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APPLICATIONS OF CELLULAR AUTOMATA AND NEURAL NETWORK METHODS FOR MODELING LARGE SCALE DISASTERS

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ABSTRACT Large-scale disasters generally involve processes that operate over a wide range of length and time scales, and provide compelling challenges. To effectively model and prevent large-scale disasters, we need to describe detailed scientific phenomena occurring at multiple scales (nano, micro, meso, macro, and mega scales) by capturing information at small scales and examining their effects on the mega scale level. Many problems will remain unresolved without the capability to bridge these scales for modeling and simulation of large-scale disasters. The study of large-scale disasters has been driven by the need for information to guide restoration, policy, and logistics because they are vital for human safety. However, the challenge is to develop more effective modeling and simulation tools that can be used for prediction and disaster management. This will require a systematic, multidisciplinary approach consisting of basic science, mathematical descriptions, and computational techniques that can address large-scale disasters across time and space scales, involving cellular automata and neural networks in multiple orders of magnitude gives an excellent results.

Key Words: modeling, cellular automata, disaster, neural networks , multiscale

I.APPLICATION OF MODELING METHODS TO LARGE-SCALE

1. DISASTERS

Multiscale modeling and simulation is concerned with the methods for computing, manipulating, and analyzing information and data at different spatial and time resolution levels. The techniques of multiscale modeling in various fields have undergone tremendous advances during the past decade because of the cost effectiveness of the hardware environment. Advances in computational methods and the distributed hardware have enabled the development of new mathematical and computational methods that enable multiple simulations. To establish the validity of a model and its application in simulations, both verification and validation aspects need to be addressed (Dolling, 1996). Verification involves checking the model for correctly solving the governing equations mathematically, whereas the validation involves checking that the right equations are solved from the perspectives of the model applications.

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Validations require advances in experimental measurement and data gathering, as well as advances in instrumentations. Figure.1 shows an overview of the multiscale methods over multiple spatial and temporal scales that can be used in developing a multiscale methodology for investigating large-scale disaster applications. Discrete modeling methods employ reduced models and integrate stochastic equations of motion. The advantages of these models include explicit atomistic detail and incorporation of stochastic phenomena.

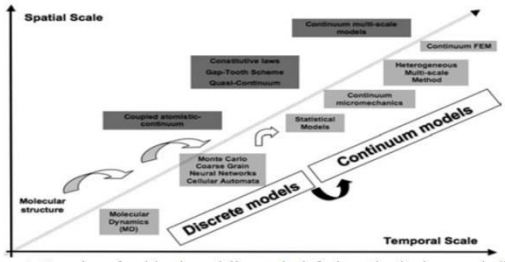

Figure 1: Overview of multiscale modeling methods for investigating large-scale disaster applications.

The disadvantages include slow convergence and difficulty in scaling. Continuum modeling methods are deterministic and offer the advantages of good convergence, are highly scalable, and provide connections to other continuum mechanics behaviors.

2. MULTISCALE MODELING TECHNIQUES

In recent years, several researchers from various fields have developed multiscale modeling techniques by taking into account various phenomena at multiple scales. For example, these include computational materials science (Gates et al., 2005; Nieminen, 2002), computational mechanics (Liu et al., 2004), biomedical engineering (Ayati et al., 2006), and nanotechnology (Fish, 2006). Traditional multiscale techniques, such as the multigrid method, domain decomposition, adaptive mesh refinement, the fast multipole method, and the conjugate gradient method (Reddy, 2006), have focused on efficiently resolving the fine scale. Recent techniques reduce computational complexity by adopting different computational approaches and different laws of physics on various space and time scales. For example, on the macroscale (> millimeters), fluids are accurately described by density, temperature, and velocity fields that obey continuum NavierStokes equations. However, on the scale of the mean free path of the fluid particles, it is necessary to use kinetic theory (Boltzmann's equations) to get a more detailed description. Averaging, where the leading order behavior of a slow time-varying variable is replaced by its time-average value, and homogenization (Fish et al., 2005), where approximate equations are obtained to leading order in the ratio of fine and coarse spatial scales, are examples of powerful analytical techniques. The quasi-continuum (QC) method (Knap and Ortiz, 2001), gap-tooth technique (Gear et al., 2003), and the heterogeneous multiscale method (HMM; Weinan et al., 2003a, b) are examples of recently developed methods. Multiscale methods offer powerful modeling and simulation techniques for the characterization and prediction of large-scale disasters. In this chapter, some of the recent development in multiscale methods from other research areas are reviewed for application to large-scale disasters.

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3. MOLECULAR DYNAMICS METHOD

Alder and Wainwright (1959) developed the molecular dynamics method (MD), which describes the behavior of a collection of atoms by their position and momentum. In this framework, the macro scale process is the molecular dynamics of the nuclei, and the micro scale process is the state of the electrons that determines the potential energy of the system. The MD simulations provide the results of structural information, transport phenomena, and time dependence of physical properties. There are various MD simulations addressing specific issues related to thermodynamics of biological processes, polymer chemistry, and material crystal structures. Most molecular dynamics simulations are performed under conditions of constant number of atoms (N), volume (V) and energy (E) or constant number of atoms (N), temperature (T), and pressure (P) to better simulate experimental conditions. The basic steps in the MD simulation include (1) establishing initial coordinates of existing atoms in the minimized structure and assigning them initial velocities, (2) establishing thermal dynamics conditions and performing equilibration dynamics to rescale the velocities and checking the temperature, and (3) performing dynamic analysis of trajectories using Newton's second law. The result of the MD simulation is a time series of conformations or the path followed by each atom. In general, MD simulations generate information about atomic positions and velocities at the nanolevel. The conversion of this position and velocity information to macroscopic quantities (pressure, energy, heat) that can be observed requires the use of statistical mechanics. Usually, an experiment is carried out on a representative macroscopic unit that contains an extremely large number of atoms or molecules, representing an enormous number of conformations. Averages corresponding to experimental measurements are defined in terms of ensemble averages in statistical mechanics. To ensure a proper average, an MD simulation must account for a large number of representative conformations.For example, the total energy (E) of a particle (atom, molecule, etc.) can be written as

$$E = T + V \quad (1)$$

Where 'T' is the kinetic energy and 'V' is the potential energy. For example, the average potential energy of the system is defined (Gates et al., 2005) as

$$V = \frac{1}{M}\sum_{i=1}^{M} V_i \quad (2)$$

Where M is the number of configurations in the molecular dynamics trajectory and Vi is the potential energy of each configuration. Similarly, the average kinetic energy (K) is given by

$$K = \frac{1}{M}\sum_{j=1}^{M}\left\{\sum_{i=1}^{N}\frac{m_i}{2V_i \times V_i}\right\} \quad (3)$$

Where M is the number of configurations in the simulation, N is the number of atoms in the system, mi is the mass of the particle i, and vi is the velocity of particle i. Once the total energy is calculated, the potential can be calculated as the difference of the energies of different particles, and the molecular forces can be calculated from the

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derivatives of the potentials.

4. COARSE-GRAINED METHODS

Due to inherent difficulties in numerical and computational boundaries in MD simulations, the size and time scales of the model may be limited. Even though, MD methods may provide the details necessary to resolve molecular structure and localized interactions, they are computationally expensive. However, coarse-grained methods may overcome these limitations by representing molecular chains as simpler, bead–spring models (Rudd, 2004). Although the coarse-grained models lack the atomistic details, they preserve many of the important aspects of the structural and chemical information. The connection to the more detailed atomistic model can be made directly through an atomistic-to-coarse-grained mapping procedure that when reversed allows one to model well-equilibrated atomistic structures by performing this equilibration by using the coarse-grained model; it helps overcome the time scale upper limits of MD simulations. Several approaches to coarse graining have been proposed for both continuous and lattice models. The continuous models seem to be preferable for dynamic problems such as might occur when considering dynamic changes in volume. The systematic development of the coarse-grain models requires determining the degree of coarse graining and the geometry of the model, choosing the form of the intra- and inters chain potentials, and optimizing the free parameters (Hahn et al., 2001). Coarse-grained models are usually constructed using Hamilton's equations from MD under fixed thermodynamic conditions. To preserve the average position and momentum of the fine scale atoms, representative atoms are enforced in the model. Coarse-grained models have shown a four orders of magnitude decrease in CPU time in comparison to MD simulations (Lopez et al., 2002).

5. MONTE CARLO METHODS

Due to the time scales (femtoseconds to microseconds) involved in the various physical and chemical phenomena in large-scale disasters, linking diverse time scales is very challenging. The kinetic Monte Carlo (KMC)-based methods can be used to address the time scales (Binder, 1995). Also, the coarse-grain models are often linked to Monte Carlo (MC) simulations to provide a solution in time. The KMC method is used to simulate stochastic events and provide statistical approaches to numerical integration. The integration scheme in the KMC method is simply implemented to integrate a function over a complicated domain D by picking randomly selected points over some simple domain D', which is a superset of D. The area of D is estimated as the area of D' multiplied by the fraction of points within domain D. The integral of a function f in a multidimensional volume V is determined by picking N randomly distributed points X1,..., XN as follows,

$$\int f\,dv \approx v\langle f\rangle \pm v\sqrt{\frac{\langle f^2\rangle - \langle f\rangle^2}{N}} \qquad (4)$$

$$\langle f\rangle \equiv \frac{1}{N}\sum_{i=1}^{N} f(x_i)$$

$$\langle f^2\rangle \equiv \frac{1}{N}\sum_{i=1}^{N} f^2(x_i)$$

There are three important characteristic steps in the MC simulation: (1) translating the physical problem into an analogous probabilistic or statistical model, (2) solving the probabilistic model by a numerical sampling experiment, and (3) analyzing the resultant data by using statistical methods. To deal with stochastic in modeling micro- and macroscale processes (discrete or continuous), MC methods can be used. Traditional MC methods are robust, but slow to converge, and require many trials to compute high-order moments with adequate resolution. Coupling discrete-stochastic models with continuous stochastic or deterministic models, where appropriate, would enable the simulation of many complex disaster-related problems.

III. CELLULAR AUTOMATA

Cellular automata (CA)-based modeling techniques are powerful methods to describe, simulate, and understand the behavior of complex physical systems (Chopard and Droz, 1998). The original CA model proposed by Von Neumann (Wolfram, 1986) is a two- dimensional square lattice in which each square is called a cell. Each cell can be in a different state at any given time. The evolution of each cell and the updating of the internal states of each cell occur synchronously and is governed by a set of rules. The cellular space thus created is a complete discrete dynamic system. Earlier work by Wolfram (1986, 1994) showed that the CA as a discrete dynamic system exhibits many of the properties of a continuous dynamic system, yet CA provide a simpler frame-work. A CA is an array (1D string or 2D grid or 3D solid) of identically programmed "cells" that interact with one another. The cells are usually arranged as a rectangular grid, honeycomb, or other form. The essential features of a CA are the State, its Neighborhood, and its Program. The State is a variable that takes a separate value for each cell, and the State can be either a number or a property. The Neighborhood is the set of cells with which it interacts. The Program is the set of rules that define how its state changes in response to its current state, and that of its neighbors. If we consider a three-dimensional space, then the CA on a cubic lattice over a period of time would occur as follows. In the lattice, each cell position is labeled as r= (i, j, k), where i, j , and k are the indices in three directions, respectively. A function ft (r) is applied to the cubic lattice to describe the state of each cell at iteration, t. This value can be Boolean 0 or 1, or it can be a continuous value by using a probabilistic function. The rule R specifies how the state changes are to be computed from an initial state configuration of f0(r) starting at t = 0. The state of the lattice at t = 1 is obtained by applying the rule to each cell in the entire lattice. CA has been successfully applied to model various physical phenomena from forest fires, game of life, and diffusion to coalescence and self-organizing systems (Chopard and Droz, 1998). The CA-based modeling techniques can be used to model for urban land- use simulations (Lau and Kam, 2005) and also to describe, simulate, and understand the spread of CBR agents into building surroundings and estimate the damage, as shown in Figure

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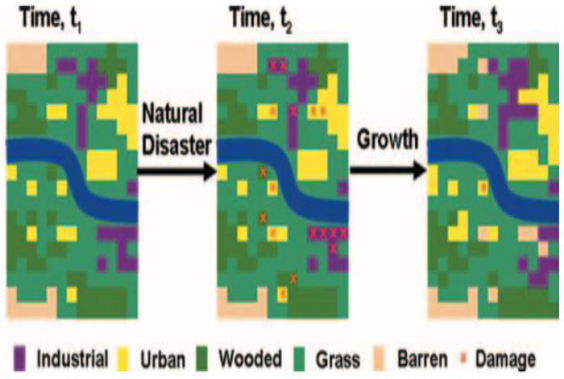

Figure 2: Progression of Damage and Spread of CBR Agents Through CA Modeling.

IV. NEURAL NETWORKS

Neural networks (NNs) are intelligent arithmetic computing elements that can represent, by learning from examples, complex functions with continuous valued and discrete outputs, as well as a large number of noisy inputs (Russell and Norvig, 1995). These networks imitate the learning process in the brain and can be thought of as mathematical models for the operation of the brain. The simple arithmetic elements correspond to the neurons—the cells that process information inside the brain. The network as a whole corresponds to the collection of interconnected neurons. Each link has a numeric weight associated with it. Weights are the primary means of long-term storage in neural networks, and learning usually takes place by updating these weights. The weights are adjusted so as to bring the network's input/output behavior more in line with that of the phenomena being modeled by the network. Each node has a set of input links from other nodes, a set of output links to other nodes, a current activation level, and a means of computing the activation level at the next step, given its inputs and weights. The computation of activation level is based on the values of each input signal received from a neighboring node and the weights on each input link. The most popular method for learning in multilayer networks is called back-propagation, first invented by Bryson and Ho (1969). In such a network, learning starts with presenting the examples to the network and comparing the output vector computed by the feed forward network with the target vector (known outcomes for the given examples). If the network output and the target vector match, nothing is done.However, if there is an error (a difference between the outputs and the target), then the weights are adjusted to reduce this error. The trick here is to assess the blame for an error and divide it among the contributing weights, thereby minimizing the error between each target output and the output computed by the network. More details can be found in Russell and Norvig (1995). Artificial NNs are capable of realizing a variety of nonlinear relationships of considerable complexity and have been applied to solve many engineering problems. The prediction of climate change parameters with varying input parameters can be modeled using NN, as shown in Figure

V.MATHEMATICAL HOMOGENIZATION

Homogenization and averaging are the mathematical/computational processes by which local properties are obtained on a coarse space/time grid from the variables on fine scales. Several analytical studies of homogenization problems in random and periodic heterogeneous.

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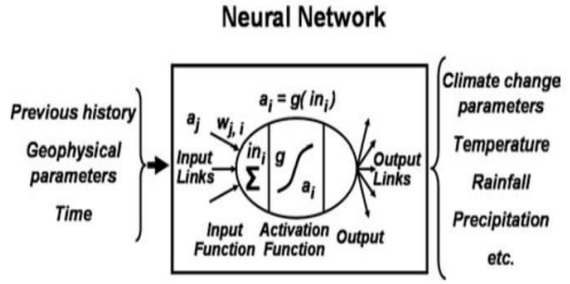

Figure 3: Neural Network Modeling and Prediction of Climate Change Parameters

Materials can be found in Schwab and Matache (2000). Homogenization was first developed for periodic structures involving boundary value problems in material sciences, continuum mechanics, quantum physics, and chemistry. Homogenization results in a coarse scale description of processes that occur on different space and time scales. Usually, the process is described by an initial boundary value problem for a partial differential equation, and the medium considered is periodical. For example, the transport process of water and solutes occurs at micro and mesoscales, and depends on the aggregate and grain size distribution, porosity, and the porous media properties. The particles and pore sizes may range from subnano, nano, to micro- and macro pores.

VI. SUMMARY

Large-scale disasters, both natural and manmade, continue to cause intense suffering anddamage to people and property around the world. Research and technological advances are focused on identifying more effective mechanisms for preventing, predicting, and responding to these disasters. Historically, the overriding concern for human safety and welfare led to the study of large-scale disasters from the perspective of restoration, policy, and logistics. However, the challenge is to develop more effective tools that can be used for prediction as well as disaster management. This will require a systematic, multidisciplinary approach consisting of basic science, mathematical descriptions, and computational techniques that can address large-scale disasters across time and space scales, involving multiple orders of magnitude. Due to the multiscale nature of large-scale disasters, multiscale modeling methods offer a promising methodology for the characterization and prediction of large-scale disasters. The idea of multiscale modeling is straightforward—one computes information at a smaller (finer) scale and passes it on to a model at a larger (coarser) scale, by leaving out degrees of freedom as one moves from finer to coarser scales.

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