

Introduction to OOMMF Micromagnetic Modeling

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Outline

Background: Micromagnetics

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Outline

Background: Micromagnetics

Practical OOMMF

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Outline

Background: Micromagnetics

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Outline

Background: Micromagnetics

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Outline

Background: Micromagnetics

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

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Outline

Background: Micromagnetics

Background

Practical OOMMF

Practical OOMMF

Pitfalls

Pitfalls

Mesh size

Mesh size

Symmetry breaking

Symmetry breaking

Field step size

Field step size

Stopping criteria

Stopping criteria

Energy minimization

Energy minimization

Advanced Topics

Advanced Topics

Extended volumes

Extended volumes

Normal mode images

Normal mode images

Sub-cell thickness variation

Sub-cell thickness variation

Movies

Movies

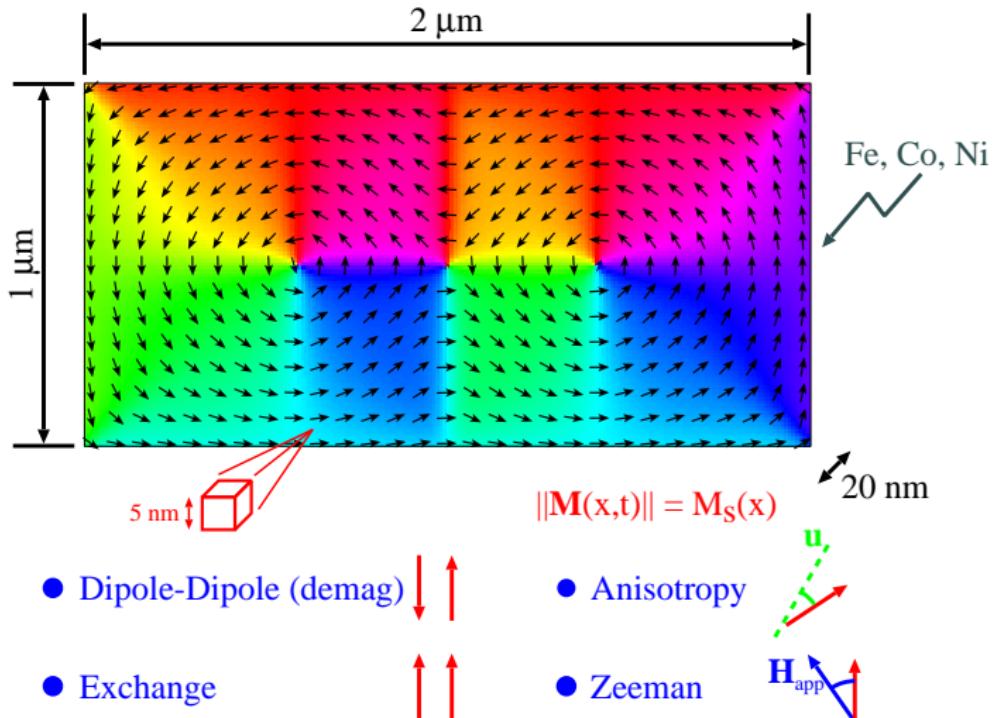
Recommendations

Recommendations

What is micromagnetics?

Micromagnetics

M.J. Donahue



$$\text{LLG: } (1+\alpha^2) \frac{d\mathbf{M}}{dt} = \gamma \mathbf{H} \times \mathbf{M} + (\alpha \gamma / M_s) \mathbf{M} \times \mathbf{H} \times \mathbf{M}$$

How can I use micromagnetics?

Micromagnetics

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Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

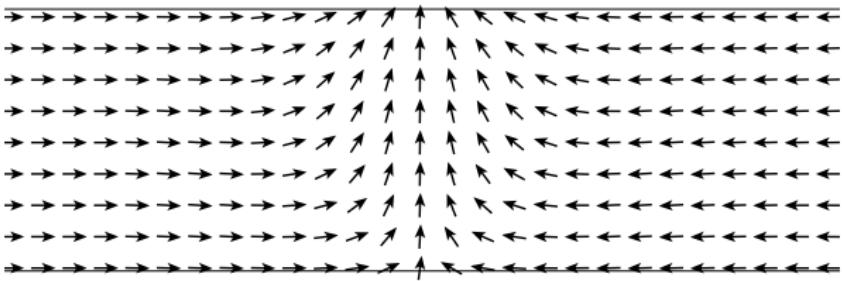
Sub-cell thickness variation

Movies

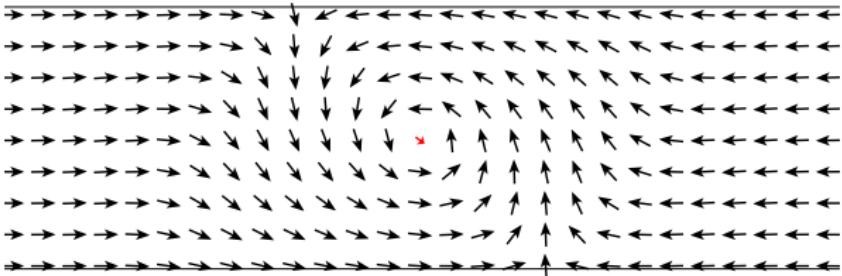
Recommendations

- ▶ Part design
- ▶ Experimental design
 - ▶ Is there anything to see?
 - ▶ Do the spatial and temporal scales match my apparatus?
 - ▶ Is the effect magnitude large enough?
- ▶ Explaining and understanding experimental results

Head-to-head domain wall types



Transverse wall



Vortex wall

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Head-to-head phase diagram

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Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

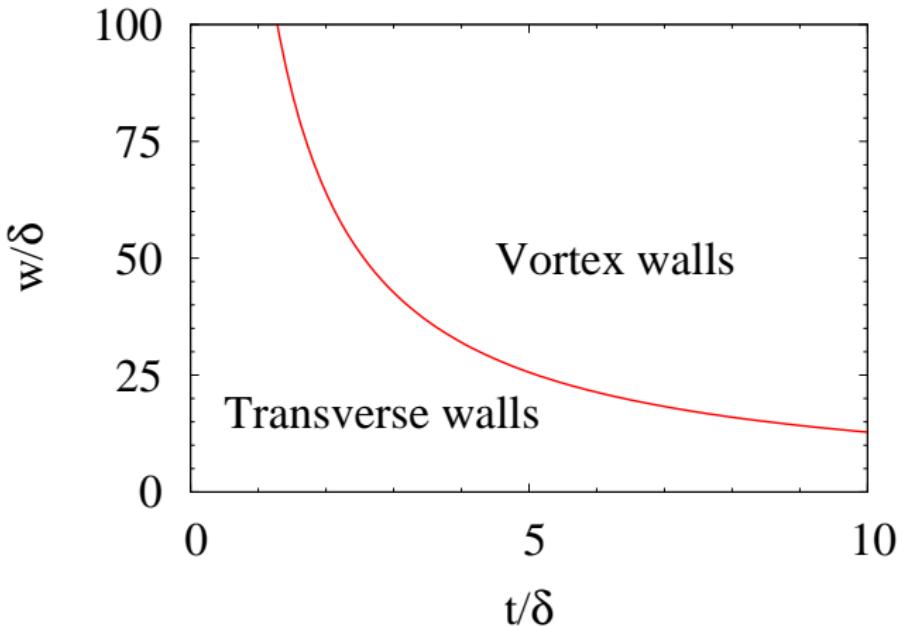
Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations



R.D. McMichael & M.J. Donahue, *IEEE Trans. Magn.*, **33**, 4167 (1997).

Size effect study

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Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

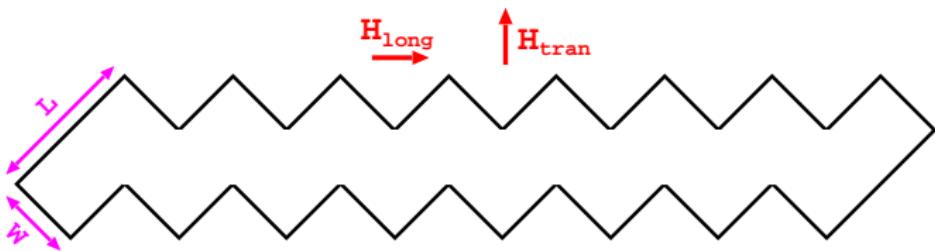
Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations



50 nm < L < 500 nm

W = 0.5 L

Thickness = 20 nm

Py material parameters:

A = 13 pJ/m

K = 0 J/m³

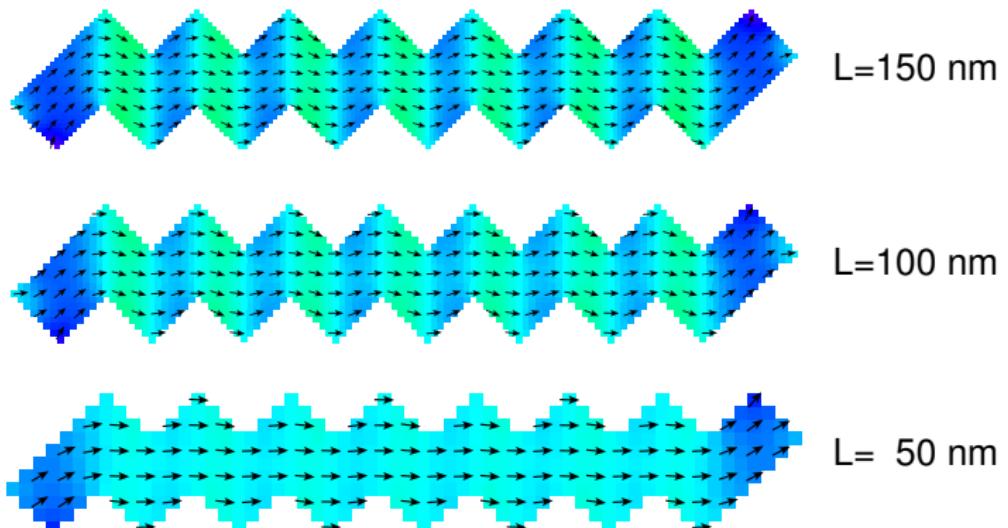
M_s = 800 kA/m

Size effect study (remanent state)

Micromagnetics

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Background



FCS da Silva, WC Uhlig, AB Kos, S Schima, J Aumentado, J Unguris & DP Pappas, "Zigzag-shaped magnetic sensors," *APL*, **85**, 6025, (2004).

Py ring, $D_O = 2 \mu\text{m}$, $t=65 \text{ nm}$

Micromagnetics

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Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

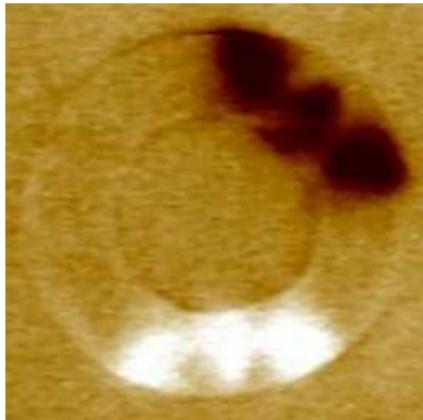
Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations



MFM image

MH Park, YK Hong, BC Choi, MJ Donahue, H Han & SH Gee, "Vortex head-to-head domain walls and their formation in onion-state ring elements," *Phys. Rev. B*, **73**, 094424 (2006).

Py ring, $D_O = 2 \mu\text{m}$, $t=65 \text{ nm}$

Micromagnetics

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Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

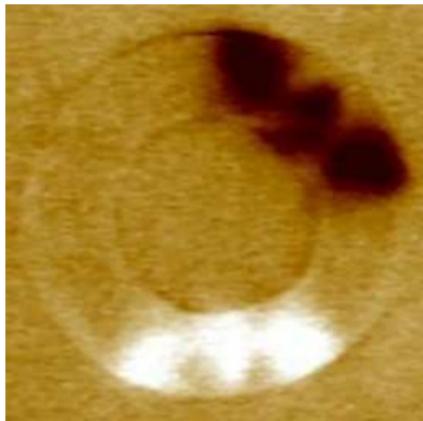
Extended volumes

Normal mode images

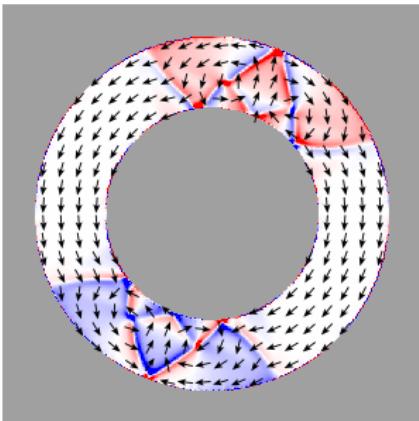
Sub-cell thickness variation

Movies

Recommendations



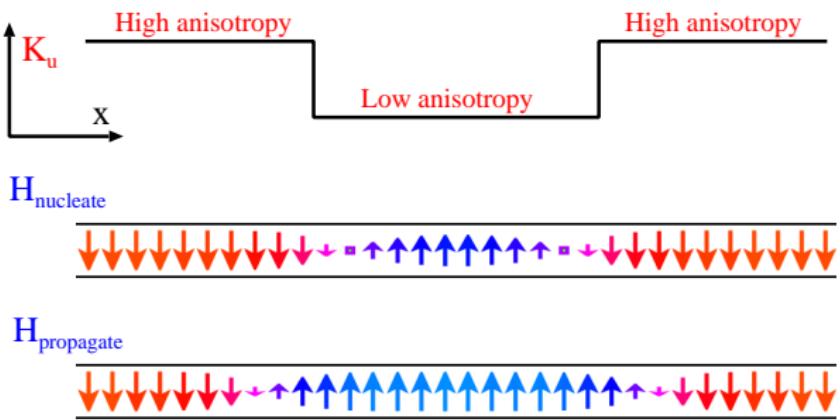
MFM image



Simulation, $\nabla \cdot M$

MH Park, YK Hong, BC Choi, MJ Donahue, H Han & SH Gee, "Vortex head-to-head domain walls and their formation in onion-state ring elements," *Phys. Rev. B*, **73**, 094424 (2006).

Pinning by simple defect (1D)



$$\mathbf{H}_{\text{propagate}} = (\mathbf{H}_{\text{u,bulk}} - \mathbf{H}_{\text{u,defect}})/4$$

$$\mathbf{H}_{\text{switch}} \geq \mathbf{H}_{\text{u,bulk}}/5$$

Background

Practical OOMMF

Pitfalls

- Mesh size
- Symmetry breaking
- Field step size
- Stopping criteria
- Energy minimization

Advanced Topics

- Extended volumes
- Normal mode images
- Sub-cell thickness variation
- Movies

Recommendations

Brown's equations

Energies:

$$E_{\text{exchange}} = \int_V \frac{A}{M_s^2} \left(|\nabla M_x|^2 + |\nabla M_y|^2 + |\nabla M_z|^2 \right) d^3r$$

$$E_{\text{anisotropy}} = \int_V \frac{K_1}{M_s^2} (\mathbf{M} \cdot \mathbf{u})^2 d^3r$$

$$\begin{aligned} E_{\text{demag}} = & \frac{\mu_0}{8\pi} \int_V \mathbf{M}(\mathbf{r}) \cdot \left[\int_V \nabla \cdot \mathbf{M}(\mathbf{r}') \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} d^3r' \right. \\ & \left. - \int_S \hat{\mathbf{n}} \cdot \mathbf{M}(\mathbf{r}') \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} d^2r' \right] d^3r \end{aligned}$$

$$E_{\text{Zeeman}} = -\mu_0 \int_V \mathbf{M} \cdot \mathbf{H}_{\text{applied}} d^3r$$

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Constraints

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

\mathbf{M} is smooth

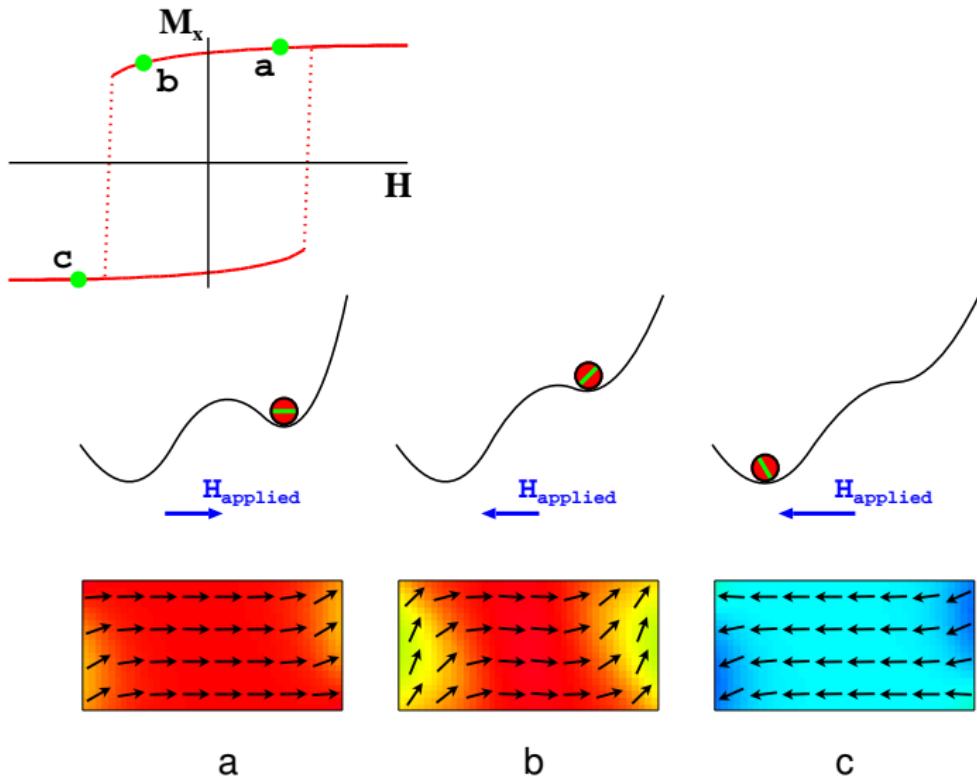
and

$$\|\mathbf{M}(\mathbf{r}, t)\| = \|\mathbf{M}(\mathbf{r})\| = M_s(\mathbf{r})$$

or equivalently

$$\|\mathbf{m}(\mathbf{r}, t)\| = \mathbf{M}(\mathbf{r}, t)/M_s(\mathbf{r}) = \|\mathbf{m}\| = 1.$$

Quasi-static micromagnetics



Magnetization dynamics

Micromagnetics

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Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Landau-Lifshitz-Gilbert:

$$\frac{d\mathbf{M}}{dt} = \frac{|\gamma_0|}{1 + \alpha^2} \mathbf{H}_{\text{eff}} \times \mathbf{M} + \frac{\alpha |\gamma_0|}{(1 + \alpha^2) M_s} \mathbf{M} \times \mathbf{H}_{\text{eff}} \times \mathbf{M}$$

where

$$\mathbf{H}_{\text{eff}} = -\frac{1}{\mu_0} \frac{\delta E_{\text{total}}}{\delta \mathbf{M}}$$

γ_0 = gyromagnetic ratio

α = damping coefficient

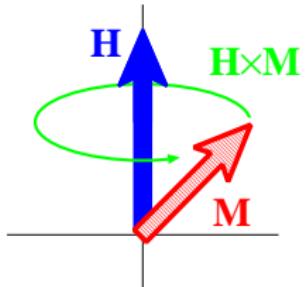
[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

Magnetization dynamics

Landau-Lifshitz-Gilbert:

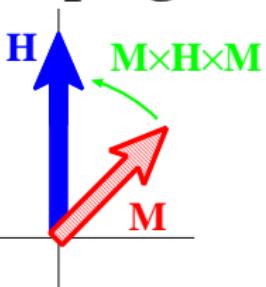
$$\frac{d\mathbf{M}}{dt} = \frac{|\gamma_0|}{1 + \alpha^2} \mathbf{H}_{\text{eff}} \times \mathbf{M} + \frac{\alpha |\gamma_0|}{(1 + \alpha^2) M_s} \mathbf{M} \times \mathbf{H}_{\text{eff}} \times \mathbf{M}$$

Precession



No energy change

Damping



Loses energy

$$\left\| \frac{d\mathbf{M}}{dt} \right\| = \frac{|\gamma_0|}{\sqrt{1 + \alpha^2}} \left\| \mathbf{H}_{\text{eff}} \times \mathbf{M} \right\|$$

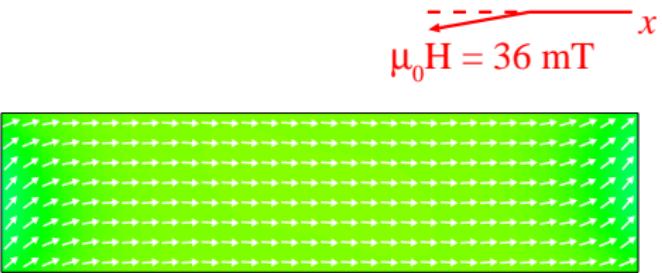
Magnetization dynamics

Micromagnets

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Time

0 ps



Background

Practical OOMMF

Pitfalls

- Mesh size
- Symmetry breaking
- Field step size
- Stopping criteria
- Energy minimization

Advanced Topics

- Extended volumes
- Normal mode images
- Sub-cell thickness variation
- Movies

Recommendations

Magnetization dynamics

Micromagnetics

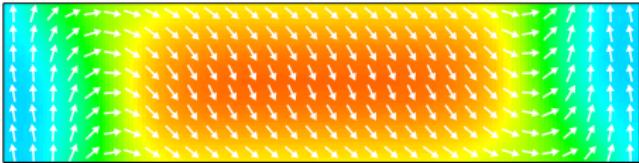
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Time

0 ps

$$\mu_0 H = 36 \text{ mT}$$

100 ps



Background

Practical OOMMF

Pitfalls

- Mesh size
- Symmetry breaking
- Field step size
- Stopping criteria
- Energy minimization

Advanced Topics

- Extended volumes
- Normal mode images
- Sub-cell thickness variation
- Movies

Recommendations

Magnetization dynamics

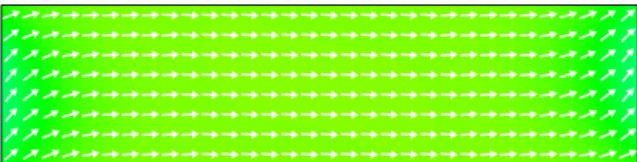
Micromagnetics

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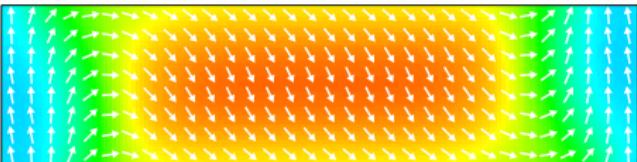
Time

0 ps

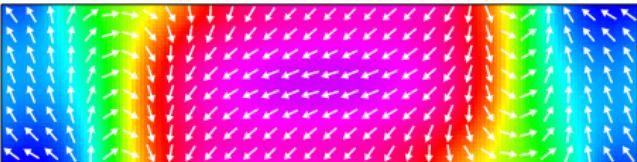
$$\mu_0 H = 36 \text{ mT}$$



100 ps



150 ps



Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

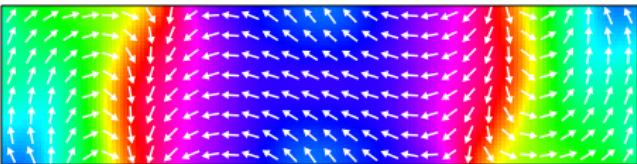
Recommendations

Magnetization dynamics

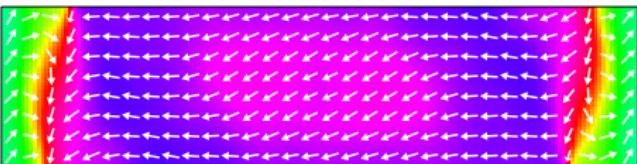
Time

$$\mu_0 H = 36 \text{ mT}$$

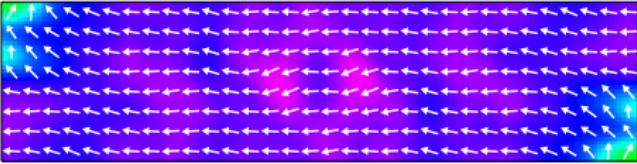
350 ps



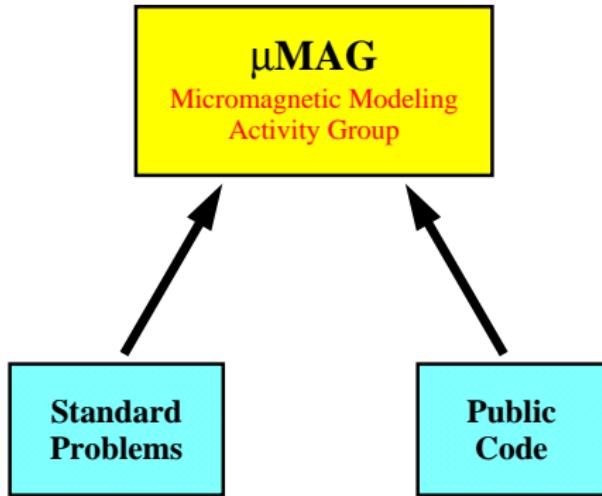
450 ps



750 ps



RD McMichael, MJ Donahue, DG Porter & J Eicke, "Switching dynamics and critical behavior of standard problem no. 4," *JAP*, **89**, 7603 (2001).



Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Center for Theoretical and Computational Materials Science

<http://www.ctcms.nist.gov/>

See also the mailing list and archives!

μ MAG standard problems

Micromagnets

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Background

Practical OOMMF

Pitfalls

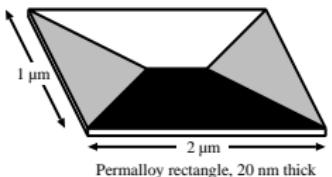
- Mesh size
- Symmetry breaking
- Field step size
- Stopping criteria
- Energy minimization

Advanced Topics

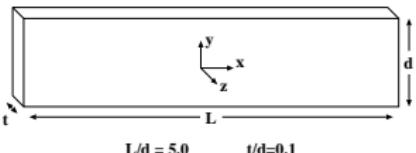
- Extended volumes
- Normal mode images
- Sub-cell thickness variation
- Movies

Recommendations

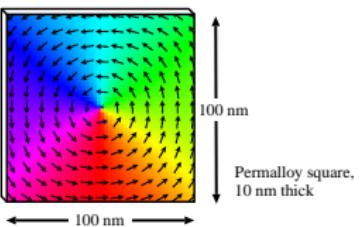
Problem 1: Hysteresis



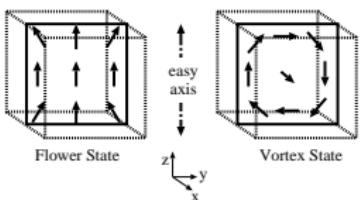
Problem 2: Hysteresis



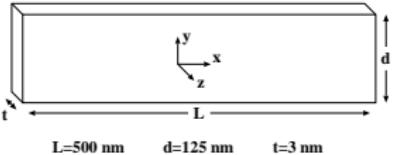
**Problem 5:
CIP Spin Torque**



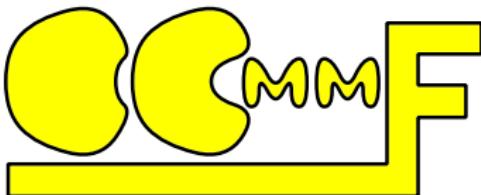
Problem 3: Energy Minimization



Problem 4: Dynamics



Portable, extensible,
public domain
programs & tools
for micromagnetics

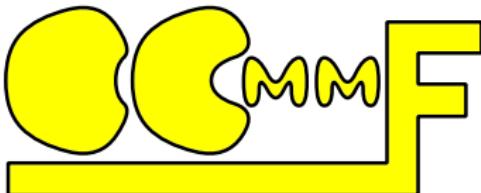


<http://math.nist.gov/oommf>

Primary developers: Don Porter, Mike Donahue (NIST)

- ▶ Finite difference code
 - ▶ Graphical User Interface
 - ▶ Windows, Unix, Mac OS X
 - ▶ Binaries and source code
 - ▶ Tcl/Tk and C++ based modular architecture
 - ▶ 250 page user's manual
 - ▶ 6000+ downloads in 2015
 - ▶ Cited in 200 journal articles in 2016
 - ▶ 2200 citations since 1997
 - ▶ Now at nanoHUB!
- ▶ Extensible architecture: numerous third party extensions

Portable, extensible,
public domain
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for micromagnetics



<http://math.nist.gov/oommf>

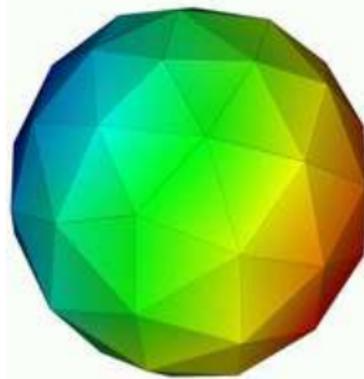
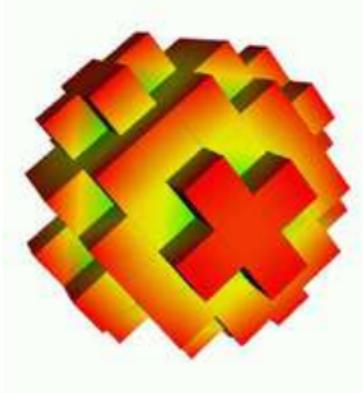
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- ▶ Finite difference code
 - ▶ Graphical User Interface
 - ▶ Windows, Unix, Mac OS X
 - ▶ Binaries and source code
 - ▶ Tcl/Tk and C++ based modular architecture
 - ▶ 250 page user's manual
 - ▶ 6000+ downloads in 2015
 - ▶ Cited in 200 journal articles in 2016
 - ▶ 2200 citations since 1997
 - ▶ Now at nanoHUB!
-
- ▶ Extensible architecture: numerous third party extensions
 - ▶ If you use OOMMF, please cite!

Finite Difference

vs.

Finite Element



- ▶ Meshing is simple
- ▶ FFT = fast demag
- ▶ Jaggy (staircase) boundaries

- ▶ Meshing is complicated
- ▶ Better boundaries
- ▶ Demag is big and slow
 - FEM-BEM
 - H-matrices (Hlib)
 - Fast multipole
 - Non-uniform FFT

Images courtesy Hans Fangohr.

Micromagnets

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Background

Practical OOMMF

Pitfalls

- Mesh size
- Symmetry breaking
- Field step size
- Stopping criteria
- Energy minimization

Advanced Topics

- Extended volumes
- Normal mode images
- Sub-cell thickness variation
- Movies

Recommendations

Outline

Background: Micromagnetics

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

How can I get OOMMF?

- ▶ OOMMF website
 - ▶ Download
 - ▶ Documentation
 - ▶ Contrib area
 - ▶ Citation page
- ▶ Nanohub
- ▶ GitHub fangoehr/oommf

Background

Practical OOMMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

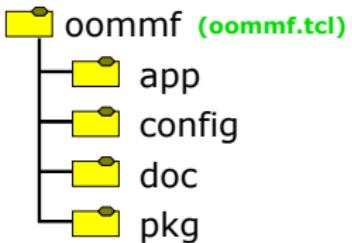
Normal mode images

Sub-cell thickness variation

Movies

Recommendations

OOMMF file layout



Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

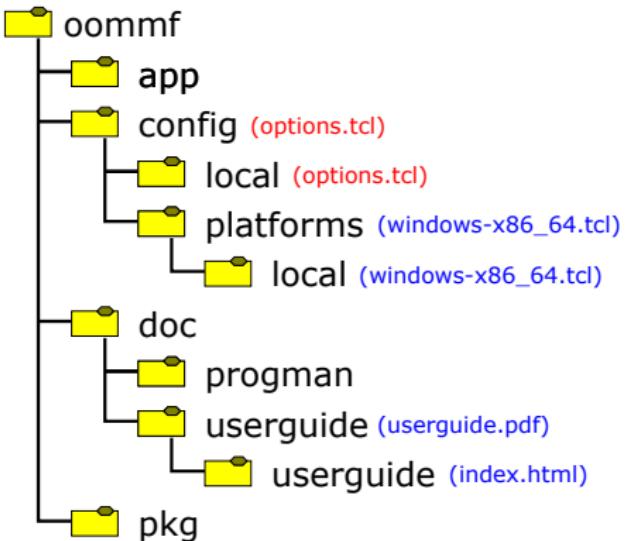
Normal mode images

Sub-cell thickness variation

Movies

Recommendations

OOMMF file layout



Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

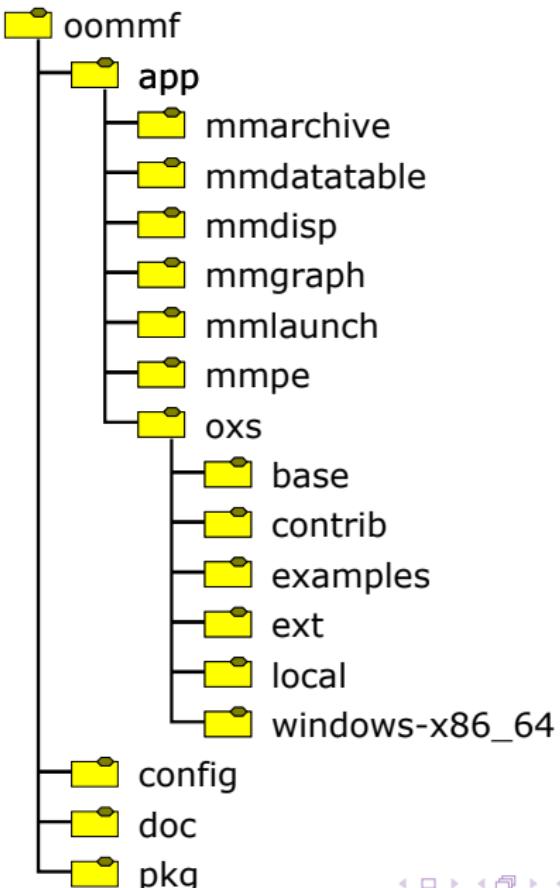
Normal mode images

Sub-cell thickness variation

Movies

Recommendations

OOMMF file layout



Widget overview

- ▶ mmLaunch
- ▶ mmDisp
- ▶ Oxsii
- ▶ mmDataTable
- ▶ mmGraph
- ▶ mmProbEd

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

OOMMF command line tools

- ▶ oommf help
- ▶ avf2ppm, avf2eps
- ▶ boxsi
- ▶ log files
- ▶ lastjob
- ▶ mifconvert

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Intro to editing MIF files

- ▶ notepad / notepad++

Background

- ▶ Tcl quickstart

Practical OOMMF

- ▶ set, \$
- ▶ expr
- ▶ []
- ▶ quoting
- ▶ subst
- ▶ incr
- ▶ for, if
- ▶ puts

Pitfalls

- Mesh size
- Symmetry breaking
- Field step size
- Stopping criteria
- Energy minimization

- ▶ MIF extensions

Advanced Topics

- Extended volumes
- Normal mode images
- Sub-cell thickness variation
- Movies

- ▶ Specify
- ▶ Parameter
- ▶ Destination
- ▶ Schedule
- ▶ Oc_Report

Recommendations

Outline

Background: Micromagnetics

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

μ MAG standard problem 1

Micromagnetics

M.J. Donahue

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

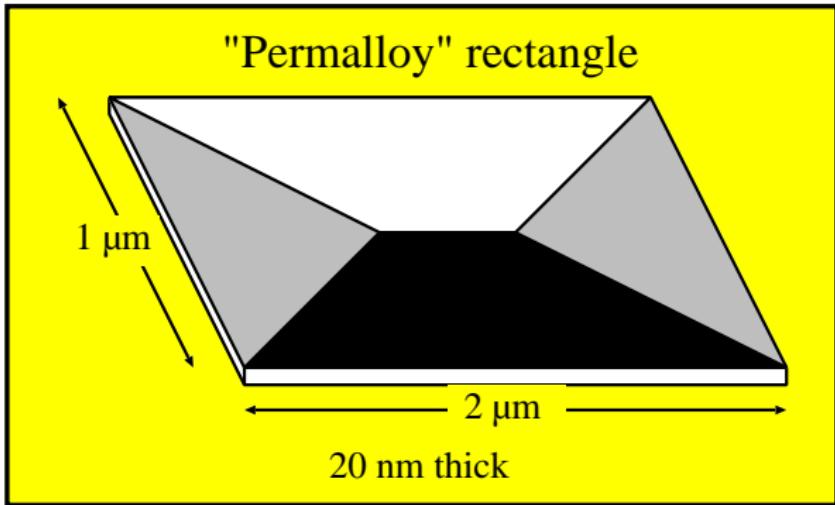
Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations



Task: Run this through a hysteresis loop.

μ MAG standard problem 1: results

Micromagnets

M.J. Donahue

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

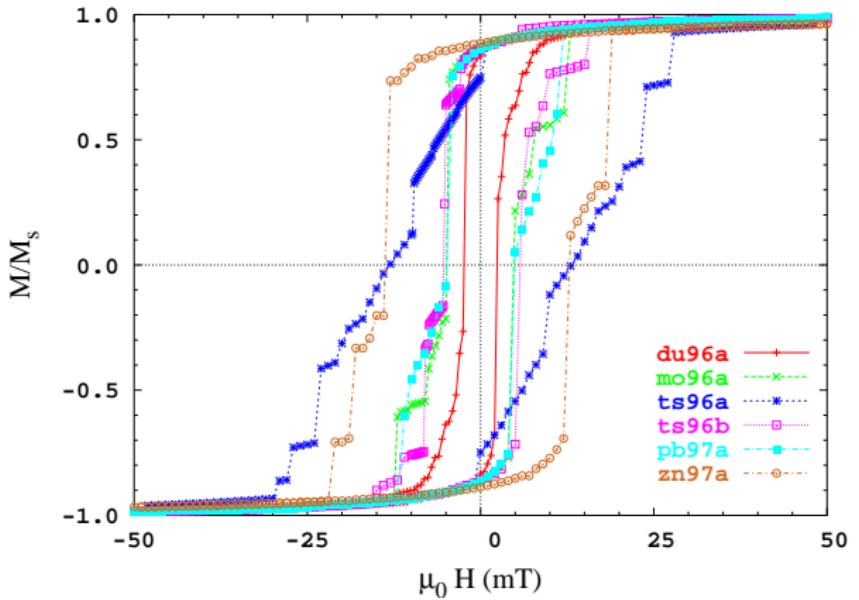
Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations



Problem: ???

μ MAG standard problem 1: results

Micromagnets

M.J. Donahue

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

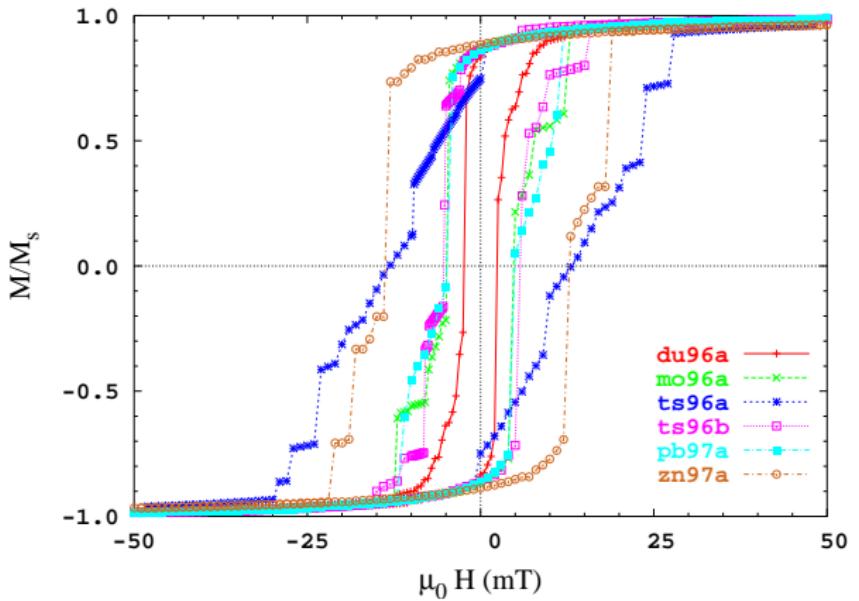
Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations



Problem: Meshes were too coarse!

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Exchange lengths

Magnetocrystalline exchange length (for hard materials):

$$\ell_{\text{ex},K} = \sqrt{\frac{A}{K_u}}$$

Magnetostatic exchange length (for soft materials):

$$\ell_{\text{ex},Ms} = \sqrt{\frac{2A}{\mu_0 M_s^2}}$$

- ▶ Don't mesh any coarser than smaller of these two values!
- ▶ Don't confuse the latter with the "characteristic length"

$$R_0 = \sqrt{2\pi} \sqrt{\frac{2A}{\mu_0 M_s^2}} \approx 2.5 \ell_{\text{ex},Ms}$$

G.S. Abo, Y.-K. Hong et al., *IEEE Trans. Magn.*, **49**, 4937 (2013).

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Example ℓ_{ex} values

Material	M_s (kA/m)	K (kJ/m ³)	A (pJ/m)	$\ell_{\text{ex},K}$ (nm)	$\ell_{\text{ex},Ms}$ (nm)
Fe	1700	48	21	21	3.4
Co	1400	520	30	7.6	4.9
Ni	490	-5.7	9	40	7.7
Permalloy	800	0	13	-	5.7
Nd ₂ Fe ₁₄ B	1280	4500	13	1.7	3.6

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

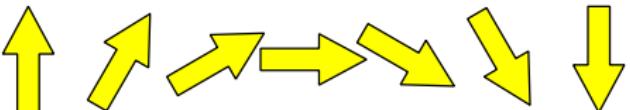
1D wall types

Bloch wall

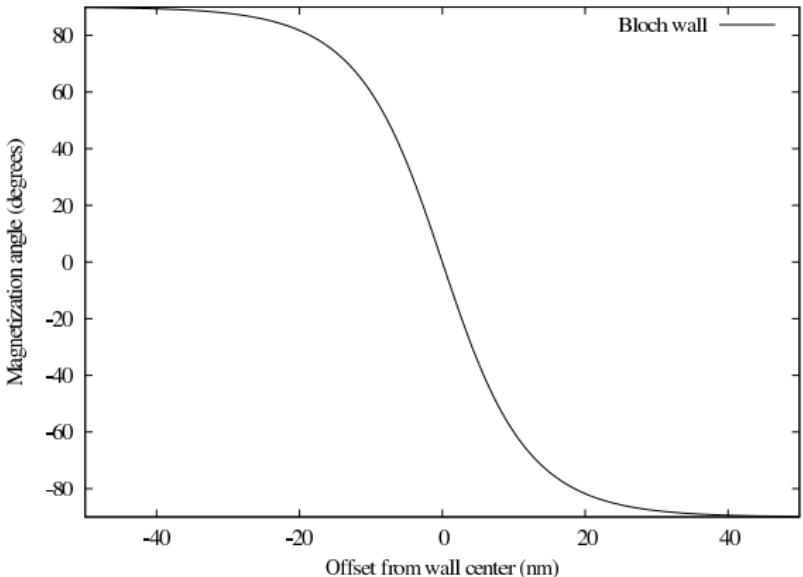


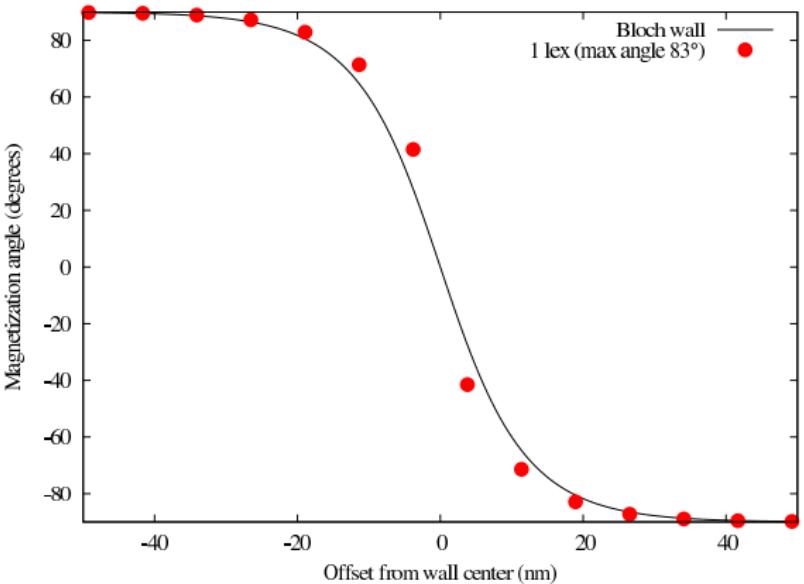
$$\nabla \cdot \mathbf{M} = 0 \quad \Rightarrow \quad \mathbf{H}_{\text{demag}} = 0$$

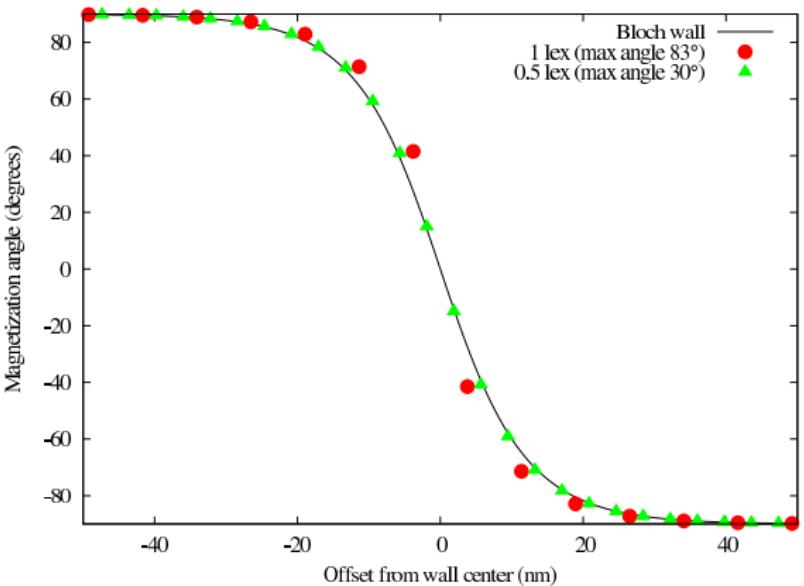
Néel wall



$$\nabla \cdot \mathbf{M} \neq 0 \quad \Rightarrow \quad \mathbf{H}_{\text{demag}} \neq 0$$

[Background](#)[Practical OOMMF](#)**Pitfalls**[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)**Advanced Topics**[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)**Recommendations**

[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

Background

Practical OOMMF

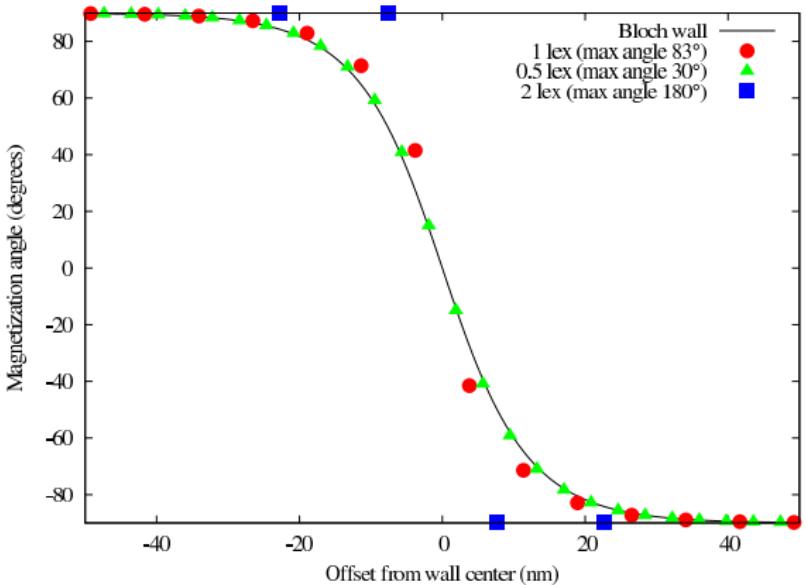
Pitfalls

- Mesh size
- Symmetry breaking
- Field step size
- Stopping criteria
- Energy minimization

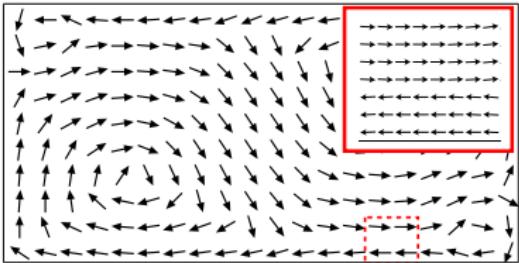
Advanced Topics

- Extended volumes
- Normal mode images
- Sub-cell thickness variation
- Movies

Recommendations



Néel wall collapse



25 nm cells

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

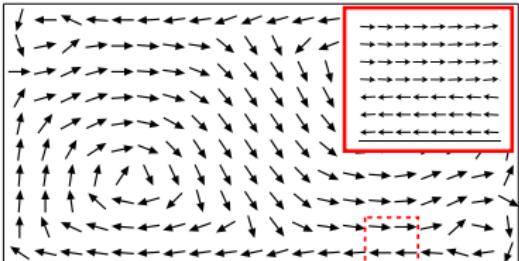
Normal mode images

Sub-cell thickness variation

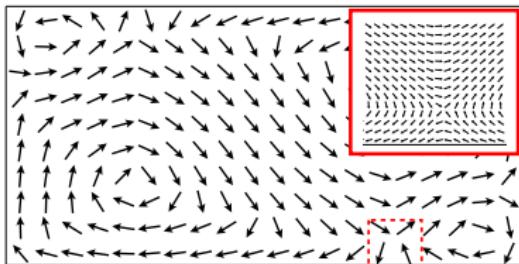
Movies

Recommendations

Néel wall collapse



25 nm cells



12.5 nm cells

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

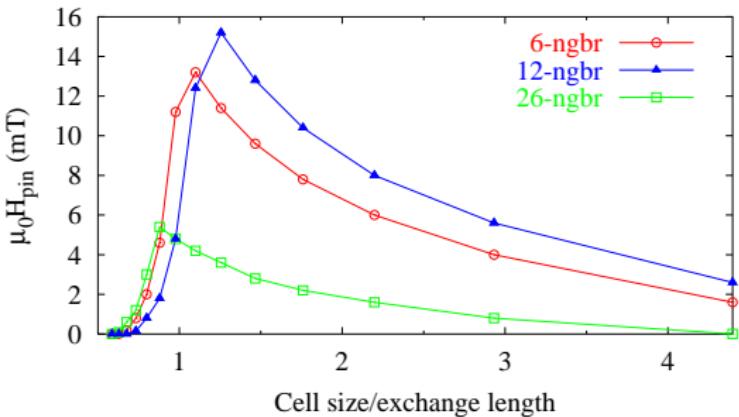
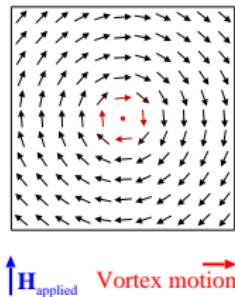
Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Vortex mobility



MJ Donahue & RD McMichael, *Physica B*, **233**, 272 (1997).

MJ Donahue & DG Porter, *Physica B*, **343**, 177 (2004).

[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

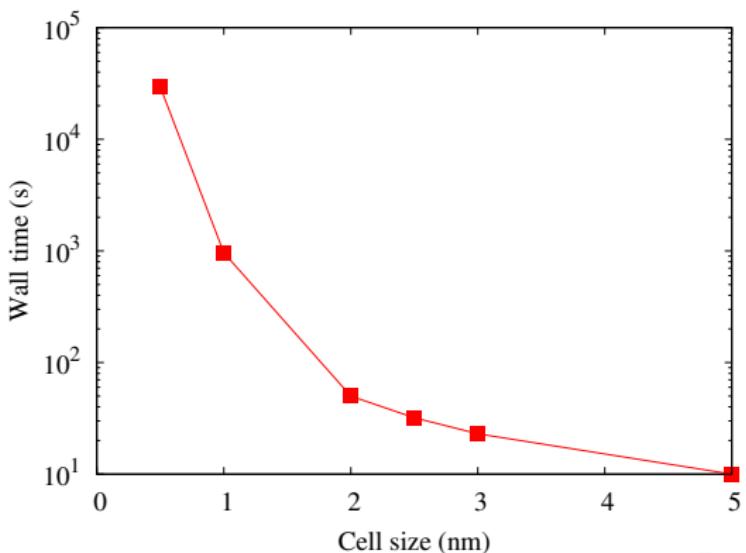
Cell size recommendations

- ▶ Don't mesh coarser than ℓ_{ex}
- ▶ Check max neighbor angle: under 30° is usually reliable, over 90° is questionable, 180° is bogus.
- ▶ Run at multiple discretizations and check for convergence (if possible!)

Over-mesh = too stiff

Standard Problem 4: Run time vs. cell size

Cellsize (nm)	Cell count	Iterations	Wall time (s)	Max angle (deg)
5.0	2500	583	10	108.1
3.0	7014	1521	23	68.0
2.5	10000	2165	32	52.2
2.0	15750	3405	50	37.4
1.0	187500	18565	961	17.7
0.5	1500000	79191	29469	8.7



Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

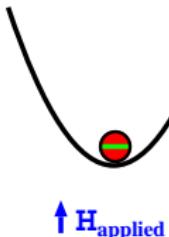
Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Symmetry breaking



Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

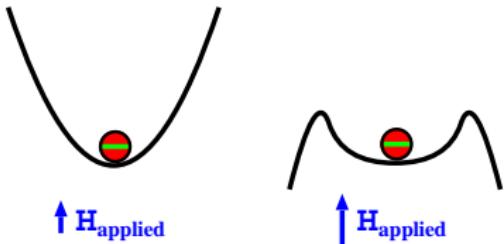
Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Symmetry breaking



Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

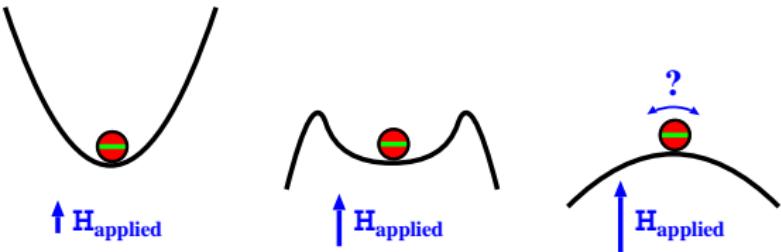
Sub-cell thickness variation

Movies

Recommendations

[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

Symmetry breaking



Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

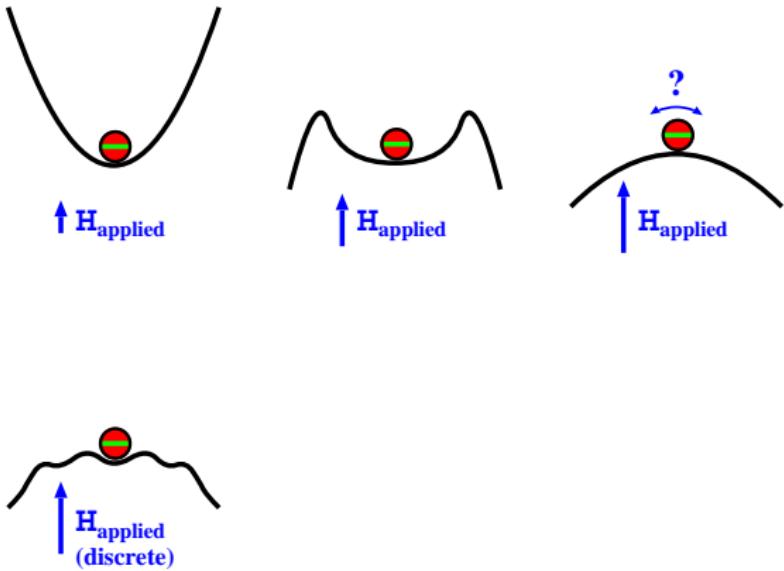
Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

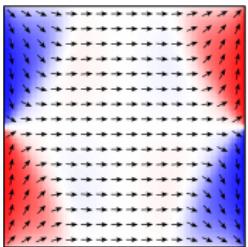
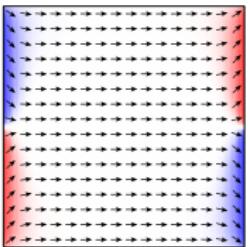
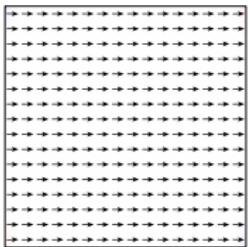
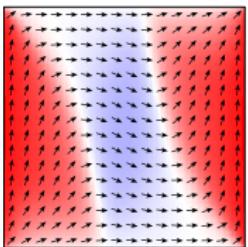
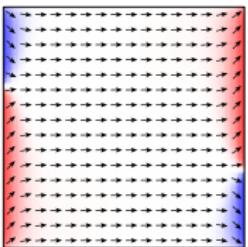
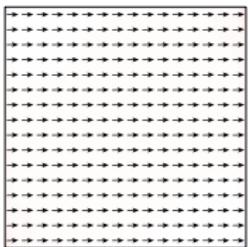
Recommendations



- ▶ Discretization introduces (false) divots
- ▶ Maximum replaced by saddle in higher dimensions

[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

Symmetry breaking

 H_{Applied}  H_{Applied}
on axis H_{Applied}
 1° off-axis

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

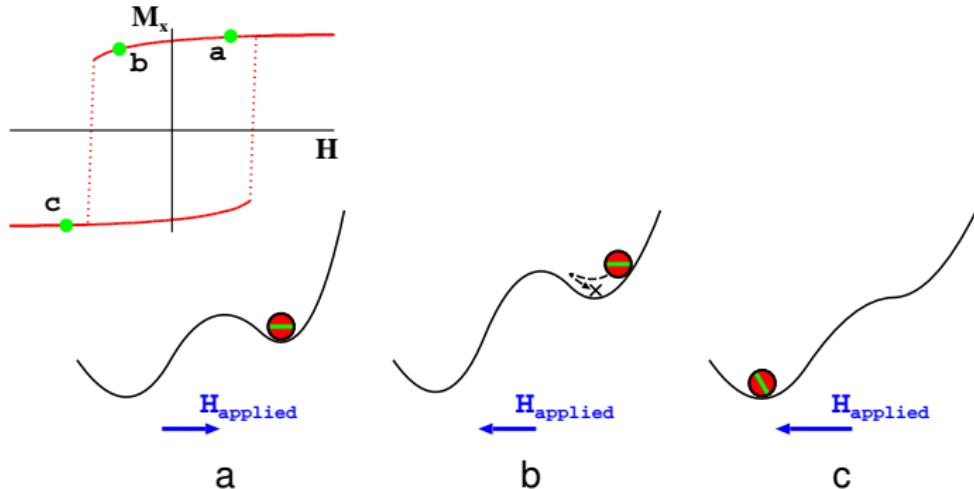
Normal mode images

Sub-cell thickness variation

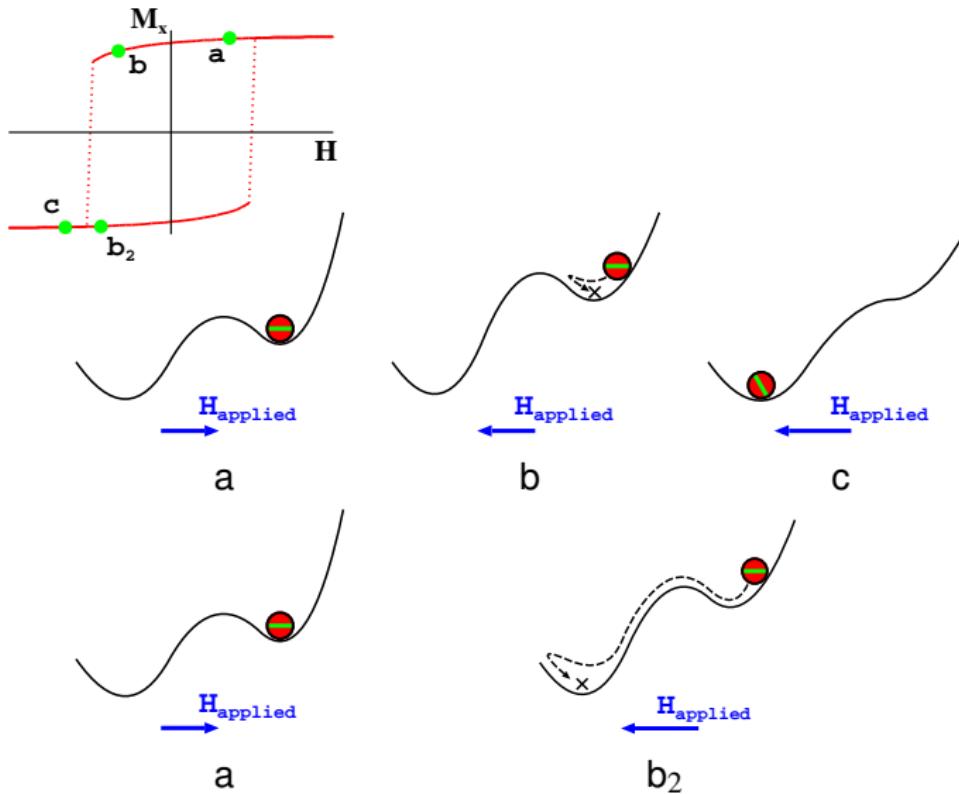
Movies

Recommendations

Big field steps \Rightarrow premature switching



Big field steps \Rightarrow premature switching



[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

Stopping too soon

Stopping criteria: $\mathbf{M} \times \mathbf{H}_{\text{eff}} < \text{stoptorque}$



[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

Stopping too soon

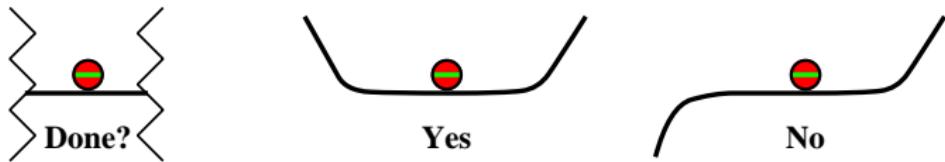
Stopping criteria: $\mathbf{M} \times \mathbf{H}_{\text{eff}} < \text{stoptorque}$



[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

Stopping too soon

Stopping criteria: $\mathbf{M} \times \mathbf{H}_{\text{eff}} < \text{stoptorque}$



Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

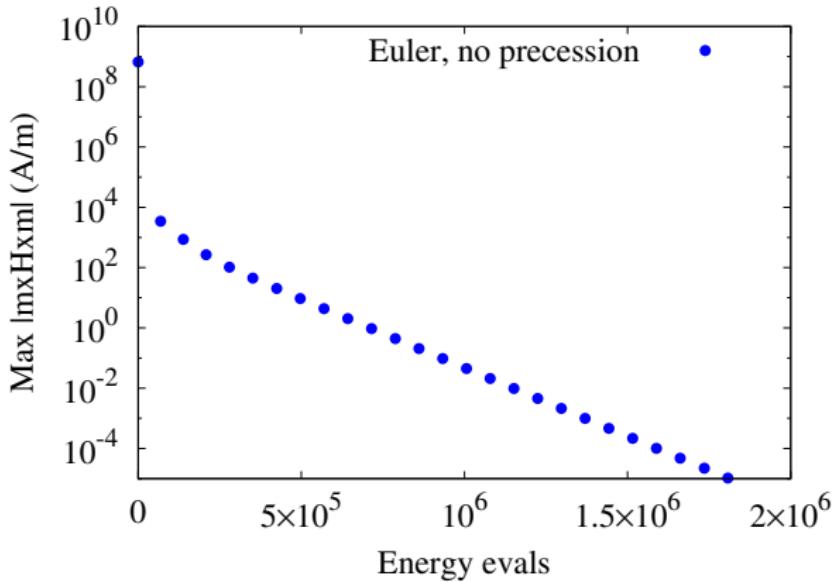
Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations



Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

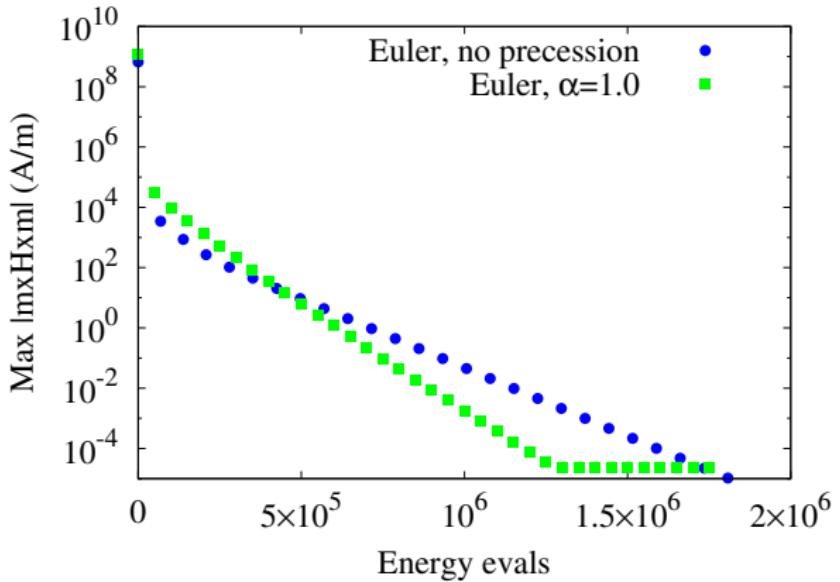
Extended volumes

Normal mode images

Sub-cell thickness variation

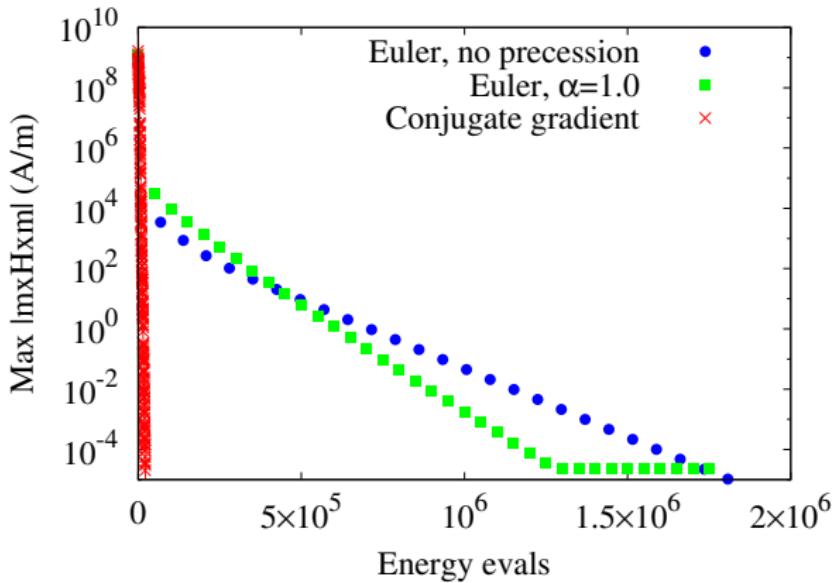
Movies

Recommendations



LLG vs. Conjugate Gradient

Standard problem 3 (energy minimization):



- ▶ Use the right tool for the job!

Outline

Background: Micromagnetics

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

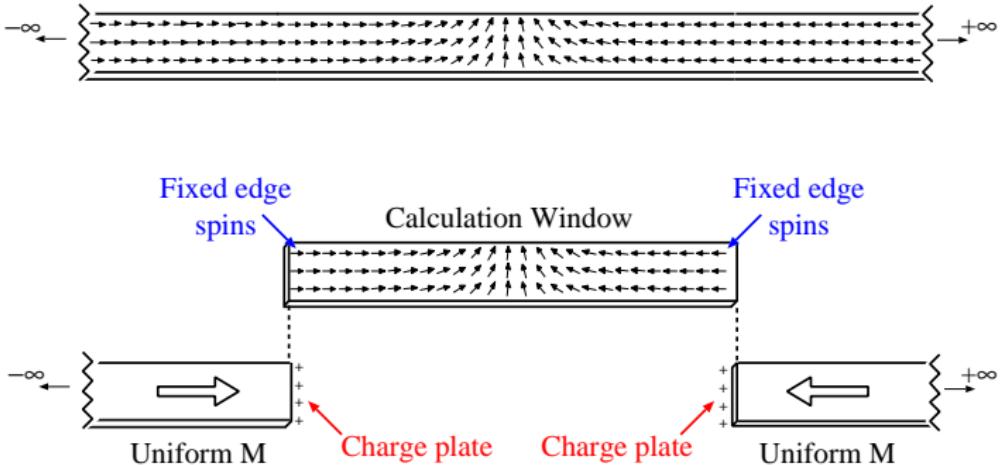
Sub-cell thickness variation

Movies

Recommendations

Infinite strips

Extended volumes



R.D. McMichael & M.J. Donahue, *IEEE Trans. Magn.*, **33**, 4167 (1997).

FMR simulations

Micromagnetics

M.J. Donahue

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

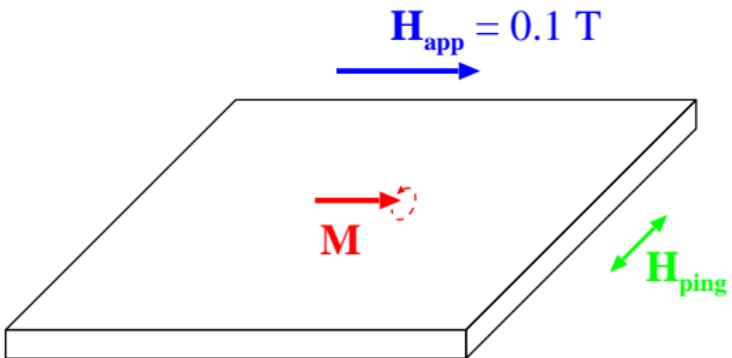
Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations



Small “ping” field induces spinwaves.

Background

Practical OOMMF

Pitfalls

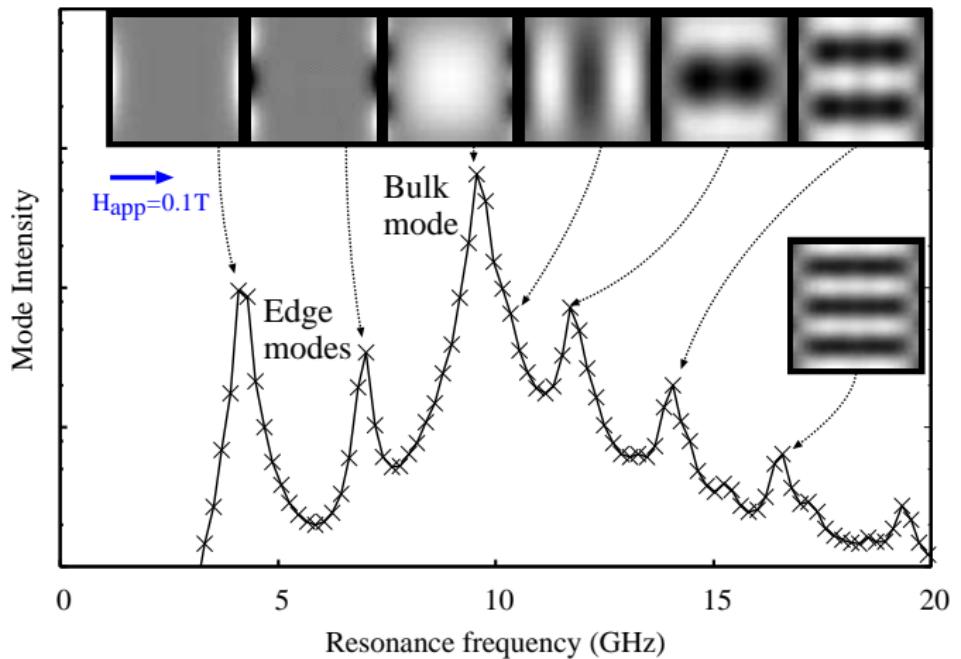
- Mesh size
- Symmetry breaking
- Field step size
- Stopping criteria
- Energy minimization

Advanced Topics

- Extended volumes
- Normal mode images
- Sub-cell thickness variation
- Movies

Recommendations

FMR spectra

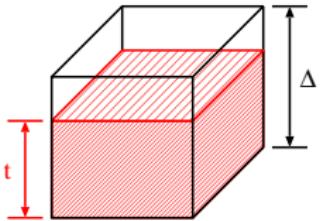


RD McMichael & MD Stiles, "Magnetic normal modes of nanoelements," *JAP*, **97**, 10J901 (2005).

[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

Sub-cell thickness variation

PROBLEM: Partially filled cell has different geometry,
so FFT can't be used to compute demag field.



Partially filled cell,
height= t , $|\mathbf{M}|=M_s$

DG Porter & MJ Donahue, *JAP*, **89**, 7257 (2001).

H Min, RD McMichael, MJ Donahue, J Miltat & MD Stiles, *PRL*, **104**, 217201
(2010).

Sub-cell thickness variation

Micromagnetics

M.J. Donahue

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

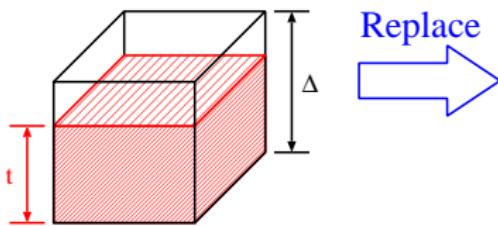
Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations



Partially filled cell,
height= t , $|\mathbf{M}|=M_s$

Full cell, height= Δ
Reduced magnetization, $|\mathbf{M}|=(t/\Delta)M_s$

DG Porter & MJ Donahue, *JAP*, **89**, 7257 (2001).

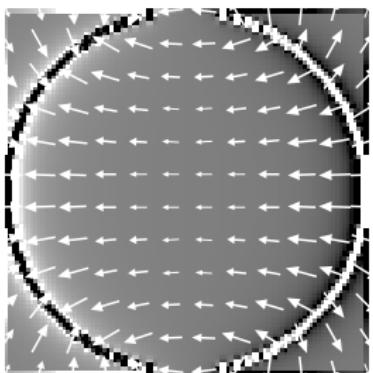
H Min, RD McMichael, MJ Donahue, J Miltat & MD Stiles, *PRL*, **104**, 217201
(2010).

Sub-cell thickness variation

Micromagnetics

M.J. Donahue

10x10x1disk



Non-uniform demag field

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Sub-cell thickness variation

Micromagnetics

M.J. Donahue

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

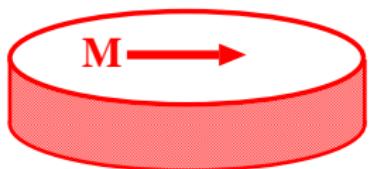
Normal mode images

Sub-cell thickness variation

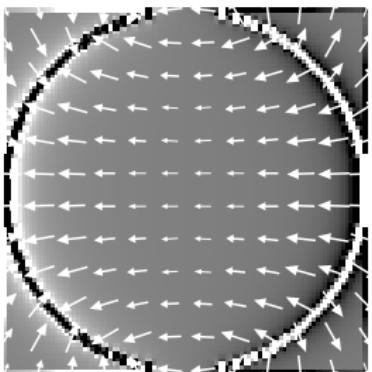
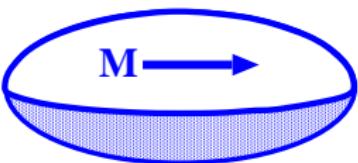
Movies

Recommendations

10x10x1disk



10x10x1 oblate spheroid



Non-uniform demag field

Sub-cell thickness variation

Micromagnets

M.J. Donahue

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

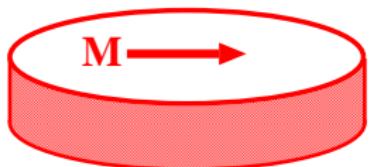
Normal mode images

Sub-cell thickness variation

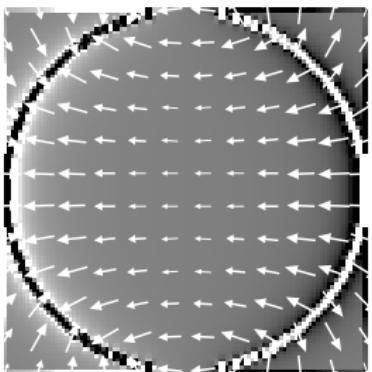
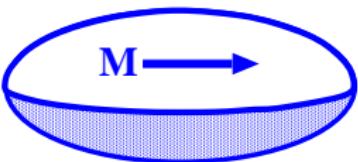
Movies

Recommendations

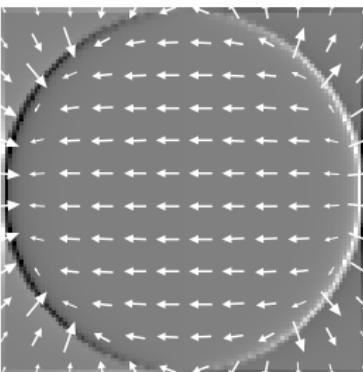
10x10x1disk



10x10x1 oblate spheroid



Non-uniform demag field



Almost uniform demag field

Making movies

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

See the OOMMF movie page:

<http://math.nist.gov/oommf/movies/oommf-movies.html>

[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

Recommendations

- ▶ Don't mesh coarser than ℓ_{ex}
- ▶ Check max neighbor angle: under 30° is usually reliable, over 90° is questionable, 180° is bogus.
- ▶ Run at multiple discretizations and check for convergence (if possible!)
- ▶ Watch for symmetries.
- ▶ Beware of problems with big field steps.
- ▶ Be careful with stopping criteria.
- ▶ LLG may not be the best for energy minimization.
- ▶ PBC only work if what happens at infinity stays at infinity.
(Think stray field, domain wall nucleation and motion.)

[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

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(Doh!)

OOMMF C++ class structure

Micromagnets

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Background

Practical OOMMF

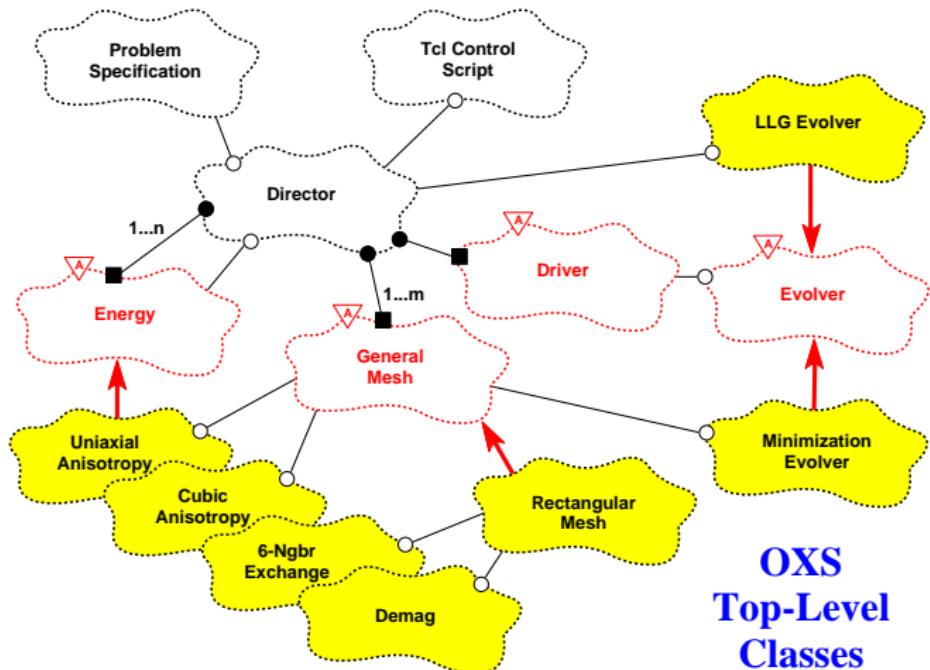
Pitfalls

- Mesh size
- Symmetry breaking
- Field step size
- Stopping criteria
- Energy minimization

Advanced Topics

- Extended volumes
- Normal mode images
- Sub-cell thickness variation
- Movies

Recommendations



[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

Adding a new energy term to OOMMF

1. Copy sample `.h` and `.cc` files to `oommf/app/oxs/local`.
2. Change names.
3. Add new code.
4. Run `pimake`.
5. Add new term to MIF input file.

NB: Modify no files in OOMMF distribution!

See Oxs Extension Modules page

<http://math.nist.gov/oommf/contrib/oxsext/>

for examples.

[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

Example extension: uniaxial anisotropy

Simple form: $E_{\text{anis}} = K_1 \sin^2 \phi$

Extended form: $E_{\text{anis}} = K_1 \sin^2 \phi + K_2 \sin^4 \phi$

where ϕ is angle between \mathbf{m} and \mathbf{u} .

Sample anisotropy header file

```
// Sample uniaxial anisotropy, derived from Oxs_Energy class.
#include "nb.h"
#include "threevector.h"
#include "energy.h"
#include "key.h"
#include "simstate.h"
#include "mesh.h"
#include "meshvalue.h"
/* End includes */

- class Oxs_SimpleAnisotropy:public Oxs_Energy {
+ class My_ExtendedAnisotropy:public Oxs_Energy {
private:
- REAL8m K1;
+ REAL8m K1,K2;
    ThreeVector axis;
public:
    virtual const char* ClassName() const; // ClassName() is
    /// automatically generated by the OXS_EXT_REGISTER macro.

- Oxs_SimpleAnisotropy(const char* name, // Child instance id
+ My_ExtendedAnisotropy(const char* name, // Child instance id
    Oxs_Director* newdtr, // App director
    Tcl_Interp* safe_interp, // Safe interpreter
    const char* argstr); // MIF input block parameters

- virtual ~Oxs_SimpleAnisotropy() {}
+ virtual ~My_ExtendedAnisotropy() {}

virtual void
GetEnergyAndField(const Oxs_SimState& state,
                  Oxs_MeshValue<REAL8m>& energy,
                  Oxs_MeshValue<ThreeVector>& field
) const;
};
```

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Sample anisotropy source file (part 1/2)

```
// Sample uniaxial anisotropy, derived from Oxs_Energy class.  
- #include "simpleanisotropy.h"  
+ #include "myanisotropy.h"  
  
// Oxs_Ext registration support  
- OXS_EXT_REGISTER(Oxs_SimpleAnisotropy);  
+ OXS_EXT_REGISTER(My_ExtendedAnisotropy);  
/* End includes */  
  
// Constructor  
- Oxs_SimpleAnisotropy::Oxs_SimpleAnisotropy()  
+ My_ExtendedAnisotropy::My_ExtendedAnisotropy(  
    const char* name,           // Child instance id  
    Oxs_Director* newdtr,     // App director  
    Tcl_Interp* safe_interp,   // Safe interpreter  
    const char* argstr)        // MIF input block parameters  
    : Oxs_Energy(name,newdtr,safe_interp,argstr)  
{  
    // Process arguments  
    K1=GetRealInitValue("K1");  
+ K2=GetRealInitValue("K2");  
    axis=GetThreeVectorInitValue("axis");  
    VerifyAllInitArgsUsed();  
}
```

Background

Practical OOMMF

Pitfalls

- Mesh size
- Symmetry breaking
- Field step size
- Stopping criteria
- Energy minimization

Advanced Topics

- Extended volumes
- Normal mode images
- Sub-cell thickness variation
- Movies

Recommendations

Sample anisotropy source file (part 2/2)

```
// Energy and field calculation code
- void Oxs_SimpleAnisotropy::GetEnergyAndField
+ void My_ExtendedAnisotropy::GetEnergyAndField
(const Oxs_SimState& state,
Oxs_MeshValue<REAL8m>& energy,
Oxs_MeshValue<ThreeVector>& field
) const
{
    const Oxs_MeshValue<REAL8m>& Ms_inverse=*(state.Ms_inverse);
    const Oxs_MeshValue<ThreeVector>& spin =state.spin;
    UINT4m size = state.mesh->Size();
    for(UINT4m i=0;i<size;++i) {
        if(Ms_inversei==0.0) {
            energyi=0.0;
            fieldi.Set(0.,0.,0.);
        } else {
            REAL8m dot = axis*spini;
            REAL8m dotsq = dot*dot;
-         energyi = -K1*dotsq;
-         REAL8m fieldmag = (2./MU0)*K1*dot*Ms_inversei;
+         energyi = ((dotsq-2)*K2-K1)*dotsq;
+         REAL8m fieldmag
+             = (-2./MU0)*((dotsq-1)*2*K2-K1)*dot*Ms_inversei;
            fieldi = fieldmag * axis;
        }
    }
}
```

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

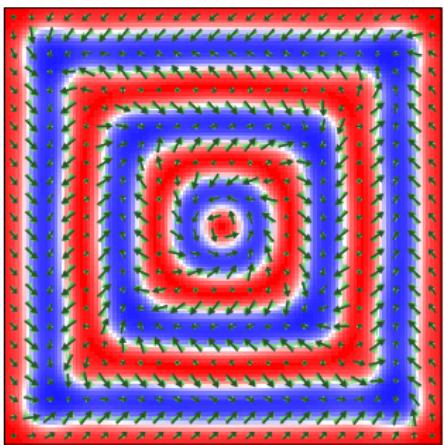
Recommendations

Remanent magnetization configuration

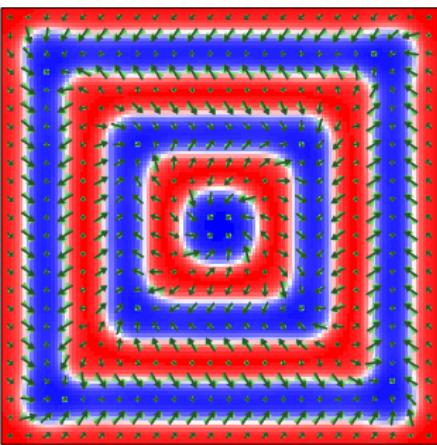
Micromagnetics

M.J. Donahue

Recommendations



Simple Anisotropy



Extended Anisotropy

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

General micromagnetic references

- ▶ W. F. Brown, Jr., *Micromagnetics* (Krieger, New York, 1978).
- ▶ A. Aharoni, *Introduction to the Theory of Ferromagnetism* (Oxford, New York, 1996).
- ▶ J. Fidler and T. Schrefl, “Micromagnetic modelling – the current state of the art,” *J. Phys.: Appl.*, **33**, R135-R156 (2000).
- ▶ H. Kronmüller and S. Parkin (eds.), *Handbook of magnetism and advanced magnetic materials, Vol. 2: Micromagnetism*, (Wiley-Interscience, Chichester, 2007).

[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

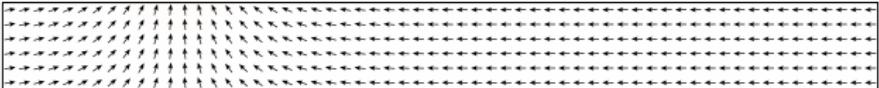
Finite element references

- ▶ B. Yang, D. R. Fredkin, "Dynamic micromagnetics by the finite element method," *IEEE Trans. Magn.* **33**, 3842 (1998).
- ▶ N. Gershenfeld, *The Nature of Mathematical Modeling*, chapter Finite elements (Cambridge University Press, 1998).
- ▶ H. Kronmüller and S. Parkin (eds.), *Handbook of magnetism and advanced magnetic materials, Vol. 2: Micromagnetism*, chapter Numerical Methods in Micromagnetics (FEM) (Wiley-Interscience, Chichester, 2007).
- ▶ R. Chang, S. Li, M. Lubarda, B. Livshitz, V. Lomakin, "FastMag: Fast micromagnetic simulator for complex magnetic structures," *JAP*, **109**, 07D358 (2011).

Thin film simulation

$$\mu_0 \mathbf{H} = 25 \text{ mT} \rightarrow$$

0 ps



Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

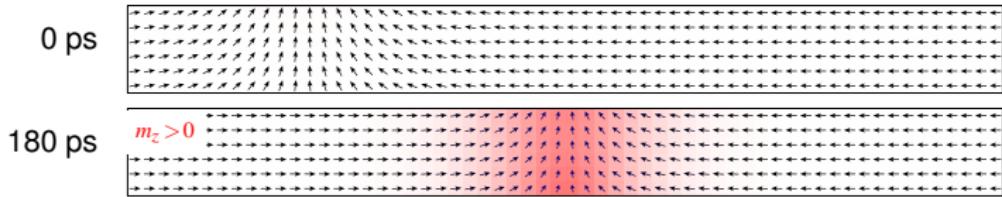
Sub-cell thickness variation

Movies

Recommendations

Thin film simulation

$$\mu_0 \mathbf{H} = 25 \text{ mT} \rightarrow$$



Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

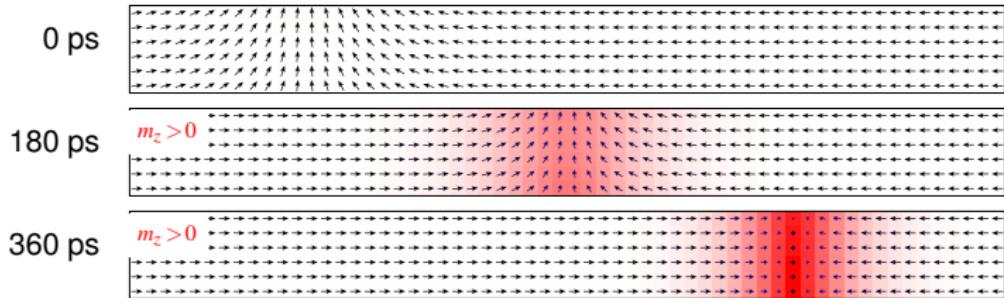
Sub-cell thickness variation

Movies

Recommendations

Thin film simulation

$$\mu_0 \mathbf{H} = 25 \text{ mT} \rightarrow$$



Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

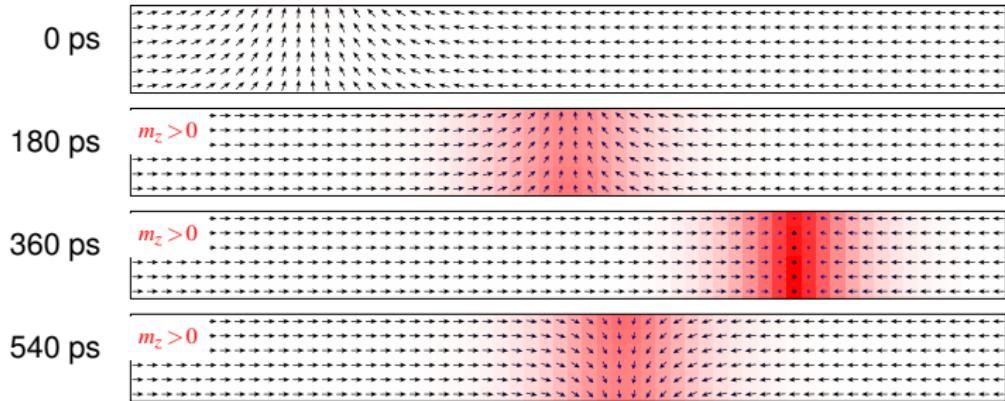
Sub-cell thickness variation

Movies

Recommendations

Thin film simulation

$$\mu_0 \mathbf{H} = 25 \text{ mT} \rightarrow$$



Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

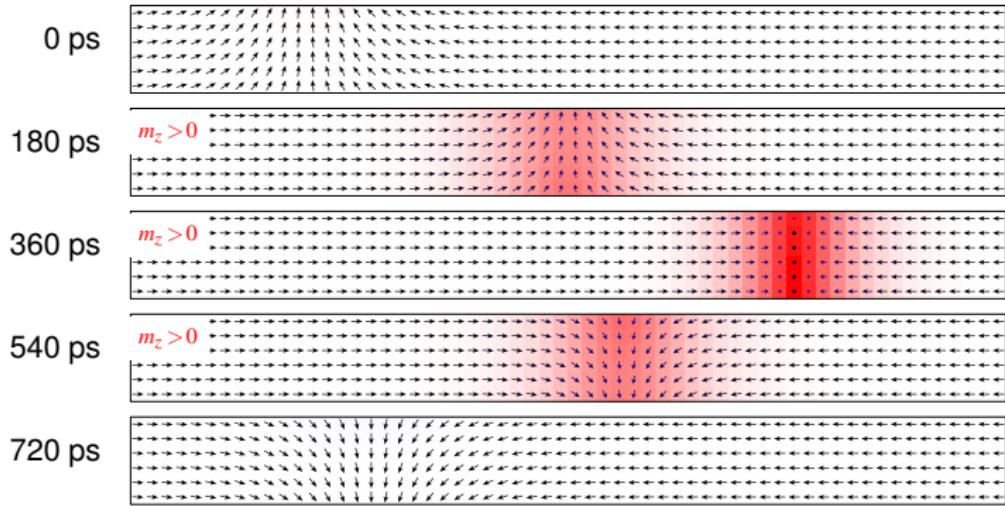
Sub-cell thickness variation

Movies

Recommendations

Thin film simulation

$$\mu_0 \mathbf{H} = 25 \text{ mT} \rightarrow$$



Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

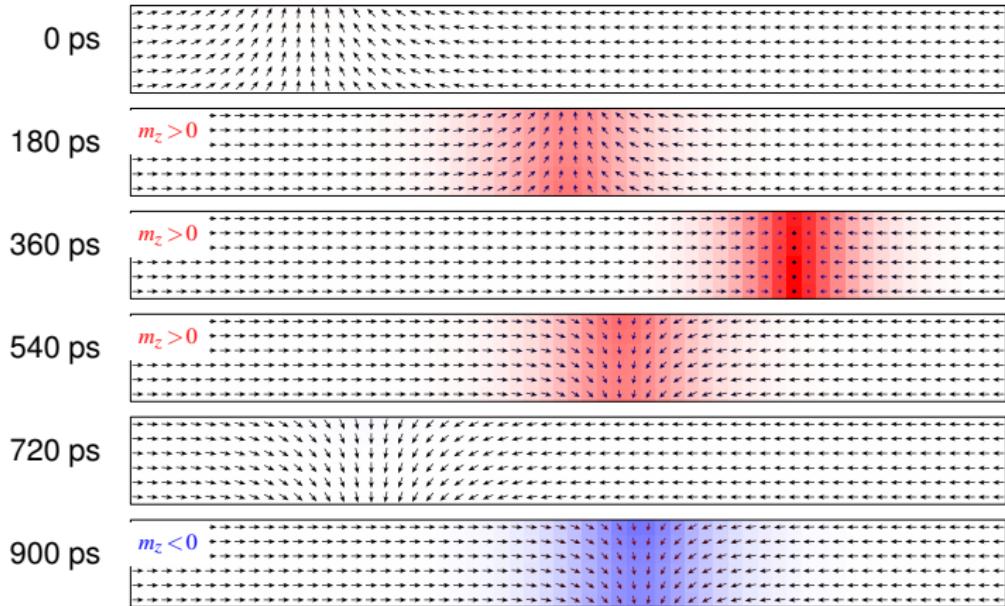
Sub-cell thickness variation

Movies

Recommendations

Thin film simulation

$$\mu_0 \mathbf{H} = 25 \text{ mT} \rightarrow$$



Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

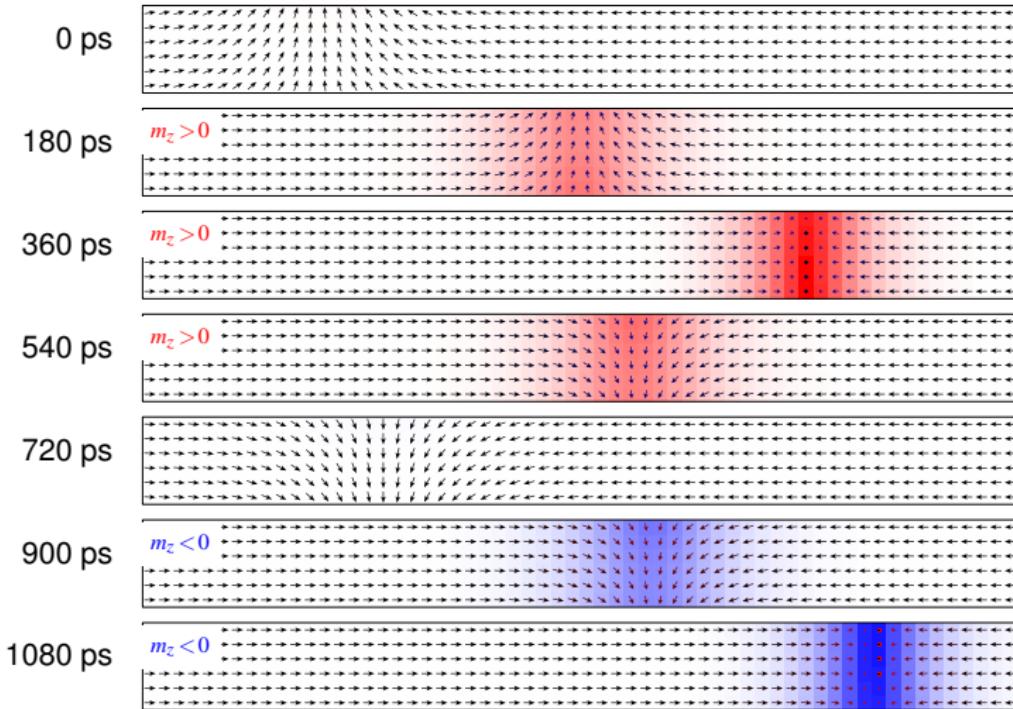
Sub-cell thickness variation

Movies

Recommendations

Thin film simulation

$$\mu_0 \mathbf{H} = 25 \text{ mT} \rightarrow$$



Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

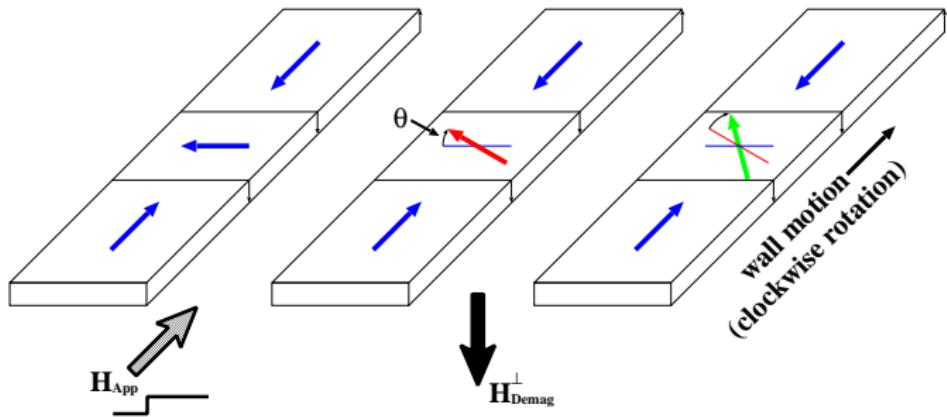
Sub-cell thickness variation

Movies

Recommendations

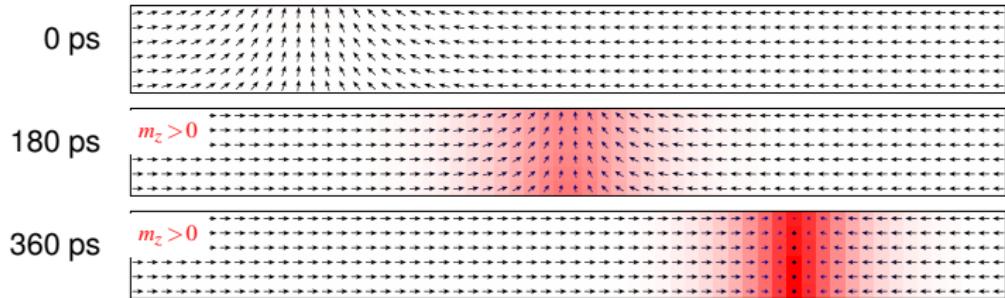
[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

Thin film wall dynamics, $m_z \geq 0$



Thin film simulation

$$\mu_0 \mathbf{H} = 25 \text{ mT} \rightarrow$$



Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

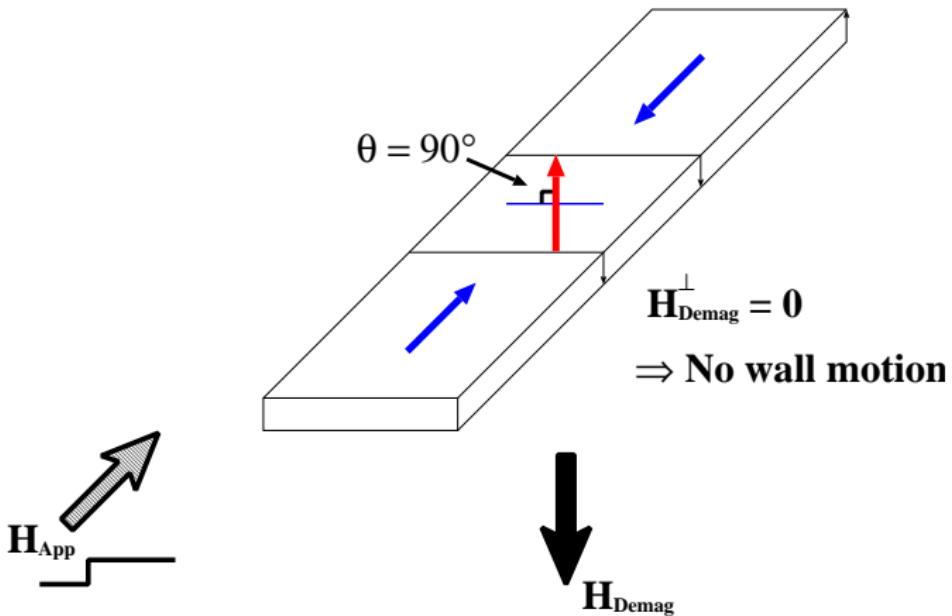
Sub-cell thickness variation

Movies

Recommendations

[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

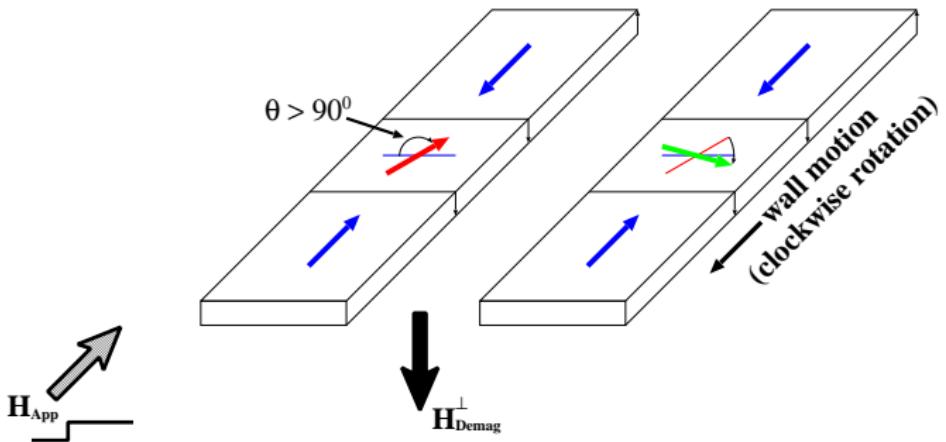
Thin film wall dynamics, $m_z \geq 0$



Thin film wall dynamics, $m_z \geq 0$

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Thin film wall dynamics, $m_z \leq 0$

Micromagnets

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Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

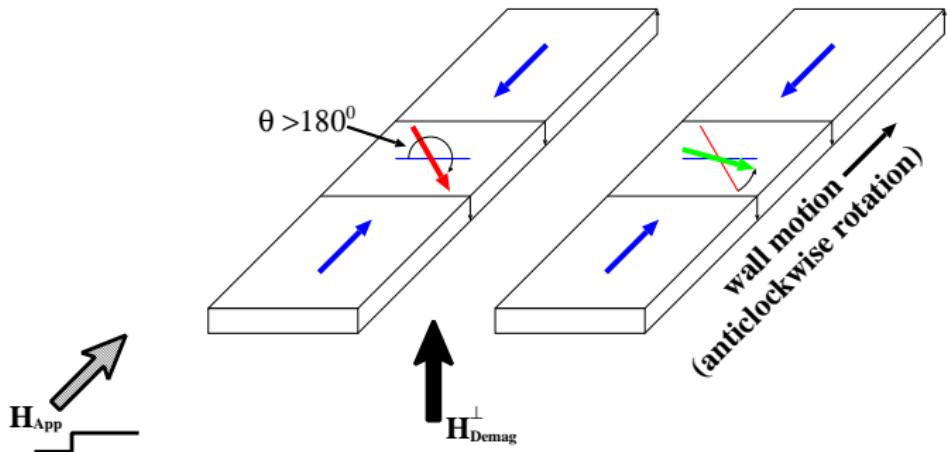
Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations



Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

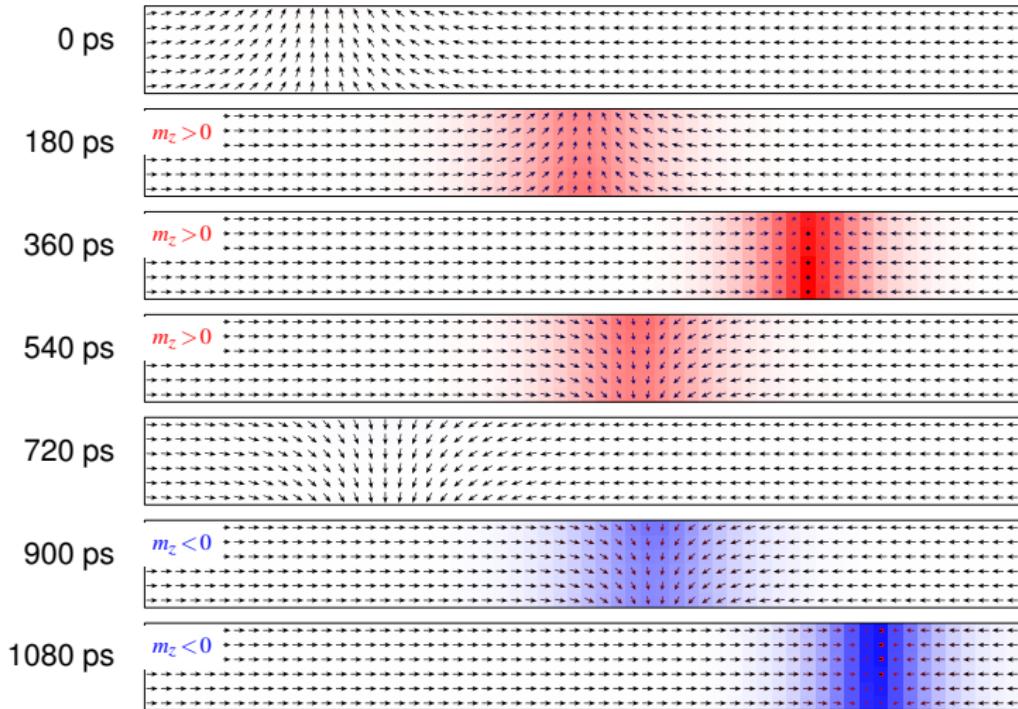
Sub-cell thickness variation

Movies

Recommendations

Thin film simulation

$$\mu_0 \mathbf{H} = 25 \text{ mT} \rightarrow$$



DG Porter & MJ Donahue, "Velocity of transverse domain wall motion along thin, narrow strips," *JAP*, **95**, 6729 (2004).

Other micromagnetic codes

- ▶ AlaMag (fast multipole, free)
- ▶ GPMagnet (commercial)
- ▶ JaMM (Java, free)
- ▶ LLG Micromagnetics Simulator (commercial)
- ▶ magpar (FE, parallel, development ceased?, free)
- ▶ Micromagus (Windows-only, commercial)
- ▶ MicroMagnum (CPU/GPU, free)
- ▶ mumax³ (FD, GPU, free)
- ▶ Nmag (FE, development ceased, free)
- ▶ ...

[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

Background

Practical OOMMF

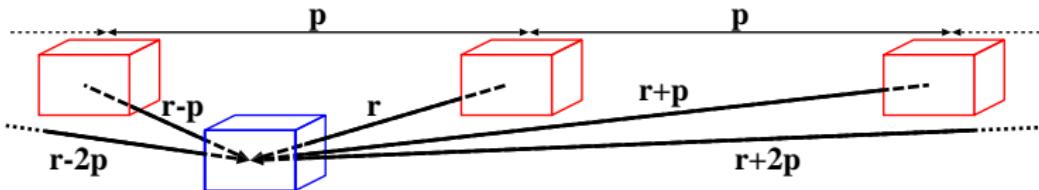
Pitfalls

- Mesh size
- Symmetry breaking
- Field step size
- Stopping criteria
- Energy minimization

Advanced Topics

- Extended volumes
- Normal mode images
- Sub-cell thickness variation
- Movies

Recommendations



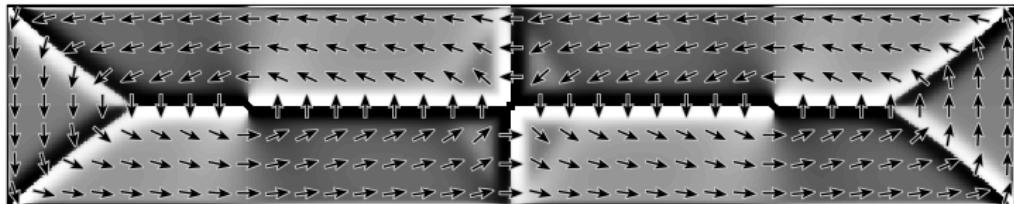
$$\mathbf{H}_{\text{demag}} = \sum_{k=-\infty}^{\infty} N(\mathbf{r} + k\mathbf{p}) \mathbf{M} = N^{pb} \mathbf{M}$$

where

 $\mathbf{p} := \text{offset vector between periods}$

KM Lebecki, MJ Donahue & MW Gutowski, "Periodic boundary conditions for demagnetization interactions in micromagnetic simulations," *JAP*, **41**, 175005 (2008).

Cross-tie walls



Remanent state: $500 \ell_{\text{ex}} \times 100 \ell_{\text{ex}} \times 6 \ell_{\text{ex}}$

Background

Practical OOMMF

Pitfalls

- Mesh size
- Symmetry breaking
- Field step size
- Stopping criteria
- Energy minimization

Advanced Topics

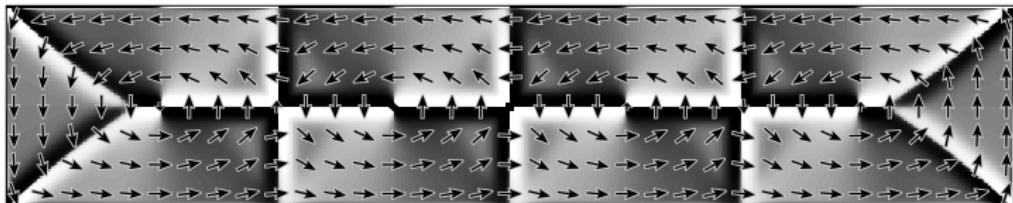
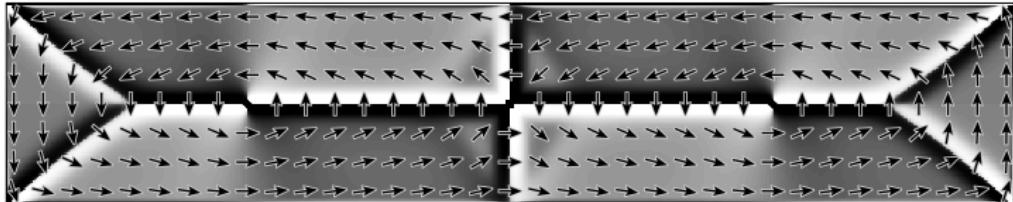
- Extended volumes
- Normal mode images
- Sub-cell thickness variation
- Movies

Recommendations

M J Donahue, "Micromagnetic investigation of periodic cross-tie/vortex wall geometry," *Advances in Condensed Matter Physics*, **2012** (2012).

[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

Remanent state: $500 \ell_{\text{ex}} \times 100 \ell_{\text{ex}} \times 6 \ell_{\text{ex}}$



M J Donahue, "Micromagnetic investigation of periodic cross-tie/vortex wall geometry," *Advances in Condensed Matter Physics*, 2012 (2012).

Multi-dimension periodic

- ▶ 1D periodic: tail sum $\sim \int_{R_2}^{\infty} 1/x^3 dx < \infty$
⇒ boundary doesn't matter.

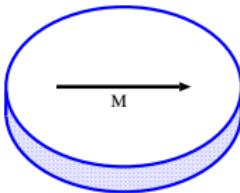
[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

Multi-dimension periodic

- ▶ 1D periodic: tail sum $\sim \int_{R_2}^{\infty} 1/x^3 dx < \infty$
⇒ boundary doesn't matter.



- ▶ 2D periodic: tail sum $\sim \iint_{R > R_2} 1/R^3 dx dy < \infty$
⇒ boundary doesn't matter.



Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

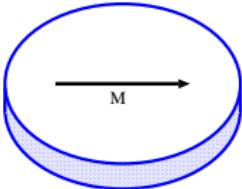
Recommendations

Multi-dimension periodic

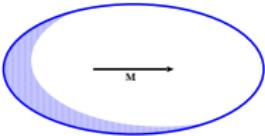
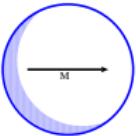
- ▶ 1D periodic: tail sum $\sim \int_{R_2}^{\infty} 1/x^3 dx < \infty$
 \Rightarrow boundary doesn't matter.



- ▶ 2D periodic: tail sum $\sim \iint_{R > R_2} 1/R^3 dx dy < \infty$
 \Rightarrow boundary doesn't matter.



- ▶ 3D periodic: Technical problem — tail sum doesn't converge \Rightarrow boundary matters.



Edge mode test

The figure consists of three parts. On the left is a plot of Mode Intensity versus Resonance frequency (GHz). The x-axis ranges from 0 to 10 GHz, and the y-axis represents Mode Intensity. Two distinct resonance curves are shown: one for 'Edge modes' (lower frequency, ~3-7 GHz) and one for 'Bulk mode' (higher frequency, ~8-10 GHz). The plot is labeled with $H_{app} = 0.1 \text{ T}$ and $\theta = 0$. Three grayscale images labeled a, b, and c are shown above the plot, corresponding to the resonance frequencies of the Edge modes. On the right is a schematic diagram of a 3D surface representing the system. It shows a grid of arrows pointing upwards, representing magnetization. A blue vector labeled H_{app} is shown at an angle θ to the surface. Another blue vector labeled H_{pmg} is shown parallel to the surface.

Staircase correction

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Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

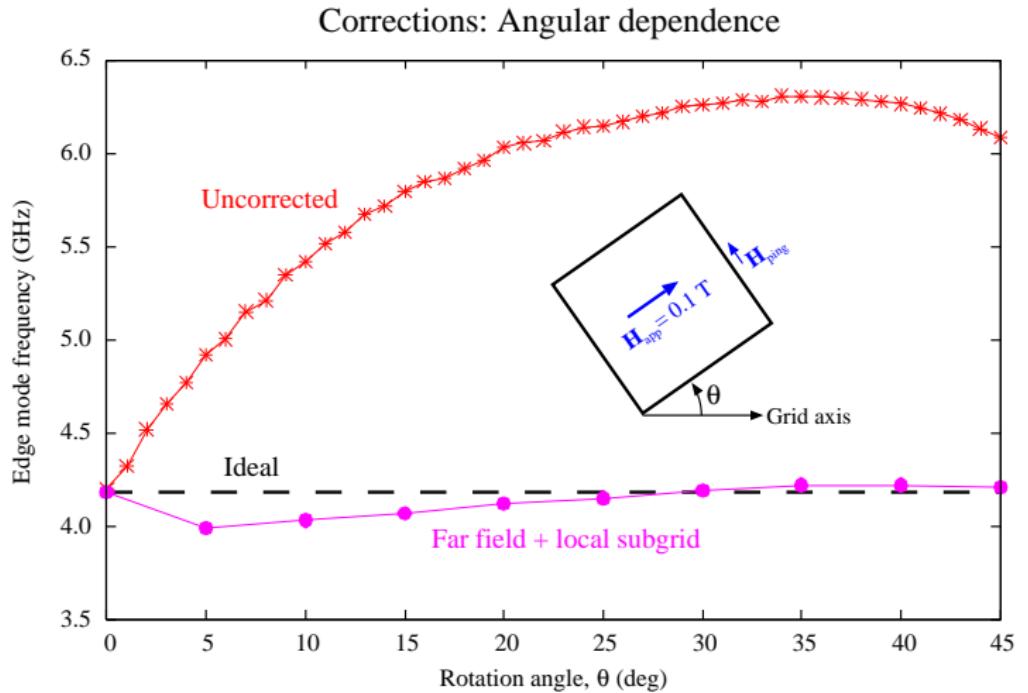
Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations



MJ Donahue & RD McMichael, "Micromagnetics on curved geometries using rectangular cells: error correction and analysis," *IEEE Trans. Magn.*, **43**, 2878 (2007).

Thermal effects

Landau-Lifshitz-Gilbert + Thermal Noise:

$$\begin{aligned} \frac{d\mathbf{M}}{dt} = & \frac{|\gamma_0|}{1+\alpha^2} (\mathbf{H}_{\text{eff}} + \mathbf{H}_{\text{th}}) \times \mathbf{M} \\ & + \frac{\alpha |\gamma_0|}{(1+\alpha^2)M_s} \mathbf{M} \times (\mathbf{H}_{\text{eff}} + \mathbf{H}_{\text{th}}) \times \mathbf{M} \end{aligned}$$

where \mathbf{H}_{th} is Gaussian random process s.t.

$$\langle \mathbf{H}_{\text{th},i}(t) \rangle = 0$$

$$\langle \mathbf{H}_{\text{th},i}(x, t) \mathbf{H}_{\text{th},j}(x', t') \rangle = 2D\delta_{ij}(x - x')\delta(t - t')$$

$$D = \frac{\alpha k_B T}{|\gamma_0| M_s}$$

[Background](#)
[Practical OOMMF](#)
[Pitfalls](#)
[Mesh size](#)
[Symmetry breaking](#)
[Field step size](#)
[Stopping criteria](#)
[Energy minimization](#)
[Advanced Topics](#)
[Extended volumes](#)
[Normal mode images](#)
[Sub-cell thickness variation](#)
[Movies](#)
[Recommendations](#)

Landau-Lifshitz-Bloch (LLB):

$$\begin{aligned}\frac{d\mathbf{m}}{dt} = & |\gamma_0| \mathbf{H}_{\text{eff}} \times \mathbf{m} + \frac{|\gamma_0| \alpha_{\parallel}}{m^2} (\mathbf{m} \cdot \mathbf{H}_{\text{eff}}) \mathbf{m} \\ & + \frac{|\gamma_0| \alpha_{\perp}}{m^2} \mathbf{m} \times (\mathbf{H}_{\text{eff}} + \boldsymbol{\eta}^{\perp}) \times \mathbf{m} + \boldsymbol{\eta}^{\parallel}\end{aligned}$$

with mean-zero noise $\boldsymbol{\eta}^{\perp}, \boldsymbol{\eta}^{\parallel}$, $\langle \boldsymbol{\eta}_i^{\parallel}, \boldsymbol{\eta}_j^{\perp} \rangle = 0$,

$$\langle \boldsymbol{\eta}_i^{\perp}(0), \boldsymbol{\eta}_j^{\perp}(t) \rangle = \frac{2k_B T (\alpha_{\perp} - \alpha_{\parallel})}{|\gamma_0| M_s^0 V \alpha_{\perp}^2} \delta_{ij} \delta(t)$$

$$\langle \boldsymbol{\eta}_i^{\parallel}(0), \boldsymbol{\eta}_j^{\parallel}(t) \rangle = \frac{2 |\gamma_0| k_B T \alpha_{\parallel}}{M_s^0 V} \delta_{ij} \delta(t)$$

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Landau-Lifshitz-Bloch (LLB) (cont.)

and

$$\mathbf{H}_{\text{eff}} = \mathbf{H} + \begin{cases} \frac{1}{2\tilde{\chi}_{\parallel}} \left(1 - \frac{\mathbf{m}^2}{m_e^2}\right) \mathbf{m}, & T \lesssim T_c \\ -\frac{1}{\tilde{\chi}_{\parallel}} \left(1 + \frac{3}{5} \frac{T_c m^2}{T - T_c}\right) \mathbf{m}, & T \gtrsim T_c \end{cases}$$

- ▶ $\|\mathbf{m}\| = 1$ constraint relaxed
- ▶ Consistent with Boltzmann distribution at all temperatures

[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

Dynamics driven by jump-noise process

$$\frac{d\mathbf{M}}{dt} = |\gamma_0| \mathbf{H}_{\text{eff}} \times \mathbf{M} + \mathbf{T}_r(t)$$

where $\mathbf{T}_r(t)$ is jump-noise process

$$\mathbf{T}_r(t) = \sum_i \mathbf{m}_i \delta(t - t_i)$$

with random jumps \mathbf{m}_i occurring at random times t_i .

- ▶ LLG damping analytically derived as average effect of jump-noise process.
- ▶ Jump-noise accounts for both stochastic thermal effects and damping.

Nudged elastic band

How to get through the mountains?



Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

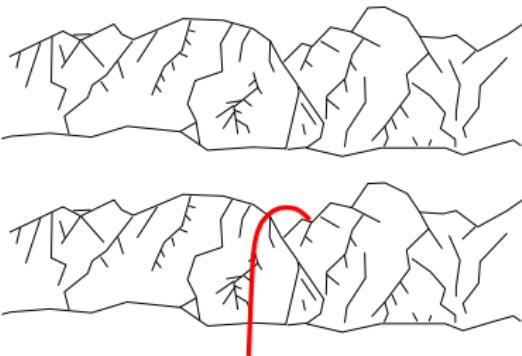
Movies

Recommendations

Nudged elastic band

How to get through the mountains?

Step 1: Throw a rope.



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Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Nudged elastic band

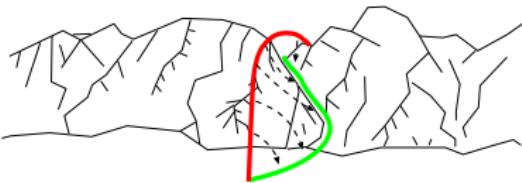
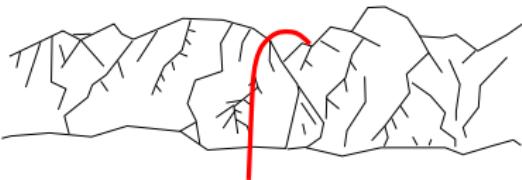
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How to get through the mountains?

Step 1: Throw a rope.

Step 2: Slide the rope down into a pass.



- ▶ Green path gives a bound on energy barrier.
- ▶ There may be more than one pass!

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

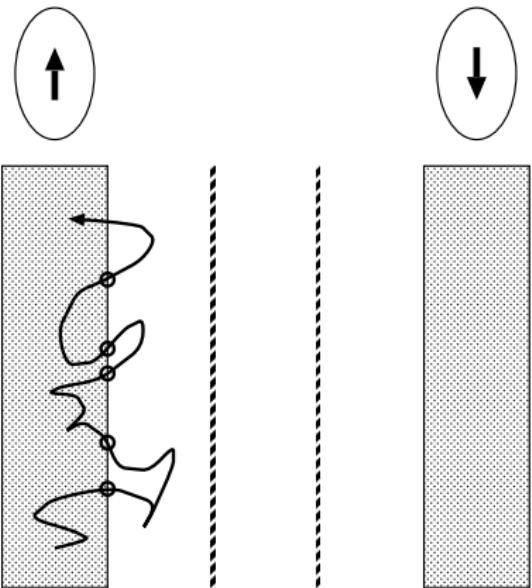
Sub-cell thickness variation

Movies

Recommendations

[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

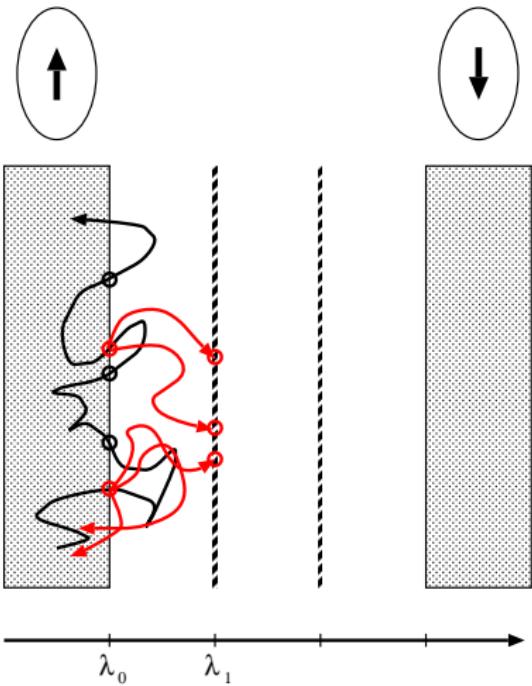
Forward flux sampling



R Allen, C Valeriani, P ten Wolde, *J. Phys.: Cond. Matter*, **21**, 463102 (2009).
C Vogler, F Bruckner, B Bergmair, T Huber et al., *PRB*, **88**, 134409 (2013).

[Background](#)[Practical OOMMF](#)[Pitfalls](#)[Mesh size](#)[Symmetry breaking](#)[Field step size](#)[Stopping criteria](#)[Energy minimization](#)[Advanced Topics](#)[Extended volumes](#)[Normal mode images](#)[Sub-cell thickness variation](#)[Movies](#)[Recommendations](#)

Forward flux sampling



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Forward flux sampling

Micromagnetics

M.J. Donahue

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

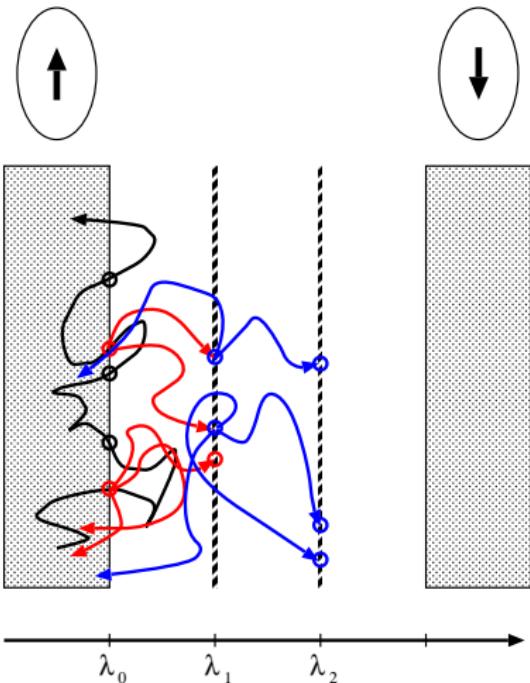
Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations



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Forward flux sampling

Micromagnetics

M.J. Donahue

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

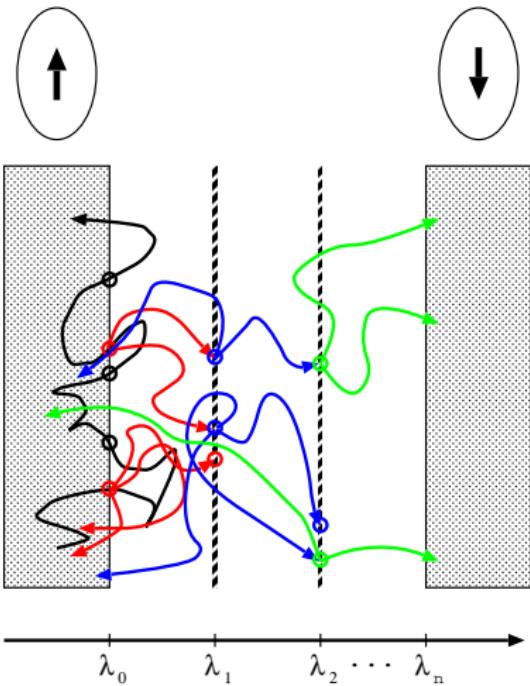
Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations



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“Local” spin-torque

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

$$\frac{\partial \mathbf{m}}{\partial t} = \gamma_0 \mathbf{H}_{\text{eff}} \times \mathbf{m} + \alpha \mathbf{m} \times \frac{\partial \mathbf{m}}{\partial t} - \mathbf{T}$$

where local form of spin-torque T given by

$$\mathbf{T}_{\text{loc}} = u \partial_x \mathbf{m} - \beta u \mathbf{m} \times \partial_x \mathbf{m}$$

with $u = \frac{JPg\mu_B}{2eM_s}$

Spin-torque with diffusion

Introduce a parallel equation for spin density $\delta\mathbf{m}$:

$$\frac{\partial \delta\mathbf{m}}{\partial t} = D \Delta \delta\mathbf{m} + \frac{1}{\tau_{sd}} \mathbf{m} \times \delta\mathbf{m} - \frac{1}{\tau_{sf}} \delta\mathbf{m} - u \partial_x \mathbf{m}$$

with diffusion constant D , spin-flip time τ_{sf} , s-d exchange time τ_{sd} linked to the first via

$$\mathbf{T} = (\mathbf{m} \times \delta\mathbf{m}) / \tau_{sd}$$

Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations

Micromagnetic simulations show

- ▶ 20% increase in vortex wall velocity
- ▶ Little effect on ATWs (asymmetric transverse walls)

D. Claudio-Gonzalez, A. Thiaville, J. Militat, "Domain wall dynamics under nonlocal spin-transfer torque," *PRL*, **108**, 227208 (2012).

Parallelization on CPU: 4 million spins

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Background

Practical OOMMF

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

Energy minimization

Advanced Topics

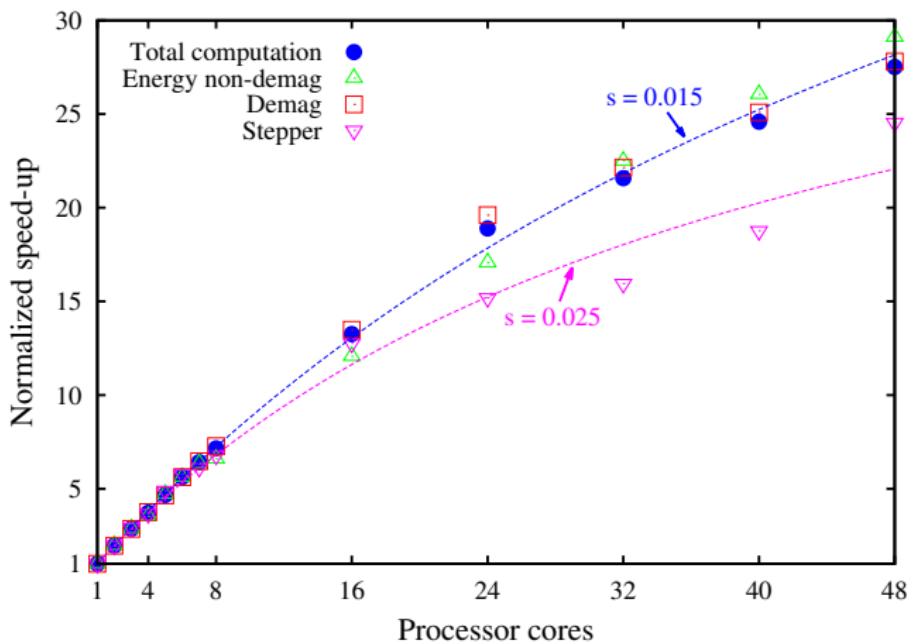
Extended volumes

Normal mode images

Sub-cell thickness variation

Movies

Recommendations



Dashed curves: $\frac{1}{s + (1-s)/n}$