Liquids present anomalies of which science has not yet understood the origin. We all know that they expand upon increase of temperature, say by increasing the temperature by one degree Celsius. At low pressures, typically the same variation of temperature, 1 degree Celsius, makes the liquid to expand more when the temperature is low than when the temperature is high. However, expansion upon temperature increases depends also on the pressure applied on the liquid. It is rather intuitive that the higher is the pressure the less the liquid expands for the same change in temperature, still the 1 degree Celsius. On the other hand, less intuitive is that for selected liquid, when the pressure is higher than some threshold, the expansion is large at low temperatures than at higher ones, inverting the trend at lower pressures.

This observation, that some theories predict to be universal, i.e., to be valid for all liquids, is, indeed, experimentally observed only for some of them. Very puzzling is the observation liquids of very similar molecular composition have very different behavior, some of them showing the inversion of expansion at high and low temperature with pressure, while other not.

The inversion of the trend of thermal expansivity with temperature beyond a given pressure threshold affects also other properties of the liquid. Consider, for example, the so-called heat capacity, measuring the amount of energy that must be provided to a liquid to increase its temperature. The heat capacity of a liquid determines, for example, its suitability as a coolant: a (cold) liquid with high heat capacity is very efficient at cooling a hot object. If it had a lower heat capacity, one had needed more liquid to cool down the same object. For liquids shown inversion in the trend of thermal expansivity, the heat capacity presents a minimum near the threshold pressure. Thus, these liquids are not the best suited to work at these pressure conditions.

Despite the intense experimental and theoretical research in the field, scientists did not understand what the chemical characteristics of the molecules are composing the liquid determining the characteristics of its thermal expansivity, the ensuing “anomaly” of the heat capacity, etc. This is because these techniques, despite their power, do not give direct access to the microscopic behavior of the system, do not allow accessing its secrets at an atomistic level. Thanks to the progress of computers power and computational techniques applied to physics and chemistry, we aim at shading light on the puzzle described above. We will use molecular dynamics, a technique consisting in simulating the behavior of atoms in a liquid. Molecular dynamics allow us "to follow the movie of dancing atoms in a glass of the liquid". Indeed, we will not follow the real atoms of the liquid, but the atoms simulated on a supercomputer, a machine able to perform thousands of billions of mathematical operations per second. Interestingly, liquids can be simulated in a computer in conditions, e.g., pressure and temperature, exceeding those accessible in experiments. Moreover, on a computer one can investigate liquids which might be difficult to synthesize in a laboratory, even liquids made by non-existing atomic species. Thus, one can single out effects that in a laboratory cannot be investigated. In other words, we will use supercomputers as a laboratory on a chip that allow use to access the intimate nature of liquids brought in conditions that might be hard to access in a real lab, finally identifying the microscopic origin of some highly puzzling liquid anomalies.