NEW COURSE: STOCHASTIC MODELS OF BIOMOLECULAR SYSTEMS, SPRING, 2002

Instructor: Daniel Dix. 777-4320, dix@math.sc.edu

Subtitle: Math 728G, Selected Topics in Applied Mathematics. This is a continuation of Math 728B, Numerical Simulation of Biomolecular Systems (Fall 2001).

Prerequisites. Undergraduate numerical analysis, ordinary differential equations, linear algebra, probability theory, and functional analysis. Elementary computer programming. No previous knowledge of chemistry or biology will be assumed or required. Previous enrollment in Math 728B is not required.

Textbooks.

(1) *Understanding Molecular Simulations: From Algorithms to Applications*, Daan Frenkel, Berend Smit, Academic Press, 1996.
(2) *Molecular Modelling: Principles and Applications*, A. R. Leach, Second Edition, Prentice Hall, 2001.
(3) *Markov Chains, Gibbs Fields, Monte Carlo Simulation, and Queues*, P. Brémaud, Springer, New York, 1999.

Topics to be Covered.

(1) General theory of dynamical systems and chaos.
(2) Ergodic theory and stationary processes.
(3) Markov processes and their large-time behavior.
(4) Stochastic differential equations, Langevin equations.
(5) Equilibrium ensembles in statistical mechanics.
(6) Monte Carlo simulations; lattice models.
(7) Computer implementations of peptide folding.

Discussion. The ordinary differential equations governing the motion of biomolecular systems are highly chaotic, exhibiting extreme sensitivity to initial conditions. This means that one can only hope to derive probabilistic conclusions from these systems. A *dynamical system* is a probability space X equipped with a one parameter group $\{\phi_t \colon X \to X\}_{t\in\mathbb{R}}$ of mappings such that the probability of an event $E \subset X$ is the same as the probability of the event $\phi_t(E)$. This structure can arise from the flow of a system of differential equations. If $X = Y \times Z$, where Z represents degrees of freedom that we do not care about then trajectories $\phi_t(x)$ project down to paths of a *stochastic process* $y(t;x) \in Y$. Such processes often are much simpler to analyze than the dynamical system. Such processes will be derived and the tools for their study will be developed.

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