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Combining Direct and Inverse problems for Reaction-Advection-Diffusion type PDE: Application to biological Keller-Segel model

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we present a method that solves simultaneously the inverse problem and the state estimation problem associated with nondegenerate anisotropic reaction?advection?diffusion systems, combined with a smooth observation operator, and showcase it on a Keller?Segel system used for the chemotaxis. The method is defined as an optimization problem that minimizes the misfit formulated with three different types of error: on the modelling choices, on the initial state assumption, and on the difference between data and the forward predictive model output. Numerical experiments in one- and two-dimensional physical domains have been performed with synthetic data to evaluate the efficiency of the proposed method, but also to describe the influence of hyperparameters on the inverse problem. Then we analyse numerically a spatiotemporally heterogeneous Keller?Segel system to model the progression of multifocal breast cancer. The central innovation is a dynamic weighting function that allows the proliferation parameter and the chemotaxis coefficient to evolve according to the current distribution of the tumour density among a fixed number of foci of distinct subtypes, calibrated from clinical doubling times.