A New Paradigm of Computer Graphics by Universal Solver for Solid, Liquid and Gas

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We propose a new algorithm for producing computer graphics of melting and evaporation process of matter. Such a computation becomes possible by a universal solver for solid, liquid and gas based on the CIP (Cubic-Interpolated Propagation / Constrained Interpolation Profile) method proposed by one of the authors. This method can also be applied to the movement, deformation and even break up of solid, liquid and gas in one simple algorithm. Therefore seamless computation of all the phases of matter becomes possible. This enables us to reproduce natural phenomena in some instances by computation. In order to demonstrate this reality, we show how precisely the computational result replicates the movies of real phenomena. The flattering motions of metal disk in water and thin name card in air are treated showing accuracy of force calculation on the surface of sub-grid scale. Although the CIP uses semi-Lagrangian form algorithm, the exact mass conservation is guaranteed by additional tool. By using this scheme, separation of a bubble in bifurcation tube and splashing of water surface are successfully simulated.

Key Words: Melting, Evaporation, Semi-Lagrangian, Conservation, Animation, Universal Solver, Natural Phenomena

1. Introduction

The key challenge of computation is to precisely replicate a real world to its extreme extent and seamlessly replace the real phenomena by computation in some instances. Toward this goal, many pioneering works have been done by physics-based computer graphics1(1)-(3). We aim to further elaborate those works to come closer to the real world. This challenge will not succeed without seamless description of all phases of matter like solid, liquid and gas in a compact and simple way.

As a first step toward this goal, we here present a new method to create computer graphics (CG) of melting and evaporation of metal under the illumination of energy beams, which have never been tried before as a CG tool. Such a process includes elastic-plastic motion for solid, viscous motion for liquid and gas together with thermal conduction. Each phase is described by equation of state. The three-dimensional simulation of such process has been beyond the capability of conventional schemes even with fastest supercomputers. The present method makes it possible with one personal computer and with computation time of several hours.

Once such universal scheme has been established, it is much easier to treat conventional fluid-structure interaction with high accuracy. Some examples demonstrate this accuracy. One is impinging of a disk on the water surface, entrapping of bubbles and flattering motion under the influence of fluid force. In order to show how accurate this scheme is, experimentally observed motion is compared. By this comparison of two movies, we confirm that the
computer graphics is now coming closer to a stage that it can replace the real phenomena.

Preceding works on CG tries to create the animation that “might” look like what we imagine as a real world. If we keep this attitude, CG of conventional fluid-structure interaction is already in a matured stage by the efforts of pioneering and innovative algorithms. However, we would have no progress if we stayed in this position. There are many difficult subjects to be resolved but to require accurate treatment. For this purpose, we need much more accurate scheme and universal scheme. The particle-based simulation initiated in 1980s and is now getting growing interest in CG\(^4\). Although the particle code is suitable for describing visualizing splashed particles\(^5\), it is still first order and not sufficient for description of precise behavior of bulk liquid. Most of the subjects presented in this paper require high-resolution and multi-phase flow scheme. In this sense, we are now in a situation that we must step further towards reality by innovative schemes.

2. Basic Algorithm

The author proposed a numerical method CIP to solve hyperbolic-type equation\(^6\)–\(^8\). After 20 years, the CIP is now proven to be applicable to hyperbolic, parabolic and elliptic equations including Schrödinger equation.

The principle of the CIP is to approximate the analytical solution inside a grid cell by polynomial or other simple functions. Suppose the wave propagates as in Fig. 1 (a) according to the advection equation

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

(1)

The profile moves like the solid line in a continuous representation and the solution at grid points is denoted by circles. If we eliminate the line as in Fig. 1 (b), however, the information of the profile inside the grid cell has been lost and it is hard to retrieve the original profile. It is likely to reconstruct a profile like that shown by the line in (c) which corresponds to the first order scheme. Higher order polynomial does not help because of being suffered from unphysical overshooting.

The CIP method predicts the time evolution of spatial derivative \(g\) differentiating the original equation like

\[
\frac{\partial g}{\partial t} + u \frac{\partial g}{\partial x} = -\frac{\partial u}{\partial x} g
\]  

(2)

as shown by the arrows in Fig. 1 (d), then the profile is limited to a specific profile. It is easy to imagine that by this constraint, the solution becomes very closer to the real solution. Most importantly, the solution thus created gives a profile consistent with the original equation even inside the grid cell. This profile can be described by cubic polynomial because \(f\) and \(g\) are given at two neighboring points. Thus the solution of Eqs. (1) and (2) is given by simply shifting a polynomial by \(u\Delta t\) as

\[
\begin{align*}
  f_{i+1}^{n+1} &= a\xi^3 + b\xi^2 + c\xi + d, \\
  g_{i+1}^{n+1} &= -\frac{u_{i+1} - u_{i}}{2\Delta x} g_i + \xi^3 - u\Delta t
\end{align*}
\]

(3)

\[
\begin{align*}
  a &= \frac{g_{i+1} + g_{i}}{\Delta x} + \frac{2(f_{i+1} - f_{i})}{D^2} \\
  b &= \frac{3(f_{i+1} - f_{i})}{D^3} - \frac{2g_i + g_{i+1}}{D} \\
  f &= \frac{g_i + g_{i+1}}{2}
\end{align*}
\]

(4)

where \(\Delta t, \Delta x\) are the time step and spatial grid spacing. Depending on upwind position, \(D = -\Delta x, iup = i-1 (u \geq 0)\) and \(D = \Delta x, iup = i+1 (u < 0)\), where \(i\) is the grid number.

Importance of such predicted gradient is demonstrated in the phase error shown in Fig. 1. The phase speed in the CIP method is accurately reproduced up to the wave of only two grid sizes.

Three-dimensional extension is straightforward by introducing cubic polynomial in \(x, y, z\) directions as

\[
F(x,y,z) = \sum_{0 \leq i,j,k \leq 3} C_{i,j,k}(x-x_i)^i(y-y_j)^j(z-z_k)^k
\]

where \(i,j,k\) denote the grid number in \(x,y,z\) direction. These 20 coefficients \(C\) are determined from the values and \(x,y,z\) -derivatives at \((i,j,k),(i-1,j,k),(i,j-1,k),(i,j,k-1)\) and values at \((i-1,j-1,k),(i-1,j-1,k-1),(i-1,j,k-1),(i-1,j,k-1),(i-1,j-1,k-1)\) for \(u,v,w > 0\). Depending on the sign of the velocity, the upwind position is chosen as in one-dimensional case.

This method is applied to a set of fluid-dynamic type
equation.
\[
\frac{\partial f}{\partial t} + (u \cdot \nabla)f = S
\]  \hspace{1cm} (5)

where \( f = (\rho, u, T, \phi) \) is the vector and \( \rho, u, T, \phi \) are density, velocity, temperature and color function, respectively. The corresponding non-advection terms are given by
\[
S = (-\rho \nabla \cdot u + Q_m - \nabla p/\rho + Q_u, -P \nabla \cdot u/\rho C_v + Q_e, 0)
\]
where \( Q_m \) represents the mass source term, \( Q_u \) includes viscosity, surface tension for fluid, elastic stress for solid and so on. \( Q_e \) includes viscous heating, thermal conduction, and heat source. \( C_v \) is the specific heat ratio for constant volume and \( P = T (\partial p/\partial T) \) is derived by thermodynamic consistency.

This universal form of equation can seamlessly describe solid, liquid and gas simultaneously. All the physical coefficients like sound speed, viscosity coefficient, thermal conductivity and so on, which are denoted by \( A(f) \) for each \( f \) species, are given by
\[
A = \sum A(f)\phi(f)
\]  \hspace{1cm} (6)
where \( \phi(f) \) is the color function of \( f \) species, which include solid, liquid and gas.

In solving all the phases, we encounter the difficulty to treat very different acoustic properties. If the computation is limited by sound speed from stability constraint, we are not able to treat compressible fluid together with nearly incompressible fluid. This effort to overcome the problems caused by high sound speed was pioneered by Harlow and Amsden [1968]\(^9\). However, most of the preceding works chose conservative form of target equations and therefore they are not stable at the air-water interface that has 1000 times density difference.

One of the authors used the non-conservative Euler or semi-Lagrangian form (Eq. (5)) to overcome this problem and separately solved acoustic part from advection part\(^10\). For this purpose, we predict the response of the pressure to the change of density and temperature as
\[
\Delta p = \left( \frac{\partial p}{\partial \rho} \right)_\rho \Delta \rho + \left( \frac{\partial p}{\partial T} \right)_\rho \Delta T,
\]  \hspace{1cm} (7)
and treat the non-advection terms related acoustic wave as
\[
\frac{\rho^{n+1} - \rho^*}{\Delta t} \equiv \frac{\Delta \rho}{\Delta t} \equiv -\rho^* \nabla \cdot u^{n+1}
\]  \hspace{1cm} (8)
\[
\frac{T^{n+1} - T^*}{\Delta t} \equiv \frac{\Delta T}{\Delta t} = -\frac{P}{\rho^* C_v} \nabla \cdot u^{n+1}
\]  \hspace{1cm} (9)
\[
\frac{u^{n+1} - u^*}{\Delta t} \equiv \frac{\Delta u}{\Delta t} = -\nabla \rho^{n+1}
\]  \hspace{1cm} (10)
where values with * means those after the advection terms are calculated in Eqs. (3) and (4). Combining Eqs. (8) – (10), we obtain
\[
\nabla \left( \frac{1}{\rho^*} \nabla p^{n+1} \right) = \frac{p^{n+1} - p^*}{\Delta t (\rho C_v^2 + p/\rho C_P^2)} + \nabla \cdot u^*
\]  \hspace{1cm} (11)
This last form of pressure equation is important, because the pressure force \( \nabla p/\rho \) is continuous at the discontinuity.

Since the density on the denominator changes by 1000 times in one grid, it is essential to guarantee such continuity, otherwise large acceleration should prevent further computation. Finite difference solution of non-advection term is solved by staggered grid system used in MAC\(^{11}\).

3. Melting and Evaporation of Metal

The elastic-plastic motion inside solid can also be described by Eq. (5) in the framework of fluid equation introducing stress tensor \( \sigma \) for non-advection term in equation of motion as
\[
Qu = \frac{1}{\rho} \frac{\partial \sigma_{ij}}{\partial x_j}, \quad \sigma_{ij} = 2G e_{ij}
\]  \hspace{1cm} (12)
where \( G \) is the Young modulus and \( e \) the strain whose time evolution can be given by velocity shear.
\[
\frac{de_{ij}}{dt} = \frac{1}{2} \left( \frac{\partial u_{ij}}{\partial x_j} + \frac{\partial u_{ij}}{\partial x_i} \right) - \frac{1}{3} \frac{\partial \varepsilon}{\partial t} \delta_{ij}
\]  \hspace{1cm} (13)
If the stress exceeds the yield stress \( Y \), the stress is limited to this value so that it behaves like plastic material.
\[
\sigma_{ij} = \sigma_{ij}/\min \left[ 1.0, \left( \sigma_{ij}, \sigma_{ij}/(2/3)^{1/2} \right) \right]
\]  \hspace{1cm} (14)

Once the computational scheme is established, only tool we need is the equation of state. Since we aim to exactly replicate the real phenomena as precisely as possible, we here use realistic equation of state (EOS) rather than model equation. The EOS is given by the Thomas-Fermi-Dirac formula with the bonding correction at the solid and is tabulated in terms of density and temperature. This procedure is very similar to SESAME EOS at Los Alamos National Laboratory.

As easily imagined, combination of all the processes thus described would make the computation very heavy if conventional algorithms were used. However, the high performance of the CIP method makes such simulation possible even in three-dimensions on one personal computer. Actually the simulation given here is about 7 hours by a Pentium M 1.6 GHz.

In the example of Fig. 2, a bunch of straight energy beam is incident on the metal surface and deposits the energy at the surface. In the course of time, temperature increases and diffuses out by thermal conduction. Before the temperature reaches the melting point, the material properties and elastic stress for solid plays important role. After melting temperature is reached or stress tensor exceeds the yield strength, it behaves like liquid dominated by viscosity and surface tension. If the temperature further increases above boiling temperature, the material evaporates and behaves like gas of compressible fluid. All the phases are recognized by density and temperature and therefore color functions such as in Eq. (5) are not needed. The used grid is the non-uniformly spaced Cartesian of 74×72×55 and the metal block is described by the mesh of 28×34×41.
The rear side view just after the beam punches the hole is shown in Fig. 3.

4. Precise Description of Force

In the example of the previous section, the phase boundary was determined based on the EOS. In most of the slow process, however, there are no phase transition and solid and liquid stay in their state forever. In this and following sections, we concentrate on such impermeable materials whose surfaces are described by color function \( \phi \). In such cases, the precise computation of the force acting on the interface becomes essential.

Fluid-structure interaction has been solved at first employing particles\( ^{12} \) at the solid surface which is so-called immersed boundary method proposed by Peskin [1977]\(^ {13} \). A simple algorithm that uses only color function has been demonstrated by Xiao et al. [1997]\(^ {14} \) and Kunimatsu et al. [2001]\(^ {15} \). The following examples treated in this paper require much more accurate representation of the force.

We shall show how to compute the force acting on the surface that has a shape of sub-grid scale. When the structure is embedded inside a grid cell, we need to estimate the force on the surface by use of the information from the grid points. If we use linear interpolation, the accuracy goes down to the first order and subtle difference of the forces on the two sides of thin material as in Figs. 5 and 6 is smeared out. As already shown in section 2, we need to know the real solution inside a grid cell but higher order polynomial constructed only by smoothness constraint cannot give sufficient solution. For this purpose, the CIP method is one of the best compact schemes.

In describing the movement of structure or interface within fluid, overlapped grid or overset grid system has been frequently used [for example Ref. (16)]. One grid system describes structure and the other does fluid. However, this is not always possible in many cases. For example, let us consider a disk impinging onto the water surface like in Fig. 5. In this case, the complicated shape of water-air interface must be solved as well as the disk movement. In this case, it is impossible to use the adaptive overset grid for two fluid, air and water. In tracing such interface, there are several methods like VOF\( ^{17} \) and level set\( ^{18} \) and so on. In this paper, we shall use the CIP method because recent version of the CIP guarantees exact mass conservation.

The merit of the CIP is demonstrated in Fig. 4. Let us use \( 10 \times 10 \) grid and store a Gaussian profile. If we display this profile in this grid system, it is shown as in (a). Let us imagine that this grid system is used for fluid computation. When the structure is within a grid cell, we need to interpolate the force acting on the solid surface based on this grid information. (b) and (c) show the result of linear interpolation with \( 30 \times 30 \) and \( 60 \times 60 \) sampling points. Thus we cannot avoid the influence of the Cartesian grid if we used only the information of grid values. Higher order interpolation does not help. On the contrary, if we use the Hermite interpolation as in the CIP method, the Gaussian profile is correctly recovered. This means that the force profile within a grid cell can be accurately interpolated from the force and its gradient predicted by the CIP method.

It is important to note that although the Hermite interpolation has been well known for a long time, it is of no use without specifying the way of predicting the gradient. In the fluid dynamic equation, the profile should change in time and hence it is important to predict the spatial gradient that accurately describes the real solution. In this sense, the CIP predicts it according to the original equation and therefore even the profile of sub-grid scale becomes an approximate solution to the original equation.

Figure 5 shows a disk falling on the water surface. The key issues of this simulation are the calculation of pressure force and air entrainment. Although the thickness of the disk is only 4 mesh-sizes in the Cartesian grid, the pressure force on the surface is accurately calculated because the pressure profile inside a grid cell is interpolated by polynomial that approximates real solution. Therefore the time evolution of the disk movement agrees well with the experiment. The second point is that water and air are successfully solved even if the density difference is 1 000 times, and entrainment of air is correctly described. The second example is similar but now the thickness of the material is zero. A flapping fall of a sheet of square paper like a name card is familiar with our daily experience, but the full numerical simulation is not so easy.

In this case, the overlapped grid is used to keep sufficient resolution along the paper surface because of the thin boundary layer. In connecting two grid systems we need the CIP procedure to keep the approximate solution between the grids as already stated. For the mesh moving with the paper, \( 30 \times 40 \times 50 \) grids are assigned, and stationary \( 50 \times 50 \times 80 \) grids are in the background. The Reynolds number is set to be 250.

Since the paper thickness is zero, we need to assign two different pressures on the grids aligned on the top and bottom surface of the paper. Since the difference of force on the both surfaces is very small, we need accurate computation. Although the advection term can be calculated with the third-order in time and space by the CIP, non-advection terms like pressure work, viscosity and so on are not accurate because the second-order derivatives are less accurate by cubic polynomial. Therefore we use the 5-th order polynomial for describing these terms. This is the straightforward extension of the CIP to the 5-th order polynomial determined from the value and its derivative on three grid points. After the polynomial is constructed, the first and the second order derivatives are simply ob-
tain the derivatives of the polynomial. This scheme is called IDO (Interpolated Differential Operator) scheme$^{(19)}$ and has the third-order accuracy in time and space including advection and non-advection terms.

Initially, the paper obliquely lies with a 15 degree angle, which we call the attack angle, from the horizontal plane. The gravity force accelerates the paper downward. Because of the attack angle, the airflow from the bottom of the paper induces horizontal motion. Since the pressure at the leading edge of the paper is higher than the rear edge, torque is generated. Then the attack angle decreases and finally overshoots to the negative value. Thus periodic flatter motion is repeated as shown in Fig. 6. When the initial attack angle of the paper is larger, the paper does not show the flatter trajectory any more but falls with straight sliding.

5. Mass-Conserving Semi-Lagrangian Method

Since the CIP uses semi-Lagrangian form$^{(20)}$, the total mass of fluid is not exactly conserved although the high accuracy of the CIP prevents large departure from the conservation. In some case, this conservation becomes important. For example, when the size of the liquid drop becomes comparable to grid size, it should be suffered from large dissipation and disappear. This is important in case we do use coarse grid in order to make a fast computation. In order to overcome this difficulty, one of the authors pro-
posed to change the profile inside a grid cell forcing mass conservation (21).

This scheme is called CIP-CSL (conservative semi-Lagrangian) scheme and is easily understood if we replace \( f \) and \( g \) in Eqs. (1) and (2) by its integration \( M = \int f \, dx \) and \( f \) as

\[
\frac{\partial M}{\partial t} + u \frac{\partial M}{\partial x} = 0, \quad (15)
\]
\[
\frac{\partial f}{\partial t} + \frac{\partial f u}{\partial x} = 0 \quad (16)
\]

Interestingly, Eq. (16) is the conservative equation for \( f \). Therefore the simple advection equation of \( M \) gives conservative law. Thus the CIP procedure can be applied to the above set of equations. Even if the conservation is broken after separate treatment of advection and non-advection terms, mass \( M \) inside a grid cell modifies the profile through the coefficients like in Eq. (4).

This scheme is applied to the mass conservation equation and color function for a rising bubble in a bifurcation tube. The grid system is the Cartesian and therefore the curved tube is embedded in this grid system. In order to accurately follow the motion of the bubble, the conservation of mass is important because the number of used grid is as small as 60 \( \times \) 40 \( \times \) 160.

Therefore the use of CSL scheme is interesting sub-
ject. Unfortunately, however, the CSL is a little diffusive and we can not use the sharpness enhancement method by tangent transformation\textsuperscript{(22)} that may deteriorate the conservation.

To get rid of the numerical smearing of the advection computation, a mass-conservative adjustment or anti-diffusion on the both sides of the interface is conducted, in which a level set function is created near the interface of the color function and the mass is redistributed along the direction normal to the interface within a transition zone of a pre-determined thickness. Since the color function is conservative, the level set is temporary used to predict the normal vector in the Cartesian grid.

A spherical bubble with the Bond number being 24 is initially placed near the bottom of the tube. Figure 7 shows the snapshot after the bubble passed through the bifurcation junction where the single bubble was broken into two. The total mass and the volume of the bubble(s) are conserved in the computation.

It is interesting to see an alternative strategy to guarantee the mass conservation coupled with the CIP method. The surface movement is traced by PLIC\textsuperscript{(23)} (piecewise linear interface calculation)-like VOF algorithm for conservation of volume, then the level set function is produced by the CIP for the calculation of curvature\textsuperscript{(24)}. This algorithm is useful for a body-fitted.

This algorithm is applied to the sloshing of water surface in the curved container as in Fig. 8. The container is abruptly decelerated and then the water surface shows sloshing motion. The air is assumed to be ideal gas and is calculated simultaneously. The grid is fitted to the outer container but only a half around of the tank is calculated with 50×90×36 grid. On the tank wall, non-slip and wetted condition are imposed. The vertical and lateral acceleration were varied as those in the corresponding experiment.

6. Conclusion

We proposed a new simple algorithm to directly solve all the phases of matter. This scheme is applied to melting and evaporation of metal under the illumination of energy beams, which have never been tried before as a CG tool. It is also used for conventional fluid-structure interaction with the solid body replaced by rigid body, then flattering motions of disk and thin name card have been successfully simulated in close agreement with observation. Improvement of the conservation was demonstrated by two algorithms.

References


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