Abstract Submitted
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Obtaining macroscopic quantities for the contact line problem from Density Functional Theory using asymptotic methods[1] DAVID SIBLEY, Department of Mathematical Sciences, Loughborough University, ANDREAS NOLD, SERAFIM KALLIADASIS, Department of Chemical Engineering, Imperial College London — Density Functional Theory (DFT), a statistical mechanics of fluids approach, captures microscopic details of the fluid density structure in the vicinity of contact lines, as seen in computations in our recent study [1]. Contact lines describe the location where interfaces between two fluids meet solid substrates, and have stimulated a wealth of research due to both their ubiquity in nature and technological applications and also due to their rich multiscale behaviour. Whilst progress can be made computationally to capture the microscopic to mesoscopic structure from DFT, complete analytical results to fully bridge to the macroscale are lacking. In this work, we describe our efforts to bring asymptotic methods to DFT to obtain results for contact angles and other macroscopic quantities in various parameter regimes. [1] A. Nold, D. N. Sibley, B. D. Goddard and S. Kalliadasis, "Fluid structure in the immediate vicinity of an equilibrium three-phase contact line and assessment of disjoining pressure models using density functional theory" Phys. Fluids 26, 072001 (2014).

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David Sibley
Department of Mathematical Sciences, Loughborough University

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