A mapping method for shock waves using ALE formulation

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Abstract: To simulate accurately a pressure wave propagation problem, a fine mesh is required in order to capture peak pressures accurately. This may require a very large size problem with several millions of elements. To reduce CPU time and prevent high mesh distortion, a two-dimensional problem for blast ignition and pressure propagation is performed first on a fixed Eulerian mesh. When the pressure wave gets closer to the structure, a three dimensional ALE simulation follows, where the fluid mesh and structure mesh at the fluid structure interface are coincident. The three dimensional problem is performed after mapping history variables from the two-dimensional to the three dimensional mesh. In this paper an ALE multi-material formulation is used for both explosive and air materials, and a classical Lagrangian formulation for the structure. The method has been implemented successfully in LSDYNA code and validated with different applications. To validate the method, this technique is used for pressure wave propagation, due to explosive detonation, and its interaction with the structure. The numerical solution, in terms of maximum displacement, is compared to experimental data performed at Aeronautical and Maritime Research Laboratory at DSTO, Australia. Good correlation has been observed between numerical results and experimental data.

Keywords: ALE, Fluid Structure Interaction, bird strike

1 Introduction

The principle of an ALE code is based on the independence of the Finite Element mesh movement with respect to the material motion. In fact, the freedom of moving the mesh offered by the ALE formulation enables a combination of advantages of Lagrangian and Eulerian methods.

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In the Lagrangian description of motion the computational domain follows the material motion, which greatly simplifies the governing equations. Lagrangian schemes have proven very accurate as long as the mesh remains regular. However, the material may undergo large deformations that lead to severe mesh distortions and thereby accuracy losses and a reduction of the critical time step, which is the amount of time necessary for an acoustic wave to cross the smallest element in the mesh (the Courant Friedrichs Levy condition).

With an Eulerian description of motion the mesh is fixed in space and the material passes through the element grid. The transport of mass between elements complicates the governing equations by introducing nonlinear transport terms. Mass conservation is not automatically satisfied. Advection algorithms need to be implemented for the mass, momentum and internal energy conservation and for tracking of all state variables.

It has been specified by Benson (Benson 1992) that the accuracy of Eulerian codes are comparable to the accuracy of Lagrangian codes in hydrodynamic applications, when using higher order advection algorithms. Furthermore, since the reference system is fixed, the Eulerian formulation preserves the mesh regularity. The main drawbacks are the computational cost per cycle and the dissipation errors generated when treating the advective terms in the governing equations.

Eulerian and ALE hydrocodes split each computational timestep into two phases. The first step is the Lagrangian phase, where the material motion and the mesh motion are identical and where the incremental motion of the material is computed. All physical phenomena as well as boundary conditions are considered during this phase.

The second step is the Eulerian phase, which is referred to as the advection, or remap phase. In this step the mesh is moved independently to the material motion and there is a transport of material between the cells. This corresponds to the treatment of the convective terms introduced in the governing equations.

Pioneering work on the ALE formulation were presented by Hughes et al. (Hughes, 1981) and Liu et al. (Liu, 1988) to solve free surface problems for incompressible viscous flow, by Benson (Benson, 1992) and Belytschko et al. (Belytschko, 1982) to treat fluid-structure interaction problems. A detailed survey of ALE Finite Element methods was presented by Donea (Donea, 1983). Hughes et al. developed a streamlined upwind Petrov-Galerkin method (Hughes, 1981), which was implemented in an ALE formulation by Liu et al. (Liu, 1988). The formulation has been applied for several applications in automotive, aerospace and biomedical industries for free surface modeling, sloshing tanks, fluid-structure coupling applications and for high velocity impact and penetration problems. An explicit ALE formulation
has been applied by Aquelet et al (Aquelet 2006), for high velocity impacts of elasto-plastic materials and for the analysis of sloshing tanks in aerospace applications.

This paper presents a new mesh relaxation method for explicit multi-material Arbitrary Lagrangian-Eulerian (ALE) Finite Element simulations. The proposed method is valid for structured and unstructured meshes and it is designed with the objective to reduce numerical dissipation errors when analyzing the propagation of shock fronts. The method aims to delay the advection phase in the vicinity of shock fronts in order to obtain an as "Lagrange like" behavior as possible near the shock, while at the same time keeping the mesh distortions on an acceptable level.

The outline of this paper is as follows. In Section 2 an overview of the governing equations in the ALE description of motion are presented. Section 3 describes the mapping strategy used to reduce computational time and performing the simulation on a very fine mesh.

In Section 4 the numerical modeling of a high explosive detonation in air using a structured ALE Cartesian grid is presented, illustrating the performance of the mapping technique. In this application the air blast loads a steel plate and a comparison with available experimental data (Boyd, 2000) was possible.

2 Lagrangian and advection phases of the Eulerian formulation

A multi-material Eulerian formulation, where soil and explosive materials can be mixed in the same element is used in the paper. Since Eulerian formulation is a particular case of the ALE formulation, a brief description of the ALE formulation is presented. A mixture theory is used to partition the material inside the element and compute the volume weighted stress from the constitutive model of each material as described in detail in (Aquelet 2006).

In the ALE description, an arbitrary referential coordinate is introduced in addition to the Lagrangian and Eulerian coordinates. The material derivative with respect to the reference coordinate can be described in equation (1). Thus substituting the relationship between material time derivative and the reference configuration time derivative leads to the ALE equations in (1)

\[
\frac{\partial f(X_i,t)}{\partial t} = \frac{\partial f(x_i,t)}{\partial t} + w_i \frac{\partial f(x_i,t)}{\partial x_i}
\] (1)

where \(X_i\) is the Lagrangian coordinate, \(x_i\) the Eulerian coordinate, \(w_i\) is the relative velocity. Let denote by \(v\) the velocity of the material and by \(u\) the velocity of the mesh. In order to simplify the equations we introduce the relative velocity \(w = v - u\). Thus the governing equations for the ALE formulation are given by the
following conservation equations, mass, momentum and energy:

\[
\frac{\partial \rho}{\partial t} + w_i \frac{\partial \rho}{\partial x_i} = -\rho \cdot \text{div}(v) \tag{2}
\]

\[
\rho \frac{\partial v_i}{\partial t} + \rho w_i \frac{\partial v_i}{\partial x_j} = \text{div}(\sigma) + f_{\text{ext}} \tag{3}
\]

\[
\rho \frac{\partial E}{\partial t} = \sigma_{ij} v_i \cdot v_j - \rho w_j \frac{\partial E}{\partial x_j} + Q_{\text{ext}} \tag{4}
\]

where \( \sigma \) is the stress tensor defined by \( \sigma = -p I_d \tau \).

\( \tau \) is the shear stress from the constitutive model, and \( p \) the pressure computed from an equation of state, \( f_{\text{ext}} \) and \( Q_{\text{ext}} \) are external load and heat flux.

The conservation equations (2) to (4) are applied for soil, and explosive materials. For soil material, the pressure is given from volumetric strain-pressure curve, obtained through experimental compression tests. For explosive gas the pressure is computed through JWL (Jones-Wilkins-Lee) equation of state.

Note that the Eulerian equations commonly used in fluid mechanics are derived by assuming that the velocity of the reference configuration is zero, \( u = 0 \), and that the relative velocity between the material and the reference configuration is therefore the material velocity, \( w = v \). The term in the relative velocity in (3) and (4) is usually referred to as the advective term, and accounts for the transport of material past the mesh. It is the additional term in the equations that makes solving the ALE equations much more difficult numerically than the Lagrangian equations, where the relative velocity is zero.

There are two ways to implement the ALE equations, and they correspond to the two approaches taken in implementing the Eulerian viewpoint in fluid mechanics. The first way solves the fully coupled equations for computational fluid mechanics; this approach used by different authors in CFD can handle only a single material in an element as described for example in (Longatte 2009). The alternative approach is referred to as an operator split in the literature, where the calculation, for each time step is divided into two phases. First a Lagrangian phase is performed, in which the mesh moves with the material, in this phase the changes in velocity and internal energy due to the internal and external forces are calculated. In the Lagrangian formulation the equilibrium equations can be describes by equations (5) and (6):

\[
\rho \frac{\partial v_i}{\partial t} = \text{div}(\sigma) + f_{\text{ext}} \tag{5}
\]

\[
\rho \frac{\partial E}{\partial t} = \sigma_{ij} v_i \cdot v_j + Q_{\text{ext}} \tag{6}
\]
In the Lagrangian phase, mass is automatically conserved, since no material flows across element boundaries, and element density is algebraically computed by (7) as the ratio of the mass element by the deformed element volume.

\[ \rho = \frac{M}{Vol} \]  

(7)

In the second phase, the advection phase, transport of mass, energy and momentum across element boundaries are computed; this may be thought of as remapping the displaced mesh at the Lagrangian phase back to its original for Eulerian formulation or arbitrary position for ALE formulation using smoothing algorithms. From a discretization point of view of (5) and (6), one point integration is used for efficiency using hourglass viscous forces to eliminate locking. The resolution is advanced in time with central difference method, which provides a second order accuracy for time integration. First nodal acceleration is computed based on nodal forces by (8):

\[ a^n = M^{-1}(F_{ext} + F_{int}) \]  

(8)

Second, velocity and displacement are updated using second order central finite difference method (9):

\[ u^{n+1/2} = u^{n-1/2} + \Delta t \cdot a^n, \quad x^{n+1/2} = x^{n-1/2} + \Delta t \cdot u^{n+1/2} \]  

(9)

Where \( F_{int} \) is the internal vector force and \( F_{ext} \) the external vector force associated with body forces, coupling forces, and pressure boundary conditions, \( M \) is a diagonal lumped mass matrix. For each element of the mesh, the internal force is computed based on the element stress computed through constitutive material model.

In the second phase, the transport of mass, momentum and internal energy across the element boundaries is computed. This phase may be considered as a ‘re-mapping’ phase. The displaced mesh from the Lagrangian phase is remapped into the initial mesh for an Eulerian formulation. To illustrate the advection phase, we consider in figure 1 a simple problem with 2 different materials, one with high pressure and the second a lower pressure. During the Lagrangian phase, material with high pressure expands, and the mesh moves with the material. Since we are using Eulerian formulation, the mesh is mapped to its initial configuration, in the advection phase, material volume called flux is moving from element to element, but we keep separate materials in the same element, with a interface between the 2 materials inside a single element.

All the physics is performed in the Lagrangian phase, stress computation, boundary conditions, contact forces, and time step. The advection phase can be seen as a
remapping phase from a deformable mesh to initial mesh for an Eulerian formulation, or to an arbitrary mesh for general ALE formulation. In the advection phase, volume flux of material through element boundary needs to be computed. Once the flux on element faces of the mesh is computed, all state variables are updated according to the following algorithm, using a finite volume algorithm (10),

\[ V^+M^+ = V^-M^- + \sum_{j=1}^{\text{faces}} \text{Flux}_jM_j \]

where the superscripts ‘-‘ and ‘+’ refer to the solution values before and after the transport. Values that are subscripted by j refer to the boundaries faces of the element, through which the material flows, and the \( \text{Flux}_j \) are the volume fluxes transported through the adjacent elements. The flux is positive if the element receives material and negative if the element looses material.

The ALE multi-material method is attractive for solving a broad range of non-linear problems in fluid and solid mechanics, because it allows arbitrary large deformations and enables free surfaces to evolve. The advection phase of the method can be easily implemented in an explicit Lagrangian finite element code. Before advection, special treatment for elements containing more than one material is needed. For a mixed element, a volume fraction of the material is computed that satisfies \( V_f \leq 1 \).

### 3 Constitutive models and equation of State

#### 3.1 Equation of State for explosive material

In High explosive process, a rapid chemical reaction is involved, which converts the material into high pressure gas. From a constitutive material point of view, the gas is assumed inviscid with zero shear, and the pressure is computed through JWL equation of state (Jones-Wilkins-Lee), a specific equation of state, commonly used for explosive material. There have been many equations of state proposed...
for gaseous products of detonation, from simple theoretically to empirically based
equations of state with many adjustable parameters.

The explosive was modeled with 8-nodes elements. The equation of state deter-
mines the relation between blast pressure, change of volume and internal energy.
The JWL equation of state was used in the following form:

\[ p = A \left( 1 - \frac{\omega}{R_1 V} \right) \exp(-R_1 V) + B \left( 1 - \frac{\omega}{R_2 \omega} \right) \exp(-R_2 V) + \frac{\omega}{V} E \]  

(11)

In Equation (11) \( p \) is the pressure, \( V \) is the relative volume:

\[ V = \frac{v}{v_0} \]

Where \( v \) and \( v_0 \) are the current and initial element volume respectively, while \( A, B, R_1, R_2 \) and \( \omega \) are material constants defined in table 1. These performance properties are based on the cylinder expansion test in controlled conditions.

<table>
<thead>
<tr>
<th>Table 1: Parameters used for C-4 explosive</th>
</tr>
</thead>
<tbody>
<tr>
<td>A (Mbar)</td>
</tr>
<tr>
<td>B (Mbar)</td>
</tr>
<tr>
<td>R_1</td>
</tr>
<tr>
<td>R_2</td>
</tr>
<tr>
<td>E_0 (Mbar– cm^3 / cm^3)</td>
</tr>
<tr>
<td>( \omega )</td>
</tr>
<tr>
<td>V_d (cm / µs)</td>
</tr>
<tr>
<td>( \rho ) (g / cm^3)</td>
</tr>
<tr>
<td>( \rho_{CJ} ) (Mbar)</td>
</tr>
</tbody>
</table>

At the beginning of the computations \( V=1.0. \) \( E \) is the initial energy per unit volume. The first term of JWL equation, known as high pressure term, dominates first for \( V \) close to one. The second term is influential in the JWL pressure for \( V \) close to two. Observe that in the expanded state, the relative volume is sufficiently important so that the exponential terms vanish, and JWL equation of state takes the form of an ideal gas equation of state:

\[ P = \frac{\omega E}{V} \]
The temperature $T$ can be computed using internal energy:

$$E = C_v \cdot T$$

Where $C_v$ is the average heat capacity. The heat capacity is held constant throughout the calculation.

### 3.2 Material model and Equation of state for air

Air is modeled using the hydrodynamic material model. The model requires an equation of state, density, pressure cut-off and dynamic viscosity to be defined. The viscosity and pressure cut-off are set to zero, because pressure cannot be negative and the viscosity forces are negligible. The ideal gas law (i.e. gamma law) is used as an equation of state for air. This polytropic equation of state is given by considering the general linear polynomial equation of state (12):

$$P = (\gamma - 1) \frac{\rho}{\rho_0} E$$

Where $\rho$ and $\rho_0 = 1 \text{ kg/m}^3$ are current and initial densities of air respectively, and $E$ is the specific internal energy per unit volume (units of pressure) and $\gamma$ is the polytropic ratio of specific heats. For the diatomic molecules comprising air, this adiabatic expansion coefficient is $\gamma = 1.4$. To be thermodynamically consistent, air must be initialized to atmospheric pressure. Note that from equation (12) at time $t=0$, for an initial pressure $P^i_0 = 0.1 \text{ MPa}$, the initial internal energy should be set to $E^i_0 = 1.25 \text{ MPa}$, since $\gamma = 1.4$, and $\rho = \rho_0$ at initial time. Setting a non-zero initial pressure in the air domain, appropriate boundary conditions are imposed at the external boundary, to avoid initial air leakage, thus a 0.1 MPa pressure boundary condition need to be assumed.

### 3.3 Constitutive material model for the structure

The structure is a composed of square shells with the same size. On Figure 2, the nodes at the interface of the air and structure meshes are sheared with the fluid to handle fluid-structure interaction phenomena.

For the structure, a classical elasto-plastic constitutive material law is used, where material properties are given in the following table:

### 4 Experimental Setup and numerical model

As mentioned earlier, the experimental test was performed at DSTO, a Defence and Sciences and Technology Organization, part of the Australian Department of Defence (Boyd 2000). A 1200 mm square, 5 mm thick mild steel plate bolted to a
heavy steel frame of 50 mm weight. A central area of 1000 mm square free is free to move under explosive loading. Space was available between the blocks for access to the bolts and also to position the instrumentation, as can be seen Figure 2. A sphere of Pentolite explosive, a mixture of 50% PETN and 50% TNT with a density of 1.65 g/cm$^3$ and a detonation of 7400 m/s. The 250 g explosive was detonated centrally using an Exploding Bridge Wire detonator. The plate to explosive standoff distance is 500 mm. The numerical model is described in figure 1, to use the symmetrical properties of the model, 2 planes of symmetry, with symmetry boundary conditions are used. The mesh of three dimensional fluid model consists of 5.6 millions hexahedra elements for explosive and air domains, with a mesh size of 0.3 cm, figure 3 describe a sketch of the model used in the simulation.

We notice the this resolution is too coarse to obtain accurate peak pressure, but can be fine enough for obtaining pressure pulse. The plate is located at 500 mm from the explosive charge. The physical dimensions of the plate is 1000 mm by 1000 mm and 5 mm thick. The mesh of the plate consists of 26,266 shell elements.

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**Table 2: Parameters used for Structure**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (g/cm$^3$)</td>
<td>7.85</td>
</tr>
<tr>
<td>Young Modulus (Mbar)</td>
<td>2.03</td>
</tr>
<tr>
<td>Poisson ratio</td>
<td>0.3</td>
</tr>
<tr>
<td>Yield Stress (Mbar)</td>
<td>27.e-4</td>
</tr>
<tr>
<td>Tangent Modulus</td>
<td>47.e-4</td>
</tr>
</tbody>
</table>

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Figure 2: Experimental setup (Boyd 2000) and Numerical model
5 Mapping algorithm for three dimensional problems

The mesh with three planes of symmetry is presented on Fig. 1. The air mesh is a Cartesian ALE grid with a cubic mesh size of 1 cm. The mass of the explosive is computed in the air mesh so that the explosive be a $1/4^{th}$ of sphere with a radius of 32.9 mm. The ignition point is applied at the center of the sphere. The high explosive material was modeled with the JWL (Jones-Wilkins-Lee) equation of state.

Using 5.6 millions elements, this resolution is too coarse to obtain accurate peak pressure, but can be fine enough for obtaining pressure pulse. The mesh of the structure plate located at 500 mm from the explosive charge, is sharing same nodes with the fluid mesh. Fluid structure coupling between the plate and the air material is automatically satisfied through common nodes. This is a simple way to define the coupling, and for complex problems, this way of coupling cannot be applied. General coupling methods have been developed by the authors in previous papers, Aquelet et al (2006). It is not the goal of the paper to develop and describe a coupling method that has already been developed in previous research papers and applied to different industrial and academic problems by the authors. The main goal of the paper, is to develop a mapping method between different meshes, in order to reduce computational time without reducing accuracy.

To reduce computational time, we first run a 2D spherical model for both explosive and air materials, for pressure wave propagation, with a radius at with the pressure wave propagation becomes non spherical, as illustrated in figure 4. The use of a two dimensional model allows a very fine mesh at the detonation process for the model to capture physical peak pressure. We know from previous simulations, to capture the measured Chapman - Jouguet pressure inside the explosive during detonation, mesh size of 0.1 mm or less needs to be used. For three dimensional problems, this mesh size requirement leads to large problems up to several millions of elements. The final results form the two dimensional model is projected or mapped into the three dimensional model In the mapping algorithm, history variables and velocity are mapped from the 2D to the 3D mesh. Pressure wave plot from the 2D simulation can be seen in figure 5.

6 Numerical results and validation

To highlight and validate the performance of the mapping method described in the paper, we consider the blast problem described in previous sections, where experimental data are available for correlations. During the first step, a two dimensional problem using a very fine mesh, to capture accurate peak pressure values, is performed. As shown in figure ??, the run is stopped when the pressure wave gets
very close to the structure, but no interaction between the fluid and structure has started. The second step of the simulation consists of mapping history variables, internal energy, pressure, fluid density, as well as nodal velocities from the two dimensional mesh to the 3D mesh. This step is well described in figure 4, where data from 2D mesh is mapped into 3D mesh. Following the mapping step, we con-

Figure 3: mesh of the air and explosive materials with 2 symmetry planes

Figure 4: mapping of the pressure for 2D to 3D model
Figure 5: Pressure wave in 2D mesh at t=150 microseconds

sider the real problem starting with a pressure wave accurately computed in 2D fine mesh. This step is automatically implemented in the LSDYNA code, Hallquist (1998) and validated for complex industrial applications, using contact algorithms, Euler Lagrange coupling and general boundary conditions. To describe the coupling between the blast wave and the structure, we plot the Von-Mises stress on the plate as shown in figure 6, we also plot displacement time history of the center of the plate in figure 7, where the maximum displacement is estimated at 28 mm. As noted in table 3, the error between numerical and experimental value of the peak displacement is estimated at 12%. This can be improved using explosive mass scaling described in Souli (2012).

Table 3: experimental and numerical data of displacement at the center

<table>
<thead>
<tr>
<th>Numerical Peak displacement</th>
<th>Experimental Peak displacement</th>
</tr>
</thead>
<tbody>
<tr>
<td>28 mm</td>
<td>33 mm</td>
</tr>
</tbody>
</table>

These simulations are of great interest for the design of structures to resist blast load and provide protection against damage from munitions and debris fragments produced by the blast. Since the ultimate objective is the design of resistant structures, numerical simulations can be included in shape design optimization with shape optimal design techniques, Souli et al (1993), and material optimisation, Erchiqui et
Figure 6: Von Mises stress at time $t=150$ microseconds

Figure 7: displacement time history at plate center
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al (2007), and Ozdemir et al (2010). Once simulations are validated by test results, it can be used as design tool for the improvement of the system structure involved.

7 Conclusion

For structure integrity and safety, several efforts have been made in defense and civilian industries, for modeling explosions and their effect on structures. Empirical loading models have been developed for predicting the effects of blast on structures. In engineering, CONWEP (1991), a code for Conventional Weapons Effects, is mainly used for preliminary design. From previous analysis, it is well known that these techniques have some limitations, particularly when the explosive charge is very close to the structure. In this paper, an ALE multi-material formulation approach for air and explosive materials and a Lagrangian approach for the structure are used for the simulation of pressure wave and its interaction with the structure. These two approaches are coupled using sheared nodes at the interface between all materials involved in the analysis. To reduce computational time without affecting the accuracy of the results, we first use a 2D model for blast wave propagation, since for a 2D model we can allow very fine mesh inside and outside the explosive material, and reduce dissipation and dispersion errors due to mesh effects. This technique used for different applications, allows to simulate problems containing several millions of elements, that we could simulate in the past only on large and expensive mainframe computers. To validate the method, the maximum displacement of the impacted structure is compared to experimental data, where the experiments has been performed at Australian Department of Defence. Good agreement for maximum displacement has been observed. The mapping strategy technique can be used for more complex problems where the structure can be defined with several complex components.

Acknowledgement

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CONWEP. Conventional Weapons Effects program, Version 2.00, (1991), US Army Engineer Waterways Experimental Station, Vicksburg, MS, USA