Implicit Solvent vs. Explicit:

- Advantages:
  - Faster (fewer atoms).
  - Reduced viscosity allows faster sampling of conformations.
- Disadvantages:
  - Approximation.

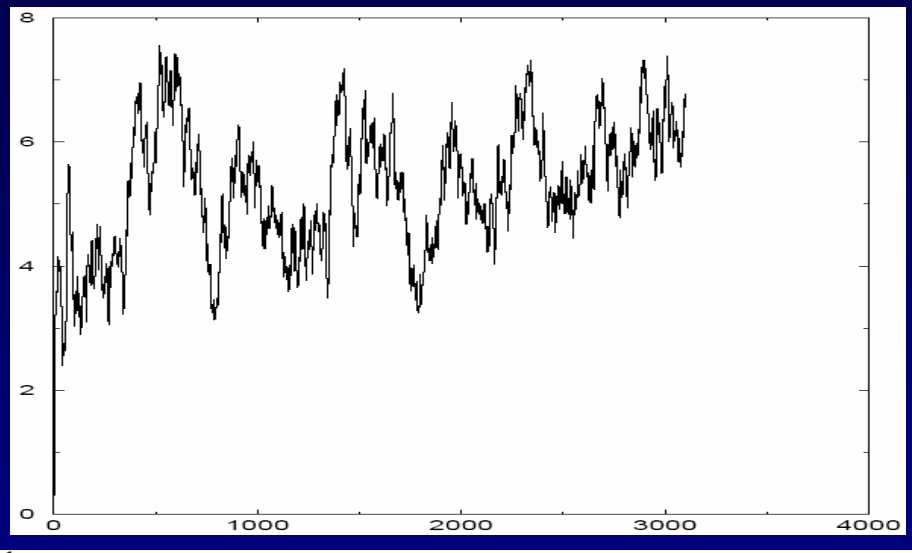
RMSD:

$$\mathrm{RMSD} = \sqrt{\frac{\sum_{1}^{N} (r_{sim} - r_{exp})^2}{N}}$$

Commonly used method for assessing the quality of a simulation.

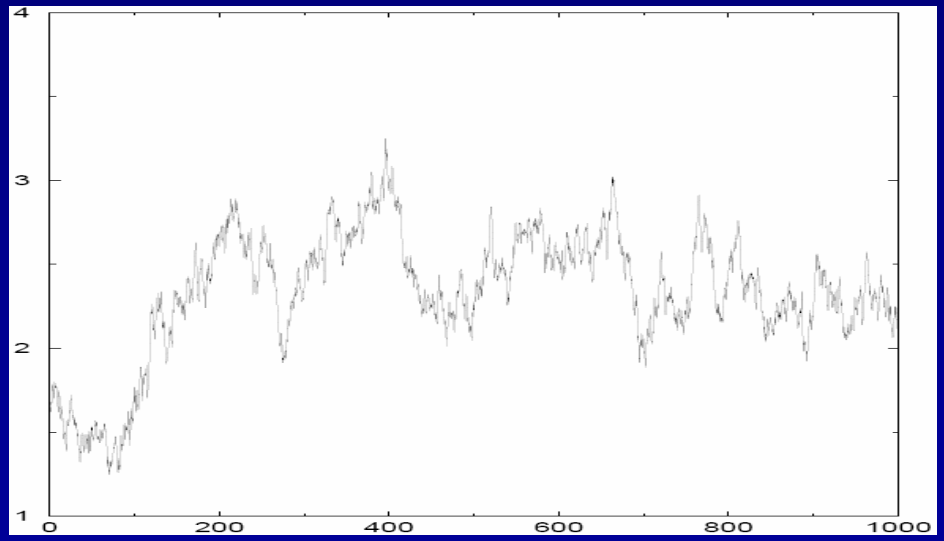
Actual Simulations:

Implicit:



(45 nucleotide RNA kissing hairpin)

Explicit:



RMSD (Å)

Time (ps)

Temperature:

$$T(t) = \frac{1}{3Nk} \sum_{i=1}^{N} \left| v(t) \right|^2$$

Where N is the number of atoms.

Temperature can be regulated by scaling (Berendsen Coupling):

$$F_i(t) = -\nabla V_i(t) + \frac{p_i}{\tau} \left[\frac{T_0}{T(t)} - 1 \right]$$

T_0 is the target temperature, p_i is the momentum of atom i, and τ is a relaxation constant (with time units – higher values cause slower coupling to bath).

Temperature Regulation:

- Advantage-
  - Required for NVT or NPT calculations.
  - Equilibration method.
- Disadvantage-
  - Trajectory does not conserve energy.
  - Trajectory is not reversible.
- In Practice-
  - A simulation is started with a small relaxation constant.
  - Once equilibration is finished, the relaxation constant is increased to lessen the effect of the thermostat.

Actual Simulation: