

# Introduction to Micromagnetic Modeling

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## Background

## Pitfalls

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

## Advanced Topics

- Extended volumes
- Normal mode images
- Sub-cell thickness variation
- Thermal
- Spin Torque
- Fast hardware
- OOMMF extensions
- Movies

## Recommendations

Talk slides available at

[http://math.nist.gov/~MDonahue/talks/  
tms2015-mmintro.pdf](http://math.nist.gov/~MDonahue/talks/tms2015-mmintro.pdf)

# Outline

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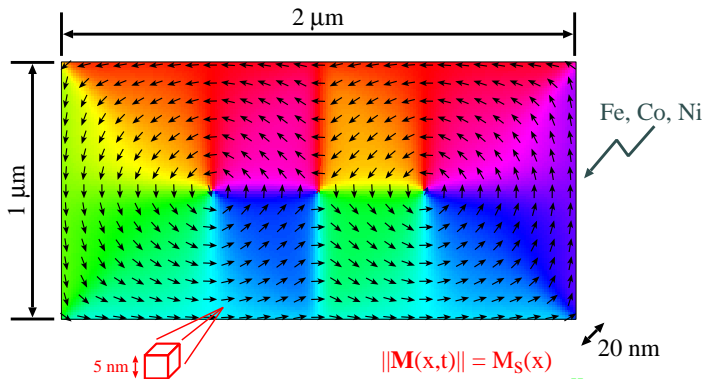
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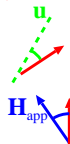
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# What is micromagnetics?



- Dipole-Dipole (demag)  $\downarrow \uparrow$
- Exchange  $\uparrow \uparrow$
- Anisotropy  $\uparrow$
- Zeeman  $\uparrow$



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

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# 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).

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# How can I use micromagnetics?

- ▶ 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

## Background

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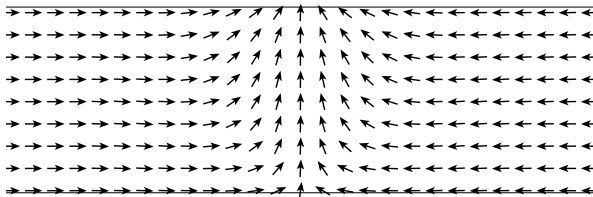
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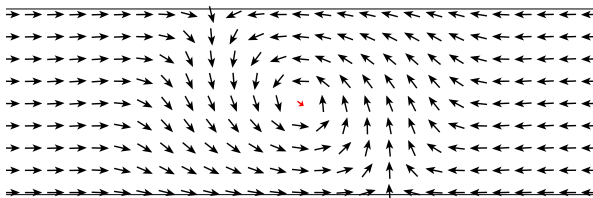
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# Head-to-head domain wall types



Transverse wall



Vortex wall

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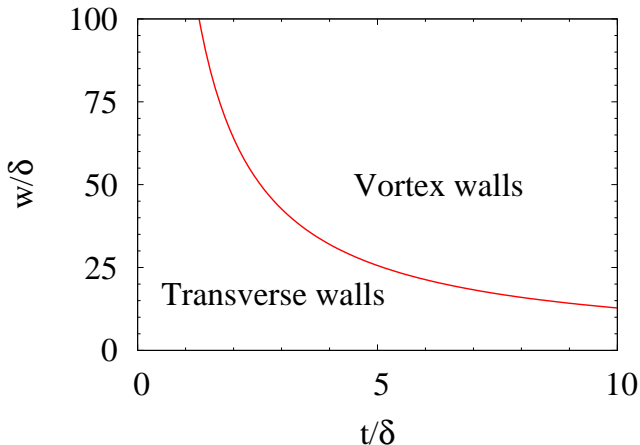
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## Recommendations

# Head-to-head phase diagram



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

# Size effect study

## Background

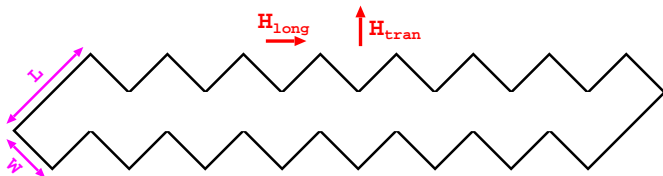
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$50 \text{ nm} < L < 500 \text{ nm}$

$W = 0.5 L$

Thickness = 20 nm

Py material parameters:

$A = 13 \text{ pJ/m}$

$K = 0 \text{ J/m}^3$

$M_s = 800 \text{ kA/m}$

## Background

## Pitfalls

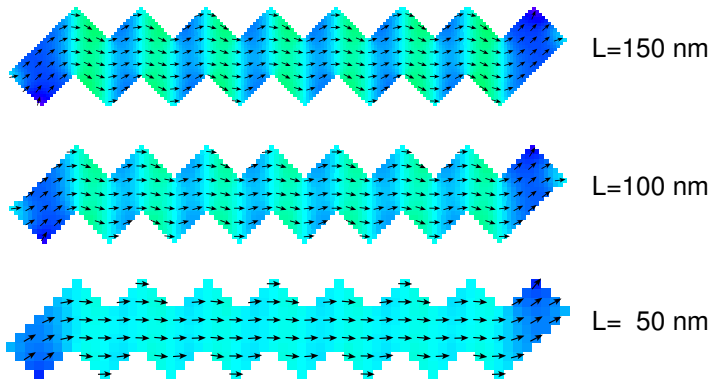
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## Recommendations

# Size effect study (remanent state)



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

## Background

## Pitfalls

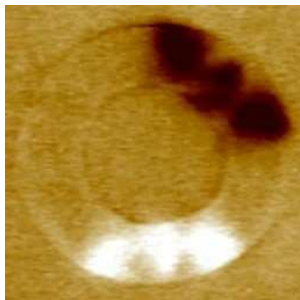
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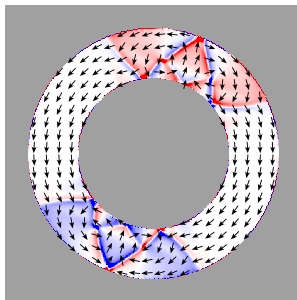
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## Recommendations

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



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).

## Background

## Pitfalls

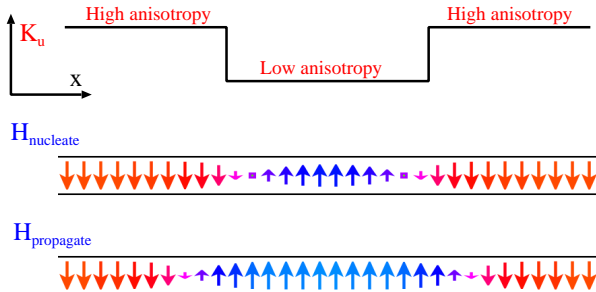
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# Pinning by simple defect (1D)



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

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

---

A. Aharoni, *Phys. Rev.*, **119**, 127 (1960).

# Brown's equations

## Energies:

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

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

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

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

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$\mathbf{M}$  is smooth

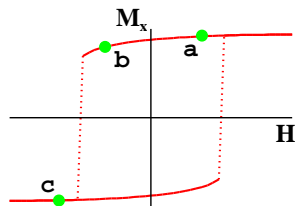
and

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

or equivalently

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

# Quasi-static micromagnetics



## Background

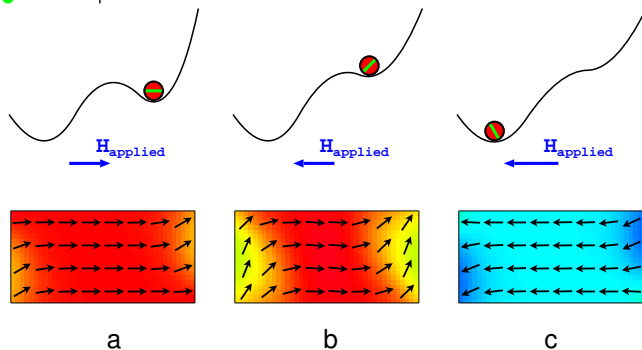
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# Magnetization dynamics

## Landau-Lifshitz-Gilbert:

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

where

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

$\gamma_0$  = gyromagnetic ratio

$\alpha$  = damping coefficient

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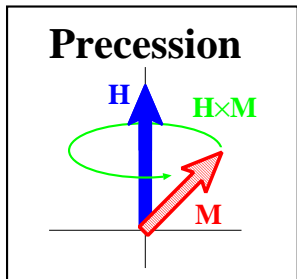
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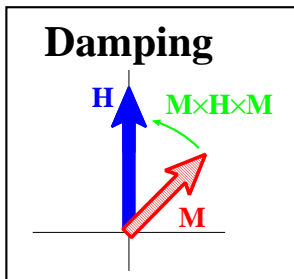
# Magnetization dynamics

## Landau-Lifshitz-Gilbert:

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



No energy change



Loses energy

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

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# Stopping criteria

Recall

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

Natural stopping criterion for dynamics is small  $|d\mathbf{M}/dt|$ , say

$$\|\mathbf{H}_{\text{eff}} \times \mathbf{M}\| / M_s < \varepsilon.$$

Natural stopping criterion for energy minimization is small

$\|\delta E_{\text{total}} / \delta \mathbf{M}\|$ , which means small  $\|\mathbf{H}_{\text{eff}}\|$  subject to constraint  $\|\mathbf{M}\| = M_s$ , so

$$\begin{aligned} \|\mathbf{H}_{\text{eff}} - (\mathbf{H}_{\text{eff}} \cdot \mathbf{M}) \mathbf{M} / M_s^2\| &= \|\mathbf{M} \times \mathbf{H}_{\text{eff}} \times \mathbf{M}\| / M_s^2 \\ &= \|\mathbf{H}_{\text{eff}} \times \mathbf{M}\| / M_s \\ &< \varepsilon. \end{aligned}$$

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# Mathematically equivalent forms for LLG

## Landau-Lifshitz:

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

## Gilbert:

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

- ▶ Note  $1 + \alpha^2$  factor in Landau-Lifshitz.
- ▶ Gilbert form is implicit, and terms on right are not orthogonal.

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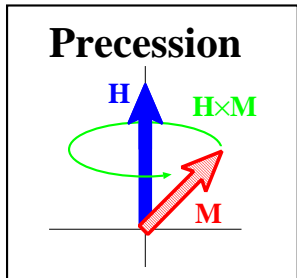
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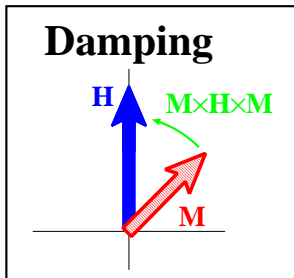
# Magnetization dynamics

## Landau-Lifshitz-Gilbert:

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



No energy change



Loses energy

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

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# Variational derivatives

Let (support  $\Delta\mathbf{M}$ )  $\subset B(x_k, \varepsilon)$ .

Then

$$\left. \frac{\delta E}{\delta \mathbf{M}} \right|_{x_k} = \lim \frac{E(\mathbf{M} + \Delta\mathbf{M}) - E(\mathbf{M})}{\|\Delta\mathbf{M}\|_1}$$

as

$$\varepsilon \rightarrow 0, \quad \|\Delta\mathbf{M}\|_\infty \rightarrow 0.$$

**Discretized form:** If

$$\mathbf{M}(x) = \sum M_i \phi_i(x),$$

then

$$\left. \frac{\delta E}{\delta \mathbf{M}} \right|_{x_k} \approx \frac{\partial E}{\partial M_k} \cdot \frac{1}{\|\phi_k\|_1}$$

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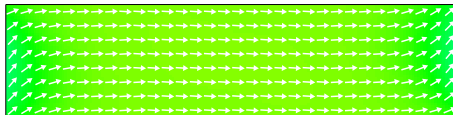
## Recommendations

# Magnetization dynamics

Time

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

0 ps



100 ps



150 ps



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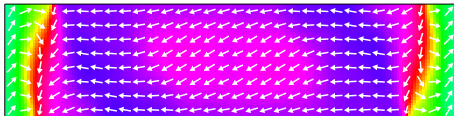
Time

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

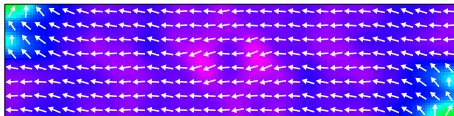
350 ps



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).

# Thin film simulation

## Background

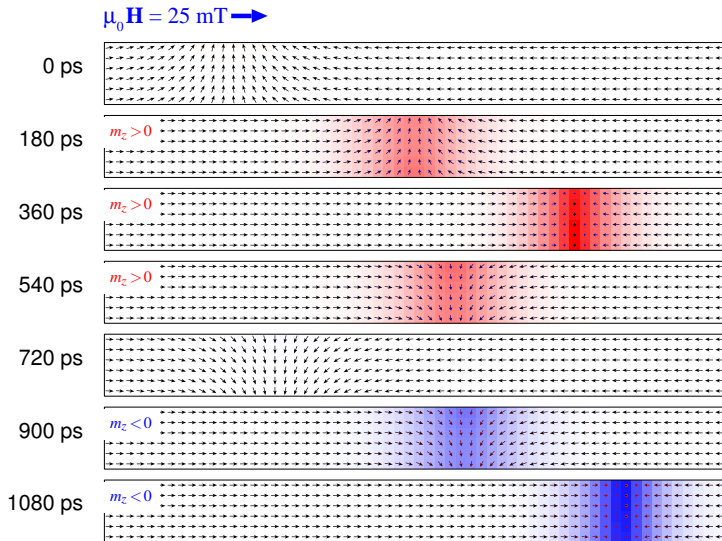
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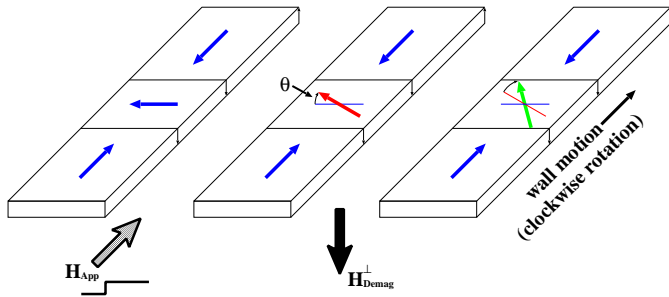
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# Thin film wall dynamics, $m_z \geq 0$



## Background

### Pitfalls

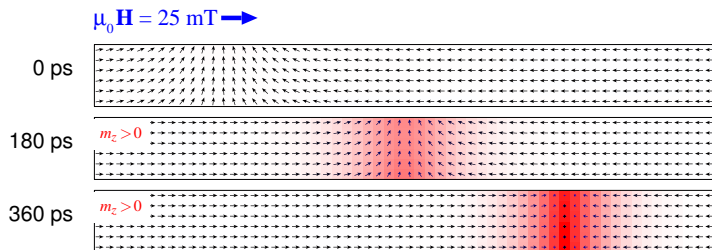
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# Thin film simulation



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# Thin film wall dynamics, $m_z \geq 0$

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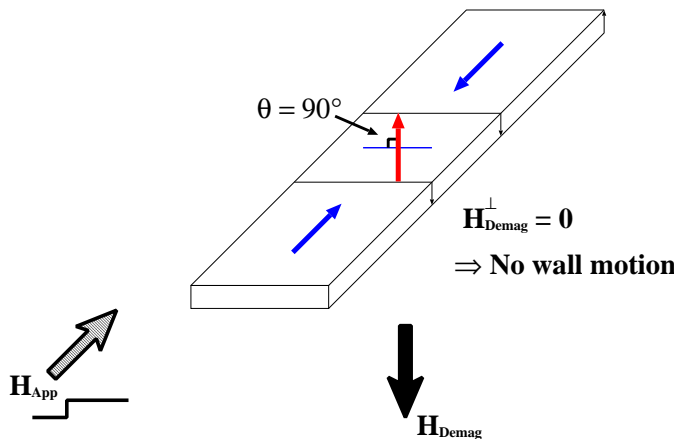
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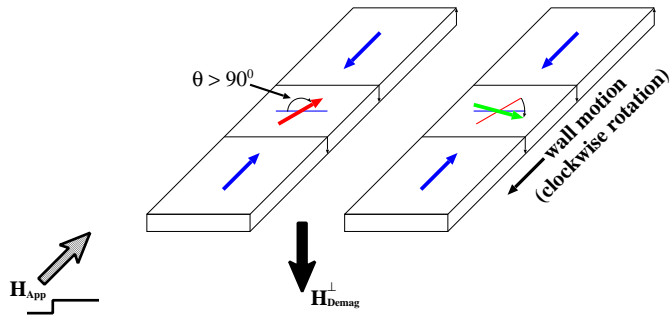
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# Thin film wall dynamics, $m_z \geq 0$



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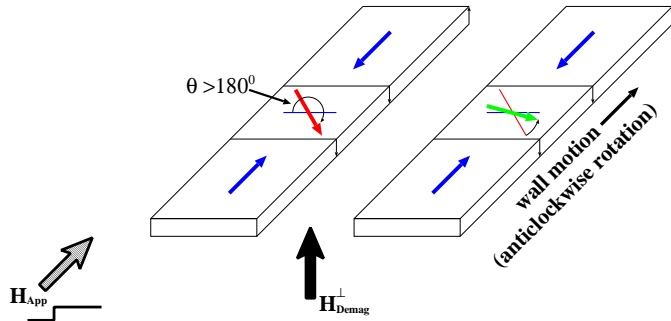
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# Thin film wall dynamics, $m_z \leq 0$



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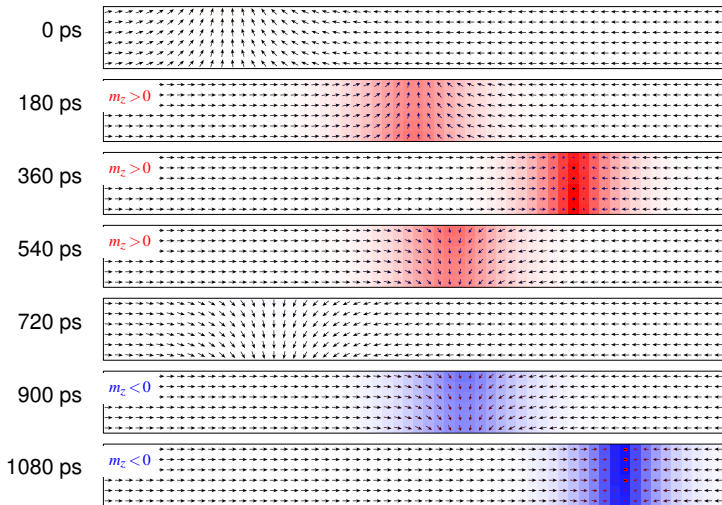
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## Thin film simulation

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



## Background

## Pitfalls

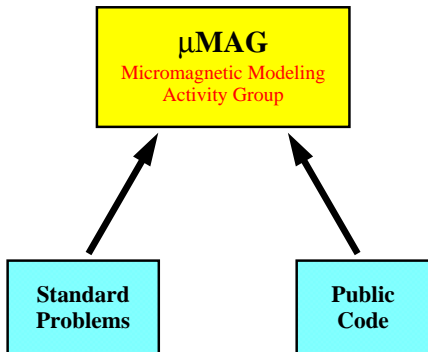
- Mesh size
- Symmetry breaking
- Field step size
- Stopping criteria
- Energy minimization

## Advanced Topics

- Extended volumes
- Normal mode images
- Sub-cell thickness variation
- Thermal
- Spin Torque
- Fast hardware
- OOMMF extensions
- Movies

## Recommendations

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



Center for Theoretical and Computational Materials Science

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

See also the mailing list and archives!

## Background

### Pitfalls

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

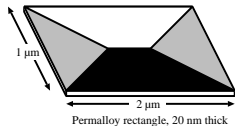
### Advanced Topics

- Extended volumes
- Normal mode images
- Sub-cell thickness variation
- Thermal
- Spin Torque
- Fast hardware
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- Movies

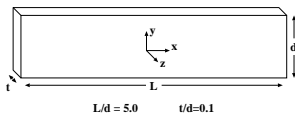
### Recommendations

# $\mu$ MAG standard problems

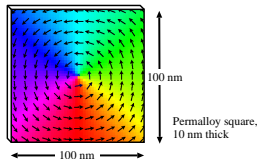
## Problem 1: Hysteresis



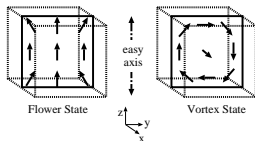
## Problem 2: Hysteresis



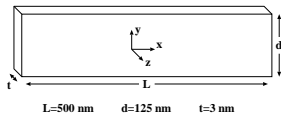
## Problem 5: CIP Spin Torque



## Problem 3: Energy Minimization



## Problem 4: Dynamics



## Background

### Pitfalls

- Mesh size
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Field step size  
Stopping criteria  
Energy minimization

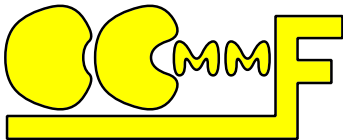
## Advanced Topics

Extended volumes  
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Sub-cell thickness variation  
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## Recommendations

## Public code

**Portable, extensible,  
public domain  
programs & tools  
for micromagnetics**



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

Primary developers: Don Porter, Mike Donahue (ITL)

- ▶ Graphical User Interface
- ▶ Windows, Unix, Mac OS X
- ▶ Binaries and source code
- ▶ Tcl/Tk and C++ based modular architecture
- ▶ 250 page user's manual
- ▶ 15000+ downloads in 2014
- ▶ 185 journal cites in 2013
- ▶ 1850 citations since 1997

▶ Extensible architecture: numerous third party extensions.

# 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)
- ▶ mumax<sup>3</sup> (FD, GPU, free)
- ▶ Nmag (FE, development ceased, free)
- ▶ ...

**If you use a code, please cite!**

## Background

### Pitfalls

- Mesh size
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- Field step size
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### Advanced Topics

- Extended volumes
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### Recommendations

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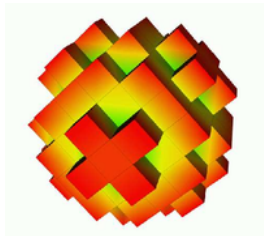
## Pitfalls

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Symmetry breaking  
Field step size  
Stopping criteria  
Energy minimization

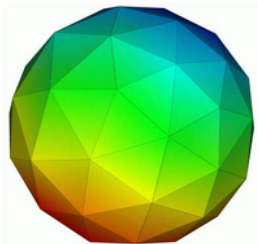
## Advanced Topics

Extended volumes  
Normal mode images  
Sub-cell thickness variation  
Thermal  
Spin Torque  
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OOMMF extensions  
Movies

## Recommendations



- ▶ 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.

## 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).

### Background

#### Pitfalls

- Mesh size
- Symmetry breaking
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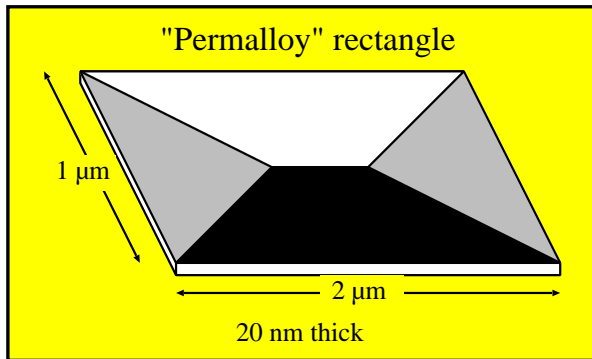
Fast hardware

OOMMF extensions

Movies

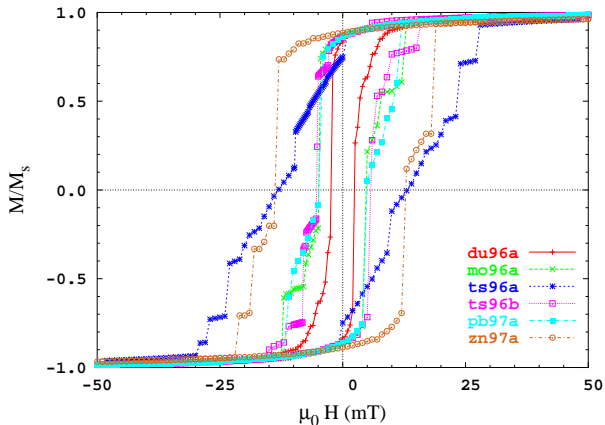
### Recommendations

# $\mu$ MAG standard problem 1



Task: Run this through a hysteresis loop.

# $\mu$ MAG standard problem 1: results



Problem: ???

Problem: Meshes were too coarse!

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## 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"

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

# Example $l_{ex}$ values

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Material	$M_s$ (kA/m)	K (kJ/m <sup>3</sup> )	A (pJ/m)	$l_{ex,K}$ (nm)	$l_{ex,M_s}$ (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 <sub>2</sub> Fe <sub>14</sub> B	1280	4500	13	1.7	3.6

# 1D wall types

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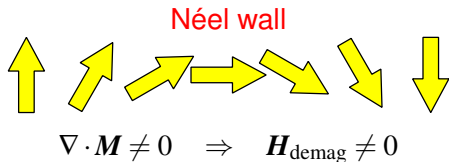
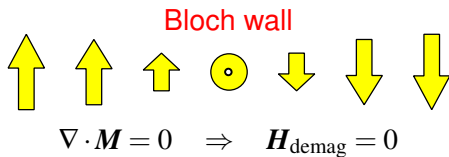
Spin Torque

Fast hardware

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# Bloch wall discretization

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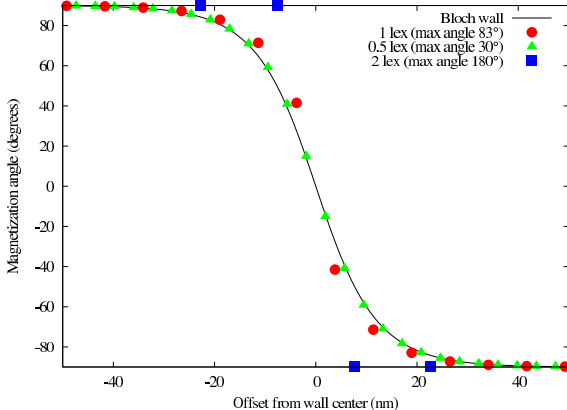
Spin Torque

Fast hardware

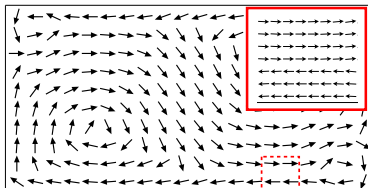
OOMMF extensions

Movies

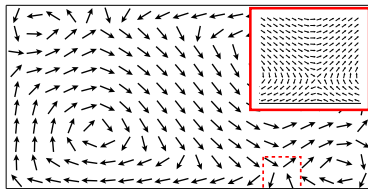
Recommendations



# Néel wall collapse



25 nm cells



12.5 nm cells

MJ Donahue, "A variational approach to exchange energy calculations in micromagnetics," *JAP*, **83**, 6491 (1998).

Background

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

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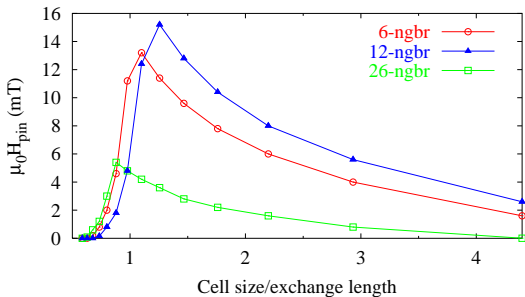
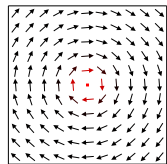
Fast hardware

OOMMF extensions

Movies

Recommendations

# Vortex mobility



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

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

# Cell size recommendations

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

## Background

### Pitfalls

#### Mesh size

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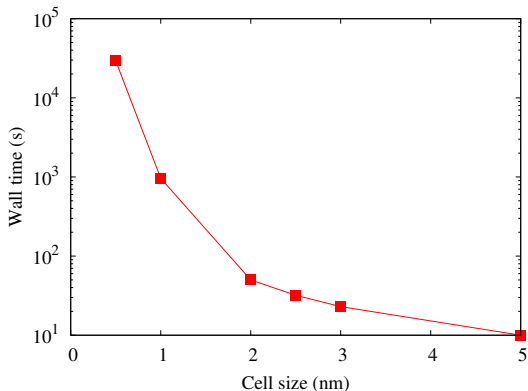
Movies

## Recommendations

# 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

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##### Mesh size

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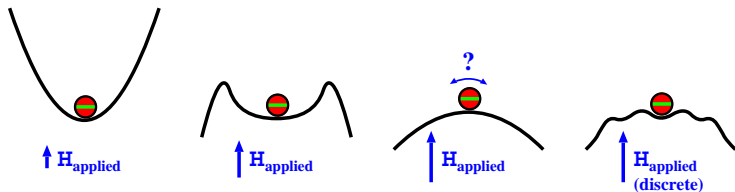
Fast hardware

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#### Recommendations

# Symmetry breaking



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

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Recommendations

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## Advanced Topics

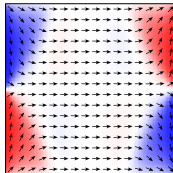
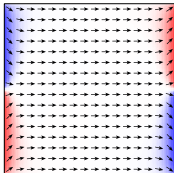
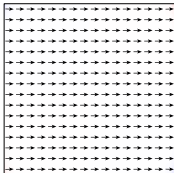
- Extended volumes
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## Recommendations

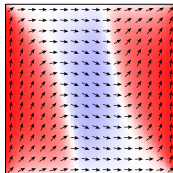
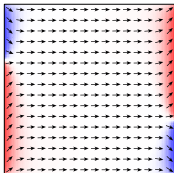
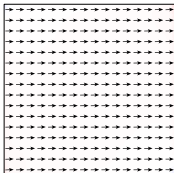
## Symmetry breaking

 $H_{\text{applied}}$ 

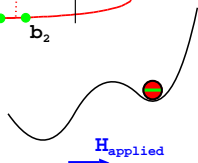
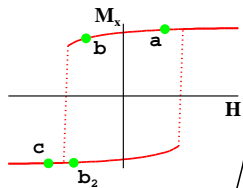
$H_{\text{applied}}$   
on axis



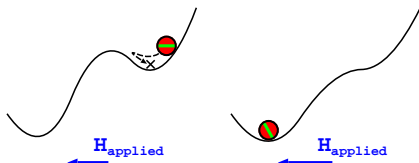
$H_{\text{applied}}$   
 $1^\circ$  off-axis



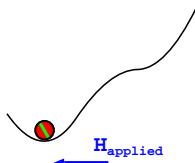
# Big field steps $\Rightarrow$ premature switching



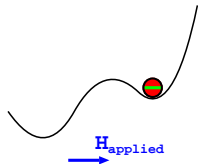
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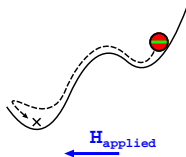
b



c



a



b<sub>2</sub>

Background

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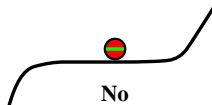
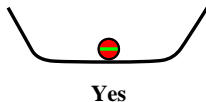
Advanced Topics

- Extended volumes
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Recommendations

# Stopping too soon

Stopping criteria:  $M \times H_{\text{eff}} < \text{stoptorque}$



## Background

### Pitfalls

- Mesh size
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- Energy minimization

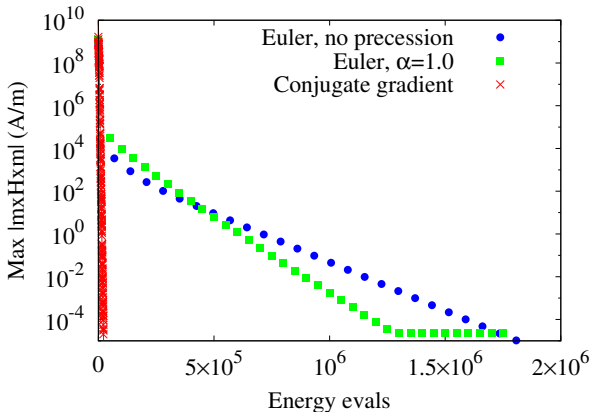
### Advanced Topics

- Extended volumes
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- Movies

### Recommendations

# LLG vs. Conjugate Gradient

Standard problem 3 (energy minimization):



- Use the right tool for the job!

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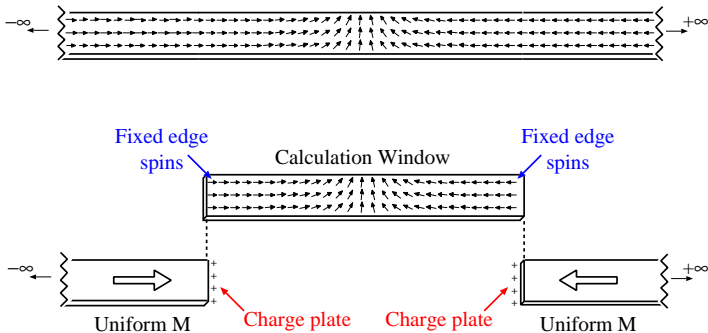
## Pitfalls

- Mesh size
- Symmetry breaking
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## Advanced Topics

- Extended volumes
- Normal mode images
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- Movies

## Recommendations



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

## Background

## Pitfalls

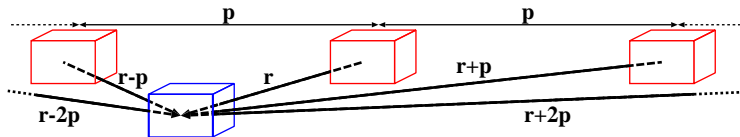
- Mesh size
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## Advanced Topics

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## Recommendations

# Periodic boundaries: 1D



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

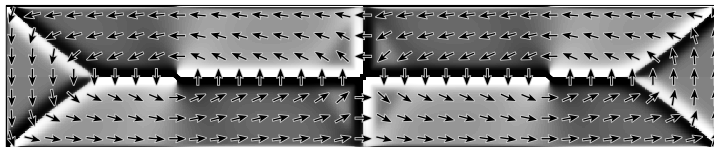
where

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

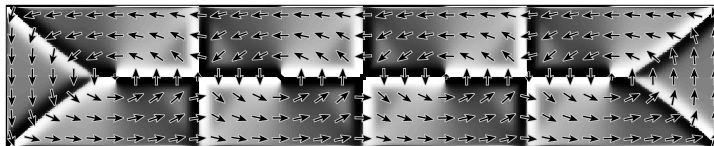
---

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

# Cross-tie walls



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



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

## Background

### Pitfalls

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

### Advanced Topics

- Extended volumes
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### Recommendations

# Multi-dimension periodic

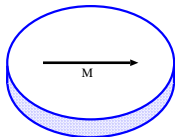
- ▶ 1D periodic: tail sum  $\sim \int_{R_2}^{\infty} 1/x^3 dx < \infty$

$\Rightarrow$  boundary doesn't matter.

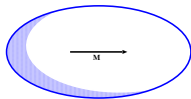
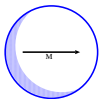


- ▶ 2D periodic: tail sum  $\sim \iint_{R>R_2} 1/R^3 dx dy < \infty$

$\Rightarrow$  boundary doesn't matter.



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



## Background

### Pitfalls

- Mesh size
- Symmetry breaking
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- Energy minimization

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### Recommendations

# FMR simulations

Background

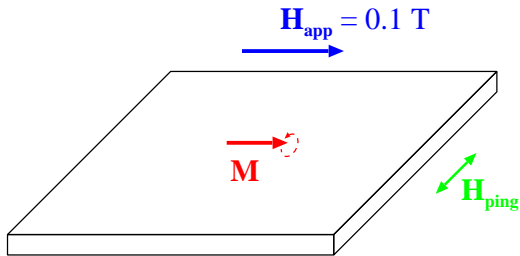
Pitfalls

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

Advanced Topics

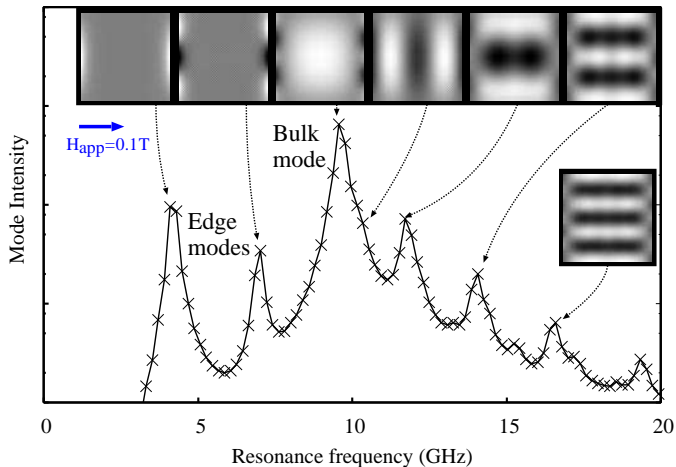
- Extended volumes
- Normal mode images
- Sub-cell thickness variation
- Thermal
- Spin Torque
- Fast hardware
- OOMMF extensions
- Movies

Recommendations



Small “ping” field induces spinwaves.

# FMR spectra



## Background

### Pitfalls

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

### Advanced Topics

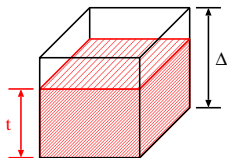
- Extended volumes
- Normal mode images
- Sub-cell thickness variation
- Thermal
- Spin Torque
- Fast hardware
- OOMMF extensions
- Movies

### Recommendations

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

# 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= $t$ ,  $|\mathbf{M}|=M_s$

## Background

### Pitfalls

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

### Advanced Topics

- Extended volumes
- Normal mode images
- Sub-cell thickness variation
- Thermal
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- Fast hardware
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- Movies

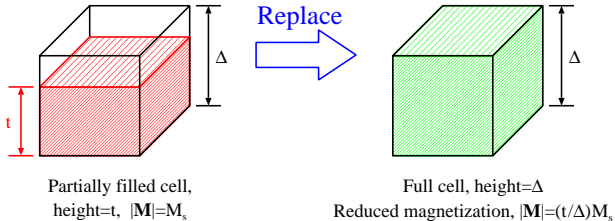
### Recommendations

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

**SOLUTION:** Use full cell so all cells have same geometry, but reduce  $M_s$  so far-field demag is correct.

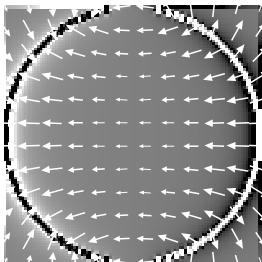
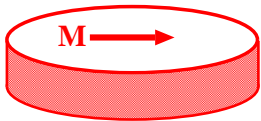


DG Porter & MJ Donahue, *JAP*, **89**, 7257 (2001).

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

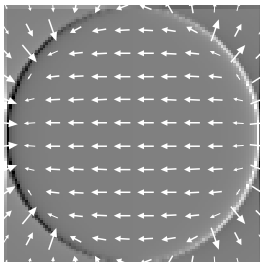
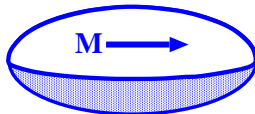
# Sub-cell thickness variation

10x10x1 disk



Non-uniform demag field

10x10x1 oblate spheroid



Almost uniform demag field

Background

Pitfalls

Mesh size

Symmetry breaking

Field step size

Stopping criteria

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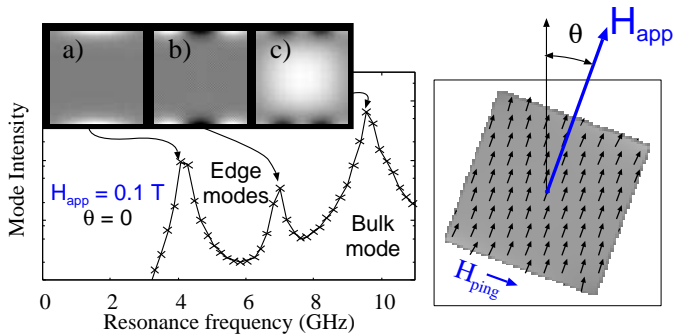
Fast hardware

OOMMF extensions

Movies

Recommendations

# Edge mode test



## Background

## Pitfalls

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

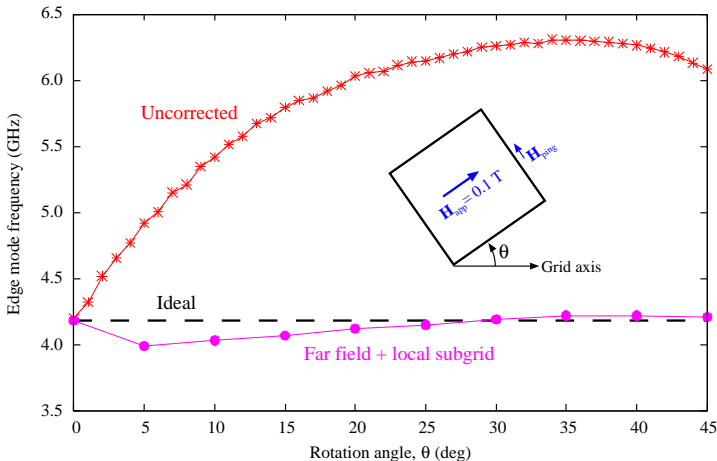
## Advanced Topics

- Extended volumes
- Normal mode images
- Sub-cell thickness variation
- Thermal
- Spin Torque
- Fast hardware
- OOMMF extensions
- Movies

## Recommendations

# Staircase correction

## Corrections: Angular dependence



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

## Background

## Pitfalls

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

## Advanced Topics

- Extended volumes
- Normal mode images
- Sub-cell thickness variation
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## Recommendations

# Thermal effects

## Landau-Lifshitz-Gilbert + Thermal Noise:

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

where  $\mathbf{H}_{\text{th}}$  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

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## Recommendations

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

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

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

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

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

and

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

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

# 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.

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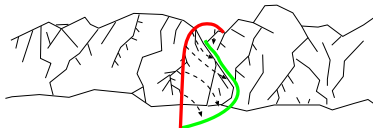
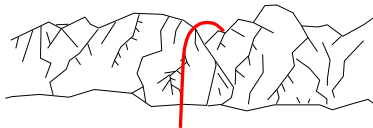
I Mayergoyz, G Bertotti, C Serpico, "Magnetization dynamics driven by a jump-noise process," *PRB* **83** (2011) 020402.

# Nudged elastic band

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!

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Symmetry breaking  
Field step size  
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Sub-cell thickness variation

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Recommendations

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## Pitfalls

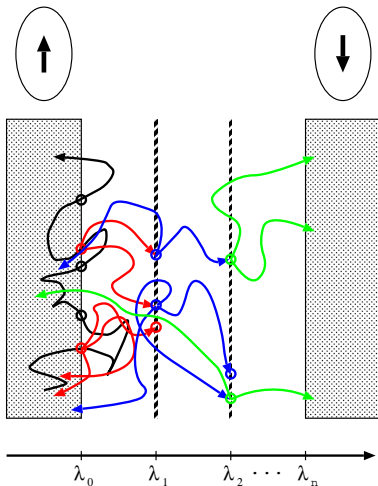
- Mesh size
- Symmetry breaking
- Field step size
- Stopping criteria
- Energy minimization

## Advanced Topics

- Extended volumes
- Normal mode images
- Sub-cell thickness variation
- Thermal
- Spin Torque
- Fast hardware
- OOMMF extensions
- 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).

# “Local” spin-torque

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

where local form of spin-torque  $\mathbf{T}$  given by

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

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

## Background

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### Recommendations

# 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  $\tau_{sf}$ , s-d exchange time  $\tau_{sd}$  linked to the first via

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

Micromagnetic simulations show

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

---

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

Background

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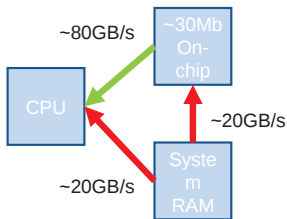
Movies

Recommendations

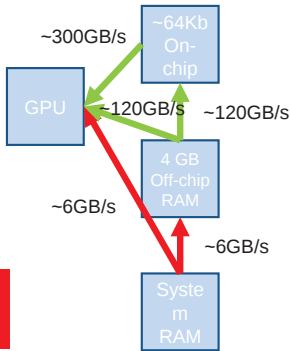
# Why GPU is awesome?



CPU



GPU



CPU has much higher chance to be memory throughput limited

GPU can transfer buffers during kernel execution

Background

Pitfalls

- Mesh size
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Recommendations

Slide courtesy Mykola Dvornik.



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- Fast hardware**
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- Movies

Recommendations

- Number of registers per thread is limited
- Transfer to/from system memory are slow
- Manual management of memory resources
- Branching is expensive
- Low inter-GPUs throughput (just like on CPU)
- Memory access should be aligned to cache line and coalesce (just like on CPU)

# More reasons why GPU is pain

- ▶ Reported GPU results are usually single-precision floating point, compared to double-precision on CPU. Double-precision on GPU is usually either slow or expensive.
- ▶ Memory on GPU is limited to 4–8 GB.
- ▶ GPU programming model quite different than CPU.

## Background

### Pitfalls

- Mesh size
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- Extended volumes
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- Movies

## Recommendations

## Background

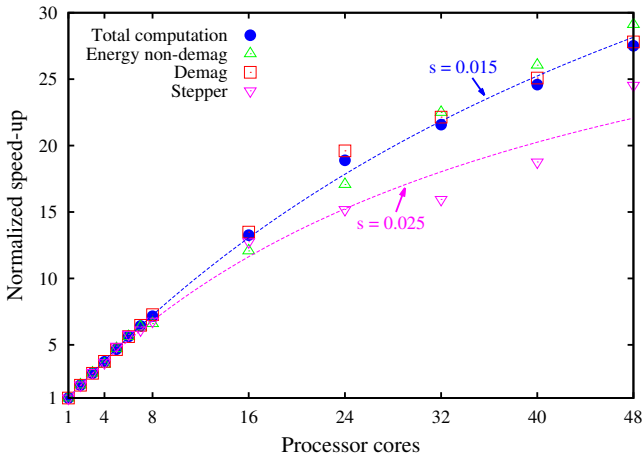
## Pitfalls

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

## Advanced Topics

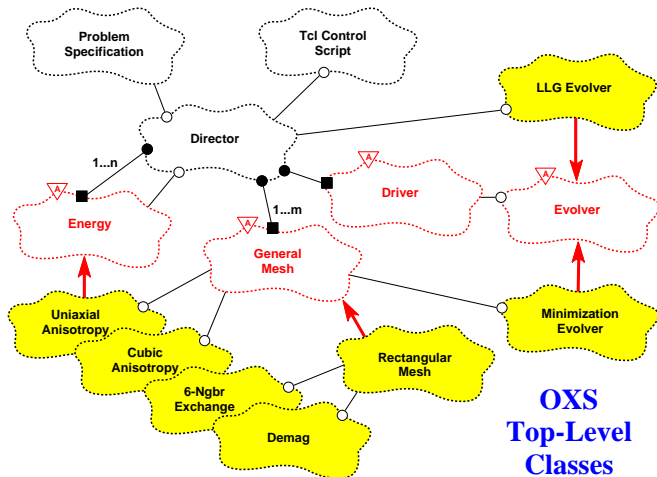
- Extended volumes
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- OOMMF extensions
- Movies

## Recommendations



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

# OOMMF C++ class structure



## Background

### Pitfalls

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

### Advanced Topics

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### Recommendations

**OXS**  
**Top-Level**  
**Classes**

## Background

## Pitfalls

- Mesh size
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## Advanced Topics

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## 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.

# 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  $\phi$  is angle between  $\mathbf{m}$  and  $\mathbf{u}$ .

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# 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

### Pitfalls

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

## Advanced Topics

- Extended volumes
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## 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

### Pitfalls

- Mesh size
- Symmetry breaking
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## 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_inverse[i]==0.0) {
      energy[i]=0.0;
      field[i].Set(0.,0.,0.);
    } else {
      REAL8m dot = axis*spin[i];
      REAL8m dotsq = dot*dot;
-     energy[i] = -K1*dotsq;
-     REAL8m fieldmag = (2./MU0)*K1*dot*Ms_inverse[i];
+     energy[i] = ((dotsq-2)*K2-K1)*dotsq;
+     REAL8m fieldmag
+     = (-2./MU0)*((dotsq-1)*2*K2-K1)*dot*Ms_inverse[i];
      field[i] = fieldmag * axis;
    }
  }
}
```

### Background

#### Pitfalls

- Mesh size
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### Recommendations

# Remanent magnetization configuration

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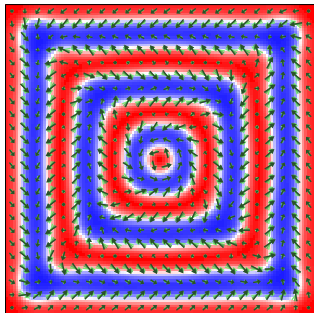
Spin Torque

Fast hardware

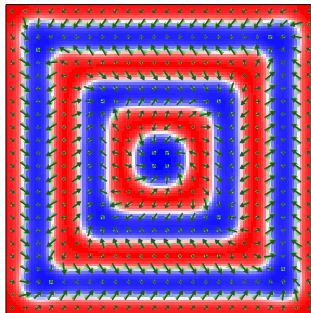
OCCMF extensions

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Simple Anisotropy



Extended Anisotropy

# Making movies

See the OOMMF movie page:

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

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**Movies**

Recommendations

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## Recommendations

# Recommendations

- ▶ Don't mesh coarser than  $\ell_{\text{ex}}$
- ▶ Check max neighbor angle: under  $30^\circ$  is usually reliable, over  $90^\circ$  is questionable,  $180^\circ$  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.)