

EMBio: science

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Main themes

- ▶ Computational mechanics of MD trajectories
- ▶ Dynamics of peptides structural changes

Computational mechanics of MD trajectories

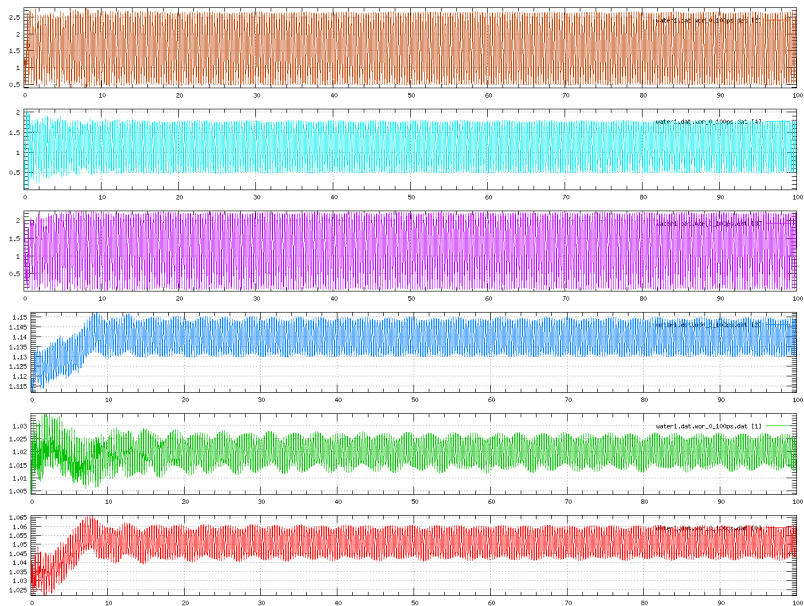
Symbolization

- ▶ representative examples of the dynamics: 2 waters (trivial and "synchronized")
- ▶ method to find approximation to generating partition
- ▶ GP for two cases

Complexities

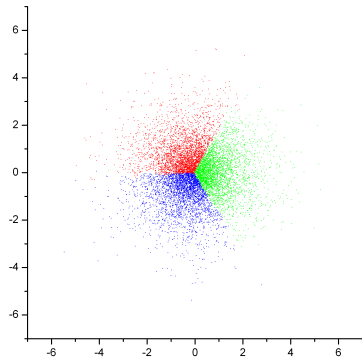
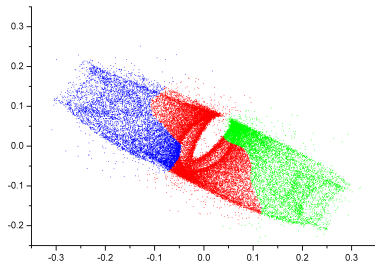
- ▶ "synchronised":
- ▶ "normal"

Dynamics



Dynamics

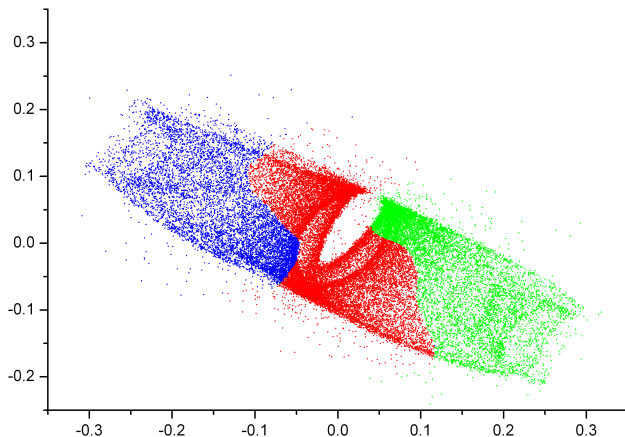
Poincare section for two cases



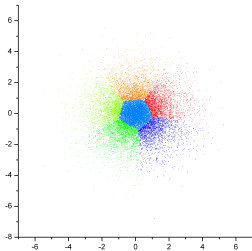
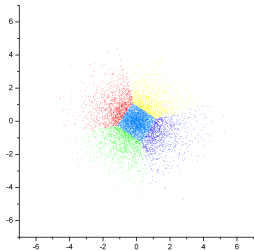
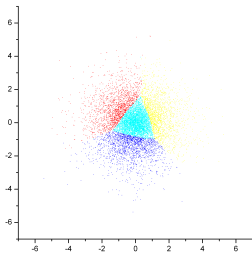
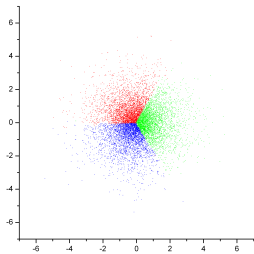
Symbolisation

Method for approximation GP by Michael Buhl and Matthew B. Kennel
[Phys. Rev. E 71, 2005]

Idea: if two short pieces of trajectory in the phase space are close they must be close in the symbolic space

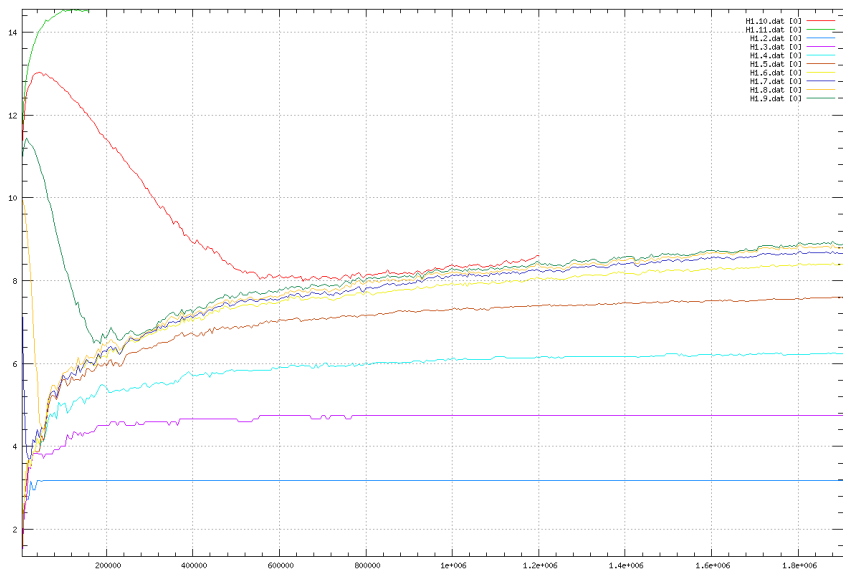


Symbolisation



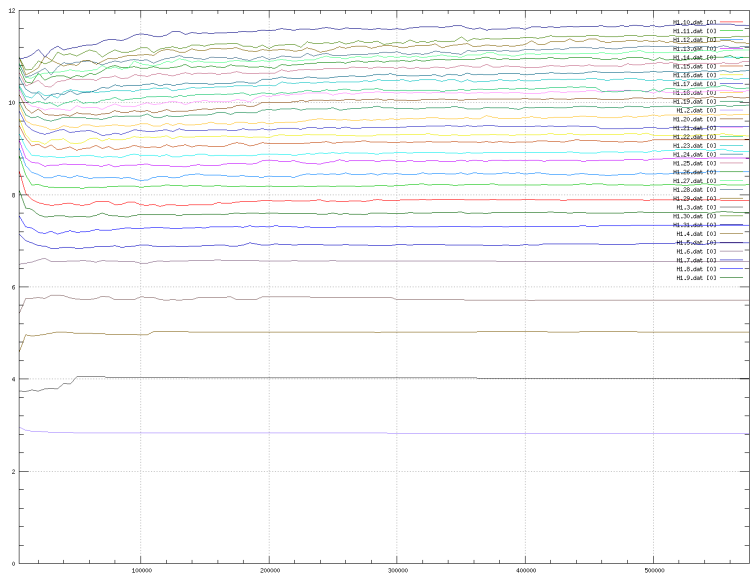
PBC water

Complexities



PBC water complexities

Complexities



2 waters complexities