Abstract Submitted
for the DFD15 Meeting of
The American Physical Society

**A framework for embedding molecular-level information in continuum-scale simulations of interfacial flows**[1] EDWARD SMITH, PANAGIOTIS THEODORAKIS, ERICH MULLER, RICHARD CRASTER, OMAR MATAR, Imperial College London — Molecular dynamics provides a means of resolving the contact-line paradox. The price to pay for this insight is computational, with droplet simulations limited to the nanoscale. In order to model problems of engineering interest, the molecular contact line must be abstracted and included as part of a continuum scale simulation. Coupling, using dynamic molecular simulation in place of empirical or approximate closure relations, provides a means of doing just this. Molecular simulation of two phase Couette flow can reproduce the key features of the moving contact line. This sheared liquid bridge has the advantage that a steady state can be obtained, providing an unlimited source of data for statistical analysis. In this talk, we will present highlights from molecular dynamics simulation of the moving contact line. Using interface tracking, the dynamics of the contact line are examined, with results compared to published experimental studies. Good agreement is observed despite the difference in scale between the molecular model and experiments. Potential applications of this method are discussed, including coupled simulation which incorporates the molecular detail for surfactant-driven spreading.

[1]EPSRC Platform Grant (MACIPh) EP/L020564/1

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Date submitted: 29 Jul 2015 Electronic form version 1.4