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Importance of scalar source term discretization on the second-order convergence of the Lattice Boltzmann Method for reaction-diffusion equation systems

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In this contribution, we discuss the importance of source term discretization on the second-order convergence of the Lattice Boltzmann Method (LBM) for diffusion and advection-diffusion systems with a strong reaction term. Despite its apparent simplicity, the second-order accuracy and implicitness of the scheme can be degraded by the inconsequent discretisation of the source terms. The research focuses on convection-diffusion models in which the source terms depend on the intensity of the transported fields in an implicit manner. Such terms frequently occur in reaction-type equations, but the findings are widely applicable to other problems.

There is a variety of source term discretisation schemes present in the literature. They can be interpreted as different ways of contributing to either zeroth or first moments of the distribution function (respectively scalar or vector fields transport equations). Change of the zeroth moment accounts for the source term for scalar fields, such as density, concentration, or temperature. Contribution to the first moments is used in many LBM schemes for the discretisation of forces in Navier Stokes equations. Moreover, some of the immersed boundary methods can be interpreted as source-terms ones. In the present work, a detailed derivation and discretisation of the reaction term in the LBM framework are presented. The derivation focuses on maintaining the second order of the numerical method, through the usage of appropriate schemes for integration of the discrete Boltzmann equation. To clarify the origins of differences in the results reported in the literature, we explicitly show the algebraic manipulations utilized during the integration of the Discrete Boltzmann equation (DBE). An in-depth insight is provided by the evaluation of error between the DBE, LBM and continuous solution. In addition, a simplification for the commonly used scheme is derived. Finally, a numerical benchmark compares different spatio-temporal refining approaches in terms of accuracy and computational costs.