Multiphase Flow CESE Solver in LS-DYNA®

Zeng-chan Zhang, Grant Cook, Jr. & Kyoung-su Im

Livermore Software Technology, an ANSYS Company, Livermore, CA 94551, USA

Abstract

In this paper, we will introduce a new capability of multiphase flow simulations in the LS-DYNA CESE compressible solvers. It is a hybrid multiphase flow model proposed by L. Michael [1]. This model is targeted for high-speed explosions, especially shock-to-detonation transition in liquid nitromethane. While the space-time conservation element and solution element (CESE) method, originally proposed by Chang [2], is designed for solving compressible flows, it is especially good for high-speed flows with complicated flow patterns. So we will use the CESE method to solve this hybrid multiphase flow model, and this approach will avoid a lot of complicated and time consuming treatments such as Riemann solvers and the Strang-splitting that are used in Ref.[1]. Our numerical examples show that we can get similar results using the CESE method. In the next sections, we will first give a brief introduction to the hybrid multiphase model, then the CESE method. Finally, we will give some numerical examples.

Hybrid multiphase model

Multiphase and multicomponent flows are very common in many engineering applications such as fuel sprays in combustion processes, ammonium-nitrate-based explosion in mining, and liquid-jet machining of materials. In past decades, many different multi-phase flow models have been proposed, and each one has its merits and limitations. A hybrid multiphase flow model proposed by L.Michael [1] is one of them. This multi-phase model is based on an augmented Euler approach to account for the mixture of the explosive and its products. It integrates the advantages of the augmented-Euler and Baer-Nunziato (BN)-type formulations while allowing for the interaction of an inert component with the reactant-product mixture, through a diffuse interface approach. Reduced versions of this formulation include modelling cases where the inert component is not present, when explicit modeling of the products of reaction is not required, or even when the phases are all non-reacting and could form free-surfaces. The main usage of this model is the numerical simulation of combustion and transition to detonation of condensed-phase commercial and military grade explosives, such as the propagation of detonations in compliantly-confined charges and the sensitization of commercial explosives by means of collapsing micro-balloons and shock-induced cavity collapse in liquid explosives.

The full conservation form system of equations for this model can be written as:

$$\frac{\partial U}{\partial t}+\frac{\partial F}{\partial x}+\frac{\partial G}{\partial y}+\frac{\partial H}{\partial z}=S \tag{1}$$

With

$$U=\begin{Bmatrix} z_1\rho_1 \\ z_2\rho_2 \\ \rho u \\ \rho v \\ \rho w \\ \rho E \\ z_1 \\ z_2\rho_2\lambda \end{Bmatrix},\qquad F=\begin{Bmatrix} z_1\rho_1 u \\ z_2\rho_2 u \\ \rho u^2+P \\ \rho uv \\ \rho uw \\ u(\rho E+P) \\ z_1 u \\ z_2\rho_2\lambda u \end{Bmatrix},\qquad G=\begin{Bmatrix} z_1\rho_1 v \\ z_2\rho_2 v \\ \rho uv \\ \rho v^2+P \\ \rho vw \\ v(\rho E+P) \\ z_1 v \\ z_2\rho_2\lambda v \end{Bmatrix},$$

$$H = \begin{Bmatrix} z_1\rho_1 w \\ z_2\rho_2 w \\ \rho u w \\ \rho v w \\ \rho w^2 + P \\ w(\rho E + P) \\ z_1 w \\ z_2\rho_2\lambda w \end{Bmatrix}, \quad S = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ z_1\nabla\cdot(u,v,w) \\ K \end{Bmatrix}$$

If two-dimensional axisymmetric cases are considered, an additional geometric source term should be included in *S*. Also, in the source term, *K* is a function giving the rate of conversion of reactants to products. Depending on the reaction rate law form used, term *K* usually depends on the temperature or pressure of the mixture, as well as the total density, the density of material 2 and λ. z_1 and z_2 are volume fractions of material 1 and 2 with respect to the volume of the total mixture with density ρ respectively, and we have $z_1 + z_2 = 1$; For example, if we consider a gas-filled cavity embedded in a liquid explosive, collapsing due to its interaction with an incident shock wave, the gas can be treated as material 1 with density, velocity and pressure given by (ρ_1, V_1, p_1), and the heterogeneous reactant-product mixture as material 2, with properties (ρ_2, V_2, p_2). The two components are separated by a material interface, and physical mixing between the two is not observed. Mechanical equilibrium (velocity and pressure) is assumed between the two materials, while thermal equilibrium (temperature) is assumed only between the components representing the reactants and products, i.e., the components that are allowed to physically mix.

Material 2 is composed of two components; the explosive reactants (material α), with properties $(\rho_\alpha, V_\alpha, p_\alpha)$ and the explosive products (material β), with properties $(\rho_\beta, V_\beta, p_\beta)$. The mass fraction of material α with respect to the explosive mixture with density ρ_2 is denoted by λ. As a result, the mass fraction of material β with respect to the explosive mixture is given by 1- λ. Velocity and pressure equilibrium between the two constituents of the heterogeneous mixture is assumed, such that $V_\alpha = V_\beta = V$ and $P_\alpha = P_\beta = P$. Effectively, all three materials in the system (i.e. material 1, α, and β) are in velocity and pressure equilibrium. Temperature equilibrium is only assumed between the constituents of the explosive mixture, i.e. $T_\alpha = T_\beta$.

This multiphase flow model is focused on high-speed explosion and it exactly matches the CESE method's key capabilities, so this multiphase flow model will be solved using the CESE method under our dual CESE framework.

CESE Method

The simulation of multiphase flows poses far greater challenges than that of single-phase and single-component flows. These challenges are due to interfaces between phases and large or discontinuous property variations across interfaces between phases and/or components. In ref.[1], a conventional Godunov (MUSCL-Hancock) scheme is used, plus a Strang-splitting to account for multiple dimensions. A hierarchical adaptive mesh refinement (AMR) is also used to increase the resolution of shocks and material interfaces. Furthermore, an energy correction step is adopted in order to suppress the numerical oscillations near the smeared material interfaces. It is not only complicated, but also time-consuming.

The space-time conservation element and solution element (CESE) method proposed by Chang [2] is especially designed for high speed compressible flows. It has several nontraditional features such as (i) a unified treatment of space and time, thereby ensuring good conservation in both space and time; (ii) simple but efficient discontinuity (shock) treatments. It is particularly useful for complex flows with shock waves and/or detonations. Here we use the CESE method to solve the aforementioned hybrid multiphase flow model under our dual mesh CESE framework.

In order to use the CESE method, Eq. (1) is rewritten as:

$$\nabla \cdot h = S \tag{2}$$

Where $h = (F, G, H, U)$ and $\nabla = (\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}, \frac{\partial}{\partial t})$. Here the time coordinate is treated as the fourth dimension in three dimensional cases. Applying Gauss's divergence theorem in the space-time domain, Eq. (2) is the differential form of the integral conservation law

$$\oiint_{s(V)} h \cdot ds = \iiint_V S \tag{3}$$

Where $s(V)$ is the boundary of an arbitrary closed space-time region V and $ds = d\sigma n$ in which $d\sigma$ and n are the length (area or volume) and unit outward normal vector of a microelement on $s(V)$ respectively.

Now the fluid domain will be divided into nonoverlapping elements (mesh). In the CESE method, there is no limitation to the element shape; for example, Fig. 1(a) shows a two-dimensional spatial mesh (triangles and quadrilaterals mixed). In our new dual CESE framework, the flow variables are solved and stored on two different sets of nodes (denoted as solution point (SP)) in two successive time steps. One set is associated with the element centers (C_i is Fig.1(a)), the other set is associated with the element vertices (A_i in Fig.1(a)) (but not necessarily coincident with it).

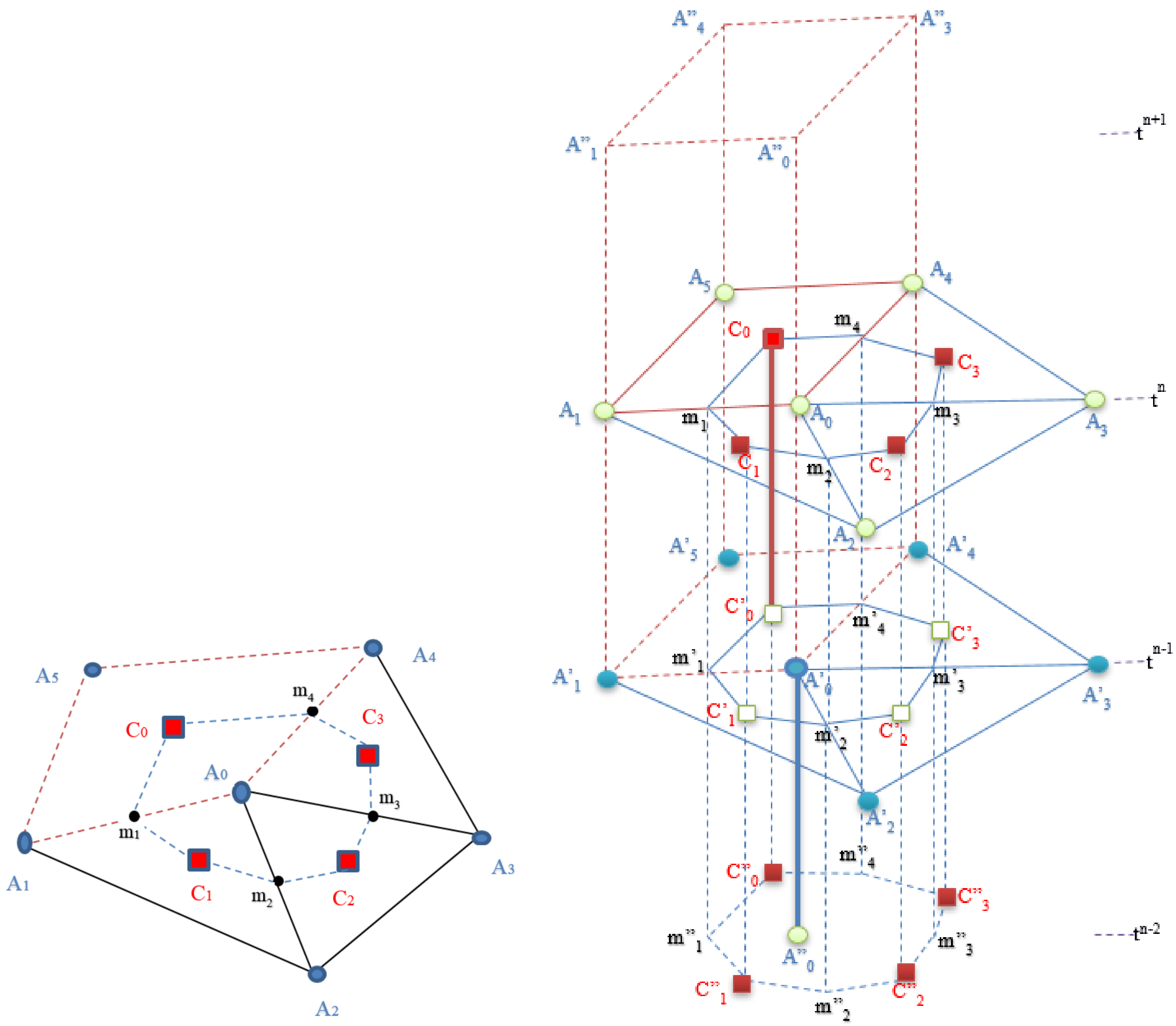
There are two important concepts in the CESE method, i.e., conservation element (CE) and solution element (SE), that is where the CESE name comes from. Associated with each solution point, there is a CE and a SE. Different definition of the CE and SE will make the CESE method a little different. Fig.1(b) shows the CE and SE definitions in our dual mesh CESE method for a two-dimensional hybrid mesh. If at $t=t^n$, the element center solution point value are updated, then the CE associated with element center C_0 is defined as the quadrangular cylinder $A'_0A'_1A'_4A'_5A_0A_1A_4A_5$, while the SE is defined as the quadrangular cylinder $A_0A_1A_4A_5A''_0A''_1A''_4A''_5$. Similarly, the CE associated with vertex A_0 at $t=t^{n-1}$ will be the polygonal cylinder $C''_0m''_1C''_1m''_2C''_2m''_3C''_3m''_4C'_0m'_1C'_1m'_2C'_2m'_3C'_3m'_4$, while the SE is defined as the polygonal cylinder $C'_0m'_1C'_1m'_2C'_2m'_3C'_3m'_4C_0m_1C_1m_2C_2m_3C_3m_4$ (see Fig.1(b)).

Inside each SE, the flow variables are approximated by a first-order Taylor expression, e.g. in two dimensional cases,

$$U(x,y,t) = U(x_0,y_0,t^n) + \Delta x U_x(x_0,y_0,t^n) + \Delta y U_y(x_0,y_0,t^n) + \Delta t U_t(x_0,y_0,t^n) \tag{4}$$

Where $\Delta x = x - x_0$, $\Delta y = y - y_0$, $\Delta t = t - t^n$ and (x_0, y_0, t^n) are the coordinates of solution point C_0 in space-time. Since the time derivative U_t can be calculated by Eq. (1), there are only three set of unknown variables that need to be approximated, i.e., U, U_x and U_y.

In each CE, the conservation law Eq. (3) is enforced to obtain the main flow variables U. For the other two set of spatial derivatives, there are different ways to get it. For example, the conservation law Eq. (3) can be applied in the sub-conservation elements (sub-CE), e.g., the sub-CE of quadrangular cylinder $m'_1A'_0m'_4C'_0m_1A_0m_4C_0$, to get some additional discrete equations to solve other two sets of unknows. Another way is to use flow variable information at neighboring points, plus some derivatives calculation strategies. Of course, when there is a discontinuity or shock in the flow field, limiters of some kind (such as some weighting strategies) are also needed to suppress the overshoot and/or undershoot. Here in our CESE solver, we developed a very simple but efficient method for calculating derivatives for shock capturing.



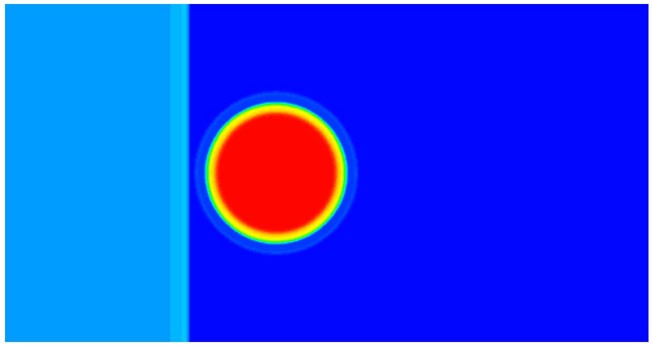
(a) (b)

Fig. 1 (a) Schematic 2D spatial mesh grids and (b) definitions of CE and SE in space & time under dual CESE framework

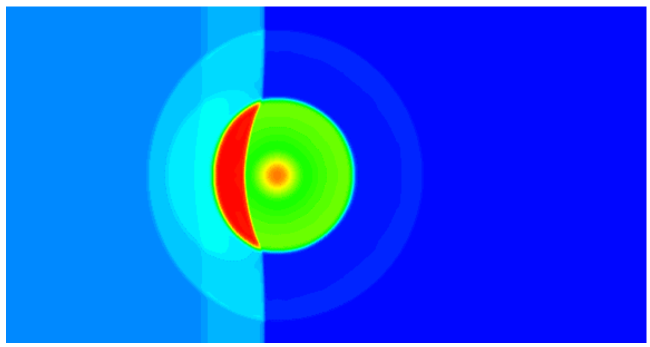
Numerical examples

1. **Planar shock interaction with cylindrical gas bubbles**

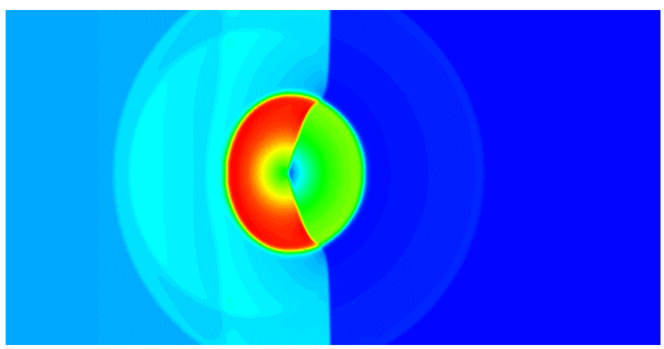
In this example, we use one of the reduce cases of the aforementioned hybrid model, i.e., two immiscible materials multiphase model, to test a planar shock wave interaction with an isolated bubble. Initially, a relatively weak shock in air with shock Mach number equal to 1.22 impacts a cylindrical bubble filled with refrigerant. Details about this problem's setup and the experimental results can be seen in Ref. [3]. The shock is initially located in front of the bubble at x=0.05 and moving from left to right. Fig. 2 shows four snapshots before and after the shock impacts the bubble. These results agree well with the results of Ref. [3], where they use a Godunov method (so some kind of Reimann solver is needed) and an energy correction technique is also needed to suppress the numerical errors near the interface. They also use adaptive mesh refinement (AMR) to increase the shock resolution. But here we only use the CESE method with a uniform mesh (with far fewer mesh elements) to get similar results.



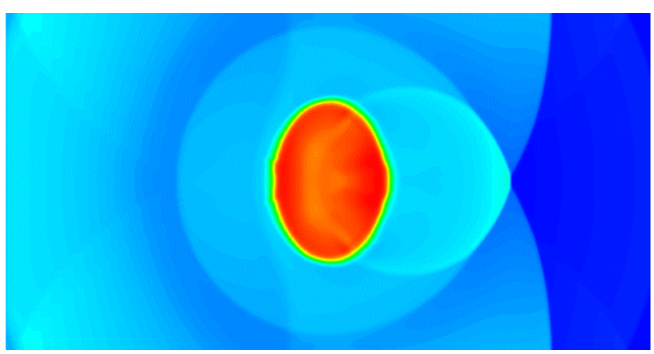
t=0.02



t=0.08



t=0.16

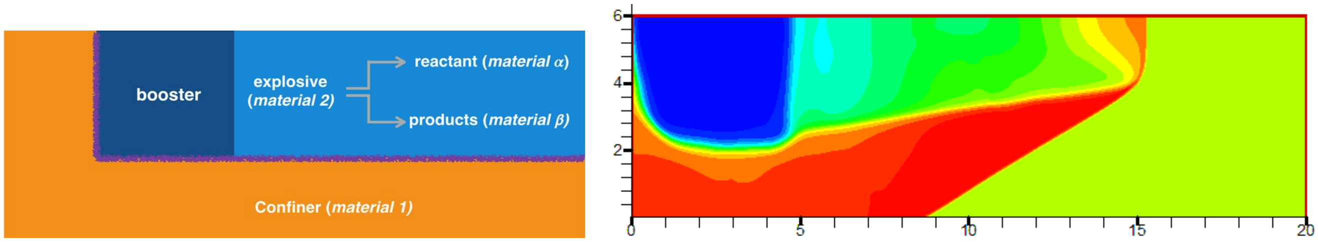


t=0.35

Fig.2 Planar shock interaction with a helium-filled bubble at four different time (density contours)

2. **Detonation propagation in a JWL rate stick with confinement**

This is the example in Ref. [1], where a slab of explosive in a stick form is confined by an inert material, as illustrated in Fig. 3 (a). The explosive (LX-17) is initiated by a booster of the same material. The equation of state (JWL) and reaction rate law parameters are scaled with respect to appropriate reference quantities. This problem is cylindrically symmetric, with axis of symmetry the centerline of the rate stick, and only the bottom half of the domain is simulated. Fig. 3 (b) shows the numerical results of density at t=11 using the CESE method, it agrees well with the results in Ref. [1], but without adaptive mesh refinement, operator splitting and an energy correction approach. Also, no Riemann solver is needed when using the CESE solver.



(a) (b)

Fig. 3 (a) Schematic of confined JWL rate-stick and (b) numerical results of density at time t=11

References

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