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Title: Numerical closure for chemically reacting systems with lateral interactions

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We investigate the relation between macroscopic state variables and microscopic evolution in a system of chemically reacting species on a lattice. In the absence of strong diffusion, mean-field approximations are invalid, and correlations between lattice sites need to be taken into account. We investigate the importance of the capturing these correlations in the context of a numerical multiscale simulation tool: the equation-free method. In this method, a (suitably chosen) macroscopic state is advanced over time via a three-step procedure: (i) lifting (creation of a consistent microscopic state); (ii) microscopic simulation of an atomistic description, such as a Gillespie model; and (iii) restriction to the macroscopic state. In particular, we discuss the intimate relation between the choice of macroscopic state variables and the corresponding lifting operator, and we illustrate the effects of the procedure on the accuracy of the obtained numerical closure.