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Numerical Simulation of Phase Transition Problems with Explicit Interface Tracking

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Abstract

Phase change is ubiquitous in nature and industrial processes. Started from the Stefan problem, it is a topic with a long history in applied mathematics and sciences and continues to generate outstanding mathematical problems. For instance, the explicit tracking of the Gibbs dividing surface between phases is still a grand challenge. Our work has been motivated by such challenge and here we report on progress made in solving the governing equations of continuum transport in the presence of a moving interface by the front tracking method. The most pressing issue is the accounting of topological changes suffered by the interface between phases wherein break up and/or merge takes place. The underlying physics of topological changes require the incorporation of space-time subscales not at reach at the moment. Therefore we use heuristic geometrical arguments to reconnect phases in space. This heuristic approach provides new insight in various applications and it is extensible to include subscale physics and chemistry in the future. We demonstrate the method on applications such as simulating freezing, melting, dissolution, and precipitation. The later examples also include the coupling of the phase transition solution with the Navier-Stokes equations for the effect of flow convection.

Keywords: Front tracking; Phase transition; Precipitation; Dissolution; Freezing; Melting

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