

1st part (Enzo Orlandini 12h):

## STOCHASTIC MODELS IN SOFT MATTER PHYSICS

### 1. Theory of stochastic processes

- a Brownian Motion
- b Langevin equation
- c Fluctuation dissipation theorem
- d Fokker-Planck equation
- e Mean first passage problems

### 2. Numerical integration of stochastic equations

### 3. Applications

- a. Polymer translocation
- b. Brownian ratchets and molecular motors
- c. Coherent motion in self-propelled (active) particles:  
bacteria suspensions and birds flocks.

2nd part (Antonio Trovato 12h):

## STOCHASTIC METHODS IN BIOMOLECULE SIMULATIONS

### 4. Monte Carlo effective dynamics

- a. Markov process
- b. Detailed balance condition and Metropolis test
- c. Density of states reconstruction: WHAM (weighted histogram) equation

### 5. Enhanced sampling techniques

- a. Umbrella sampling and simulated tempering
- b. Multiple Markov processes
- c. Generalized ensemble techniques
- d. Wang-Landau algorithm
- e. Metadynamics

### 6. Applications

- a. A brief survey on the physics of proteins
- b. Coarse grained protein modeling
- c. Protein folding
- d. Protein aggregation