Research Article

MCA Model for Simulating the Failure of Microinhomogeneous Materials

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A special cellular automaton (CA) model called mechanical cellular automaton (MCA) is built, in which inhomogeneity of material cell can be evaluated by Weibull's distribution function. In MCA, such material physical parameters as energy or strength and anisotropy defined by the different transferring energies along different directions are adopted. To simulate a crack or a weak zone, a cluster of weak energy cells are disposed. By the MCA, examples of failure evolving process of material containing one crack, two parallel cracks, and two cracks by bridge conjunction are simulated. The results show for inhomogeneous materials that their failure behaviors are much different from homogeneous ones, self-organization must be considered, and traditional homogeneous mechanics cannot be applied by copying word to word.

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1. INTRODUCTION

As an efficient method for self-organization, cellular automaton is proposed by von Neumann and Burks [1], and is gradually developed into a dynamical evolving method in statistical mechanics [2]. It is considered as a powerful tool to analyze evolutionary theory of life game [3]. Considering the complexity of a system, Wolfram has made great contribution to computation of CA model [4, 5].

Based on the rationale of CA, the effects of spatial heterogeneities of environment and/or asymmetries in the interactions among the individuals are analyzed [6] and applied in material science. For example, particle-size distributions (PSDs) of soil samples are analyzed by fractal methods and different scaling domains, characterizing different ranges of particle sizes, are identified based on CA. Modelling and controlling of microstructure as well as grain size during thermal processing operations are essential for tailoring the properties of polycrystalline materials; to investigate them, a cellular automaton model, with advanced features for continuous tracking of grain boundary and precise estimation of curvature, is developed [7], in which namely parabolic growth behavior and the time invariant nature of grain size distributions are accurately described by Weibull's distribution function. It is shown that the predicted

topological features during the grain growth closely resemble experimental observations in succinonitrile polycrystals.

Also, because of the parallel evolving function of CA, it is a useful technique for improving the classical numerical method. For example, reversible computing is a paradigm, in which it can reflect physical reversibility [8]. A new cellular automaton (CA) model which reproduces isotropic time-evolution patterns observed in the Belousov-Zhabotinsky reaction is proposed by Nishiyama et al. [9]. Lattice Boltzmann method, finite element method, and cellular automata are coupled by Kwon and Hosoglu [10], and are tested by wave propagation problems in 1D and 2D [11]. A three-dimensional cellular automaton (CA) model is coupled with finite-element (FE) heat flow calculation in order to predict the solidification grain structures in a Ni-base superalloy [12], in which Gaussian distribution of nucleation sites is adopted and the Kurz-Giovanola-Trivedi model is extended to multicomponent alloys to account for the growth kinetics of dendrite tip. Much more, a cellular automata finite element (CAFE) model is developed to simulate the strain localization phenomena that occur during various plasto-metric tests, as well as real industrial processes [13].

Compared with other materials, rock mass is one kind of most complicated materials in the world, because of discontinuity, rheology, anisotropy, inhomogeneity, and so

on. Generally, rock mass has obvious scale-feature behavior, and it can be divided into macro- and microscales simply.

In macroscale, a commonly used model for fault-tolerant computation based on cellular automata is built by McCann and Pippenger [14], in which the degree (the number of neighboring cells on which the state transition function depends) needed to achieve fault tolerance is concerned when the fault rate is high (nearly 1/2), both some traditional transient fault models (where faults occur independently in time and space) and a recently introduced combined fault model including manufacturing faults (which occur independently in space, but which affect cells for all time) are considered. Earthquake can be defined as a spatially extended dissipative dynamic system that naturally evolves into a critical state with no characteristic time or length scale. A two-dimensional CA model capable of reproducing some prominent features of earthquake data is presented [15]. Else, a proposed model with continuous state and discrete time, comprising cell-charges and aiming at simulating earthquake activity with the usage of potentials, is proposed by Georgoudas et al. [16]. It is tested as well as calibrated using the recorded events of the area in Northeastern Greece, centred at Xanthi, Thrace as initial conditions. The simulation results are found in good quantitative and qualitative agreement with the Gutenberg Richter (GR) scaling relations.

In microscale, a new theory of physical cellular automaton (PCA) for simulating the failure evolving process of microheterogeneous materials is first set up by Tan et al. [17] according to the basic law of transferring energy. PCA breaks through the localization of traditional cellular automaton, and it is shown that the simulating results by PCA can agree with the laboratory results perfectly. By using PCA model, the anisotropic and discontinuous rock mass failure process and corresponding acoustic emission (AE) are effectively simulated [18, 19]. Much more, a PCA model considering elastoplastic property of rock has been developed by Feng et al. [20] to simulate the 2D heterogeneous rock specimens under uniaxial cyclic load compression test, and the influences of inhomogeneity, softening coefficients, specimen sizes, and spatial distributions of material parameters.

In this paper, the failure evolving processes of inhomogeneous rock containing single crack, discontinuous cracks bridge, and double parallel cracks are simulated by building a special CA model called mechanical cellular automaton (MCA).

2. MODEL DESCRIPTIONS

2.1. Basic model of CA

In a cellular automaton (CA), there are identical elements, usually located in a regular array that can be one-dimensional, two-dimensional, or even higher dimensional. The update rules are as follows: the elements or cells of a CA are spread over the nodes of a rectangular grid, each of them capable to be in one of a finite set of possible states. The neighborhood of each cell can be defined as the set of the four nearest neighbors (North, South, East and West), the set of the eight nearest neighbors (N, NE, E, SE, S, SW, W, NW), or other bigger neighborhoods.

FIGURE 1: The relation between CA components.

Conventional CA models employ spatial lattices; each lattice element takes one of a set of discrete values. The lattice evolves over discrete time steps, with element values changing according to rules relating to the surrounding elements. CA models are typically used to investigate “complex systems” [5], which exhibit extreme sensitivity to initial conditions, boundary conditions, history and element properties, and may have many different outcomes due to the existence of multiple local equilibria. Thus, a cellular automaton is a discrete dynamical system, and is composed of cells, cell lattices, neighbor rules, and so on. The state of a cell is determined only by the states of itself and its neighbors at previous step. CA has some advantages of time evolution, space discretization, locality and parallelization, and so on. In order to build a cellular automaton, the relationships between model components are needed to be clear (Figure 1).

2.2. MCA model for microheterogeneous materials

Many kinds of material (e.g., rock, concrete, etc.) are typical microheterogeneous ones; damages may occur firstly in weak zones under certain load conditions. From their initial damage to regional fracture, it is a typical self-organization process. As a dynamical evolving technique, CA provides a base for simulating the fracture process of microheterogeneous materials in methodology, because CA is a kind of mathematical model to simulate the self-evolving process of a system caused by element interacts one to another nonlinearly in it under a random initial condition [1], but traditional CA cannot simulate microscale failure evolving process effectively in physical meaning because of the complexity of microheterogeneous properties of rock-like materials. After the equivalent physical and mechanical properties for all cells are given in a form of energy, the rock failure process as well as nonlinear dynamic behavior scan can be simulated by transformation of energy from one cell to the others, based on the basic evolving rules, and thus it is called mechanical cellular automaton (MCA).

In MCA, a cell is defined by mapping a real minor homogenous region inner material. As shown in Figure 2, a material specimen like rock can be divided into $N \times N$ elements or grids in terms of homogeneity of material, and every element is considered as one cell. According to the rationale of self-similarity of microstructure of rock,

FIGURE 2: Cell grids.

FIGURE 3: Damage evolving process of a cell.

enough cells can approach the real microstructure of rock equivalently.

For a cell located at (x_i, y_i) , if its deposited energy is regarded as strain energy, and is denoted as $Ge(x_i, y_i, t_i)$ at time t_i , then it can be calculated by

$$Ge(x_i, y_i, t_i) = \frac{1}{2} \sigma_i \varepsilon_i = \frac{1}{2} \frac{\sigma_i^2}{E_i}, \quad (1)$$

where σ_i is the maximum stress in the i th cell at time step t_i , and E_i is Young's modulus of the i th cell.

Given the threshold of the i th cell damage energy $Ge_{th}(x_i, y_i)$, the corresponding failure strength $[\sigma_i]$ of the i th cell is equivalent to

$$[\sigma_i] = (2E_i \cdot Ge_{th}(x_i, y_i))^{1/2}. \quad (2)$$

If the i th cell at time step t_i satisfies

$$Ge(x_i, y_i, t_i) \geq Ge_{th}(x_i, y_i) \quad \text{or} \quad \sigma_i \geq [\sigma_i], \quad (3)$$

the cell is damaged and the energy stored in it releases and transfers to other neighbor cells. The total damaged cell number at step t_i is counted by $Nd(t_i)$.

To simulate rock damage gradually, a cell is divided 4 or more subcells obeying the rule of multiplier $4k$, in order to

FIGURE 4: $\varphi(u)$ of different m .

FIGURE 5: Moore's neighbor cells.

satisfy the cell dividing symmetry for four quadrants in a plane, where $k = 0, 1, 2, \dots$. Obviously, the larger the value k , the more the subcell numbers. So a cell damage grade is considered as a gather of subcell fracturing, as shown in Figure 3. In terms of the rationale of damage mechanics, the damage variable for a cell can be described as

$$D(x_i, y_i, t) = 1 - \frac{n(t)s^*}{s_i}, \quad (4)$$

where s_i is the i th cell area, s^* is one subcell area, and $n(t)$ is the count of damaged subcell at time step t . If $D(x_i, y_i, t) = 0$, it indicates that the cell i is in the undamage state; if $D(x_i, y_i, t) = 1$, it indicates that the cell i is in complete damage state; if $0 < D(x_i, y_i, t) < 1$, it indicates that the cell i is in partial damage state. By counting the energy releases of all damaged cells and subcells at time t , we can obtain the equivalent energy releases diagram versus time step.

The damage process of microheterogeneous material can be simulated by the following procedures.

Step 1. According a probability distribution to initialize the primary energy $Ge(x_i, y_i, t_i)$, the damage threshold energy $Ge_{th}(x_i, y_i)$, the potential probability $P(i)$ of transferring energy from cell i to neighbor cells after cell i being damaged, which indicates the heterogeneous property of material. Also the weak zones are dominated by decreasing the $Ge(x_i, y_i, t_i)$ value. After a cell fractures, the dissipative energy is in the form of acoustic emission, heat dissipation as well as light,

FIGURE 6: A crack set up by MCA.

which can be expressed by energy dissipative efficient $NH(t)$ in order to simulate a dissipative system.

Step 2. Input energy from boundaries. In each evolving step, a cell is chosen randomly and is endowed with certain energy. This can simulate the cell energy obtained in the period of no any cell failure.

Step 3. Check the energy of each cell in the cell space, if the energy of a cell satisfies (3), then this cell is taken as in the failure state; its energy is counted as zero and transfers to the neighborhood cells. If all cells are checked no failure, that is, every cell energy is less its damage threshold, then a complete evolving step runs out.

Step 4. Repeat the process from Steps 1 to 3, until simulation task arrives at the goal.

2.3. Inhomogeneity

For a very heterogeneous material like rock, it is not suitable to describe the mechanical behavior and fracture process by using an oversimplified model. Generally, a statistical approach is useful to characterize the heterogeneity of rock. Previous work [18] indicates that Weibull's function can describe very well the distribution of material parameters of rocks, and the homogeneous efficient m can be adopted in Weibull's distribution function

$$\varphi(u) = \frac{m}{u_0} \left(\frac{u}{u_0} \right)^{m-1} e^{-(u/u_0)^m}, \quad (5)$$

where u is the strength or the damage energy threshold of material, $\varphi(u)$ is the density of distribution, u_0 is the average strength or damage energy threshold of material for all cells. The efficient m indicates homogeneous extent of material, that is, the larger for value m , the more homogeneous for materials, as shown in Figure 4.

2.4. Anisotropy

Such material as rock behaves not only inhomogeneity but also anisotropy in microscale, each microelement in the interior of such material like rock behaves different potential of transferring energy along different direction.

FIGURE 7: AE simulations of coal by CA [21].

(a) Step 0

(b) Step 1

(c) Step 5

(d) Step 10

FIGURE 8: Failure process of a specimen containing one crack.

Weak element is inferior for transferring energy, but strong element is superior for transferring energy. The potential of transferring energy is a function of Young's modulus, which can be denoted by the concept of connecting weight for transferring energy. Assume that the connection weight of energy cell i transferring to the neighborhood cell j at time t is $w(i, j)$, for Moore's neighborhood cells (Figure 5), it satisfies

$$\sum_{j=1}^8 w(i, j) = 1. \quad (6)$$

If $w(i, j) \neq w(i, k)$ ($j = 1, 2, \dots, 8$; $k = 1, 2, \dots, 8$; $j \neq k$), it is called typical anisotropy. After cell i releases its total energy

FIGURE 9: CSNBD specimens after failure (see [22] by Al-Shayea).

FIGURE 10: Failure process of specimen containing two parallel cracks.

ΔGe at time step t , the total energy of cell j at time step $t + 1$ is expressed as

$$Ge(x_j, y_j, t + 1) = Ge(x_j, y_j, t) + w(i, j) \cdot \Delta Ge. \quad (7)$$

Obviously, $w(i, j)$ is another type of expression for anisotropy.

2.5. Crack

There exist many cracks in such materials as rock and concrete, which cause their strengths to decrease obviously. Also, a failure inner material originates from the crack zone firstly. In MCA model, a crack is set up by a weakening zone in cell space accordance with the crack length and direction,

as shown in Figure 6. The cells in a crack obey the following evolving rules.

- The cells in crack zones are assigned in low damage energy threshold $Ge_{Th}(x_i, y_i)$. Generally, the damage energy threshold is considered as only 1/100 of average damage energy threshold of the whole cells.
- All cells in crack zone have high absorbing energy potential and less releasing energy potential. This can be done by given absorbing energy weight in a large value of 0.8–1.0 and releasing energy weight in a small value 0.01–0.1, which means the crack cell can absorb most energy but release less energy like a “black body”.

3. SIMULATIONS FOR SPECIMENS CONTAINING CRACKS

As a valid approach, CA is used to simulate the force-epoch and AE-epoch of coal specimen (Figure 7) successfully by Tan et al. [21]. This supplies primary evidence that MCA may be used to simulate the crack extending in rock.

In this article, a specimen of microheterogeneous material like rock of 10 cm wide and 10 cm high divided by 50×50 cells is taken. Weibull's distribution is utilized for approaching inhomogeneity. Let the average Young modulus $E = 1e06$ MPa and homogeneous efficient $m = 8$, the average failure strength $[\sigma] = 200$ MPa and homogeneous efficient $m = 4$. Three cases are considered: only one crack of length 2 cm, two parallel cracks in 2 cm space and 2 cm long, two cracks in 2 cm long by bridge conjunction.

For only one crack case as shown in Figure 8, the initial damage occurs mainly in the region near crack end although some damage occur closing the midregion of crack also. As simulating step increases, the damage extends along the two ends in the direction of near inclination 30° , which is in accordance with the results of limestone rock compressive split test by Al-Shayea [22], as shown in Figure 9.

For two parallel cracks, because of the interaction of cracks, although some damages occur near the crack ends, the large-scale damages occur in the regions vertical to the cracks (i.e., in two sides of the two parallel cracks) as shown in Figure 10. The results indicate multinatural fissures or cracks take a lead rule in the failure process of rock. This result is similar to the wing crack pattern II/III of crack coalescence which is a sandstone-like material containing two parallel inclined frictional cracks under uniaxial compression experimented by Wong and Chau [23] (Figure 11), but much more disorder damage zones near cracks occur because of microheterogeneous property of rock. If this idea has been generalized to the macroscale, for an example in underground engineering, a group of caves take controllable action for surrounding rock mass failure zones, which is valuable for the reinforcement of underground engineering.

For the case of two cracks by bridge conjunction, as shown in Figure 12, by analogy to a single crack case, the damages occur in the regions of crack ends. But as the failure

FIGURE 11: Nine different patterns of rock crack coalescence (see [23] by Wong and Chau).

evolves, the bridge zone is destroyed by high energy concentration at last. The damage extends asymmetrically along two ends of cracks, and failure zone forms irregularly because of inhomogeneity also. This case is similar to shear crack pattern of crack coalescence to a sandstone-like material containing two cracks by bridge conjunction under uniaxial compression generally (Figure 11), which is experimented by Wong and Chau [23]. But some damage zones also occur far away from cracks, this also because of microheterogeneous property of rock. Thus, for inhomogeneous materials, their failure behaviors are much different from the homogeneous ones, so homogeneous mechanics cannot be adopted by copying word to word.

FIGURE 12: Failure process of specimen containing two cracks by bridge conjunction.

4. CONCLUSIONS

Some kinds of materials (e.g., rock, concrete, etc.) have many complicated properties such as inhomogeneity, anisotropy, discontinuity both in microscale and macroscale. Their damage process is a typical self-organization evolving one. A special CA model called MCA has been built, in which inhomogeneity of material cells is evaluated by Weibull's distribution function, the failure index can be represented by energy or strength, anisotropy is defined as the difference of transferring energy along different direction, and the crack is constructed by a cluster of weak energy cells.

By MCA, three cases of crack: only one crack, two parallel cracks, and two cracks by bridge conjunction, are simulated. The results show, for only one crack, that the damage extends along the directions of crack end near inclination 30° which is in accordance with the result fracture mechanics. For two parallel cracks, because of the interaction of cracks, although some damages occur near the crack ends, the large-scale damages occur in the regions vertical to the cracks.

For the case of two cracks by bridge conjunction, although the damage evolution is analogous to one single crack case, but the bridge is destroyed by high energy concentration at last, the damage extends asymmetrically along two ends of cracks, so an irregular failure zone forms, just because of inhomogeneity. Thus, for inhomogeneous materials, their failure behaviors are much different from homogeneous ones, so traditional homogeneous mechanics is limited for application.

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