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Do Big and Little Earthquakes Start Differently?

John E. Vidale

The general question for short-term earthquake prediction is whether or not the rupture plane of an earthquake undergoes some preparatory process that may be detected in the seconds, days, or years prior to failure. This crucial question has separated optimistic and pessimistic seismologists for decades. The unexpected 1992 Landers earthquake (magnitude M = 7.3), for example, ruptured a plane that spanned several hundred square kilometers, so detection of a preparatory process across a significant fraction of that plane would have waved a red flag indicating impending earthquake mayhem to the appropriate authorities.

In the 1970s, rock dilatancy (that is, the expansion of rock caused by formation of voids) was proposed to provide such a danger flag (*1*). Dilatancy is caused by tensile cracks opening just before shear failure and has been well documented in the laboratory. It causes swelling and changes in seismic wave velocities and possibly attenuation just before rock fractures. Observations from the former U.S.S.R., New York, and California, including the Palmdale Bulge, suggested that large volumes of rock underwent dilatant changes that could have been measured with seismic or geodetic methods. Subsequent studies, most recently and most precisely with repeating earthquakes for the case of the 1989 Loma Prieta earthquake (*2*), show that signals of dilatant changes before earthquakes are far smaller than first suspected and not easy to see.

It is not hopeless to look for precursors to earthquakes, however. There is clearly more to earthquake loading than gradual plate tectonic movement steadily pushing faults toward failure. Such a simple model would predict that earthquakes would correlate with Earth tides, which is not observed (*3*) and is not expected from models of slip initiation, on the basis of laboratory observations of friction (*4*). In addition, there are observations of decreased and increased seismicity (*5*) preceding large earthquakes. There are also recent claims of precursors with the potential to predict earthquakes (*6*, *7*). These schemes rely on electrical and electromagnetic signals in the days before an earthquake occurs, but a wide range of possibilities have been entertained in the last few decades. Any short-term precursory patterns that proved reliable would require a preparatory stage to seismic failure.

Shifting science. An earthquake that struck in 1992 caused this rupture, which shifted Reche Road in Landers, California. After the rupture, the edge of the far section was aligned with the center line of the near section. Knowledge of how such earthquakes are initiated may reveal whether the existence of a preparatory stage could be used for earthquake prediction. [AP/Wide World]

Because the demonstration of an aseismic preparatory process has proven elusive, researchers have tackled the more resolvable problem of whether big and small earthquakes, such as M = 7 compared to M = 4, start differently (*8*). One hypothesis is that such a difference might indicate that larger earthquakes start by spreading across a larger "prepared" zone. The preparation zone might differ from a normal interseismic fault surface in a variety of ways. It might be the locus of very slow strain or anomalous variation in porosity and fluid pressure, or it may show symptoms of self-organized criticality. If larger earthquakes start from larger prepared zones, then a few seconds of warning could be gained by estimating the eventual size of an large earthquake shortly after it starts, and seismologists could hunt for prepared zones as a method of earthquake prediction.

A slow initial stage in earthquakes is expected from frictional models. These models can also explain many features of foreshocks and aftershocks as well as the lack of earthquake correlation with the tides (*4*). In this model, the slow beginning is the result of rupture initiation in a zone that is too small for stable crack propagation. Indeed, a difference between the start of big and little earthquakes has been inferred (*9*, *10*), with the sense that rupture starts more slowly for larger earthquakes. However, the inferred size of the zone, 15% of the ultimate rupture surface (*9*), conflicts with other studies that find that large and small events start similarly (*11*) and with the lack of strain precursors to earthquakes (*12*), unless precursory strains are quite small.

The simplest interpretation of the lack of a correlation between earthquakes and Earth tides is that earthquake nucleation zones exist. However, our ability to detect the precursors to earthquakes relies on their area or volume being large enough to be reliably found. The area in frictional models depends on the scale length of the roughness of the fault surface, which is not well-known and therefore is difficult to estimate. It is clear from the properties of the smallest earthquakes that their entire seismic rupture spans only tens of meters (*13*), so their nucleation zones must be even smaller.

The chore ahead is to determine whether earthquakes of all magnitudes start from similarly tiny nucleation zones, which would probably cause prohibitive difficulties for short-term earthquake prediction. Alternatively, if nucleation size is a roughly constant fraction of rupture length (*9*), we may be able to spot the nucleation of large earthquakes before damage is inflicted. So far, the more tenacious obstacle to progress is the difficulty of directly detecting aseismic nucleation, even for potentially large zones like Landers (*14*).

With the latest seismic results, debate continues unabated about whether it is practical to predict earthquakes days ahead of time or even possible to predict the magnitude of an earthquake as late as when it is well under way.

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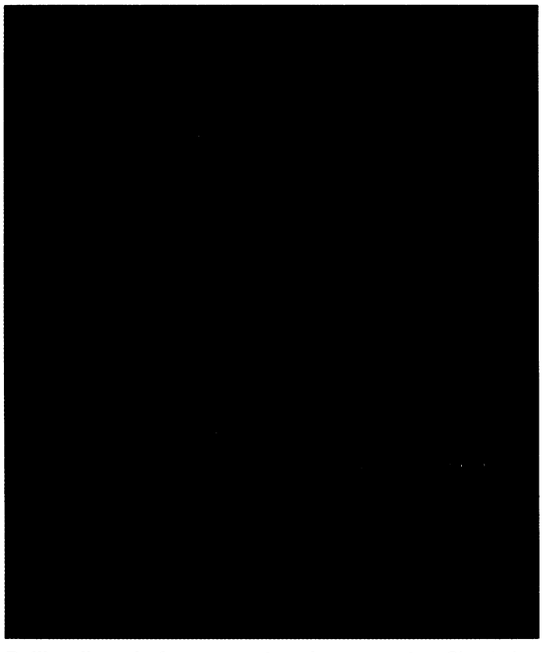
Bio-Molecular Dynamics Comes of Age

Herman J. C. Berendsen

Molecular dynamics (MD) as a computational technique for simulating the motion of atoms has been around since the late 1960s and has been applied to proteins since the mid-1970s. Limited computer resources and limited accuracy of available expressions for molecular force fields have for a long time fed doubts about the applicability of MD to real biological problems, but the tide is turning. Present-day computers, a thousandfold more powerful than those in the late 1970s, can simulate a system of tens of thousands of atoms as it evolves over times of nanoseconds (*1*). Thus, all of the necessary solvent molecules and long-range interactions can be included and most of the local fluctuations can be equilibrated to yield information on realistic time scales. Once a particular application has been validated by critical comparison with experiment, MD yields a wealth of insight into the atomic details of a biomolecular process.

Molecular dynamics methods have the advantage that they are not limited to equilibrium states but can be used to simulate nonequilibrium processes. Motions on a molecular scale, which are not often accessible to experiment, are sampled by MD. Hence, validation is generally indirect and subject to statistical traps. In 1994, Gaub's group succeeded in measuring the adhesion force between a single ligand and a receptor (*2*, *3*). Now, on page 997 of this issue, Grubmüller *et al.* (*4*) report on a simulation of the atomic force microscope (AFM) experiment by MD and find excellent agreement with experiment for the rupture force between ligand and receptor. The system studied is the binding of biotin (a vitamin with 16 heavy atoms) to streptavidin, a 159-residue protein that normally occurs as a tetramer with specific and strong binding to biotin. The tetramer was studied with AFM, along with the similar protein avidin and with biotin analogs; the simulations were performed on the smaller monomer in a complex with biotin and surrounded by a sphere of water, the total system comprising nearly 11,000 atoms.



Pulling ligands from receptors by computer. Simulation of molecular rupture as an AFM tip pulls the biotin ligand, causing unbinding and rebinding at different sites. The biotin is attached to a mechanically compliant agarose bead, shown as a spring. Careful computer pulling reveals binding pathways, identifies bottlenecks in the binding process, predicts rupture forces, and estimates free energies of binding. [Computer graphics: H. Grubmüller, University of Munich]

In the experiments, biotin molecules were attached to an agarose bead, and the rupture (or adhesion) force was 160 pN for avidin and 250 pN for streptavidin. To get an impression of the size of these piconewton forces, consider that a force of 300 pN (or much less in an aqueous environment) will rupture a hydrogen bond between two isolated water molecules, but more than 30,000 pN is needed to rupture a covalent carbon-carbon bond. Grubmüller *et al.* (*4*) simulated several pulling rates and found that their values could be accurately and linearly extrapolated to zero pulling rate, yielding the experimental force of 250 pN. It is most interesting that over a path of 9 Å, the ligand keeps sticking to the protein through continuous rearrangement of hydrogen-bonding networks. In the region where the rupture force (that is, the maximum free energy gradient) occurs, the free energy is dominated by enthalpic effects. It is therefore not surprising that the experimental rupture force for several ligands appears to be correlated with the enthalpy, rather than the free energy, of binding (*3*), although proper understanding of this observation needs some further thought.

The feasibility of following a molecular "unbinding" process within 1 ns is consistent with our own experience that local structural rearrangements in proteins, including those that involve water reorganization, can be reasonably probed in 1 ns. The full trajectory of configurations over 1 ns contains the necessary information to analyze the possible internal dynamics of a protein in solution. From such a trajectory it is possible to determine those collective degrees of freedom in which the molecules can really move. It turns out that 90% of the molecular displacement can be described by only a few (10 to 30) collective degrees of freedom. This reduces in principle the description of the mechanics of a protein to a few "essential" degrees of freedom and allows much more efficient probing of the available configurational space (*5*).

Not all motions are grasped in a nanosecond, however: Secondary structure elements, even isolated helices, are often slower to fold or unfold. But tens of nanoseconds (computationally feasible in a few years time) will suffice to bring such processes within reach. Further folding into tertiary structures is farther away and still beyond sight; MD is not a theoretical panacea ex-

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