Lab/State Partnership

- State: Alabama
- Alabama-ORNL Collaboration: Adaptation of Fast Multipole Code for Atomic-scale Micromagnetics
- Lab Partnership PI: Pieter B. Visscher
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- Total DOE Funding: \$149,662 (3 years)
- Duration of Award: 3 years (9/15/98-9/15/01-5/15/02)
- Reporting period (9/15/98-5/15/02)

Electrical and Thermal Transport Properties of New and Novel Solid State Systems

Laboratory Partnership Abstract

Project Summary:

Understanding the molecular-scale dynamics of magnetic materials is a long-standing problem of fundamental physics, as well as being of great importance in the technology of information storage (tapes and disks). The new "GMR" read heads exploit the phenomenon of "exchange bias" at the interface between a ferromagnetic and antiferromagnetic material. The theory group at Oak Ridge National Laboratory has made recent progress in understanding the structures of these interfaces, but is limited by the fact that the computation of long-ranged magnetostatic interactions is extremely time-consuming, even on modern parallel computers, because the time required is proportional to the square of the number of particles. Prof. Visscher's group at Alabama has developed improved hierarchical "fast multipole" methods for dealing with this problem, in computation time that rises only linearly with the number of particles. This project involves applying these new methods to the large-scale computations done by the ORNL group.

Institutions and Personnel Involved

- Universities Involved with project
 - University of Alabama
- Faculty
 - Prof. Pieter B. Visscher (tenured)
- Postdocs: 0
- Graduate Students: 2
 - Xuebing Feng
 - Xiaoguang Deng
- Undergraduate Students: 0

DOE Lab Collaborators

Dr. William H. Butler (until August 2001)

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DOE Patent Clearance Granted

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Scientific Productivity

- 5 publications (1 Phys. Rev. B, 4 J. Appl. Phys.)
- 15 conference presentations (1 invited)
- 2 extramural seminars
- 4 proposals funded
- 5 proposals rejected
- 1 proposal pending

Accomplishments

This project was directed at the study of dynamics of magnetization in magnetic systems, particularly magnetostatic interactions. Important results have been obtained in four areas:

- (1) development of new and efficient fast-multipole methods for dealing with long range magnetostatic interactions

Mourad Benkhalil, a postdoc with the Alabama group, made several visits to Oak Ridge to work with Thomas Schultness on the inclusion of FMM methods in the ORNL codes. Serendipitously, an opportunity to leverage these methods even more widely has appeared in the form of the magnetic thrust of DOE's Computational Materials Science Network (CMSN), PTD by Bruce Harmon (Ames) and Malcolm Stocks (ORNL). P. Visscher, Dmitri Apalkov, and Xuebing Feng (a graduate student at Alabama) are working with Greg Brown (a postdoc partially supported by CMSN at ORNL) and Schultness (ORNL) to develop FMM micromagnetic codes for general CMSN use. The main Alabama contribution to this work is (a) the simplification of FMM codes through the use of recursive and hierarchical methods, and (b) the development of simpler Cartesian (as opposed to the usual spherical-harmonic) expansions for the FMM.

Accomplishments (2)

- (2) Direct evidence for the importance of interactions in novel nanostructured materials synthesized at ORNL

This work [T. C. Schultness et al, J. Appl. Physics, v. 89, 7594, 2001] involved the simulation of material synthesized by Lynn Boatner's group at ORNL using ion implantation of iron in yttrium-stabilized garnet. The hysteresis curves were calculated with and without magnetostatic interactions, and it was found that magnetostatic interactions can make this material (whose inclusions have a very high degree of crystalline orientation) mimic the behavior of an isotropic material. Thus the inclusion of such interactions is very important for the correct characterization of these new materials.

Accomplishments (3)

- (3) progress in understanding how damping on macroscopic scales arises from energy transfer to short-wavelength spin waves

We applied renormalization-group methods [Feng and Visscher, J. Appl. Phys., v. 89, 6988, 2001 (http://arxiv.org/abs/hep-th/0006101)] to calculate the dependence of Landau-Lifshitz damping on cell size, which results from energy loss to short wavelength spin waves. This is an important effect, especially at the very high switching speeds of latest-generation magnetic media, because intrinsic mechanisms such as spin-lattice relaxation are ineffective over short times.

- (4) Quaternion algorithm for micromagnetics

In a paper accepted by Phys. Rev. B [Feng and Visscher, Phys. Rev. B, 2002, http://arxiv.org/abs/hep-th/0109041] we have developed and tested a new algorithm for micromagnetic simulation which facilitates visualization of local processes in the reference frame of the local magnetization. Instead of following the changes in the magnetization vector M , it follows changes in the quaternion (rotation matrix) which describes the precessing local frame in which M is constant.

Accomplishments (4)

- (5) Understanding spin-wave instabilities in switching

A very puzzling switching mode was discovered in simulations by Safonov and Bertram in 1999, in which a magnetic element becomes unstable homogeneously, rather than at the ends or in some geometric pattern such as curling. We have developed new ways of visualizing this process (<http://bama.ua.edu/~vinscher/munag> has a J.Appl. Phys. Paper and some movies) and have been able to calculate the instability growth factor (Lyapunov exponent) and show that it becomes positive when the Safonov-Bertram instability occurs.