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Corresponding Author	Family Name	Rizvi	
	Particle		
	Given Name	Zarghaam Haider	
	Prefix		
	Suffix		
	Role		
	Division	Geomechanics and Geotechnics	
	Organization	Kiel University	
	Address	Kiel, Germany	
	Email	zarghaam.rizvi@ifg.uni-kiel.de	
Author	Family Name	Mustafa	
	Particle		
	Given Name	Syed Husain	
	Prefix		
	Suffix		
	Role		
	Division	Department of Computer Science and Engineering	
	Organization	Aligarh Muslim University	
	Address	Aligarh, India	
	Email		
Author	Family Name	Sattari	
	Particle		
	Given Name	Amir Shorian	
	Prefix		
	Suffix		
	Role		
	Division	Geomechanics and Geotechnics	
	Organization	Kiel University	
	Address	Kiel, Germany	
	Email		
Author	Family Name	Ahmad	
	Particle		
	Given Name	Shahbaz	
	Prefix		
	Suffix		

	Role		
	Division	ZachryDepartment of Civil Engineering	
	Organization	Texas A&M University	
	Address	College Station, USA	
	Email		
Author	Family Name	Furtner	
	Particle		
	Given Name	Peter	
	Prefix		
	Suffix		
	Role		
	Division		
	Organization	Vienna Consulting Engineers	
	Address	Vienna, Austria	
	Email		
Author	Family Name	Wuttke	
	Particle		
	Given Name	Frank	
	Prefix		
	Suffix		
	Role		
	Division	Geomechanics and Geotechnics	
	Organization	Kiel University	
	Address	Kiel, Germany	
	Email		
Abstract	Cemented geomaterial due to inherent porosity and composition difference has many stress localization spots. These spots when they exceed the material limit locally form centres for crack nucleation and propagation. A vast pool of numerical and analytical methods is available, but these methods fail to solve the problem of wave motion at the granular level. The problem offers a daunting task in static or pseudodynamic loading but becomes highly challenging in a dynamic loading scenario. Here, in this paper, we present the lattice element method from the family of discrete element method to solve the problem of mechanical waves in rock mass or cemented granular material under dynamic excitation. The method offers a robust solution to the problem of crack initiation and propagation in a dynamic loading scenario. The lattice element method is capable of handling the nucleation, propagation, coalescence and branching of the cracks with relative ease. The method could be extended to impact loading and multiphysics scenarios in a straight-forward manner.		
Keywords		d - Dynamic loading - Granular physics - Computational fracture mechanics	

Dynamic Lattice Element Modelling of Cemented Geomaterials



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Zarghaam Haider Rizvi, Syed Husain Mustafa, Amir Shorian Sattari, Shahbaz Ahmad, Peter Furtner and Frank Wuttke

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Z. H. Rizvi (S) · A. S. Sattari · F. Wuttke

Geomechanics and Geotechnics, Kiel University, Kiel, Germany

e-mail: zarghaam.rizvi@ifg.uni-kiel.de

S. H. Mustafa

Department of Computer Science and Engineering, Aligarh Muslim University, Aligarh, India

ZachryDepartment of Civil Engineering, Texas A&M University, College Station, USA

P. Furtner

Vienna Consulting Engineers, Vienna, Austria

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Z. H. Rizvi et al.

1 Introduction

For the natural or artificial cemented granular media, such as rock, soil and concrete, the location and distribution of the grains and bonds dramatically affects the dynamic characteristics. Microstructural contact laws based on Hertz contact model and multibody dynamics relying on Newton's' law for accelerating bodies offer a solid foundation for development and optimization of new knowledge for both mathematical and numerical solution of such a complex problem. The first attempt to numerically model the granular media with multibody interaction with circular particle and computation of macroscopic deformation was shown by Cundall and Strack [1]. Zhang and Evans [2] provided a rich review of different model setup schemes for the Discrete Element Method (DEM) and the limitation of such a model. The DEM models offer an implacable solution for large deformation problems but are limited in its ability for modelling of the microscopic intergranular interaction and nucleation, propagation, fingering, coalescence and branching of the cracks in cemented granular media. A more challenging scenario arises in case of cemented granular media developing cracks subjected to a dynamic load. Modelling of such a system considering the mesoscale geometry, which primarily influences the wave motion and cracks propagation behaviour is a daunting task. The extended finite element method (XFEM) that allow for arbitrary cohesive crack propagation and the embedded strong discontinuity finite element method (ED-FEM) both treat with the cracks in a mesh independent approach due to their enrichment. The computation costly tracking algorithms are often used with these methods, mainly to solve the problematic crack phenomena in dynamics, such as bifurcating, also shown in Nikolić et al. [3]. The phase field models for the granular system requires mammoth computational resource and many fitting parameters are included in an ad hoc manner. Therefore, Lattice element method, derived from condense physics matter which offers an accurate and computationally efficient solution is considered here.

The Lattice Element Method (LEM), was first introduced by Hrennikoff [4] and later by Kawai [5], in which they developed the truss framework to discretize the elastic continua. The lattice model is defined as an assembly of discrete cohesive link elements for the representation of a structural solid. This simplification of continua is not a rudimentary assumption for modelling of complex solids or structures and the approach results to a lighter computational cost. Moreover, efficient representation of some aspects, which are not easily tackled with simplicity and successful description of the localized failure and cracking mechanisms are the most critical features that led to the rapid development of lattice models shown in Nikolić et al. [6]. Failure and cracking mechanisms can be simulated straightforwardly usually by detecting if any lattice element, which represents the cohesive force between the particles, has reached a specific failure criterion. These failure criteria could be based on Linear Elastic Fracture Mechanics (LEFM) shown in Wuttke et al. [7], Rizvi et al. [8–10] or the classical failure models Khan et al. [11]. Once the critical failure value is reached, a cohesive fracture is initiated, leading to the gradual separation of the crack surfaces across the cohesive zone. This simple assumption helps in bypassing

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the issue of the singularity of the stress at the crack tip, which is present in linear elastic fracture mechanics. Additionally, with lattice models, it is possible to simulate multiple cracks without worrying about numerous crack interactions.

Despite being applied mostly to quasi-static loading conditions, the lattice elements can also be used for simulation of impact problems as well as shown in Nikolić et al. [3]. The broad applicability of this model is ranging from the quasi-static uniaxial loading and shearing of geomaterials to the dynamic fragmentation due to explosion, impact and collision of solids. The model is suitable for impact simulations in which cracks occur as a result of large movements of the rigid Voronoi particles. However, the applicability of these models is limited to a very regular type of grain sizes. Karavelić et al. [12] Here, we present a lattice element model for a full grain size range capable of capturing wave motion in plain and cracked cemented granular matter at a meagre computational cost.

2 Mesh Generation and Mathematical Formulation

To generate the granular assembly, a random set of points are generated in a Euclidean plane and the nearest neighbour points are computed using the Voronoi tessellation algorithm (Fig. 1). For a set of random points $P = \{p_1, \ldots, p_n\} \subset \mathbb{R}^2$, where $2 < n < \infty$ and $x_i \neq x_j$ for $i \neq j, i, j \in I_n$. The region by Eq. (1) is the Voronoi polygon for the node p_i .

$$V(p_i) = \{x ||x - x_i|| \le ||x - x_j|| \text{ for } j \ne i, j \in I_n \}$$
 (1)

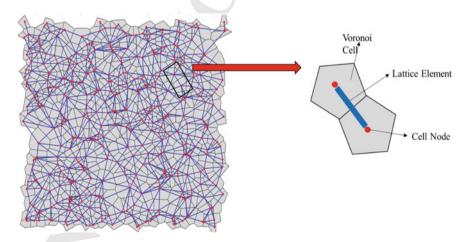


Fig. 1 Cell nodes, Voronoi cells and Lattice elements. Voronoi Algorithm is used to find the nearest neighbours and Delaunay triangulation to connect the neighbouring nodes to form the lattice elements

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4 Z. H. Rizvi et al.

The set of all the polygons thus generated for the nodes p_i are the Poission Voronoi diagram. The dual tessellation of the Voronoi diagram is generated to form the connections among the neighboring Voronoi cells. This triangulation scheme is called the Delaunay triangulation. Mathematically, V(P) be the Voronoi diagram generated by a set of n distinct points $P = \{p_1, \dots, p_n\} \subset \mathbb{R}^2, 3 \le n < \infty$ that satisfies the non-collinearity assumption (D_1) ; $Q = \{q_1, \dots, q_{nv}\}$ be the set of Voronoi vertices in V; and $\{x_{i1}, \ldots, x_{ik1}\}$ be the location vectors of the generator points whose Voronoi polygons share a vertex q_i .

$$T_i = \left\{ x | x = \sum_{j=1}^{k_i} \lambda_j x_{ij}, \text{ where } \sum_{j=1}^{k_i} \lambda_j = 1, \lambda_j \ge 0, j \in I_{k_i} \right\}$$
 (2)

$$D = \{T_1, \dots, T_{nv}\}\tag{3}$$

Equation (3) represents the *Delaunay triangulation* of the represented points.

The material properties are assigned to the Voronoi cells and then transferred to the elements thus generated by the Delaunay triangulation scheme shown in Rizvi et al. [13] and Shrestha et al. [14]. Material damping is not considered here.

For the dynamic simulation, the equation of motion for each element is solved with Newmark beta method. For a forced undamped system, the equation of motion is given as

$$M\ddot{u} + Ku = F(t) \tag{4}$$

where M and K are the mass and the stiffness matrices terms and F(t) is the applied time dependent force.

Mass Matrix Generation 2.1

The mass matrix or the consistent mass matrix (CMM) is generated either by lumping the mass at the nodes or by following the variation mass lumping (VMM) scheme. The VMM scheme is also implemented in the finite element method for dynamic simulations.

The element mass M^e is computed using the following equation:

$$M_e = \int \rho \left[N_v^e \right]^T N_v d\Omega \tag{5}$$

If the shape function are identical, that is, $N_v^e = N^e$, the mass matrix is called the consistent mass matrix (CMM) or M_c^e .

$$M_c^e = \int_0^l \rho A[N^e]^T N^e dx = \frac{1}{4} \rho l A \int_{-1}^1 \left[\frac{1-\xi}{1+\xi} \right] \left[1-\xi \ 1+\xi \right] d\xi \tag{6}$$

where ρ is the density assigned to the Voronoi cells and A and l are the area and the length of the lattice elements.

The elemental mass matrix is symmetric, physical symmetric, and complies with the condition of conservation and positivity. To obtain the global mass matrix, a congruent transformation is applied. In contrast to the stiffness matrix, translational masses never vanish. All the translational masses are retained in the local mass matrix. The global transform is achieved through the following equation:

$$\bar{M}_c^e = \left[T^e\right]^T \left[M_c^e\right] \left[T^e\right]$$

$$M_c^e = \frac{1}{6}m^e \begin{bmatrix} 2 & 1 & 0 & 0 \\ 1 & 2 & 0 & 0 \\ 0 & 0 & 2 & 1 \\ 0 & 0 & 1 & 2 \end{bmatrix}$$

2.2 Element Stiffness Matrix

The force displacement component of a truss element is given by the spring relation

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$$\{F\} = [K]\{U\}$$
 (9)

The vectors $\{F\}$ and $\{U\}$ are the member joint force and member joint displacement, respectively shown in Fig. 2. The member stiffness matrix or the local stiffness

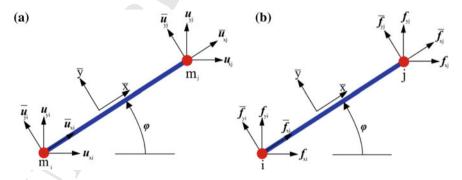


Fig. 2 a Bar element with diagonally lumped mass moving in 2D. b The transformation of node displacement and force components from the local system \bar{u}_x , \bar{u}_y to the global system u_x , u_y

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6 Z. H. Rizvi et al.

matrix is [K]. For a truss element it is given by 133

$$[K] = \frac{EA}{L} \begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$
 (10)

After applying the congruent transformation, the member stiffness matrix in global 136 coordinates are given as 137

$$\left[K^{e}\right] = \left[T^{e}\right]^{T} \left[K\right] \left[T^{e}\right] \tag{11}$$

$$K^{e} = \frac{E^{e} A^{e}}{L^{e}} \begin{bmatrix} l^{2} & lm & -l^{2} & -lm \\ lm & -m^{2} & -lm & -m^{2} \\ -l^{2} & -lm & l^{2} & lm \\ -lm & -m^{2} & lm & m^{2} \end{bmatrix}$$
(12)

where $l = \cos \varphi^e$, $m = \sin \varphi^e$ and φ^e is the orientation angle as shown in Fig. 2.

The equation of motion for the linear system of equations is solved with the Newmark beta method due to its unconditional stability. The displacement and the velocity terms for the next time are calculated as follows:

$$u_t = u_{t-\Delta t} + \Delta t \dot{u}_{t-\Delta t} + \left(\frac{1}{2} - \beta\right) \Delta t^2 \ddot{u}_{t-\Delta t} + \beta \Delta t^2 \ddot{u}_t \tag{13}$$

$$\dot{u}_t = \dot{u}_{t-\Delta t} + (1 - \gamma)\Delta t \dot{u}_{t-\Delta t} + \gamma \Delta t \ddot{u}_t \tag{14}$$

We follow the average acceleration approach with $\beta = 1/4$ and $\gamma = 1/2$.

The Newmark beta method solves the algebraic form of the equation of motion (EOM) of undamped forced vibration at the end time interval $t + \Delta t$.

$$F_{t+\Delta t} = M\ddot{u}_{t+\Delta t} + Ku_{t+\Delta t} \tag{15}$$

The stiffness and the mass matrices are computed in the following fashion to 155 reduce in the form of Eq. (9) 156

$$\hat{\mathbf{K}} = \mathbf{K} + a_0 \mathbf{M} \tag{16}$$

where \hat{K} is the *effective stiffness matrix* and $a_0 = \frac{6}{\gamma \Delta t^2}$. Similarly, the effective load vector at time $t + \Delta t$ is calculated as in (17). 159

$$\hat{F}_{t+\Delta t} = F_{t+\Delta t} + M(a_0 u_t + a_2 \dot{u}_t + a_3 \ddot{u}_t)$$
(17)

Here, $a_2 = \frac{1}{\gamma \Delta t}$ and $a_3 = \frac{1}{2\gamma}$. 163

The above simplification leads to the algebraic form

$$\left\{\widehat{F}_{t+\Delta t}\right\} = \left[\widehat{K}\right] \left\{U_{t+\Delta t}\right\} \tag{18}$$

From the above equation, displacement of each node is calculated for every time step.

The natural frequency of the system is calculated as given below

$$\omega^2[M]\phi = [K]\phi \tag{19}$$

$$\omega^2 = \text{eig}([M]^{-1}[K]) \tag{20}$$

3 Results and Discussion

Three different systems are generated with the defined boundary conditions, as shown in Fig. 3a–c. A granular assembly is generated with the Voronoi tessellation and Delaunay triangulation, as explained in Sect. 2. For the first scenario (Fig. 3a), 550 cell points have been used. The other two simulations are performed with 6400 points. MATLAB programming environment is used for computation. As reported earlier in literature Nikolic et al. [3, 6], Rizvi et al. [8] the mesh dependence response of the method is not significant and will be dealt in detail in future works.

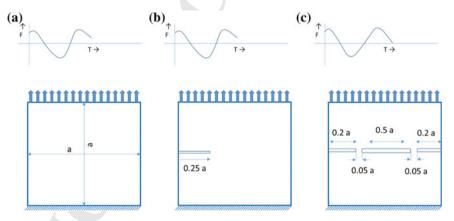


Fig. 3 The schematic diagrams of the boundary conditions for the simulations. **a** A cemented square plate with side a=1 cm. **b** A square cemented granular plate with a single crack of 0.25 a length. **c** Two granular systems connected with two bridges of 0.05 a length each. A harmonic force is applied at the top and the bottom is held fixed

AQ3₂₀₄ 8 Z. H. Rizvi et al.

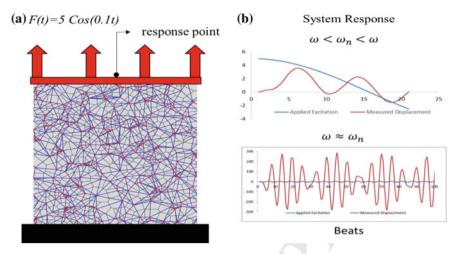


Fig. 4 a Assembly of the granular system and the applied loading with the boundary condition. b Response of system at excitation frequency away from the resonance frequency (top) and (bottom) near to the resonance frequency ω_n . Beat formation is recognisable at frequencies close to the excitation frequency

The above-generated system is subjected to a time-harmonic excitation, as shown in the figure below. The response of the system is measured at the top. The bottom nodes are fixed, and the excitation is applied to the top nodes.

The natural frequency of the system is calculated from Eq. (20). The system is excited to a frequency far from the resonant frequency. Figure 4b shows the response of the system. The excitation force is shown with a blue line, and the computed response at the top is plotted in red. As the excitation frequency is brought closer to the natural frequency of the system, beats are observed (Fig. 3b). This confirms the validity of the method.

Figure 5 shows the movement of mechanical waves in a cemented granular system. A time depended on force, as shown in Fig. 3 is applied at the top surface, and the displacement of the nodes are plotted. This indicates the formation of high and low displacement zones. The phenomenon of wave movement is puffed rice grains has been investigated, and the creation of a band has been reported in Guillard et al. [15]. A similar pattern is observed here too (Fig. 4). After the first cycle at time t = 25, the system does not return to its original position. A residual negative strain in the system remains. A further investigation with voids and different density particles will be reported elsewhere.

Figure 6 shows the response of a cracked cemented granular assembly subject to the same cosine loading (Fig. 3b). The presence of a crack modifies the wave path, and the existing crack behaves as a stress concentrator. A similar result is reported with existing cracks in a homogeneous plate with the Boundary Element Method (BEM) shown in Rizvi et al. [16]. However, it is impossible to capture the intra and intergranular response with BEM. The simulation in Fig. 6 shows the modification in

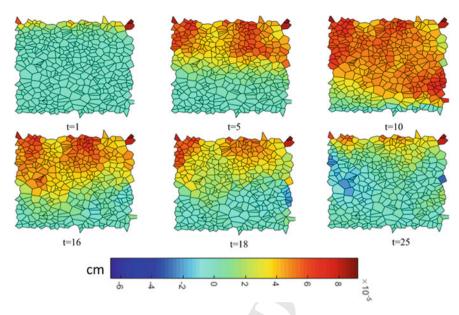


Fig. 5 Propagation of waves in the cemented granular media. The figure shows the response of a cosine excited wave of the system. The red colour shows the maximum amplitude and the blue the minimum

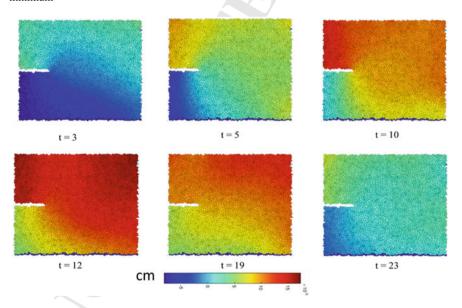


Fig. 6 Propagation of waves in the cemented granular media. The figure shows the response of a cosine excited wave of the system. The excitation is applied at top and bottom is held fixed. The red colour shows the maximum amplitude and the blue the minimum

10 Z. H. Rizvi et al.

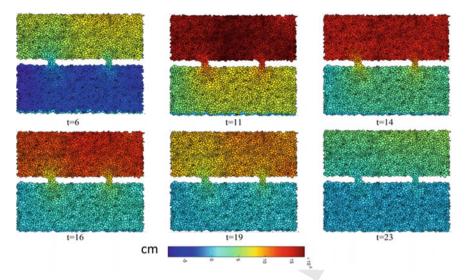


Fig. 7 Mechanical wave propagation in two granular cemented blocks with two contact points. The excitation is applied at top of the top block and bottom is held fixed. The dynamic lattice element method is capable of capturing this complex response with ease

the near and far field of the existing crack. The method combined with conventional lattice element methods is capable of modelling crack initiation and propagation. These results will be reported elsewhere.

Figure 7 shows two cemented granular blocks connected with two granular pillars. The top surface of the top block is excited with the harmonic force, as explained in Fig. 3c. The bottom surface of the base block is held fixed. The waves started at the top block travels through the granular pillars to the lower block. The movement of mechanical waves in such a non-trivial system is captured with relative ease.

4 Conclusion

The dynamic lattice element method is reported here for cemented granular medium, and the following conclusions are drawn from this study.

- Lattice element method coupled with average acceleration Newmark beta method
 is capable of solving the mechanical wave movement with relative ease and at a
 low computational cost.
- 2. The pre-existing cracks modify the near and far field displacement and act as stress concentrators and distributors.
- 3. Wave motion in cemented granular media with existing cracks are modelled easily, which offers computational and mathematical challenges in other numerical and analytical methods.

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272 273 **Acknowledgements** Z. H. R, F. W and P. F want to acknowledge the *Marie Curie* project *ExchangeRisk* (Grant No. 691213) for financial support. A. S. S acknowledge the Grant GeoMInt (03G0866B). Z. H. R acknowledges and thanks *Vienna Consulting Engineers ZT GmbH* for hosting the research work. ZHR and SHM prepared and communicated the manuscript.

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