Stress and Strain Analysis in Molecular Dynamics Simulation of Solids[9]

O. R. Walton[10]. As the authors correctly point out, an expression for the stress due to a system of particles with forces acting between them can be obtained by discretizing the definition of stress in terms of integrals, so that they become summations over forces in an averaging volume. The relationship between stress and interparticle forces (noting that the momentum flux density tensor is equivalent to the stress tensor) is well established, and has been utilized in molecular dynamics calculations for decades. There are two components to the stress tensor, the *kinetic* contribution due to the motion of the atoms or particles (see Chapman and Cowling, 1952), and the *potential* contribution due to the forces of interaction between particles (Irving and Kirkwood, 1950). Evans (1979) pointed out that the stress tensor represented as a sum over particles and interparticle forces

$$\sigma = \frac{1}{V}\sum_i m_i(\mathbf{v}_i - \mathbf{u}_i)(\mathbf{v}_i - \mathbf{u}_i) + \frac{1}{V}\sum_{i>j}\mathbf{F}_{ij}\mathbf{R}_{ij}$$

(where m_i is the mass, $\mathbf{v}_i$ is the velocity of the atom due to microscopic vibrations, i.e., temperature, and $\mathbf{u}_i$ is the average velocity field at the location of particle i and $\mathbf{F}_{ij}$ is the force acting between particle i and j, and $\mathbf{R}_{ij}$ is the vector from the c.g. of particle i to the c.g. of particle j) need not be symmetric, if the forces are noncentral (as can happen for nonspherical molecules or for macroscopic particles interacting via elastic contact forces with friction). The first term in the above expression is the *kinetic* contribution and the second is the *potential* contribution to the stress. The second term is equivalent to what most engineers would consider to be the stress in a material at rest. Cundall and Strack (1983) derive an expression for the stress in a granular material which can easily be shown to be equivalent to the potential contribution to the stress in the above expression. The above summation has been used in the molecular dynamics community for the past three or four decades. Modern texts on molecular dynamics (e.g., Hoover (1986) or Rapaport (1995)) simply treat the above expression as the *definition* of the stress tensor (or pressure tensor).

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A Critical Study of the Applicability of Rigid-Body Collision Theory[11]

A. Chatterjee[12] and A. Ruina[13]. Stoianovici and Hurmuzlu (1996) present an interesting critique of rigid-body collision theory, based on experiments with, and simulations of, slender steel rods colliding with a massive steel object. However, the authors group certain ideas which we feel should be viewed as distinct. We feel their concluding dismissal of rigid-body collision theory is too harsh. In essence, we value the authors' experimental results, but disagree with some of their conclusions. This note is meant to be a partial defense of rigid-body collision theory, in the light of their study.

The authors study rods at various orientations, dropped vertically onto a massive anvil. High-speed photography is used to measure pre and post-collision velocities. It is found, experimentally and through simulations, that bending vibrations in the rod make the collisional interaction complicated. Their study is interesting both because experimental data for two-dimensional or three-dimensional collisions of objects other than spheres and disks is scarce, and because the fairly complicated experimental results are explained nicely with the help of a discrete dynamical model for the rods along with a spring/nonlinear dashpot contact model. Their observed coefficient of restitution varies strongly with orientation for a given slender rod, as well as for rods of different slenderness ratios at a fixed orientation. In their conclusions, the authors say:

> "*Is the coefficient of restitution relatively constant for highly rigid material and low-impact speeds?* The most important outcome is that the rigid-body theory (the invariance of the coefficient of restitution) has a very limited applicability even for highly rigid material and low-impact speeds."

In our opinion, it appears too restrictive to identify "rigid-body theory" with "invariance of the coefficient of restitution." The two (distinct) ideas each have their own strengths and weaknesses. While some pitfalls of special rigid-body collision models are revealed nicely by the authors' data, the most basic aspects of the rigid-body approach are preserved accurately in the system they study. While the dramatic variation they report in the coefficient of restitution is interesting, it is equally interesting to note the consistency of their data with general rigid-body collision modeling.

The system they studied clearly satisfies some of the standard fundamental assumptions of rigid body collision modeling: (i) the changes in the overall rigid-body velocities of the bodies, from just *before* to just *after* the collision, may be described by impulse-momentum relations for rigid bodies, i.e., an equation of the form

$$\mathbf{P} = \mathbf{M}\cdot\Delta\mathbf{V}, \tag{1}$$

where $\mathbf{P}$ is the impulse transmitted, $\mathbf{M}$ is a local inertia tensor, and $\mathbf{V}$ is the relative velocity at the contact point (see, e.g., Smith, 1991) (ii) collision contact forces and accelerations are very large, changes in velocities are bounded, and displacements are very small, (iii) the time of interaction is very small compared to the time scale of overall motions ($\sim$1 msec versus $\sim$100 msec), (iv) contact occurs over a small region that may be approximated as a point for purposes of impulse-momentum calculations, (v) a well-defined common tangent plane exists at the "point of contact," and (vi) kinetic energy is not created in a collision. These assumptions are in fact not very restrictive and are a reasonable model for a large variety of collisions that are of practical interest, including collisions of fairly stiff manipulators.

However, most rigid-body collision models are actually based on *far* more stringent, albeit often implicit, assumptions, about the rigidity of the bodies *during* the collision (e.g., see discussion in Chatterjee, 1997).

Examples of such models include that of Routh (1897), rediscovered recently by Keller (1986), based on infinite tangential stiffness and Coulomb friction, as well as Maw, Barber, and Fawcett's approach (1976), based on Mindlin and Deresie-

[11] Stoianovici, D. and Hurmuzlu, Y., 1996, "A Critical Study of the Applicability of Rigid-Body Collision Theory," ASME JOURNAL OF APPLIED MECHANICS, Vol. 63, pp. 307–316.

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wicz's solution (1953) for spheres under oblique contact forces. Note that the fundamental difference between these two approaches (Routh 1897; Maw et al., 1976) lies in the assumptions about the contact mechanism. Philosophically, the models (Routh 1897; Maw et al., 1976) are very similar. These models rest on an assumption of rigidity that is stronger than that implicit in Eq. (1), since they assume that the interference at any instant *during* the collision can be calculated from the rigid-body motions alone (part (b)). We refer to such "more" rigid bodies as *force-response rigid* (see Chatterjee, 1997). The rods studied by the authors are *not* force-response rigid, because the significant bending vibrations in the rods affect the contact conditions; the interference, and hence the contact force at any instant *during* the collision, is *not* given by the overall rigid-body motions of the rods alone. Similarly, for a constrained system like a manipulator, if significant compliance is present at the bearings, the interference in the contact region depends both on rigid-body motions as well as the joint compliances, and thus is not known solely in terms of the rigid-body motions. Bodies like slender rods, or robotic manipulators, will typically *not* be force-response rigid. However, the assumptions outlined in the second paragraph will still hold. Equation (1) will still be good. We refer to bodies where these assumptions hold to reasonable accuracy as *impulse-response rigid* (Chatterjee, 1997).

Why should one care about rigid-body collision models for general impulse-response rigid bodies, given the apparently viable detailed modeling approach demonstrated by the authors? A possible reason is that in real situations, where the body of interest physically exists, detailed modeling may be too time consuming. Another possible reason is that the body of interest may not be as "clean" as a slender steel rod with hemispherical ends. It might be a robotic manipulator, with each link an assembly of many component pieces that are screwed, glued, press or snap-fitted together, connected to each other with bearings with their own clearances and other unknown characteristics. Many such features, each hard to control precisely during manufacture, will be exactly the features hardest to model during the collisional interaction of such composite bodies. Yet, the *net* response to impulses of such composite bodies will still be well described by Eq. (1). A third reason why detailed modeling might not be possible is that the body of interest may not yet actually exist physically, as is often the case in multibody dynamics simulation environments. In all of these situations, a reasonable approach might be to try and characterize all possible outcomes of a given collision, a task for which rigid-body collision models are quite well suited.

Next, consider the "coefficient of restitution." As Goldsmith clearly states in his classic text (1960), the coefficient of restitution has doubtful fundamental validity. The authors' data clearly demonstrates that e, if such there be, cannot be a property of a material or a body alone. Thus far there is little to argue about. However, it *is* true that for a *given* collision, a ratio of normal components of relative velocities, from before to after a collision can, in principle, be measured. It is also true that for frictionless collisions, the measured ratio *will* be between zero and one. The authors' data clearly demonstrates that for a given collision configuration and given direction of pre-collision relative velocity, and within some range of magnitudes, the normal velocity ratio is roughly independent of velocity magnitude. This independence on velocity magnitude is, we feel, a key feature of the data that bears emphasis. That is, in their experiments the "coefficient of restitution" does depend on body orientation but *does not* depend substantially on velocity magnitude (in the range of their observations).

Thus, while the particular outcomes of the authors' experiment could not have been predicted in advance by rigid-body collision models, the results could indeed have been captured *a posteriori* by reasonable collision models of the form

$$\mathbf{V}_{\text{postcollision}} = \mathbf{f}(\mathbf{M}, \mathbf{V}_{\text{precollision}}, \text{parameters}),$$

for reasonable values of collision parameters. Finally, their graphs of the coefficient of restitution as a function of angle (one dimensionless quantity against another), for different slenderness ratios of the rods (another dimensionless parameter), could, in principle, be incorporated into a simple, special purpose rigid-body collision model of the form given above, which *would* work well for the class of rods studied here, and which might then be used efficiently in numerical simulations of more complicated motions of these rods spanning several collisions.

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