Multiscale Simulation of Evaporation Using the Multiscale Universal Interface

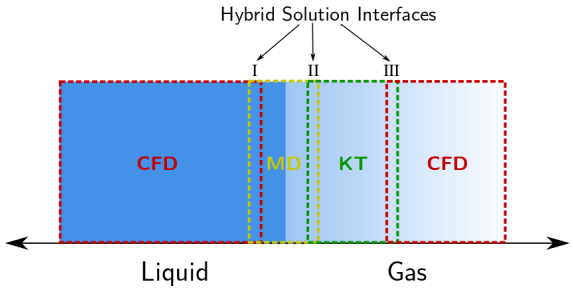
S. M. Longshaw[a], R. Pillai[b], L. Gibelli[b], D. R. Emerson[a], and D. A. Lockerby[c]

[a]Scientific Computing Department, STFC Daresbury Laboratory, United Kingdom
[b]School of Engineering, The University of Edinburgh, United Kingdom
[c]School of Engineering, The University of Warwick, United Kingdom

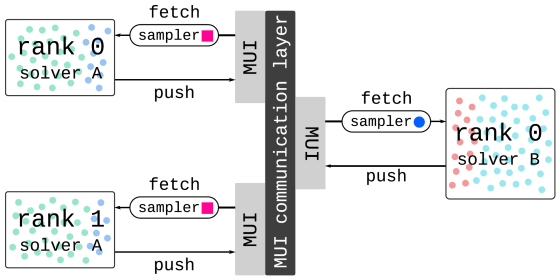
This work uses a new open-source code coupling library, the Multiscale Universal Interface (MUI)[1], to connect together solvers built in OpenFOAM, mdFoam+[2] (a molecular dynamics solver) and dsmcFoam+[3] (a direct simulation Monte Carlo solver) with a view to then connecting these to parametrise a macroscopic CFD simulation.

The purpose is to simulate the process of evaporation, using a CFD solver to handle macroscopic phase change simulation but improve its existing capability by replacing fixed condensation and evaporation coefficients with the results from underlying, coupled micro to mesoscopic simulations. Specifically, molecular dynamics is needed to accurately capture the start of the interface between liquid and gas phases, whilst direct simulation Monte Carlo is needed for the Knudsen (evaporation) layer directly following the interface, this is shown in Figure (a).

The use of the MUI library is key to this work and will be a focus in the delivered talk. MUI is a light-weight header-only C++ library, with wrappers available for Fortran, C and Python. It allows MPI parallelised solvers to communicate by way of the MPI Multi-Program Multi-Data (MPMD) paradigm. This is a portable way to enable scalable coupling on HPC architectures. MUI allows coupling between Eulerian and Lagrangian methods by employing a non-domain specific approach that uses data exchange at points in space, combined with spatial and temporal interpolation methods, this is shown in Figure (b).



(a) Capturing the evaporation process using coupled CFD, Molecular Dynamics and direct simulation Monte Carlo simulations with three interfaces.



(b) General work-flow for the Multiscale Universal Interface coupling library.

References

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[3] C. White, M. K. Borg, T. J. Scanlon, S. M. Longshaw, B. John, D. R. Emerson, J. M. Reese (2018) dsmcFoam+: An OpenFOAM based direct simulation Monte Carlo solver. Computer Physics Communications, 224: 22-4.