The 8th European Congress on Computational Methods in Applied Sciences and Engineering
ECCOMAS Congress 2022
5 – 9 June 2022, Oslo, Norway

A DISCRETE DIFFERENTIAL GEOMETRIC FORMULATION OF MULTIPHASE SURFACE INTERFACES FOR SCALABLE MULTIPHYSICS EQUILIBRIUM SIMULATIONS

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Key Words: *Mean curvature, Surface tension, Multiphase surface interfaces, Three-phase contact angle, Discrete differential geometry (DDG)*

In many multiphase systems (e.g. gas-liquid-solid) where surface tension forces dominate over viscous forces, the model can be reduced to a surface interface curvature-driven mechanical problem. In such systems an accurate estimate of the mean curvature of phase interfaces is essential. Conventional numerical methods formulated in Cartesian coordinates are incapable of simulating certain complex systems over the space and timespans of interest [1] due to the large number of discrete elements needed. Here we demonstrate how modern developments in the field of discrete differential geometry can be applied to greatly reduce the computational resources required in such simulations.

In particular, we demonstrate a generalised formulation which builds on the conventional cotan-formula [2] that can be used to reconstruct the exact mean normal- and geodesic curvatures of convex interfaces in equilibrium essential to many scalable systems of interest. An essential extension of conventional formulations is a discrete differential geometric formulation of three-phase contact angles which is accomplished through the Gauss-Bonnet Theorem. Our formulation can also provide error estimates needed for a particular mesh refinement to retain a predetermined accuracy in the simulations. This coordinate free formulation can be applied to any data structure used for multiphysics simulations when the underlying space of the interface is manifold (i.e. triangulable). Three test cases of surface energy minimization flow in

three-phase systems will be presented:

(i) Capillary rise in a tube (modelled as an idealised spherical cap).
(ii) Particle-particle liquid bridges (modelled as ideal Catenoids).
(iii) Sessile microdroplet (comparisons to non-ideal physical experiments).

For all these test cases, near exact results could be demonstrated even for very sparse refinements of the mesh. A comparison to the conventional Surface evolver [3] is also provided for the third test case. Finally, methods are proposed for incorporating the equilibrium formulation into a hybrid Euler-Lagrangian framework for scalable multiphase simulations of capillary force models with discontinuous pressure gradients [4, 5].

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