Kolloquium für Mechanik

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Datum: Freitag, 22.01.2021
Zeit: 15:00 Uhr
Format: ONLINE-SEMINAR

Titel: Enforcing physical bounds in finite volume and discontinuous Galerkin phase-field simulations

Abstract

The Cahn–Hilliard equation is (besides the Allen–Cahn equation) the prototype phase-field model for immiscible mixtures of two fluids. This fourth-order nonlinear parabolic PDE describes phase separation at a constant temperature in the presence of a mass constraint and the dissipation of free energy, eventually building two ‘pure’ bulk phases, which are separated by a smooth interface. The order parameter, u, which is the main unknown, is physically meaningful only if it attains values within a certain interval, e.g., in [-1,1] when u is chosen as the difference of mass fractions of either fluid component. Whether analytical solutions u satisfy the corresponding bound preservation inequalities, -1 ≤ u(t,x) ≤ 1, depends on the chosen potential function Ψ(u) appearing in the equation. Such potentials that guarantee bound preservation do not allow input values of u outside the admissible range and thus lead to the termination of a simulation if overshoots or undershoots occur in the numerical solution. To enforce the global bounds of -1 and 1 for finite volume solutions or for element averages of discontinuous Galerkin (DG) solutions, the numerical fluxes must be constrained in an appropriate manner. To this end, we propose a novel flux limiter that has to be applied after each time step and that is computed by local (time-explicit) iterations. In the case of DG, after the mean values are bound-preserved, the higher-order solution parts can be controlled by a subsequent slope limiter.

Alle Interessenten sind herzlich eingeladen.
Prof. Dr.-Ing. Bettina Frohnepfel