RESEARCH ARTICLES

Numerical simulation of particulate materials using discrete element modelling

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Discrete element method (DEM) is a numerical technique pioneered by Cundall[1] for problems in rock mechanics where the continuity between the separate elements does not exist. Discrete numerical simulations with particles are currently used in several different scientific disciplines. The DEM is capable of handling a wide range of material behaviour, inter-body interaction force laws and arbitrary geometries. DEM models granular materials which can freely make and break contacts with their neighbours and is capable of analysing interacting deformable bodies undergoing large absolute or relative motions. DEM-related research has proved to be very meaningful for enhancing the understanding of granular materials. This tool has been used for developing and validating constitutive relationships of particulate materials such as soil, rock, grain or ceramic powder by using appropriate particle properties, sizes, shapes, and gradation. Moreover, DEM is the best tool for explaining the experimentally observed facts from a more fundamental approach. Perhaps one of the major advantages of the discrete particle model approach is that what is being done during a simulation is obvious at all the times. The discrete element model incorporates induced anisotropy, shear dilatancy and stress path dependency from more fundamental principles and has proven its usefulness to generate insights into the processes involved with particulate media. DEM is an explicit finite difference code and because of the explicit nature of the algorithm, it is necessary to use a very small time-step of simulation to guarantee numerical stability and accuracy. Many researchers are attempting to expose the advent of the effective use of the supercomputer and parallel computing for engineering problems by modifying the discrete element simulation codes. This will allow a major step forward in handling a very large number of particles for the more realistic simulations of particulate solids. In this paper, an overview of the discrete element modelling is presented along with some of its applications in engineering.

1. Introduction

The continuum assumption is used as a basis for the idealization of many materials such as soils, rocks, rockfills, aggregates, concrete and other engineering materials. Numerical solution techniques such as finite element, finite difference and boundary element methods are founded on the continuum assumption and have been proved as extremely useful tools for the engineer to solve many complex engineering problems. However, the continuum mechanics models are phenomenological and are primarily concerned with mathematical modelling of the observed phenomenon without detailed attention to their fundamental physical significance. In particulate materials forces are transferred through contacts between the particles. Problems occur with the continuum assumption due to the particulate material's inherent granular nature and the consequent deformation and failure modes. This discrete behaviour makes the constitutive relationship of particulate media complex and many laboratory tests are necessary to understand the behaviour before the physical processes in these materials can be modelled. In materials dominated by particulate behaviour it is advantageous to treat the medium as an assemblage of particles rather than as a continuum as it permits the exploration of actual mechanisms involved. Also, there are many situations especially in large deformation problems and fracture in engineering materials where continuity cannot be assumed and other techniques must be utilized.

An alternative approach is discrete element model (DEM), which is capable of analysing multiple interacting deformable continuous, discontinuous or fracturing bodies, undergoing large displacements and rotations. The method is general in its ability to handle a wide range of material constitutive behaviour, interaction laws and arbitrary geometries. Currently, there are two-dimensional models available with particles as circular discs, ellipses and polygons and three-dimensional models with particles as spheres, blocks/bricks, and ellipsoids. Also DEM has progressed from the early rigid and simply deformable elements to its present state of complex elements which place at its disposal the full range and the power of the finite element method. The method solves for the dynamic equilibrium equations for each body subjected to body and boundary forces. Highly dynamic effects can also be simulated including stress wave propagation, vibration and damping[2].

DEM has evolved from various disciplines such as physics of particles[3,4], from geomechanics[1,5,6] and from structural engineering[7,8]. Theoretical background for the

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method is derived from the fields of aero-elasticity[9], the finite element method[10] and the finite difference method[11]. Discrete numerical simulations with particles are currently used in several different scientific disciplines, to examine a wide range of physical systems with inherent 'granularity' (stellar dynamics, hydrodynamics, molecular dynamics, and electrostatic plasma; Hockney and Eastwood[12]). The DEM approach has been applied to problems on an atomic scale, to modelling of sedimentary rocks[13,14], and to slope stability problems in which particle dimensions are up to many feet[15]. The method is used in process engineering to study the flow of granular media in hoppers or down-inclined chutes[16,17]; the development of stresses around tunnel openings in jointed rocks[18]; nonlinear static and dynamic soil structure interaction problems[19]; and the stress and flow response of naturally fractured fluid reservoirs[13]. Cundall and coworkers extended the DEM to soil using two-dimensional discs[20] and three-dimensional spheres[21] and subsequently these models were extended to handle particles of any shape. Numerical simulations using DEM have been attempted by several workers[1,14,20,22–26] to model granular media.

An excellent source of references with respect to DEM is contained in refs 27 and 28.

2. Discrete element method

DEM is a numerical technique pioneered by Cundall[1] for rock mechanics problems where the continuity between the separate elements does not exist. In DEM, the equilibrium contact forces and displacements of a stressed assembly of discs are found through the medium of disturbances originating at the boundaries, which is a dynamic process. The speed of propagation is a function of physical properties of the discrete medium. DEM is based on the idea that this time-step may be chosen so small that during a single time-step disturbances cannot propagate from any disc further than its immediate neighbours. It is this key feature of DEM which makes it possible to model the interaction of large number of elements without excessive memory requirements.

One of the important elements of the DEM model is the explicit incorporation of Coulomb's frictional behaviour at contacts between elements. Slippage between elements is permitted, when the tangential or shear force at a contact exceeds a critical value, $F_s^{\max}$, defined by:

$$F_s^{\max} = c + \tan\phi_\mu \quad F_n , \tag{1}$$

where F_n is the normal force at the contact, and c and ϕ_μ are the cohesion and the angle of internal friction at contacts, respectively.

2.1 *Calculation cycle of DEM*

A typical calculation cycle of DEM is shown in Figure 1. Each DEM cycle involves application of Newton's second law of motion, the velocities $\dot{x}$ and $\dot{\theta}$ which will be used in the force–displacement are obtained from the current resultant force and the moment acting on the disc, given by:

$$\begin{aligned} m\ddot{x} &= \Sigma F_i , \\ I\ddot{\theta} &= \Sigma M , \end{aligned} \tag{2}$$

where F_i is the unbalanced force on each element, M is the resultant moment on each element, m is the mass of the element, I is the moment of inertia of the element and $\dot{x}$ and $\ddot{\theta}$ are the element accelerations. For each element, accelerations are integrated over a small time-step to give velocities ($\ddot{x}$ and $\ddot{\theta}$) and displacements (x and θ). The time-step chosen is small enough that the velocities and accelerations are constant over it. This is followed by a force displacement law through which the unbalanced forces on each individual element are calculated. A simple

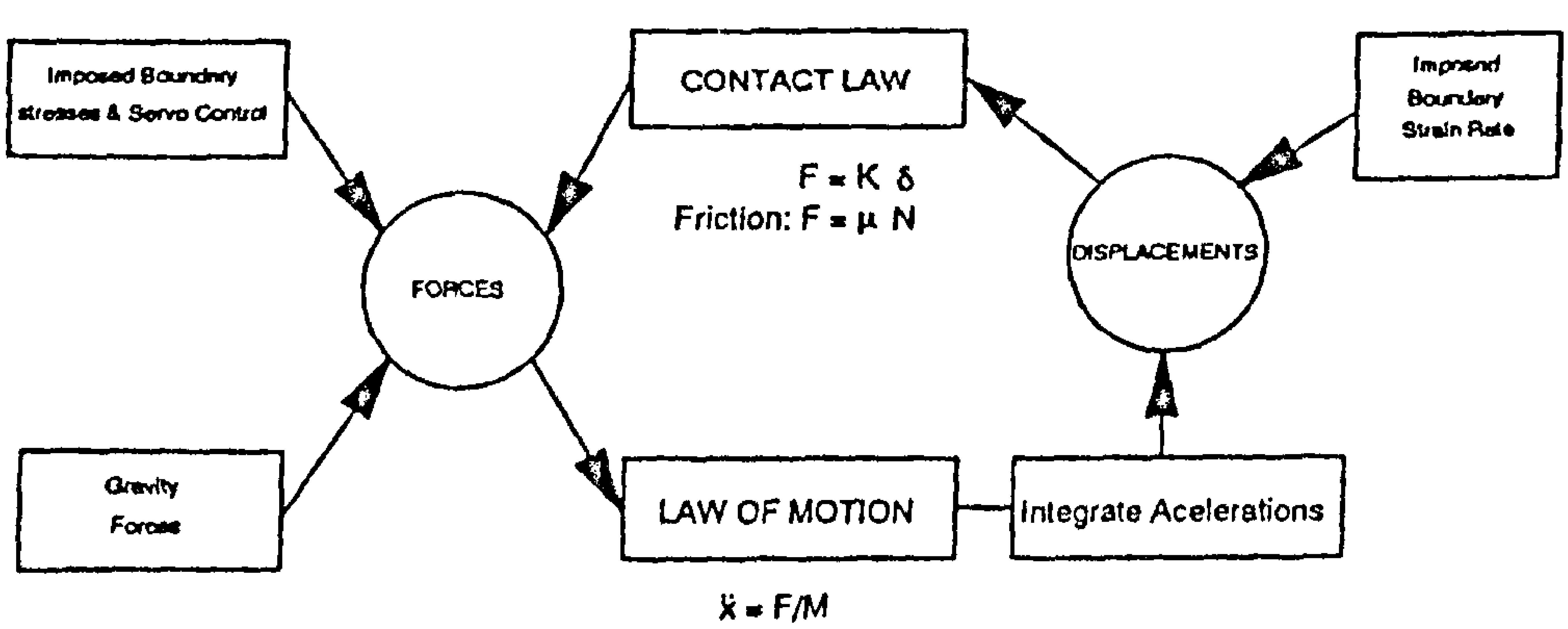

Figure 1. A typical calculation cycle in DEM.

interaction law at the contact of the two interacting discs can be written as:

$$(F_n)_{new} = (F_n)_{old} + \Delta F_n; (F_s)_{new} = (F_s)_{old} + \Delta F_s,$$

$$\Delta F_n = K_n \Delta n; \Delta F_s = K_s \Delta s, \quad (3)$$

where F_n and F_τ are the normal and shear contact forces, K_n and K_s are the element stiffness in normal and shear directions, and Δn and Δs are the normal and shear relative displacements at a contact. ΔF_n and ΔF_s are the incremental normal and shear contact forces respectively. The components Δn and Δs of the relative displacements at a contact are obtained by integrating the relative velocity component with respect to time. The relative velocity components are calculated by projecting relative velocity at the contact point in normal and tangential directions to the contact plane.

The calculations presented are repeated till the unbalanced forces on the particles are very small or zero for static problems. Interaction relationships for other types of contacts such as rock joints may include cohesion, dilation, damage to asperites and stress-dependent friction. Also there is no restriction on where one element may make contact with another. The connectivity or interaction of element to element is computed automatically in the algorithm, since the elements can rapidly change neighbouring elements upon motion or fracturing.

Rheological elements of the discrete element model for a simple disc element are shown in Figure 2. In DEM artificial damping is incorporated to dissipate the kinetic energy so as to bring the assembly to static equilibrium under imposed boundary conditions. DEM includes two forms of viscous damping such as contact damping and global damping. Contact damping (C_n) operates on relative velocities at the contacts and is visualized as resulting from dashpots acting at normal and shear directions at the contact as shown in Figure 2. The contact damping coefficients are taken to be proportional to contact stiffnesses. Global damping (C_m and C_1) operates on the absolute velocities of discs and is visualized as the effect of dashpots connecting each particle to the ground. Coefficients of global damping are taken proportional to absolute velocities of both translational (C_m) and rotational movement (C_1). Friction damping (C_s) occurs during sliding when the absolute value of the shear force at each contact is at the value of F_s^{max}. The use of additional damping other than friction is necessary in order that the assemblies reach a state of equilibrium for all conditions. If neither contact nor global damping were included, the assemblies could only reach equilibrium if slip occurred.

Although the assembly is dynamic, static equilibrium is achieved by applying the boundary stresses in terms of small increments for all the static problems. Equilibrium contact forces and displacements are found in an assembly of particles, stressed by imposed boundary conditions through a series of calculation cycles which trace the movement of each particle. These movements are the results of diffusion of the disturbance due to external application of forces and displacements. Because of the unbalanced forces, the particles try to rearrange themselves so as to achieve equilibrium. Following the application of Newton's second law, a test for existence of physical contacts is performed. If the contact exists between two elements, incremental normal and tangential contact displacements are calculated from rigid body movements of each element, and the linear and angular velocities at each element centre during a fixed time interval. It may be noted that the linear force displacement law discussed above is not inherent in the method. A nonlinear law such as that of Hertzian contact could equally well be employed and has been used in many simulations presented in the next section. Calculations are repeated till the unbalanced forces on the particles are very small or zero. A general purpose DEM can treat nonlinearities which may arise from large displacement, rotation, slip, separation and material behaviour. The incremental motion of the elements may give rise to interactions between elements and thus strain rates are generated within the elements. From the constitutive behaviour of the material, the element will experience elastic or viscoelastic behaviour or possibly fracturing. Fracturing of a discrete element is relatively easy because all interactions with other elements occur through boundary forces[2]. Thus once the

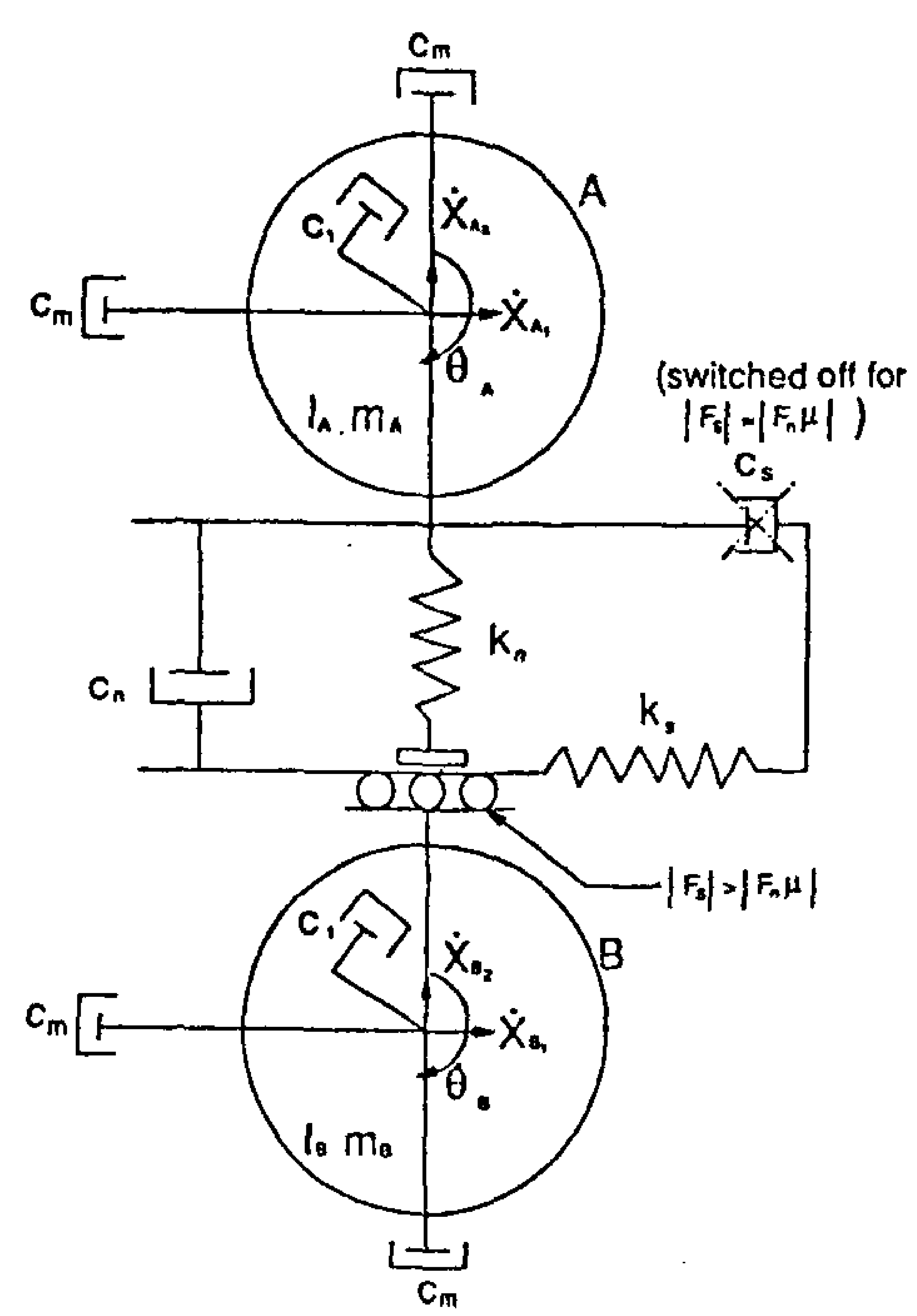

Figure 2. Rheological elements of DEM along with the damping mechanisms adopted in DEM.

geometric bookkeeping of creating two elements from one has been accomplished, the standard discrete element algorithms will take care of determining new contacts and forces. It must be mentioned here that the structure for fracturing is relatively straightforward, however the rules for fracturing are not well developed[29].

2.2 *Method of analysis*

The method of analysis consists of mainly three steps[30]:

1. Contact processing and detection: The essence of contact detection is the determination of the surfaces and volumes of intersection between two bodies. Once the contact geometry has been determined, one can easily enforce the contact conditions. In this case the program should determine the contacts automatically within itself. This is done through a contact algorithm which checks every face/point contact of every element with every face/point of every other element.
2. Contact and interaction forces: The numerical modelling of contact between bodies is a rather complex subject. It is however noted that any form of interaction law or numerical technique can be accommodated within the discrete element framework. A most significant feature of the contact problems involving friction is that deformations, in general, depend on the loading history and thus the loading process is followed with time. The earlier contact interaction law described is a linear interaction model.
3. Element motion in which the dynamic equation of motion is applied for rigid body motion as applied to a single discrete element acted upon by an arbitrary set of point forces. Adopting an incremental displacement approach linearizes these equations.

3. Validation tests

DEM consisting of 2-dimensional discs was developed and validated by Cundall and Strack[31]. They have compared the force vector plots obtained from the discrete element model consisting of 2-dimensional discs with the corresponding force vector plots obtained by photo-elastic experiments by De Josselin de Jong and Verruijit[32] as shown in Figure 3. The correspondence between the plots was sufficiently good to conclude that the discrete element model simulates well the contact interaction and is a valid tool for fundamental research in understanding micromechanical behaviour of particulate media. Sitharam[14] has presented several other validation tests using the DISC model.

The power of the technique can be appreciated from the idealized uniaxial compression test illustrated in Figure 4 (ref. 2). The left-hand plate moves towards the specimen against a second fixed plate. When the stress in the specimen exceeds a user-defined limit, fracture occurs. Further compression causes large motion and repeated fracturing, with some fragments flying off with high velocity. It should be noted that the fracturing proceeds without intervention. The fracture orientation, new element generation and new interactions are automatically calculated within the program. This relatively straightforward discrete element analysis would be extremely difficult with conventional FEM analysis.

4. Applications in engineering

Many applications of DEM are reported in the literature. In this section only selected applications of DEM in engineering in general and structural engineering in particular, geomechanics encompassing both soil and rock mechanics applications, and granular flow problems have been pre-

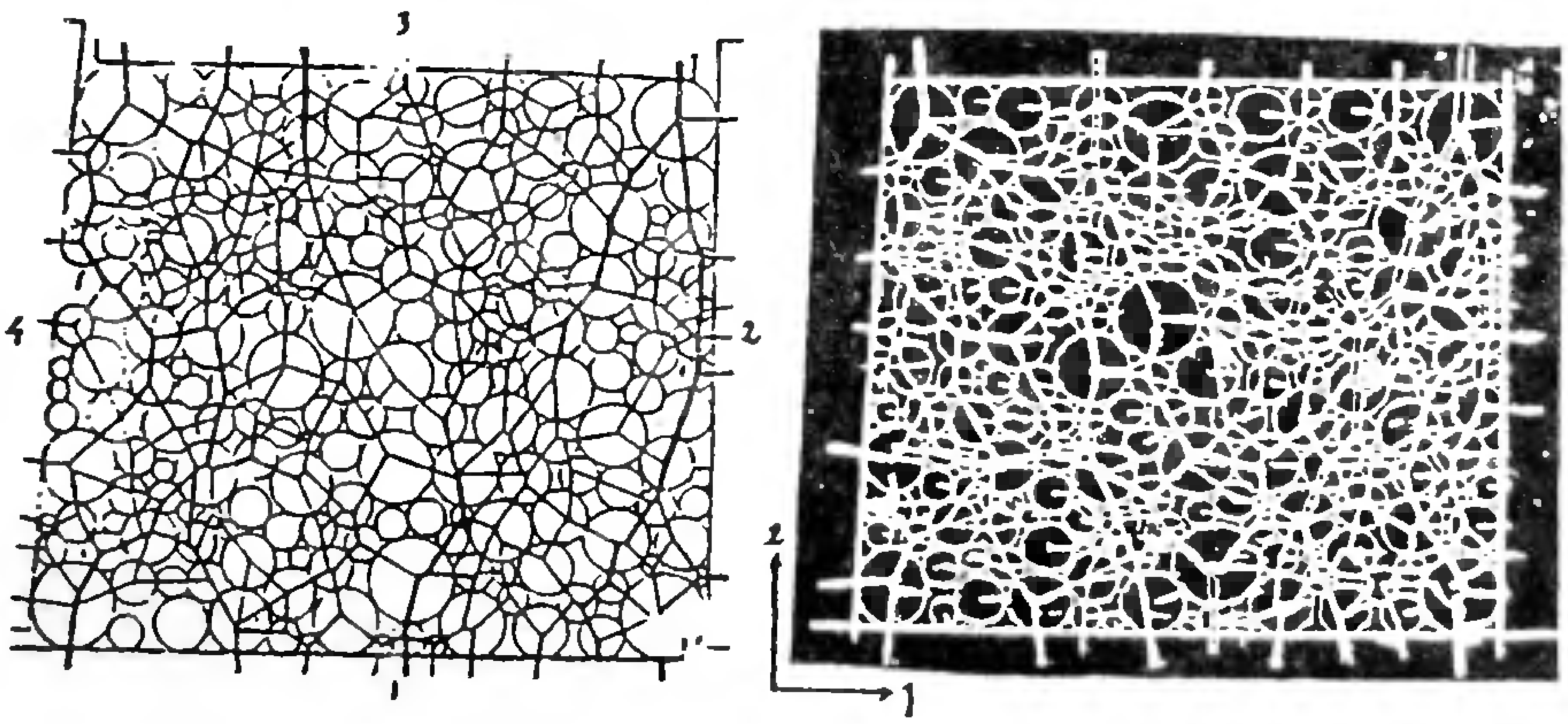

Figure 3. Comparison of force vector plots obtained from the discrete element model[31] consisting of two-dimensional discs with the corresponding force vector plots obtained by photo-elastic experiments by De Josselin de Jong and Verruijit[32].

sented. Especially in rock mechanics and soil mechanics applications, the joint/contact behaviour is the controlling parameter and the intact rock/soil element deformations may have little effect. In such cases the rigid body DEM is an excellent tool. The following selected DEM applications from the literature are presented to highlight the power of discrete element modelling.

Figure 5 shows the three-point loading of a concrete beam consisting of bonded discs[33]. Figure 5 *a* shows the force distribution prior to cracking and Figure 5 *b* shows the particle configuration after some bond breakage has occurred. This test was simulated using particle flow code in two dimension (PFC2D) of Itasca[33]. The particles may represent individual grains in a material such as sand, or they may be bonded together to represent a solid material such as concrete or rock. Fracturing was modelled when bonds break under load.

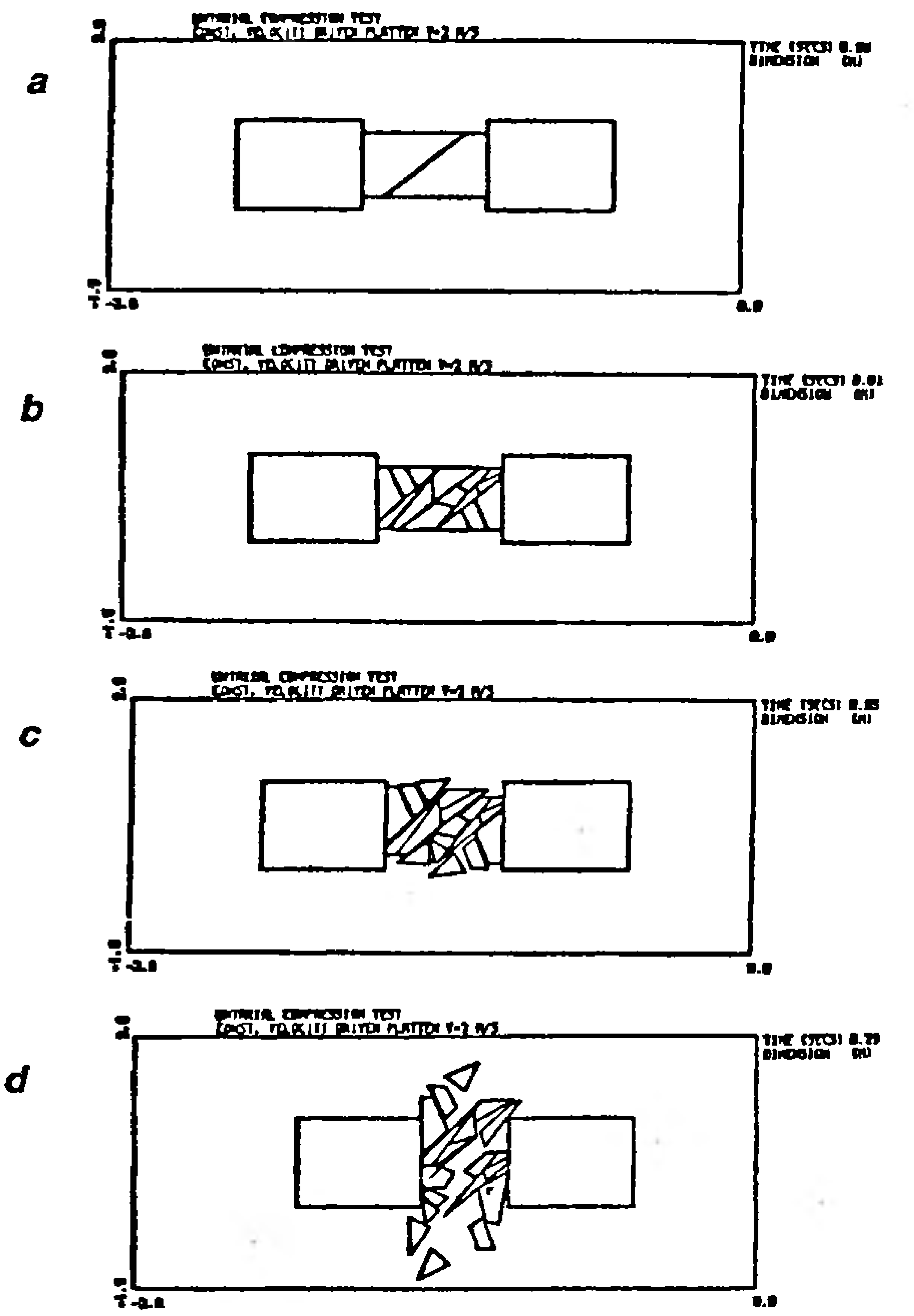

Figure 4. Idealized uniaxial compression test simulation-using DEM (Mustoe *et al.*[50]).

The example described here presents simple results of a particulate mechanics approach to understand the constitutive behaviour of granular materials to give a flavour of this emerging branch of materials science. The essence of the modelling approach is illustrated in Figures 6 and 7 (ref. 35). Figure 6 shows the computer-generated assembly of two-dimensional disc particles at the start of the simulation and several stages of compaction from initially generated no touching discs. By applying isotropic stress on the boundary particles of the initially generated assembly, compaction was initiated. One can clearly see how contact forces generate as the sample gets compacted and finally a homogeneous sample with uniform distribution of contact forces between the discs is achieved using DEM (see Figure 6 *d*). Figure 7 *a* shows the stress–strain curves for a biaxial test conducted on the compacted assembly. Based on micromechanics, stress has been represented by the contribution from arrangement of particles and their orientations (known as fabric), and contact forces including normal and shear forces are presented in Figure 7 *b*. For the details one can refer to Sitharam[35]. The beauty of particulate simulation using DEM is the availability of micro-parameters at all stages of the simulation. Using the micro-parameters such as average coordination number, contact forces (both normal and shear) and their orientations and displacement trajectories, one can look for better understanding of the material behaviour and develop or validate relationships between micro- and macro-parameters (stress, strain, etc.). For these simulations, we have used only linear contact law. However, the stress–strain curve observed was nonlinear. Nonlinear behaviour is attributed to rearrangement of particles (change in fabric) and the macroscopic averaging of the movement of particles over a large assembly of particles. In real granular systems, nonlinear contact interaction may be ascribed to surface asperities or slight irregularities in particle shape. Although a nonlinear con-

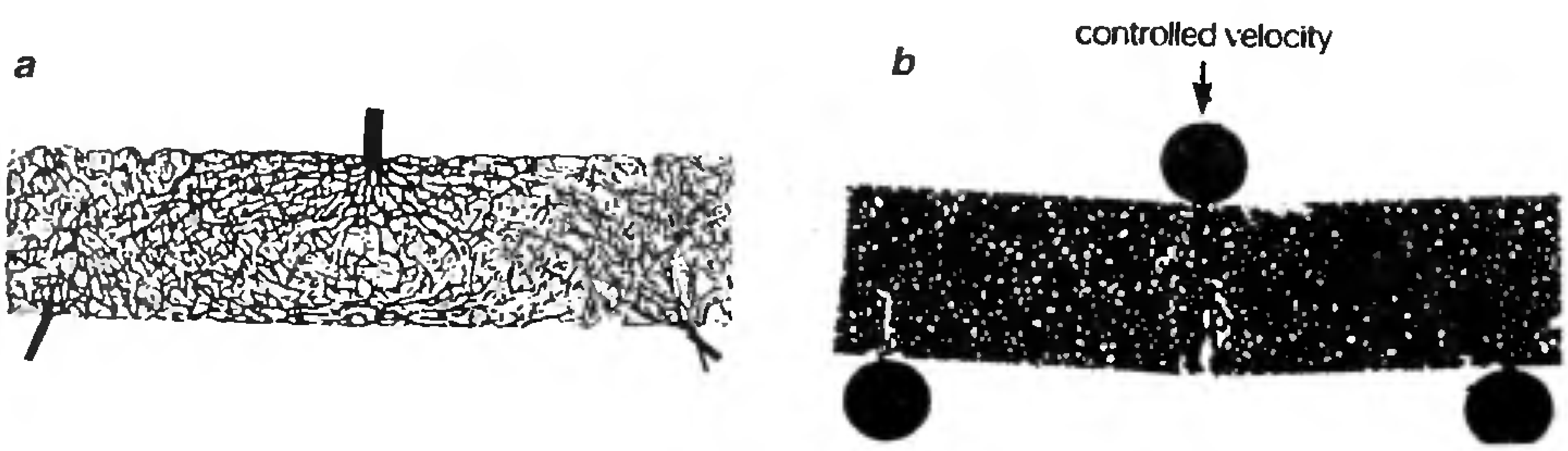

Figure 5. Three-point bending test of a concrete beam consisting of bonded discs[33].

tact interaction model such as Hertzian contact theory characterizes the relationship between contact force and inter-particle displacement in a more realistic manner, we have observed that the stress–force–fabric relationship for a homogeneous assembly is independent of the contact interaction model adopted for two-dimensional systems[14,22]. However, it is still of interest to further explore the outcome of such implementation for three-dimensional particulate assembly.

DEM has been applied to dynamical problems, such as granular flow problems[36–38], impact problems[39], and geo-dynamical problems[40,41]. Examples of granular flows include transportation of food grains, pharmaceuticals and coal through hoppers, chutes, and conveyer belts and also fluidized bed reactors. For these examples, a dynamic process was simulated using DEM by not considering the global and mass damping options.

Other applications include packing of granular materials, particulate segregation and mixing, and particulate drying. It has also been extensively applied to quasi-static problems, both two- and three-dimensional, with discs and spheres, respectively[30,39,42–44]. Ohnishi and Kono[45], Hart, Cundall and Lemos[15] and Harper and Last[13] have applied DEM to the analyses of rock masses.

Figure 8 shows a simulation of the progressive caving of a mine using a two-dimensional rigid block code UDEC (universal discrete element code)[34]. This code can be used to study two-dimensional analysis of jointed rock or granular media with different particle shapes and sizes. The program can also be used for stability analysis of dams on jointed rock foundations, design and construction

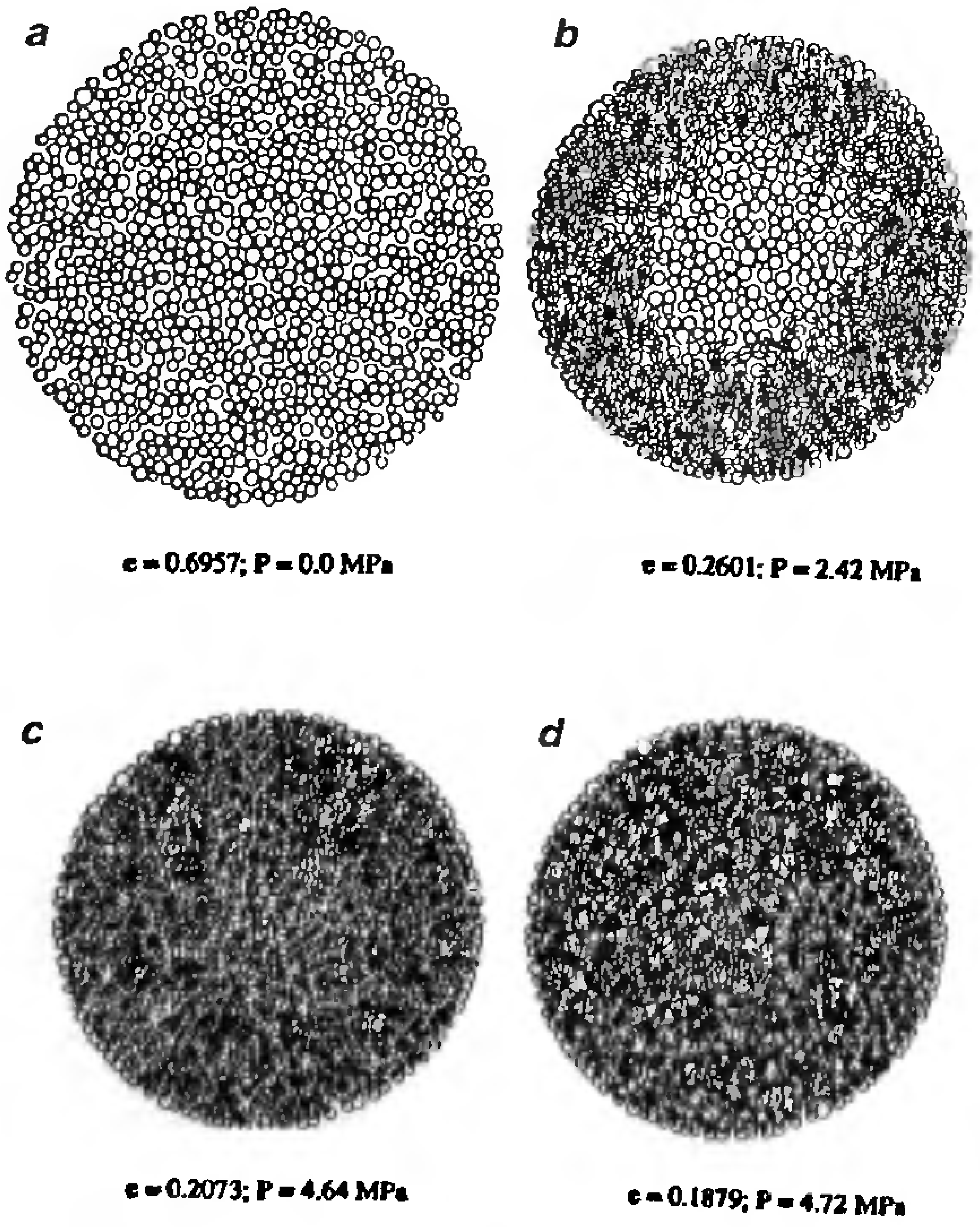

Figure 6. Compaction simulation of discs[51].

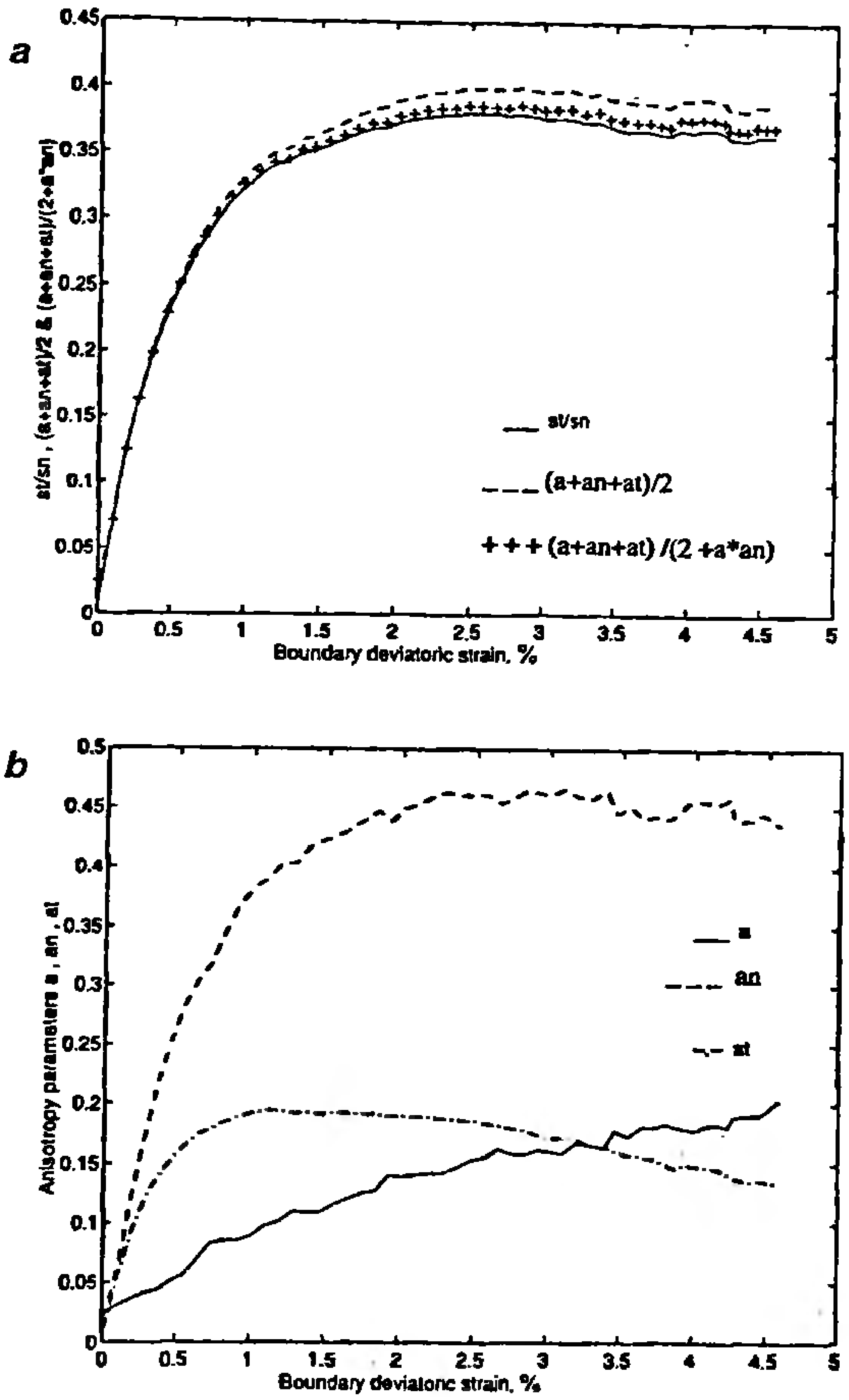

Figure 7. Stress-strain plots and their micro-parameter constitutions in terms of anisotropy coefficients.

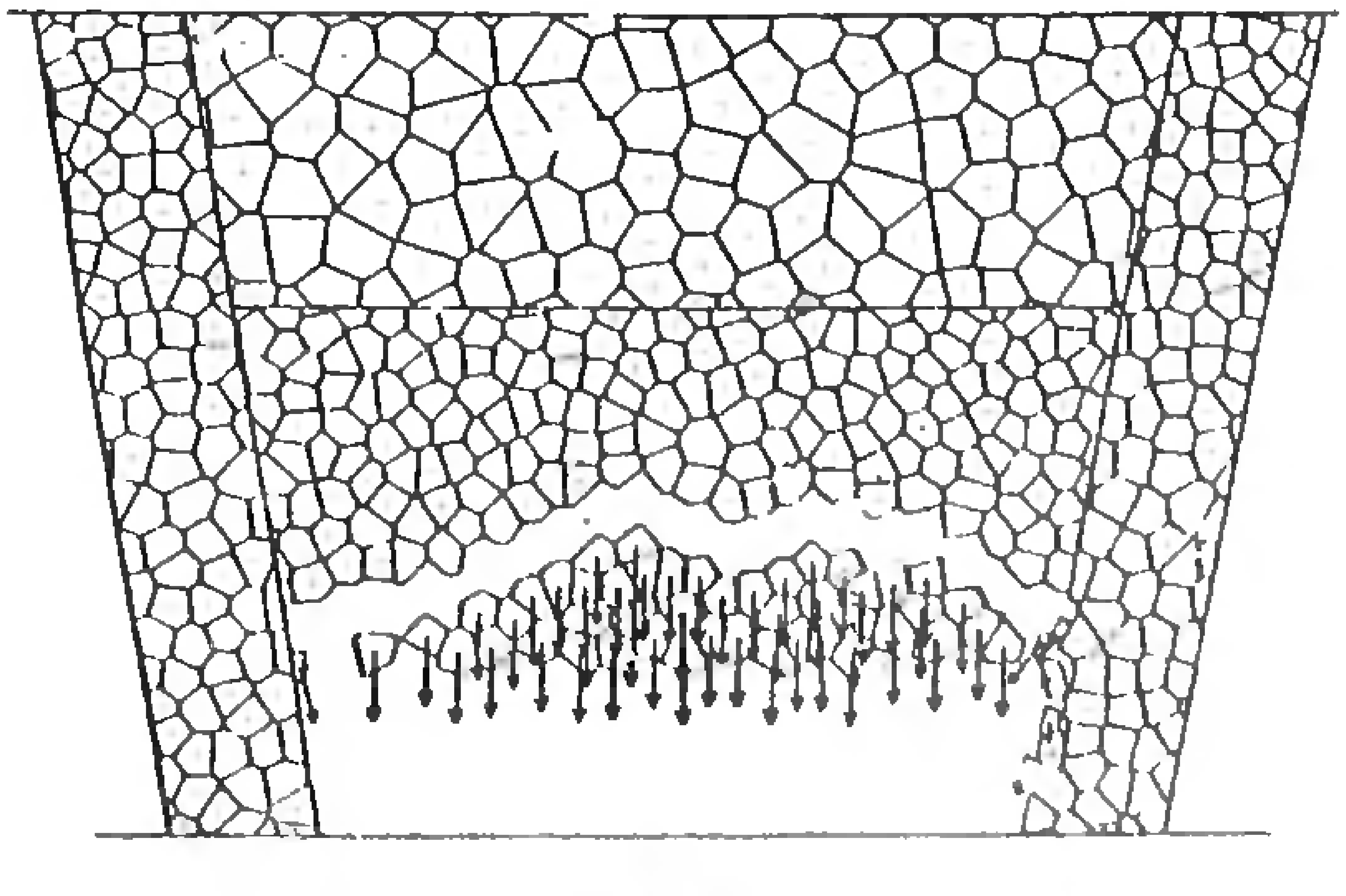

Figure 8. Progressive caving of mine[34].

of open cuts and underground excavations and also for mine extraction sequences, support requirements and mining methods. Figure 9 shows a simulation of failure of an unlined tunnel using UDEC. Figure 10 shows an application of three-dimensional DEM using 3DEC of Itasca for modelling of an excavation through jointed rock. Figure 10 shows the perspective view of 3DEC model with several foreground blocks hidden to expose the tunnel. The model contains 616 deformable blocks (with 56,700 degrees of freedom) and 33 joints have been modelled. It requires approximately 7 h on an 80486 computer to reach a solution for excavation-induced stress effects for each excavation step[46].

To apply DEM to a full-scale situation in geotechnical engineering, one could utilize real-sized particles for the entire problem with suitable material properties and full-scale loads. However this is impossible considering the computational intensity required for handling a very large number of particles. Nevertheless, application of the DEM to realistic geotechnical problems may be possible with appropriate measures[47]. The key to applying the DEM to a full-scale problem lies in ensuring proper nonlinear stress–strain–strength soil behaviour and maintaining stress similitude in the simulation. Ting *et al.*[47] have used the centrifuge modelling principle, in which a small-scale model of the full-scale problem is constructed using the same 'soil' in the model as the prototype to assure proper soil behaviour. To guarantee stress similitude, the gravitational acceleration is increased by a factor α equal to the length reduction. However in rock mechanics, full-scale simulations are being carried out (as shown in Figure 10) in real field scale problems[46,48]. A bearing capacity test conducted by Ting *et al.*[47] on the 8500 disc bin by translating a 0.04 m wide (model unit) rigid 'footing' vertically at 0.5 m/s for 0.0225 s has been reported here. After 0.0225 s (0.28 of the footing width), the footing was stopped and the bin allowed to equilibrate until 0.03 s. Figure 11 *a* shows the initial 8500 disc bin and footing. Figure 11 *b* shows the actual displacement vectors of disc particles at the end of the test. The ultimate footing pressure applied compares favourably with the ultimate bearing capacity from Terzaghi's theory for sand with angle of internal friction $(\phi) = 26°$ and density $(\gamma) = 2000$ kg/m^3. Also, the incremental normal stress contours at the end of the bearing capacity test compare well with Boussinesq's stress contours (not shown here).

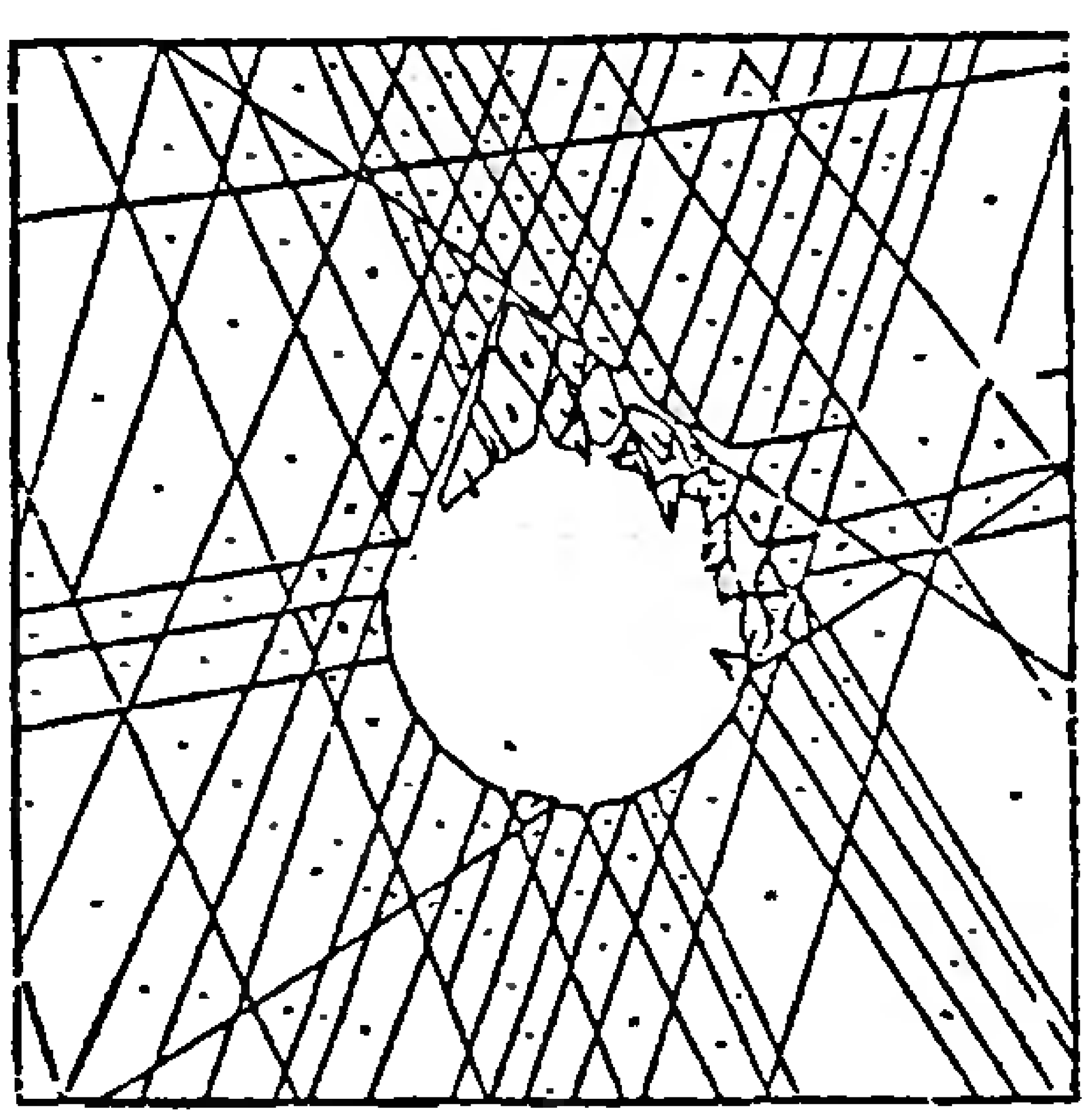

Figure 9. Failure of an unlined tunnel using UDEC[33].

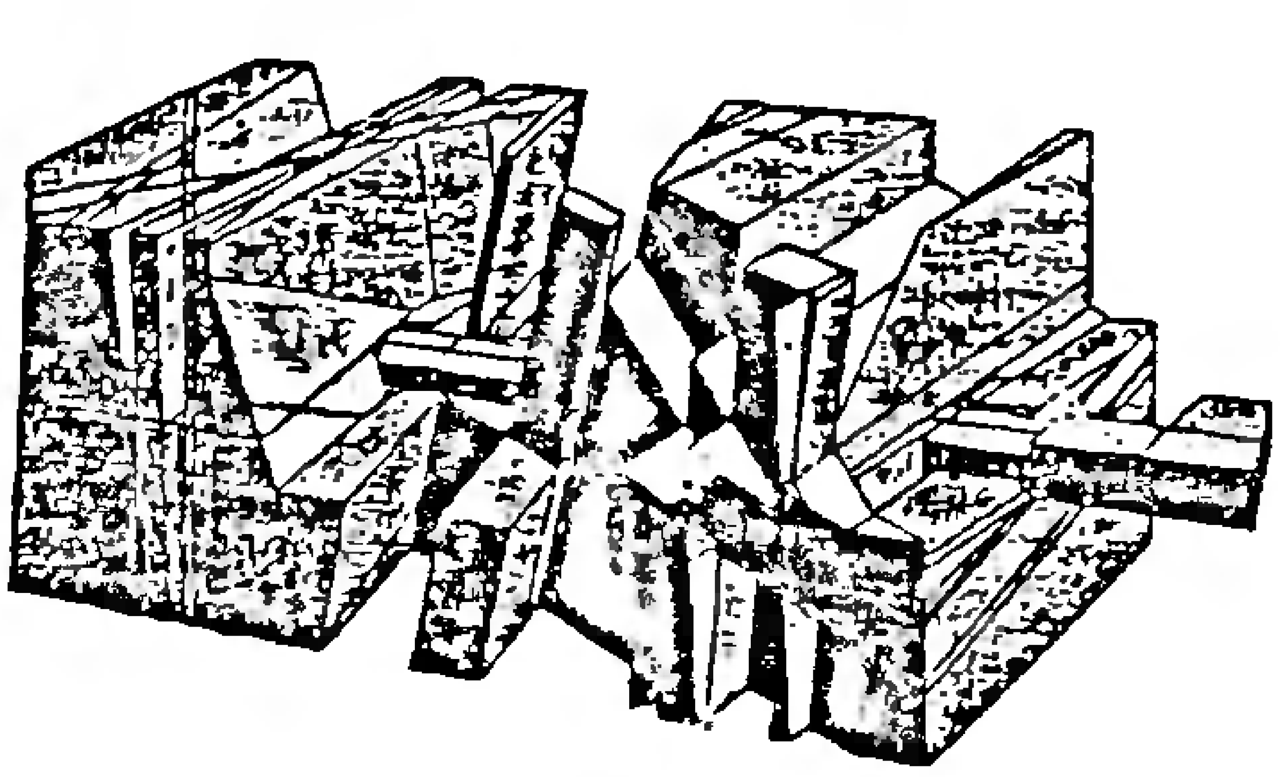

Figure 10. Modelling of a tunnel (excavation) through jointed rock using 3DEC[46].

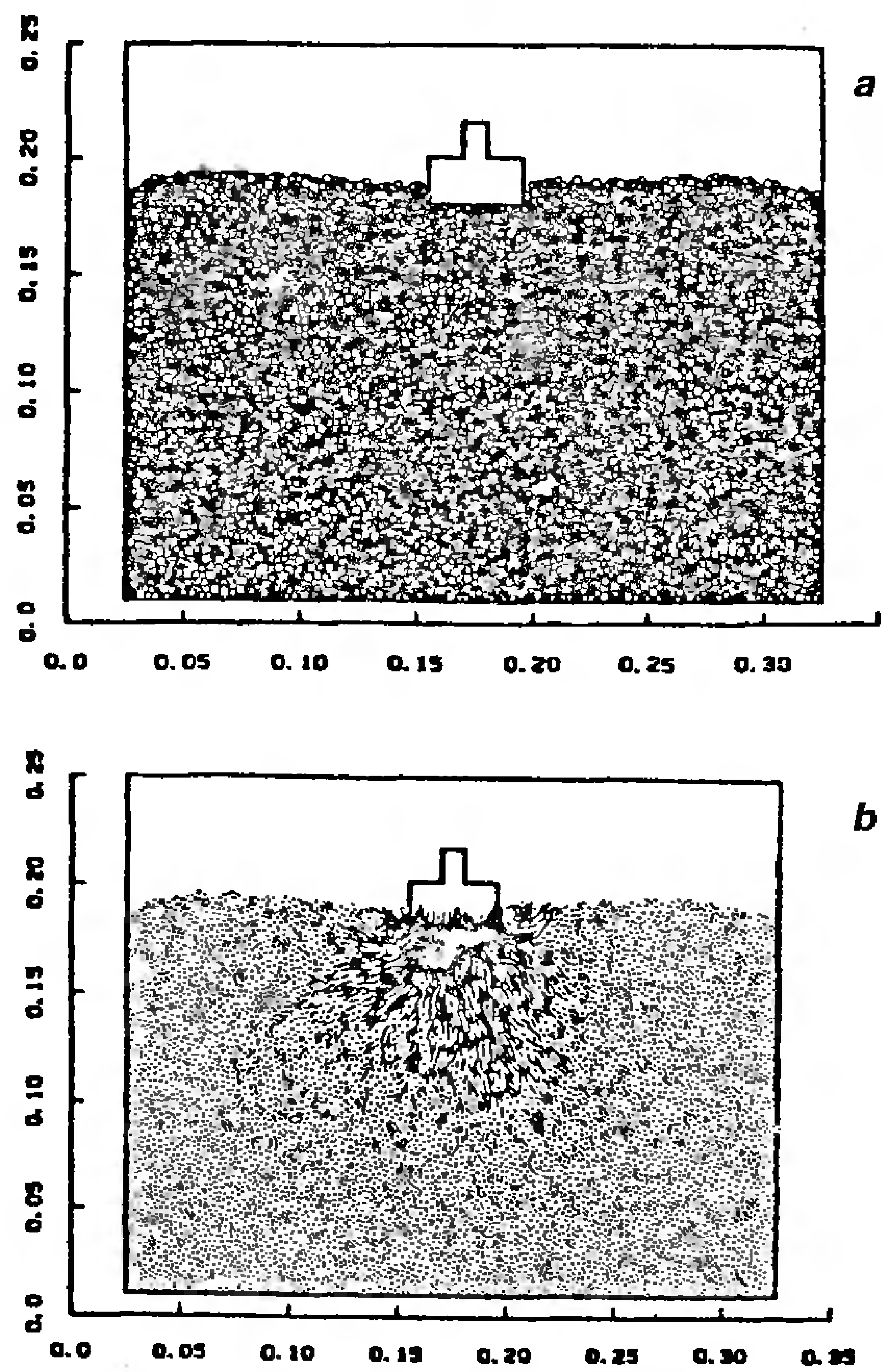

Figure 11. *a*, Footing response on a granular soil; *b*, Trajectories of disc particles below a footing[47].

Simulation of a injection test in a particulate medium has been carried out to model hydrofracturing in granular media using a two-dimensional disc model coupled with fluid flow[14]. These tests are carried out to study the fracture initiation pressures and on fracture orientations in cohesionless granular media where conventional fracture mechanics concepts are not applicable. Figure 12 shows the results of injection-induced deformation in the two-dimensional assembly of discs. Figure 12 *a* indicates the fracture initiation in the isotropic disc assembly due to injection in a central pore or a void. This fracture is stable and is slowly growing as the injection pressure is gradually increased. Figure 12 *b* and *c* show the fracture propagation due to further increase in injection pressures. Contact-force redistribution takes place because of reduction in contact forces around the fracture, which causes concentrated deformations dominated by plastic slip and parting. The grains on the wall of the fracture are not free floating, they are pushed against the walls of the fracture by the pressure drop across them. This is a demonstration of the stabilizing effect of fluid flow. It is also pointed out here that the particulate medium around the fracture is dilating and yielding as a consequence of the very low effective stress arising because of high pore pressure. In an isotropically compacted assembly, there is no preferential direction for fracture propagation; the fracture, once initiated because of large deformation around the injection point, creates its own anisotropy and propagates in the path of least resistance.

A simulation of multiple interacting fractures in a discrete element particulate system is shown in Figure 13 *a* and *b*. The figure also shows the interaction of multiple (two) fractures in an isotropically compacted system. Figure 13 *a* shows the contact force distribution in a discrete element system when the two fractures are interacting with each other. Figure 13 *b* shows the displacement trajectories corresponding to the stage of Figure 13 *a* from the initially compacted system.

Figure 14 shows the dynamic nonlinear response of structural foundations, in particular the penetrating pile in a sand bed[40]. In this figure, the first column clearly shows the stages of penetration of a pile in a two-dimensional circular particle system. The second and third columns highlight the disc trajectories and contact force in the system. This example highlights the failure pattern formed below a penetrating pile and 2 : 1 slope, which is generally assumed in all geotechnical designs. This clearly shows that the observed failure mechanism is realistic and

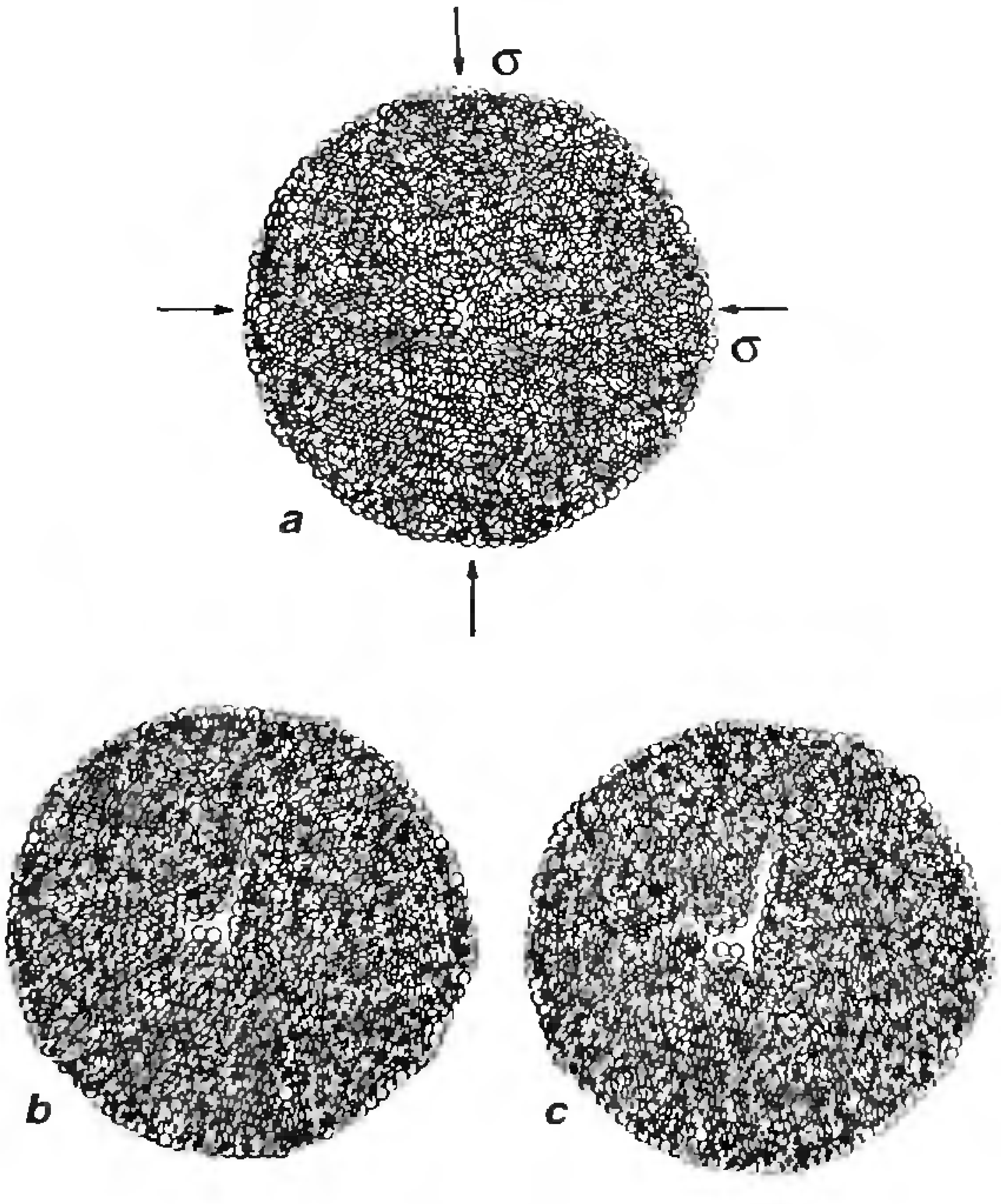

Figure 12. Hydrofracture initiation and propagation simulation in a two-dimensional disc assemblage[14].

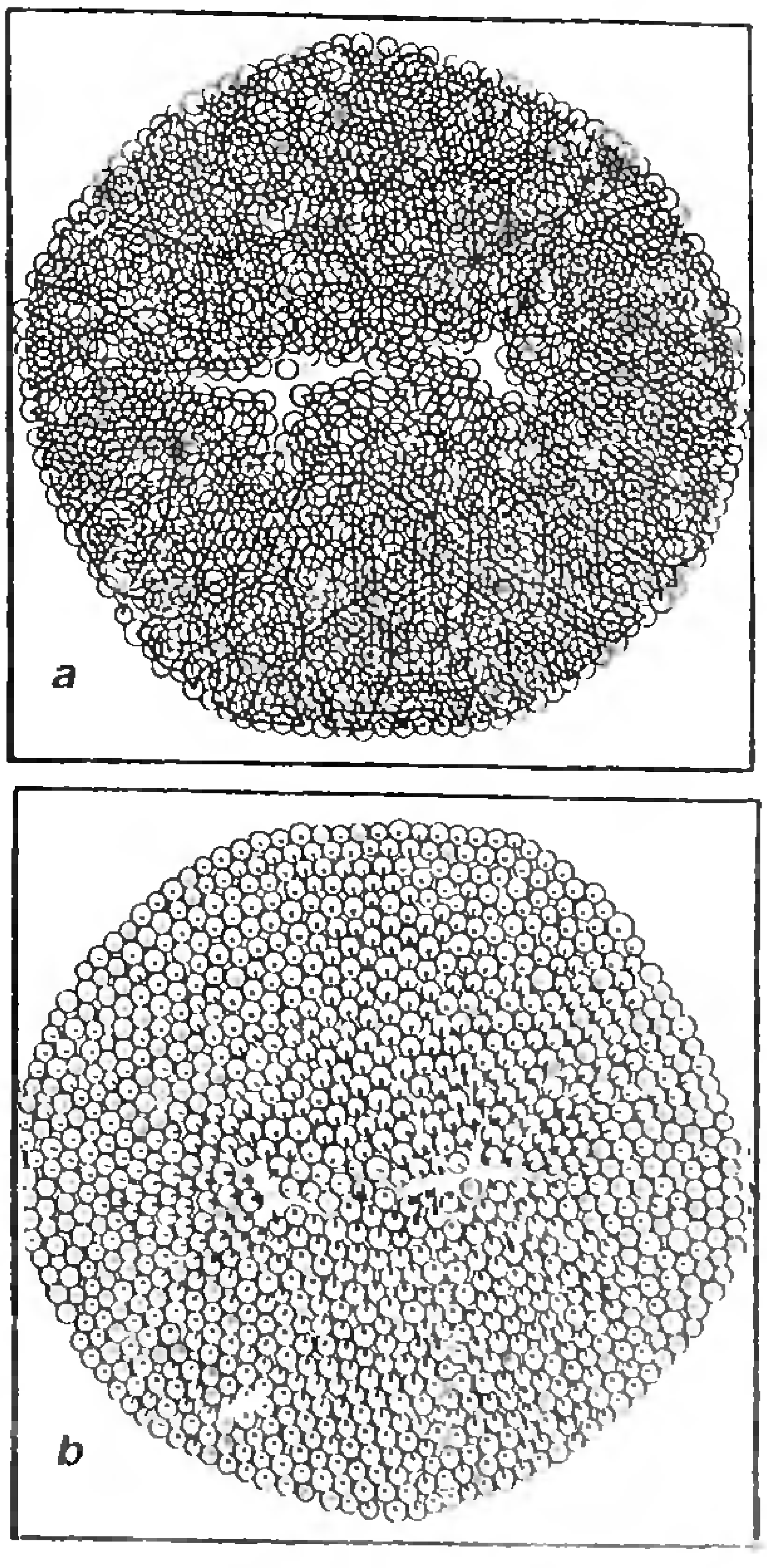

Figure 13. Multiple fracture interactions in a discrete element system[14].

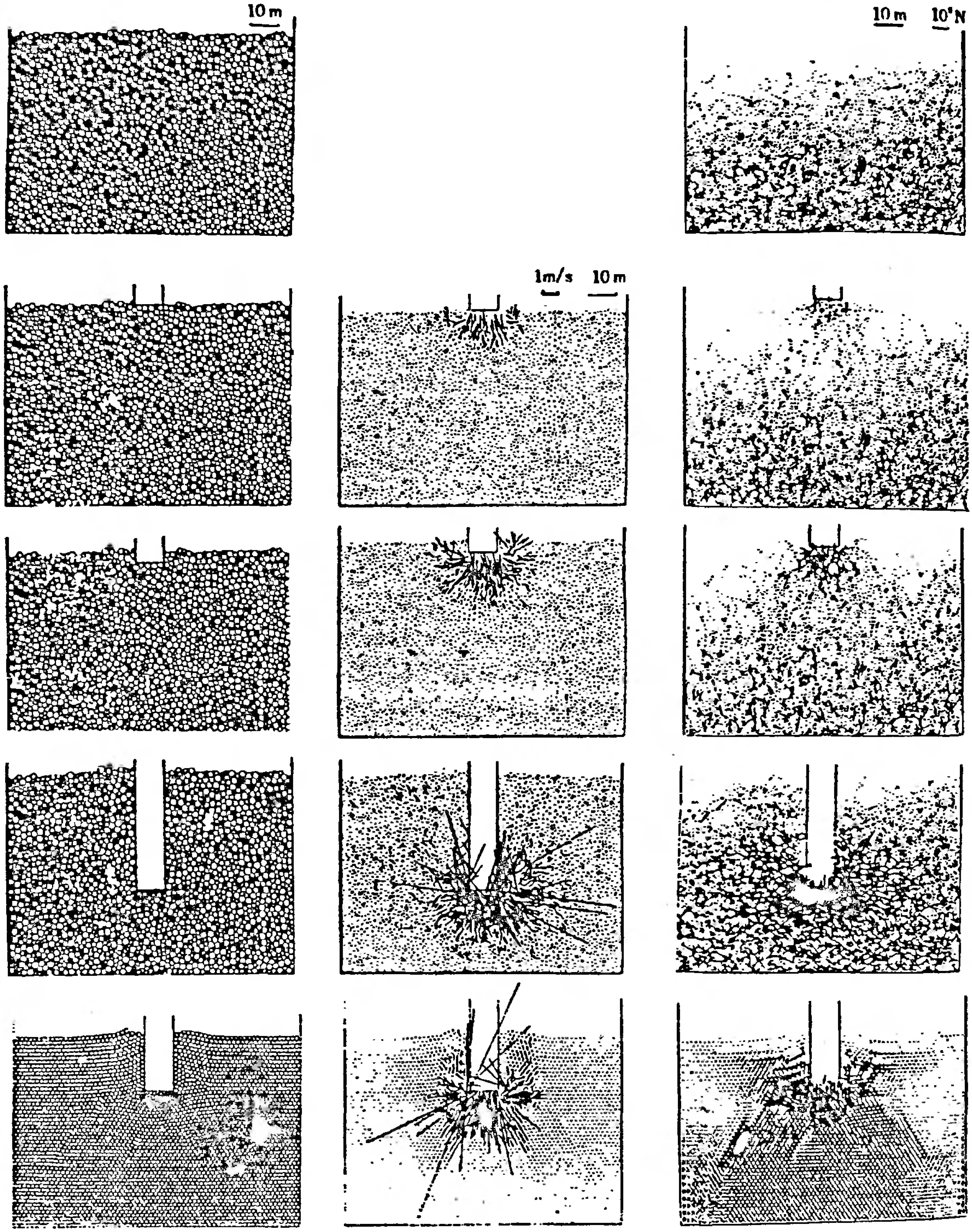

Figure 14. Simulations of a penetrating pile in sand[40].

the failure surfaces formed with almost 2 : 1 slope from the point above the pile tip (see bottom most picture in column 3 of Figure 14).

5. Other practical applications

Other areas in which useful practical results may be obtained using the DEM include:

1. Soil–structure interaction problems.
2. Dynamic pressures behind a flexible retaining wall.
3. Ice mechanics and other related applied mechanics problems.
4. Fundamental aspects of particulate mechanics and constitutive behaviour of soils and rocks.
5. Soil-reinforcement interaction in reinforced earth structures, viz. reinforced retaining walls and soil beds.
6. Design of stone or gravel column in soft clays.
7. Analysis and design of earth anchors.
8. Fracture mechanics and large displacement nonlinear problems.

Many new applications using DEM are being carried out, e.g. simulation of comminution in ball mills, slurry flow, flow of powders and grains, and physical animation for computer graphics. Materials other than those discussed earlier, such as ice plates, masonry and jointed rocks are also ideal candidates for modelling using DEM.

6. General remarks

One can envisage many advantages and uses for the DEM. The power of DEM in simulating the real processes and in identifying the mechanisms is evident. Thus it is an useful tool in understanding the physics of the processes and problems. DEM clearly simulates deformation mechanisms in jointed and particulate media in a more realistic way than any of the continuum-based models. Because it can monitor internal stresses and contact behaviour unobtrusively, sample reproducibility can be guaranteed, and it is ideal for use in understanding fundamental particulate material behaviour. In addition, since external stresses and stress paths can be controlled precisely it can be used for developing and validating constitutive relationships of any particulate materials such as soil, rock, grain or ceramic powder by using appropriate particle properties, sizes, shapes and gradation. Moreover, DEM is the best tool for explaining the experimentally observed facts from a more fundamental approach.

The results of compaction of 1000 disc particles (Figure 6 *a*; after Sitharam[35]) to a dense system takes about 6 h to perform on an 80486 microcomputer. More than the discrete element calculation cycles, bookkeeping of the particles and their contacts are very time consuming. The computing power of today's state-of-the-art computer technology offers the possibility to consider even more realistic three-dimensional systems with spheres, ellipsoids and blocks to simulate particulate materials, which was prohibitively complex and expensive a few years ago. However, due to the explicit nature of the algorithm, it is necessary to use a very small time-step of simulation to guarantee numerical stability and accuracy. To obtain proper aggregate behaviour, enough particles must be used to ensure sufficient number of contacts along any shear surface or structural interface. Many researchers are attempting to expose the advent of the effective use of the supercomputer and parallel computing by modifying the discrete element simulation codes. Slowly consensus is emerging on the use of a parallel processing machine with good graphics to simulate particulate materials using DEM rather than vector processing machines[49]. It may be expected that these studies will allow a major step forward to the more realistic simulations of particulate solids and a better understanding of the constitutive behaviour of particulate materials.

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