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

S. Mohorianu[1,a], M.-L. Craus[1,2,b]

[1]National Institute of Research and Development for Technical Physics, Romania,
47Mangeron Boulevard, Iasi, Ro-700050, Romania

[2]IUCN, Frank Laboratory for Neutron Physics (FLNP)
6, Joliot Curie, Dubna, 141980, Russia

E-mail: [a] sergium@phys-iasi.ro; [b] craus@phys-iasi.ro, kraus@nf.jinr.ru

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 the distances between atoms and characteristics of their bonds, implicitly 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, goin 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 ferro-, ferrimagnetic and ferroic perovskites, enumerating here (nano)cobaltites, (nano)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. In 2010 we introduce parallel computing applications on the simulation of the structure, magnetic and transport properties to explain the structure-properties relationships for some new nanomagnetic materials. 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.

Keywords: computational material science, magnetic properties-structure relationship, parallel and distributed technologies

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Introduction. Computational materials science - an interdiscipli-nary field that demands parallel and distributed computing technologies

Mathematical modeling aims to describe through mathematics the different aspects of the real world, their dynamics and their interaction. Numerical simulation provides accurate and certified solutions to complex mathematical models by means of scientific computing. Modeling and numerical simulation have become the road-map for mathematics to develop and analyze novel techniques to solve problems in basic sciences. New science called around 2000 by D. Raabe as *computational materials science* [Raabe, 1998], part of a much larger branches, the *computational sciences applied*, requires: *(1)* massive data calculations with *(2)* complex algorithms and *(3)* sophisticated methods. There are many different ways to represent knowledge in a computational framework. The builder of computational models needs an awareness of both: *the range* and *the scope* of representational choice. *New materials and structures by design* is now a modern concept that grows, to be particularly important for the material sciences and engineering. The outstanding success of magnetic materials for the last two decades may be ascribed to three relevant accomplishments in the last 15-20 years: *i)* overall improvements in general expertise and techniques in sample synthesis; *ii)* a dramatic refinement and development of new methods and probes for magnetic materials characterization; *iii)* the increasing importance of nano-level studies, which has led to the ingenious ways of producing nanoparticle samples and the advent of powerful new techniques for element specific studies, layer-by-layer and even leading to atomic resolution, suitable for investigating magnetism of nanoclusters, bi- and trilayer systems and even single atoms at surfaces and/or interfaces. The success at the nano-level has opened-up new frontiers: - *magnetism of nanoclusters*; - *surface and interface magnetism*; - *low dimensional magnetism*; - *interacting nanostructure magnetism*, and others. In terms of theoretical research the rapid development of theoretical methods based on congruity of computer simulation has allowed the calculation of increasingly complex details of the formation and interaction of magnetic moments and has permitted a refined interpretation of experimental data. These continuing work begun in 2005's by works on some *nanomagnetic materials*. The new aspects studied in the last year, our latest research, specialize in improving techniques for high-level simulation in the design of nanomaterials with controlled magnetic properties. New achievements and performance of computing resources have allowed the use of parallel algorithms, distributed calculation appearance in our laboratories. As an interdisciplinary field to simulate the magnetic properties-structure relationship for new magnetic materials that requires advanced knowledge in several areas was not available to everyone from the beginning. The starting point of a *computer simulation* is the development of an *idealized model* of a physical system of interest. Theoretical studies to introduce *parallel computing* in simulation of processes and phenomena encountered in *the design of magnetic materials* have been made yet since the 2000's. Analyzing the actual condition and the capacity of the laboratory, we started to build a parallel computational system only after years 2010 [Mohorianu, Craus, 2010]. So, in the late years we conducted an analysis of endowment and human resource capacity and we got to the conclusion that we can achieve a laboratory infrastructure to support a system of parallel computing for simulation and design of magnetic materials [Mohorianu, 2013]. The *theoretical modeling for the magnetic properties of nanomaterials* turns out to be a quite difficult task. That is because it involves the study of a lot of variables and some apparently non-connected phenomenon that may happen. According with the complexity of the problem we need to create an appropriate theoretical instrument in order to explain and to predict how the *nature* works in our particular problem. It is already well known that *magnetism* is a very complex and intriguing phenomenon. Early experiments to elucidate magnetic phenomena and magnetic materials behavior were based on the measurement of forces and torques exerted on *"samples"* placed into magnetic fields produced by current flow through wires. Our modern understanding of electronic structure is based on the concepts of *charge* and *spin*. The key to this development was the understanding of atomic spectra by means of quantum theory concepts of *exchange* and *spin–orbit coupling*. Most of the common theory is based on these observations. We try to

correlate all these theories and try to exploit some of the newest IT instruments to generate *"recipes"* for the experimentalist to produce faster and cheaper magnetic nanomaterials. It seems that today's magnetic materials are not only the bulk materials, but atomic engineered *wires*, *particles* or *thin film* and *multi layer structures* that often have one, two, or three dimensions on the nanometric scale as we show in figure 1. The massive growth of magnetic technologies is due to scientific and technological developments in four key areas: *a)* the development of *new magnetic materials*; *b)* the *progress in theoretical developments*; *c)* the developments of *new experimental techniques* and *d)* the developments in *simulation techniques*. As things are going now modeling and simulation techniques can be used in all stages in the development and improvement of new magnetic materials, from the initial formation of concepts to synthesis and characterization of properties. In this article we describe how a *S*imulation and *D*esign *M*ethod *(SDM)* attempt, based on our last results is applied on some new type nanomaterials, demonstrating the adaptation of parallel and distributed computing simulators. Our new simulation and design methods allow that by searching on the correlation for the most recent material properties to enhance the actually known magnetic properties. Our IT simulation results are now proposed to be checked in labs with the experimental data and we expect a good agreement.

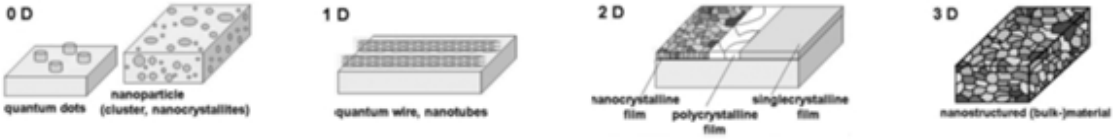

Fig. 1. Nano-materials and nano-structures. Dominant dimension classification

Applied problem. Experimental and Theoretical Approach

Currently nanomagnetism research involves investigating the basic magnetic, magneto-optical, galvano-magnetic, magneto-transport phenomena associated with reduced dimensionality. The idea of extracting valuable information from data is not new. It is new distributed computer processing and data storage technologies, which allow gigabytes, even terabytes of data to remain on-line, available for processing by client/server applications. It's new as well, creating algorithms to study micromagnetism, parallelizing these algorithms, the use of some *Artificial Neural Network* applications and the development of advanced algorithms for knowledge discovery. The parallelization of some of these algorithms is one of our last attempts. The challenges of simulating the relationship structure-magnetic properties of nanomagnetic materials appeared lately. Simulation and design in case of magnetic material structure was started for some *perovskites like materials*. We studied: *cobaltites oxide* with perovskite structure, *multiferroics* materials of type $ReTO_3$ and ReT_2O_5 (Re-rare earth, T- transition metal), *manganites type* $La_{1-x}Re_xMnO_3$. As a result a variety of magnetic different behavior appears in response to external conditions: temperature, chemical doping, magnetic or electric fields, pressure. The *NMAG* [NMag package] *MPI* package was implemented in the laboratory in order to simulate of new magnetic materials in bulk presentation, micro or nano magnetic: perovskites generic $CaTiO_3$, enumerating here cobaltites and manganites as nanoferrimagnetics, nanomultiferroics and nanoferromagnetic materials. We construct a database (*DB)* with many of these materials. The basic idea is to obtain a fine correlation between the *material structure* and/or *composition* and *the magnetic material properties* using either *ANN* or some *micromagnetics soft* as IT instrument. The analyst has a near-infinite number of approaches that can be taken in the course of a simulation/numerical experiment. The approach that is used will depend on *1) the* ***kind*** *of material to be analyzed*, *2) the* ***form*** *of the material*, *3) the* ***problem type*** *that is required to be solved*, *4) the* ***experimental*** *or instrumental technique* that can be employed, and *5) the* ***known limitations*** *of the instrumental / simulation method*. Nanometer-sized magnetic '*object*' are theoreticaly placed at the limit between classical and quantum magnetism so, detecting their magnetic properties is technologically very challenging and from the computational point of view a very difficult task. Thus, we experimen-

tally implemented a *Parallel Computational System (PCS)* working with some academic software packages that were adapted to our current modelling problems. Accumulation based on logistics and scientific development in recent years allowed the creation and development of some modern computational strategies in our laboratory.

Method. Paradigms

Our latest research specializes in improving techniques for high-level simulation programs in the design of nano-materials with controlled magnetic properties. We have tried adapting across multiple platforms, several programs: *OOMMF* (finite differences), *Magpar* (finite elements) and other codes (*Mumax, MicroMagnum*). We presented here as an example what we use in some work constructing the parallel computing network. The package built on *Linux (Python language)*, called *NMag (finite elements)* used. This is on an open source platform, working across a network of parallel computers or *P*rocessor *E*lements *(PE). Nmag's* numerical core as part of the *nsim* (multi-physics library) has been designed to carry out numerical computation on several CPUs simultaneously. The protocol is the wide spread *Message Passing Interface* (*MPI)*. The best ones in this application are probably *MPICH1*. We give data from the package builder on a test for a fairly small system: 4114 mesh nodes, 1522 surface nodes, BEM size 18MB. *NMag* uses the hybrid finite element method/boundary element method to compute the demagnetization field. The *HLib* library is available for academic use, and we have installed it, does not support *parallel execution*. It is thus stored on the master node, and cannot be distributed over several nodes. Simulations using the *Hlib* library can *use MPI* yet, which means parallelized execution. The meshes used in micromagnetic simulations were obtained with *NetGen* and usually represent idealized geometries [NetGen], for example a nano-wire might be modeled using a completely smooth cuboid mesh.

Results

The present work gives some few milestones on how to design new nanomagnetic materials (wires), using simulation methods strictly correlated with the experimental validation. We start from a simple and suitable geometry of the experimental data. So, we considered for the first round of the simulation process a nanomagnetic wire whose magnetic properties have been specified. We enter the specific length values with a 50 nm radius and 1000 nm in length. This calibration was set to work on the simulation tool. *Netgen* produces a mesh network shown in figure 2, with *(P)=703* points; *(E)=1940* elements; *(SE)=1256* SurfacesElements in this case. Same geometry was studied for different wire symmetries, once taking *Ox* axis of symmetry then taking *Oz*. Differences occur for different symmetries. Thus, taking Oz as axis we have: *P=695; E=1902; SE=1252*. In an another step we built a new configuration of *two*, *six* and *twelve* were built to simulate the *interactions between wires* including *short range magnetic interactions*, and *exchange coupling*, see figure 3.

Fig. 2 Netgen mesh for a nanowire

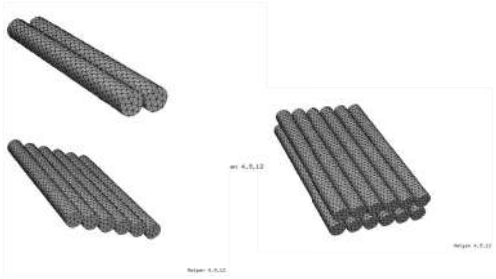

Fig. 3. Magnetic interaction nanowire prepared

So, we were expected some differences in the simulation results. Part of this work seek to establish the necessary parameters for the theoretical model, capable to explain and later to obtain in experimental laboratory help to give new magnetic nanomagnetic wires with *predicted* properties: Curie and transition temperature variation with concentration and implicit the *structure* dependence, or magnetic hysteresis. We give here as example what *NMag* computes the hysteresis loop shown in figure 4, for a series of nano-wires, for this magnetic 'objects' with *K1* (magnetic uniaxial anisotropy) being *(a) 0*, *(b) 10* and *(c) 100 (J/m^3)*. *Nmag* uses the hybrid finite element method/boundary element method (hybrid *FEM/BEM*) to compute the demagnetisation field. For our parallel network we obtain for *4 PE's* a relatively close *score* of *2.03 SS (Simulation – Speedup)* that agree the *Amdahl's low*. The genuine progress on the computational methods, on the experimental IT-based technique, dedicated to the magnetic materials simulation, now allow us a better understanding of our experimental data.

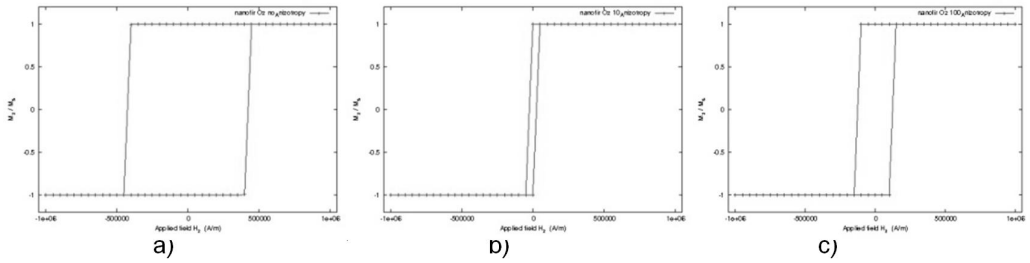

Fig. 4. The computed hysteresis loop (magnetic nanowires with *K1* a) zero; b) 10; c) 100 *(J/m^3)*)

Conclusions

Low dimensional magnetic systems, such as thin films, wires, multilayers, and surfaces exhibit many scientifically interesting and technologically useful properties. Modeling has now a very important position in the development and improvement of new materials for applications. *Modeling* and *simulation techniques* affect all stages in the development and improvement of new materials, from the initial formation of concepts to synthesis and characterization of material properties. We have been applied successfully in the identification and classification of some nanomagnetic characteristics from a large amount of data. These methods prove themselves to be better candidates for *the discovery of new aspects between structure and properties of magnetic nanomaterials.* Our extensive research practice in the properties study of magnetic materials, closely depending on new theories and theoretical models describing their properties led us to an intensive use of the *numerical experiment* in our research. Our methods based on *numerical experiment* and *theoretical modeling* involves *checking with the experimental data* and *validation stage*. Simulations in magnetic material usually require large computing power in order to produce realistic results in an acceptable execution time. Today *parallel computation* becomes a standard way to achieve this, for new complex and realistic simulation programs. Regular algorithms can be realized as parallel programs in a straightforward way but when especially more complex algorithms are involved some more effort is needed to exploit the specific algorithms and the parallel hardware platform to get fast and efficient runs.

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