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STRUCTURE-PRESERVING NUMERICAL SCHEMES FOR THE ALLEN–CAHN AND CAHN–HILLIARD MODELS WITH DYNAMIC BOUNDARY CONDITIONS

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ABSTRACT

The Allen–Cahn and Cahn–Hilliard equations are phase-field models that describe phase separation dynamics and can be derived as gradient flows of Ginzburg–Landau-type energies. To account for dynamics on the surface, dynamic boundary conditions such as Allen–Cahn-type [1] and Cahn–Hilliard-type [2] conditions have been introduced, extending these models to coupled bulk-surface systems.

In this work, we propose structure-preserving numerical schemes for the Allen–Cahn and Cahn–Hilliard models with dynamic boundary conditions. The proposed schemes preserve two important physical properties of the continuous systems: dissipation of the bulk-surface total energy and, whenever applicable, conservation of mass. We first reformulate the models within a variational framework and apply the finite element method for spatial discretization. For the temporal discretization, we follow the discrete gradient approach [3] and construct schemes that inherit the underlying energy structure of the continuous models at the discrete level.

The resulting schemes satisfy discrete energy dissipation laws independently of the choice of time-step size and preserve the corresponding mass conservation properties. The preservation of these physical properties is established theoretically and further confirmed through numerical experiments.

Keywords Dynamic boundary conditions · Allen–Cahn equation · Cahn–Hilliard equation · Phase-field models · Structure-preserving numerical scheme · Energy stable scheme · Discrete gradient method

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