지진하중에 의한 구조물 파괴형상 변화에 대한 메조스케일 해석

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ABSTRACT

A lattice model of a typical bridge column section is analyzed, and results are presented. The lattice is built as an ensemble of line elements and masses, that can capture strain rate dependency of concrete material.

The research mainly breaks up into two parts: First, a micro level analysis of the material is executed, and control parameters of the governing equations are derived by matching the results with the common macroscopic properties of concrete material. Then, the properties exhibited by the micro model, which extends the classical material properties are applied to the mesoscale model. Hence, the analysis of the target structure can be performed. In the mesoscale analysis, ramp-like impulse loads are applied at different velocity, so that the contribution of the material level rate dependency to the global behavior of the structure can be tracked.

1. Introduction

Traditionally, civil structures have been analyzed by exploiting the results of classical mechanics. Although effective and arguably cheap in computation, the method vastly ignores features that might affect the quality of the outcome from the analyses. Especially, in the realm of dynamic simulation, the trend intensifies. Filling the holes has often been a loop of adding relatively expensive techniques developed in numerical science. One distinct example would be the inclusion of rate dependency into crack-prone materials. Many studies have reported the contribution of the rate dependency may be significant in catastrophic dynamic situations, such as earthquakes, wind, explosion, and etc. Empirical and experimental results are available in limited quantity, and yet a general formulation that can reliably be incorporated into the grand picture can hardly be obtained.

A new trend of research is emanating on the bleeding edge of applied mechanics, with the

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advent of cheap and fast computers. As the state of the art approach, focus is fixed at atomic or molecular level of materials. By investigating the micro structure of materials under stress and heat, it may lay ground for the determination of the advanced properties omitted in macro level formulation. Such efforts are already making a debut in civil engineering field. However, even with the molecular dynamics formulation, that is known to be efficient, the number of particles that can be packed in a model is known to be confined within the boundary of several million. Knowing that the typical metal atoms are distanced within picometer range, a 2-D rectangular equivalence of the specimen would be sized at approximately 10^{-5} meters, or 0.01 mm at maximum, which is ridiculously small considering the ordinary size of civil structures. Thus, a bridge that can connect the macro and micro level models becomes necessary.

Note that, true molecular dynamic formulation would require *ab initio* data, which takes into account fundamental laws of physics including quantum mechanics. Also, even a less rigorous approach that can output physically interesting data would call for *a priori* knowledge about atomic/molecular structure of the material. For the sake of computation time and engineering efficiency, the above mentioned details are abandoned in this study. Instead, virtual particles are used, that can simulate simple yet practical behavior of engineering materials.

2. Formulation of microscopic model

Instead of using the typical configuration of simplified and real molecules, a brute force approach is used, on the ground of the following assumptions:

1. Microscopic composition of different molecules and congregates are unknown, so that it is assumed that a virtual particle can capture the properties of the actual mixture, in average sense.
2. Since, a virtual particle is employed; control parameters in potentials do not possess physical meaning. The parameters should be determined by fitting a moderately sized micro model to a known macroscopic behavior.
3. Concrete materials are assumed to be a mixture of covalently bonded particles (i.e. a ceramic-like material). In addition, it is assumed that van der Waals force acts on neighboring particles. Van der Waals force is assumed to be different in source from the covalent force, in that no explicitly bonded linkage is required between interacting particles.
4. For the bonded link, a quadratic potential that follows Hook's law is used, and for the unbound link, Lennard Jones potential is used.

The potential used for the covalent bond is

$$U_b = kr_{ij}^2 \tag{1}$$

, where U_b is the bonded potential. k is the spring constant that determines the stiffness of the connection, $r_{ij} = |\mathbf{q}_i - \mathbf{q}_j|$, and $\mathbf{q}_i$ and $\mathbf{q}_j$ are position vectors of particles. The potential is also cutoff at a critical length r_c, so that the spring force is released and local fracture can be simulated.

The Lennard Jones (LJ) potential is the potential under spotlight, in that the popularity of the potential in molecular dynamics is well-known. However, it is also well noted that the LJ potential may be suitable for simulation of some rare gases and long range Coulomb interaction[1], and may not be the perfect approximation of the interaction between crystalline molecules. For the purpose of simulating concrete, the LJ potential is used in case the covalent bonding is broken, so that unbound particles would still repulse other particles in collision. The LJ potential can be expressed as

$$U_u = 4\alpha\left[\left(\frac{a}{r_{ij}}\right)^{12} - \left(\frac{a}{r_{ij}}\right)^{6}\right] \tag{2}$$

where α, and a are control parameters that determine the shape of the potential. Note that, the potential well is located at $r_0 = 2^{1/6}a$.

For the time dependent integration of the system, the Verlet technique[2] is used, such that

$$\begin{aligned} \mathbf{q}_i(t+\Delta t) &= \mathbf{q}_i(t) + \Delta t \times \dot{\mathbf{q}}_i(t) = \mathbf{q}_i(t) + \Delta t \times \mathbf{p}_i(t)/m_i \\ \mathbf{p}_i(t+\Delta t) &= \mathbf{p}_i(t) + \Delta t \times \dot{\mathbf{p}}_i(t) = \mathbf{p}_i(t) + \Delta t \times \mathbf{F}_i(t) \end{aligned} \tag{3}$$

, where $\mathbf{q}_i$ is the position vector, $\mathbf{p}_i$ is its momentum, m_i is the mass of the particle, and F_i is the force derived from the potential. The derivation can be achieved by

$$F_i = \sum -\frac{\partial(U_b + U_u)}{\partial r_{ij}} \tag{4}$$

It is worth mentioning at this stage, that the time step should be small enough to capture the vibrations induced by the LJ potential. For small amplitude, the potential can be expanded around $r_0 = 2^{1/6}a$ so that the radial frequency $\omega = (72\alpha)/(m_i r_o^2)$ can be obtained. From this, it can be deduced that $\Delta t \approx 0.01\omega^{-1}$ would be enough for the simulation.

3. Numerical simulation in micro level

One important, although often neglected aspect should be included as an initial condition in the simulation. The numerical experiment executed in this study assumes the room temperature condition, not the absolute zero temperature condition. The room temperature

condition prescribes that the initial velocity, or momentum p_i are not identically zero, as is almost always assumed at the beginning of classical analysis. The temperature (momentum) distribution should follow the Maxwell–Boltzmann law, which means that the initial velocity of the molecules should be randomized. This condition poses a significant problem on actual simulation, in that

1. The randomized velocity may incur rigid body motion of the system if the sums of all the velocities are non–zero.
2. It is extremely difficult to randomize the velocity filed, so that the Maxwell–Boltzmann's distribution is satisfied.

Hence, a compromise is made by using the average momentum and temperature, that is

$$\left\langle \frac{p_i^2}{2m_i} \right\rangle = \frac{p^2}{2m} = \frac{3k_B T}{2} \tag{5}$$

, where <> denotes the average value, p and m are the fixed initial average values for all particles, and k_B is Boltzmann's constant. In this scheme, magnitude of the momentum is not randomized; instead, directions should be randomized in one complete circular range. Also, for the total number of N particles, only $N/2$ is direction–wise randomized, while the other half is populated with the opposite direction of the counterpart. So that, the unfortunate situation of rigid body motion can be prohibited.

The simulation starts with the equilibrating phase. During the phase, the randomized directions result in randomizing velocities of each particle, while propagating the given energy throughout the system. Then the analysis proper begins, with imposed boundary conditions.

5. Fitting the model with the experimental (global) data.

Three control parameters remain after fixing the remaining two. Mass m is determined by dividing the mass of the control volume by the number of particles, such that

$$m = \frac{\rho V}{N} \tag{6}$$

, where ρ is the mass density (2320 kg/m^3 [3]), V is the volume, and N is the total number of particles. Control parameter a can be fixed by setting the potential well at $r_0 = 2^{1/6}a$ equal to the initial distance between particles, which are uniformly distributed in square grid.

The spring constant k should strongly correlate to Young's modulus (27.6 GPa for normal

strength concretes at 28 days[4]), while the cutoff length r_c should correlate to the peak point on stress-strain curve (approximately 0.006 in Nawy Nawy[4]). Parameter α in LJ potential poses a challenge. It should mainly control the strain softening in stress-strain curve. Hence, sample the stress at strain of 0.008 in Nawy, then use the strain-stress point as a target.

With the three sampled values, the model can be first slowly loaded with force to determine the initial elastic modulus to fix k, then the remaining strain-stress points should be matched by adjusting r_c and α.

6. Results reserved for the presentation.

Due to massive amount of calculation, and the animated nature of the results, presentation of the analysis results is reserved for the conference. The study itself is not, by any means, comprehensive. Hence, technical details of what has been done will also be presented at the conference.

Conclusions will be drawn, and discussion about future research will follow the presentation

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