Implementation of a high performance parallel finite element micromagnetics package

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Abstract

A new high performance scalable parallel finite element micromagnetics package has been implemented. It includes solvers for static energy minimization, time integration of the Landau-Lifshitz-Gilbert equation, and the nudged elastic band method.

Key words: micromagnetics, finite element method, parallel computing
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1. Introduction

The large computing resources required by large scale micromagnetic simulations as well as the availability of powerful parallel computers and clusters of workstations have been the motivation to implement a new micromagnetics package. The finite element method is very popular for its flexibility in modeling arbitrary geometries, which makes it a very suitable especially in the light of the importance of the microstructure of modern magnetic materials.

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2. Finite Element Micromagnetics

Our new implementation is mainly based on the open source toolbox PETSc [1] for parallel data handling and high level solvers, the BLAS and LAPACK libraries for low level linear algebra, and MPI for communication between the processors. The METIS library [2] is used for mesh partitioning, TAO [3] for energy minimization, and PVODE [4] for the (preconditioned) time integration. All these packages are free and open source, optimized for parallel computers and clusters, and highly portable to various architectures.

The micromagnetics program can be split into four parts: First, a short serial initialization part, which is executed on just one single processor. It reads various configuration and data files of the finite element mesh, material parameters, solver options, etc. Before the mesh is partitioned into parts to be distributed to an arbitrary number of pro-

cessors (mesh partitioning using Metis), the finite element mesh can be refined globally to obtain a better space discretization.

Then, the data are distributed to all processors and the parallel initialization continues with an analysis of the finite element mesh, setup of all required data structures, and the calculation of the "micromagnetic matrices".

The total Gibbs free energy is given by [5]

$$E_{\mathrm{tot}} = \int_{\Omega} \Bigg(A(\nabla \boldsymbol{u})^2 + K_1\big(1 - (\boldsymbol{a}\cdot\boldsymbol{u})^2\big) - \boldsymbol{J}\cdot\boldsymbol{H}_{\mathrm{ext}} - \frac{1}{2}\boldsymbol{J}\cdot\boldsymbol{H}_{\mathrm{demag}} \Bigg)\, dv \quad , \tag{1}$$

where $\boldsymbol{J}(\boldsymbol{x},t) = J_{\mathrm{s}}(\boldsymbol{x})\cdot\boldsymbol{u}(\boldsymbol{x},t)$ describes the magnetic polarization as a function of space and time with the constraint $|\boldsymbol{u}| = 1$. A is the exchange constant, K_1 is the first magnetocrystalline anisotropy constant and $\boldsymbol{a}$ the unit vector parallel to the easy axis, $\boldsymbol{H}_{\mathrm{ext}}$ the external field, and $\boldsymbol{H}_{\mathrm{demag}}$ the demagnetizing field.

The discretization of Eq. (1) is based on the standard Galerkin discretization on tetrahedral meshes with linear basis functions.[6] Thus, the resulting sparse matrices are well suited for parallel computers and clusters of workstations.

In the third part, the requested solver is started to carry out the simulation. All required data (energies, magnetization distributions, etc.) are stored in log files (in compressed format to save disk space) or directly written as graphics images.

Finally, the simulation stops if some exit condition is met. The final results are logged and all data structures freed before the program exits.

3. Performance

We have tested the performance of the energy minimization method, which uses the limited memory variable metric (LMVM) algorithm of the TAO package, for nucleation and domain wall motion problems in hard magnetic FePt nanoparticles and SmCo high temperature permanent magnets. Careful profiling and optimization lead to excellent parallel efficiency with almost linear scaling on up to 24 processors (Fig. 1) on a Compaq SC45 cluster. On eight processors a "superlinear" behavior due to caching effects is observed.

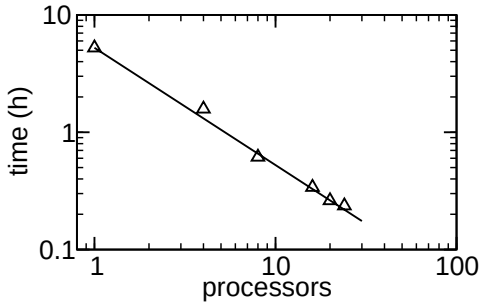

Fig. 1. Execution time of a static energy minimization problem (nucleation in FePt nanoparticles) as a function of the number of processors. The solid line represents the ideal scaling behavior.

4. Conclusions

We have developed a scalable parallel finite element micromagnetics package, which is entirely based on free open source software packages. The implementation of static energy minimization, time integration, and the nudged elastic band method makes it a universal tool for micromagnetic simulations. It has been successfully applied to the simulation of nucleation and domain wall motion problems in hard magnetic materials and showed very efficient parallelization and speedup.

References

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