

## Hybrid MC (§14.2 in F+S)

Main differences between MD + MC:

- MD updates all particle positions at once, MC only one at a time
- MD moves have 100% "acceptance" MC can be much less
- MC can execute unphysical moves, overcome time scale issues, jump over barriers

Why not try to combine the two?

\* Force-bias MC: attempt to move particles in the direction of forces pushing them; Increased acceptance, higher cost

\* Hybrid MC: "Bad" MD as MC

- Perform MD simulations w/ time step too long for energy conservation
- After system has evolved for some time, accept/reject w/ Metropolis  $P_{acc} = \min(1, \exp(-\beta \Delta U))$ , reset velocities

E.g. Forrest + Suter Mol. Phys. 82:293 (1994)

- Time step + evolution time need to be optimized. Only modest improvements in efficiency found.