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From parallel to distributed computing as application to simulate magnetic properties-structure relationship for new nanomagnetic materials

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Modern materials science is based in principle on the fundamental experience that the properties of materials are not peremptorily determined by their average chemical composition but they are to a large extent influenced by their microstructure. Now, it is obvious that the outstanding success of magnetic materials for the last two decades may be ascribed to three relevant accomplishments: -overall improvements in general expertise and techniques in sample synthesis; -a dramatic refinement and development of new methods and probes for magnetic materials characterization; -the increasing importance of nano-level studies that led to the ingenious ways of producing nanoparticle samples, new techniques for element specific studies, going down to atomic resolution studies and even to single atoms at surfaces and interfaces. In the last projects completed in recent years we have analyzed and studied magnetic materials mostly micro and nano scale of perovskite, enumerating here cobaltites, ferrimagnetics, ferroics, manganites and other nanomagnetic materials. Almost all of them, listed up require massive data processing. At that time, it became obvious to us that it needs another embodiment, namely in the processing data activity. We were at the beginning, in the 2010 years to introduce parallel computing applications on the simulation of the structure, magnetic and transport properties and to explain the structure-properties relationships for the new nanomagnetic materials that were fashionable in those years. Knowing quite substantial intersection of the parallel computing and distributed, we think it is of common sense to introduce our applicative work in magnetism and magnetic materials science modeling properties, in the context of distributed computing applications. Our latest research specializes in improving techniques for high-level simulation in the design of nano-materials with controlled magnetic properties. We used a package built on Linux, called Nmag (with acquiescence) on an open source platform, across a network of parallel computers.

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