting to examine phase error of various schemes using the method proposed by Purnell [9] and Utsumi et al. [12]. Fig. 1 summarizes those results. As is well known, phase speed of conventional schemes depart from the exact one, that is shown by the solid line, around \( k\Delta x = \pi/2 \). Surprisingly, however, the CIP can reproduce the correct phase speed even up to \( k\Delta x = \pi \). This is remarkable because \( k\Delta x = \pi \) means that one wavelength is described by 2 grid size. Let us consider the case where values of the 3 points are zero. Even in this case, one wave can exist. The CIP
gives correct spatial gradients, which are non-zero at these points, and therefore it recognize the existence of the wave inside the grid cell. Any code that uses only the information of the value, that is zero now, cannot correctly recognize the wave even if higher order polynomial is employed. The superiority of the CIP also appears in numerical damping and dissipation [12]. The importance of propagated gradients can be clearly demonstrated in comparison with the cubic spline [9]. Although the cubic spline uses the same cubic polynomial and the information of gradient as the CIP, it cannot reproduce the result of the CIP, because the gradient of the spline is determined merely from smoothness requirement. As is easily recognized, such a constraint that is independent of the original equation will not help to retrieve the profile inside the grid cell. It is important to note that the computation time does not seriously increase by the addition of spatial gradient because coefficients of cubic polynomial can be used also for gradient calculation. Actually the CPU time required for a simple advection problem in one dimension is cubic-lagrange/CIP = 1.0, spline/CIP = 1.68 (Thomas method is used to solve matrix), RCIP/CIP = 1.77, PPM/CIP = 2.31. RCIP is the rational function CIP [14].

2.2. Burgers turbulence

The CIP method is applied to Burgers equation:

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = v \frac{\partial^2 u}{\partial x^2}.
\]  (3)

After imposed random-noise initial perturbation, we observe the power spectrum calculated from various schemes as shown in Fig. 2 where \( v = 1/250 \) and velocity is \( u = 20 + \delta u \) and \( \delta u \) is random number of \( \pm 5 \) size. The CIP can reproduce the spectrum regardless of mesh size. It should be noticed that the end point of the highest \( k \) corresponds to \( k \Delta x = \pi \) which corresponds to the wavelength of 2 grid size. As shown in Fig. 1, the CIP can accurately trace the phase speed of this wave and this is the reason why the spectrum does not change regardless of mesh size. Since the spectrum method does not converge in this situation, we shall compare our result with UTOPIA scheme and K–K scheme [5]. UTOPIA and K–K schemes give similar result. Although K–K scheme can produce a
universal spectrum for stationary turbulence that is $u = \delta u$ without main flow [6], it suffers from significant diffusion for streaming flow because of fourth order dissipation term.

2.3. Interface tracking: a sharpness preserving method

Various kinds of methods have been developed so far to achieve a compact and correctly defined interface by introducing extra programming. Among those mostly used algorithms are the level set methods and the VOF (volume of fluid) methods [4] for front capturing, and others for front tracking [11]. Level set method that was firstly proposed by Osher and Sethian [8] gets around the computation of interfacial discontinuity by evaluating the field in higher dimensions. The interface of interest is then recovered by taking a subset of the field. Practically, the interface is defined as the zero level set of a distance function from the interface.

We devised an interface tracking technique [14] which appears efficient, geometrically faithful and diffusionless. The method is a combination of the CIP advection solver and a tangent function transformation. Let us consider the time evolution of color function which is described by Eq. (1), where the color function $f$ represents the interior of material by 1 and the outside by 0.

Solving the above equation by finite difference schemes in an Eulerian representation will produce numerical diffusion and tend to smear the initial sharpness of the interfaces. In our method, rather than the original variable $f$ itself, its transformation, say $F(f)$, is calculated by the CIP method. We specify $F(f)$ to be a function of $f$ only, which means that the new function $F(f)$ is also governed by the same equation as (1). Hence, we have

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

and all the algorithms proposed for $f$ (schemes for advection equation) can be used to $F(f)$. Hopefully, by the considerable simplicity, this kind of techniques would be very attractive for practical implementation. We here use a transformation of a tangent function for $F(f)$.

Although $f$ experiences a rapid change from 0 to 1 at the interface, $F(f)$ shows a quite regular behavior. Because most of the values of $F(f)$ are concentrated near $f=0$ and 1, the function transformation improves locally the spatial resolution near the large gradients. Thus, the sharp discontinuity can be described quite easily. This method does not involve any interface construction procedure.
and is quite economical in computational complexity. It should be noted that the present method is more attractive in 3-D computation since the extension of the scheme to 3-D is straightforward.

Fig. 3 shows an example of this treatment. The initial sharpness of a bullet is well preserved and the discontinuities are advected with a correct speed.

2.4. Conservative semi-Lagrangian scheme

It is quite useful to look for conservative semi-Lagrangian scheme because semi-Lagrangian method can be quite effective on parallel computers, suits for multi-phase flow, and enables the advection calculation with large time step free from CFL condition. Although the semi-Lagrangian scheme has been successfully used in short-term atmospheric problems, the loss of exact conservation makes the scheme inappropriate for long-term problems and oceanic problems.

Furthermore, there exist subjects that require exact conservation of mass. One of the typical example is the black-hole formation and emission of gravity wave. In this case, small fraction of mass is converted into gravity wave and strict mass conservation is essential. Another example is plasma simulation in which Vlasov equation in six-dimensional phase space must be solved and total density of particle must be conserved, otherwise large electric field appears. The CIP method can be constructed to exactly conserve the total mass in Vlasov system of equally spaced grid in phase space [7]. However, the use of non-equally spaced grid or other general grids can save the computational cost and is worthy for investigation.

In this sense, the effort to establish exact conservation in semi-Lagrangian form would be a challenging task. Toward this goal, we proposed two schemes CIP-CSL4 [10] and CIP-CSL2 [13]. In CIP-CSL4, the fourth-order polynomial is chosen as an interpolation function and the time development of $f$ and $g$ is calculated simply by shifting the interpolation function $F_i(x)$ by $u \Delta t$ in the same way as Eq. (2) of the CIP method. Since the order of polynomial is increased, we have now freedom to choose another constraint to determine the polynomial. We use the constraint to the integrated value to guarantee the mass conservation. Thus this scheme is able to describe a structure of one-grid size as shown in Fig. 4 even without tangent transformation.

The CIP-CSL2 uses a set of equations:

$$
\frac{\partial D}{\partial t} + u \frac{\partial D}{\partial x} = 0, \quad \frac{\partial f}{\partial t} + \frac{\partial (uf)}{\partial x} = 0.
$$

$$
(5)
$$
These two equations are similar to the equations for $f$ and $g$ in Eq. (1) by replacing $f$ by $D = \int f \, dx$ and $g$ by $f = \partial D / \partial x$. Therefore, we can use all the procedures of the CIP method for the integral value of $f$. We can impose the conservation of integrated value easily by this change.

3. Semi-Lagrangian approach to hydrodynamic equations

3.1. Pressure-projection algorithm in primitive Euler scheme

Before presenting a method to solve all the phases of materials, we must at first construct a unified equation to describe all the phases. For this purpose we use the following set of hydrodynamic-type equations:

$$\frac{\partial f}{\partial t} + (u \cdot \nabla)f = S.$$  

(6)
Here, $f = (\rho, \mathbf{u}, T)$, $S = (-\rho \nabla \cdot \mathbf{u} + Q_m, -\nabla p/\rho + Q_u, -P_{TH} \nabla \cdot \mathbf{u}/\rho C_v + Q_E)$, and $\rho$ is the density, $\mathbf{u}$ the velocity, $p$ the pressure, $T$ the temperature, $Q_m$ represents the mass source term, $Q_u$ represents viscosity, elastic stress tensor, surface tension, etc., and $Q_E$ represents viscous heating, thermal conduction and heat source. Here, $C_v$ is the specific heat for constant volume and we define $P_{TH} = T(\partial p/\partial T)_\rho$ which is derived from the first principle of thermodynamics.

The underlying physics included in the above equations for continuum dynamics is complex and may include processes which possess quite different time scales of variation. It should be expedient to separate the solution procedure into several fractional steps.

The CIP method uses the primitive Euler method to solve Eq. (6) with a separate treatment of advection term like conventional semi-Lagrangian formulation, thus the formulation into a simultaneous solution of incompressible and compressible fluid is readily obtained.

Original CCUP (CIP-combined unified procedure) method was proposed only for a special equation of state, but here we rebuild it with more general EOS [14]. That is, for small change of density and temperature, the pressure change can be linearly proportional to them as

$$\Delta p = \left( \frac{\partial p}{\partial \rho} \right)_T \Delta \rho + \left( \frac{\partial p}{\partial T} \right)_\rho \Delta T,$$

where $\Delta p$ means the pressure change $p^{n+1} - p^*$ during one time step and $^*$ is the profile after advection. This applies also to $\rho, T$. From this relation, once $\Delta \rho, \Delta T$ are predicted, $\Delta p$ will be predicted based on Eq. (7). Needless to say, $\partial p/\partial \rho, \partial p/\partial T$ are given by EOS. Since the CIP separates the non-advection terms from the advection, we can concentrate on the non-advection terms related to sound waves which are the primary cause of the difficulty in liquid having large sound speed. Thus we obtain

$$\nabla \left( \frac{1}{\rho^*} \nabla p^{n+1} \right) = \frac{p^{n+1} - p^*}{\Delta t^2 (\rho C_v^2 + (P_{TH}^2/\rho C_v T))} + \nabla \cdot \mathbf{u}^*.$$

This equation shows that, at the sharp discontinuity, $\mathbf{n} \cdot (\nabla p/\rho)$ is continuous. Since $\nabla p/\rho$ is the acceleration, it is essential that this term is continuous since the density changes by several orders of magnitude at the boundary between liquid and gas. In this case, the denominator of $\nabla p/\rho$ changes by several orders and pressure gradient must be calculated accurately enough to ensure the continuous change of acceleration. The equations derived by the ICE [3] in the framework of conservative Euler seems to be quite similar to Eq. (8) but the continuity of $\nabla p/\rho$ in the formers is not guaranteed.

3.2. Application to hydro planning

Figs. 5 and 6 show two examples of fluid-structure interaction calculated by the procedure given in the previous section. A thin aluminum cylinder is thrown over water surface. As our experience tells, the cylinder slides over the surface and then jumps up. In Fig. 5, the cylinder has a round bottom shape while the bottom is flat in Fig. 6.

The present simulation code can replicate well the overall behavior of aluminum disk observed in the experiment.
4. Matrix-free incompressible-flow calculation

Since the CIP is superior in the calculation of advection equation, we can apply the procedure to conventional characteristic equations. Then, if this equation can be solved with large CFL,
compressible and incompressible flow can be solved without matrix solution of pressure. As a simple application, we deal with shallow water equation. Let \( h \) be the height of water surface, then shallow water equations are simply written in one dimension as

\[
\frac{\partial}{\partial t} \begin{pmatrix} h \\ u \end{pmatrix} + \begin{pmatrix} u h \\ g u \\ \frac{\partial h}{\partial x} \end{pmatrix} = \frac{\partial W}{\partial t} + A(W) \frac{\partial W}{\partial x} = 0.
\] (9)

Eq. (9) leads to two equations for the Riemann invariants,

\[
\frac{D^\pm}{Dt} \left( \Gamma \pm \frac{u}{2} \right) = 0, \quad \frac{D^\pm}{Dt} \equiv \frac{\partial}{\partial t} + \lambda^\pm \frac{\partial}{\partial x}.
\] (10)

where \( \Gamma \equiv \sqrt{gh} \), \( \lambda^\pm = u \pm \Gamma \) and \( g \) represents the gravity. The form of Eq. (10) is the same as Eq. (1), so the CIP method can be applied to Eq. (10). Since the phase speed of the gravity waves \( \Gamma \), which is equivalent to sound waves in hydrodynamics, is so fast, time step is restricted by the CFL (\( = \lambda^\pm \Delta t/\Delta x \)) condition of gravity wave when conventional explicit Eulerian schemes are employed. Therefore, the semi-Lagrangian approach [1,2] to the characteristic equations has been used for solving gravity wave to make time step be much longer than CFL condition. This algorithm is tested with initial perturbation of \( h \) in Gaussian form.

\[
h(x, t = 0) = 1.0 + 0.01 \exp \left\{ - \left( \frac{x - X_{\text{max}}/2}{50.0} \right)^2 \right\},
\] (11)

The mesh size of \( \Delta x = 0.25 \) and the number of meshes is 4000. The numerical solution is shown in Fig. 7 and agrees well with analytical solution even for very large CFL = 320.0.

Next, we shall extend the scheme to two dimensions. We use directional splitting here and repeatedly apply the procedure of one dimension to each direction. The initial condition is set as follows.

\[
h(x, y, t = 0) = 1.0 + 0.001 \exp \left\{ - \left( \frac{x - X_{\text{max}}/2}{50.0} \right)^2 - \left( \frac{y - Y_{\text{max}}/2}{50.0} \right)^2 \right\}.
\] (12)
Mesh size is $\Delta x = \Delta y = 1.0$, the number of meshes is $(NX,NY) = (400,400)$. We take CFL = 1.4, 5.0 and 14.0, and calculate up to $t = 100.0$. The contours for each CFL are shown in Fig. 8. Even in two dimensions, the method can give a symmetrical wave propagation under large CFL condition. Therefore we conclude that the present method is applicable to the cases in which the change of characteristic speed can be neglected for one time step, that is, perturbations are small. This does not restrict the applicability of the present method. If the speed of gravity wave is much larger than fluid velocity, variation of characteristic speed becomes smaller and large CFL can be used. The same can be said for incompressible flow because sound speed is much faster than fluid velocity.

Considering the conventional solution to incompressible flow, the use of the Poisson equation for pressure and its implicit solution do not trace the exact movement of sound wave profile, and the wave form in the solution above Lipschitz condition ($\Delta u \Delta t / \Delta x = 1$) is smeared out by strong damping. If the phenomena in the time scale of $\Delta u \Delta t / \Delta x < 1$ is important for the system, these should be correctly treated in the time scale of $\Delta u \Delta t / \Delta x < 1$. If not, we can still use larger time step $\Delta u \Delta t / \Delta x \gg 1$ suffering the exact shape of solutions. Since the present scheme is applicable to multi-dimensional shallow water equations, it is possible to apply it to hydrodynamics directly in future.

References


