Local Hyperdynamics

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After a brief introduction to the accelerated molecular dynamics approach for reaching long times in infrequent-event systems, I will present a new, local formulation of the hyperdynamics method that makes it suitable for very large systems. In standard hyperdynamics, the requirement that the bias potential be zero everywhere on the dividing surface bounding the state has the consequence that for large systems the boost factor decays to unity, regardless of the form of the bias potential. In the new method, the bias force on each atom is obtained by differentiating a local bias energy that depends only on the coordinates of atoms within a finite range D of this atom. This bias force is thus independent of the bias force in distant parts of the system, providing a method that gives a constant boost factor, independent of the system size. Although the resulting dynamics are no longer conservative, for a homogeneous system (all atoms equivalent) using a simplifed bond-boost bias potential, the bias forces in any local region are equivalent to those in a system accelerated by a specific boost factor, except for additional error forces that balance in a time average. For inhomogeneous systems, the errors relative to an exactly accelerated dynamics should decay roughly as 1/D. I will demonstrate that for some realistic atomistic systems that the method gives escape rates in excellent agreement with direct molecular dynamics simulations.