THEORY AND COMPUTATIONAL METHODS FOR BIOLOGICAL PHYSICS

Dr. Velia Minicozzi

1) STATISTICAL MECHANICS
Definition of *ensemble*: micro-canonical, canonical and gran-canonical *ensemble*. *Ensemble* equivalence. The equipartition theorem. Chemical potentials. The Maximum Entropy Method.

2) CLASSICAL MOLECULAR DYNAMICS
Discretization of the Hamilton-Jacobi equations. The Liouville time evolution operator. Molecular dynamics as a canonical transformation. Multiple-Time-Step. Systolic and list methods.

3) STOCASTIC METHODS FOR THE EVALUATION OF THE PARTITION FUNCTION
The Monte Carlo method. Markov chains, the detailed balance principle, the Markov theorem, the Metropolis algorithm. Hybrid Monte Carlo. Brownian motion and the Langevin equation. The Fokker-Planck equation and its asymptotic solution.

4) FERMNIC SYSTEMS IN CONDENSED MATTER
Born-Oppenheimer approximation. The Thomas-Fermi model. Hartree-Fock approximation. *Ab initio* simulations: the density functional theory. The Car-Parrinello method.

5) APPLICATION TO BIOMOLECULES
Introduction to biomolecules modelling. Empirical force-fields: all atoms and coarse grained (Martini). Velocity-Verlet and leap-frog algorithms. Time reversibility. Algorithms to minimize energy. Simulations in the NVT and NPT *ensembles*. Ewald summation. Correlation functions and their computation in molecular dynamics. The diffusion coefficient.

6) PARALLEL PLATFORM PROGRAMMING TOOLS
Code structure for the molecular dynamics OF biomolecules. Agent-oriented programing.