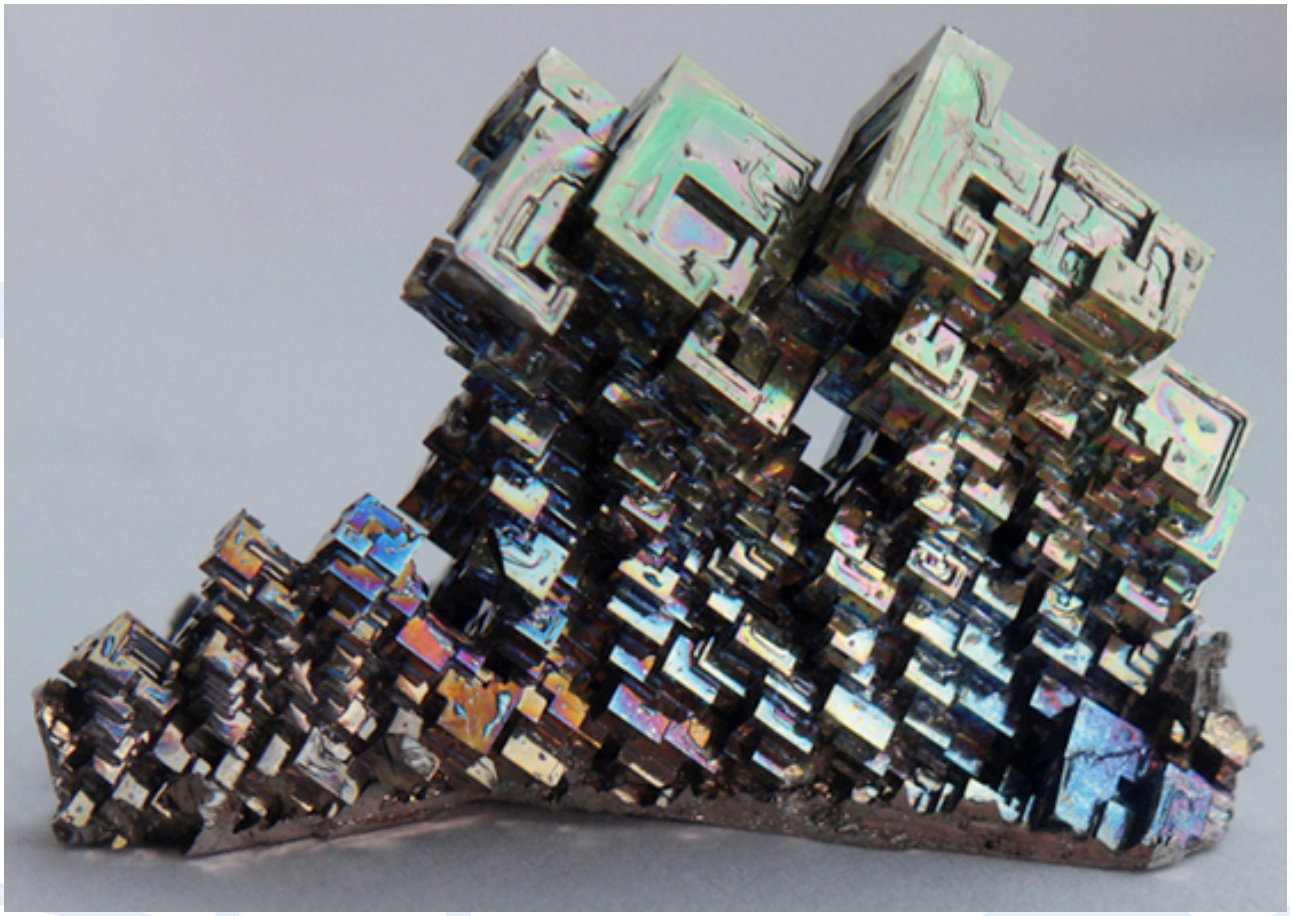
Simulations "sharpen" their tools



The community of physicists validates the precision of numerical methods

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For several years now, numerical simulations have been recognised as an important method of scientific investigation in the field of the physics of materials (amongst others). With simulations, reality is reproduced, by means of computer calculations, to a necessary degree of approximation (which may produce errors) that experts refer to as "precision". An article in Science, authored by a large group of scientists from 44 international institutions, marks the beginning of a major process of validation of algorithms and methods which, though different, converge on the same "problems". The first test was carried out on the equations of state of elemental crystals: the software and methods examined (including the most commonly used today) showed great consistency of predictions, confirming their precision. Among the authors of the article are a number of SISSA research fellows and professors.

In science, there is theory: a fairly general "statement" that describes the world. For example (simplifying somewhat) take the statement "the Earth rotates around its own axis and around the Sun". To test this theory, we need to produce predictions that we are able to compare by means of measurements (when these are possible). And to do this, we need more specific models translated into a mathematical language. However, there may be several, slightly different models or even models based on radically different methodologies that predict the same thing. For example, going back to our "theory" presented above, we know that it implies that day and night alternate on the Earth, so we can decide to calculate when the Sun will rise tomorrow and then check the correctness of of the prediction in real life. This can be done in several ways. By using a record of all the sunrise times over the past months, we can try to identify regular patterns and produce a mathematical function that describes the past and provides an estimate of the future, including the time at which the sun will rise tomorrow – all without knowing anything about the Earth or its rotation speed, etc. Alternatively, we can use mathematical methods to reconstruct the physical system of the Earth revolving around the Sun (entering data on the planet's diameter, rotation speed, axis inclination, etc.), and calculate tomorrow's sunrise time using this method.

The results of the two methods can be compared with real-life observation and with each other. Two types of error can occur: the theory is wrong, the Earth does not revolve around the Sun and it is only by chance that the predictions coincide or do not coincide with reality, but sooner or later some major inconsistency will emerge and the theory will have to be reviewed (imagine that our starting theory had been "the Sun revolves around the Earth"). This is a problem of "accuracy" and concerns our knowledge of reality (and much broader processes of review, debate and reasoning within the scientific community). However, another type of problem may arise: the theory is correct, but the mathematical tools we are using are wrong, for a variety of reasons. In this case, we talk about "precision" a measurement that can be obtained, for example, by comparing the results of the different methods: if they are consistent (in our case they yield the same sunrise time) then we can consider them to be reliable and continue to use them.

This, though in a far more complex manner, is what was done by the scientists (including Stefano de Gironcoli and Andrea Dal Corso, professors at SISSA/CNR-IOM Democritos, Emine Küçükbenli SISSA research scientist, and Paolo Giannozzi, professor at the University of Udine) for the numerical simulation methods that are widely used in the physics of materials. Indeed, today physicists study the nature of matter by simulating its properties with different methods and

software. "During an important conference held a few years ago, we came to the conclusion that it was time to do something we had not done before – at least not systematically – and which chemists, in a field quite close to ours, had already started to do, that is, to test the precision of our instruments", explains de Gironcoli.

"We started with simple things, but clearly we still have a long way to go. Nonetheless the results were positive" continues de Gironcoli. The group of scientists started from the basis of physics, the equation of state, and tested it on the simplest materials: crystals made up of one element only (doing it for all elements of the periodic table). We tested no less than 40 methods, implemented with 15 different software packages.

Among them is also Quantum ESPRESSO, one of the most important software packages currently in use, produced by a consortium in which also SISSA and the University of Udine participate. "We are very satisfied: not only do different software packages implementing the same methods yield the same results, but now we also get the same results with the most commonly used main classes of methods (there are two)" comments Giannozzi. Obviously, this is only the start - the group is already considering extending the test to more complex materials – but it is still an important confirmation: "precision is high", concludes de Gironcoli, "so we can relax a little and concentrate on accuracy, that is, on theoretical speculation". Among the other institutions taking part in the study, coordinated by the Ghent University (Belgium), are Harvard University (USA), the Universities of Oxford and Cambridge (UK), the École Polytechnique Fédérale de Lausanne (Switzerland), the Max-Planck Institute of Microstructure Physics (Germany), to name just a few.

USEFUL LINKS:

- **Original paper in Science: http://goo.gl/ZoJE2b**

IMAGES:

- **Bismuth crystals - Credits: Maxim Bilovitskiy (Wikimedia commons: https://goo.gl/4fRRNa)**

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