DYNAMIC FRACTURE OF NONLINEAR SOLIDS WITH MULTI-PARTICLE MODELING

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ABSTRACT

Some sorts of fracture are particularly challenging to model because deformations of the materials can nowhere be described as small. The fracture of rubber is of this type. In order to understand such systems, it is valuable to have a numerical method that is able to treat nonlinear deformations and fracture in a single framework, and to make it as simple as possible to introduce new physical ideas about how the physical mechanisms of fracture. The technique of muli-particle modeling achieves this goal. It models a solid as a collection of mass points interacting with each other by two– and three–body forces. The mass points need not be viewed as atoms, but may be mesoscopic. With proper choice of interaction laws, the muli-particle system can be arranged to reproduce desired nonlinear elastic theories in the continuum limit, and to have physically sensible failure properties at small scales. This method has been employed to study supersonic mode I cracks in rubber.

1. INTRODUCTION

Recent experiments in rubber [1]have presented the problem of understanding supersonic tensile cracks in a highly nonlinear solid. Some of the relevant experimental observations are:

1. The speeds of shear and longitudinal waves have been measured in our rubber samples over a range of extensions. From these data, it is possible to determine a unique continuum theory for the rubber, valid over the range of extensions for which measurements were performed.

2. The speed of cracks moving in rubber has been measured, and the crack tips have been photographed. The crack tip speeds lie between the shear and longitudinal wave speeds of the stretched rubber far ahead of the tip, and the shape of the tip is wedge-like, suggesting a Mach cone.

3. However, there is no direct experimental information on how the energy density of the rubber behaves for extensions sufficient to rip polymers apart and allow the crack to propagate.

A numerical method able to deal with this problem should have the following characteristics:

1. It must be capable of reproducing the desired continuum theory in the range of extensions where it is valid.

2. It must be capable of accepting the very large nonlinearities that occur in the vicinity of the tip.

3. It should be simple to explore various ideas for the physics in the highly nonlinear region. The method should make it easy to implement new ideas rapidly, and one should be able to investigate the physical ideas rapidly without concern about whether the numerical method is introducing unphysical instabilities.

These conditions are met by the technique of multi-particle modeling. The idea of multi-particle modeling is to treat the system as a set of interacting nodes obeying Newton's laws. In molecular dynamics, these nodes would be atoms, and the forces between them would be inter-atomic forces. In multi-particle modeling, the nodes can be much further away from each other than atoms, and represent lumped masses. The forces between them are chosen from a mixture of different considerations. First, the forces must be consistent with any facts known from the continuum description of

the solid. Second, the forces should be as simple as possible. Finally, the forces should incorporate reasonable guesses about the interactions of nodes in highly nonlinear regimes, such as at a crack tip, where no direct experimental information is available. Considerations such as these certainly cannot specify a numerical scheme uniquely, but they leave less freedom than one might expect.

One great advantage of multi-particle modeling is that numerical artifacts are very easy to eliminate. Newton's laws acting upon a collection of particles provide a well-posed initial value problem. No matter how nonlinear the problem may be in certain regions in space, one simply does not have to worry about matters such as whether the continuum limit is elliptic or hyperbolic. I will illustrate the method by discussing some of the methods used to study supersonic cracks in rubber.

2. COORDINATE SYSTEM AND ENERGY FUNCTIONAL

Adopt a description of a highly deformed rubber sheet with

$$\vec{r} \mapsto \vec{u}. \tag{1}$$

The original location of all mass points is given by $\vec{r}$ and the location of points after the rubber is moved and stretched is given by $\vec{u}$. Note that $\vec{u}$ is measured from the origin, not from the original location of the mass point $\vec{r}$. Let $W(e)$ be the effective energy per area of the sheet after it contracts as it will along z, and e is the 2–d strain tensor,

$$e_{\alpha\beta} \equiv \tfrac{1}{2}\left[\sum_{\gamma} \frac{\partial u_\gamma}{\partial r_\alpha}\frac{\partial u_\gamma}{\partial r_\beta} - \delta_{\alpha\beta}\right] \tag{2}$$

$$\Rightarrow \sum_{\gamma} \frac{\partial u_\gamma}{\partial r_\alpha}\frac{\partial u_\gamma}{\partial r_\beta} = 2e_{\alpha\beta} + \delta_{\alpha\beta} \tag{3}$$

Since there are two coordinate systems floating about, one must specify which "area" one means in talking about energy per area. Area is measured back in the reference coordinate system. That is, the total potential energy of the system is given by

$$U = \int d\vec{r}\, W\left(e\left(\vec{r}\right)\right). \tag{4}$$

The assumption is that W depends upon $\vec{r}$ only through $\vec{u}$, and through $\vec{u}$ only through the strain tensor. Furthermore, for an isotropic material, only rotationally invariant functions of the strain tensor are allowed. In the theory of a two–dimensional sheet, there are only two possible combinations:

$$J_1 = e_{xx} + e_{yy}; \quad J_2 = e_{xx}e_{yy} - e_{xy}^2. \tag{5}$$

A specific energy functional that describes sound speeds in rubber samples well[2] is the Mooney–Rivlin theory[3]:

$$\frac{W}{\rho} = a\left[J_1 + bJ_2\right] = a\left[\left(e_{xx} + e_{yy}\right) + b\left(e_{xx}e_{yy} - e_{xy}^2\right)\right]. \tag{6}$$

3. MULTI-PARTICLE SCHEME

For the problem of fracture, there are great advantages to thinking in terms of molecular dynamics. From a continuum viewpoint, it is difficult to understand how to construct a physically sensible theory where material gives way. From an atomic viewpoint it is easy; when two atoms are separated

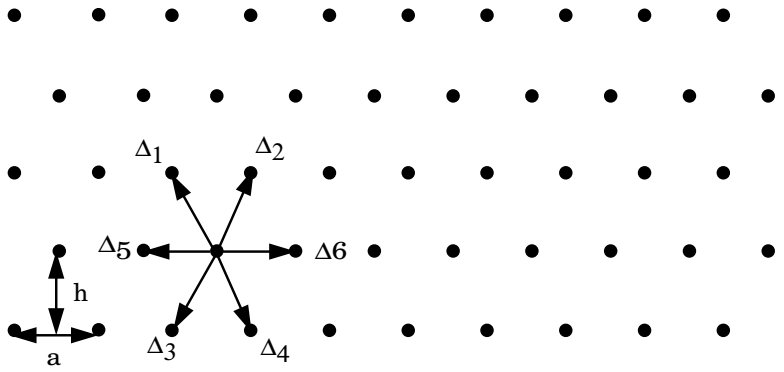

Figure 1: Diagram showing triangular lattice to be used in these simulations.

by more than a certain distance, they stop applying force to one another. Therefore, I search for a simple set of microscopic interactions that produces the Mooney–Rivlin theory of Eq. (6).

The theory involves J_1 and J_2, and these involve quadratic and quartic functions of displacements u. It is possible to construct such theories by considering the following combinations of rotationally invariant operations on nearest-neighbor vectors.

$$F_i = \frac{1}{6} \sum_{j \in n(i)} \left(\vec{u}_{ij} \cdot \vec{u}_{ij} - \Delta^2 \right) \tag{7}$$

$$G_i = \frac{1}{9} \sum_{j \in n(i)} \left(\vec{u}_{ij} \cdot \vec{u}_{ij} - \Delta^2 \right)^2 \tag{8}$$

$$H_i = \frac{1}{27} \sum_{j \neq k \in n(i)} \left(\vec{u}_{ij} \cdot \vec{u}_{ik} + 2\Delta^2 \right)^2 \tag{9}$$

The sums are carried out over the 6 nearest neighbors of point i shown in Fig. 1. To form a correspondence with continuum theory, let

$$u^\alpha_{ij} \approx \sum_\beta \Delta^\beta_{ij} \frac{\partial}{\partial x^\beta} u^\alpha(\vec{r}) \tag{10}$$

Inserting Eq. (10) into each of Eqs. (7) and (8) gives in turn

$$F_i \approx \frac{1}{6} \sum_{j \in n(i)} \left(\sum_{\alpha\beta\gamma} \Delta^\beta_{ij} \frac{\partial u^\alpha}{\partial x_\beta} \frac{\partial u^\alpha}{\partial x_\gamma} \Delta^\gamma_{ij} - \Delta^2 \right) \tag{11}$$

$$= \frac{1}{6} \sum_{j \in (i)} \left(\sum_{\beta\gamma} \Delta^\beta_{ij} \left[2e_{\beta\gamma} + \delta_{\beta\gamma} \right] \Delta^\gamma_{ij} - \Delta^2 \right) \tag{12}$$

$$= (e_{xx} + e_{yy})\Delta^2 = J_1 \Delta^2 \tag{13}$$

$$G_i \approx \frac{1}{9}\sum_{j\in n(i)}\left(\sum_{\alpha\beta\gamma}\Delta_{ij}^{\beta}\frac{\partial u^{\alpha}}{\partial x_{\beta}}\frac{\partial u^{\alpha}}{\partial x_{\gamma}}\Delta_{ij}^{\gamma}-\Delta^2\right)^2 \tag{14}$$

$$= \tfrac{1}{9}\sum_{j\in n(i)}\left(\sum_{\alpha\beta\gamma}\Delta_{ij}^{\beta}\left[2e_{\beta\gamma}+\delta_{\beta\gamma}\right]\Delta_{ij}^{\gamma}-\Delta^2\right)^2 \tag{15}$$

$$= \left[(e_{xx}+e_{yy})^2+\frac{4}{3}\left(e_{xy}^2-e_{xx}e_{yy}\right)\right]\Delta^4 \tag{16}$$

$$= \left[J_1^2-\frac{4}{3}J_2\right]\Delta^4 \tag{17}$$

$$H_i \approx \tfrac{1}{27}\sum_{j\neq k\in n(i)}\left(\sum_{\alpha\beta\gamma}\Delta_{ij}^{\beta}\frac{\partial u^{\alpha}}{\partial x_{\beta}}\frac{\partial u^{\alpha}}{\partial x_{\gamma}}\Delta_{ik}^{\gamma}+2\Delta^2\right)^2 \tag{18}$$

$$= \tfrac{1}{27}\sum_{j\neq k\in n(i)}\left(\sum_{\alpha\beta\gamma}\Delta_{ij}^{\beta}\left[2e_{\beta\gamma}+\delta_{\beta\gamma}\right]\Delta_{ik}^{\gamma}+2\Delta^2\right)^2 \tag{19}$$

$$= \left[(e_{xx}+e_{yy})^2+\frac{20}{9}\left(e_{xy}^2-e_{xx}e_{yy}\right)+4\right]\Delta^4 \tag{20}$$

$$= \left[J_1^2-\frac{20}{9}J_2+4\right]\Delta^4 \tag{21}$$

Therefore

$$J_1=\frac{F_i}{\Delta^2} \tag{22}$$

and

$$J_2=\frac{9}{8}\frac{1}{\Delta^4}\left(G_i-H_i+4\right) \tag{23}$$

The microscopic theory can now be completed. Take

$$U=\sum_i\left[AF_i+B\left\{G_i-H_i+4\right\}\right]. \tag{24}$$

Then

$$\frac{W}{\rho} = \sum_i\left[AF_i+B\left\{G_i-H_i+4\right\}\right]/\sum_i m, \tag{25}$$

$$\rightarrow \int d\vec{r}\left[\Delta^2 AJ_1+\frac{8}{9}\Delta^4 BJ_2\right]/\int d\vec{r}\rho \tag{26}$$

and

$$A=\frac{\rho a}{\Delta^2} \quad \text{and} \quad B=\frac{9\rho ab}{8\Delta^4}. \tag{27}$$

A specific implementation of these ideas is

$$U = U^{(1)} + U^{(2)}$$

with

$$U^{(1)} = \sum_{\substack{i \\ j \in n(i)}} f_{ij} \tag{28}$$

$$U^{(2)} = \sum_{\substack{i \\ j \neq k \in n(i)}} h_{ij} h_{ik} g_{ijk}. \tag{29}$$

Here

$$f_{ij} \equiv f(u_{ij}), \quad h_{ij} \equiv h(u_{ij}), \quad \text{and} \quad g_{ijk} \equiv g(\vec{u}_{ij} \cdot \vec{u}_{ik}), \tag{30}$$

with the following specific forms for f g, and h :

$$f(u) = \begin{cases} \frac{1}{6}A(u^2 - \Delta^2)(u - \Delta)/u_s + \frac{1}{9}B(u^2 - \Delta^2)^2 + 4 & \text{for } 0 < u < u_s + \Delta \\ \frac{1}{6}A(u^2 - \Delta^2) + \frac{1}{9}B(u^2 - \Delta^2)^2 + 4 & \text{for } u_s + \Delta < u < u_c \\ \frac{1}{6}A(u_c^2 - \Delta^2) + \frac{1}{9}B(u_c^2 - \Delta^2)^2 + 4 & \text{for } u \geq u_c \end{cases} \tag{31}$$

$$h(u) = \frac{1}{1 + e^{(u - u_c)/u_s}} \tag{32}$$

$$g(X) = -\frac{1}{27}B\left(X + 2\Delta^2\right)^2, \tag{33}$$

where u_c is the separation at which bonds fracture, and u_s is a short–distance cutoff.

4. APPLICATION

These numerical ideas have been employed to study supersonic cracks in Mooney–Rivlin rubber, and an image appears in Figure 2. The crack in this figure runs at around 20% more than the longitudinal wave speed. The shape of the tip looks very much like the photographs displayed in Reference [2]. Note, however that in Reference [2], all crack speeds are intersonic, while this one is supersonic. This feature of the simulations, and many others remain yet to be worked out, and compared with experiment. However, the basic ideas discussed here are sufficient to permit fruitful numerical study of this difficult nonlinear problem.

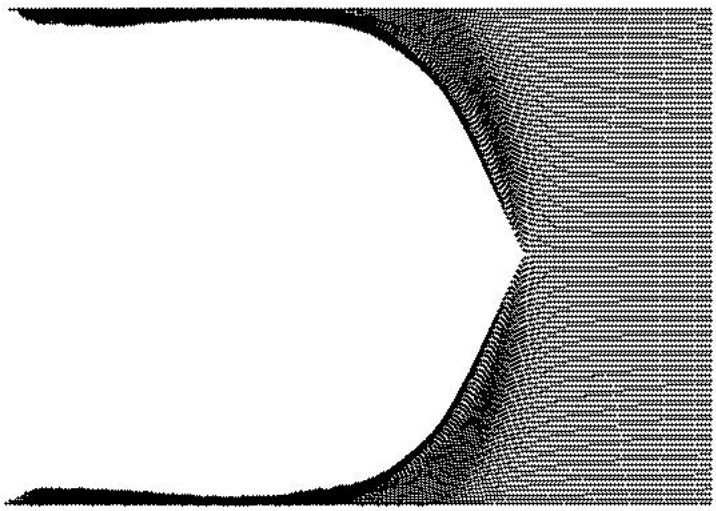

Figure 2: Supersonic crack in Mooney-Rivlin rubber, studied with the method of multi–particle modeling described above. Parameters are chosen to match the experiments in [1, 2]

5. ACKNOWLEDGEMENTS

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[1] R. D. Deegan, P. Petersan, M. Marder, and H. L. Swinney, "Oscillating fracture paths in rubber," *Physical Review Letters*, vol. 88, p. 014304, 2002.

[2] P. J. Petersan, R. D. Deegan, M. Marder, and H. L. Swinney, "Cracks in rubber under tension exceed the shear wave speed," *PRL*, vol. In press, 2004.

[3] L. R. G. Treloar, *The Physics of Rubber Elasticity*. Oxford: Oxford University Press, third ed., 1975.