Implementation of a High Performance Parallel Finite Element Micromagnetics Package

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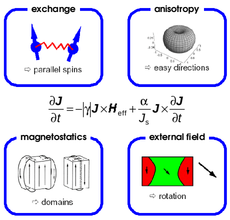
Introduction

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. There are several commercial and free open source packages available, but all of them are based on the finite difference method. 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.

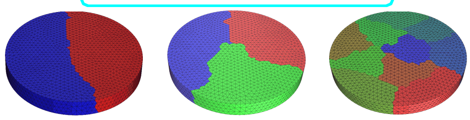
Finite Element Micromagnetics



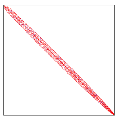
The implementation is based on unstructured tetrahedral finite element meshes with linear test functions.

Exchange interactions, magnetocrystalline anisotropy, magnetostatics (using a hybrid FEM/BEM method) and external fields are taken into account.

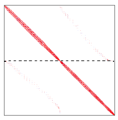
Mesh Partitioning



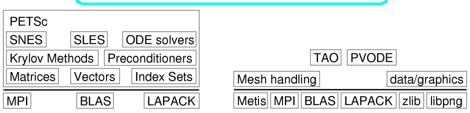
Mesh partitioning for 2 processors, 3 processors and 10 processors using the METIS library.



The elements and nodes are distributed to the processors. Suitable numbering gives the typical band structure of FE stiffness matrices left: stiffness matrix for a single proc. right: distributed to two proc.



Library Structure



The micromagnetics package is based on PETSc, the "Portable, Extensible Toolkit for Scientific Computation". PETSc uses MPI for message passing, BLAS and LAPACK for low level linear algebra. The "Toolkit for Advanced Optimization" is used for energy minimization and PVODE for the time integration of the Landau-Lifshitz-Gilbert equation. METIS handles the mesh partitioning, zlib is used for the compression of output data and libpng for the generation of PNG graphics files.

Solvers

- Energy minimization using TAO
- Landau-Lifshitz-Gilbert time integration using PVODE
- Nudged Elastic Band Method

Features

- Debugging and optimized compilation
- Easy activation of optional components
- Consistency checking - assert statements
- Memory allocation tracking
  PetscMalloc, PetscFree, memory usage statistics
- C++ compatible - required by TAO
- Problem independent parallelization
- Profiling - timing in every subroutine
- Performance evaluation - timing, FLOP count (PVODE missed!)
- Mesh import
  - Patran neutral file (no surface triangles)
  - AVS inp file (Patran neutral file not required)
- Mesh analysis
  - element and node volumes (max,min,avg)
  - edge lengths (max,min,avg)
  - element quality check
  - model bounding box
  - volume by property id
- Mesh distortion - mimic surface/interface roughness
- Mesh refinement - full regular refinement before partitioning:
  $x8^n$ number of nodes and elements
- Micromagnetics
  - Uniaxial/cubic anisotropy
  - Exchange
  - Magnetostatic field (hybrid FEM/BEM)
  - External field (quasistatic, sweeping, rotating)
- Dynamic LLG integration using PVODE
- Static energy minimization using TAO
- Data output
  - Geomview output
  - Log file(compatible with vecu*, Diffpack program, analog.sh)
  - PNG files
  - sampling line

Anisotropy Energy

The magnetocrystalline anisotropy energy for uniaxial anisotropy is given by

$$E_{\rm ani} = \int_\Omega \sum_j K_1 (1 - (\boldsymbol{a} \cdot \boldsymbol{u}_j \eta_j)^2)\, dv \quad . \tag{3.23}$$

The gradient is given by

$$\frac{\partial E_{\rm ani}}{\partial u_{i,l}} = \int_\Omega \sum_j K_1 \frac{\partial}{\partial u_{i,l}} \left(1 - \left(\sum_k^{\{x,y,z\}} (a_k \cdot u_{j,k} \eta_j)\right)^2\right) dv \tag{3.24}$$

$$\begin{aligned} \frac{\partial}{\partial u_{i,l}} \left(\sum_k^{\{x,y,z\}} (a_k \cdot u_{j,k}\eta_j)\right)^2 &= 2 \sum_k^{\{x,y,z\}} (a_k \cdot u_{j,k}\eta_j) \cdot \sum_m^{\{x,y,z\}} (a_m \delta_{ij} \delta_{lm} \eta_j) = \\ &= 2 \sum_k^{\{x,y,z\}} (a_k \cdot u_{j,k}\eta_j) \cdot a_l \eta_i \end{aligned} \tag{3.25}$$

and we get the result

$$\frac{\partial E_{\rm ani}}{\partial u_{i,l}} = -2K_1 a_l \int_\Omega \sum_j \sum_k^{\{x,y,z\}} a_k u_{j,k} \eta_j \cdot \eta_i \, dv \quad . \tag{3.26}$$

This can be rewritten in matrix notation as

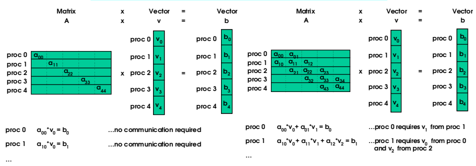
$$\boldsymbol{g}_{\rm ani} = G_{\rm ani} \cdot \boldsymbol{u} \tag{3.27}$$

with

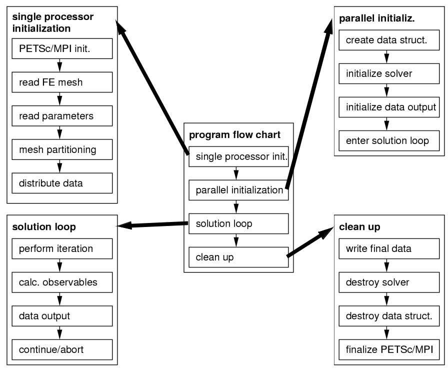
$$G_{{\rm ani},i,l} = -2K_1 a_l \int_\Omega \sum_k^{\{x,y,z\}} a_k \eta_j \cdot \eta_i \, dv \quad . \tag{3.28}$$

For energy minimization as well as the calculation of the effective field, the gradient of the total energy is required. As an example, one contribution - the magnetocrystalline anisotropy energy - is discretized using linear test functions. The calculation of the gradient leads to a simple matrix-vector expression. Thus, the gradient of the magnetocrystalline anisotropy energy can be easily calculated by a simple multiplication of the magnetization vector with a sparse matrix.

Parallel Linear Algebra

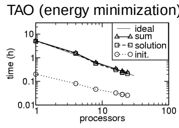


Program Structure



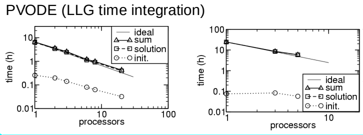
Performance

TAO (energy minimization)



- TAO: speedup 23.9 on 24 processors superlinear behavior on 8 processors (caching effects)
- PVODE:speedup 16 on 20 processors

PVODE (LLG time integration)



tested on Compaq SC45: 11x ES45 with 4x EV68@1 GHz 16 GB RAM

Requirements/Licensing

- Hardware/Software platform, which is supported by PETSc
  IBM RS6000 including IBM SP, SGI running IRIX, 64 bit SGI including Origin and PowerChallenge, Convex Exemplar running HPUX, HP running HPUX, Sun Sparcstations running Solaris, Cray T3D/E, DEC Alpha OSF (Tru64), Intel processors running Linux, FreeBSD, Windows, Mac OS X, PC Running BeOS
- MPI, PETSc, GNU make, C,C++ compilers, METIS, TAO, SUNDIALS, zlib, libpng
- Licenses: all software free and open source mostly under GPL/BSD style OSI approved licenses

URLs: PETSc: http://www-fp.mcs.anl.gov/petsc/ METIS: http://www-users.cs.umn.edu/~karypis/metis/ TAO: http://www-fp.mcs.anl.gov/tao/ SUNDIALS: http://www.llnl.gov/CASC/sundials/
Werner Scholz, Scalable Parallel Micromagnetic Solvers for Magnetic Nanostructures, dissertation, Vienna University of Technology, 2003

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