



Controversy over spin glasses laid to rest

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Víctor Martin-Mayor and Peter Young head research groups that are studying the phase transition for a particular type of spin glasses, called Heisenberg spin glasses. The controversy over the behaviour of this particular type of spin glasses lasted over 20 years until finally settled by the work of these research groups.

Spin glasses are magnetic alloys that have one salient feature: their properties are never stable over time. When you cool a spin glass below its critical temperature, its properties will continue to change for years. This “aging” phenomenon is not peculiar to spin glasses alone: many other systems of great industrial relevance, such as polymers and structural glasses, also suffer from it. Nevertheless, spin glasses are regarded by scientists as a particularly simple model system for the study of aging.

“We are concerned with the change of ordering properties of the atomic magnets for a particular type of spin glasses, namely Heisenberg spin glasses, at their critical temperature. In order to explore the ordering changes we need to analyse low-enough temperatures. In order to get significant results,

our simulated systems need to be large enough. That’s why the full name of our project is Heisenberg Spin Glasses: Large Lattices at Low Temperatures,” says **Víctor Martin-Mayor**.

In Heisenberg spin-glasses (named after **Werner Heisenberg**, one of the greatest physicists ever who did pioneering work in quantum mechanics), the atomic magnets can be visualized as “arrows” of fixed length, or as points in the surface of a sphere. In “normal” spin glasses (called Ising spin glasses), the magnetic moments can point only to the north pole or to the south pole of this sphere. In Heisenberg spin glasses, on the other hand, they can point anywhere. Some materials are better described as Ising-like, while others are Heisenberg-like. Experiments show that the two types of materials behave rather differently.

The HSG (Heisenberg Spin Glasses) project started in fall 2007, after Martin-Mayor, researcher at the Complutense University of Madrid (Universidad Complutense de Madrid) in Spain, and his group had published the results of their research on Heisenberg spin glasses. These results were soon added to by the research conducted by **Peter Young** and his student **L.W. Lee** at the University of California in the USA. It was clear that neither of the two sets of results were conclusive, but all involved felt that a full understanding was within reach. Instead of competing the researchers decided to collaborate. “The 2007 DECI call for proposals was opened just

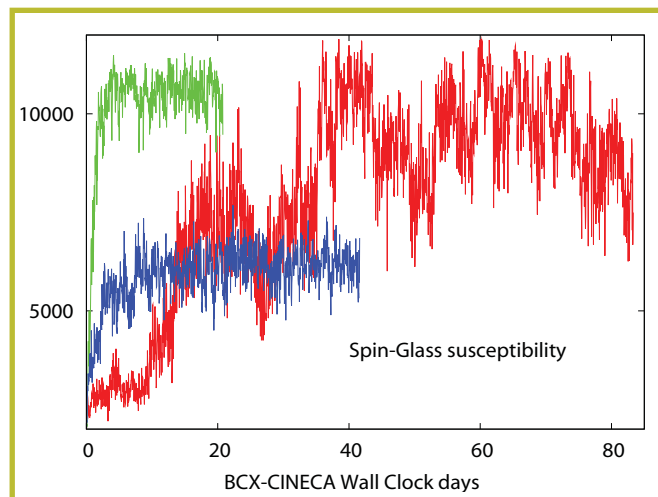


Fig.2 Real simulation data on the time evolution of the spin glass susceptibility. The horizontal axis in the plot is human, wall clock time. For some samples, it was necessary to have 80 CPUs working for almost 90 days before the results were stable with time.

at the ideal moment for us. We had a well-framed problem, and knew how to solve it. We just needed the computational resources and DECI was ready to provide them,” recalls Martin-Mayor.

Martin-Mayor, Young and their research groups are interested in the nature of the phase transition for Heisenberg spin glasses. The changes from liquid to vapour, for example when boiling water, or from liquid to ice when freezing water, are phase transitions. The general feature of these two phenomena is a change of order at the microscopic level. When water is heated until it reaches the boiling point, the water molecules start a fast, random motion. This changes if the water is kept cooling until it freezes: at 0 °C water molecules order into a crystalline structure.

“Phase transitions are a kind of microscopic revolution that happens at a critical temperature. Above the critical temperature, molecules or atoms are significantly more disordered than below it. Phase transitions are ubiquitous in the physics of condensed matter. They receive a lot of attention from scientists, since many interesting things happen close to the

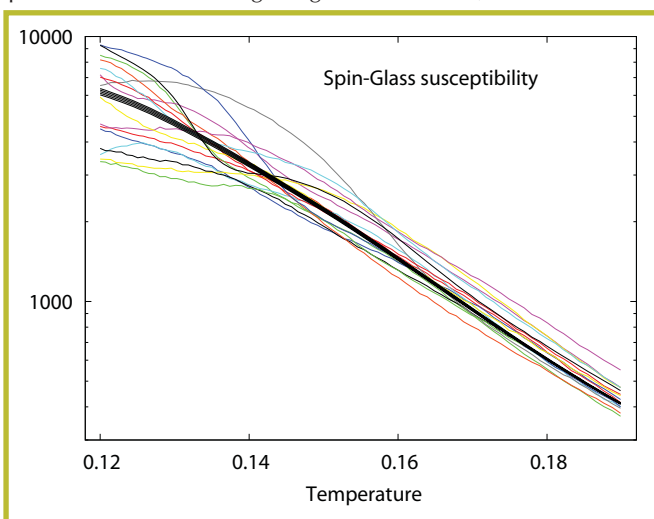


Fig.1 The temperature dependency of the spin glass magnetic susceptibility for some 10 samples to compare with the average behaviour. A Logarithmic scale is needed to represent the extreme sample-to-sample variability.

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critical temperature, while the system properties are relatively constant at other temperatures. Furthermore, sudden changes in material properties triggered by small changes in temperature can be used by engineers. For instance, information is imprinted in a hard disk by ordering the microscopic magnets the disk is made of," explains Martin-Mayor.

Significant number of CPU hours used for simulations

Research into spin glasses is computer-intensive in two ways. "To start with, we are considering disordered magnetic alloys. At a microscopic level, two samples of the very same spin glass material are not identical. These differences can be quite significant as far as the ordering magnetic pattern is concerned. In order to get significant results, we need to simulate hundreds or even thousands of samples," says Martin-Mayor.

"In terms of scientific results, we have obtained conclusive evidence of a spin glass transition in Heisenberg spin glasses. Furthermore, we have demonstrated that there is a single phase transition in the system, even if two quite different types of ordering arise. The controversy over the behaviour of this particular type of spin glasses has lasted for some 23 years now, and we think that it has basically been settled by our work. As originally conceived, the project has been successfully concluded. DEISA gave us enough momentum to complete our research. Our results were reported in a research paper that was written in May 2009, and have already appeared in the journal *Physical Review B*," he continues.

Computing and future developments

The computing time needed in order to obtain significant results even for a single sample can be prohibitive, especially if the system is large or the temperature is low. Physicists have invented a clever way to combat dynamical slowing down, by allowing the temperature of the sample to be a dynamical variable: sometimes it is high, sometimes it is low. This is traditionally done by simulating on the same CPU as many copies of the systems as values can take its temperature. Pairs of copies exchange their temperature periodically, according to certain rules. "This was just too slow for us, since the total CPU time has to be divided between the

many copies of the system," notes Martin-Mayor.

According to Martin-Mayor, the obvious solution was to have a large number of processors (79 plus a central controlling processor) working on different copies of the same sample. The processors needed to be synchronized very often to exchange their temperatures and, less often, to check dynamically the magnetic properties. "To our knowledge, this had not been attempted before, and for good reason. We needed a large number of well communicated CPUs in order to simulate a single sample, but then we needed to simulate hundreds of samples. These kind of computational resources are not easily available for scientists in our area. The DECI call for proposals that would give us access to DEISA resources was an opportunity that we simply could not miss."

"Thanks to DEISA, we have made an important step forward in the understanding of this particular phase transition. We were granted 1.3 million CPU hours in the CINECA supercomputing centre, in Bologna, Italy. We got enough computers to put our research to work. Even if quite large, the thermalization time turned out to be feasible with our parallel computation. We got some 40 samples from CINECA, from a final total of 164. The work was then completed with an extra allocation of some 4.7 million CPU hours in the Red Española de Supercomputación, a network of supercomputing centres in Spain. Our experience with DEISA was crucial in getting such generous time allocations, as we could demonstrate to the Access Commission that our research was working in reality," Martin-Mayor points out.

In the future, Martin-Mayor intends to extend the research program in two ways: "First, Heisenberg spin glasses are, in a sense, an ideal limit. Real materials always have some traces of anisotropic interactions. In order to integrate our theoretical work with experiments, we need to understand in detail the effect of these residual interactions. Second, we have gathered information on the equilibrium spin glass phase, which is clearly relevant to the nonequilibrium experimental work. I think that, since we have already cleared up the phase diagram, it would be of great interest to undertake new simulations of very large systems in order to investigate their aging behaviour."

"In addressing the nonequilibrium, speed is an issue. Nowadays, we roughly need 1 microsecond to update a single spin. To get close



Fig.3 Researcher Víctor Martin-Mayor in the garden in front of the Physics Department of the Complutense University of Madrid, Spain. Picture © Carlos Díaz Guerra

to experimental conditions, we would need to simulate a large number of spins (1 million or so), performing on each some 10 000 million updates. This is roughly equivalent to 300 years of a single CPU. In order to approach that goal, parallel computations are clearly needed. We need to get many CPUs collaborating in the simulation of a single sample, in order to significantly speed up the computation. Technically, this is considerably more demanding than our previous work in DEISA, where each CPU worked on an independent copy of the system," explains Martin-Mayor.

"We do basic research. We seek to advance knowledge on glasses and are convinced that this knowledge will be of practical usefulness in the future, but it is not easy to guess when and where. If I had to make a bet, my money would be in computer science. Computers are being used to solve many problems, where many mutually contradicting goals need to be balanced. The theory of spin glasses has already proven useful to the analysis of difficult optimization problems, and my feeling is that some powerful tools will be made available to engineers in the future as a result," he concludes.

More Information

www.deisa.eu/science/deci/projects2007-2008/HSG

DEISA and TeraGrid Present Joint Summer School Program

European-US Summer School on HPC Challenges in Computational Sciences organized by DEISA and TeraGrid sites

The European Union Seventh Framework Programme's Distributed European Infrastructure for Supercomputing Applications (DEISA), and the United States National Science Foundation's TeraGrid, present a joint EU-US school on High Performance Computing (HPC) Challenges in Computational Sciences, Oct. 4-7, 2010, in Acireale, Catania, Italy.

High-level speakers from the US and Europe will address the following areas in computational science with high relevance for HPC simulations:

- * HPC Challenges and Technology
- * Challenges by Scientific Disciplines
- * Programming
- * Performance Analysis & Profiling
- * Algorithmic Approaches & Libraries
- * Data Intensive Computing and Visualization



Leading scientists in the fields of astrophysics, materials science, nanotechnology, quantum chromo dynamics, and plasma physics will present discipline-related talks. The program will benefit graduate students and postdoctoral scholars who use high performance computing to conduct research.

For all further details (programme, speakers, venue), visit:

www.deisa.eu/Summer-School

Apply via the web by August 29, 2010:

US Applicants:

www.teragrid.org/deisa-tg_form

EU Applicants:

www.deisa.eu/Summer-School/application

(EU applicants may also contact their respective DEISA site)

Applications are being accepted from advanced graduate students and postdoctoral scholars at US and EU institutions through Aug. 29, 2010. Awards will be announced by September 6, 2010. Successful applicants will receive free lodging and meals. US attendees' travel expenses will be paid by TeraGrid.

DEISA Training Courses

14-16 September 2010 at EPCC

-14 September:

Introduction to the DEISA Infrastructure

-15 September:

Performance Optimisation on CrayXT Systems

-16 September:

Parallel Programming with Coarray Fortran

DEISA is running a series of three training courses at EPCC, The University of Edinburgh, in September 2010. All the courses will be based around a series of lectures with associated practical programming exercises.

Courses are free to all EU academics, and you can register for all the courses or just for selected days. Note that the first course is primarily aimed at DEISA users with accepted DECI-6 projects; the other courses are of general interest to all HPC users.

More detailed agendas:

www.deisa.eu/usersupport/training/training-events

Registration form:

www.epcc.ed.ac.uk/training-education/course-registration-form/

Location of EPCC:

www.epcc.ed.ac.uk/contact-us/maps/

DEISA PRACE Symposium 2011



Helsinki, Finland
6-7 April, 2011

at the National Museum of Finland

follow www.deisa.eu and www.prace-project.eu for more details

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