Solving combined state and parameter estimation problems for complex reaction-advection-diffusion systems

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Résumé

In this study, we develop a method that integrates state and parameter estimation in complex, anisotropic reaction-advection-diffusion systems, illustrated through applications to the Keller-Segel and Turing models. This approach addresses inverse problems by simultaneously estimating state variables and model parameters, minimizing a misfit that includes error from model assumptions, initial conditions, and discrepancies between data and model output. Unlike traditional methods that often require interpolation or a large number of forward model evaluations, our method leverages a deterministic approach, optimizing computational efficiency by decoupling state and adjoint variables. For practical application, we solve the inverse problem iteratively, adapting state and parameter values with sparse temporal data, and avoiding classical Newton-based schemes for enhanced convergence in high-dimensional contexts. Numerical experiments in 1D and 2D domains demonstrate the approach's robustness, particularly regarding the tuning of hyperparameters and handling of epistemic uncertainty. This framework extends the reliability of model calibration across diverse fields, from biological systems to material sciences, by ensuring more accurate parameter fitting with reduced computational cost.

Mots-Clés: Numerical analysis, Parameter estimation, State estimation, Advection, reaction, diffusion systems, Numerical simulation

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