



## Three Dimensional Modeling of Dynamic Compaction in Granular Materials

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### ABSTRACT

The current work is focused on the simulation of Deflagration-to-Detonation Transition (DDT) in granular materials and energetic solids. The study of various cases of dynamic compaction is considered important because of its application in various fields; including solid rocket technology, mining, military, manufacture of weapons and commercial grade explosives, study of effects of low temperature environments on pyrotechnics. When a solid energetic material is damaged due to ageing or improper handling, porous regions are created which increase the chances of detonation due to subsequent mechanical impact. Much of the heating produced during compaction is due to the intergranular friction between grains. The compaction in granular materials is illustrated in Figure 1.

The bulk compaction model proposed by Gonthier et al. (1998) has been extended to provide a simple multidimensional hydrodynamic model of the compaction process. This is the first step to providing a full comprehensive model for the simulation of 3-D, reacting, multi-granular, DDT problems. Developmental costs were minimized by utilizing an existing off-the-shelf CFD code which has been modified to handle the 3-D compaction model. This entailed the modification from solution of the five standard gas dynamic equations to the solution of the eight compaction equations which include the evolution equations for solid volume fraction, no-load volume fraction and particle density. The 3D compaction model written in strong conservation form for generalized curvilinear coordinates is given by

$$\frac{\partial Q}{\partial \tau} + \frac{\partial F}{\partial \xi} + \frac{\partial G}{\partial \eta} + \frac{\partial H}{\partial \zeta} = b$$

$$Q = J \begin{Bmatrix} \rho\phi \\ \rho\phi u \\ \rho\phi v \\ \rho\phi w \\ \rho\phi e_0 \\ \rho\phi^2 \\ \rho\phi\tilde{\phi} \\ n \end{Bmatrix} \quad S = J \begin{Bmatrix} \rho\phi\beta_k \\ \rho\phi u\beta_k + p\phi k_x \\ \rho\phi v\beta_k + p\phi k_y \\ \rho\phi w\beta_k + p\phi k_z \\ \rho\phi e_0\beta_k + p\phi\theta_k \\ \rho\phi^2\beta_k \\ \rho\phi\tilde{\phi}\beta_k \\ n\beta_k \end{Bmatrix}$$

where  $k=\xi, \eta, \zeta$  for flux vector  $S=F, G, H$  respectively and  $J$  is the Jacobian matrix of the coordinate transformation. The dependent variables in the above model are  $\rho\phi, \rho\phi u, \rho\phi v,$

$\rho\phi w, \rho\phi e_0, \rho\phi^2, \rho\phi\tilde{\phi}$  and  $n$  where  $\rho$  is the density,  $\phi$  is the solid volume fraction,  $\tilde{\phi}$  is the no-load volume fraction and  $n$  is the particle density.

The source vector  $b$  is defined as

$$b = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \frac{\rho\phi 2(1-\phi)(P-\beta)}{\mu} \\ \frac{\rho\tilde{\phi}}{\tilde{\mu}} \max[(f-\tilde{\phi}), 0] \\ 0 \end{Bmatrix}$$

As given in [4] the function  $f$  represents the yield surface for the inelastic volume fraction and  $\tilde{\mu}$  characterizes the relaxation time for  $\tilde{\phi}$  to return to the yield surface. The mathematical model given above is to be closed using some constitutive relations which include:

$$f = f(\phi), \quad \omega = \omega(\phi - \tilde{\phi}), \quad \beta = \rho\phi\omega(\phi - \tilde{\phi}),$$

$$P = P_s(\rho, T), \quad e = e_s(\rho, T) + B, \quad B = \int_0^{\phi - \tilde{\phi}} \omega(\phi') d\phi'$$

with final closure provided by the Hayes equation of state[3].

An analysis of the eigenstructure has been made. The eigenvalues were found to be  $\lambda_{1-6} = \beta_k, \lambda_7 = \beta_k - c,$  and  $\lambda_8 = \beta_k + c$  where  $\beta_k$  is the contravariant velocity across face  $k$  and  $c$  is the acoustic speed.

The conservative variable right eigenvectors  $T_k$  are

$$T_{k,1} = \{0, 0, 0, 0, 0, 0, 0, 1\}$$

$$T_{k,2} = \{0, 0, 0, 0, -\rho\phi\omega, 0, \rho\phi, 0\}$$

$$T_{k,3} = \{\rho, \rho u, \rho v, \rho w, -\frac{p(\Gamma+1)}{\Gamma} + \rho(H + \phi\omega), 2\rho\phi, \rho\tilde{\phi}, 0\}$$

$$T_{k,4} = \{\alpha\phi k_x, \alpha\phi u k_x, \alpha\phi v k_x + \rho\phi k_z, \alpha\phi w k_x - \rho\phi k_y,$$

$$\alpha\phi(H - \frac{c^2}{\Gamma})k_x + \rho\phi(vk_z - wk_y), \alpha\phi^2 k_x, \alpha\phi\tilde{\phi} k_x, 0\}$$

$$T_{k,5} = \{\alpha\phi k_y, \alpha\phi u k_y + \rho\phi k_z, c^2 - \alpha\phi v k_y, \alpha\phi w k_y + \rho\phi k_x,$$

$$\alpha\phi(H - \frac{c^2}{\Gamma})k_y + \rho\phi(wk_x - uk_z), \alpha\phi^2 k_y, \alpha\phi\tilde{\phi} k_y, 0\}$$

$$T_{k,6} = \{\alpha\phi k_z, \alpha\phi u k_z + \rho\phi k_y, \alpha\phi v k_z - \rho\phi k_x, \alpha\phi w k_z,$$

$$\alpha\phi(H - \frac{c^2}{\Gamma})k_z + \rho\phi(uk_y - vk_x), \alpha\phi^2 k_z, \alpha\phi\tilde{\phi} k_z, 0\}$$

$$T_{k,7} = \left\{ \frac{\rho\phi}{n}, \frac{\rho\phi}{n}(u - ck_x), \frac{\rho\phi}{n}(v - ck_y), \frac{\rho\phi}{n}(w - ck_z), \right. \\ \left. \frac{\rho\phi}{n}(H - c\theta_k), \frac{\rho\phi^2}{n}, \frac{\rho\phi\tilde{\phi}}{n}, 1 \right\}$$

$$T_{k,8} = \left\{ \frac{\rho\phi}{n}, \frac{\rho\phi}{n}(u + ck_x), \frac{\rho\phi}{n}(v + ck_y), \frac{\rho\phi}{n}(w + ck_z), \right. \\ \left. \frac{\rho\phi}{n}(H + c\theta_k), \frac{\rho\phi^2}{n}, \frac{\rho\phi\tilde{\phi}}{n}, 1 \right\}$$

where total enthalpy

$$H \equiv e + \frac{1}{2}(u^2 + v^2 + w^2) + \frac{p}{\rho}$$

the Gruneisan Coefficient,

$$\Gamma = \frac{1}{\rho} \left( \frac{\partial p}{\partial e_s} \right)_\rho$$

the acoustic speed,

$$c^2 = \left( \frac{\partial p}{\partial \rho} \right)_{e_s} + \left( \frac{p}{\rho} \right) \Gamma$$

and some other simplifying coefficients

$$\psi \equiv c^2 - \Gamma[H - (u^2 + v^2 + w^2)] + \eta + \Gamma\varpi(\phi - \tilde{\phi})$$

$$\eta \equiv c^2 - (\Gamma + 1) \frac{p}{\rho}$$

have been introduced.

The governing equations presented above are discretized in space using an approximate Riemann solver of the Roe type. Development of an approximate solver hinges on the determination of approximate Roe averages for the eigenvalues, right eigenvectors and wave strengths so that the following jump conditions are satisfied.

$$\|Q\| = \sum_{i=1}^8 \hat{\sigma}_i \hat{r}_i \quad \|S\| = \sum_{i=1}^8 \hat{\sigma}_i \hat{\lambda}_i \hat{r}_i$$

In the above,  $\hat{\cdot}$  denotes the averaged terms. Determination of these algebraic averages is the key step in the development of Riemann solver. For computational efficiency, a parallelization strategy has been developed, which uses the domain decomposition inherent in the block structured grid, in combination with message passing routines for communication with processors.

In order to have good understanding of the accuracy of the proposed computational tool, validation studies will be undertaken. Gonthier, Cox and Reynolds solved a one dimensional, steady continuum model to predict dynamic compaction and localized heating of a granular material with non-uniform porosity. One of the 1D test cases is presented in Figure 2. For this case, the material on the left has been compacted such that  $\phi_L=0.999$  while the material at right has free pour volume fraction  $\phi_R=0.655$ . When the piston impacts at the dense left region, the heat fluxes greater than 2000 MW/m<sup>2</sup> are generated as the transmitted wave traverses the variable porosity region and subsequently propagates through the porous material. Sample calculations of 1D dynamic compaction are presented.

## FIGURES AND TABLES

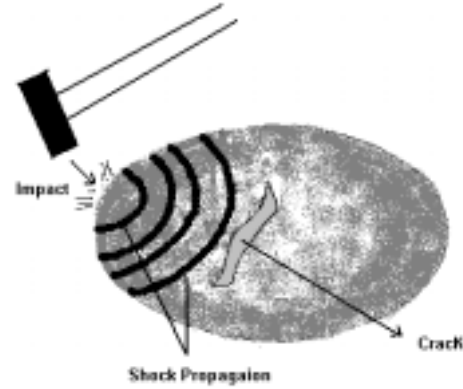


Figure1: Schematic of Compaction

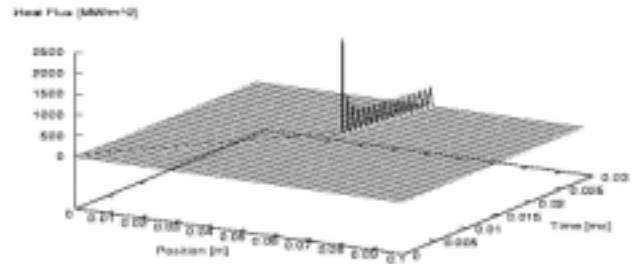


Figure: 1-D Heat Flux Results

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