4th YSM-SPIP in Sendai/Prologue Series IV of FSPIP

New statistical enumeration methods for self-avoiding walks

Nobu C. Shirai[1,2] , Macoto Kikuchi[2,1,3]
[1] Graduate School of Science Osaka University
[2] Cybermedia Center Osaka University
[3] Graduate School of Frontier Biosciences Osaka University

We develop statistical enumeration methods for self-avoiding walks [1] using a powerful sampling technique called the multicanonical Monte Carlo method [2, 3]. Using these methods, we estimate the numbers of the two dimensional N-step self-avoiding walks up to $N = 256$ with statistical errors. The developed methods are based on statistical mechanical models of paths which include self-avoiding walks. The criterion for selecting a suitable model for enumerating self-avoiding walks is whether or not the configuration space of the model includes a set for which the number of the elements can be exactly counted. We call this set a scale fixing set. We selected the following two models which satisfy the criterion: the Gō model [5, 6] for lattice proteins and the Domb-Joyce model [4] for generalized random walks. There is a contrast between these two models in the structures of the configuration space. The configuration space of the Gō model is defined as the universal set of self-avoiding walks, and the set of the ground state conformation provides a scale fixing set. On the other hand, the configuration space of the Domb-Joyce model is defined as the universal set of random walks which can be used as a scale fixing set, and the set of the ground state conformation is the same as the universal set of self-avoiding walks. From the perspective of enumeration performance, we conclude that the Domb-Joyce model is the better of the two. The reason for the performance difference is partly explained by the existence of the first-order phase transition of the Gō model.

References

[1] Shirai N C and Kikuchi M 2012 arXiv:1212.2181
[2] Berg B A and Neuhaus T 1991 *Phys. Rev. B* **267** 249
[3] Berg B A and Neuhaus T 1992 *Phys. Rev. Lett.* **68** 9
[4] Domb C and Joyce G S 1972 *J. Phys. C: Solid State Phys.* **5** 956
[5] Gō N and Taketomi H 1978 *Proc. Natl. Acad. Sci. USA* **75** 559
[6] Gō N 1983 *Ann. Rev. Biophy. Bioeng.* **12** 183
[7] Iba Y, Chikenji G and Kikuchi M 1998 *J. Phys. Soc. Jan* **67** 3327
[8] Chikenji G, Kikuchi M and Iba Y 1999 *Phys. Rev. Lett.* **83** 1886