数学与系统科学研究院

计算数学所学术报告

(定期学术报告)

报告人： 雷锦志博士

(清华大学周培源应用数学研究中心)

报告题目：

从统计物理的观点看蛋白质折叠

邀请人： 卢本卓副研究员

报告时间： 2010 年 4 月 29 日(周四)

下午 4:00—5:00

报告地点： 科技综合楼三层 311

计算数学所报告厅

Abstract：

In this talk, I will introduce an approach to the

protein folding problem from the point of view of statistical physics. Protein folding is a stochastic process by which a polypeptide folds into its characteristic and functional 3D structure from random coil. The process involves an intricate interplay between global geometry and local structure, and each protein seems to present special problems. First, I will discussion on kinetics versus thermodynamics in protein folding, and introduce the statistical physics basis of protein folding. Secondary, I will introduce CSAW (conditioned self−avoiding walk), a model of protein folding that combines the features of self−avoiding walk (SAW) and the Monte Carlo method. In this model, the unfolded protein chain is treated as a random coil described by SAW. Folding is induced by hydrophobic forces and other interactions, such as hydrogen bonding, which can be taken into account by imposing conditions on SAW. Conceptually, the mathematical basis is a generalized Langevin equation. Despite the

simplicity, the model provides clues to study the universal aspects while we overlook details and concentrate only on a few general properties. To illustrate the flexibility and capabilities of the model, we consider several examples, including helix formation, elastic properties, and the transition in the folding of myoglobin. From the CSAW simulation and physical arguments, we find a universal elastic energy for proteins, which depends only on the radius of gyration R_g and the residue number N. The elastic energy gives rise to scaling laws $R_{g}\sim N^{\nu }$ in different regions with exponents $\nu =3/5,3/7,2/5$, consistent with the observed unfolded stage, pre−globule, and molten globule, respectively. These results indicate that CSAW can serve as a theoretical laboratory to study universal principles in protein folding.

欢迎大家参加！