A potential-based particle method for failure modeling in solids

Roberto Brighenti, Nicholas Corbari, Andrea Carpinteri
Department of Civil-Environmental Engng & Architecture, University of Parma, Parma (Italy)
brigh@unipr.it

ABSTRACT. Continuum mechanics is typically based on the fundamental notion of a mesoscopic volume element, whose physical characteristics can be considered as averaged properties over discrete particles, obeying deterministic relationships. Recent works on granular-like materials have found that a continuum description may not be appropriate for these cases, since inhomogeneities at the particle level, such as force chains and microscopic breaking, can occur. The above discussed aspects point out the particle nature of materials and suggest to use a different approach, namely a discrete one, to describe their mechanical behaviour; moreover such a new approach can be suitably used for both continuum-like or granular-like materials by properly setting the nature of the reciprocal forces exerted between particles. Such an approach is usually identified also as the discrete-element method (DEM). By properly modelling the material as an assemble of small discrete elements, the mechanical behaviour and the failure evolution of the material under mechanical actions can be properly described.
In the present paper, a computational discrete element method for continuum or particle-like materials, based on the concept of potential-based force interaction law for the quantification of the mutual forces exchanged by small portions of the material interacting each other, is developed. After illustrating the basic concepts related to the discrete nature of materials and their mechanical modelling, a simple particle based approach is presented by adopting a Lennard-Jones like potential function to quantify the particles interaction. Finally, an example related to the failure of a brittle solid is analysed in order to underline the capability of the proposed approach.

SOMMARIO. La meccanica del continuo è normalmente basata sullo studio dei materiali considerandone il loro comportamento mesoscopico, riferito cioè ad un elemento di volume le cui caratteristiche fisiche possono essere considerate come valori medi delle proprietà meccaniche delle particelle costituenti il materiale stesso. Studi recenti relativi ai materiali granulari hanno mostrato come una loro descrizione di tipo continuo non sia appropriata a causa della particolare natura delle forze che si esercitano tra gli elementi costituenti. Gli aspetti salienti della natura particellare dei materiali, granulari possono anche essere adottai per i materiali macroscopicamente continui, ovviamente con una opportuna descrizione delle forze che si esercitano tra le particelle per i diversi materiali considerati. Tale approccio viene normalmente indicato come metodo degli elementi discreti (DEM). Descrivendo in modo opportuno il materiale continuo come un insieme di piccole particelle solide, il suo comportamento meccanico e la descrizione dei processi di rottura dovuti ad azioni meccaniche possono essere ottenuti e quantificati in modo appropriato.
Nella presente nota viene sviluppato un modello computazionale basato su un approccio discreto per la simulazione di materiali continui o granulari; l'interazione tra le particelle viene considerata mediante forze mutue valutate a partire da una funzione potenziale, opportunamente tarata sulla base dei parametri meccanici macroscopici del materiale. Dopo una presentazione dei concetti essenziali relativi alla natura discreta dei materiali ed alla loro modellazione meccanica, viene sviluppato un semplice modello discreto basato sull'impiego di una funzione potenziale tipo Lennard-Jones per il calcolo delle forze interparticellari. In

conclusione viene presentato un caso di rottura per frattura di un solido costituito da materiale fragile e vengono evidenziate le peculiarità dell'approccio proposto.

KEYWORDS. Particle method; Material failure; Fracture; Potential forces.

INTRODUCTION

The mechanical simulation of solid materials must take into account that their behaviour can range from incoherent up to compact cases, typical of granular (or powder) and of polycrystalline materials, respectively [1].

In the light of the above consideration, a material cannot be simply associated univocally to one of the two extreme classes, but it can be characterized by an intermediate behaviour, since the nature of the forces between the discrete particle elements can be regarded to range from adhesion-like (such as in powders materials) up to strong covalent bond (for compact materials).

The description of the behaviour of materials has recently been tackled by considering different scales of observation: the very microscopic one, such as in the so-called ab initio approach (multi-body electronic structure theory, density functional theory, quantum chemistry, …) in which the force field arising between atoms are considered [2]; the atomistic dynamics and statistics approaches (referred to as molecular dynamics, MD, or kinetic Monte Carlo models, suitable to describe kinetically dominated mechanisms) in which the effective bonds between molecules are properly described through potentials [3, 4]; mesoscale approaches based on the mean field rate theoretical methods that typically mimic average dynamical properties [5]; finally, at the macroscopic scale, continuum-based thermodynamics or constitutive kinetic models, typically formulated by using variational methods. Multiscale analysis of solids has also been proposed in recent papers [6, 7].

In the context of the last cited scale, the classical continuum mechanics approach can be collocated, typically based on the fundamental notion of a mesoscopic volume "element", whose characteristics can be considered as averaged properties over discrete particles obeying deterministic relationships. On the other hand, the unavoidable particle nature of real materials suggests - in competition with classical continuum models - the possibility to use a different approach, namely a discrete one, to describe their mechanical behaviour at different scales.

By considering the particle-like nature of solids, such a new approach can be suitably used for either continuum-like [8, 9] or granular-like materials [10, 11], by properly setting the law governing the mechanical forces existing between particles. Such an approach is usually identified also as the discrete-element method (DEM) or particle finite element method. By properly modeling the material as an assemble of discrete small elements, its mechanical behaviour as well as its failure process under mechanical actions can be described at a local level; such description allows us to get the overall response of the material at the macroscale, which is the main interest of materials science and mechanics of materials [12].

In the present paper, taking into account the particle-like nature of materials, a computational discrete element method - based on the concept of potential-based force interaction between particles - is developed.

After illustrating the basic concepts related to the material discrete nature and its mechanical modeling, a simple particle based approach is developed by adopting a proper potential to describe the interaction forces.

Finally some examples related to the failure of brittle or quasi-brittle solids are examined in order to underline the capability of the proposed approach.

PARTICLE METHODS IN MECHANICS OF SOLIDS

The mechanics of compact materials can be applied by a proper description of the bonding forces existing between particles in which the solid can be ideally subdivided. Such an approach is straightforward for granular-like solids where the composing particles can be immediately identified as the grains present in the matter. Continuous solids can be idealized as a cluster of elements, properly 'connected' by forces that act when particles tend to approach each other (analogously as in cohesionless granular materials) or when they tend to move far away one to another.

In the following, the use of a force potential for the description of the actions between particles (in which the solid is assumed to be discretized) at the mesoscopic scale is illustrated.

Interparticle forces

By adopting a nanoscale insight of solids, their mechanical behaviour can be assumed to be governed by the equilibrium conditions of a system of N atoms (each one identified by the position vector $\mathbf{x}_i$), whose equilibrium configuration corresponds to the state leading to the minimum of the total energy of the system.

By denoting with $E_{tot}(\mathbf{x}) = E_{tot}(\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N)$ the function which defines the total energy of the system (at a greater scale, such atoms can be identified with macroscopic particles), the equilibrium configuration is identified by the following relationship [3]:

$$\frac{\partial E_{tot}(\mathbf{x})}{\partial \mathbf{x}} = \mathbf{0} \tag{1}$$

In the context of the so-called molecular dynamics (MD) simulation, an inter-atomic potential can be considered in order to quantitatively determine the forces acting between atoms. In computational simulations at the nanoscale, the atoms are most often represented by point-like elements, which in general interact through many-body interactions potential. In that way, the highly complex description of electron dynamics is abandoned and an effective picture is adopted. In order to find out the equilibrium configuration of particles, ad hoc interatomic potentials - which values depend on material parameters and by the mutual positions of the atoms in the current configuration - are required. These parameters and functions give a complete set of information about the energy of the system, as well as the forces acting on each particle.

Having assumed to consider a continuum material as an assemble of several discrete particles, the above interatomic relationship can be assumed to be applicable also at different scales. In this new context the atoms are represented by finite small volumes of material (particles), and the interacting forces, described through proper constitutive relationships, are represented by mechanical actions.

From the above assumption, it can be considered that each couple of particles interact by exerting equal and opposite forces between them (Fig. 1). Such reciprocal forces allow the material to assume either a compact structure if they are strong enough to avoid the particles to 'easily' separate each other, or a granular-like structure when they allow the particles to detach one another for low values of the acting forces.

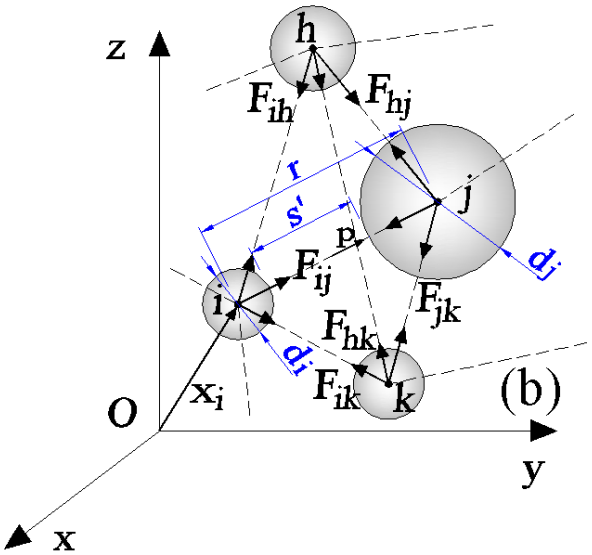

Figure 1: Scheme of the pair-wise interparticle forces.

By taking into account the macroscale level, it can be assumed - analogously to the atomic description of solids – that the material is characterized by the total potential energy functional $\Pi(\mathbf{x})$. Such an energy can be written as follows:

$$E_{tot}(\mathbf{x}) = \Pi(\mathbf{x}) = \Phi_{tot}(\mathbf{x}) - \mathbf{P}_i \cdot \mathbf{x}_i \tag{2}$$

where $\Phi_{tot}(\mathbf{x})$ and $\mathbf{P}_i$ are the strain energy of the system and the force applied to the particle *i*, respectively. The state of minimum energy can be obtained by setting to zero all the derivatives of $E_{tot}(\mathbf{x})$ with respect to the position vectors $\mathbf{x}_i$,

$$\frac{\partial E_{tot}}{\partial \mathbf{x}_i} = \frac{\partial \Phi_{tot}(\mathbf{x})}{\partial \mathbf{x}_i} - \mathbf{P}_i = 0 \tag{3}$$

By performing a power series expansion of the total energy starting from the equilibrium configuration (identified by the position vectors synthetically indicated as $\mathbf{x}_0$)

$$E_{tot}(\mathbf{x}) \cong \left\{ E_{tot}(\mathbf{x}_0) + \left.\frac{\partial E_{tot}}{\partial \mathbf{x}}\right|_{\mathbf{x}_0} (\mathbf{x}-\mathbf{x}_0) + \frac{1}{2}(\mathbf{x}-\mathbf{x}_0)^T \left.\frac{\partial^2 E_{tot}}{\partial \mathbf{x}^2}\right|_{\mathbf{x}_0} (\mathbf{x}-\mathbf{x}_0) + ... \right\} - \mathbf{P}_i \cdot \mathbf{x}_i \tag{4}$$

the stationary condition expressed by Eq. (3) can be rewritten in the following way:

$$\frac{\partial E_{tot}}{\partial \mathbf{x}} \cong \left.\frac{\partial E_{tot}}{\partial \mathbf{x}}\right|_{\mathbf{x}_0} + \left.\frac{\partial^2 E_{tot}}{\partial \mathbf{x}^2}\right|_{\mathbf{x}_0} (\mathbf{x}-\mathbf{x}_0) + ... - \mathbf{P} = \mathbf{0} \tag{5}$$

$$\text{i.e. } \left.\frac{\partial^2 E_{tot}}{\partial \mathbf{x}^2}\right|_{\mathbf{x}_0} (\mathbf{x}-\mathbf{x}_0) = \left.\frac{\partial^2 \Phi_{tot}}{\partial \mathbf{x}^2}\right|_{\mathbf{x}_0} (\mathbf{x}-\mathbf{x}_0) = \mathbf{P} - \left.\frac{\partial E_{tot}}{\partial \mathbf{x}}\right|_{\mathbf{x}_0} = \mathbf{K}(\mathbf{x}-\mathbf{x}_0) = \mathbf{P}$$

where the stiffness matrix can be identified through the second derivatives of the strain energy function :

$$\mathbf{K}_{ij} = \frac{\partial^2 E_{tot}}{\partial \mathbf{x}_i \partial \mathbf{x}_j} = \frac{\partial^2 \Phi_{tot}}{\partial \mathbf{x}_i \partial \mathbf{x}_j} = \begin{bmatrix} \dfrac{\partial^2 \Phi_{tot}}{\partial x_i \partial x_i} & \dfrac{1}{2}\dfrac{\partial^2 \Phi_{tot}}{\partial x_{i-1} \partial x_1} & \dfrac{1}{2}\dfrac{\partial^2 \Phi_{tot}}{\partial x_{i-2} \partial x_1} & .... \\ \dfrac{1}{2}\dfrac{\partial^2 \Phi_{tot}}{\partial x_{i-1} \partial x_1} & 0 & 0 & .... \\ \dfrac{1}{2}\dfrac{\partial^2 \Phi_{tot}}{\partial x_{i-2} \partial x_1} & 0 & 0 & .... \\ .... & .... & .... & .... \end{bmatrix} \tag{6}$$

Several potentials can be used to represent the mechanical interactions between particles. Among them, we can mention the Morse potential [13], the Lennard-Jones (LJ) potential [14], the classical strain energy based potential widely used in continuum mechanics.

The above cited pair-wise potential, known as the Lennard-Jones (LJ) potential, is usually employed to describe the forces between particles at the nanoscale, but it has also been used for the description of solids at the macroscopic scale [8, 9]. It can mathematically be written as follows:

$$\Phi_{LJ}(r_{ij} = \left|\mathbf{x}_i - \mathbf{x}_j\right|) = D \cdot \left[\left(\frac{R}{r}\right)^{2n} - 2\left(\frac{R}{r}\right)^{n} \right] \tag{7}$$

where R is the distance at which the potential reaches its minimum, D is the depth of the potential well, and r is the actual distance between two considered atoms (or particles); the typical assumption $n = 6$ leads to the so-called 12-6 Lennard-Jones potential.

It has been shown that it does not give us adequate description of all the properties of metals. For example, the above recalled LJ potential imposes the Cauchy relationship $C_{12} = C_{44}$ (C_{12}, C_{44} are the elastic constants corresponding to the force relationship established by the potential) that has been demonstrated to be wrong for most of the metals. Moreover, pair-wise potentials fail to estimate the structure relaxation and reconstruction around point defects (vacancies and self-interstitials) in metals. The vacancy formation energy obtained by means of pair-wise potentials is overestimated, and has been found to be equal to about the bulk cohesive energy. The best potential for simulations of metals is a many-body potential.

A suitable interatomic potential for metals is a many-body one which includes a pair-wise interaction only as a part of the full potential. This first part (V_1) of the many-body potential accounts for the core-core interactions (or ion-ion interactions), whereas the second part (V_2) incorporates the complex nature of the metallic cohesion by an additional term as follows:

$$V = V_1 + V_2 = \frac{1}{2}\sum_{i,i\neq j}^{N} \Phi_{LJ}(r_{ij}) + \sum_{i=1}^{N} U(n_i) \tag{8}$$

The above concept related to the development of forces at the atomic scale in solids based on interatomic potentials can conveniently be used to also tackle the problem of the mechanical description of solids at the macroscale [8] at which the matter can be assumed to be formed by particle elements. Moreover, such an approach – once the potential has properly been set – can be used to describe the behaviour of a generic solid, i.e. compact or granular up to the case of fluids in which the particles are characterized by a particular kind of interacting forces.

In the case of granular materials, for which the simple scheme of multi-interacting bodies can be adopted, a suitable force-particle distance description could be as that shown in Fig. 2a where the corresponding potential is also displayed. By indicating with $d_i/2$ and $d_j/2$ the radii of the particles i and j (assumed for the sake of simplicity to have a spherical shape), respectively, the distance between the surfaces of the particles can be expressed as follows: $s' = r - (d_i/2 + d_j/2)$, where r is the distance between the centres of the particles.

As can be noted from Fig. 2a, a quadratic potential implies a linear force-distance relationship when the particles are in contact ($s' < 0$), whereas the force becomes equal to zero when the contact disappears ($s' \geq 0$). The stiffness K of such a contact force corresponds to the slope of the F against s' relationship when $s' < 0$ (Fig. 1).

A regularised counterpart (smooth) potential and the corresponding force for such a class of materials can be introduced in order to obtain suitable relationships for computational purposes (Fig. 2b).

In order to have a realistic description of the forces, an infinite repulsive force value can reasonably be assumed to appear when the two elements compenetrate by a given amount $\delta = \alpha \cdot (d_i + d_j)/4$ (where α is a proper coefficient, and $\bar{r} = (d_i + d_j)/4$ is the average particles radius). The effective surface distance can be expressed as follows: $s = r - r_0 = r - (2 - 2\alpha)(d_i + d_j)/4$, where $r_0 = -2\delta + (d_i + d_j)/2 = (2 - 2\alpha)(d_i + d_j)/4$ is the distance between the centres of the particles at which $F(r_{ij} = r_0) \to -\infty$. Such a regularised (smooth) potential can mathematically be described through the following relationship:

$$\Phi(s = r_{ij} - r_0 = \left|\mathbf{x}_i - \mathbf{x}_j\right| - r_0) = \frac{c}{n-1} \cdot \frac{1}{s^{n-1}} \tag{9}$$

where c, n are constants ($n > 2$), and the corresponding pair forces relationship can be expressed as follows:

$$\mathbf{F}(s = r_{ij} - r_0 = \left|\mathbf{x}_i - \mathbf{x}_j\right| - r_0) = \frac{\partial \Phi(s)}{\partial s} = -\frac{c}{s^n}\mathbf{p} \tag{10}$$

where $\mathbf{p}$ is the unit vector identified by the two particles centers (Fig. 1).

The coefficient c in Eq. (10) can be determined, for example, by setting the value of the stiffness when the two spheres are in contact, i.e. when $s' = 0$ or $s = 2\delta$, i.e. $K(s = 2\delta) = \partial \mathbf{F} / \partial s\big|_{s=2\delta} = K_0$.

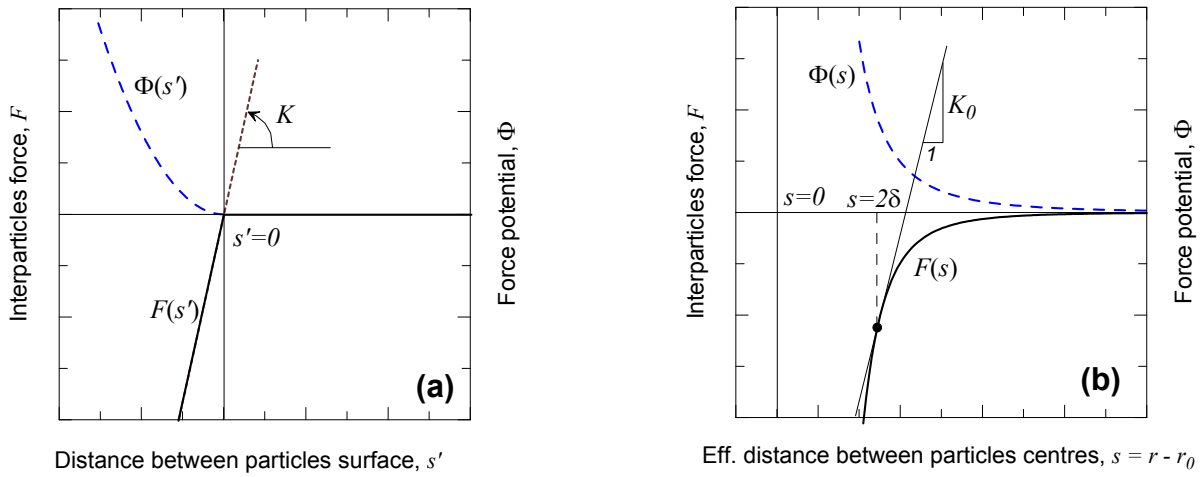

Figure 2: (a) Interparticles potential and corresponding forces for an ideal granular material without cohesion; (b) corresponding regularised counterpart .

If a compact solid material is examined instead, a suitable choice for the potential consists in adopting the Lennard-Jones one [8]. By assuming, as in the previous case, that an infinite repulsive force takes place when the two elements co-penetrate by the amount δ, the Lennard-Jones-like potential can be rewritten (Fig. 3a):

$$\Phi_{LJ}(s = r_{ij} - r_0 = \left|\mathbf{x}_i - \mathbf{x}_j\right| - r_0) = D \cdot \left[\left(\frac{R}{s}\right)^{2n} - 2\left(\frac{R}{s}\right)^{n} \right] \tag{11}$$

where D is a constant, and $s = R$ corresponds to the value of s for which the potential attains its minimum or, equivalently, the interaction force becomes equal to zero, $F(s = R) = 0$. As can be observed in Fig. 3b, the $F(s)$ relationship corresponds to the force-displacement behaviour of a softening material, since - once the force attains its maximum for $s = s_d$ - $F(s)$ decreases tending to zero by increasing the distance s. The corresponding stiffness $K(s)$ is also depicted in Fig. 3b: it presents high values when $s \to 0$; afterwards it decreases by increasing s up to the value $s = s_d$, at which it becomes equal to zero; subsequently it attains negative values giving rise to the above mentioned softening behaviour. For computational purposes, the $K(s)$ relationship can be assumed as is plotted in Fig. 3b (thick dotted line), i.e. by adopting only values greater or equal to zero (for $s > s_d$ $K(s)$ is assumed to be zero).

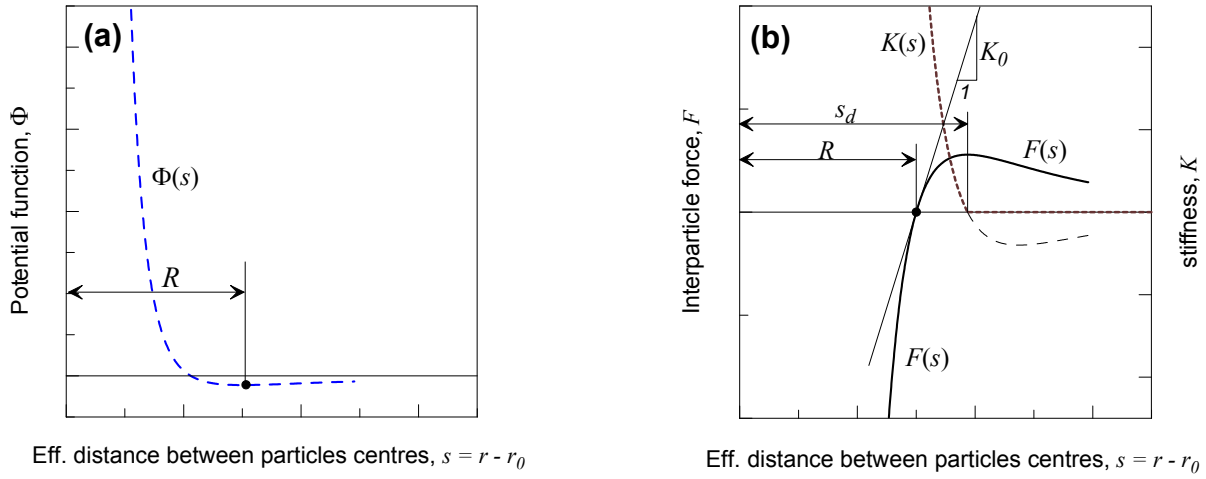

Figure 3: (a) A graphical schematic representation of the Lennard-Jones potential for $n = 2$; (b) the related forces and stiffness.

The last assumption corresponds to non-interacting particles if they are located at a distance, measured between their centres, greater than $r_0 + s_d$.

By setting the stiffness $K(s)$ to be equal to K_0 when $F(s) = 0$, i.e. when $s = R$, the constant D in Eq. (11) can be computed:

$$D = \frac{K_0 R^2}{2n^2} \tag{12}$$

Moreover, the distance at which the force $F(s)$ reaches its maximum can also be determined by setting $K(s) = dF(s)/ds = 0$. This condition leads to the following value of the effective distance s_d between the particle centres:

$$s = s_d = \frac{R \cdot (2n+1)^{1/n}}{(n+1)^{1/n}} \tag{13}$$

The force $F(s)$ can be assumed to exist between each couple of particles belonging to the body under study. Their reciprocal interaction obviously becomes smaller and smaller as their distance s increases as is shown in Fig. 3b. It can reasonably be assumed that such an interaction completely vanishes for a sufficiently large distance. In other words, it can be assumed the existence of a cut-off distance s_c for which the force becomes equal to zero. From the above discussion, such a non-interacting distance corresponds to $s_c = s_d$.

Setting of the potential function

The Lennard-Jones potential function, which is used herein to describe the reciprocal forces between particles, requires the knowledge of the stiffness K_0, corresponding to the value attained by $dF(s)/ds$ when $F(s)$ is equal to zero. Such a value can be determined by considering the nature of the material under study.

In case of granular-like materials, such a stiffness can be associated with the contact stiffness between two particles in reciprocal contact.

For a continuum material, once the arrangement of the particle and the non-interacting distance s_d of the discrete model have been assumed, it is possible to determine the stiffness K_0 by equating the elastic energy stored in a representative volume of the real material and that in the corresponding discretized one by using particles elements, considering a uniaxial strain field. The term K_0 obviously depends on the adopted non-interacting distance s_d, i.e. on the number of particles (in a given volume of material) that exchange reciprocal forces each other.

NUMERICAL IMPLEMENTATION

The above described model has been implemented in a nonlinear computational algorithm, in which the equilibrium configuration is determined by considering the forces existing on the particles due to their reciprocal interaction (by taking into account their evolving reciprocal position as usually done in the total Lagrangian formulation framework related to the mechanics field) and the actions due to the presence of constraints such as rigid boundaries, prescribed forces or displacements acting in some given portion of the boundary of the body, etc. The inertial and the damping forces are also included in the equilibrium system in the case of dynamic problems that arise when collisions take place between particles or with other bodies [15, 16].

The Lennard-Jones potential has been used (with $n=2$) for the assessment of the interparticle forces, whereas the non-interacting distance between two particles *i* and *j* has been assumed equal to $s_c = s_d = 5\cdot(d_i + d_j)/4$, i.e. five times their average radius. The above choice has been verified to be appropriate by performing several numerical analyses, even if greater s_d values lead to similar mechanical behaviour of the solid being examined.

APPLICATION TO A FRACTURE MECHANICS PROBLEM FOR BRITTLE MATERIALS

In the present section, a simple mixed mode fracture mechanics problem simulated through the above discussed particle method is analysed. A rectangular cracked thin plate under upward displacements, prescribed to its upper edge and fixed at the bottom (Fig. 4a), is examined up to the final failure (complete cracking and fragmentation of the material).

The plate is modelled as a 2D structural component with an elastic modulus equal to $2\cdot10^4\,MPa$, whereas its tensile strength is taken equal to $5\ MPa$.

As can be observed in fig. 4b, the obtained crack pattern adequately represents the expected fracture behaviour of the brittle plate. The initial crack propagates under nearly pure Mode I, and some small parts of the plate can be observed to be ejected out of the plate.

CONCLUSIONS

In the present paper, a discrete approach for the mechanical description of the behaviour of solids has been developed. Starting from a typical discrete approach, commonly used at the nanoscale observation of matter such as the computational molecular dynamic method, the basic principles typically used at such a scale is also extended to the meso and macroscale.

The particle nature of macroscopically continuum materials enables us to describe their macroscopic behaviour through the description of the laws governing the mechanical interactions between particles.

Such a new point of view, usually identified as the discrete-element method (DEM), can suitably be used for both continuum-like or granular-like materials by properly setting the nature of the forces exchanged between particles.

A computational discrete element method for continuum or particle-like materials, based on potential-based force interaction between small portions of the material, has been developed.
After illustrating the basic concepts related to the discrete nature of materials and its mechanical modeling, a simple computational particle based approach is developed by adopting a Lennard-Jones like potential to quantify the interaction forces.
Finally, an example related to the fracture failure of a brittle plate is examined in order to underline the capability of the proposed approach. The fracture behaviour and the fragmentation of the material during the fracture process is correctly described by the computational approach here proposed.

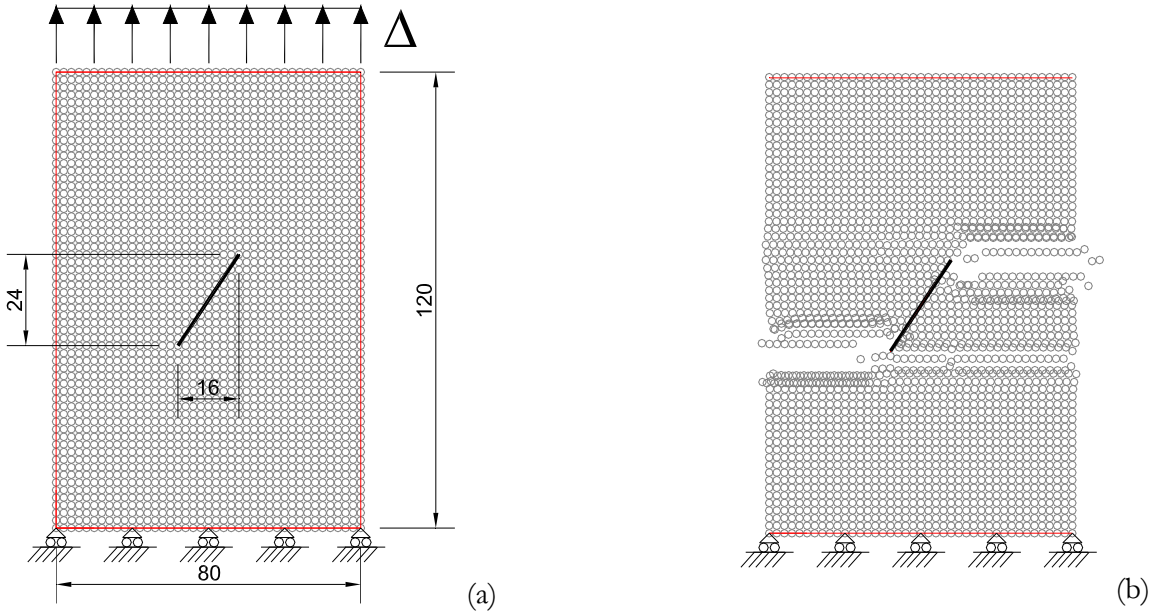

Figure 4: (a) Rectangular cracked plate under remote tension discretized by 2501 particles (dimensions in mm); (b) particle arrangements corresponding to the final failure of the plate for $\Delta = 10^{-4}\, m$.

REFERENCES

[1] W. A. Curtin, R. E. Miller, Modelling Simul. Mater. Sci. Eng., 11 (2003) R33–R68.
[2] K. Ohno, K. Esfarjani, Y. Kawazoe, Computational Materials Science: From Ab Initio to Monte Carlo Methods. Springer Series in Solid-State Sciences, (2000).
[3] B. Liu, H. Jiang, Y. Huang, S. Qu, M.-F. Yu, Physical Rev. B, 72 (2005) 035435-1–035435-8.
[4] B. Liu, Y. Huang, H. Jiang, S. Qu, K.C. Hwang, Comput. Methods Appl. Mech. Engng., 193 (2004) 1849.
[5] V. Yamakov, E. Saether, E.H. Glaessgen, A New Concurrent Multiscale Methodology for Coupling Molecular Dynamics and Finite Element Analyses. NASA/TM-2008-215328 (2008).
[6] H.S. Park, W.K. Liu, Comp. Meth. App. Mech. Engng, 193 (2004) 1733.
[7] X. Zeng,· X. Wang,· J.D. Lee,· Y. Lei, Comput Mech, (2010) 205.
[8] A. Krivtsov, Meccanica, 38 (2003) 61.
[9] G. Wang, M. Ostoja-Starzewski, Comput. Mat. Sci., 33 (2005) 429.
[10] M. Obermayr, K. Dressler, C. Vrettos, P. Eberhard, J. Terramechanics, 48 (2011) 347.
[11] E. Onate, S.R. Idelson, F. Del Pin, R. Aubry, Int. J. Comput. Meth., 1 (2004) 267.
[12] V. R. Coffman, J. P. Sethna, G. Heber, M. Liu, A. Ingraffea, N.P. Bailey, E.I. Barker, Modelling Simul. Mater. Sci. Eng., 16 (2008) 1.
[13] R. N. Costa Filho, G. Alencar, B.S. Skagerstam, J. S. Andrade, Europhysics Letters, 101 (2013) 1009.
[14] W.K. Liu, S. Jun, D. Qian, In: Handbook of Theoretical and Computational Nanotechnology, M. Rieth and W. Schommers Eds, American Scientific Publishers, Stevenson Ranch, CA (2005).
[15] A Tasora, M Anitescu, Comp. Meth. App. Mech. Engng, 200 (2011) 439.
[16] A. Tasora, M. Anitescu, J. Comput. Nonl. Dyn., 5 (2010) 1.