The Hong Kong Polytechnic University
Department of Applied Mathematics

Colloquium

Structure-preserving, operator splitting numerical schemes for reaction-diffusion system in the energetic variational approach

By
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Abstract

A few positivity-preserving, energy stable numerical schemes are proposed and analyzed for certain type reaction-diffusion systems involving the Law of Mass Action with the detailed balance condition. The energetic variational formulation is applied, in which the reaction part is reformulated in terms of reaction trajectories. The fact that both the reaction and the diffusion parts dissipate the same free energy opens a path of an energy stable, operator splitting scheme for these systems. At the reaction stage, equations of reaction trajectories are solved by treating all the logarithmic terms in the reformulated form implicitly due to their convex nature. The positivity-preserving property and unique solvability can be theoretically proved. Moreover, the energy stability of this scheme at the reaction stage can be proved by a careful convexity analysis. Similar techniques are used to establish the positivity-preserving property and energy stability for the standard semi-implicit solver at the diffusion stage. As a result, a combination of these two stages leads to a positivity-preserving and energy stable numerical scheme for the original reaction-diffusion system. It is the first time to report an energy-dissipation-law-based operator splitting scheme to a nonlinear PDE with variational structures. Several numerical examples are also presented.

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Date: 4 November 2021 (Thursday)
Time: 9:00-10:00 (Hong Kong Standard Time GMT +8)
Venue: Online Talk via Zoom (Meeting ID: 972 3751 5690)
Speaker: Prof. Cheng Wang, University of Massachusetts Dartmouth
Host: Dr. Xiao Li, The Hong Kong Polytechnic University
Click to join:
https://polyu.zoom.us/j/97237515690?pwd=K2svR0d0bnRRcS9lOUl3VTZCd0dnQT09

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