PRESS RELEASE

From the evolution of the planets to electronics: studying heat transfer with computers is easier now

Thermal conductivity plays a fundamental role in many natural and technological processes. New research will enable this complex phenomenon to be studied more accurately and efficiently using powerful super computers, thereby opening up interesting application and research perspectives.

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“Our goal? To radically innovate numerical simulations in the field of thermal transport to take on the great science and technology issues in which this phenomenon is so central. This new study, which has designed a new method with which to analyse heat transfer data more efficiently and accurately, is an important step in this direction”. This is how Stefano Baroni describes this new research performed at Trieste’s SISSA by a group led by him, which has just been published in the Scientific Reports journal. The research team focused on studying thermal transfer, the physics mechanism by which heat tends to flow from a warmer to a cooler body. Familiar to everyone, this process is involved in a number of fascinating scientific issues such as, for example, the evolution of the planets, which depends crucially on the cooling process within them. But it is also crucial to the development of various technological applications: from thermal insulation in civil
engineering to cooling in electronic devices, from maintaining optimal operating temperatures in batteries to nuclear plant safety and storage of nuclear waste. "Studying thermal transfer in the laboratory is complicated, expensive and sometimes impossible, as in the case of planetology. Numerical simulation, on the other hand, enables us to understand the hows and whys of such phenomena, allowing us to calculate precisely physical quantities which are frequently not accessible in the lab, thereby revealing their deepest mechanisms", explains Baroni. The problem is that until a short time ago it was not possible to do numerical simulations in this field with the same sophisticated quantum methodologies used so successfully for many other properties: "The equations needed to compute heat currents from the molecular properties of materials were not known. Our research group overcame this obstacle a few years ago formulating a new microscopic theory of heat transfer". But a further issue needed resolving. The simulation times required to describe the heat transfer process are hundreds of times longer than those currently used to simulate other properties. And this understandably posed a number of problems. “With this new research, bringing together concepts demonstrated by previous theories - especially that known as the Green-Kubo theory - with our knowledge of the quantum simulation field we understood how to analyse the data to simulate heat conductivity in a sustainable way in terms of computer resources and, consequently, cost. And this opens up extremely important research possibilities and potential applications for these studies”. With one curiosity which Baroni reveals: “The technique we have formulated is adapted from a methodology used in completely different sectors, such as electronic engineering, to study the digitilization of sound, and quantitative social sciences and economics, to study the dynamics of complex processes such as financial markets, for example. It is interesting to see how unexpected points of contact and cross fertilization can sometimes arise amongst such different fields".

The paper: [http://rdcu.be/yUPc](http://rdcu.be/yUPc)

IMAGE: IStock

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