1 Model problem

1.1 Advection-diffusion

In general, we are interested in performing a bifurcation analysis for models at which an exact, closed model at the macroscopic level is not available. However, as a toy problem, we start using an example where the macroscopic model is already known. On the macroscopic scale the evolution of a probability density ρ is given by a PDE of the advection-diffusion type

$$\frac{\partial \rho(x,t)}{\partial t} + \mu \frac{\partial (f(x)\rho(x,t))}{\partial x} = \frac{\sigma^2}{2}\frac{\partial^2 \rho(x,t)}{\partial x^2}. \tag{1}$$

The advection represents gradient-driven flow, according to an advection coefficient μ and a force $f(x) = -\frac{\partial V}{\partial x}$. In this example $V(x)$ is chosen to be a bi-stable potential $V(x) = x^4 - x^2$. The microscopic model consists in simulating an ensemble of N particles evolving according to the corresponding SDE

$$\mathrm{d}\mathbf{X_t} = \mu f(\mathbf{X_t})\mathrm{d}t + \sigma \mathrm{d}\mathbf{W_t}, \tag{2}$$

where $\mathbf{W_t}$ are N independent, standard Brownian motions.

1.2 Discretization

We look for solutions of the Fokker-Planck-equation (1) in two ways:

- By explicitly solving eq. (1) using the discretization scheme

$$\rho_i^{n+1} = \rho_i^n + \Delta t \left(\frac{\sigma^2}{2\Delta x^2} \left(\rho_{i+1}^n - 2\rho_i^n + \rho_{i-1}^n\right) - \mu \frac{f(x)}{\Delta x}(\rho_i^n - \rho_{i-1}^n) \right) \tag{3}$$

  for the value of ρ at position $x = i\Delta x$ and time $t = (n+1)\Delta t$. This is a first-order upwind scheme for the advective part combined with the Forward-Time Central-Space-method for the diffusive part.

- By simulating an ensemble of N particles evolving according to the SDE . The position X^{n+1} of each particle at time $t = (n+1)\Delta t$ is simulated using the Euler-Maruyama scheme

$$X^{n+1} = X^n + \mu f(X^n)\Delta t + \sigma\sqrt{\Delta t}\cdot \xi^n \tag{4}$$

  with $\xi^n \sim \mathcal{N}(0,1)$.

2 Method

2.1 Coarse time stepper

To simulate the time evolution of the density $\boldsymbol{\rho}(t)$, we construct a coarse time stepper $\boldsymbol{\Phi}_T^N$ which allows the performance of time-steps at the macroscopic level, using only the stochastic simulation of the position vectors of the N particles at the microscopic level, generated by eq. (4).

To achieve this, we will define two operators (lifting in subsection 2.1.1 and restriction in subsection 2.1.2) that relate the microscopic and macroscopic levels of description. Once these lifting $\mathcal{L}$ and restriction operators $\mathcal{R}$ have been constructed, a coarse time-stepper $\mathbf{\Phi}_T^N$ to evolve the macroscopic state $\boldsymbol{\rho}$ over a time interval of length $n\Delta t$ is constructed as a three-step-procedure (lift–evolve–restrict):

$$\boldsymbol{\rho}(t+n\Delta t) = \mathbf{\Phi}_T^N(\boldsymbol{\rho}) = (\mathcal{R} \circ \mathcal{E}(n\Delta t) \circ \mathcal{L}(\omega))(\boldsymbol{\rho}(t)) \tag{5}$$

where $\mathcal{E}(n\Delta t)(\boldsymbol{\rho}(t))$ is the simulation of the SDE for N particles over n timesteps.

2.1.1 Lifting: $\boldsymbol{\rho} \rightarrow \mathbf{X}$

Given the density $\boldsymbol{\rho}$, we need to sample a position vector X_i for every particle $i \leq N$. We compute X from a N-dimensional vector $\mathbf{U}$ with uniform random elements $U_i \in [0,1]$ such that $\boldsymbol{\rho}(X_i) = U_i$, using the inverse transformation method. The particle does not only gets an inital position, but also a seed for generating random steps in the simulation.

2.1.2 Restriction: $\mathbf{X} \rightarrow \boldsymbol{\rho}$

The restriction operator $\mathcal{R} : \mathbb{Q}^N \rightarrow \mathbb{Q}^k$ maps the microscopic state $\mathbf{X}$ (determined by the position vectors of N particles) to a density $\boldsymbol{\rho}$, discretisized in k bins. This is done by counting the number of particles in every bin Δ_j for $1 \leq j \leq k$:

$$\frac{1}{N}\sum_{i=1}^{N} w^i \cdot \chi_{\Delta_j}(X^i) = \rho_j \tag{6}$$

with

$$\chi_{\Delta_j}(X) = \begin{cases} 1 & \text{if } X \in \Delta_j, \\ 0 & \text{if } X \notin \Delta_j. \end{cases} \tag{7}$$

and setting all weights $w_i = 1$ for $1 \leq i \leq N$.

The reason why we explicitly introduced these weights in the restriction operator will be clarified in section **??** where we will need to evaluate the coarse time stepper $\mathbf{\Phi}_T^N(\boldsymbol{\rho} + \varepsilon\mathbf{v})$, now applied to the density shifted with a certain perturbation $\varepsilon\mathbf{v}$. To evaluate the perturbated restriction-operator we will use the weights w_ε^i, determined such that

$$\frac{1}{N}\sum_{i=1}^{N} w_\varepsilon^i \cdot \chi_{\Delta_j}(X^i) = \rho_j + \varepsilon v_j. \tag{8}$$

We do this by computing the weight per bin as $w_\varepsilon^j = 1 + \frac{\varepsilon v_j}{\rho_j}$ and assign this value to each particle in Δ_j. So, small perturbations on the density lead to small perturbations in the weights. The advantage of this weighted restriction operator lies in the possibility to use the same realizations $\mathbf{X}$ in the unperturbated (6) and the perturbated (8) restriction-operator.