Development of Phase Field Methods with OpenFOAM® and its Application to Dynamic Wetting Processes

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1. Motivation
   ▪ Wetting process in chemical reactor of foam structure
     ➢ Mathematical consistent modeling of moving contact lines on irregular solid surface
     → Resolve stress singularity at no-slip wall

2. Phase Field Methods
   ▪ Cahn-Hilliard (CH) or Allen-Cahn (AC) equation for phase field advection
     CH: \( \frac{\partial C}{\partial t} + (\mathbf{u} \cdot \nabla)C = \kappa \nabla^2 \left( C(C-1)(C+1) - \nabla^2 C \right) \)
     AC: \( \frac{\partial C}{\partial t} + (\mathbf{u} \cdot \nabla)C = -\frac{\gamma}{\epsilon} C(C-1)(C+1) + \nabla^2 C \)
   ➢ \( C \): phase field; 1 for liquid and -1 for gas; it varies continuously over the diffuse interface
   ➢ CH or AC is coupled with momentum equation through surface tension, linear momentum, viscous stress and buoyancy terms

3. Development and Implementation
   ➢ Platform: OpenFOAM® (an open source CFD software package); interDyMFoam as starting point
   ➢ In Cahn-Hilliard, the mobility (4th order derivative) is for now treated in segregated manner with time-step sub-cycling
   ➢ In Allen-Cahn, Lagrange multiplier implemented to enforce phase volume conservation property
   ➢ In momentum equation, relative density flux term due to diffusion of components (central to volume conservation)
   ➢ Surface tension term is implemented as surface tension energy density

4. Validation (using Cahn-Hilliard)
   ▪ 2D Static mesh simulation
   ▪ 3D Adaptive Mesh Refinement (AMR) simulation interface region (refinement level = 2)

5. Outlook
   ➢ Compensation scheme for wall energy relaxation model
   ➢ Block-coupled solution approach to phase field transport in Cahn-Hilliard equation
   ➢ Chemically and geometrically heterogeneous surface
   ➢ Pinning effect of droplet on inclined surface
   ➢ Representative complex sponge structure

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