Bonded potentials? What’s the definition of bonded potential? Page1.

We call CG segments as superatoms? Page 2.

Bonded interactions = Bonded potentials? Page 2.

|  |  |
| --- | --- |
| Traditional method | Our Method |
| Bonded interactions are taken as those in atomistic model | ? |
| monomer along the chain | CG segments along the chain |
| Bonded potentials: bond stretch, angle bend and torsion potentials (use to reproduce local intrachain structures) | Need to produce the intrachain segment pair correlations functions (then? After get PFC? What we can get next?) closure? Non-bonded pair potentials? |
| Non-bonded potentials are obtained sequentially or even independently | Bonded and non-bonded CG potentials are coupled and need to be obtained simultaneously. （why at the same time?）Page43 |

Second Method Calculation Order:

Page5: a set of m different integers with[1, N-1]

Page5: can you explain the second method calculation order in details?

The only difference between the first method and second method is that define a set of m different integers??

Page6: the set one, I don’t understand.

Page6: how to get the analytical solution?