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

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

\[
\mathcal{H}(\vec{p}, \vec{r}) = \exp \left( -\frac{\mathcal{H}}{2\alpha} \sum_i p_i^2 - \beta U(r_1, \ldots, r_N) \right)
\]

The parameter \( \alpha \) is a free parameter in the simulation unrelated to the real mass of the molecule.

The basic hybrid move is the following:

1. Generate \( \vec{p}_i \) as independent Gaussian variables of variance \( \alpha \)  
   Correction: \( Q \rightarrow Q/\beta \)

2. Perform \( N_{MD} \) molecular-dynamics iterations (using e.g. Verlet) with time step \( \Delta t \) starting from \( \{r_1, \ldots, r_N\} \) and \( \{p_1, \ldots, p_N\} \)
   At the end we obtain \( \{r'_1, \ldots, r'_N\}, \{p'_1, \ldots, p'_N\} \)

3. Perform a standard Metropolis check
   If \( H_{\text{tot}} \) is the full Hamiltonian, compute
   \[
   \Delta H = H_{\text{tot}}(r'_1, p'_1) - H_{\text{tot}}(r_1, p_1)
   \]
   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
   \[(r_1, \ldots, r_N, p_1, \ldots, p_N) \mapsto (r'_1, \ldots, r'_N, p'_1, \ldots, p'_N)\]
   Verlet is reversible and phase-space conserving.
   Therefore, the proposal is symmetric.
   We can thus use the usual Metropolis check.

\textbf{Note}: in the Verlet approach, \(H_{\text{tot}}\) is “almost” conserved, so that \(\Delta H\) is small.

\(\downarrow\)

These moves have a high acceptance rate.