Possible Project 4

The aim is to explore the splitting method of SDEs and Langevin dynamics.

- Make a study notes of "Rational Construction of Stochastic Numerical Methods for Molecular Sampling". In particular, understand how the scheme in equation (3) is asymptotically second order.
- Make a survey of the article "The computation of averages from equilibrium and nonequilibrium Langevin molecular dynamics".
- This is the bonus part. Use the ideas in the two papers to analyze the coordinate splitting method of SDEs. In particular, for SDE

  $$dX = -\nabla V dt + \sqrt{2\epsilon} dW$$

  One example is to split the right hand side as

  $$A_i = -\partial_i V dt + \sqrt{2\epsilon} dW_i.$$

  This in fact has some flavor of the coordinate descent method. (You may consider other splittings, but the requirement is that the computational cost should be low.)

  (1). Explore whether there is some order of these operators that gives high accuracy. Explore whether the new splitting has ergodicity. (2). Compare with the splitting method with coordinate descent (random) numerically.