P 16 Volume-surface reaction-diffusion systems: analysis, numerics, control, and optimality issues
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Volume-Surface Reaction-Diffusion (VSRD) systems arise in many timely applications such as molecular-biology, chemistry, fluid dynamics, crystal growth, see e.g. [15, 12, 13]. In the first funding period, the PhD project "Asymmetric stem-cell division" of Bao Q. Tang yielded multiple pioneering results (see [9, 11, 7, 10]) concerning the mathematical modeling, the analysis, the large-time behavior and the numerical simulation of VSRD models, which are motivated by the asymmetric localization of the protein Lgl prior to asymmetric stem-cell division in Drosophila SOP precursor cells, see [17, 14, 2]. The developed analytic framework is robust with respect to model generalizations and carries over to many related VSRD systems describing e.g. cell-biological signaling processes, see [12] and references therein.

State of the art. A prototypical linear VSRD system was formulated in [11] and describes four conformations of Lgl: L and P in the cytoplasm (i.e. the cell volume) and l and p on the cell cortex (i.e. the cell surface):

$$
\begin{aligned}
L_t - d_L\Delta L &= \alpha P - \beta L, & x \in \Omega, & \qquad d_L\,\partial_\nu L = -\lambda L + \gamma l, & x \in \Gamma, \\
P_t - d_P\Delta P &= -\alpha P - \beta L, & x \in \Omega, & \qquad d_P\,\partial_\nu P = \chi_{\Gamma_2}\xi p, & x \in \Gamma, \\
p_t + d_p\Delta_{\Gamma_2} p &= \sigma l - \xi p, & x \in \Gamma_2, & \qquad d_p\,\partial_{\nu_{\Gamma_2}} p = 0, & x \in \partial\Gamma_2, \\
l_t + d_l\Delta_\Gamma l &= \lambda L - (\gamma + \sigma\chi_{\Gamma_2})l, & x \in \Gamma, &
\end{aligned}
\tag{1}
$$

with positive diffusion coefficients d_L, d_P, d_l, and d_p, positive and constant reaction rates α, β, γ, λ, σ and ξ and a unit out normal ν. The system is closed by initial conditions for all four variables. The function χ_{Γ_2} is a possibly smoothened characteristic function localizing the activity of p onto the boundary part $\Gamma_2 \subset \Gamma = \partial\Omega$. The VSRD systems (1) conserves the total mass of Lgl: $\int_\Omega(L+P)\,dx + \int_\Gamma l\,dA + \int_{\Gamma_2} p\,dA = const$.

Besides global well-posedness, a rigorous Quasi-Stationary-State-Approximation to a reduced model system was proven. Discretizing this VSRD model, a first order, conservative and positivity preserving finite element scheme was studied in [7] and successfully applied to numerically illustrate the complex dynamics described by this four-species VSRD model system [11]. Since phosphorylation of Lgl is potentially a nonlinear process [2], in [9], a reduced two species VSRD model with nonlinear reactions

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\begin{aligned}
u_t - \delta_u\Delta u &= 0, & x \in \Omega, & \qquad \delta_u\partial_\nu u = -\alpha(k_u u^\alpha - k_v v^\beta), & x \in \Gamma, \\
v_t - \delta_v\Delta_\Gamma v &= \beta(k_u u^\alpha - k_v v^\beta), & x \in \Gamma, & \qquad \alpha, \beta \geq 1
\end{aligned}
\tag{2}
$$

was shown to have global, bounded solutions and exponential convergence to equilibrium. The key theorem in [9] proves an entropy entropy-dissipation inequality for (2).

Concerning the general theory of nonlinear reaction-diffusion systems, basic questions like global existence, regularity and large-time behavior constitute many open problems due to the lack of comparison principles and related properties known for scalar parabolic equations. Recent

progress in the study of nonlinear RD systems has been made by applying improved duality methods [3, 16, 6] and by developing entropy methods for nonlinear RD systems (see e.g. [4, 5]). The later requires the existence of suitable entropy functionals, which is nontrivial in cases of reaction networks without detailed balance condition. The existence of suitable relative entropies and entropy methods was shown for linear complex balance reaction networks in [10].

Thesis project to be supervised by Klemens Fellner A first direction of the project is devoted to extending the obtained results to models which additionally describe buffer- and feedback mechanisms, see e.g. [17]. Such models are necessarily nonlinear systems without detailed balance equilibria. Nonlinear models also require the generalisation of the numerical scheme analysed in [7], for instance, in terms of suitable conservative, (hybrid) mixed and discontinuous Galerkin finite element methods see e.g. [8, 18]. Given the complexity of realistic model systems, a main goal will address systematic adaptivity of the FEM based on a posteriori error estimates.

A second direction of the project aims to study optimal control problems, especially boundary control, where we shall consider reaction rates as control variables. Considering a two-species RD system as starting point, we may investigate the controllability of a desired equilibrium state (and/or speed of convergence) in terms of reaction rates, which can be controlled only on a subpart of the domain. Indeed, since crucial protein concentrations are located on the cell cortex, this naturally leads to boundary control problems. Here, an optimal control approach shall also be attempted to identify the activity of this protein from given equilibria concentrations, and thus provide feedback to the biological modeling, see e.g. [1].

Further topics. A further direction of the project concerns the optimality of entropy entropy-dissipation inequalities in order to obtain optimal convergence rates. A possible approach leads to minimizing a non-convex functional under conservation law constraints.

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