Molecular and Particle Dynamics Simulation, Cours 3

CIRM school: Stochastic Dynamics out of Equilibrium, April 3 - 7, 2017

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- Lecture 1. Molecular dynamics models goals and purposes, numerical methods by splitting, analysis and examples.
- Lecture 2. Ensembles for molecular simulation (microcanonical, canonical), stochastic differential equations (Brownian/Langevin dynamics), examples.
- Lecture 3. Numerical methods for Langevin dynamics: splitting algorithms, error analysis, superconvergence, examples.
- Lecture 4. Constraints in molecular dynamics, SHAKE and RATTLE discretization, geodesic integration, isokinetic MD, examples.
- Lecture 5. Application of thermostat methods in fluids; examples such as shear flows and vortex dynamics.
- Lecture 6. More general statistical sampling from molecular dynamics, applications to Bayesian inference.

Lectures based largely on the book :

B. Leimkuhler and C. Matthews, 'Molecular Dynamics', Springer, 2015. http://www.springer.com/us/book/9783319163741 (available via Springer-Link) (intended for MSc or starting PhD students).

Supplemented by the following references:

L3: B. Leimkuhler, C. Matthews, G. Stoltz, The computation of averages from equilibrium and nonequilibrium Langevin molecular dynamics, IMA J Num. Anal., 36 (1): 13-79, 2016. doi: 10.1093/imanum/dru056,
Arxiv: http://arxiv.org/abs/1308.5814

L4: B. Leimkuhler and C. Matthews, Efficient molecular dynamics using geodesic integration and solvent-solute splitting, Proc. Roy Soc A, 472, 2016, doi: 10.1098/rspa.2016.0138

L5: B. Leimkuhler and X. Shang, Pairwise adaptive thermostats for improved accuracy and stability in dissipative particle dynamics, preprint, 2016.

L6: X. Shang, Z. Zhu, B. Leimkuhler and A. Storkey, Covariance-Controlled Adaptive Langevin Thermostat for Large-Scale Bayesian Sampling, NIPS 2015; C. Matthews, J. Weare and B. Leimkuhler, Ensemble preconditioning for Markov Chain Monte Carlo simulation, preprint, 2016.