Simplified Fast Multipole Methods for Micromagnetic Modeling

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This project was supported by NSF grants # ECS-008534 and DMR-0213985, and DOE grant # DE-FG02-98ER45714
Overview

• Context: Fast multipole method (FMM), calculates magnetostatic fields hierarchically

• Previous improvements:
  • Cartesian (simpler than spherical) harmonics
  • recursive calculation of kernels using self-similarity (PBV & DMA, J. Appl. Phys. 93, 15 May 2003. )

• Improvements described here:
  • Simple way to treat periodic systems (MRAM, thin films)
  • Compute fields from surface charges on discrete cells, not from uniform magnetization inside
Basic idea of FMM

Rationale -- MRAM example:

Subdivide rectangular elements into grid (N~10^5 cells)

H~M/r^3+Quad/r^4…

FMM lumps cells together hierarchically:

\[ \begin{align*}
\text{M} & \quad \text{quad, oct, …} \\
\text{Quad.} & \quad \text{(add multipole moments)}
\end{align*} \]
Basic FMM operations

A FMM (fast multipole method) needs functions to

- Compute Taylor expansion of the potential of a point charge at an arbitrary point

  \[ V(\mathbf{r}) = \frac{1}{n_x! n_y! n_z!} \sum_{n_x, n_y, n_z} V_{n_x n_y n_z} x^{n_x} y^{n_y} z^{n_z} \]

- Compute multipole moment of a charge or \( \mathbf{M} \) distribution

  \[ Q_{n_x n_y n_z} = \int x^{n_x} y^{n_y} z^{n_z} \rho(x, y, z) \, dx \, dy \, dz \]

- Convolute the multipole moment with the field of a point charge to get the field of the multipole

- Shift the origin of a Taylor expansion

This gives an O(N) algorithm for computing the magnetostatic field.
Application to periodic system

Want Taylor expansion of potential about center of one cell:

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Need potential of “cored array” of multipoles like

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But . . . it’s enough to know potential of cored array of point charges!

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Just convolute this with the multipole moment of periodic cell.
Conclusion: to do FMM efficiently in a periodic system, we need only calculate the potential of a cored array of point charges:

Traditional Methods:

• Ewald sum (disadvantage: order $N^2$)
• FFT (disadvantage: requires uniform periodic grid)

Instead, use iterative method that uses functions already part of an FMM code.
Conclusion: to do FMM efficiently in a periodic system, we need only calculate the potential of a cored array of point charges:

Convolute with weight array \( w(\mathbf{r}) = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \)

Still missing: shell from \( R \) to \( \sim 2R \) – add “by hand”
Iterative algorithm to calculate the potential of a cored array of point charges

- Start with any estimate of $V^{\text{cored}}(r)$
- Rescale to coarse grid (V of black 1’s)
- Convolute with $w(r) = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$
- Add $V^{\text{shell}}(r)$
- Repeat

Formally,

$$V^{\text{cored, new}}(r) = \frac{1}{2} V^{\text{cored, old}}(r/2) \ast w + V^{\text{shell}}(r)$$

Converges very fast.
Numerical result for cored potential

\[ V^{\text{cored}}(x, y, 0) \]

\[
V^{\text{cored}}(x, y, z) = \frac{0.110572}{4!} (2x^4 + 2y^4 + 2z^4 - 6x^2y^2 - 6y^2z^2 - 6z^2x^2) + \\
\frac{0.0219011}{6!} \left( 2x^6 + 2y^6 + 2z^6 - 15x^4y^2 - 15y^4z^2 - 15z^4x^2 - \\
15x^2y^4 - 15y^2z^4 - 15z^2x^4 + 180x^2y^2z^2 \right) + O(r^8).
\]

Agrees numerically with brute-force summation.

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Charge-based calculation of magnetostatic field

• Magnetization of a cubical cell can be treated as
  (1) Uniform magnetization \( M \) (dipole moment per unit volume) over cell, OR
  (2) Uniform surface charge (density = normal component of \( M \)) on each face of cell
• These are mathematically equivalent, but may not be equivalent in any given approximation
• Trivial example where charge-based method is more efficient: uniformly magnetized infinite thin film.
  – Magnetization method gives poorly convergent sum of dipole fields
  – Surface charge method gives zero (correct answer) immediately – there are no charges anywhere
• Many real problems are close enough to this case that the charge method is significantly more efficient.
Implementing charge-based field calculation in FMM context

FMM requires hierarchical description of system

- cubical cells are the lowest objects on the hierarchical tree, in usual M-based scheme
- In charge-based scheme, charged faces of cells are treated as children of the cells – tree is extended at the bottom

Whole system or “root” cell

boundary cell may “own” up to 6 faces

cells in the bulk “own” 3 faces

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Advantages of charge-based field calculation in FMM context

  – Kernel (used to calculate interactions between nearby objects) describes average field of charged square (rather than magnetized cube) over another cube.

• Uniformly-magnetized regions are treated efficiently.
Test case: MRAM element

50x20x1 cells, in “C” state

Magnetization vector shown (red); charge not shown

Charge concentration at top corners

Charge concentration
Accuracy of charge-based vs magnetization-based FMM calculation

Detail of upper left corner of MRAM, showing both M (red) and charge (black)

Field error in a 50x20x1-cell MRAM element (averaged over element, relative to average field)

Relative Error

Big charges at external faces

Tiny charges at faces, if M nearly uniform

Charge-based FMM

Magnetization-based FMM

Multipole order
Conclusions

• New method for iterative calculation of the magnetostatic field of an infinite array of periodic images
  • Well adapted to Fast Multipole Method
  • Easy to implement, uses functions that already exist in FMM code
• Charge (rather than magnetization) based calculation of magnetostatic field is much more accurate in many cases, especially where there is flux closure (MRAM, thin film)
Spin-Polarized Current Induced Switching.

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Motivation

• study spin-polarized current induced switching in thin film multilayered Co/Cu/Co structures;

• include the influence of the reflected current induced torque in the thick Co-layer.
Cornell experiment


- device dimensions $\sim 60 \text{ nm} \times 130 \text{ nm}$;
- layer thickness:
  Cu (80 nm) / Co (40 nm) / Cu (6 nm) / Co (2.5 nm) / Cu (15 nm)/ Au(60 nm);
- effect of the current induced magnetic field is assumed to be small compared to the effect of the spin-polarized current on the spin moments.
Micromagnetic Calculation

Modified Landau-Lifshitz (LL) equation:

\[
\frac{dM}{dt} = -\gamma M \times H - \frac{\alpha \gamma}{M_S} M \times (M \times H) + \frac{J \beta}{M_S^2} \sum_{\text{SpinPartners}} M \times (M \times M_{SP})
\]

\(\gamma = 17.6 \ (\text{KOe ns})^{-1}\) is the gyromagnetic ratio;
\(\alpha = 0.07\) is the LL damping coefficient;
\(H\) is the total magnetic field;
\(M_S\) is the saturation magnetization;
\(J\) is the current density;
\(\beta\) is a constant, which characterizes the magnitude of the current-induced torque.
Treatment of the Current Induced Torque

These cells affect the magnitude of spin torque in the blue cell. They are called “Spin Partners” for the blue cell. The radius of the cylinder is 6 nm (the discretization size is 3 nm).

\[
\frac{d\mathbf{M}}{dt}_{\text{current}} = \frac{J\beta}{M_S^2} \sum_{\text{SpinPartners}} \mathbf{M} \times (\mathbf{M} \times \mathbf{M}_{SP})
\]
Magnetic Field

\[ H(r) = H^{\text{ext}} + H^{\text{stat}} + H^{\text{rand}} + \sum_{\delta} J_{\text{ex}} M(r + \delta) + \frac{H_K}{M_S} (M(r) \cdot \hat{e}) \hat{e} \]

- \( H^{\text{ext}} \) is the external (applied) field;
- \( J_{\text{ex}} = 0.42 \) is the exchange integral (dimensionless), corresponding to exchange constant \( A = \mu_0 J M_S^2 a^2 = 1 \times 10^{-11} \text{ J/m} \);
- \( M_S = 1440 \text{ emu/cc} \) \( (4\pi M_S = 18.2 \text{ KOe}) \) is the saturation magnetization (Co);
- \( \hat{e} \) is a unit vector along the crystallographic easy axis (z-axis);
- \( H_K = 0.5 \text{ KOe} \) is the effective anisotropy field;
- \( H^{\text{stat}} \) is the magnetostatic field (includes both demag field and the magnetostatic field due to the other layer of Co).
- \( H^{\text{rand}} \) is the effective random field describing Langevin noise.
System Geometry

Relaxed to thermal equilibrium (T = 24 K) system is shown.
Switching Process (T=300 K)

- $\beta J = -0.3 \text{ ns}^{-1}$
- $T = 300 \text{ K}$
- $H_{\text{ext}} = 1.0 \text{ Koe}$
- switching time $\sim 0.4 \text{ ns}$
- pulse duration is 1.7 ns
M-J Hysteresis Loops

For one-domain model:

\[ \beta J_{\text{crit}}^{+/−} = \frac{\alpha \gamma}{N_{sp}} \left[ \mu (2\pi M_s + H_K) + H_{\text{ext}} \right] \]

\[ = -0.168, \ 0.21 \text{ns}^{-2} \]

\[ H_{\text{ext}} = 1 \text{ kOe}, \text{ sweep rate is 0.25 ns}^{-2} \]
Conclusions

• One-domain assumption is wrong in some cases, complete micromagnetic treatment is required
• switching is achieved by domain wall motion
• thermal fluctuations are important to nucleate the reversed domain

Future work

• Study the probability of reversed domain nucleation versus temperature;
• compare the results with experimental data and adjust the model;
• calculate the current induced torque from electron wave functions (W. Butler and J.Velev)