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Sustaining pressure gradients in molecular dynamics simulations of fluid-flow through slab geometries

Mohamed T. Elewa[*1], **Lars Pastewka**[2] **and Peter Gumbsch**[1,3]

[1] Institute for Applied Materials - Karlsruhe Institute of Technology, Straße am Forum, Karlsruhe, 76131, Germany, mohamed.hassan@kit.edu
[2] Department of Microsystems Engineering (IMTEK), University of Freiburg, Georges-Köhler-Allee 103, Freiburg, 79110, Germany, lars.pastewka@imtek.uni-freiburg.de
[3] Fraunhofer IWM, Wöhlerstraße 11, Freiburg, 79108, Germany, peter.gumbsch@iwm.fraunhofer.de

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Lubricated machinery is often operated in the boundary lubrication regime where roughness induces significant local variations in pressure. Deviations from the classical description of the flow are attributed to the significance of molecular effects. Non-equilibrium molecular dynamics simulations provide a crucial tool to investigate the microscopic behaviour of lubricants. However, Modeling of pressure gradients in molecular dynamics simulations do not arise naturally for periodic domains with flat walls (slab geometry).

We report the *'pump'* method that allows introducing a physical pressure gradient in periodic molecular domains with slab geometry setup to achieve a pressure-driven flow. The method offers the flexibility to control either the pressure difference (thermodynamic force)[1] or the mass flux (thermodynamic current)[2] directly. The imposed force/flux is in the form of a perturbation field which preserves the dynamic fluctuations of the system and conserves the linear momentum balance.

The robustness of the method is tested by application on molecular n-alkane fluids with different wetting conditions. The method's validity is assessed by measuring the steady-state transport coefficients and comparing with the continuum predictions and shear-driven simulations.

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