**School of Molecular Kinetics: Set of Lectures**

**Henri Orland**

**Introduction to Stochastic Modeling of Molecular Processes**

1. **Basic formalism**

- Introduction

- Langevin equation - Brownian dynamics

- Fokker-Planck equation

- Quantum Mechanics analogy: the Schrodinger approach

- The discrete case: the Master equation

- Kinetic Monte Carlo

2. **Barrier crossing**

- Kramers formula

- Path integral representation

- Transition path time distribution

- The semi-classical limit: dominant paths

- Transition paths

- Some examples

**3. Non-equilibrium work relations**

- Jarzynski theorem: Hamiltonian and Diffusive case

- Crooks relation

- Examples of application

**Dmitrii Makarov**

**Kinetics and Rate Theory**

1. **Reversible first order reactions**

* Bulk kinetics vs. stochastic single molecule trajectories
* Experimental methods for measuring kinetics

1. **Introduction to rate theory**

* Correlation function methods and their numerical implementation
* Transition State Theory (TST)
* Multidimensional harmonic TST
* Transmission factor

1. **Reduced dynamics**

* When can complex dynamics be reduced to simple two- (or few-) state kinetics?
* Diffusion-controlled reactions and “target search” problems

1. **Quantum effects (if time permit)**

* Quantum tunneling
* Zero-point energy
* Electronically nonadiabatic transitions
* Other quantum mechanical effects in chemical kinetics

**Ron Elber**

**Molecular Dynamics for Kinetics**

1. **Molecular Dynamics simulation and equilibrium of rare events**

* Ergodic hypothesis and molecular dynamics
* Verlet algorithm and conservation of phase space
* Sampling rare configurations, umbrella sampling and free energy perturbation.

1. **Enhanced sampling approaches for sampling configurations**

* Replica Exchange
* Meta Dynamics
* Temperature Accelerated Molecular Dynamics
* Minimum Free Energy Pathways

1. **Enhanced sampling of trajectories and trajectory fragments**

* Direct rate calculations
* Transition Path Sampling
* Transition Interface Sampling
* Markov State Models
* Milestoning