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Discrete-element modelling: methods and applications in the environmental sciences

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This paper introduces a Theme Issue on discrete-element modelling, based on research presented at an interdisciplinary workshop on this topic organized by the National Institute of Environmental e-Science. The purpose of the workshop, and this collection of papers, is to highlight the opportunities for environmental scientists provided by (primarily) off-lattice methods in the discrete-element family, and to draw on the experiences of research communities in which the use of these methods is more advanced. Applications of these methods may be conceived in a wide range of situations where dynamic processes involve a series of fundamental entities (particles or elements) whose interaction results in emergent macroscale structures. Indeed, the capacity of these methods to reveal emergent properties at the meso- and macroscale, that reflect microscale interactions, is a significant part of their attraction. They assist with the definition of constitutive material properties at scales beyond those at which measurement and theory have been developed, and help us to understand self-organizing behaviours. The paper discusses technical issues including the contact models required to represent collision behaviour, computational aspects of particle tracking and collision detection, and scales at which experimental data are required and choices about modelling style must be made. It then illustrates the applicability of DEM and other forms of individual-based modelling in environmental and related fields as diverse as mineralogy, geomaterials, mass movement and fluvial sediment transport processes, as well as developments in ecology, zoology and the human sciences where the relationship between individual behaviour and group dynamics can be explored using a partially similar methodological framework.

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1. Introduction

In recent years, forms of individual-based method have developed in a wide range of research areas. Some examples of this breadth are provided later in this paper, and in

One contribution of 12 to a Theme 'Discrete-element modelling: methods and applications in the environmental sciences'.

the series of papers that follow it in this thematic issue. A reason for these approaches generally appears to be that they allow a fairly rigorous analysis of the behaviour of small-scale 'entities' that appear, in some sense, to be 'fundamental'. Interaction of large numbers of these entities then allows larger-scale aggregate-system behaviour to be studied, and facilitates understanding of phenomenological system properties and large-scale relationships, which tend to be emergent from the interacting behaviour of large numbers of the basic entities. It is not uniformly feasible in all areas of science that real, basic underlying entities can be defined, but a reductionist path which seeks to achieve this, and then promises descriptive and explanatory power at the macroscale, is a challenging route to explore. In some cases, and for some purposes, this can even be true in the biological and social sciences.

The following papers form a contribution to this inter-disciplinary field. Their focus is on discrete-element methods (DEMs) (or models), which are examples of individual-based approaches which have developed almost quasi-independently in several different research communities. These communities are concerned with basic entities, or 'particles', which when interacting *en masse* generate interesting constitutive properties, behaviours and mass phenomena. They include geotechnical engineering, hydraulic engineering, mining engineering, chemical engineering and powder technology. They are concerned with rock and soil mechanics (landslides, rock and snow avalanches, soil load-bearing properties); with the transport of sediment by fluids, for example, in rivers and along coasts; with blasting behaviour in quarries and the hopper flow of ores; and with particulate mixing behaviour in manufacturing processes. Some are able to treat the 'fundamental' particles as rigid balls without significant loss of realism, while others must deal with entities that deform under stress. At a different scale, the molecular-dynamics community is also using DEMs, with the fundamental entity in this case being the atom. Some of these fields are more advanced than others in their applications of the DEM, while others may see new opportunities on being exposed to research in the fields where greater technical development has already occurred. Thus, it seems timely to draw together these experiences, and this is the purpose of the current collection. Particularly for the environmental sciences, where the potential of DEM and its allied methods is high, but where applications appear currently to be lagging behind, it is hoped that this will be beneficial.

The collection of papers in this theme issue is therefore an outcome of a workshop arranged through the National Institute for Environmental e-Science (NIEeS), funded by the Natural Environment Research Council and based in Cambridge, UK. This deliberately brought together members from the wide range of research communities noted above, to discuss and examine theoretical and computational issues, validation problems, and application opportunities. It also focused on the potential for e-science applications in the broad field of DEM. Some of the issues for discussion in the environmental science applications of DEM included: the generic aims of DEM modelling as a methodology; common features and differences amongst the models required in applications to different kinds of problem; relationships between DEM and macroscale approaches, and the possibility of formal or pragmatic methods for effecting this transition; consideration of methods for particle tracking of multiple discrete elements to describe aggregate behaviour; comparison of strategies for code development and implementation; the potential for e-science applications (code sharing, visualization tools, Grid applications); the portability of code between different applications (such as molecular-dynamics and engineering problems), and the potential for this sharing to develop; and general challenges for the dispersed and diverse community of DEM users.

2. Reductionism and emergence

As noted above, a general theme in the use of DEMs is the relationship between reductionism and emergence. Science often follows a reductionist route in the search for explanation, and the environmental sciences are no exception. For example, accounting for the spatial and temporal variations in river-bedload transport rates requires an understanding of the threshold of individual grain motions in complex sedimentary environments with mixed grain sizes in non-random spatial arrangements, which are convolved with turbulent flow fields having three-dimensional flow structures. Macro-scale regularities and generalizations are often emergent from, and understood through, the behaviour of multiple individual instances, such as this interacting motion of river-bed material particles (see Heald *et al*. 2004). This is classically illustrated by the relationship between the gas laws and the kinetic theory. But properties of the emergent behaviour are often not readily understood without reduction to the level of the relevant individuals, because the macroscale parameters depend on statistical properties of the aggregated individuals, and it is practically impossible to sample reliably in order to determine their values at the macroscale. However, it is now possible, in many cases, to model the behaviour of large number of individuals and their interactions, and then recover parameter values as emergent characteristics of the ensemble.

Consider the case of a mudflow, for example. It is difficult to create a forward model of a mudflow, because measuring the necessary rheological properties of such a complex pseudo-Bingham fluid is practically impossible at the relevant scale. However, it is possible to effect inverse modelling with a discrete-element model or a smoothed-particle hydrodynamic model, and adjust model parameters that represent the rheology until the mudflow run-out distance and depositional lobe dimensions are adequately simulated. This system-scale rheology is then an emergent constitutive property of the model which can be related to some of the sedimentary characteristics of the observed flows, in order that other models can be calibrated on the basis of these more readily recoverable data. A key purpose of discrete-element modelling may therefore often be to estimate emergent, constitutive macroscale properties of systems that are difficult to measure practically at their natural scale. Appeals to DEMs, enabling such inverse modelling, have increased significantly in recent years. However, methods including and linked to DEM (such as smoothed-particle hydrodynamics and lattice Boltzmann methods (see Heyes *et al*. 2004)) are less widely known than, say, mature methods such as computational fluid dynamics (CFD), and software is correspondingly less readily available. In addition, more philosophical issues related to the realism of the fundamental 'entities' identified, the implication of this for the relationship between modelled and measured constitutive properties, and the validation of models based on experimental data at both the individual and system scales, have been the subject of less widespread debate.

It would be mistaken to assume, however, that the 'entity' and the 'system' are the only scales of interest. As in much environmental modelling, internal behaviour of both real and modelled systems must be examined to ensure that the physics operates correctly at intermediate scales. In hydrological modelling it is now well known that some models can appear to predict catchment output hydrographs reasonably well, while representing internal processes and patterns (such as soil wetness) incorrectly. It is thus necessary to evaluate relationships between model internal predictions and the behaviour of real systems; internal microstructures generated by a discrete-element model may be critical in determining its emergent macroscale behaviour. Experimental methods are then needed to validate internal behaviour in precisely those regions where measurement is most difficult. Laboratory-scale models which can be monitored using positron-emission-particle tracking (PEPT) methods (using radioactive tracers) are therefore as important in environmental applications of DEM as they are in chemical engineering and powder technology (Kuo *et al*. 2002). Consider the example of tumbler experiments used to examine rates of grain-size reduction by attrition during fluvial transport. In chemical and mining engineering, DEM models of various types of tumbler are relatively common (see http://www.cmis.csiro.au/cfd/dem/index.htm), and it is feasible to use them to examine attrition. However, these models often illustrate mixing patterns within a tumbler (McCarthy *et al*. 2000) that imply that particles may become trapped in regions which limit their capacity for interaction. The aggregate statistical properties of grain-size change may therefore disguise the fact that particles fail to participate in the attrition process equally, and such output data have to be understood in the context of this internal system behaviour.

3. Technical issues

There are several technical issues that require attention when DEMs are used to model environmental phenomena (which can cover a rather wide range of spatial and temporal scales). Some of these are noted briefly here, and papers in this issue consider them, and others, in more detail.

(*a*) *Contact models*

A key requirement in a DEM is a model of the particle interaction at the moment of contact. In the simplest case, the elements are spheres that collide at a point, and rebound in a trajectory that can be calculated by integrating Newton's laws, knowing the direction and velocity of the approach, and the forces at the collision. Non-spherical particles introduce an immediate complexity in terms of defining the geometry of the collision (see Latham & Munjiza 2004), although models involving various realistic non-spherical shapes such as super-quadrics are being developed. Various contact interaction models have been proposed, usually with some combination of normal, tangential and dissipative forces. Commonly, the collision is not assumed to occur at an instant and at the point contact, but instead the particles are allowed to overlap in a numerical sense, usually by less than *ca.* 1%, and the overlap is used to derive a repulsive normal force; this is a so-called 'soft-particle' model. A typical collision model is illustrated by Cleary & Prakash (2004) as

$$F = -k_{\mathrm{n}}\Delta x + C_{\mathrm{n}}v_{\mathrm{n}}.$$

The first term is a linear spring with a stiffness k, which defines the repulsive, normal elastic force as a function of particle overlap Δx, while the second term is a dissipative force which moderates this in the manner of an in-parallel dashpot, and whose damping coefficient C is related to the coefficient of restitution. A tangential force is also required which depends on the surface friction of the particles; in Campbell *et al.* (1995), the surface friction coefficient for rock is taken as 0.5. More complex models do exist, and it is also possible to use a simpler 'hard-particle', or Hertzian, model in which the collisions are binary, instantaneous and involve no assumed 'overlap'.

The question of the most appropriate contact interaction model for use in environmental applications of DEM is significant, as Tüzün *et al.* (2004) illustrate. DEM simulations of granular flows forming heaps, or in hoppers, show different patterns of voidage, contact force distributions, and 'shear banding', depending on the particle interaction model employed. Shear banding is more strongly developed when there is a 'continuous interaction' model of the kind requiring particle overlap than in an instantaneous elastic collision. Experimental validation in conjunction with DEM modelling is thus required at least at two different scales (although as noted above, intermediate scales of validation are also important if laboratory models of field prototypes can be interrogated internally). At the macroscale, measurement of the emergent or constitutive behaviour of a simulated process is required in order to test the model's performance (the distance of run-out of a landslide, or the spatial pattern of deposit thickness). At the microscale, experiments are needed to identify realistic particle interaction behaviour on collision, and to ensure that the DEM implementation contains appropriate representations of the collision physics. There is no reason to suppose that a DEM model of pancake ice formation (Hopkins & Shen 2001) requires the same contact interaction model as a model of a debris flow. Representation of the collision physics appropriately is also strongly dependent on the scale of application. As Yong *et al.* (2004) demonstrate, at the molecular scale, and for some kinds of particle, hysteretic interaction behaviour occurs as surface adhesion takes place and a 'jump-to-contact' phenomenon at collision requires tensile failure at separation. When DEMs are applied at the macroscale, for example, to simulate geological folding and faulting processes, the constituent elements may be 'conceptual' rather than 'real' and, in this circumstance, the contact interaction law required to capture inter-element behaviour is much less clear (see § 4). These examples illustrate that environmental science applications can span a very wide range of scales, that the realism of entities may vary, and that the relationship between model parameters and measurable properties may be tenuous.

DEM simulations may fail to conserve system-scale energy and momentum as a result of the treatment of particle–particle collisions. For example, Hopkins & Louge (1991) present evidence of emergent microstructures in two-dimensional (2D) disc models, which conflicts with theoretical approaches to such systems that assume isotropic and homogeneous distributions. The microstructures imply that DEM simulation must be at a scale to permit averaging across the local anisotropy they define, when comparison is made between the model output and theory. This of course raises a question of whether a 2D model can properly represent this phenomenon. However, it also highlights a possibility that modelled energy dissipation in inelastic disc collisions fails to ensure adequate system-scale conservation of energy and momentum. Granular simulations must be fully dissipative, or they may require rescaling to stabilize the total kinetic energy. Spring-and-dashpot models of interparticle behaviour, which are phenomenological approaches to computational problems, may fail to ensure large-scale energy and momentum conservation in the mass as a whole. Explicit modelling of the energy and momentum conservation at collision is a solution that would ensure system-wide conservation, but may introduce significant implications for the computational overhead. Preservation of energy and interaction symmetry requires careful treatment of multi-particle collisions. Pairs of particles cannot be assumed to act in isolation, implying a search process to discover multi-particle interactions where more than two bodies collide simultaneously. Algorithms which integrate energy and momentum over such collisions will guarantee conservation, and any conservation errors that do arise will then be attributable to loss of precision associated with numerical truncation.

(*b*) *Computational issues*

Computational requirements in DEM simulations are inevitably demanding. The method requires efficient algorithms to track the positions, velocities and directions of large numbers of particles, to detect the particle pair that will create the next collision and to calculate the collisional behaviour. Decisions in each of these areas reflect the need to balance the computational effort between efficiency of search algorithms and simplicity of collision mechanics. This is evident in the comparison by Hopkins & Louge (1991) of hard- and soft-particle collision models and associated tracking and detection algorithms (the latter model requires several time-steps to integrate the forces at collision, so requires a more efficient detection algorithm). The algorithms employed in DEM codes may differ less than one might expect, since many codes have developed from a limited number of original sources (for example, the code developed by Cundall that now underpins the Itasca PFC3D code (see http://www.itascacg.com/pfc.html for details) (Cundall & Strack 1979)). Furthermore, code development may have lagged behind evolution in computing power, so that decisions about this balance made to reflect earlier computing constraints may still be 'locked-in'. However, DEMs lend themselves to parallelization (Todorov & Smith 2004), and offer opportunities for e-science applications based on code sharing and distributed computing. As particle numbers in a simulation increase, so the time-step must reduce to ensure that single collisions occur within a time-step, but even with small numbers (n) of particles, it is possible for a particle to pass through a solid boundary if the time-step is so long that it 'fails to detect' the boundary as it approaches, and its centre passes outside the domain between one time increment and the next. The reduction in time-step with increasing n has had a severe effect on the scales of realistic simulation, particularly for environmental phenomena. Thus, when Campbell *et al.* (1995) simulated long-run-out landslides using only a 2D model involving discs, they were restricted to a single run with one million 'particles' because it required a year of computer time. This indicates the need to explore the effect of simulation 'size' on stability of the output from a model, as shown in figure 1. Here, a series of experiments was run in which a Gaussian distribution of spherical particle sizes was dropped vertically onto a rough surface to form a natural bed. This was repeated with increasing numbers of particles. In each experiment, for each particle the sum of the radii of touching particles was calculated, and the distribution of this quantity for all particles in the simulation was obtained. The median appears to stabilize beyond about 1000 particles, indicating that edge effects are significant up to this scale of simulation.

A key requirement in the coding of a DEM model is the search procedure employed to identify collisions, for which a range of computational algorithms exist and continue to be researched (Munjiza & Latham 2004). In models employing hard-particle

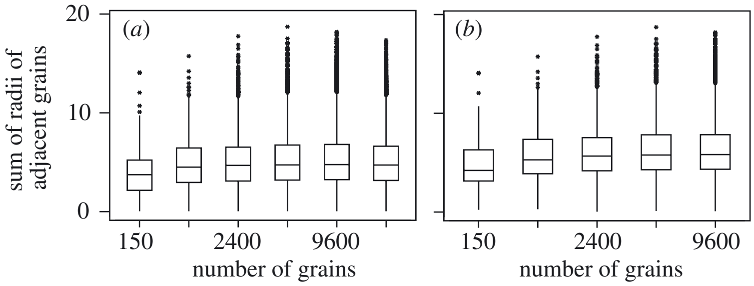

Figure 1. Results of a series of DEM simulations in which spheres with a narrow range of sizes were dropped into a box to create a bed several grains thick. At the end of each simulation, for each particle the sum of the radii of all touching particles was calculated, and each box-and-whisker plot shows the median, inter-quartile range and range of this sum. In (a) this is for all grains, while in (b) it is for the surface particles only.

collisions, one strategy is to maintain a list of future collisions in order of their likely occurrence, and update it after the next collision in the list has happened; however, this is computationally expensive. More efficient methods are needed for soft-particle models, since the execution of the collision is itself computationally expensive. Algorithms that scale linearly with the number of particles are generally best suited to systems of similarly sized particles, implying that models which can simulate realistic grain-size distributions (ranging from gravel to silt-sized particles in the case of river-bed sediment, for example) are likely either to require the additional power of distributed computing methods, or to await the development of hypo-linear search algorithms in which central-processing-unit time scales as a power of the number of particles, where the power is less than 1.0 (Munjiza & Latham 2004). One of the limitations of DEM in its application to natural materials is that they consist of very wide ranges of grain size. It is common for river-bed sediment, or material in a debris flow, to include particles ranging in size from silts and clays to gravels, pebbles and even boulders. Some particle-tracking algorithms require a spatial grid in which cells are approximately the size of a particle (so that only one particle can exist at a time in a cell). However, this is inefficient when there is a wide particle size range, since larger particles must occupy several cells. Indeed, when this arises, it may be appropriate to evaluate the relative merits of mechanistic DEMs and cellular automata.

(c) *Allied methods*

The NIEeS Workshop considered the potential in environmental modelling not only of DEM, but also of a range of allied methods applicable to macroscale systems and problems, including lattice Boltzmann methods and additional off-lattice methods related to DEM, such as smoothed-particle hydrodynamics (SPH) (Heyes *et al*. 2004). Cases where particles deform under stress require combined DEM–FEM methods, where the finite-element component handles particle deformation. An example of this is provided by Ransing *et al*. (2004), while Dupin *et al*. (2004) provide a review of the lattice Boltzmann method and empirical examples of hydrodynamics and the transport of dense suspensions of deformable droplets, analysed using this method. SPH uses the (gridless) Lagrangian form of the hydrodynamics equations to model a fluid as a collection of discrete elements (Monaghan 1992). These elements are initially distributed with a specified density distribution, and are translated according to the conservation equations. Other continuous variables are determined by a smoothing of the nearby particle distribution using a weighting function. This so-called 'smoothing kernel' defines the simulation resolution according to its smoothing length, which relates to the number of adjacent particles across which smoothing takes place. Cleary & Prakash (2004) provide examples of the application of SPH to problems as diverse as dam breaks, tsunamis and lava flows. This adds to the small number of applications of SPH to environmental phenomena, which include that of Bursik *et al.* (2003), who simulated debris-laden floods occurring over digital elevation models (also, confusingly, abbreviated to DEMs). The flows were modelled by separating advection and diffusion terms, then solving the advection term in a cellular automaton model and the diffusion term using smoothed-particle hydrodynamics. The gridless nature of SPH enables it to model flow over complex topography, even in cases where the fluid breaks up into separate streams, and even splashes. Thus it can model unsteady, rapidly varying flow.

(*d*) *Describing macroscale behaviour*

There are certain dilemmas faced by those applying DEMs when interpreting model outputs. One is that, unsurprisingly in these many-body simulations, there is sensitivity to initial conditions that causes individual simulations to differ in detail. A simple numerical experiment will reveal that repetitions result in different patterns of particle motion, as small deviations in collision angle occur because of numerical error. One implication of this is that macroscale structure in a single output may be accidental, and needs to be checked by repeated model runs in order that consistency of macroscale statistical descriptions can be confirmed. However, when simulations with large numbers of particles are undertaken, this is not always practicable, and it is then necessary to assume that the constitutive descriptions are made at a scale so much greater than that of the individual particles that single experiments average across the effects of local divergence due to the chaotic dynamics (using the analogy of a long-term run of a climate model, this is comparable to assuming that a 30-year average climate can be reliably inferred even if a specific weather condition on a given date cannot).

A second challenge for the analysis of DEM simulations, particularly those involving complex three-dimensional (3D) flows of many particles over convoluted boundaries, is that the outcome of the simulation may involve transient collective effects on groups of particles within the body of the flow. While visualization techniques are very helpful in identifying and describing such cases, a range of different methods may be needed to permit extraction of useful quantitative information. Selection of a fixed plane in which to view the motion may miss the relevant structures, even where the system boundaries have a special symmetry. On the other hand, 3D visualizations may require continual changes of viewpoint, and may not allow a direct view of internal structure. At the same time, traditional analysis techniques such as the Fourier transform may not adequately capture temporally transient or spatially localized phenomena. The Fourier technique is best suited to time-series whose frequency structures are statistically stationary, for example. However, isolated events, such as the occurrence of small-scale avalanching, may be best described using statistical mechanical approaches. A technique such as wavelet analysis may prove beneficial, as this can capture the local coupling in such an event of phenomena, such as the velocity field to the voidage, without the need for prior knowledge of where or when such an event might occur (Tüzün *et al.* 2004). This then provides insight into the temporal lead-lag relationships between different local properties, and improves physical understanding of the underlying, internal, mesoscale mechanisms involved in the motion of groups of particles.

4. Scales of phenomena

As illustrated by some of the examples discussed above, the simultaneous treatment of environmental processes acting at different scales may require innovative modelling solutions. One of these is the coupling of mechanistic physical mathematical methods with simpler cellular methods (cf. Bursik *et al.* 2003), particularly across a transition in scale and process representation. For example, different methods are needed to model bedload transport and river channel change, although there must be a feedback between them. Heald *et al.* (2004) show that we can use DEM simulations to generate increasing bedload fluxes with increasing levels of the driving fluid stress, and that these fluxes match empirical evidence, and theoretical mass flux models, suggesting that such models can be regarded as the emergent character of interacting multiple particle transport. However, at the reach scale, and especially in relation to morphological change as bed material experiences entrainment, transport and re-deposition over a mobile boundary, DEMs may be too computationally demanding. Nevertheless, it is a goal of fluvial geomorphology to model the interrelationship of local bed particle motion and reach-scale morphological change. This could be based on a sediment transport model with improved sedimentological content (including distributional properties of grain size, exposure, pivoting angle, bed surface porosity, bed surface roughness, for example), all of which could in turn be derived from small-scale DEM models of the deposition of grains of a specified size distribution. Then, given limited grain-size data, multi-dimensional look-up tables of properties correlated with grain-size distributions could generate the necessary distribution functions to parametrize a sediment transport model to be used in routing sediment through a cellular automata model at the reach scale. This illustrates one of the ways in which mechanistic models that cannot be applied at the reach scale for practical reasons can nevertheless generate information to drive simpler models in a physically meaningful way.

A second scale-related issue involves that of the realism of the entities that are treated as elements or particles in a discrete-element model. In large-scale geological simulation the elements are pseudo-particles, which represent entities in a generalized manner. For example, using the DEM to simulate tectonic deformation, and the structural geology of folding and faulting, requires the elements to represent large lumps of rock which are not necessarily representative of any naturally occurring particle size, but are a convenient way to discretize the rock body (Morgan 1999; Morgan & Boettcher 1999). The implication is that the frictional contacts are not strictly frictional, but rather that friction has to subsume the effects of the shearing of small-scale asperities around the natural blocks of rock that they represent. This makes choice of a friction coefficient applicable at this scale more uncertain, and less amenable to measurement. This problem also applies when an allied method to DEM, such as SPH (Cleary & Prakash 2004), is applied, as this may represent constitutive properties in a manner that does not relate closely to any quantity that can be obtained from conventional measurement practices (for example, the viscosity required in an SPH model of a mudflow or lava flow).

5. Examples of discrete approaches in the environmental and related sciences

As noted above, a wide variety of research fields now explores variants of individual-based methods and, while the interaction rules and the consequences of proximity may differ markedly, the philosophical objectives of such modelling are often similar (namely, to determine emergent system-scale properties from multiple individual interactions). How much we might expect to see similar emergent phenomena as each of the elements becomes more complex depends on how much the dynamics are dominated by the network of interactions, as opposed to being driven by the internal state of each individual element. There are nevertheless some common problems in this diversity, such as algorithms for contact identification, and the transition from mechanistic to cellular approaches. The following sections provide illustrations of problems in the environmental and related sciences that are currently being addressed using DEMs, and papers in this Theme Issue illustrate applications to several of these problems. DEMs simulate dynamic processes, and illustration in textual documents is difficult; accordingly, where possible website details are provided where animations of simulations can be viewed.

(*a*) *Physical processes*

The study of physical processes in environmental sciences, where solid particle interactions occur, is a fruitful arena for the application of DEMs. This is the case across a very wide scale range, and begins with environmental applications at the molecular level. For example, the potential for storing high-level radioactive waste in crystalline ceramics requires improved understanding of the nature of radiation damage in such materials, and large-scale molecular-dynamics simulations (with up to 300 000 atoms) can assist in developing this. Trachenko *et al*. (2002) and Geisler *et al*. (2003) have used large-scale molecular-dynamics techniques (involving up to 300 000 atoms) to simulate response to a high-energy (30 keV) recoil of an atom after alpha decay (see http://www.esc.cam.ac.uk/movies/). Realistic recoil events have been simulated with the mineral zircon, $ZrSiO_4$, which is a natural example of a material that may contain radioactive elements. In particular, the local structure resulting from a recoil event has been shown to involve a lower-density core region surrounded by a shell of polymerized SiO_4 tetrahedra (figure 2). A simulation begins with a perfect crystal of zircon at 300 K. If one of the atoms is simulated to undergo radioactive decay, a high-energy recoil then sends oxygen atoms flying in many directions, with additional displacements of the silicon atoms. After some time the thermal motion allows a healing of some of the disorder. This polymerized shell may act as a barrier between the low-density region and the rest of the matrix, suggesting that storage of radioactive waste could be feasible since the recoil events provide a form of self-encapsulation.

Soil mechanical and geotechnical problems are other areas where DEM approaches can be valuable, particularly in terms of providing understanding of the internal micro-mechanics of particulate systems under stress. For example, Thornton &

Antony (2000) illustrate the use of DEM to study quasi-static stress–strain behaviour in a polydisperse system of soft elastic spheres with interface friction and adhesion, under both compression and tension. Stress waves in particulate systems arise from the micro-mechanics of transmission of local dynamic loading along discrete paths, related to variation in fabric (Sadd *et al*. 2000), and this can be studied using DEM for dry and cohesionless, cemented and fluid-saturated media, although this range of conditions demands new interparticle contact relations that are both appropriate representations of the prototype and efficient for coding purposes. Bonded particle models can be employed to investigate shear failure in soils and rocks, and to simulate landslides and faulting. Increasing shear stress in such a model causes bonds to break and acoustic emissions to occur. This provides seismic signals that are derived from known sources of bond failure and crack formation in the model, and this makes it possible to explore the recovery of tectonic information from the inversion of seismic signals (Hazzard *et al*. 2002).

A productive area for discrete-element modelling is in the investigation of sediment transport. This is especially the case in fluvial systems, and Heald *et al*. (2004) illustrate how variable bedload fluxes as a function of increasing fluid stresses can be simulated successfully using DEMs. This follows from earlier research into local conditions for grain entrainment, local sediment sorting, and sediment transport rates by grain-size fraction by McEwan *et al*. (2001), Schmeeckle *et al*. (2001) and Schmeeckle & Nelson (2003) (see http://www.eng.abdn.ac.uk/~eng548/abdndpm/intro.html and http://www.public.asu.edu/~mschmeec/). Bi-directional sediment transport processes in the surf zone on beaches have also been studied using DEM, and this has exposed limitations in widely employed theoretical bases for littoral transport models (Drake & Calantoni 2001). Calantoni *et al*. (2004) have also taken the question of grain shape further than in other sediment transport studies by examining the use of a dual-sphere representation of grains, providing a computationally efficient means of exploring the effects of particle shape on the transport process.

Geomechanical behaviour and sediment transport and flow come together in the simulation of slope processes, such as landslides, rockfalls, debris avalanches and mudflows. The behaviour of particles under shear on a 'sand pile' (Tüzün *et al*. 2004) illustrates the grain interactions typical of scree-slope surfaces, and DEM simulations offer considerable potential for the study of the morphology and sedimentology of these features. A related area is in the study of rock slopes (Allison & Kimber 1998), where DEMs which employ arbitrarily shaped joint-bounded blocks have made it possible to examine rock-slope mechanics and rock-slope evolution realistically. Compressive and shear strength laboratory measurements on rock samples are unrepresentative of the properties relevant to macroscale (joint-controlled) behaviour at the field scale, and DEM simulations suggest a means of generating macroscale constitutive properties which can then be correlated with field measurements of joint characteristics (such as spacing, continuity, infill and seepage rates). Some of the most interesting applications of DEMs to large-scale environmental processes have been to the question of the long run-out behaviour of some landslides that become debris avalanches (Campbell *et al*. 1995; Cleary & Prakash 2004). Much debate focuses on the causes of excess run-out distances, with various hypotheses including air entrapment, basal water pressures, thixotropic behaviour and acoustic fluidization. DEMs have been able to show that bed roughness inducing a relatively thin basal shear layer can translate much of the body of an avalanche over long

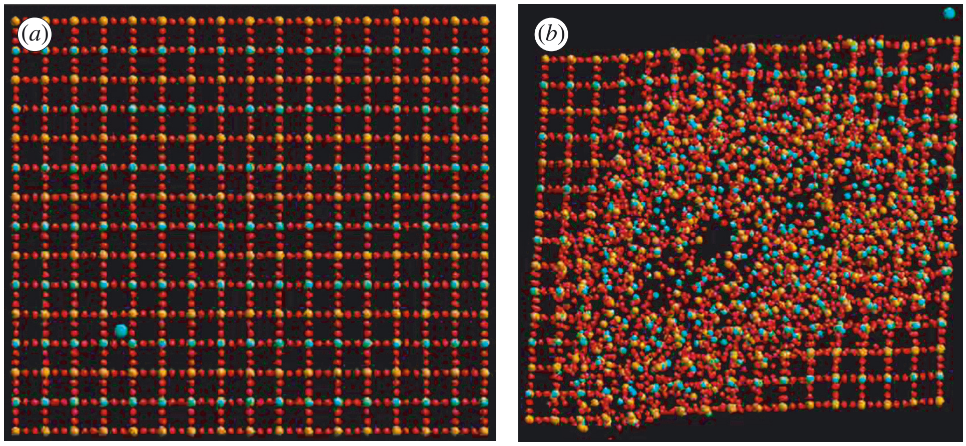

Figure 2. Molecular-dynamics simulation of a high-energy (30 keV) recoil event following alpha radioactive decay in zircon. (*a*) The pristine crystal structure. (*b*) A portion of the structure 2 ns after the recoil event, just after the initial burst of kinetic energy has left the core region. Note the large amount of damage formed as atoms collide, and the large shear of the structure that forms with the damage.

distances with relatively limited mixing and low apparent friction. However, there remain many interesting questions about such particle flows. For example, the roles of wide ranges of grain size and shape are poorly understood, although insights may be gained from hopper-flow studies in mining engineering (Mustoe & Miyata 2001); see http://egweb.mines.edu/dem/. Also, particle flows may experience unsteady or periodic flow behaviour, and experimental studies coupled with DEM simulations suggest that this may relate to 3D flow effects also induced by side-wall friction at a bumpy boundary (Hanes & Walton 2000). Clearly, there is a valuable opportunity here to use the DEM and allied methods, especially SPH, in hazard management. Debris flows (and pyroclastic volcanic flows and snow avalanches) are particularly dangerous natural hazards, and understanding the variations in run-out distance with differences in slide volume and path geometry and topography can contribute to planning and hazard management. However, as the above examples suggest, this potential is likely to be best realized by combining numerical simulation, laboratory experiments and field measurements in innovative ways.

There are many other physical environmental processes where DEM and related methods may make important contributions to understanding and predictive capability. In glaciology, for example, it has been possible to treat both sea ice and river ice cover using a DEM involving discs or polygonal slabs. Hopkins & Shen (2001) have simulated the evolution of pancake ice under a wave regime in this way. Pressure ridging in sea ice has also been simulated, and Hopkins *et al*. (1996) have developed an innovative approach to prediction of river-ice break-up by coupling a fluid dynamic model of unsteady flow to a DEM model of surface ice cover, represented as polygons joined by a visco-elastic glue which breaks under loading, to produce interacting polygonal plates (see http://www.crrel.usace.army.mil/sid/hopkins_files/Discrete_Elements/discrete.htm). Again, this is an illustration of a case where DEMs can be productively deployed in a hazard management context, particularly in engineering design of bridges in order to minimize the build-up of ice jams which are both damaging to structures and a cause of extreme melt-season flooding. Some of these applications, especially those of ice pressure-ridging, have similarities with the largest scales of environmental phenomena to which DEM has been applied: the tectonic evolution of folds and faults (Morgan 1999; Morgan & Boettcher 1999). Here, as in the rock-slope evolution case noted above, a key benefit of the DEM method is that it provides a realistic basis on which to explore the nature of processes whose time-scale of operation precludes direct field measurement (see http://terra.rice.edu/department/faculty/morganj/). Of course, there remain major advantages in combining numerical methods with experimental studies, and then using field observation of macroscale emergent structural properties in rock outcrops as a means of validating the overall output of the model, and to assist in up-scaling interparticle collision parameters to the 'conceptual' particle scale required in these applications of DEM.

(*b*) *Plant sciences*

Considerable opportunities are offered in plant ecology by individual-based models that capture the growth behaviour and life history of single plants, representing the control exercised on these processes by interaction with their neighbours and the environment. These are not concerned with *motion* of individuals, but require rules based on the complex dependencies of individual plants on their biotic and abiotic environment. Although seed transport may determine plant propagation and dispersal, its success is governed less by interaction amongst the seeds, than by the mechanism of transport and the quality of the deposition site, including its soil properties and the availability of water and nutrients. Nevertheless, in some contexts (eg in riparian environments) a combination of DEMs for sediment transport and individual-based models for vegetation should form a powerful combination for study of this kind of system. Where direct competition between plants is considered, individual based models are particularly good for the illumination of evolving spatial patterns. For example, the SORTIE model of forest dynamics (see http://www.sciencemag.org/feature/data/deutschman/) (Pacala *et al*. 1996; Deutschman *et al*. 1997, 1999) models local competition between trees for a critical environmental resource, namely light (energy supply). Different species show different responses to light availability at different life history stages. Light availability for each tree is a function of solar elevation and shading, and is used to determine for each species the relative radial growth rate of the trunk, which is then allometrically related to other attributes such as height and canopy width (which influences shading of adjacent individuals). This therefore represents an 'interaction model' for an individual in a discrete ecology.

In the interaction of many individuals, some species that are more sensitive than others to reduced light availability may be shaded out as their growth falters and they receive less and less light. Thus, it is possible to simulate the evolution of a stand of woodland as local species interaction takes place. Shade-tolerant species will dominate eventually if there is no disturbance, whereas when there is frequent disturbance (for example, by fire, windthrow, landslides or river erosion), shade-intolerant species are more prominent as they can take advantage of light availability in the gaps created by disturbance. The spatial pattern, and the areas occupied by different species, thus represent emergent aggregate system properties which are the result of the interaction of individuals under particular sets of conditions; as these change over time, they define a plant community succession which emerges from the behavioural properties of individuals. Similar models have been used by Köhler & Huth (1998) for modelling the effects of tropical forest management and logging. Light availability will not always be the key (or the only) resource constraint on tree growth, of course. Where there is strong competition for water, the annual incremental trunk growth may primarily reflect the water uptake, and distinguishes between adjacent trees of different species. Furthermore, for herbs and shrubs, it may be practically difficult to model individual behaviour, and instead an 'entity' may have to be defined which is a 'community' of species rather than an individual plant. This partly parallels the difficulty in using DEM to model sediment transport where the grain-size range is large (from gravel to silt), and suggests a similar combination of 'classical' DEM and cellular automata approaches. However, the plant sciences have a research agenda here to link organism (individual) and ecology (structure) in novel ways.

(*c*) *Zoology*

The same is true of zoology, where dynamic spatio-temporal aggregate behaviour is generated by interactions amongst individuals: the flocking or schooling of birds and fish are well-known examples. Models of this behaviour are often based on three simple steering rules for the individual members of a flock (Reynolds 1987). (See also http://www.red3d.com/cwr/papers/1987/boids.html.) These rules are

(i) separation, or steering to avoid the crowding of local flock members,

(ii) alignment, a steering behaviour towards the average heading of local members,

(iii) cohesion, which is steering towards the average position of the local members.

With a simple definition of the range within which flock members are considered to be 'local', these rules reproduce remarkably well the movement through time and space of a flock or school, simply by constraining the paths navigated by each individual. The parallel here is with a group of particles governed by both long-range attractive forces, which bind the flock together, and a shorter-range repulsion that allows for collision avoidance. One might thus expect there to be some resemblance of the statistical properties of a large flock to that of a flowing fluid. However, the extra internal states available to the individual 'particles' cannot be neglected—the requirements to conserve momentum or energy in an interaction no longer tightly constrain the possible motion, as the internal structure of the animal is complex and under independent control, and the apparent forces of interaction may have complex forms that are governed more by behavioural requirements (the search for food, avoidance of predators) than by simple physics. Emergent phenomena at the flock level may still be observed however. An obvious example is the V-shaped pattern adopted by flying geese, where the pattern apparently minimizes energy expenditure (Lissaman & Shollenberger 1970). More complex cases involve collective effects, such as the almost simultaneous changes in direction of an entire flock of birds or school of fish. Here the results may depend on the existence of a 'small world' network structure of interactions: a general network property in which the local interactions of individuals can spread signals rapidly through a whole group (Watts & Strogatz 1998).

The emergent population dynamics of animals and birds has also been successfully modelled using spatially explicit, individual-based approaches. For example, Pettifor *et al*. (2000) have considered the population consequences of the individual behaviour of species of geese—although the approach also applies to oystercatchers and other wading birds. The grazing behaviour of individual birds at particular breeding sites is represented in individual-based models of food intake (determined by peck frequency and size), which determines growth and health, and these in turn strongly influence reproductive success (or failure). The resource limits of a given breeding site then interact with the changing competition for resource defined by population size, and the temporal dynamics of the population can be predicted. Such models can then be used to predict how populations will respond to environmental and other changes that alter the resource availability—as a result of climatic changes, sea-level change or alterations in land-use pressure and management. The impact of spatial location is thus significant in animal populations, which both condition and are conditioned by the landscape and its vegetation. Spatial heterogeneity and patchiness in the landscape can lead to very pronounced differences in the dynamics of populations (a field that has received much study of recent years in the guise of metapopulation ecology (see Hanski 1999)). However, competition for territory, competition between species or predator–prey interactions can lead to the spontaneous generation of spatial structure in spite of uniformity in the underlying space (Rand & Wilson 1995). Such emergent phenomena are even more evident when we analyse human populations.

(*d*) *Social simulation*

In the biological sciences, individual-based models have been developed since the late 1980s (Huston *et al*. 1988; DeAngelis & Gross 1992) and many different models have been constructed (Grimm 1999) by using a range of techniques to cope with the spatial aspects (McGlade 1999). In the social sciences, early attempts to describe the emergence of structure using simple rules met with some success, a good example being that of Schelling (1971), in which simple preferences for types of neighbour in the interaction between two types of individual were sufficient to segregate those types spatially. Individual-based models able to represent people or organizations directly are generally referred to as agent-based models, or multi-agent systems (Woolridge 2002). These also originated in the late 1980s (Doran 1987), with complex social structures being simulated in the mid 1990s (Doran & Palmer 1995; Epstein & Axtell 1996).

The essence of multi-agent modelling is to add to the reactive behavioural rules of an individual-based model the ability of agents to reason about the environment and about the motivation and opinions of other agents. Such opinions may be based on incomplete or erroneous data, and thus generate apparently irrational or sub-optimal behaviour. Agents can also have extensive memory of past situations and learn from previous experience. An ambitious future for such models is toward integrated systems in which a full suite of individually based vegetation types, embedded in a realistic physical environment which provides both resources and constraints, interacts with animal populations which 'remember' locations of food sources and co-operate in herding or hunting, and in which intelligent human individuals exploit the plant and animal resources through hunting and agriculture. The principal difficulties in building such a scheme rest in there being sufficient computing power to make it realistic and in being able to define the rules of human and animal behaviour to obtain believable results. However, the latter demands an equivalent to the microscale experimental investigation that defines interaction models in DEM, such as social-survey methods that can reveal behavioural traits and rules. Even then, analysis of the model output will present its own challenges; it is likely to be difficult to relate emergent structures in space and time to particular properties of the underlying individual behaviour and interaction. Nevertheless, multi-agent modelling may offer the social sciences an opportunity to combine research into individual behaviour with modelling to explore the emergence and evolution of structures such as communities, regions and groups: emergent aggregate structures created by, as well as determining, the behaviour of the many individual humans within them (Holland 1998; Gilbert 1995).

While the realism of such models continues to be limited both by computing power and the general difficulties of constructing artificial intelligence, instructive models can still be built. Anthropological examples can be found in Köhler & Gumerman (1999), and individual-based modelling is already very well developed in the health and safety literature. Here, manageable numbers of individual 'agents' are incorporated in simulations of the evacuation from offices, buildings, aircraft and ships during emergencies (Helbing & Molnár 1995; Helbing *et al.* 2000), with observed human behaviour being used to define rules of both normal and panic-driven behaviour in a crowd. Animated figures in these computer models move through corridors and down stairs—that is, in four-dimensional (x, y, z, t) space-time—responding to stimuli, driven by goals, and interacting with those about them. Their aggregate behaviour is reflected in the time-series of departures from the space they are evacuating, and in the spatial pattern of their movements to exits; of course, the objective here is to design the pattern of exits in order to maximize the speed with which such evacuations occur, and influence the character of the time-series. It is not unreasonable to anticipate the development of similar modelling strategies to assist in the development of management of evacuation procedures in the face of environmental hazards such as floods, earthquakes and volcanic eruptions.

Crowded situations where physical interaction between people is direct are in some senses similar to particulate simulations from the physical sciences (although the internal states of the individuals may lead to very different types of flow: sudden panic by claustrophobic individuals, for example). But the density of human individuals is generally much lower than that of typical physical particle systems, and the network structures built by social interaction and individual needs are more likely to govern emergent large-scale properties. Little is yet known about how much of the large-scale structure of human society might be captured by models of this type, nor how much of this structure depends on the accuracy with which the representation of individuals reflects that of real people. Nevertheless, the future may involve descriptions and models of individual human behaviour and both its organizational consequences (into social institutions and living environments) and its response to crises (such as natural or socially produced hazards). This will require significant computing resources and sophisticated code development, and innovative experiments to explore the sensitivity of emergent structures to different assumptions about behavioural rules.

6. Conclusions

The foregoing discussion indicates the significant philosophical and practical gains to be made through adopting off-lattice (Lagrangian) discrete-element approaches to the investigation of a wide range of environmental processes and problems. The examples quoted show that considerable progress has already been made in several applications. Certain questions need to be addressed before these methods can be applied successfully elsewhere, and it is hoped that, as well as providing some exemplar studies in sediment transport (Heald *et al*. 2004; Calantoni *et al*. 2004) and mass flow processes (Tüzün *et al*. 2004; Cleary & Prakash 2004), this Theme Issue can help to provide some answers to these. There are issues to evaluate before further penetration of DEM and its allied approaches into a wider range of environmental science investigations occurs. These include the definition of models of individual contact behaviour (Yong *et al*. 2004), the representation of realistic particle shape and particle behaviour (Latham & Munjiza 2004; Ransing *et al*. 2004; Calantoni *et al*. 2004) and accessibility to high-quality, tested, and open-access software (Munjiza & Latham 2004; Todorov & Smith 2004; Munjiza 2004). There is also a need to give serious consideration to the computational and validation problems associated with simulation of large-scale particle-based processes, which may require a scale- and problem-related classification of approaches. This would help to distinguish circumstances where explicit mechanical methods give way to, or are coupled with, computationally efficient cellular automata methods, and the cases where DEM, SPH and lattice Boltzmann methods might be most appropriate (Heyes *et al*. 2004; Dupin *et al*. 2004; Cleary & Prakash 2004).

Critical scientific requirements in all DEM applications include the need for validation at various levels. This requires, firstly, microscale validation of assumptions about individual particle behaviour during interaction. The interaction mechanics will depend on the character of the elements: whether they are 'real' or 'conceptual' representations of the prototype, and whether they are hard, soft, elastic, ductile, 'sticky', etc. Secondly, mesoscale validation is desirable of the internal character of local aggregate motion of particles (for example, anisotropic structures, or 3D flow behaviour). This may require that individual Lagrangian particle paths are tracked in the numerical model, and measured in an experiment using a method such as PEPT. Finally, macroscale (emergent) patterns and structures in the ensemble of particles must match some observable properties in a prototype (Tüzün *et al*. 2004). Such external validation involves defining constitutive properties of the mass, but in many cases these properties may require tuning in the model in order to match observed structures. Thus, the risk of circular logic in which calibration and validation converge has to be avoided. This implies that models that are computationally demanding may need to be run several times in order to examine the effects of sensitivity to initial conditions, parameter values, repeatability and equifinality. There is as yet little evidence in the DEM literature of the attention to uncertainty that now characterizes CFD applications in the environmental sciences. The CFD experience is instructive in one other, important sense. It has shown that environmental problems, which usually involve rather large scales and very complex boundary and initial conditions, are best tackled by a combination of numerical experiment, scaled laboratory experiment and detailed field campaigns. This is equally likely to be necessary as DEM applications become more common in the environmental sciences.

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