Computing the Effective Hamiltonian for Different Time Scales

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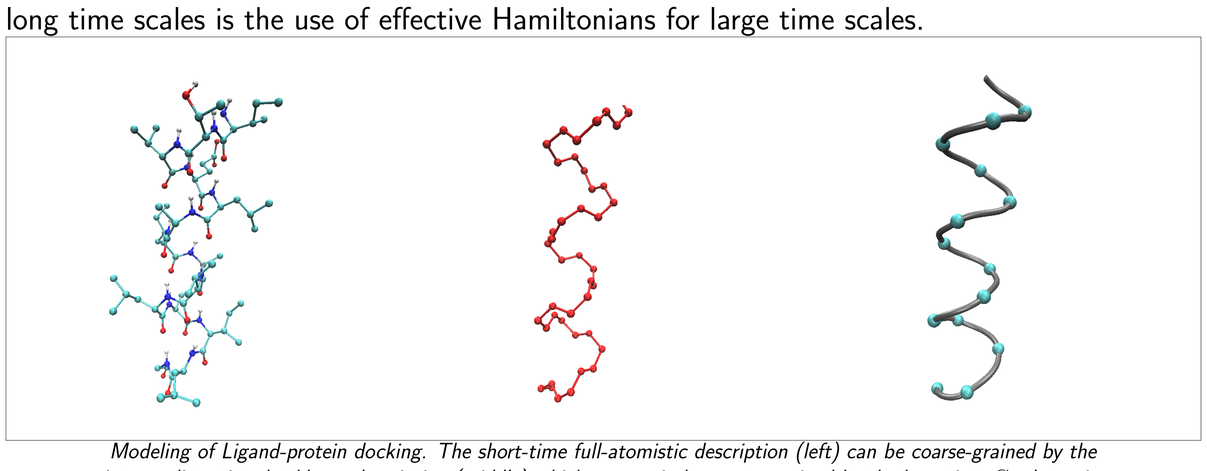
Motivation

High-dimensional proteins are capable of forming metastable conformations. The transition from one conformation to another happens on much longer time scales, compared to the dynamics of the constituents of a protein. Transitions between the conformations dominantly influence macroscopic quantities of the system. For large proteins the conformational timescales are expensive to simulate by use of atomistic molecular dynamics methods. One ansatz for simulating long time scales is the use of effective Hamiltonians for large time scales.



Modeling of Ligand-protein docking. The short-time full-atomistic description (left) can be coarse-grained by the intermediate-time backbone description (middle) which can again be coarse-grained by the long-time C_α dynamics (right) [1].

Having the effective Hamiltonian dynamics for large time scales at hand leads to the opportunity of choosing greater temporal discretisation constants and therefore enable the simulation of conformation changes efficiently [2].
In this poster a variational ansatz to compute the effective Hamiltonian for different time scales is presented. Since the method relies on choosing the temporal scale and basis functions initially, there is a great potential for the application of machine learning techiques and optimisation ansatzes, to obtain optimal coarse-graining models.

Microcanonical Ensemble

The system is considered to be given in a microcanonical setting, following the Hamiltonian equations of motion

$$\frac{d}{dt}x(t) = J\nabla_x H(x(t)),$$

where $x(t)$ is the phase-space trajectory containing all positions and momenta of the system of interest, J is the Poisson matrix and $H = V + T$ is the temporally constant Hamiltonian of the system. It is decomposed into a potential part V and a kinetic part T.
Because of the validity of the Hamiltonian equation of motion, a constant scalar quantity of the system is given by the scalar product

$$S(x(t)) = \left\langle \frac{d}{dt}x(t) - J\nabla_x H(x(t)) \,\middle|\, \frac{d}{dt}x(t) - J\nabla_x H(x(t)) \right\rangle = \text{const.}$$

Analytical knowledge of the Hamiltonian enables canonical setting study furthermore.

Variational Ansatz

Based on a set of ansatz functions f_i, which can be chosen to be an orthonormal set of basis functions or can be chosen on the basis of previous or intuitive results, the Hamiltonian can be set up as a general superposition of these basis functions

$$H = \sum_i c_i f_i$$

with variable coefficients c_i. The functional to minimise is thus given by

$$F(x(t)) = \frac{1}{T}\int_0^T S(x(t))dt$$

with a simulation time T as large as possible. Differentiating the functional F with respect to the coefficients c_i leads to an optimisation problem of the form

$$c = \underset{c'}{\operatorname{argmin}} ||Ac' - d||_2$$

with a matrix A, the vector of coefficients c and a right side d. The optimisation problem is solved by use of singular value decomposition.
One set of basis functions could be given by Hermite polynomials

$$g_0(w) = 1 \qquad g_1(w) = w \qquad g_2(w) = w^2 - 1 \qquad \cdots$$

which form a complete orthonormal basis of the set of square-integrable functions with respect to a gaussian kernel. For initialising a multidimensional basis, the product of basis functions can be considered. In the case of a two-dimensional system, this would be given by

$$f_i(q,p) = f_{i_q,i_p}(q,p) = g_{i_q}(q)\cdot g_{i_p}(p).$$

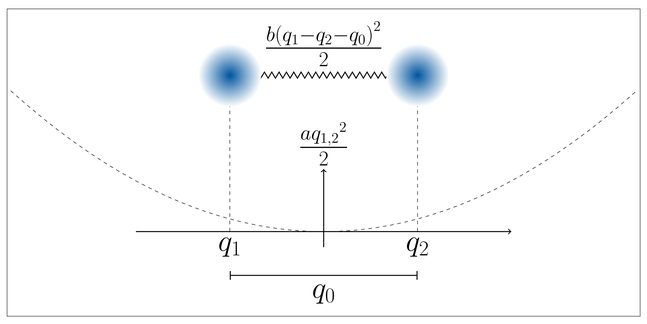
In the sense of a numerical computation the basis has to be truncated at a maximal index to allow for finite-dimensional computation on a computer.

Model System

To analyse the computation of effective Hamiltonians, a model system of two confined particles in one dimension interacting by a strong attracting quadratic force is considered

$$H = \frac{{p_1}^2}{2} + \frac{{p_2}^2}{2} + \frac{a{q_1}^2}{2} + \frac{a{q_2}^2}{2} + \frac{b\left(q_1 - q_2 - q_0\right)^2}{2} \qquad 0 < a \ll b \qquad q_0 \geq 0.$$

$p_{1,2}$ are the momenta of the two particles, $q_{1,2}$ are the positions of the two particles, q_0 is the separation distance between the two particles and a, b are coefficients describing the strengths of the attracting and confining forces.



Model of two externally weak confined particles attracted to each other by a strong quadratic potential.

The given dynamics can be separated into fast oscillations between the two particles and a slow oscillation of the center of mass of both particles within the confining potential.

Smoothing

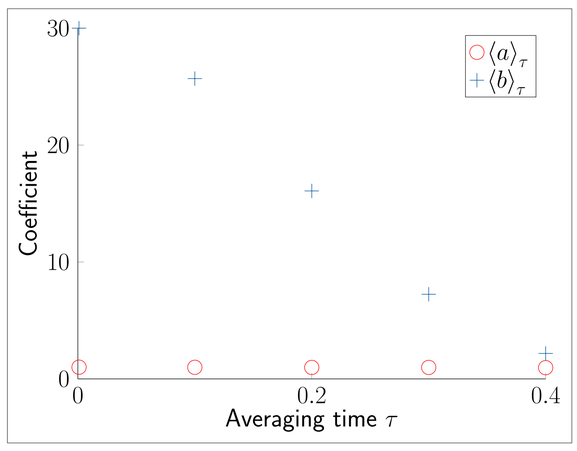
Within the computation of the matrix elements of A and the right side b one has to compute the temporal derivative of the phase-space trajectory $x(t)$. At this point, a temporal averaging scheme for the derivative of the momenta $p_{1,2}(t)$, to smear out the fast modes of the system, can be performed. This is done by gaussian smoothing

$$\langle \dot{p}_{1,2} \rangle_\tau (t) = \frac{1}{\sqrt{\pi\tau^2}} \int_{-\infty}^{\infty} e^{-\frac{\theta^2}{\tau^2}} \dot{p}_{1,2}(t+\theta)\, d\theta$$

with a smoothing window size parameter τ. The corresponding numerical Hermite-Gauss quadrature is used to perform the numerical integration efficiently.

Numerical Results

The method stated above is used to compute the effective Hamiltonian for different averaging times τ, where the parameters of the underlying system are given by $a = 1$, $b = 30$ and $q_0 = 0$.



Plot of the effective coeffficients for different averaging times τ.

With increasing averaging time τ the coefficient of the fast dynamics is decreasing and therefore the corresponding fast oscillations are filtered effectively.

Conclusions and Outlook

A method is presented to smear out fast dynamics of Hamiltonian systems. This method enables for slow mode effective Hamiltonian computation.
The Kullback-Leibler divergence [3] can be used, to quantify the error of the effective system. The dependence of the accuracy of the system with respect to the choice of basis functions can be studied furthermore.

References

[1] J. Schneider *Student Program Description*. CAMMP Week Pro. MATHCCES, 2017.

[2] N. Aguirre *Scientific Discussion*. Complex High-Dimensional Energy Landscapes. IPAM, 2017.

[3] A. Chaimovich and M. S. Shell *Coarse-graining errors and numerical optimization using a relative entropy framework*. The Journal of Chemical Physics, 134:094112, 2011.