AB-INITIO GREEN-KUBO SIMULATION OF THERMAL TRANSPORT IN LIQUIDS AND GLASSES: A CHALLENGE TO THEORETICAL PHYSICS AND TO HPC TECHNOLOGY

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The ab-initio computation of thermal conductivities from the Green-Kubo theory of linear-response has long been hampered by two misconceptions. First, the Green-Kubo theory of heat transport was deemed to be incompatible with modern simulation techniques based on electronic-structure theory, because it is based on such concepts as energy densities and currents, which are ill-defined at the quantum-mechanical level. Second, it is commonly thought that the application of this theory would require very long molecular-dynamics simulations, much longer in fact than the typical heat-flux auto-correlation times one is required to evaluate. In this talk I will describe the efforts done at SISSA over the past few years to overcome this state of affairs, which resulted in a methodology allowing us to compute thermal conductivities from equilibrium ab-initio molecular dynamics, no less than in a deeper understanding of the theory of hydrodynamic fluctuations and their numerical analysis through the statistical theory of stationary time series. This methodology sets a number of challenges to the current HPC technology, which I will briefly discuss.