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To cite this article: K-t Wu et al 2008 J. Phys.: Conf. Ser. 96 012135

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A Novel Numerical Method for Interface Disposal

Kai-teng Wu\textsuperscript{1,2*}, Jian-guo Ning\textsuperscript{3}, Lian-ming Mu\textsuperscript{1,2}

1 Key Laboratory of Numerical Simulation of Sichuan Province, Neijiang Teacher's College, Neijiang 641112, China;

2 Department of Mathematics, Neijiang Teacher's College, Neijiang 641112, China;

3 State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology, Beijing 100081, China

E-mail: ktengwu@njtc.edu.cn

Abstract. This paper suggests a novel Eulerian approach to dealing with interfaces. The normal direction of interface and transport velocity can be easily determined. It is also shown that the method is able to simulate shock waves and their propagation process with complex boundaries.

1. Introduction
As either type of Euler or Lagrange methods has its own disadvantages and applicable scenarios, Euler-Lagrangian methods have been evolved gradually, which made use of their excellences and overcame their shortcomings. Nevertheless, it is still inevitable in these methods to face the problem of interface description and transport computation as in the Eulerian method. Moreover, only field variables may be computed in the Eulerian method, such as velocity, mass, pressure, etc. The position of interfaces keeps unclear in the mesh. Much effort has been put in the interface description and transport computation, and many approaches have been developed. Although some results have been obtained, it keeps unsolved in problems for 3D.

Although Hirt in [1] and S.Cardovelli in [2] early gave Volume of fluid (VOF) method, which was used preferably in numerical simulation of 2D problems. Numerical simulation of more practice problems was researched by 3D methods, for example, penetrate-slanting and explosive with complex boundaries in air are difficult. Although Ning et al in [3-5] obtained some results in discussing and researching to these problems, in fact, there exists more difficulties to solve practice cases. In this paper, modified numerical methods are given, which can simulate shock waves and their propagation in 3D explosive fields with complex boundaries by numerical experiments.

2. Numerical method
Governing equations of hydrodynamic model consist of mass conservation, momentum conservation, energy conservation and equation of state. These partial differential equations are unsteady problem of isothermal inviscid compressible fluid without body force in [6] for 3D.

\* To whom any correspondence should be addressed.
2.1. Fundamental equations

(1) **Mass-conservation equation**

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0.
\]

(2) **Momentum-conservation equation**

\[
\frac{\partial \rho \mathbf{U}}{\partial t} + \nabla \cdot (\rho \mathbf{U} \mathbf{U}) = -\nabla \cdot \mathbf{P}.
\]

(3) **Energy-conservation equation**

\[
\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E \mathbf{U}) = -\nabla \cdot \mathbf{q}.
\]

where \(\mathbf{q} = \mathbf{S} \cdot \mathbf{U} + \mathbf{U} \cdot \mathbf{q} \), \(\mathbf{S} = \mathbf{S}_{ij} \delta_{ij} \hat{\mathbf{r}}\), \(\mathbf{q} = \mathbf{q}_{ij} \delta_{ij} \hat{\mathbf{r}}\), \(\mathbf{S}_{ij} \delta_{ij} \hat{\mathbf{r}}\), \(\mathbf{q}_{ij} \delta_{ij} \hat{\mathbf{r}}\), and \(\mathbf{q}_{ij} \delta_{ij} \hat{\mathbf{r}}\) are the first order artificial viscosity coefficients, \(c\) is a constant depending on the medium, \(\rho\) is the density, \(\mathbf{U}\) is velocity increment.

2.2. Artificial viscosity

In order to calculate shock wave and to improve the stability of solution, artificial viscosities are introduced in [6]

\[
q_i = \rho [\Delta u_i - \Delta u_i] \left\{ a_n (|\Delta u_i| - \Delta u_i) + b_n c \right\},
\]

where \(a_n\) and \(b_n\) are respectively the second order and the first order artificial viscosity coefficients, \(c\) is a constant depending on the medium, \(\rho\) is the density, \(\Delta u_i\) is velocity increment.

3. Interface Disposal technique

Though Euler methods accommodate numerical calculation of large medium distortion problems, it is difficult to discuss interfaces of mediums. Here D.L.Youngs in [7] interface techniques for 2D are generalized numerical simulation for 3D. The interface in mixed mesh is denoted by an approximative plane, whose normal direction is confirmed by distributing of volume ratio of 26 meshes around donor cell, position of the plane, by the self volume ratio of donor cell again. And transport volume of acceptor cell from the donor cell is calculated. At the same time, mass, momentum and energy of passing mesh boundary can also be calculated.

3.1. Normal direction of interface

From Youngs interface technique in [7], normal direction of interface is denoted with volume of medium in mixed mesh, its form as following

\[
\hat{n} = \frac{\Delta f}{|\Delta f|},
\]

where \(n_x = \frac{\partial f_x}{2\Delta x}\), \(n_y = \frac{\partial f_y}{2\Delta y}\), \(n_z = \frac{\partial f_z}{2\Delta z}\), and \(f_x, f_y, f_z, f_N, f_S, f_T, f_B\) are the volume-ratio of six side faces of cuboid cell(Fig.1), for example, \(f_E\) can be defined as following

\[
f_E = A_1(f_1 + f_2) + A_2(f_1 + f_2) + A_3(f_1 + f_2) + A_4(f_1 + f_2) + A_5(f_1 + f_2) + A_6(f_1 + f_2),
\]

where the volume-ratio \(f_i, (i=1,\ldots,27)\) of each side face of cuboid cell can be obtained by former one-step computation. The revised coefficients \(A_i, (i=1,\ldots,5)\) are auto-regulated by interface cases.

So normal cosine \((\alpha, \beta, \gamma)\) of interface plane equation can be written as following

\[
\alpha = -\frac{n_x}{\sqrt{n_x^2 + n_y^2 + n_z^2}}, \beta = \frac{n_y}{\sqrt{n_x^2 + n_y^2 + n_z^2}}, \gamma = -\frac{n_z}{\sqrt{n_x^2 + n_y^2 + n_z^2}}.
\]
3.2. Interface equation
The ratio of volume of the mixed mesh is suited to the position of interface plane adjusted with above the normal direction (9), and equation of the plane is gained.

To suppose an equation of interface plane be
\[ d = \alpha(x-x_0) + \beta(y-y_0) + \gamma(z-z_0) = 0 \]  
(9)

An equation of a plane, paralleling interface plane out mesh
\[ d = \alpha(x-x_1) + \beta(y-y_1) + \gamma(z-z_1) = d \]  
(10)

here \( \vec{n} \) is normal vector of interface plane, \( \alpha, \beta, \gamma \) are normal cosine of \( \vec{n} \). Mesh nodes number are arranged from Fig.2, coordinates of these nodes are \( p_i(x_i,y_i,z_i) \) respectively, thus let distant from at point \( P \) to plane (10) be
\[ f(P_i) = \frac{|\alpha(x_i-x_1) + \beta(y_i-y_1) + \gamma(z_i-z_1) - d|}{\sqrt{\alpha^2 + \beta^2 + \gamma^2}} \]  
(11)

where \( x_0-x_1 = (1 + \text{sign}\alpha) \Delta x/2 \), \( y_0-y_1 = (1 + \text{sign}\beta) \Delta y/2 \), \( z_0-z_1 = (1 + \text{sign}\gamma) \Delta z/2 \), \( \text{sign}\theta \) is sign function.

3.3. Computation of medium volume
Let interface plane of A-medium in mixed mesh be
\[ \alpha(x-x_1) + \beta(y-y_1) + \gamma(z-z_1) = 0 \]  
(12)
then interface plane of B-medium in mixed mesh is
\[ \alpha(x-x_1) + \beta(y-y_1) + \gamma(z-z_1) = 0 \]  
(13)

When mixed mesh is the donor, the flux of A-medium passing boundary may be calculated in the following formulas. To suppose interface velocity be \( u(x,y,z) \) (Fig.4), and each side of surface of the cuboid be \( \hat{x}, \hat{y}, \hat{z} \) respectively, then the transport volume \( \Delta V = \Delta x \Delta y \Delta z \) . Let \( n_i = |\alpha \hat{x}| \), \( n_2 = |\beta \hat{y}| \), \( n_3 = |\gamma \hat{z}| \), and transform according to \( n_1 \leq n_2 \leq n_3 \) , 8 points are arranged again, we obtained \( (\hat{x}_k, \hat{y}_k, \hat{z}_k) \) , \( (k=1,2,\cdots,8) \) , so.

Let function \( G(x,y,z) = \alpha(x-x_1) + \beta(y-y_1) + \gamma(z-z_1) + d \) , to solve a special-value of each node \( k(\hat{x}_k, \hat{y}_k, \hat{z}_k) \)
\[ m_k = \frac{[1 - \text{sign} G(\hat{x}_k, \hat{y}_k, \hat{z}_k)]/2}{(k=1,2,\cdots,8)} \]

4. Improvement Computation of Eulerian Transport
On correlation with interface description, the computation of transport quantities needs more precision. Generally speaking, accurate calculation of all variables in computation field can be gained by transport quantities nearest interface including mixed and free cells.
Donor-acceptor model is adopted in this paper. For Fig.3, velocity $u_{i+1,j,k}$ at a point in neighborhood boundary of $\Omega(i,j,k)$ and $\Omega(i+1,j,k)$ is calculated by linear interpolation method.

$$u_{i+1,j,k} = u_{i,j,k} \Delta x_{i+1} + u_{i+1,j,k} \Delta x_i. \quad (14)$$

If $u_{i+1,j,k} \geq 0$, then $\Omega(i,j,k)$ is donor mesh, $\Omega(i+1,j,k)$ is acceptor mesh, otherwise, $\Omega(i,j,k)$ is acceptor mesh, $\Omega(i+1,j,k)$ is donor mesh. The donor mesh can be noted as $\Omega(id,i,j,k)$, the acceptor mesh can be noted as $\Omega(ic,i,j,k)$. If $\Omega(i,j,k)$ is donor mesh, $\Omega(id,i,j,k)$, $\Omega(i+1,j,k)$ is $\Omega(ic,i,j,k)$, at the same time, there is the following definition $ie = 2 \times id - ic$, thus $\Omega(ie,i,j,k)$ is mesh after donor mesh of contrary direction of transport. Shadow part (Fig.3) will be transported. Average velocity $\hat{u}_{idc,j,k}$ of transportation may be solved by the following interpolation formulations

$$\hat{u}_{idc,j,k} = \frac{1}{1 + \frac{\Delta t}{\Delta x_i} \left( u_{id,j,k} - u_{idc,j,k} \right)} \frac{u_{id,j,k} \Delta x_{i+1} + u_{idc,j,k} \Delta x_i}{\Delta x_{id} + \Delta x_{ic}}. \quad (15)$$

Transportation velocity from mixed mesh to mixed mesh need to be revised. When two neighborhood meshes $\Omega(id,j+1,k)$, $\Omega(id,j-1,k)$ are filled with two media, transportation velocity of first medium in $\Omega(id,j,k)$, $\Omega(ic,j,k)$ is obtained by the following linear interpolation formulations

$$\bar{u}_{id,j,k} = u_{id,j,k} + \frac{\Delta y_j (1 - V_{id,j,k,1})}{\Delta y_j + \Delta y_{j+1}} (u_{id,j+1,k} - u_{id,j,k}), \quad (16)$$

$$\bar{u}_{ic,j,k} = u_{ic,j,k} + \frac{\Delta y_j (1 - V_{ic,j,k,1})}{\Delta y_j + \Delta y_{j+1}} (u_{ic,j+1,k} - u_{ic,j,k}). \quad (17)$$

To substitute into (15), viz. transportation velocity of first medium is

$$\hat{u}_{idc,j,k} = \frac{1}{1 + \frac{\Delta t}{\Delta x_i} \left( \bar{u}_{idc,j,k} - \bar{u}_{id,j,k} \right)} \frac{\bar{u}_{id,j,k} \Delta x_{i+1} + \bar{u}_{idc,j,k} \Delta x_i}{\Delta x_{id} + \Delta x_{ic}}. \quad (18)$$

Similarly, transportation velocity of second medium can be obtained.

5. Numerical Simulation

5.1. Initial value and boundary condition

The air density is $\rho_{air} = 1.293 \times 10^{-3} \text{g/cm}^3$. The explosive density is $\rho_0 = 1.65 \text{g/cm}^3$, TNT masses is $0.5$ units, explosive velocity $D_{ej} = 6970 \text{m/s}$.

The boundary conditions are dealt with row false meshes added out boundary mesh. Ground, protective wall and symmetry faces (front boundary) are taken as rigidity boundaries. In addition, these numerical experiments have the same initial condition: a number of cells is $170 \times 85 \times 25$. 

5.2. Computation model and state equation
Computation model is a garage with explosive hidden trouble, and the computational field is a cuboid: $82.5\text{m} \times 40\text{m} \times 10\text{m}$. A position of TNT explosive is at the origin point $(78.88,36.38,2.88)$.

The state equation of explosive is the JWL (Jones-Wilkins-Lee) type in [6]

$$P_s = A\exp(-R_1 V) + B\exp(-R_2 V) + CV^{-\omega s},$$

(19)

$$E_s = \frac{A}{R_1}\exp(-R_1 V) + \frac{B}{R_2}\exp(-R_2 V) + \frac{C}{V^{\omega s}},$$

(20)

Where $P_s$ is the pressure, $E_s$ is the internal energy, $V$ is the relative volume. The volume ratio of the product to the initial volume is $V/V_0$. The subscript $s$ indicates isentropic process. $A, B, C, R_1, R_2, \omega$ are known constants.

The state equation of air

$$P = (k - 1)\rho e.$$

(21)

Where $k$ is the isentropic index of air, and the $k, \rho, e$ are the isentropic index, pressure, density and specific energy respectively.

5.3. Numerical experiments and analysis of its results

From Fig.4-7, these figures have shown laws of shock waves shaping and existence of vortex-flow. We have obtained clearly propagation process of shock waves and the strength of the shock waves becomes weaker as time increasing, i.e, the peak of the pressure is reduced gradually. By these figures, we can also see that the pressure of detonation products decreases gradually. When it is equal to the atmospheric pressure, the detonation products no longer supports the explosive wave. Due to the inertia, the detonation product particles move on, and their pressure falls under the atmospheric pressure. So for the higher pressure of the surrounding air, the detonation products gradually stop and move back, then their pressure will increase gradually.

Generally, the shape of the complex boundaries near the explosion center affects the super-pressure of points behind protective wall more obviously. The super-pressure value will decrease with the increase of the angle between the positive direction of the land and the edge of complex boundary. While the shape of the complex boundary away from the explosion center affects the super-pressure less obviously, the value of the super-pressure will not change much with the change of the angle between the positive direction of the land and the edge of complex boundary.
6. Conclusions

Based on its algorithm for two second Cartesian coordinate systems, definition of the function of volume of fluid, approximating interface to plane, and revised coefficients are introduced, Youngs’ method is developed for 3D coordinate system. We obtain computing methods and its codes MMIC3D, which can simulate form of shock waves and their propagation in 3D explosive fields with complex boundaries. By testing of numerical experiments, Youngs’ methods are proved to be effective in 3D coordinate systems.

The numerical simulation of explosion field for 3D is the investigative task with important academic and practical meanings. Furthermore, we added the post-process of images, so the display of the numerical experiment result became much clear, more actual, more visual and more convictive in [7] in this paper. Here, we adopted MMIC3D code to simulate the explosive field with complex boundary and study the influence of the rigid boundary. We also acquire the relation between physical quantities and time corresponding to complex boundary. We yet provide some useful results for the project design. At the same time, it is impossible to solve all problems about explosive fields by experiment. Therefore, explosive problems will be discussed by ways of experiments, numerical experiments and their combinations.

Acknowledgement: This work was supported by the National Natural Science Foundation of China (10472042, 10672151), and Application Basic Research Foundation of SiChuan (05JY029-152).

Reference