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Toward an Ultimate Goal for Universal Solution by CIP Method - 3D Space and 6D Phase Space Solver -

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1 Introduction

In recent years, with the computing environment being improved, a demand for high-precise stable numerical methods is rapidly increasing in various fields of technology. The Cubic Interpolated Pseudoparticle/Propagation (CIP) scheme which has been developed by Yabe *et al.* [1, 2, 3, 4, 5, 6]for solving hyperbolic equations attracts a great deal of attention [7]. The CIP scheme is a low diffusion and stable scheme, and can solve hyperbolic equations by the 3rd order accuracy in space [8], and this scheme has been successfully applied to various complex fluid flow problems, covering both compressible and incompressible flow, such as laser-induced evaporation , shock wave generation, elastic-plastic flow, bubble collapse, milk-crown and so on (see for review [9, 10]).

For these types of problems such as welding and cutting processes, we need to treat topology and phase changes of the structure simultaneously. In freezing, condensation, melting and evaporation, the grid system aligned to the solid or liquid surface has no meaning and sometimes the mesh is distorted and even broken up. To solve these problems requires new tools for combined analysis of materials in different phase state, e.g., solid, liquid and gas. A universal treatment of all phases by one simple algorithm is essential.

Toward this goal, we take Eulerian-approach based on CIP method mentioned above. The CIP method 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 materials from solid state through liquid and two-phase state to gas without restriction on the time step from high-sound speed.

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2 Universal Treatment

2.1 CIP method

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. We here explain its strategy by using an advection equation,

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} = 0. \tag{1}$$

When the velocity is constant, the solution of Eq.(1) gives a simple translational motion of wave with a velocity u. The initial profile (solid line of Fig.1(a)) moves like a dashed line in a continuous representation. At this time, the solution at grid points is denoted by circles and is the same as the exact solution. However, if we eliminate the dashed line as in Fig.1(b), then the information of the profile inside the grid cell has been lost and it is hard to imagine the original profile and it is natural to imagine a profile like that shown by solid line in (c). Thus, numerical diffusion arises when we construct the profile by the linear interpolation even with the exact solution as shown in Fig.1(c). This process is called the first-order upwind scheme. On the other hand, if we use quadratic polynomial for interpolation, it suffers from overshooting. This process is the Lax-Wendroff scheme or Leith scheme.

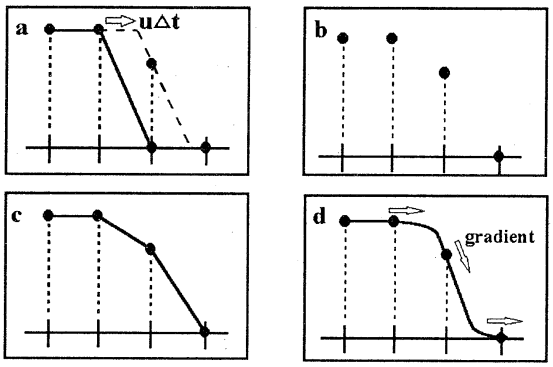

Figure 1: The principle of the CIP method. (a) solid line is initial profile and dashed line is an exact solution after advection, whose solution (b) at discretized points. (c) When (b) is linearly interpolated , numerical diffusion appears. (d) In the CIP, spatial derivative also propagates and the profile inside a grid cell is retrieved.

What made this solution worse ? It is because we neglect the behavior of the solution inside a grid cell and merely follow after the smoothness of the solution. From this experience, we understand that a method incorporating the real solution into the profile within

a grid cell is quite an important subject. We propose to approximate the profile as shown below. Let us differentiate Eq.(1) with spatial variable x, then we get

$$\frac{\partial g}{\partial t} + u\frac{\partial g}{\partial x} = -\frac{\partial u}{\partial x}g, \tag{2}$$

where $g \equiv \partial f/\partial x$ stands for the spatial derivative of f. In the simplest case where the velocity u is constant, Eq.(2) coincides with Eq.(1) and represents the propagation of spatial derivative with a velocity u. By this equation, we can trace the time evolution of f and g on the basis of Eq.(1). If g could be predicted to propagate like that shown by the arrows in Fig.1(d), the profile after one step would be limited to a specific profile. It is easy to imagine that by this constraint, the solution becomes much closer to the initial profile that is the real solution. Most importantly, the solution thus created gives a profile consistent with Eq.(1) even inside the grid cell. Importance of this consistency has been demonstrated in the previous paper[11].

If both the 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 is readily obtained by shifting the profile by $u\Delta t$ like $f^{n+1} = F(x - u\Delta t), g^{n+1} = dF(x - u\Delta t)/dx$.

$$\begin{aligned}
a_i &= \frac{g_i + g_{iup}}{\Delta x_i^2} + \frac{2(f_i - f_{iup})}{\Delta x_i^3}, \\
b_i &= \frac{3(f_{iup} - f_i)}{\Delta x_i^2} - \frac{2g_i + g_{iup}}{\Delta x_i}, \\
\Delta x_i &= x_{iup} - x_i \\
iup &= i - \mathrm{sgn}(u_i)
\end{aligned} \tag{3}$$

$$\begin{aligned}
f_i^{n+1} &= a_i\xi_i^3 + b_i\xi_i^2 + g_i^n\xi_i + f_i^n, \\
g_i^{n+1} &= 3a_i\xi_i^2 + 2b_i\xi_i + g_i^n,
\end{aligned} \tag{4}$$

where we define $\xi_i = -u_i\Delta t$ and $\mathrm{sgn}(u)$ stands for the sign of u.

2.2 Conservative Semi-Lagrangian Scheme

It is well known that the CIP method shows good conservation of mass, although the method is written in a non-conservative form. However, in some special cases, there still exist problems which require exact conservation of mass. For example, when we treat the black-hole formation and plasma dynamics, small fraction of mass and charge generates a gravity wave and a large electric field, respectively, and therefore, the exact conservation of mass is necessary to success the numerical analysis. For the solution of Vlasov equation, it is possible to constitute and improve the CIP method so as to exactly conserve the mass [12]. However, it is impossible to apply this numerical technique to the solution of general hyperbolic equations. Therefore, the development of the conservative CIP method is desired earnestly.

Under such situation, recently, authors have succeeded in the development of new conservative schemes called as CIP-CN4 [13] and CIP-CN2 [14] which are based on the concept of the CIP scheme and succeeded the excellent numerical features of the CIP scheme. In order to include these various families of the schemes, we here extend the name CIP to mean Constrained Interpolation Profile and CN means Conservative scheme in Non-conservative form. CN4 and CN2 use the 4-th order and quadratic polynomial, respectively. The scheme has been applied to many problems of the linear and nonlinear one-dimensional hyperbolic equations in the previous papers [13, 14].

Since semi-Lagrangian schemes [15, 16, 17] can be used for high CFL (Courant-Friedrichs-Lewy) condition in explicit form and are stable for multi-phase flow calculations [18] but only shortcoming is the lack of exact mass conservation, exactly conservative semi-Lagrangian schemes like the CIP-CN2 and CN4 have many promising future applications.

As already seen, the CIP adopted additional constraint, that is spatial gradient, to represent the profile inside the grid cell. For being endowed with the conservative property, we here add another constraint as

$$\rho^n_{i-1/2} = \int_{x_{i-1}}^{x_i} f^n dx. \tag{5}$$

Therefore the spatial profile must be constructed to satisfy this additional constraint. If this could be realized, f would be advanced in the non-conservative form with exact conservation in a form of ρ which could be advanced maintaining mass conservation.

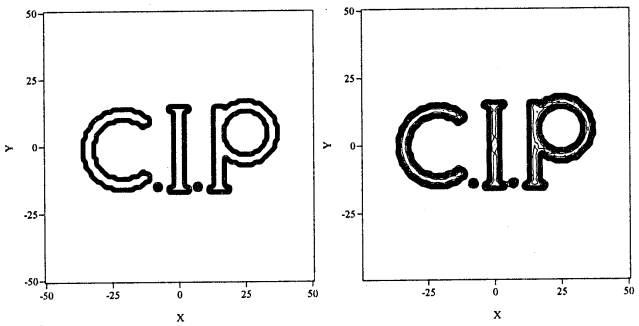

Figure 2: Contour plots after one complete revolution of a solid-body which consists of three characters of "C.I.P" and all the lines composing the charecters are thiner than 3 grid points. (Left) Initial profile (Right) profile after one complete revolution.

Keeping this point in mind, then the ith function piece $F_i(x)$ must be determined so as to satisfy the following constraints:

$$\begin{cases} F_i(x_{i-1}) = f(x_{i-1}) \,, \quad F_i(x_i) = f(x_i) \\ \partial F_i(x_{i-1})/\partial x = g(x_{i-1}) \,, \quad \partial F_i(x_i)/\partial x = g(x_i) \\ \int_{x_{i-1}}^{x_i} F_i(x)dx = \rho_{i-1/2}. \end{cases} \tag{6}$$

In order to meet the above constraints, the 4th-order polynomial can be chosen as the interpolation function $F_i(x)$. Thus 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.(4) of the CIP method. This method is called CIP-CN4 because it uses the 4-th order polynomial. Figure 2 demonstrates the advantage of improved accuary by 4-th order and exact conservation. These characters in Fig.2 is rotated within fixed grid system and dots after the character "C" and "I" are one-grid size. It is surprising, material of one grid size has been preserved even after revolution.

In the CIP, the time evolution of f and $g = \partial f/\partial x$ is used as constraints to define a cubic polynomial, while in the CIP-CN4, constraints are now $f, \partial f/\partial x$ and $\int f dx$ giving 4-th order polynomial. It would be intresting to find a way to apply the CIP to the integrated value of f instead of f itself. The motivation to employ this analogy stems from the following advection equation.

$$\frac{\partial D}{\partial t} + u\frac{\partial D}{\partial x} = 0. \tag{7}$$

Interestingly, if we take a spatial derivative of Eq.(7) and define $D' \equiv \partial D/\partial x$, we obtain a conservative-type equation

$$\frac{\partial D'}{\partial t} + \frac{\partial (uD')}{\partial x} = 0. \tag{8}$$

Then we come to an idea to use $D' = f$ in Eq.(8) and $D = \int f\, dx$ in Eq.(7). This procedure is exactly the same as Eq.(1) by simply replacing f by $\int f\, dx$, together with Eq.(2) in which g is replaced by f. Thus all the CIP procedure can be used for a pair of $\int f dx$ and f instead of f and $\partial f/\partial x$

By this analogy, we shall introduce a function :

$$D_i(x) = \int_{x_i}^{x} f(x')dx'. \tag{9}$$

We shall use a cubic polynomial to approximate this profile.

$$D_i(x) = A1_i X^3 + A2_i X^2 + f_i^n X \tag{10}$$

where $X = x - x_i$. The role of spatial gradient g in the CIP method is now played by f that is spatial gradient of $D(x)$ in the present scheme. By using the above relation, a profile of $f(x)$ between x_i and x_{iup} is then given by taking the derivative of Eq.(10.

Then we apply the splitting algorithm of the CIP to

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} = -f\frac{\partial u}{\partial x}, \tag{11}$$

in which advection part is calculated by

$$f_i^{n+1} = 3A1_i\xi^2 + 2A2_i\xi + f_i^n, \tag{12}$$

where $\xi = -u\Delta t$. Although we separately treat the conservative equation Eq.(8), mass conservation is recovered by Eq.(5) in constructing the spatial profile inside a grid cell.

Although this scheme is quite promising, we will not use it for the calculations given in the following sections, since the original CIP is sufficient for these applications.

2.3 Hydrodynamic Equations

In order to solve all the materials in a universal form, we must find an appropriate equation for solid, liquid and gas. We use full hydrodynamic equations for these materials, which can be written in a form :

$$\frac{\partial \mathbf{f}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{f} = \mathbf{S} \tag{13}$$

where $\mathbf{f} = (\rho, \mathbf{u}, T)$, $\mathbf{S} = (-\rho\nabla \cdot \mathbf{u} + Q_m, -\nabla p/\rho + Q_u, -P_{TH}\nabla \cdot \mathbf{u}/\rho C_v + Q_E)$, and ρ 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 as

$$\begin{aligned} TdS &= dU + pdV = \left(\frac{\partial U}{\partial T}\right)_V dT + \left(\frac{\partial U}{\partial V}\right)_T dV + pdV \\ &= C_v dT + T\left(\frac{\partial p}{\partial T}\right)_V dV \end{aligned} \tag{14}$$

where S is the entropy, U the internal energy, $V = 1/\rho$ the specific volume. The last relation in Eq.(14) is derived from the Helmholtz free energy $F = U - TS$ and thermodynamic consistency : $(\partial p/\partial T)_V = -(\partial^2 F/\partial V \partial T) = (\partial S/\partial V)_T = 1/T\,[p + (\partial U/\partial V)_T]$. Here, P_{TH} is not merely the pressure. In the special case of ideal fluid, however, P_{TH} is exactly the pressure p because the pressure linearly depends on temperature. Next simpler example is the two phase flow described by the Clausius-Clapeyron relation :

$$p = p_0 \exp\left(-\frac{L}{RT}\right), \quad P_{TH} = T\left(\frac{\partial p}{\partial T}\right) \propto L \tag{15}$$

where R is the gas constant. In this case, P_{TH} becomes proportional to the latent heat L. Therefore, P_{TH} describes the heat loss due to latent heat when the ratio of gas increases in two-phase flow. More general form of C_v and P_{TH} will be given by semi-analytical formula or tabulated data.

The CIP method solves the equations like Eq.(13) by dividing those into non-advection and advection phases as given in previous papers. A cubic-interpolated profile propagates in space in the advection phase and then nonadvection phase is calculated by finite difference methods.

As shown in the previous papers, we can trace shock waves correctly with the CIP method although it uses fluid equations written in a non-conservative form or in primitive Euler representation.

2.4 Universal Solver

Since we are treating hydrodynamic equations in a non-conservative form, it is easy to extend it to include both incompressible and compressible fluids. Let us consider again

the origin of the difficulty. In the gas phase where density is sufficiently low, the pressure is in proportion to the density. Therefore, we may solve the density first in Eq.(13) and then after temperature is obtained, we use EOS(equation of state). However, near the solid density, the pressure rises very sharply. If we use the same procedure there, the pressure can change easily by 3-4 orders of magnitude even with small error of density around few tens of percent. Therefore, the strategy to solve the density first is broken in this area. This is the reason why the universal treatment of solid, liquid and gas has been a difficult task.

In attacking this problem, the physicist in incompressible fluid invented an interesting technique. We will translate the strategy they used from a different view point and reconsider the technique. If the pressure is very sensitive to the density, we had better solve pressure at first. If we have a way to solve pressure at first, then we get density very accurately at the solid density. Since the pressure is proportional to density in the gas phase, this strategy does not harm the solution there either. Then how to realize this strategy ? Our method starts with the thermodynamic relation :

$$\Delta p = \left(\frac{\partial p}{\partial \rho}\right)_T \Delta \rho + \left(\frac{\partial p}{\partial T}\right)_\rho \Delta T \tag{16}$$

where Δp means the pressure change $p^{n+1} - p^*$ during one time step and * is the profile after advection. This applies also to ρ, T. From this relation, once $\Delta\rho, \Delta T$ are predicted, Δp will be predicted based on Eq.(16). Needless to say, $\partial p/\partial \rho, \partial p/\partial T$ are given by EOS.The advantage of the CIP is the separate treatment of the non-advection term. We should note that this merit is quite important to get the final result.[5, 19]

$$\nabla\left(\frac{1}{\rho^*}\nabla p^{n+1}\right) = \frac{p^{n+1} - p^*}{\Delta t^2(\rho C_s^2 + \frac{P_{TH}^2}{\rho C_v T})} + \frac{\nabla \cdot \mathbf{u}^*}{\Delta t} \tag{17}$$

where $C_s^2 = (\partial p/\partial \rho)T$.

It is very important to note that in Eq.(17), ρ is inside the derivative on the lefthand side. At the interface between materials having large density difference, the continuity of acceleration $\nabla p/\rho$ is very important because the denominator ρ can change by several orders of magnitude in one grid. Equation (17) guarantees the continuity of $\nabla p/\rho$ at the discontinuity. By this procedure, we can treat all the material at once by simply changing its equation of state. We note again that this property is a consequence of the separate treatment of advection and non-advection terms, otherwise the continuity of $\nabla p/\rho$ is not guaranteed and a large density can not be traced.

It is interesting to examine the meaning of this pressure equation. If $\nabla \cdot \mathbf{u}$ term is absent, this equation is merely the diffusion equation.The origin of this term is as follows. During time step Δt, the sound wave propagates for a distance $C_s \Delta t$. In the next step, the signal also propagates backwardly and forwardly since sound wave should isotropically propagate . Then statistically, 50% propagates backwardly and another 50% forwardly. This process is similar to random walk. The diffusion coefficient of the random walk is given by the quivering distance $\Delta x = C_s \Delta t$ as $D = \Delta x^2/\Delta t$. This leads to the diffusion equation

for pressure. From this consideration, we understand how the effect of sound waves is implemented.

2.5 Elastic-Plastic Model

Elastic motion can be included also in Eq.(13) as

$$Q_u = \frac{1}{\rho}\frac{\partial s_{ij}}{\partial x_j}, \tag{18}$$

where s is the stress tensor. The time development of stress is calculated to be

$$\frac{ds_{ij}}{dt} = 2G\left(\frac{1}{2}\frac{d\epsilon_{ij}}{dt} - \frac{1}{3}\frac{d\epsilon_{kk}}{dt}\delta_{ij}\right),$$
$$\frac{d\epsilon_{ij}}{dt} \equiv \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i},$$

where u is the fluid velocity and G is the Young modulus. When the stress exceeds the von-Mises yield condition, the elastic material changes into plastic material , that is fluid dominated by viscous stress. Figure 2 shows an example of elastic-plastic flow in which both ball and plate are moving through air in the fixed grid system.

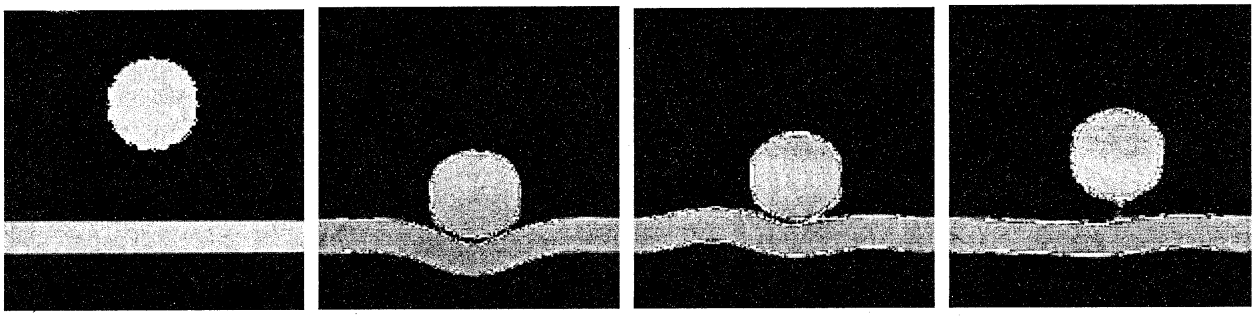

Figure 3: Example of elastic-plastic flow. The system is described by 100×100 Cartesian fixed grid and only 10 grids are used for the width of plate. Plate and ball are moving through fixed grid system. Black part is filled with air and is also calculated.

3 Summary

We have proposed a new tool to attack the simultaneous solution of all the materials. The success of the code is due to a high ability of tracing sharp interface even with fixed grid and flexibility of extension to various materials and physics. The code has been applied to various subjects including fluid-structure interaction , laser-induced melting and evaporation, milk crown formation and so on. Furthermore, the method is easily extended

to solve advection equation in phase-space. At each time step, the distribution function and its first derivatives are advected in phase space by the Cubic Interpolated Propagation (CIP) scheme. Although a cell within grid points is interpolated by a cubic-polynomial, any matrix solutions are not required. The scheme guarantees the exact conservation of the mass. The numerical results show good agreement with the theory. Even if we reduce the number of grid points in v-direction, the scheme still give the stable, accurate and reasonable results with memory storage comparable to particle simulations. Owing to this fact, the scheme has succeeded to be generalized in a straightforward way to deal with the six-dimensional, or full-dimensional problems [12].

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