Development and application of a three-dimensional GPGPU-parallelized FDEM for modelling rock fragmentation by blast

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Abstract. Numerical modelling of rock fragmentation by blast is an important step to the optimum fragmentation. Combined finite-discrete element method (FDEM) has recently been proven to be one of the most promising methods for modelling the fracture and fragmentation of rocks under various loading conditions including rock blasting. However, almost all FDEM modellings of rock blasts are conducted in two-dimension. Correspondingly, this study implements a three-dimensional (3D) hybrid finite-discrete element method (HFDEM) parallelized on the basis of the general-purpose graphic-processing-unit (GPGPU) to model the fracture and fragmentation process of rock by blast. The main components of HFDEM3D include robust fracturing algorithm, efficient contact activation approach and various implementations of gas and rock interactions, which are firstly briefly reviewed here and introduced in detail in authors’ various former publications. The GPGPU-parallelized HFDEM3D is then applied to model the rock fracture and fragmentation process by the detonation of a single borehole and simultaneous and consecutive detonations of multiple boreholes.

1. Introduction
Blasting has been widely employed in the mining industry for many centuries and it remains a popular method of rock fragmentation to the present day. However, current mining production blasting techniques are far from the optimum fragmentation. The space for improving production blasting in mining engineering is huge and the economic potential is enormous. Numerical modelling of rock fragmentation by blast is an important step to the optimum fragmentation. Various numerical methods have been implemented by various researchers to untangle the blasting problem and predict the blast induced damage and fragmentation, which include finite element methods (FEM) (e.g. [1]), discrete element methods (DEM) (e.g. [2]), discontinuous deformation analyses (DDA) (e.g. [3]) and combined finite-discrete element method (FDEM) (e.g. [4]). Among them, FDEM has been proven to be one of the most promising methods for modelling rock fracture and fragmentation by blast. Compared with FEM, FDEM is more robust in modelling rock failure, especially fracture, fragmentation, and fragment movements resulting in tertiary fractures. Compared with DEM, FDEM is more versatile in dealing with irregular-shaped, deformable and breakable particles. Compared DDA, FDEM is more efficient in dealing with contact detection and contact interaction. In recent decade, the authors and their team have been developing a hybrid finite-discrete element code for modelling rock fragmentation process by blast and have successfully applied it in modelling the rock fracture and resultant fragment muck-piling by mining production blasting [5], the formation of the crushed and cracked zones, long radial cracks and craters by crater blast [6], the rock fracture and fragmentation process and the resultant excavation damage zone development induced by controlled contour blasting during tunnelling with high horizontal...
in-situ stress [4], and the stress wave propagation and rock fracture process by destress blasting in controlling the excavation-induced rockbursts in deep underground with high in-situ stresses. However, all of these modellings were conducted in two-dimension. Correspondingly, this study is intended to further extend it to develop a three-dimensional hybrid finite-discrete element method for modelling rock fragmentation process by blast.

2. Development of GPGPU-parallelized HFDEM3D for modelling rock fragmentation by blast
A hybrid finite-discrete element method (HFDEM) code has been being developed by the authors [5] on the basis of the open-source combined finite-discrete element libraries [7]. To improve its computational efficiency, HFDEM code is parallelized by the authors [8] on the basis of general-purpose graphic-processing-unit (GPGPU) using compute unified architecture device C/C++. Detailed computing performance analysis shows that the GPGPU-parallelized HFDEM can achieve maximum speed-ups of 286 times [8]. Besides GPGPU parallelisation, a number of schemes are further implemented to further speed up the GPGPU-parallelized HFDEM, which mainly include the efficient contact activation [9], local damping as well as mass scaling, hyperplane separation theorem following a pioneering work [10], adaptive as well as semi-adaptive contact activation [11] and fast inertial relaxation engine. Although not all of them can be used for modelling dynamic fracture and fragmentation of rock such as that in rock blast, the GPGPU-parallelized HFDEM with these schemes implemented is several thousand times faster than the sequential Y library, which paves the way for 3D modelling of rock fragmentation by blast.

2.1. Robust 3D fracturing algorithms
In the GPGPU-parallelized HFDEM3D code, the numerical model is considered to consist of a single discrete particle or a number of interactive discrete particles. Each discrete particle is of a general shape and size and is termed as a deformable discrete element in contrast to the rigid discrete element in DEM. Each discrete element is then discretized into finite elements to analyze deformability, failure and fracture, thus imposing no additional requirements on handling the geometry and interaction of individual discrete particles, which have advantages over purely discrete element method such as PFC and UDEC.

As shown in Fig. 2, six-noded initially zero-thickness cohesive elements are inserted into the boundaries of four-noded solid tetrahedral elements according to either intrinsic or extrinsic cohesive zone models. The constitutive behaviors of the inserted cohesive element under uniaxial tension and shear loading conditions are depicted in Fig. 2, in which the normal and shear cohesive tractions, ($\sigma^{coh}$ and $\tau^{coh}$, respectively), acting on each face of the cohesive elements are computed using Eqs. 1 and 2 following tensile and shear softening behaviors, respectively:

$$\sigma^{coh} = \begin{cases} \frac{2\alpha}{\alpha_{overlap}}T_s & \alpha < 0 \\ g(\alpha)f(D)T_s & 0 \leq \alpha \leq \alpha_p \\ f(D)T_s & \alpha > \alpha_p \end{cases}$$

where

$$g(\alpha) = \left[\frac{2\alpha}{\alpha_p} - \left(\frac{\alpha}{\alpha_p}\right)^2\right]$$

Figure 1. Six-noded initially zero-thick cohesive element inserted between four-noded tetrahedral elements and its constitutive behaviours under uniaxial tensile and shear loading conditions.
\[ \tau^{\text{coh}} = \begin{cases} 
(g(s)[f(D)c - \sigma^{\text{coh}} \tan \emptyset] & 0 \leq |s| \leq s_p \\
(f(D)c - \sigma^{\text{coh}} \tan \emptyset) & s_p < |s| \end{cases} \]

where \( \sigma_p \) and \( s_p \) are the elastic limits of the opening displacement \( o \) and the shear displacement \( s \), respectively, \( \sigma_{\text{overlap}} \) is the representative overlap when \( o \) is negative, \( T_i \) is the tensile strength of the cohesive element, \( c \) is the cohesion, and \( \phi \) is the internal friction angle. Positive \( o \) and \( \sigma^{\text{coh}} \) values indicate crack opening and a tensile cohesive traction, respectively. Eq. 2 represents the Mohr-Coulomb shear strength model with a tension cut-off. The cohesive tractions \( \sigma^{\text{coh}} \) and \( \tau^{\text{coh}} \) are applied to the opposite directions of the relative opening and sliding in the cohesive element, respectively.

### 2.2. Efficient contact activation approaches

In the GPGPU-parallelized HFDEM3D, the discrete particles are discretised into tetrahedral elements, whose contacts are modelled using the penalty method. For example, when any two tetrahedral elements subjected to contact detection are found to overlap each other, the contact potential due to the overlapping of two elements is exactly computed. The normal contact force is then computed for each contacting couple, which acts normally to the contact surface and is proportional to the contact potential. The proportional factor is called the normal contact penalty. After the normal contact force and its acting point are obtained, the nominal normal overlap and relative displacement vector at the acting point are readily computed. After normal contact force is determined, the magnitude of the tangential contact force vector is computed according to the classical Coulomb friction law. The tangential contact force is applied parallel to the contact surface in the opposite direction.

All tetrahedral elements in the model domain are subjected to contact interaction force calculations above, which is the so-called full contact activation approach [9]. It is, however, inefficient and rather time consuming, especially in the case that no failures of the particles occur. Moreover, the authors have noticed that it is not physically reasonable and contradictory to the continuous deformation of intact rocks using continuum solid elements. Correspondingly, the authors [9] proposed an adaptive contact activation approach, in which, only the tetrahedral elements in the model boundary and those in the vicinity of newly failed cohesive elements become contact candidates and are added to the contact detection list. Compared with the full contact activation approach, the advantage of the adaptive contact activation approach is that the contact detection and contact force calculations are necessary only for the initial material surfaces until the failures occur, which not only makes the dramatic savings of the computational time but also are more physically sound resulting in smooth stress distributions in intact rocks. Both the full and adaptive contact activation approaches have been applied by the authors [9] to simulate the uniaxial compression test of a homogeneous limestone under quasi-static conditions, which are compared with each other revealing minor differences but the simulation with the adaptive contact activation approach is 10.8 times faster than that with the full contact activation approach.

However, the adaptive contact activation approach suffers from numerical instabilities characterized by spurious fracture mode when modeling hard rocks under quasi-static conditions and both hard and soft rocks under dynamic loading conditions with high loading rates such as those in the split Hopkinson pressure bar tests. It has been proven by the authors [10] that the spurious fracture mode is due to the unphysical mesh movement caused during the shear softening of cohesive elements when the relative sliding distance \( |s| \) becomes larger than \( s_p \), i.e. in the shear softening regime in which the effect of missing contacts starts to be non-negligible anymore. Moreover, with the increase of the relative sliding distance \( |s| \) in the shear softening regime, the shear resistance force exponentially decreases as shown in Eq. 2 in the case of \( |s| > s_p \), which further derives the unphysical movement of mesh due to missing contacts. Correspondingly, a semi-adaptive contact activation approach was developed by the authors [10] to overcome the numerical instability, in which we adaptively activate the contact calculation for the tetrahedral elements in the close vicinity of the cohesive elements which enters the shear softening regime (\( |s| > s_p \)) with \( f(D) \) of the cohesive element in Eq. 2 dropping to a certain threshold value (\( 1.0 \geq f_{\text{threshold}} \geq 0.0 \)) regardless of the pure mode II fracturing or the mixed-mode fracture. The
advantage of the semi-adaptive contact activation approach is that it behaves exactly the same as the adaptive contact activation approach until \(D\), which means that the simulation with semi-adaptive contact activation approach is faster than the full contact activation approach. Therefore, the semi-adaptive contact activation approach is proposed not only as a countermeasure to overcome the spurious fracturing mode but also a fast contact calculation scheme. Most importantly, the semi-AACAA can ensure the high precision of stress wave in the intact rock, which is the basis for any dynamic simulations including rock blasting problems.

2.3. Various implementations of gas and rock interactions

One of the biggest challenges in modelling the fracture and fragmentation of by blast is to simulate how the fracturing rock interacts with the explosive detonation-generated high pressure gas resulting in the flow of the gas through fracture and fragmentation. In the GPGPU-parallelized HFDEM3D, following most of existing methods for rock blasting modelling, the pressure-time histories generated from field observations and empirical equations are implemented to model the detonation-induced pressure although the approach has many limitations and involves in various crude approximations. For example, in authors’ early study [6], the chemical reaction in blast is modelled using the commercial explicit finite element code AUTODYN to generate a relationship between the blast-induced instantaneous gas pressure and the time. A similar gas pressure vs time relationship has been implemented into the GPGPU-parallelized HFDEM3D. As the detonation gas expands, the rock around the borehole fails to form the crushed zone and cracks, and then the detonation gas flows through the crushed zone and the cracks propagating out of the crushed zone. Meanwhile the detonation gas exerts pressures on the cracks and the crushed zone to result in further fracture and fragmentation. In order to model this process, a relatively simple model for gas flow through the fracturing rock is implemented, which is actually based on the detonation wave speed and the distance of the observation point from the detonation point. The explosive gas is presented only within the gas zone, which is best defined as a circle around the borehole. The spatial and temporal distribution of the gas pressure in the circle are determined on the basis of the distance of the circle from the detonation point and the instant time.

However, the simple model for gas flow through the fracturing rock suffers from the drawbacks of applying the gas pressure on any cracks inside the circle around the borehole no matter these cracks are connected to the borehole or not. In the GPGPU-parallelized HFDEM3D, the simple model for gas flow through the fracturing rock is improved so that the gas pressures are applied on the cracks only directly connected to the blast-hole. Moreover, Duvall’s type pressure function is implemented into to model the pressure rise and decay period during the blasting process, as shown in Eq. 3:

\[
P = P_0 \xi (e^{-\alpha t} - e^{-\beta t}) \quad \text{where} \quad \xi = 1 / \left( e_0^{-\alpha t} - e_0^{-\beta t} \right) \quad \text{and} \quad t_0 = \left[ 1 / (\beta - \alpha) \right] \log(\beta / \alpha)
\]

(3)

where \(P\) and \(P_0\) are the current and peak blasting pressures acting on the blast-hole wall and cracks connected to the blasthole, and \(\alpha\) as well as \(\beta\) are constants related to explosives. By using Eq. 3, the pressure rising and decay time can be adjusted by changing the decay time ratio \(\beta / \alpha\) and \(t_0\).

Numerical modelings have shown the empirical and theoretical gas pressure vs time relationships introduced above are able to result in promising rock fracture and fragmentation but the explosive gas flow process is greatly simplified, which may overestimate/underestimate the role of the explosive gas in producing long radial cracks. Moreover, the algorithm of tracing the connections between radial cracks and corresponding boreholes becomes complicated or even impossible when fragmentations are generated. Correspondingly, the authors are attempting to implement a 3D fluid-structure interaction solver (FSI) into the GPGPU-parallelized HFDEM3D. Currently, we are testing a 2D FSI solver in literature [12] and are hoping to extend it into 3D and then implement it into HFDEM3D. Promising progresses have been achieved in implementing the 2D FSI solver although verifications and calibrations are needed.
3. GPGPU-parallelized 3D modelling of rock fragmentation process by blast
The GPGPU-parallelized HFDEM3D introduced in Section 2 is applied to model rock fracture and fragmentation process by the detonation of a single borehole, and simultaneous and consecutive detonation of multiple boreholes. To save pages, only brief explanation is given in this section.

3.1. Modelling rock fracture process by the detonation of a single borehole
Fig. 2 illustrates the numerical model for the detonation of a single borehole in the cylinder blasting experiment [13], in which a borehole with a length of 20mm and a diameter of 20mm is drilled in a cylinder rock sample and then charged with explosive. The corresponding detonation process and resultant rock fracturing process are simulated using the GPGPU-parallelized HFDEM3D, as illustrated.
in Fig. 3. The one cross-section and three slices clearly show the detonation process of the explosive along the borehole, the formation of the crushed and cracked zone, and the long radial crack propagation surrounding the borehole.

3.2. Modelling rock fracture by simultaneous detonations of multiple boreholes
Six sub-parallel boreholes are detonated at the same time in a rock mass as shown in Fig. 4. The one cross-section illustrates the detonation process along the length of the borehole while the three slices are cut perpendicularly to the long borehole showing the interactions of the stress waves and resultant rock fractures induced by each borehole.

![Figure 4](image)

**Figure 4.** Modelling of rock fracture by the simultaneous detonation of multiple boreholes

3.3. Modelling rock fracture and fragmentation by consecutive detonations of multiple boreholes
Fig. 5 depicts the numerical model for consecutive detonations of multiple boreholes in ring blast, in which one ring of boreholes is drilled upward in a fan-shape pattern. As modelled in Fig. 6, explosives are charged into the boreholes and the rings are blasted in sequence. The central borehole is firstly ignited from the bottom and then the explosives in the borehole are burning upwards with a detonation wave.

![Figure 5](image)

**Figure 5.** Numerical model for the consecutive detonation of multiple boreholes
Figure 6. Modelling of rock fracture by consecutive detonation of multiple boreholes
velocity. As soon as the borehole is detonated, high compressive stress waves are generated in the detonated area and propagate outwards resulting in fracturing. After that, the explosives in the left and right boreholes of the central borehole are detonated simultaneously from the bottom of the borehole and the subsequent boreholes are detonated so on from the centre to the left and right sides until the boreholes in the far left and far right sides are detonated. The blast-generated rock fragments then collapse and fall into the crosscuts.

4. Conclusions
A three-dimensional (3D) hybrid finite-discrete element method (HFDEM) is first implemented to model the fracture and fragmentation process of rock by blast. The HFDEM3D code is several thousand times faster than its former version after the parallelisation on the basis of general-purpose graphic-processing-unit (GPGPU) and the implementation of various speeding up schemes, which paves the way for 3D modelling of rock fragmentation by blast. The main components of HFDEM3D are then briefly reviewed, which include the robust fracturing algorithms, efficient contact activation approaches and various implementations of detonation-generated gas and rock interactions detailed by the authors in various former publications. After that, the GPGPU-parallelized HFDEM3D is applied to model the rock fracture and fragmentation process by the detonation of a single borehole and the simultaneous and consecutive detonations of multiple boreholes.

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