Department of Physics

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Colloquia

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What I cannot compute, I do not understand: fathoming heat transport from the struggle to simulate it

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The Green-Kubo theory of heat transport has long been deemed incompatible with modern simulation methods based on electronic-structure theory, because it is based on such concepts as energy density and current, that are ill-defined at the quantum mechanical level. When a physical quantity that can be easily measured in the lab cannot be computed from the fundamental laws of nature, not even in principle, it's that our theoretical understanding of the physical phenomenon is likely incomplete. I will argue that this is the case for heat transport, and I will describe some recent efforts that are permitting to fill this gap through the introduction of a novel gauge invariance principle for thermal conductivity. These advances are finally allowing to compute heat transport coefficients using ab initio molecular dynamics, a feat that has been made possible also leveraging the statistical theory of stationary time series, and that I will illustrate with a few demonstrations performed on simple, molecular, and binary fluids.

Stefano Baroni is full professor of theoretical condensed matter physics at SISSA. In the late nineties he has been the director of the European Center for Atomic and Molecular Physics (CECAM, then in Lyon), and founding director of the DEMOCRITOS National Simulation Center in Trieste in the early 2000's. He is the main inspirer of the Quantum ESPRESSO project and founding director of the Quantum ESPRESSO Foundation. He is credited for the development of density-functional perturbation theory and several other innovations in electron-structure theory and quantum simulations, which he has applied to semiconductor physics, surface science, molecular spectroscopy, quantum nano-fluids, and, recently, to thermal transport. He is a fellow of the American Physical Society, Division of Computational Physics.

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