Multiscale Membrane Models

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Proposition

1. The Martini force field is the best coarse-grained force field to simulate the biomolecular system; however, its combination with the all-atom force field is less satisfactory. (Chapter 1)
2. Ganglioside can destabilize the phase separation of ternary lipid membranes in temperature ranging from 280 K to 325 K. (Chapter 2)
3. The combination of the Martini force field with the GROMOS force field can increase the sampling efficiency in the Hamiltonian replica exchange framework. (Chapter 3)
4. The virtual site dual resolution scheme is capable of increasing the computational efficiency, especially in vesicle simulation, without sacrificing too much all-atom accuracy. (Chapter 4)
5. The virtual site hybrid force field is also able to investigate the vibrational dynamics of lipids in vesicle and the phase separation in the planar ternary membrane. (Appendix I and II)
6. In the coarse-grain and all-atom hybrid force field, the trade-off between accuracy and efficiency is almost unavoidable. Nothing is free; one can barely achieve both of them simultaneously.