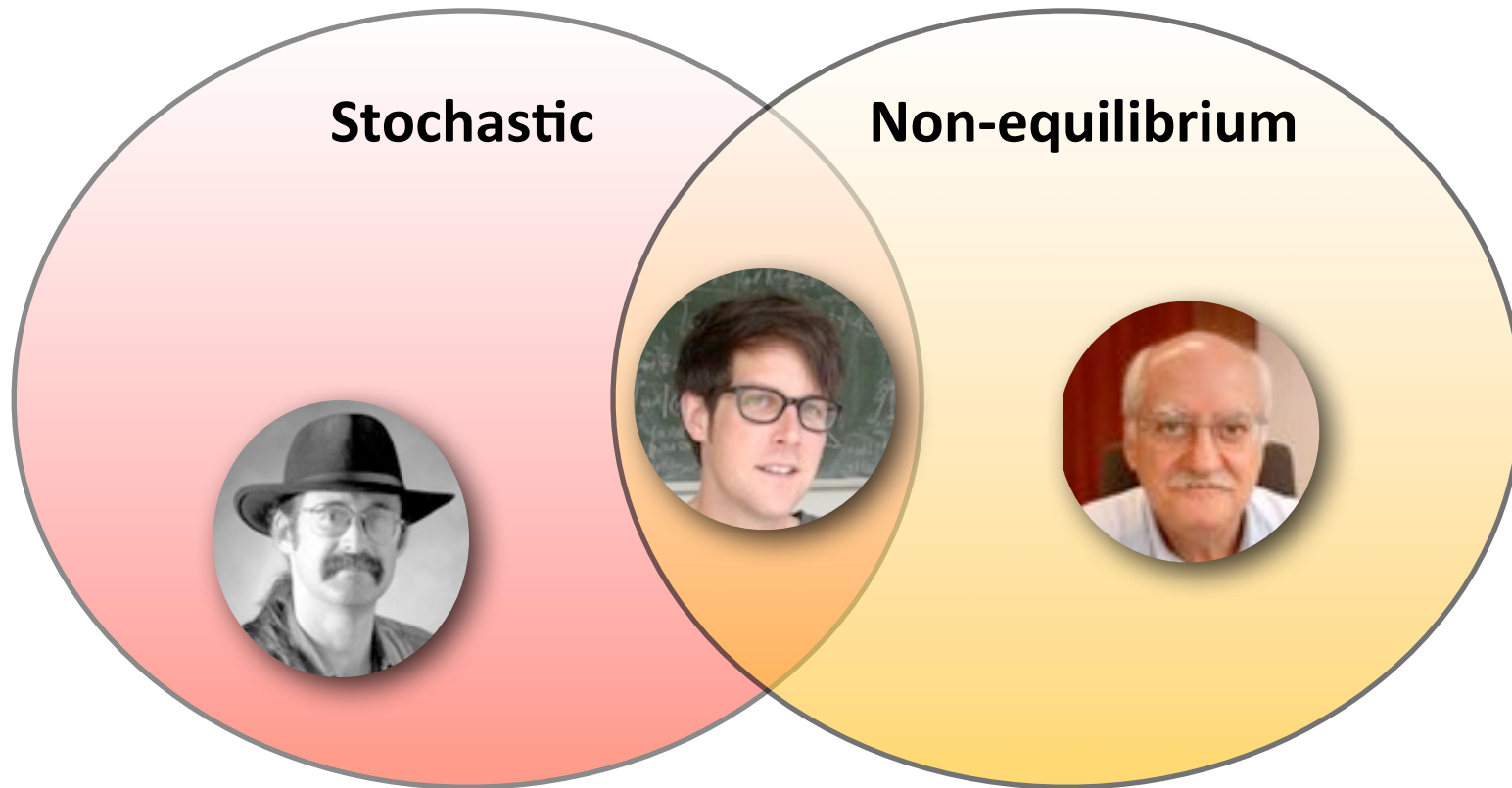


# Stochastic methods and Non-equilibrium states/processes



# From Atomically Detailed Trajectories to Equations for the Density: Coarse Graining by Milestoning



*Ron Elber*

- Milestoning: dynamical coarse graining for rare events/slow processes
- High dimensional milestoning: many collective variables
- Membranes, DNA-fragmentation
- Milestoning in non-equilibrium?

# Tackling Long Timescales in Molecular Dynamics



*Carsten Hartmann*

- Rare events sampling - optimal control
- Increase rate of rare events with non-equilibrium driving à la Jarzynski
- Statistical problem of exponential averages: optimum bias by entropy minimization

# Time-dependent Non-equilibrium Molecular Dynamics



*Giovanni Ciccotti*

- MD beyond stationary states (equilibrium and non-equilibrium): time dependent situations
- Based on generalization of linear response
- Onsager-Green-Kubo-Jacucci-McDonald-Ciccotti
- Hydrodynamic relaxation at fluid-fluid interface

# Statistical Mechanics of Hamiltonian AdResS



*Pep Español*

- Adaptive Resolution Simulation
- Change level of coarse graining dynamically - add/remove DOFs
- Do the switching at the level of Hamiltonian

# Stochastic methods (for dynamics)

- Langevin dynamics
- direct simulation Monte Carlo
- kinetic Monte Carlo
- lattice Boltzmann
- dissipative particle dynamics
- multicollision dynamics
- milestoning

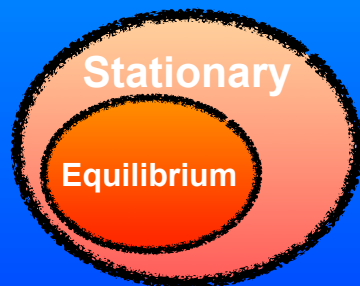
**1. Select coordinates to keep**

**2. Postulate propagation rules that mimic dynamics**

**3. Tune rules to reproduce important properties**

**More systematic approaches to coarse grain dynamics?**

# Non-equilibrium processes

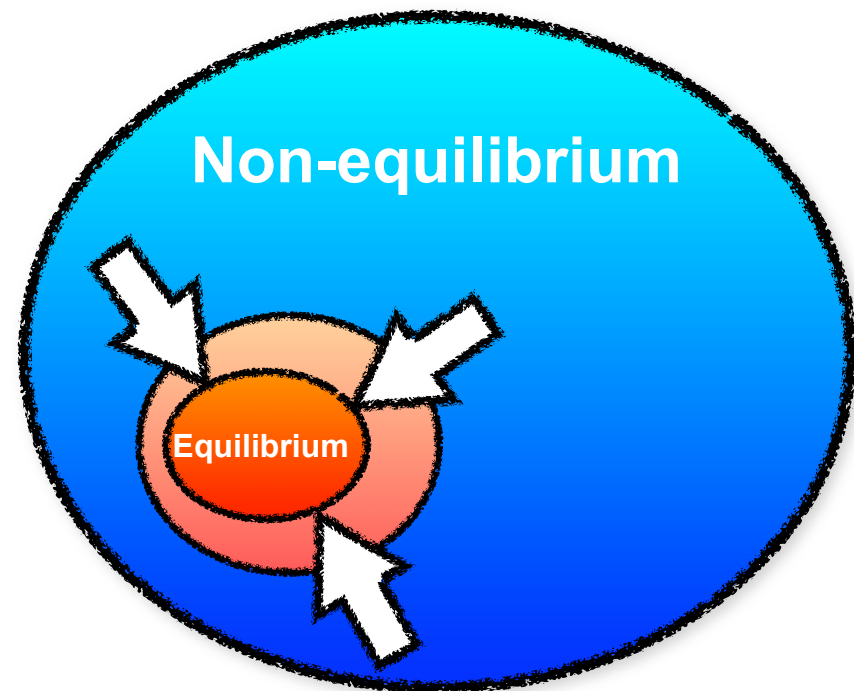


# No microscopic theory à la Boltzmann-Gibbs for non-equilibrium processes!

Exact non-equilibrium results:

- \* Linear response theory
- \* Jarzynski equation
- \* Crooks fluctuation theorem
- \* Hatano-Sasa equation
- \* Mapping to equilibrium system

$$\langle \exp(-\beta W) \rangle = \exp(-\beta \Delta F)$$



- Can we use above relations to develop (efficient) algorithms?
- Do we need a microscopic theory? After all, we have simulation!