# Coarse-Grained Polymer Models: On-Lattice vs. Off-Lattice

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## Abstract

We investigated coarse-grained polymer models such as the HP on-lattice and the AB off-lattice formulations for heteropolymers ("proteins"). The poster will focus on the results of **two problems**.
**Firstly**, we will give results of investigations concerning **designing sequences** in the HP model **on lattices**. To this end we perform exact enumerations of the whole sequence-conformation space of HP proteins on different lattices up to a certain chain length.
**Secondly** we try to show **how "far"** ("close") lattice models are **from** ("to") **"reality"**, or from similar off-lattice models, respectively. Therefore we simulate off-lattice AB model-like proteins with different potentials and compare putative ground states with those from on-lattice simulations.

## The Models I

**The HP On-Lattice Model** [1]**:**
HP proteins are the simplest models of amino acid chains which consist of only two types of amino acids: **hydrophobic** (H) and **polar** (P).
The chain of monomers is modelled by a **self-avoiding walk**. The model is restricted to **regular lattices** and contains an **attractive interaction** between two H proteins which are neighbours on the lattice, but not covalently bound.
The total energy of a HP protein is then the sum of all H–H contacs on the lattice:

$$E_{HP} = - \sum_{\binom{\text{nn-pairs } (i,j)}{\text{not connected}}} s_i s_j \,, \qquad (1)$$

with $s_i = 1$ for hydrophobic (H) amino acids and $s_i = 0$ for polar (P) ones.

## Results of exact enumeration

Here we present results concerning the **designingness** of sequences on regular lattices using the **HP Model**. It is known, that on cubic lattices, there are sequences with a unique ground state conformation [2].
What happens with the designingness, when we go over to other lattice types? Table 1 shows the numbers of designing sequences on different lattice types.

| sequence length | total # of independent sequences | # of designing sequences 2d cubic | 2d triang | 3d cubic | 3d fcc |
|---|---|---|---|---|---|
| 5 | 20 | 0 | 1 | 0 | 0 |
| 6 | 36 | 7 | 0 | 0 | 0 |
| 7 | 72 | 10 | 0 | 0 | 0 |
| 8 | 136 | 7 | 0 | 2 | 0 |
| 9 | 272 | 6 | 0 | 0 | 0 |
| 10 | 528 | 6 | 1 | 0 | 0 |
| 11 | 1056 | 62 | 3 | 0 | – |
| 12 | 2080 | 87 | 1 | 2 | |
| 13 | 4160 | 173 | 0 | 0 | |
| 14 | 8256 | 386 | – | 1 | |

Table 1: Number of designing sequences on different lattices

So, we clearly see, that designingness is a property depending on the lattice type. In the specific case of the fcc lattice, not even one designing sequence has been found.

## The Models II

**The AB Off-Lattice Model** [3]**:**
AB Models are the "**off-lattice version of HP Models**". We have again two types of monomers representing hydrophobic (A) and polar (B) amino acids. The monomer chain is again modelled by a walk through space but not restricted to any lattice. We use **two versions** of the model:
**1.** The **special case** of "**B=A**" with pure Lennard–Jones potential between all monomers

$$E_{LJ} = \sum_{i,j>i+1} \left( \frac{1}{r_{ij}^{12}} - \frac{2}{r_{ij}^{6}} \right) . \qquad (2)$$

**2.** AB Model with different Lennard–Jones Potential between different types of monomers and **additional bending term**

$$E_{AB} = \sum_{i,j>i+1} \left( \frac{4}{r_{ij}^{12}} - \frac{4C(\cdot_i,\cdot_j)}{r_{ij}^{6}} \right) + \frac{1}{4} \sum_k (1 - \cos\theta_k) \qquad (3)$$

where $k$ numbers all angles $\theta$ between monomers $\cdot_i$ and $\cdot_j$. $C(\cdot_i,\cdot_j)$ has the value $+1$ for $(A,A)$ pair (strong attraction), $+0.5$ for $(B,B)$ pair (weak attraction) and $-0.5$ for $(A,B)$ and $(B,A)$ pair (weak repulsion).

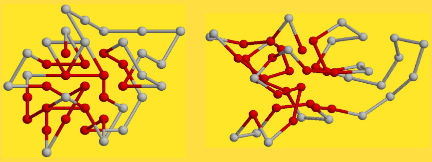

Figure 1: Lowest-energy conformations of a (HP)AB protein with 48 monomers on the fcc lattice (**left**) and off-lattice ($E = E_{AB}$) (**right**)

## Methods

1. **Exact Enumeration**
2. **Pruned-Enriched Rosenbluth Method (PERM)** [4]
   - Chain growth algorithm
   - Rosenbluth method + "Go with the winners"
3. **Metropolis Monte Carlo**
4. **Energy Landscape Paving (ELP)** [5]
   - Minimizer (thermodynamically incorrect)
   - give additional contribution to energies already visited ("paving" of energy landscape) → leave local minimas thereby
4. **Comparison with Help of Radial Distribution Function**

## References

[1] K.F. Lau and K.A. Dill, Macromol. **22**, 3986 (1989).
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[5] U.H.E. Hansmann and L.T. Wille, Phys. Rev. Lett. **88**, 068105 (2002).

This work is supported by the Deutsche Forschungsgemeinschaft (DFG) under contract No. JA483/24-1.

## Off-Lattice vs. On-Lattice

Finally we present the results of the ground state search as well as the "crystallization process" for some example polymers.

### 1. Homopolymer $N = 50$:

Here we try to find some hints whether the ground state of off-lattice homopolymers with simple Lennard-Jones potential (Eq.(2)) fits the fcc lattice. Therefore firstly we compare (putative) ground state energies (see Table 2).

| | |
|---|---|
| Ground state energy on fcc | $E_{LJ} = -188.5$ |
| Ground state energy off-lattice | $E_{LJ} = -191.3$ |

Table 2: (Putative) ground state energies of the Homo50mer on an fcc lattice and off-lattice

Secondly, we compare the radial distrubution of the monomers in that states (see Figure 2).

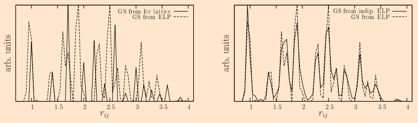

Figure 2: The comparison of the radial distribution function of the fcc ground state vs. the above mentioned off-lattice ground state (**left**) and two independently found off-lattice ground states (that one with energy $E = -191.3$ and another with energy $E = -189.0$) (**right**) (both with arbitrary normalization).

Finally, we try to show how the conformation "crystallizes" (in a sense), when cooling down. Therefore we simulated at different temperatures and measured the radial distribution over all conformations (Figure 3).

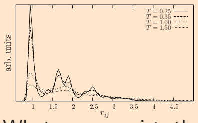

Figure 3: The radial distribution function over all generated conformation at certain temperatures (with normalization $\propto r_{ij}^{-2}$)

What we see ist the formation of preferred regions for the sites of monomers, if one like, a "crystallisation process" while "cooling down" the environment.
That means for off-lattice homopolymers with pure Lennard-Jones potential:

- there seems to be a unique ground state
- the ground state does not fit the fcc lattice
- but forms something like a crystal lattice

### 2. An Example for Heteropolymers $N = 48$:

For heteropolymers we did similar investigations. Obviously, because of the different interaction between different monomer types, the polymer as a whole does not fit to any regular lattice. So we concentrate on the hydrophobic core.

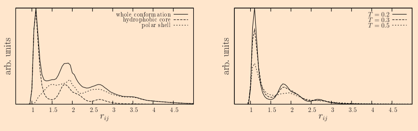

Figure 4: **Left:** The comparison of the radial distribution of the monomers of the whole conformation vs. those from the hydrophobic core and the shell monomers (accumulated over the whole simulation). A **ground state** of the simulated sequence is shown in the central **Figure 1**.
**Right:** This subfigure shows the "crystallisation" analogously to Figure 3 (both with normalization $\propto r_{ij}^{-2}$)

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