DynamO Workshop

Protein-like systems

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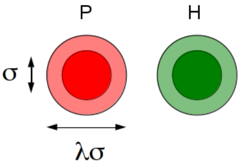
Section Outline

Heteropolymer models

Replica exchange

Histogram reweighting

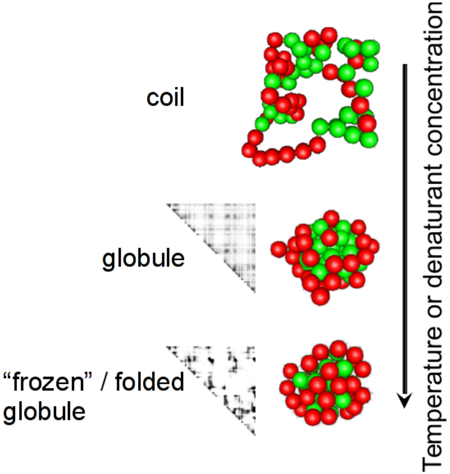
Heteropolymer models



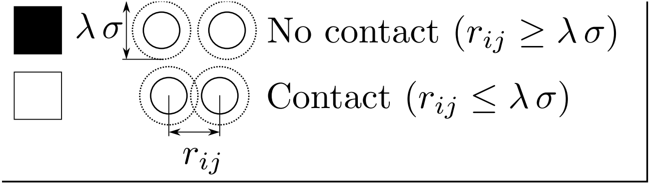
$$\varepsilon_{HH} = -1$$

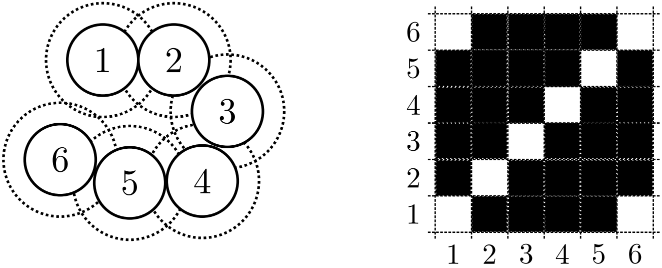
$$\varepsilon_{HP} = -1/2$$

$$\varepsilon_{PP} = 0$$



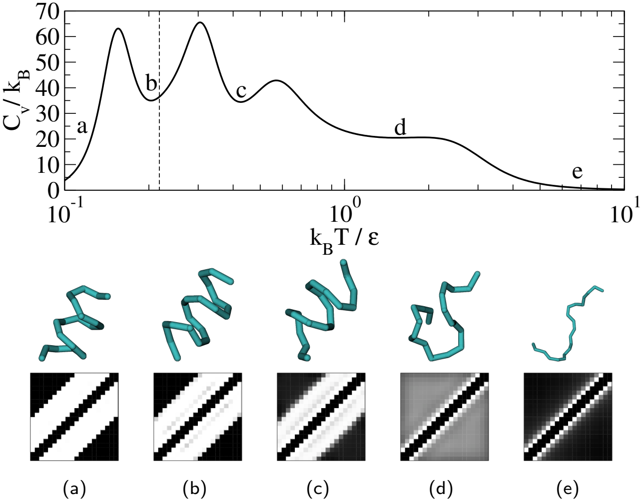
Contact maps





6-mer with 1-6 contact

Square-well homopolymer: $N_c = 20$, $\sigma/l = 1.6$, $\lambda = 1.5$

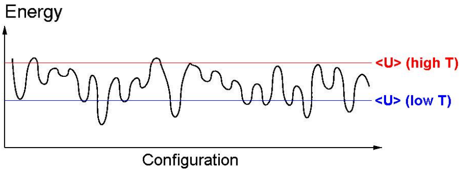


Bannerman et al., *Phys. Rev. E* (2009).

Section Outline

Replica exchange

- "Rough" energy landscapes are hard to sample at low temperature (get stuck in local minima)
- High-temperature simulations can glide over barriers



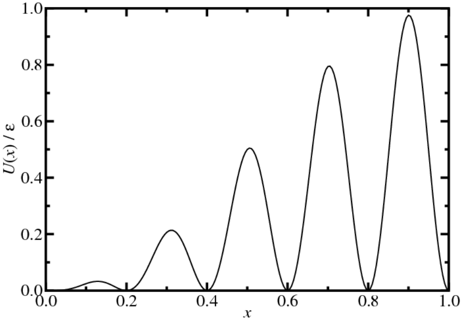
- Exchange complete configurations (with energies U_0 and U_1) between simulations run in parallel at different reciprocal temperatures (β_0 and β_1, respectively)

$$\frac{\mathcal{P}(n)}{\mathcal{P}(o)} = \frac{e^{-\beta_0 U_1} \times e^{-\beta_1 U_0}}{e^{-\beta_0 U_0} \times e^{-\beta_1 U_1}} = e^{-(\beta_0-\beta_1)(U_1-U_0)}$$

QL Yan and JJ de Pablo, *J. Chem. Phys.* 111, 9509 (1999)
A Kone and DA Kofke, *J. Chem. Phys.* 122, 206101 (2005)

Replica exchange: Simple example

- Model one-dimensional system (after Frenkel and Smit)
- Single particle in unit box (with periodic boundary conditions)
- External potential $U(x)$
- Start $x = 0$
- $\Delta x = \pm 0.005$
- 10^6 MC moves

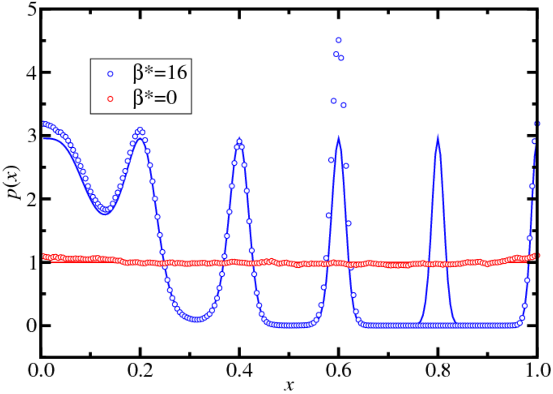


$$U(x) = \left[\sin \frac{\pi x}{2} \sin 5\pi x\right]^2$$

$$p(x, \beta) \propto e^{-\beta U}$$

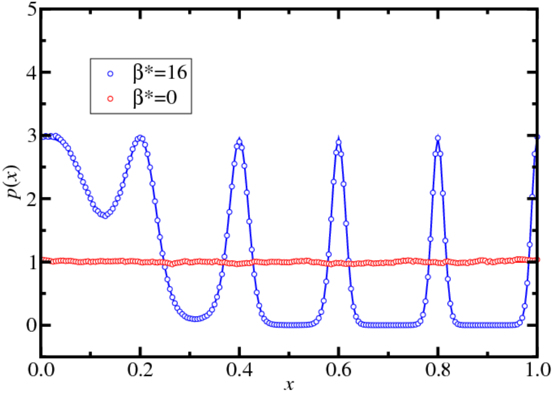
Replica exchange: Simple example

- Without parallel tempering
- Simulations (point); exact (lines)



Replica exchange: Simple example

- With parallel tempering
- Five reciprocal temperatures ($\beta^* = 0$, 4, 8 , 12, and 16)
- 10% swap moves with neighboring temperatures



Replica exchange with DynamO

Create a series of configuration files at different temperatures:

```
dynamod -m 2 --i1 20 --f1 1 -T 0.15 -o config.0.start.xml.bz2
dynamod -m 2 --i1 20 --f1 1 -T 1.5  -o config.1.start.xml.bz2
dynamod -m 2 --i1 20 --f1 1 -T 1    -o config.2.start.xml.bz2
```

Execute `dynarun` with the replica exchange simulation engine:

```
dynarun config.*.start.xml.bz2 --engine 2 -i 1 -f 100
```

Section Outline

Histogram extrapolation

- Consider an NVT simulation at β_0, where we collect the

$$\mathcal{P}(E;\beta_0) = \frac{\Omega(N,V,E)}{Q(N,V,\beta_0)} e^{-\beta_0 E}$$

$$\mathcal{H}(E;\beta_0) \propto \Omega(N,V,E) e^{-\beta_0 E}$$

- Estimate for the density of states:

$$\Omega(N,V,E) \propto \mathcal{H}(E;\beta_0) e^{\beta_0 E}$$

- Using the estimate for $\Omega(N,V,E)$, we can estimate the histogram at any other β

$$\mathcal{P}(E;\beta) = \frac{\Omega(N,V,E)}{Q(N,V,\beta)} e^{-\beta E}$$

$$\mathcal{H}(E;\beta) \propto \Omega(N,V,E) e^{-\beta E}$$

$$\propto \mathcal{H}(E;\beta_0) e^{-(\beta-\beta_0) E}$$

Histogram extrapolation: Other properties

- Other properties can be extrapolated by collecting the joint probability distribution at β_0

$$\mathcal{P}(X, E; \beta_0) = \frac{\Omega(N, V, E, X)}{Q(N, V, \beta_0)} e^{-\beta_0 E}$$
$$\mathcal{H}(X, E; \beta_0) \propto \Omega(N, V, E, X) e^{-\beta_0 E}$$

- Estimate for the modified density of states:

$$\Omega(N, V, E, X) \propto \mathcal{H}(X, E; \beta_0) e^{\beta_0 E}$$

- Using the estimate for $\Omega(N, V, E)$, we can estimate the histogram at any other β

$$\begin{aligned}\mathcal{H}(X, E; \beta) &\propto \Omega(N, V, E, X) e^{-\beta E} \\ &\propto \mathcal{H}(X, E; \beta_0) e^{-(\beta - \beta_0) E}\end{aligned}$$

Histogram interpolation

- Consider the case where we perform NVT simulations at several temperatures β_1, β_2,..., β_n where we collect the histograms:

$$\mathcal{H}(X, E; \beta_k) \propto \Omega(N, V, E, X) e^{-\beta_k E}$$

- Estimate for the density of states as a weighted sum:

$$\ln \Omega(N, V, E, X) \propto \sum_k w_k \ln(\mathcal{H}(X, E; \beta_k) e^{\beta_k E})$$

  where $\sum_k w_k = 1$.
- The uncertainty in $\ln \mathcal{H}(X, E; \beta_k)$ is roughly $[\mathcal{H}(X, E; \beta_k)]^{-1/2}$
- Determine the weights w_k by minimizing the uncertainty of the estimate of the density of states.