# Bridging the molecular-continuum divide: multi-scale modelling of flows in nano systems

## Background

The set of Navier-Stokes-Fourier (NSF) equations is the traditional model for the transfer of heat and momentum in fluid flows. While it has proven successful for flows ranging from liquids in capillaries to the atmosphere of planets, remarkably it can be an extremely poor predictor when the flow system is either very small (i.e. in micro/nano devices) or very low pressure (e.g. high-altitude air vehicles, spacecraft re-entry), or if the process depends on interactions at the molecular level (e.g. protein folding). These predictive failures arise from a limiting assumption underlying conventional fluid mechanics: **scale-separation** — macroscopic flow behaviour is assumed to be independent of the microscopic dynamics of the fluid material [1]. Scale-separation is not guaranteed in micro and nano scale flows: in these cases we need to account for the effect of the fluid's molecular nature on the overall (macro) flowfield. The design of future technologies that exploit micro and nano scale flow components will require the ability to resolve phenomena across scales of at least 8 orders of magnitude in space, and 10 orders of magnitude in time — a formidable multiscale problem.

## Project outline and aims

Recent advances in physical and computational modelling suggest possibilities for efficient and scalable simulations of molecular-continuum systems. One such approach [2] uses a stochastic model for molecular motion as a basis for solving the continuum gas dynamics equations. What is as yet unknown, is how well this approach can capture the unexpected behaviour caused by non-scale-separation in gas flows in micro channels – this is a canonical test case of critical importance. In this mini project we will investigate this stochastic model in some detail, and implement it numerically. The primary aims of the project are to:

a) determine the accuracy of the method in capturing specific flow phenomena that are beyond the understanding of conventional fluid dynamics;
b) evaluate the scalability of the approach to systems of greater complexity.

The student taking this mini project will be contributing to a multi-disciplinary UK team funded by a £2.4m EPSRC Programme Grant (ref: EP/I011927/1) on modelling non-equilibrium fluid dynamics at the micro/nano scale. As such, there may be opportunity to continue this work as part of a funded PhD.

## About the student

The student taking this challenging project opportunity must be confident in mathematics and have some rudimentary programming experience (e.g. in Matlab). No prior experience in fluid dynamics is required. If you have any queries, please contact: Dr Duncan Lockerby (d.lockerby@warwick.ac.uk).

## References


[1] Reese JM, Gallis MA, Lockerby DA. 2003. New directions in fluid dynamics: non-equilibrium aerodynamic and microsystem flows. *Phil. Trans. Roy. Soc. A.* **361** 2967-2988

[2] Jenny P, Torrilhon M, Heinz S. 2010. A solution algorithm for the fluid dynamic equations based on a stochastic model for molecular motion. *J. Comp. Phys.* **229** 1077-1098