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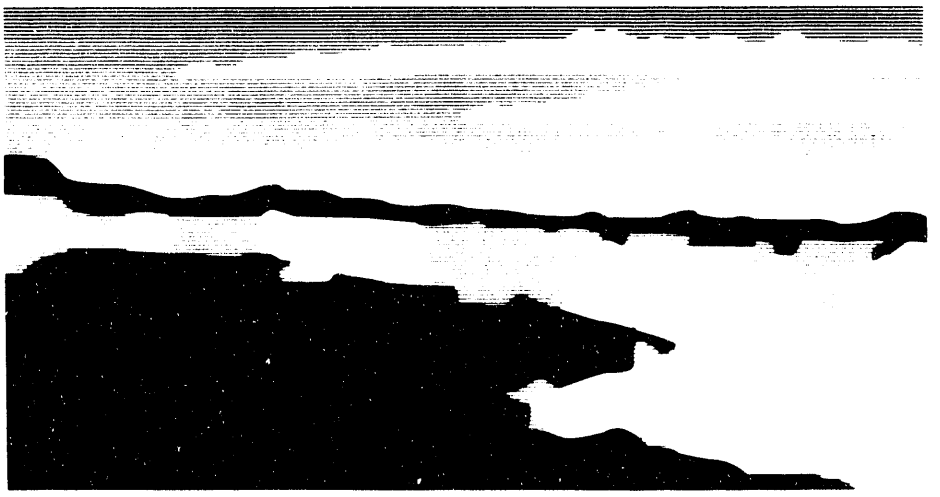

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Fracture simulations via massively parallel molecular dynamics

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ABSTRACT

Fracture simulations at the atomistic level have heretofore been carried out for relatively small systems of particles, typically 10,000 or less. In order to study anything approaching a macroscopic system, massively parallel molecular dynamics (MD) must be employed. In two spatial dimensions (2D), it is feasible to simulate a sample that is 0.1 μm on a side. We report on recent MD simulations of mode I crack extension under tensile loading at high strain rates. The method of uniaxial, homogeneously expanding periodic boundary conditions was employed to represent tensile stress conditions near the crack tip. The effects of strain rate, temperature, material properties (equation of state and defect energies), and system size were examined. We found that, in order to mimic a bulk sample, several tricks (in addition to expansion boundary conditions) need to be employed: 1) the sample must be pre-strained to nearly the condition at which the crack will spontaneously open; 2) to relieve the stresses at free surfaces, such as the initial notch, annealing by kinetic-energy quenching must be carried out to prevent unwanted rarefactions; 3) sound waves emitted as the crack tip opens and dislocations emitted from the crack tip during blunting must be absorbed by special reservoir regions. The tricks described briefly in this paper will be especially important to carrying out feasible massively parallel 3D simulations via MD.

INTRODUCTION

Some of the earliest atomistic simulations of crack propagation by Ashurst and Hoover[1] and Moran[2] involved on the order of one thousand atoms in two dimensions (2D). In these molecular dynamics (MD) simulations of plane-strain tensile loading of a notched triangular-

lattice sample, time and distance scales were extremely small, of the order of picoseconds and nanometers, which invokes a common criticism of the attempts to relate MD simulations to "real-world" laboratory experiments. Moreover, the interaction potential used in these early calculations was very simplistic (two quadratic regions of equal and opposite force constants joined at an inflection point - similar in shape to the familiar Lennard-Jones pair potential; beyond the quadratic regions, the potential is zero, representing a broken bond). Consequently, the blunting of the crack tip by emission of dislocations was seen only at temperatures that were a sensibly large fraction of the melting point. Also, the narrowness of the sample in the transverse direction to the notch further inhibited realistic mechanisms for crack propagation. Moran noted in 1983 that some more intelligent kind of boundary region (such as coupling to a continuum region) was required in order to make further progress in MD simulations. In more recent work, Cheung and Yip[3] have studied the brittle to ductile transition in α-Fe, using a constant-force boundary treatment. Again, their calculations showed that dislocations are emitted from the crack tip, though the size of their 3D system (3000 atoms, or 10 nanometers on a side) was far too small to achieve anything like realistic crack propagation.

In order to model the interior of an "infinite" (i.e., macroscopic) sample being pulled on at its edges, as in a tensile experimental setup, one can either attempt in an MD simulation to apply a constant force to atoms in boundary reservoir regions, or one can constrain reservoir atoms to move at a constant velocity. In either case, as we have found by trying it out, the "clamp" regions at the edges notify the interior notched region of this tension by sending out sound waves toward the center. After a time (of the order of the distance from the boundary to the notch, divided by the sound speed), the velocity profile across the sample can be well approximated by a linear function of distance from the notch outward, which corresponds to a constant initial strain rate. Following this acceleration phase, the material begins to be strained - that is, atoms are forced to expand homogeneously in tension. At a critical strain $\varepsilon_{crit} = \dot{\varepsilon} t_{crit}$ the crack begins to open up. The critical time t_{crit} depends on the inverse of the imposed strain rate $\dot{\varepsilon}$, so that lower strain rates, which are closer to those experimentally achievable in laboratory experiments, cause greater expense in MD simulations if nothing is done to circumvent this so-called "induction time." Next, as we will show, the opening of the crack causes emission of sound waves (which can rattle around in the computational MD volume if left unattended, even in systems where periodic boundary conditions are imposed). Later, plastic flow causes the crack tip to blunt, as dislocations are emitted from the crack tip and slippage occurs . The mobile dislocations and their attendant sound waves eventually reach the edge of the computational cell and must be dealt with in the simulation, so that they do not come back to the region of crack propagation and perturb it in an unphysical way. All of these considerations lead to the adoption

of three schemes to make MD fracture simulations resemble more closely the interior response of a material to uniaxial tension: constant strain-rate (linear expansion-velocity profile) initial conditions, absorbing reservoir-region boundary conditions, and kinetic-energy quenching of pre-strained free surfaces.

FRACTURE BOUNDARY CONDITIONS

We have employed uniaxial, homogeneously expanding periodic boundary conditions to mimic the interior region of a macroscopic sample being pulled apart at the edges. This kind of boundary condition was first proposed by Holian and Grady to study fragmentation of a fluid.[4] A constant Lagrangian strain rate (in the x-direction, say) is imposed by adding to the x-component of each atom's thermal velocity a term proportional to its x-coordinate, namely $\dot{\epsilon}x$. The sidelength of the computational box in the x-direction increases with time as

$$L_x(t) = L_x(0)\left[1 + \dot{\epsilon}(0)t\right] \quad , \tag{1}$$

so that, for example, the righthand periodic boundary moves at a constant velocity $\frac{1}{2}\dot{\epsilon}(0)L_x(0)$. When particles cross the periodic boundaries, their velocities must be adjusted in magnitude by twice the boundary velocity, with the sign chosen so as to preserve the sense of expansion. Wagner and coworkers subsequently verified by MD simulations that spallation experiments, which cause fracture by shock waves and their subsequent release, produce linear velocity profiles about the spall plane.[5] They then used this same kind of homogeneous expansion to map out the failure stress (and strain) as a function of strain rate.

In our earliest fracture simulations over a year ago, we began by imposing a high strain rate on a notched 2D Lennard-Jones (LJ) crystal. Expanding periodic boundary conditions and a commensurate linear velocity profile were imposed in the direction transverse to the direction of the notched free surface (the notch angle was chosen to be 20^o so that its surface was atomistically rough). In LJ units of inverse time, a strain rate of unity would imply that atoms move apart from each other with a relative velocity about 10% the speed of sound; in our earliest experiments, the strain rate of 10^{-2} in LJ units (about 10^{10} per second in engineering units) was therefore well below the sonic expansion limit. We quickly discovered that even this rate is too much for the notched sample to bear. At an initial temperature of about 1/4th melting, ductile holes were nucleated throughout the sample, wherever the local thermal fluctuations led to low density. Rather than opening up the crack at the notch tip , the entire sample pulled apart plastically, like taffy. When we reduced the temperature to almost zero, we obtained

qualitatively similar results. At 1/4th the melting temperature, but at a strain rate one order of magnitude lower, we observed somewhat less pronounced catastrophic plastic failure. By reducing the temperature to nearly zero, however, we found that the crack began to open up in a brittle fashion, namely, by bond-breaking at the notch tip in response to a critical stress concentration. The induction time to reach this critical strain of 2.5% was about 25 LJ time units. Sound waves were emitted by the bond-breaking process (the measured velocity of the waves was about 90% of the longitudinal sound speed). Soon after the crack opened up by about 10 lattice spacings in the forward direction, pairs of dislocations were emitted from the crack tip, moving off along the slip lines at $\pm 60^{o}$ at a velocity of around half the longitudinal sound speed. These mobile dislocations themselves emit sound waves. Accompanying the dislocation emission, the crack would bend slightly and finally bifurcate. As sound waves from periodic images of the crack converged on the central region, the crack would arrest its forward motion, and the crystal would fall apart homogeneously, opening up penny-shaped voids ahead of the notch.

Our preliminary simulations were carried out on the Connection Machine CM-200 for 2D crystals consisting of 32,000 or 65,000 atoms. Because of the interference of sound waves from the periodic images, we increased the system size to 300,000 atoms, using the new, larger CM-5. Then, at the strain rate of 10^{-3} (LJ units), the crack could propagate much farther before sound waves and emitted dislocations from the periodic images would cause crack arrest. Since we had not yet found the strain rate at which purely brittle crack opening could be seen, we carried out simulations at a strain rate of 10^{-4} ($\approx 10^{8}$/s). As expected, the induction time before crack extension occurred went up an order of magnitude. The frequency of dislocation emission went down considerably, but did not disappear - the brittle regime must therefore be at even lower strain rates. The induction time now becomes a serious issue in further fracture studies, since we would like to focus our computational energies and resources on the crack propagation itself.

To test the effect of the interaction potential on the crack process, we also looked at the Morse pair potential and the embedded-atom-method (EAM) many-body potential, which is appropriate to metals, and which has significantly lower vacancy and surface formation energies. The Morse potential was chosen to mimic the EAM equation of state, including bulk sound speed (roughly half that of the LJ system; these potentials are described, along with their affect on plastic flow, elsewhere.[6]) The results for crack length as a function of time are shown in Figure 1. Other than differences in the slope (crack velocity) that can be explained on the basis of sound speeds of the three materials, not much new is seen in brittleness vs. ductility, at least at these strain rates, though the EAM system clearly exhibits more plasticity than its Morse counterpart.

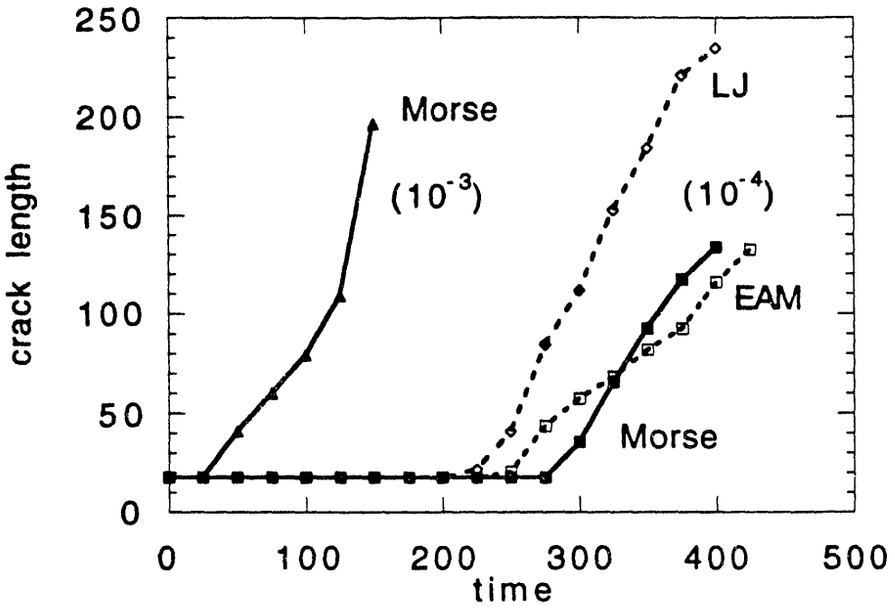

Figure 1. Crack extension as a function of time for 2D Morse, EAM, and LJ crystals at a strain rate of 10^{-4} (in LJ units of inverse time), and for the Morse crystal at a strain rate of 10^{-3}.

We studied the dependence of these fracture simulations on system size (or in other words, on boundary conditions) by comparing the results of imposing a strain rate of 10^{-4} on two LJ crystals differing only in their widths transverse to the notch direction. The first was composed of 300,000 atoms and had an aspect ratio of unity, while the second was twice as wide and contained 600,000 atoms. The two systems are shown at a time of 350 (approximately 75 LJ time units after crack initiation) in Figure 2a (300,000) and 2b (600,000). In Figure 2a, the full periodic system is shown, while in Figure 2b, only the central half is shown at the same scale. In the latter, the dislocation cores from the forked crack show up as dark clusters moving out at $\pm 60^{\circ}$ from the vertical (crack propagation direction). The dark, flat patterns immediately above the forked crack are sound waves that have been emitted from the slippage accompanying the dislocation cores. The sound waves emitted from the crack opening due to bond breakage have already bounced off the top free surface and appear as a family of concave upward arcs that intersect concave downward arcs from later bond-breaking events. In the smaller system in Figure 2a, sound waves moving sideways from neighboring periodic images have converged throughout most of the lower part of the sample, forming a cloud of dark spots. Notice that in

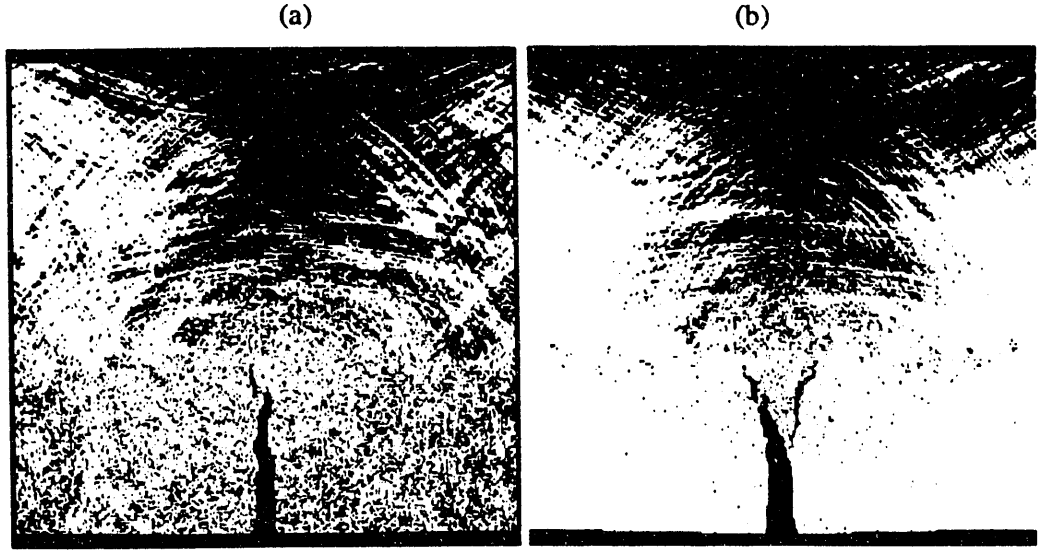

Figure 2. Fracture simulation in 2D LJ crystal under periodic boundary conditions at a strain rate of 10^{-4} (in LJ units of inverse time); (a) 300,000 atoms, aspect ratio = 1, entire sample shown; (b) 600,000 atoms, aspect ratio (horizontal/vertical) = 2, middle half of sample shown - same area as in (a).

this case, the crack has been prevented from forking and is, in general, narrower than in Figure 2b. Otherwise, many of the features are the same. This comparison shows dramatically the importance of treating the boundary regions intelligently in MD simulations of fracture. If care is not exercised, the conclusions drawn from samples that are too narrow will be qualitatively, as well as quantitatively, wrong.

RESERVOIRS AND OTHER TRICKS

The preceding simulations have motivated us to examine, albeit in a rather Edisonian fashion, a variety of treatments of the reservoir regions, whose principal purpose is to absorb sound waves and mobile dislocations that have been generated in the process of crack propagation. The first continuous-potential, nonequilibrium MD simulation, carried out by

Vineyard and coworkers[7] for a radiation damage cascade, introduced not only the Stoermer central-difference integration method, but also the use of surface reservoir atoms, whose sole purpose was to damp outgoing shock waves arising from the atom initiating the collision cascade (having been struck by a high-energy neutron). The surface atoms were attached to fixed lattice sites by harmonic springs, and their velocities were damped by viscous dashpots tuned to the critical damping of longitudinal sound waves. In our case, we need to be able to absorb dislocations, too, so that, were we to use the Vineyard group's approach of fixing atoms in the reservoir, we would be preventing dislocation outflow. Thus, in all the methods we considered, we assumed that the reservoir was open, that is, atoms could enter or leave the reservoir region at will, but once they had crossed over into "no-man's land," anything could be done to their equations of motion. Apart from initial conditions and these boundary conditions, atoms in the central sample region - "The Meat" in the sandwich - always obey Newton's equations of motion. A variety of energy or temperature controls are now available, beyond simple viscous damping of velocities. We will now outline the methods we have tried and our assessment of them. They were all tried out in 1D simulations of a velocity pulse in a harmonic chain; once the most successful method was found, it was tried in a 2D simulation. (Some of them were tried out in 2D and found to be unsuccessful, but the expense of exploring methods and the parameter space associated with them forced us to return to 1D for these systematic studies.)

Velocity rescaling. The kinetic energy of the reservoir region can be controlled at each time-step so as to conform to a fixed temperature by rescaling velocities. The kinetic energy is related to the imposed temperature T and the expansion velocity profile $\boldsymbol{u}$ [see Eq.(1)] by

$$K = \sum_{i=1}^{N} \tfrac{1}{2} m_i |\mathbf{u}_i - \mathbf{u}(x_i)|^2 = K_0 = \tfrac{1}{2} dNkT \quad ,$$
$$\mathbf{u}(x_i) = \dot{\varepsilon}(t) x_i \hat{\mathbf{x}} \quad , \quad \dot{\varepsilon}(t) = \frac{\dot{L}(t)}{L(t)} = \frac{\dot{\varepsilon}(0)}{1 + \dot{\varepsilon}(0) t} \quad . \tag{2}$$

(Here N is the number of atoms in the reservoir.) The inclusion of the position-dependent velocity profile in the direction of expansion is crucial, especially for wide reservoir regions, as we found by trial and error. Nevertheless, such a thermostatting method looks like a hard wall to incoming velocity wavetrains, even though the effect of rescaling is a perturbation on each atom in the reservoir of order $N^{-1/2}$. Thus, we tried another, possibly more gentle thermostat.

Nose'-Hoover thermostatting. Instead of imposing a rigid constraint on the kinetic energy in the reservoir, applying the deterministic feedback method of Nose'-Hoover[8] ensures that the time-average kinetic energy is the imposed value, K_0. However, even this more gentle approach

to controlling the temperature due to incoming pulses behaves like a hard wall, reflecting them back into the sample region.

Light-mass reservoir atoms. We thought that making the reservoir atoms light would absorb incoming wavetrains, but again, this mismatch causes reflections just like a hard wall.

Viscous damping. The velocities of atoms in the reservoir (subtracting off their local imposed expansion velocity) are damped by a force that is linearly proportional to velocity, with a single constant damping coefficient for the whole reservoir. Even though this approach worked tolerably well for Vineyard, it did not work well in our case, primarily because of the mismatch in dynamics across the reservoir-sample interface. It also has the disadvantage that it can be applied only in the case of nearly zero temperature, which is not yet a disadvantage in our present search for the brittle-ductile transition in 2D. This led us to the method that has proved most successful.

Ramped viscous damping. We imagined that, like a sandy beach in Barbados, waves would be more gently absorbed if the damping coefficient applied to atoms in the reservoir gradually increased linearly from zero (Newton's equations of motion) at the sample interface to a value that critically damps the highest frequency oscillations at the outer extremity of the reservoir. 1D simulations of a wavetrain in a harmonic chain showed that, indeed, essentially all frequencies could be absorbed by 10 to 20 reservoir atoms, with little reflected noise. Preliminary 2D fracture simulations show that waves are indeed nicely damped and not much reflected by this reservoir technique. Further tests are underway.

Having found a likely method for eliminating unwanted reflections from the outer boundaries of fracture simulations, we needed to resolve the induction-time problem, namely, the need to pre-strain the notched crystal to the point of imminent crack propagation before applying the initial expansion velocity profile. This will be essential to simulations at lower strain rates than 10^8/s, and especially so in 3D. Imposing a homogeneous strain of, say, 2.5% is straightforward: one simply scales coordinates by 1.025. However, at the notched lower and smooth upper free surfaces, the atoms will tend to rush back towards their fellows in the bulk, causing a compressive sound wave to snap back into the material. This led us to consider annealing the surfaces by three dynamical MD-like methods. (Another popular approach, simulated annealing, is stochastic in nature: random Monte Carlo moves are made, one atom at a time, until the minimum potential energy is achieved. Especially in our case, where homogeneous strains are being annealed, the correlated motion allowed by dynamical methods is inherently preferable.)

1) Viscous damping slowly bleeds kinetic energy away until the sample reaches a minimum in potential energy and a minimum state of stress. Unfortunately, at very low temperatures, it takes a great deal of time for the system to move towards a potential minimum, and then that motion is opposed by the frictional velocity-dependent force.

2) Steepest-descent annealing assumes that near the potential minimum, the displacements will be small, so that the force on an atom can be expanded in a Taylor series:

$$\begin{aligned} 0 = \mathbf{F}_i(\mathbf{x}_i) &= \mathbf{F}_i(\mathbf{x}_i^{\,0}) - \frac{\partial \mathbf{F}_i}{\partial \mathbf{x}_i}(\mathbf{x}_i^{\,0}) \cdot \left(\mathbf{x}_i - \mathbf{x}_i^{\,0}\right) + \cdots \\ \Rightarrow \quad \mathbf{x}_i &= \mathbf{x}_i^{\,0} + \frac{\mathbf{F}_i(\mathbf{x}_i^{\,0})}{m_i \omega_i^{\,2}} + \cdots \quad . \end{aligned} \tag{3}$$

The frequency ω_i in the above equation is, of course, not easily available since it depends in general on the many-body dynamical matrix of quasiharmonic lattice dynamics. "Steepest descent" is thus replaced by "blind descent," and the coefficient multiplying the acceleration is usually chosen to be a suitably small constant. We found that this method, being the safest approach to the minimum annealed configuration, converges well but is much too slow.

3) Kinetic-energy quenching was tried first by Bill Moran[2] (and independently reinvented by Ravelo for surface reconstruction studies). Starting at the pre-strained state with zero initial velocities, standard MD is performed, with a much larger time-step than is customary. After a while, the potential energy reaches a minimum and then begins to rise, at which point the kinetic energy peaks and begins to decline. When this is detected, the velocities of all particles are set to zero, and the procedure is continued until the maximum force on any particle in the system has fallen below some small absolute value. This procedure is less cautious in its approach to a global-minimum annealed configuration than "blind descent." The final state that would have been reached by steady adiabatic expansion is actually more closely achieved by kinetic-energy quenching than the other methods, and also reached in much less time than in adiabatic expansion, typically a few hundred steps. At the slowest strain rate we have studied to date, we find that adiabatic expansion takes on the order of 50 times longer in computer time than the annealing by kinetic-energy quenching.

CONCLUSIONS

Massively parallel molecular dynamics simulations make it possible to study fracture at the atomistic level in samples that are far more macroscopic in extent than ever before. Nevertheless, the severe time and space limitations of MD require that clever boundary conditions be applied so as to mimic a large system embedded in an "infinite medium." Crack initiation is achieved most efficiently by imposing a linear velocity profile transverse to the propagation direction (pointed to by a notch in the sample). We have shown that even apparently innocent reflected sound waves can affect crack morphology by inhibiting or healing bifurcations, for example. We have therefore investigated a number of reservoir methods for absorbing sound waves and dislocations emitted from the crack tip. The best method that minimizes the mismatch between reservoir and sample appears to be a linear ramping of the viscous damping coefficient for reservoir-atom velocities that differ from the imposed linear expansion-velocity profile. We also studied ways to anneal the free surfaces of a sample prestrained to the point of incipient crack propagation, eliminating the induction time of building up to the critical strain by adiabatic expansion. Kinetic-energy quenching of a prestrained crystal can save a factor of 50 in computing time. These tricks become more and more important at lower strain rates and will be crucial to the study of realistic fracture in 3D systems.

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