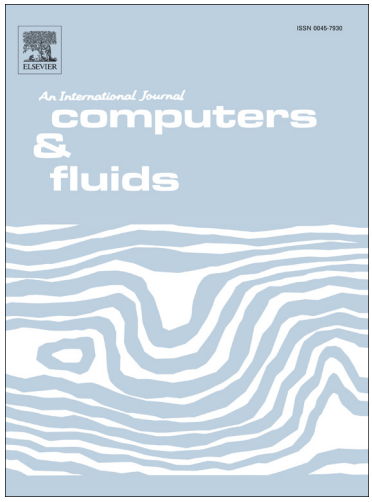

Enhancing nano-scale computational fluid dynamics with molecular pre-simulations: unsteady problems and design optimisation

David M. Holland, Matthew K. Borg, Duncan A. Lockerby, Jason M. Reese

PII: S0045-7930(15)00096-1
DOI: http://dx.doi.org/10.1016/j.compfluid.2015.03.023
Reference: CAF 2842

To appear in: *Computers & Fluids*

Received Date: 31 December 2014
Revised Date: 27 February 2015
Accepted Date: 26 March 2015

Please cite this article as: Holland, D.M., Borg, M.K., Lockerby, D.A., Reese, J.M., Enhancing nano-scale computational fluid dynamics with molecular pre-simulations: unsteady problems and design optimisation, *Computers & Fluids* (2015), doi: http://dx.doi.org/10.1016/j.compfluid.2015.03.023

Enhancing nano-scale computational fluid dynamics with molecular pre-simulations: unsteady problems and design optimisation

David M. Holland[a], Matthew K. Borg[b], Duncan A. Lockerby[a,*], Jason M. Reese[c]

[a]*School of Engineering, University of Warwick, Coventry CV4 7AL, United Kingdom*
[b]*Department of Mechanical & Aerospace Engineering, University of Strathclyde, Glasgow G1 1XJ, United Kingdom*
[c]*School of Engineering, University of Edinburgh, Edinburgh EH9 3JL, United Kingdom*

Abstract

We demonstrate that a computational fluid dynamics (CFD) model enhanced with molecular-level information can accurately predict unsteady nano-scale flows in non-trivial geometries, while being efficient enough to be used for design optimization. We first consider a converging-diverging nano-scale channel driven by a time-varying body force. The time-dependent mass flow rate predicted by our enhanced CFD agrees well with a full molecular dynamics (MD) simulation of the same configuration, and is achieved at a fraction of the computational cost. Conventional CFD predictions of the same case are wholly inadequate. We then demonstrate the application of enhanced CFD as a design optimisation tool on a bifurcating two-dimensional channel, with the target of maximising mass flow rate for a fixed total volume and applied pressure. At macro scales the optimised geometry agrees well with Murray's Law for optimal branching of vascular networks; however, at nanoscales, the optimum result deviates from Murray's law, and a corrected equation is presented.

Keywords: Nanofluidics, Computational Fluid Dynamics, Molecular Dynamics, Hybrid Methods, Design Optimisation, Murray's Law

1. Introduction

Many emerging applications of nanofluidic technology take advantage of different physical effects that dominate at small scales; examples can be found in air and water purification [1, 2], and in micro chemical reactors [3, 4]. The design of these technologies would be greatly facilitated by being able to perform numerical simulations that predict mass flow rates and heat transfer. Computational fluid dynamics (CFD) is regularly used to model and create optimal every-day engineering designs efficiently. However, the assumptions used to derive the continuum fluid equations become invalid in highly-confined systems, making the equations inaccurate. On the other hand, Molecular Dynamics (MD) can be used to perform highly detailed simulations of nano-scale systems; it has been successfully used to study the behaviour of protein folding [5], crystal formation [6] and chemical reactions [7]. The drawback is that MD is extremely computationally intensive, especially when used to model systems comprising hundreds of thousands of molecules that would be required for to engineering applications.

The continuum fluid assumptions become inaccurate

*Corresponding author
Email address: duncan.lockerby@warwick.ac.uk (Duncan A. Lockerby)