A Decomposition of Droplet Simulation Using Molecular Dynamics

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Nowhere in fluid dynamics do the limits of continuum computational fluid dynamics (CFD) modelling become more apparent than a droplet on a surface. It is here that the application of molecular dynamics (MD) can provide unique insights. Although it is possible to model droplets at the molecular scale, as in Fig 1a, it is not clear if MD simulation of these nano-droplets will ever be large enough to behave in a similar manner to their macroscale counterparts.

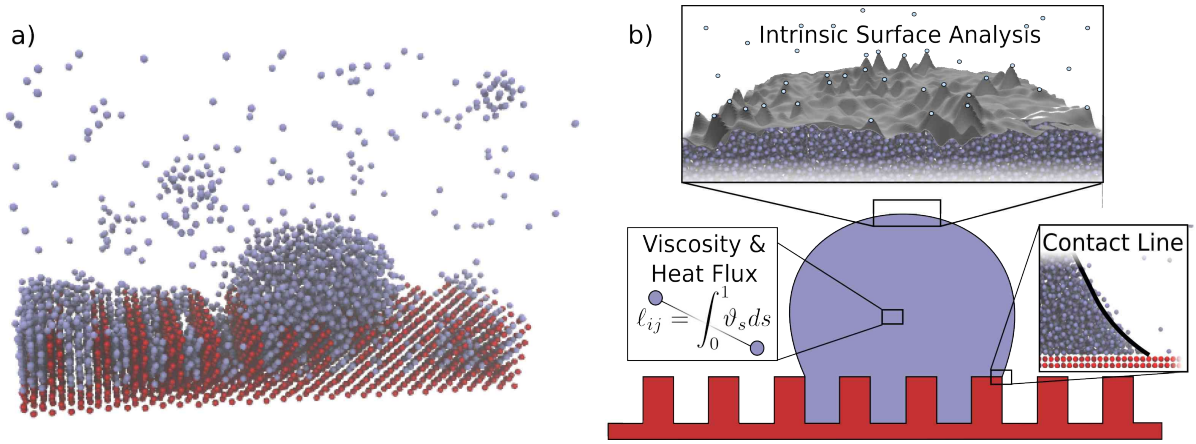

Figure 1 – a) Full MD droplet and b) multiscale model using MD for key details

As the most fundamental classical method, MD captures the full underlying structure of the fluid so that complex phenomema are reproduced with no additional models. In this talk we present molecular models for each of the key physical processes in an evaporating droplets, Fig 1b, including the moving contact line between liquid, vapour and gas [1], the liquid-vapour interface [2] and the bulk fluid properties [3]. We discuss how we use MD to extract the key empherical coefficients for use in CFD, including surface tension, Fourier's law, viscosity and a model for the contact line.

However, the holy grail for multi-scale modelling is to bring these various cases together in a single model which uses molecular detail only where it is needed. We finish with a discussion of progress in this direction [4], and discuss domain decomposition coupling with specially designed software, www.cpl-library.org, to link MD and CFD together for multiphase flow.

ACKNOWLEDGEMENTS: E. R. Smith was supported by EPSRC Grant EP/L020564/1

REFERENCES:

1. Smith E. R., Müller E. A. , Craster R. V., and Matar O. K. ‘A langevin model for fluctuating contact angle behaviour parametrised using molecular dynamics’ **2016** Soft Matter, 12, 48
2. Braga C., Smith E. R, Nold A., Sibley, D. N, and Kalliadasis S.. ‘The pressure tensor across a liquid-vapour interface’ **2018** J. Chem. Phys 149, 044705
3. Smith E. R, Daivis P. and Todd B. ‘Measuring Heat Flux Beyond Fourier's law’ **2019** J. Chem. Phys 150, 064103
4. Smith E. R., Theodorakis P. E., Craster R. V., and Matar O. K ‘Moving contact lines: linking molecular dynamics and continuum-scale modelling’ **2018**, Langmuir, 34, 42, 12501