Coarse-graining via EDP-convergence for linear fast-slow reaction-diffusion systems

Artur Stephan

1 Weierstraß-Institut für Angewandte Analysis und Stochastik, Mohrenstraße 39, 10117 Berlin, Germany

In [7], a fast-reaction limit for a linear reaction-diffusion system consisting of two diffusion equations coupled by a linear reaction is performed. The linear reaction-diffusion system is understood as a gradient flow of the free energy in the space of probability measures equipped with a geometric structure, which contains the Wasserstein metric for the diffusion part and cosh-type functions for the reaction part. The fast-reaction limit is done on the level of the gradient system by proving EDP-convergence with tilting. The limit gradient system induces a diffusion system with Lagrange multipliers on the linear slow-manifold. Moreover, the limit gradient system can be equivalently described by a coarse-grained gradient system, which induces a scalar diffusion equation with a mixed diffusion constant for the coarse-grained slow variable.

© 2021 The Authors. Proceedings in Applied Mathematics & Mechanics published by Wiley-VCH GmbH.

1 Linear fast-slow reaction system

Considering two species $X_1$ and $X_2$ that diffuse in a bounded medium $\Omega \subset \mathbb{R}^d$ and react linearly $X_1 \rightleftharpoons X_2$, the evolution of their concentrations $c = (c_1, c_2)$ can be described by the linear reaction-diffusion system

$$
\dot{c}_1^\varepsilon = \delta_1 \Delta c_1^\varepsilon - \frac{1}{\varepsilon} \left( \sqrt{\frac{\alpha}{2}} c_1^\varepsilon - \sqrt{\frac{\beta}{2}} c_2^\varepsilon \right), \quad \dot{c}_2^\varepsilon = \delta_2 \Delta c_2^\varepsilon + \frac{1}{\varepsilon} \left( \sqrt{\frac{\beta}{2}} c_1^\varepsilon - \sqrt{\frac{\alpha}{2}} c_2^\varepsilon \right),
$$

(LRDS)

complemented with no-flux boundary conditions and initial conditions, where $\delta_1, \delta_2 > 0$ are diffusion coefficients for species $X_1$ and $X_2$, respectively, and $\alpha, \beta > 0$ are reaction rates describing the reaction speed of the linear reaction $X_1 \rightleftharpoons X_2$. We are interested in the limit $\varepsilon \to 0$, i.e. if the reaction is much faster than the diffusion.

Reaction systems and reaction-diffusion systems with slow and fast time scales have attracted a lot of attention in the last decades. In [1] the following fast-reaction limit for $\varepsilon \to 0$ is proved: Let $\dot{c}_1^\varepsilon$ and $\dot{c}_2^\varepsilon$ be weak solutions of (LRDS). Then $\dot{c}_1^\varepsilon \to c_1$ and $\dot{c}_2^\varepsilon \to c_2$ in $L^2([0,T] \times \Omega)$ as $\varepsilon \to 0$, and we have $\frac{\dot{c}_1}{\delta_1} = \frac{\dot{c}_2}{\delta_2}$. Moreover, defining the coarse-grained concentration $\dot{\hat{c}} = \frac{\dot{c}_1 + \dot{c}_2}{2}$, then $\dot{\hat{c}}$ solves the diffusion equation $\dot{\hat{c}} = \delta \Delta \hat{c}$ with a new mixed diffusion coefficient $\delta = \frac{\delta_1 + \delta_2}{\alpha + \beta}$.

2 Gradient structure for linear reaction-diffusion systems

In [7], we were not primarily interested in convergence of the solutions of (LRDS). Instead, we perform the fast-reaction limit on the level of the underlying variational structure, which then implies convergence of solutions as a byproduct. The idea is that reaction-diffusion systems such as (LRDS) can be written as a gradient flow equation induced by a gradient system $(Q, \mathcal{E}, \mathcal{R}_X^\varepsilon)$, where

- the state space $Q$ is the space of probability measures $Q = \text{Prob}(\Omega \times \{1, 2\})$
- the driving functional is the free energy $\mathcal{E}(\mu) = \int_{\Omega} \sum_{j=1}^2 E_B \left( \frac{\partial w_j}{\partial x_j} \right) w_j \, dx$ for measures $\mu \in \mathcal{P}(\Omega)$, with the Boltzmann function $E_B(r) = r \log r - r + 1$ and the (in general space dependent) stationary measure $w = (w_1, w_2)^T$.
- the dissipation potential $\mathcal{R}_X^\varepsilon$ determining the geometry of the underlying space is given by two parts $\mathcal{R}_X^\varepsilon = \mathcal{R}_X^{\text{diff}} + \mathcal{R}_X^{\text{react,}\varepsilon}$ describing the diffusion and reaction separately.

The diffusion part $\mathcal{R}_X^{\text{diff}}(\mu, \xi) = \frac{1}{2} \int_{\Omega} \sum_{i=1}^2 \delta_i |\nabla \xi_i|^2 \, d\mu_i$ induces the Wasserstein distance on $Q$ following the pioneering work of Otto and coauthors [3]. Later Mielke [4] proposed a quadratic gradient structure with the same driving functional also for reaction-diffusion systems with reversible reactions satisfying detailed balance. A different but related gradient structure is the so-called cosh-type gradient structure, where the reaction part is given by $\mathcal{R}_X^{\text{react,}\varepsilon}(\mu, \xi) = \frac{1}{2} \int_{\Omega} \mathcal{C}^\varepsilon(\xi_1(x) - \xi_2(x)) \sqrt{\text{det} \nabla^2 \mu} \, dx$, with $\mathcal{C}^\varepsilon(r) = 4(\cosh(r/2) - 1)$. Setting $\mathcal{R}_X^\varepsilon = \mathcal{R}_X^{\text{diff}} + \mathcal{R}_X^{\text{react,}\varepsilon}$, the reaction-diffusion system (LRDS) can now be formally written as a gradient flow equation $\dot{\mu} = \partial_\varepsilon \mathcal{R}_X^\varepsilon(\mu, -\nabla \mathcal{E}(\mu))$. 

* Corresponding author: e-mail artur.stephan@wias-berlin.de, phone +49 30 203 72 415

This is an open access article under the terms of the Creative Commons Attribution License, which permits use, distribution and reproduction in any medium, provided the original work is properly cited.
3 EDP-convergence with tilting

In [7] an effective gradient system \((Q, \mathcal{E}, R^*_\text{eff})\) is constructed such that \((Q, \mathcal{E}, R^*_0) \to (Q, \mathcal{E}, R^*_{\text{eff}})\) as \(\varepsilon \to 0\). For this, the notion of EDP-convergence as introduce in [2] was used. It is based on the dissipation functional \(\mathcal{D}^\varepsilon(\mu) = \int_\Omega R^*(\mu, \hat{\mu}) + \mathcal{R}_\varepsilon^*(\mu, \eta - \mathcal{D}\mathcal{E}(\mu)) \, dt\), which, for solutions \(\mu\) of the gradient flow equation describes the total dissipation between initial time \(\mathcal{E}(\mu(0))\) and final time \(\mathcal{E}(\mu(T))\), and can now be defined for general trajectories \(\mu \in L^1([0, T], Q)\). Here, the primal dissipation potential \(R^*_\varepsilon\) is taken as the Legendre transform of \(R^*_\varepsilon\) with respect to the second variable. The notion of EDP-convergence with tilting requires \(\Gamma\)-convergences of the energies \(\mathcal{E}^\varepsilon \rightharpoonup \mathcal{E}_0\) and of the dissipation functionals \(\mathcal{D}^\varepsilon_\eta \rightharpoonup \mathcal{D}^0_\eta\) in suitable topologies, such that for all tilts \(\eta\) the limit \(\mathcal{D}^0_\eta^*\) has the form \(\mathcal{D}^0_\eta^*(\mu) = \int_\Omega R^*_{\text{eff}}(\mu, \hat{\mu}) + \mathcal{R}^*_{\text{eff}}(\mu, \eta - \mathcal{D}\mathcal{E}_0(\mu)) \, dt\) instead of \(\mathcal{D}^\varepsilon_\eta\).

Importantly, the effective dissipation potential \(R^*_{\text{eff}}\) in the \(\Gamma\)-limit is independent of the tilts, which in our situation correspond to an external potential \(V = (V_1, V_2)\) added to the energy \(\mathcal{E}\), i.e. \(\mathcal{E}^V := \mathcal{E} + V\). On the level of the PDE, the original reaction-diffusion system (LRDS) is extended to a reaction-drift-diffusion system of the form

\[
\frac{d}{dt} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \text{div} \left( \begin{pmatrix} \delta_1 \nabla c_1 + \delta_1 c_1 \nabla V_1 \\ \delta_2 \nabla c_2 + \delta_2 c_2 \nabla V_2 \end{pmatrix} \right) + \frac{1}{\varepsilon} \left( \sqrt{\frac{\varepsilon - V_1}{\varepsilon}} \frac{\varepsilon - V_1}{2} - \sqrt{\frac{\varepsilon - V_2}{\varepsilon}} \frac{\varepsilon - V_2}{2} \right) \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}.
\]

4 Effective gradient system and coarse-grained gradient system

The main result of [7] asserts tilt EDP-convergence of \((Q, \mathcal{E}, R^*_\varepsilon)\) to \((Q, \mathcal{E}, R^*_{\text{eff}})\) as \(\varepsilon \to 0\) and the effective dissipation potential is given by \(\mathcal{R}^*_{\text{eff}} = \mathcal{R}^*_{\text{diff}} + \chi_{\{\varepsilon = 0\}}\) (where \(\chi_{\{\cdot\}}\) is the characteristic function of convex analysis). The effective dissipation potential describes diffusion but restricts the chemical potential \(\xi = -\mathcal{D}\mathcal{E}^V(\mu)\) to a linear submanifold given by \(\xi_\mu = \frac{\mu}{\hat{\mu}}\), where the stationary measure \(w^V = (w_1^V, w_2^V)\) is given as the minimum of \(\mathcal{E}^V\) on \(Q\).

The induced gradient flow equation of the gradient system \((Q, \mathcal{E}, R^*_{\text{eff}})\) is then given by a system of drift-diffusion equations on a linear submanifold with a space and time dependent Lagrange multiplier \(\lambda\)

\[
c_1 = \text{div} \left( \delta_1 \nabla c_1 + \delta_1 c_1 \nabla V_1 \right) - \lambda, \quad c_2 = \text{div} \left( \delta_2 \nabla c_2 + \delta_2 c_2 \nabla V_2 \right) + \lambda, \quad \frac{c_1}{w_1^V} = \frac{c_2}{w_2^V}.
\]

Similarly to the space-independent situation of linear [6] or nonlinear [5] fast-slow reaction systems, the effective gradient system can be equivalently described in terms of coarse-grained slow variables. The coarse-grained gradient system is given by \((\hat{Q}, \hat{\mathcal{E}}, \hat{R}^*)\), where \(\hat{Q} = \text{Prob}(\Omega)\) is the coarse-grained state space, the driving functional and the dissipation functional are given by

\[
\hat{\mathcal{E}}(\mu) := \mathcal{E}^V(\mu_1, \mu_2) = \int_\Omega \hat{\mu} \log \hat{\mu} + \hat{\mu} \hat{V}, \quad \hat{R}^*(\hat{\mu}, \hat{\xi}) := R^*_{\text{eff}}((\mu_1, \mu_2), (\hat{\xi}, \hat{\xi})) = \frac{1}{2} \int_\Omega |\nabla \hat{\xi}|^2 d\hat{\mu},
\]

with the reconstructed measure \((\mu_1, \mu_2) = \left( \frac{w_1^V}{w_1^V + w_2^V} \hat{\mu}, \frac{w_2^V}{w_1^V + w_2^V} \hat{\mu} \right)\), a mixed diffusion coefficient \(\hat{\mathcal{D}}^V = \frac{\delta_1 w_1^V + \delta_2 w_2^V}{w_1^V + w_2^V}\), and the mixed potential \(\hat{V} = -\log \left( \frac{\hat{\mu}}{w_1^V e^{-V_1} + \frac{w_2^V}{w_1^V + w_2^V} e^{-V_2}} \right)\). The gradient flow equation induced by \((\hat{Q}, \hat{\mathcal{E}}, \hat{R}^*)\) is given by

\[
\dot{\hat{c}} = \text{div} \left( \hat{\mathcal{D}}^V \nabla \hat{c} + \hat{\mathcal{D}}^V \mathcal{C} \nabla \hat{V} \right),
\]

which is in accordance with [1] in the potential-free case.

Summarizing, the results from [7] show how to obtain a coarse-grained model for a multi-scale problem by performing structural convergence on the level of the gradient system.

Acknowledgements This research has been founded by Deutsche Forschungsgemeinschaft (DFG) through grant CRC 1114 “Scaling Cascades in Complex Systems”, Project C05 “Effective models for materials and interfaces with multiple scales”. Open access funding enabled and organized by Projekt DEAL.

References

[1] D. Bothe and D. Hilhorst. A reaction-diffusion system with fast reversible reaction. *J. Math. Anal. Appl.*, **286**, 1, 2003.

[2] P. Dondl, T. Frenzel, and A. Mielke. A gradient system with a wiggly energy and relaxed EDP-convergence. *ESAIM Control Optim. Calc. Var.*, **25**, 68, 2019.

[3] R. Jordan, D. Kinderlehrer, and F. Otto. The variational formulation of the Fokker-Planck equation. *SIAM J. Math. Analysis*, **29**.1, 1998.

[4] A. Mielke. A gradient structure for reaction-diffusion systems and for energy-drift-diffusion systems. *Nonlinearity*, **24**, 1329–1346, 2011.

[5] A. Mielke, M. A. Peletier, and A. Stephan. EDP-convergence for nonlinear fast-slow reaction systems with detailed balance. *Nonlinearity*, **34**, 5762, 2021.
[6] A. Mielke and A. Stephan. Coarse-graining via EDP-convergence for linear fast-slow reaction systems. *Math. Models Meth. Appl. Sci.*, 30, 09, pp. 1765-1807, 2020.

[7] A. Stephan. EDP-convergence for a linear reaction-diffusion system with fast reversible reaction. *Calculus of Variations and Partial Differential Equations*, 60, 226, 2021.