A Level Set-Boundary Element Method for Simulation of Dynamic Powder Consolidation of Metals

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Abstract. In this paper, the level set method is coupled with the boundary element method to simulate dynamic powder consolidation of metals based on linear elastostatics theory. We focus on the case of two particles that are in contact. The boundaries of the two particles are expressed as the zero level curves of two level set functions. The boundary integral equations are discretized using the piecewise linear elements at some projections of irregular grid points on the boundaries of the two particles. Numerical examples are also provided.

1 Introduction

The application of large amplitude stress waves for materials processing and powder compaction has been of increasing interest in recent years [3,7]. The technique is also used for materials synthesis where the stress wave can promote metallurgical reactions between two or more pure powders to produce alloy phases. When powder consolidation is of interest, it is important to understand the interaction, deformation, and bonding of particles in response to the stress wave. But the understanding of the dynamic process is far more complete. There are few papers on numerical simulations in the literature. A finite element method [1] gives some microscope analysis of a few particles. However, it seems that one can not afford to generate a body fitting grid for thousands particles at every time steps.

In this paper, we develop a boundary element–level set method to simulate the solidification process of metal particles. The choice of the boundary element method is based on the fact that we are only interested in the motion (deformation) of the boundaries of the particles, and the boundary integral equations are available and well understood. The use of the level set method [6] is to eliminate the cost of the grid generation and to simplify simulations for three dimensional problems. The projections of irregular grid points serve as a bridge between the boundaries of the particles and the underline Cartesian grid.

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2 The Boundary Integral Equations

We consider a simplified model that involves only two interacting particles, see Fig. 1 for an illustration. We assume that a small but fixed traction/pressure is applied to a portion of the boundary of a left particle while a portion of a second particle is fixed against a wall. We expect the particle will deform and want to know the position of the particles and the traction along the boundaries. For a problem with many particles, we can decompose the particle as groups of two particles using domain decomposition techniques.

We assume that the deformation is small, then from the linear elastostatics theory, see for example, [2], the traction $\mathbf{p}$ and the deformation $\mathbf{u}$ in the vector form

$$\mathbf{u} = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}, \qquad \mathbf{p} = \begin{bmatrix} p_1 \\ p_2 \end{bmatrix} \tag{1}$$

are coupled by the following boundary integral equations:

$$\begin{aligned} \mathbf{c}\,\mathbf{u}(\xi) + \int_\Gamma \mathbf{p}^*(\xi,\mathbf{x})\,\mathbf{u}(\mathbf{x})\,d\,\Gamma(\mathbf{x}) = & \int_\Gamma \mathbf{u}^*(\xi,\mathbf{x})\,\mathbf{p}(\mathbf{x})\;d\Gamma(\mathbf{x}) \\ & + \int_\Omega \mathbf{u}^*(\xi,\mathbf{x})\,\mathbf{b}(\mathbf{x})\;d\Omega(\mathbf{x}), \end{aligned} \tag{2}$$

where $\mathbf{b}$ is the body force, $c^i_{lk} = \frac{1}{2}\delta_{lk}$, where δ_{lk} is the Kronecker delta, $\mathbf{p}^*$ and $\mathbf{u}^*$ are the Green's functions

$$\mathbf{p}^* = \begin{bmatrix} p^*_{11}\ p^*_{12} \\ p^*_{21}\ p^*_{22} \end{bmatrix}, \qquad \mathbf{u}^* = \begin{bmatrix} u^*_{11}\ u^*_{12} \\ u^*_{21}\ u^*_{22} \end{bmatrix}, \tag{3}$$

with

$$\begin{aligned} u^*_{lk} &= \frac{1}{8\pi\mu(1-\nu)}\left((3-4\nu)\log\frac{1}{r}\,\delta_{lk} + r_{,\,l}\,r_{,\,k}\right), \\ p^*_{lk} &= -\frac{1}{4\pi(1-\nu)\,r}\left(\frac{\partial r}{\partial n}\left[\,(1-2\nu)\,\delta_{lk} + 2r_{,l}\,r_{,\,k}\,\right] + (1-2\nu)\,(n_l\,r_{,\,k} - n_k\,r_{,\,l})\right), \end{aligned}$$

where

$$r = |\,\xi - \mathbf{x}\,|, \qquad r_{,\,k} = \frac{\partial r}{\partial x_k}.$$

The Lamé's constant can be expressed in terms of the more familiar shear modulus G, modulus of elasticity E and Poisson's ratio ν by the following formulae,

$$\mu = G = \frac{E}{2(1+\nu)}; \qquad \lambda = \frac{\nu E}{(1+\nu)(1-2\nu)}. \tag{4}$$

In our simulation, the body force is zero. $\Gamma = \Gamma_k$, $k = 1$ or $k = 2$, is one of the boundaries of the two particles. We want to evaluate the displacement of $\mathbf{u}$ along the boundaries so that we can determine the location of the boundaries.

3 Numerical Method

We use a rectangular domain $\Omega = [a,\ b] \times [c,\ d]$ to enclose the two particles and generate a Cartesian grid

$$x_i = a + ih_x, \quad i = 0, 1, \cdots m, \tag{5}$$

$$y_j = c + jh_y, \quad j = 0, 1, \cdots n. \tag{6}$$

We use the zero level sets of two functions $\varphi_1(x, y)$ and $\varphi_2(x, y)$ to express the two particles respectively

$$\varphi_k(x, y) \begin{cases} \leq 0 \text{ inside the } k\text{-th particle,} \\ = 0 \ \text{ on the boundary of the } k\text{-th particle,} \\ \geq 0 \ \text{ outside the } k\text{-th particle,} \end{cases} \tag{7}$$

where $k = 1$ or $k = 2$. Since the two articles are immiscible, they share part of common boundary.

To use the boundary element method, we need to have some discrete points on the boundaries. We choose some of the *projections* of irregular grid points on the boundaries. An irregular grid point (x_i, y_j) is a grid point at which one of the level set functions $\varphi_k(x_i, y_j)$ changes signs in the standard five point stencil centered at (x_i, y_j).

The projection of an irregular grid point $\mathbf{x} = (x_i, y_j)$ on the boundary is determined by

$$\mathbf{x}^* = \mathbf{x} + \alpha\,\mathbf{q}, \quad \text{where} \quad \mathbf{q} = \frac{\nabla\varphi_k}{||\nabla\varphi_k||_2}, \tag{8}$$

and α is determined from the following quadratic equation:

$$\varphi_k\left(\mathbf{x}\right) + ||\nabla\varphi_k||_2\ \alpha + \frac{1}{2}\left(\mathbf{q}^T He(\varphi_k)\,\mathbf{q}\right)\ \alpha^2 = 0, \tag{9}$$

where $He(\varphi_k)$ is the Hessian matrix of φ_k evaluated at $\mathbf{x}$. All the first and second order derivatives at the irregular grid point are evaluated using the second order central finite difference schemes.

3.1 Contact of Two Particles

We use two level set functions to represent two immiscible particles and update their positions. On the part of the contact, both the level set functions should be zero.

Given two level set functions whose zero level curves intersect with each other, that is, $\varphi_{1,ij} \leq 0$ and $\varphi_{2,ij} \leq 0$, we modify the level set functions in the following way

$$\varphi_{k,ij} \longleftarrow \varphi_{k,ij} + \delta \tag{10}$$

where

$$\delta = \frac{|\varphi_{1,ij} + \varphi_{2,ij}|}{2}. \tag{11}$$

After such adjustment, the two level set functions can only have contact but not overlap, see Fig. 1 for an illustration. Note that it may be necessary to re-initialize the level set functions after such an adjustment.

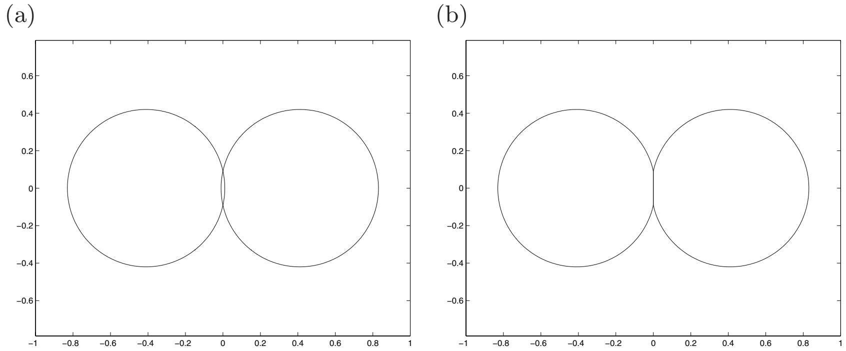

Fig. 1. Contact adjustment of the boundaries of two particles. (a): Two zero level set functions that overlap with each other. (b): The zero level curves (boundaries) of two particles after the adjustment

3.2 Set-up the Linear System of Equations

Since the projections on the zero level sets are not equally spaced, we use the piecewise linear basis functions to approximate $\mathbf{u}$ and $\mathbf{p}$, and discretize the boundary integral equation to get second order accurate method. For example, the displacement $\mathbf{u}$ between two nodal points can be interpolated using

$$\mathbf{u}(\xi) = \phi_1 \mathbf{u}^1 + \phi_2 \mathbf{u}^2 = [\phi_1,\ \phi_2] \begin{bmatrix} \mathbf{u}^1 \\ \mathbf{u}^2 \end{bmatrix}. \tag{12}$$

In the expression above, ξ is the dimensionless coordinate varying from -1 to $+1$ and the two interpolation functions are

$$\phi_1 = \frac{1}{2}(1-\xi); \qquad \phi_2 = \frac{1}{2}(1+\xi). \tag{13}$$

Given a projection (x_l^*, y_l^*) on one of the boundaries $\varphi_k = 0$, the next point (x_{l+1}^*, y_{l+1}^*) is determined as the closest projection in a small neighborhood of (x_l^*, y_l^*) that satisfies

$$\nabla \varphi_k(x_l^*, y_l^*) \cdot \nabla \varphi_k(x_{l+1}^*, y_{l+1}^*) \geq 0,$$

where $k = 1$ or $k = 2$. The gradient at the projection is computed using the bi-linear interpolation from those at the neighboring grid points evaluated with the standard central finite difference scheme. We refer the reader to [4,5] for detailed information on the bi-linear interpolation between projections and grid points.

The matrix-vector form of the linear system of equations at a particular node i can be written as

$$\mathbf{c}^i \mathbf{u}^i + \sum_{j=1}^{N} \hat{\mathbf{H}}^{ij} \mathbf{u}^j = \sum_{j=1}^{N} \mathbf{G}^{ij} \mathbf{p}^j, \tag{14}$$

where N is the total number of nodes or the projections that are used to set up the equations, $\hat{\mathbf{H}}^{ij}$ and $\mathbf{G}^{ij}$ (both are $2 \times\ 2$ matrices), are influence matrices. To avoid an ill-conditioned system and reduce the size of the linear system of equations, we use **ONLY** the projections of irregular grid points from one particular side. For example, we use the projections of irregular grid points where $\varphi_1(x_i, y_j) \leq 0$ and those projections of irregular grid points where $\varphi_2(x_i, y_j) \geq 0$. In this way, along the contact of the two particles, we can use just one projection at irregular grid points.

We use Gaussian quadrature of order four, which is an open formula, to evaluate the integrals $\mathbf{G}^{ij}$ and $\hat{\mathbf{H}}^{ij}$ for $i \neq j$. If $i = j$, the integral is a singular Cauchy principal integral and we use the *rigid body condition*

$$\hat{\mathbf{H}}^{ii} = - \sum_{j=1, j \neq i} \hat{\mathbf{H}}^{ij} - \mathbf{c}^i, \tag{15}$$

to evaluate the diagonal entries. The details about the boundary element method can be found in Chapter 3 of Brebbia and Dominguez's book [2].

3.3 Velocity Evaluation

In order to use the level set function, we need to evaluate the velocity at the grid points in a computational tube. At those grid points where the projections are used to set up the linear system of equations, we directly shift the velocity to the grid points. At those grid points where the projections are not used, for example, $\varphi_1(x_i, y_j) > 0$, we use the velocity at the closest projection from the other side where $\varphi_1(x_i, y_j) \leq 0$.

After we have evaluated the velocity $\mathbf{u}_k = \left[u_{k,1}\ u_{k,2} \right]^T$ at irregular grid points, we need to extend the normal velocity

$$V_k = u_{k,1} n_x + u_{k,2} n_y, \qquad k = 1 \quad \text{or} \quad k = 2, \tag{16}$$

where $(n_x, n_y) = \nabla \varphi_k / ||\nabla \varphi_k||_2$ is the unit normal direction, to all grid points inside a computational tube $|\varphi_k| \leq \delta$ surrounding the boundary of the particle, where $\delta = Ch$ is the width of the computational domain. This is done through an upwind scheme

$$\frac{\partial V_k}{\partial t} \pm \nabla V_k \cdot \frac{\nabla \varphi_k}{||\nabla \varphi_k||_2} = 0, \tag{17}$$

$k = 1$ or $k = 2$, which propagates V_k along the normal direction away from the interface. The sign is determined from the normal direction of the level set function.

3.4 Update the Level Set Functions

Once we have obtained the normal velocity in the computational domain, we can update the level set functions by solving one step of the Hamilton Jacobi equation

$$\frac{\partial \varphi_k}{\partial t} + V_k ||\nabla \varphi_k||_2 = 0, \qquad k = 1 \quad \text{or} \quad k = 2. \tag{18}$$

The zero level sets $\varphi_k = 0$ then gives the new location of the boundaries of the two particles.

We summarize our algorithm below:

- Set up the problem that includes input of the material parameters, initialization of the two level functions that represent the two particles.
- Adjust the level set functions at grid points where the two level set functions are both non-negative to treat the contact part.
- Find the projections of irregular grid points inside the first particle and outside the second particle.
- Find the next point for each projection on the boundaries to form the line segment needed in the boundary element method.
- Set-up the system of equations using the Gaussian quadrature of order four at all selected projections for each level set function. If **p** is known then **u** is unknown and vise versa. At contact, both **p** and **u** are unknowns. Use the rigid body condition to compute the diagonal entries.
- Shift the velocity to irregular grid points.
- Extend the normal velocity to a computational tube with a pre-selected width δ.
- Update the two level set functions by solving the Hamilton-Jacobi equation.
- Repeat the process if necessary.

4 Numerical Examples

We have done a number of numerical experiments. The results are reasonable good and are within the regime of the linear elasticity.

Example 1. The material parameters for the first and second particles are

$$G_1 = \mu_1 = 26, \quad \nu_1 = 0.33, \quad G_2 = \mu_2 = 83, \quad \nu_2 = 0.27.$$

The boundaries of the initial two particles are the circles

$$(x - 0.31)^2 + y^2 = 0.32^2; \qquad (x - 0.21)^2 + y^2 = 0.22^2,$$

before the adjustment. From the left, we apply a constant p

$$p(x, y) = C \cos(\pi x/2\epsilon), \quad \text{for} \quad |x| \leq \epsilon,$$

on the part of the boundary of the left particle, where we take $C = 5$ and $\epsilon = 0.1$. On the right, we fix the displacement $\mathbf{u} = \mathbf{0}$ if $|x - x_{max}| \leq 0.05$ along the part of the boundary of the right particle, where x_{max} is the largest x coordinates of the projections of irregular grid points. Fig. 2 is the computational result using our method.

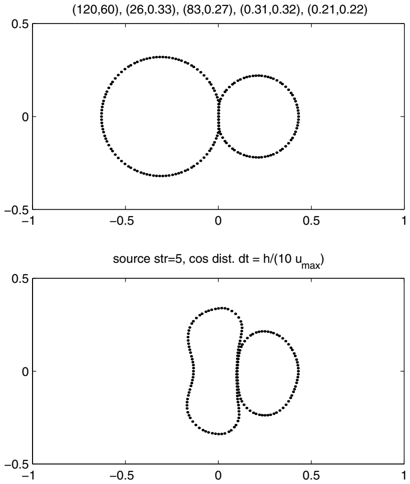

Fig. 2. Numerical result of Example 1 using a 120 by 60 grid. The upper half picture is the original particles; the lower half is the computed result

Example 2. The material parameters for the first and second particles are

$$G_1 = \mu_1 = 83, \quad \nu_1 = 0.33, \quad G_2 = \mu_2 = 26, \quad \nu_2 = 0.27.$$

The boundaries of the initial two particles are the circles

$$(x + 0.21)^2 + y^2 = 0.22^2; \qquad (x - 0.31)^2 + y^2 = 0.32^2,$$

before the adjustment. The rest of set-up is the same as Example 1. Fig. 3 is the computational result using our method.

5 Conclusion and Acknowledgment

A new numerical method that couples the boundary element method with the level set method is proposed in this paper to simulate multi-particles of liner elasticity. The new method can handle the contact of two particles easily.

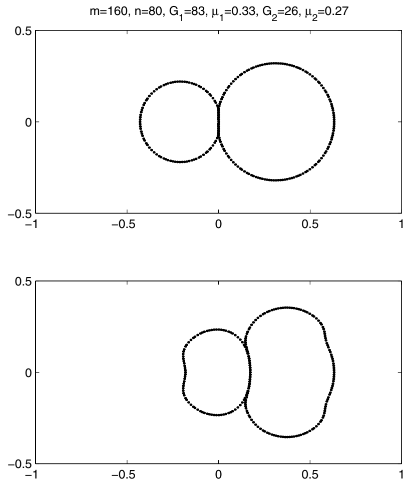

Fig. 3. Numerical result of Example 2 using a 160 by 80 grid. The upper half picture is the original particles; the lower half is the computed result

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