# Vibrations, diffusions, and currents (oh my!) - Untangling the mechanisms of heat transport in fluid mixtures

**Cillian Cockrell**[1], Kostya Trachenko[2]

[1]Bangor University, Bangor, United Kingdom, [2]Queen Mary University of London, London, United Kingdom

Much progress has been made towards understanding the mysterious liquid state in recent years. Microscopic theories resolving the thermodynamic properties of liquids in terms of collective modes (likened to the phonons of solid state physics) have been enormously successful. In particular, liquid heat capacity is determined uniquely by the mean free path of transverse phonons. Transverse phonons in liquids are scattered by atomic diffusion events, which macroscopically amounts to the continuum flow of matter. The more viscous a fluid, the less frequently transverse phonons are scattered, and (all else being equal) the greater its heat capacity. Likewise, a more inviscid fluid has a shorter mean free path and a lower heat capacity. The thermodynamics and transport of liquids therefore share an interesting interrelationship.

The transport of heat, on the other hand, is considerably more complex. We recall the two mechanisms of heat transport: conduction and convection. Unlike shear momentum, matter advects heat as it flows. Conduction describes the "intrinsic" transfer of heat, driven by gradients of temperature. The lattice thermal conductivity of solids is still admissible to phonon theories, with scattering events acting to reduce the conductivity, as they reduce the viscosity of liquids. In liquids, where the dominant mechanism of scattering is atomic mobility itself, a confounding factor is introduced – when an atom is displaced, it takes energy with it. This introduces a competition where atomic displacement impedes vibrational heat transport but facilitates hydrodynamic heat transport. The waters are further muddied in fluid mixtures, where, even in a barycentric frame, partial mass currents advect heat in a seemingly non-conductive way.

Here, we shall examine these competing mechanisms of heat transport in molecular dynamics simulations of several molten salt systems, whose strong interactions and large mass ratios make analysis delightfully complicated indeed. This causes us to question what we mean by conduction, and how best to assign transport coefficients to atomistic trajectories. Understanding these systems is rather pressing – their thermodynamics and transport properties are of great practical relevance due to the candidacy of molten salts as energy storage media, pyroprocessing hosts, and coolant and fuel carrier fluids in molten salt nuclear reactors. Strongly interacting fluids such as molten salts, and the extent to which their properties are governed by phonons, serve as important and fascinating milestones of how much progress has been made in understanding liquids and how much work remains to be done.