HYBRID ALGORITHMS

We wish to simulate a system with potential $U(r_1, \dots r_N)$

The idea is to enlarge the configuration space adding "momenta"

$$\pi(\vec{p}, \vec{r}) = \exp\left(-\frac{\beta}{2Q} \sum_i p_i^2 - \beta U(r_1 \dots r_N) \right)$$

The parameter Q is a free parameter in the simulation unrelated to the real mass of the molecule

The basic hybrid move is the following

ⓐ Generate $\bar{p}_i$ as independent Gaussian variables of variance Q **Correction: Q-> Q/beta**

ⓑ Perform N_{MD} molecular-dynamics iterations (using e.g. Verlet) with time step Δt starting from $\{r_1 \dots r_N\}$ and $\{p_1 \dots p_N\}$
At the end we obtain $\{r_1' \dots r_N'\}, \{p_1' \dots p_N'\}$

ⓒ Perform a standard Metropolis check
If H_{tot} is the full Hamiltonian, compute

$$\Delta H = H_{tot}(r_i', p_i') - H_{tot}(r_i, p_i)$$

and perform a standard Metropolis accept/reject check

This algorithm can be easily justified

1) The enlargement of the configuration space is harmless:
averages over the coordinates are the same

2) We use MD to generate a proposal

$$(r_1 \dots r_N, p_1 \dots p_N) \longrightarrow (r'_1 \dots r'_N, p'_1 \dots p'_N)$$

Verlet is reversible and phase-space conserving
Therefore, the proposal is <u>symmetric</u>
We can thus use the usual Metropolis check

<u>NOTE</u>: in the Verlet approach H_{tot} is "almost" conserved, so that ΔH is small

$\Downarrow$

These moves have a high acceptance rate.