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Flow and heat transfer processes at fluid-solid interfaces on molecular scale

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Using Molecular Dynamics simulations, we investigate the fluid dynamics, and thermodynamic properties of liquids in the immediate vicinity of smooth and rough solid surfaces. Surface roughness is modelled using fractal theory to capture the stochastic nature and multiple scales inherently found on real solid surfaces.

Starting with an atomically perfect nanochannel, we find the thermal conductivity of confined liquid argon to be approximately three times greater than the thermal conductivity of its bulk counterpart. This increase is attributed to phonons (lattice vibrations) that propagate over relatively longer distances, enabled by the structural order and greater relaxation time of confined liquids. As the diameter of the nanochannel increases, the thermal conductivity decays and quickly converges to the experimentally measured value of bulk argon.

While the flow velocity in a Poiseuille flow is often assumed to vanish at the boundary, a high boundary velocity is observed next to smooth solid walls. With the introduction and increasing depth of surface roughness, the boundary velocity diminishes, quickly realising the no-slip condition that is often used in Computational Fluid Dynamics (CFD) (Figure 1). We show that this is due to the breakup and mixing of the stratified liquid structures found next to smooth surfaces, resulting in momentum transfer and reduction of the velocity.

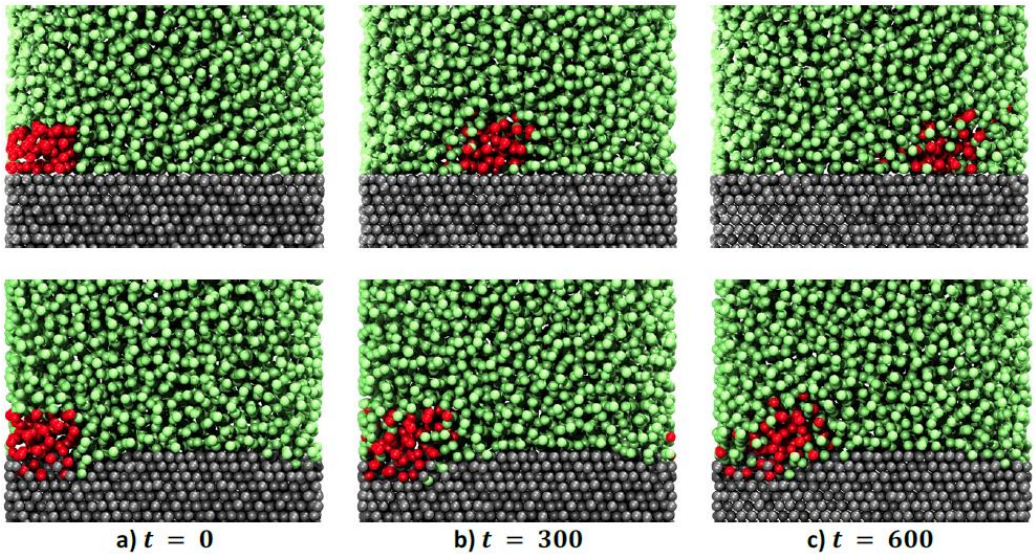

Figure 1 Motion of an arbitrary selection of liquid atoms close to a smooth (top row) and rough (bottom row) solid surface. While the atoms glide over the smooth surface with relatively low resistances, almost no motion is observed next to the rough surface