

# Introduction to Micromagnetic Modeling

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Talk slides available at

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

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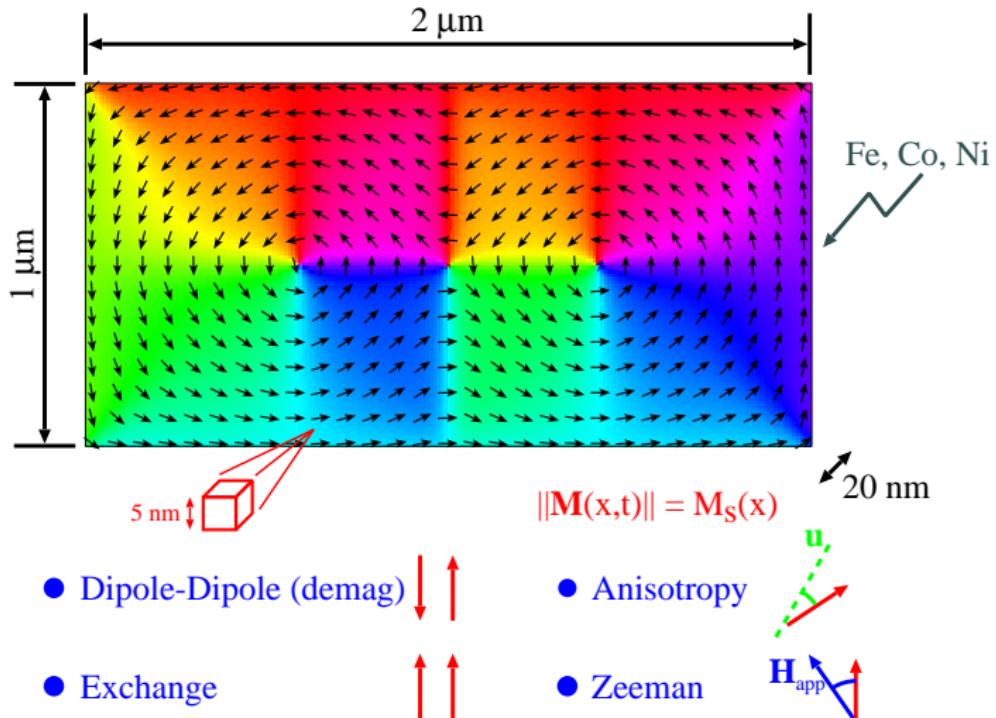
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## What is micromagnetics?



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

# 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

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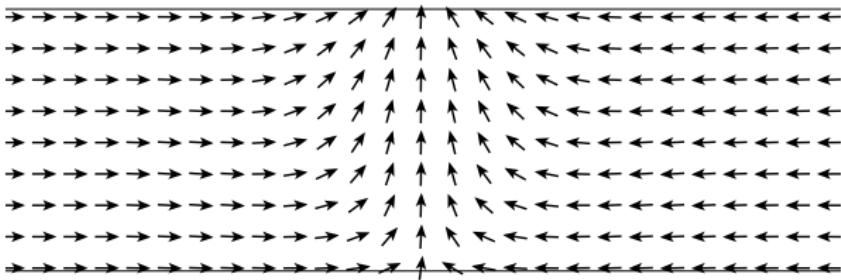
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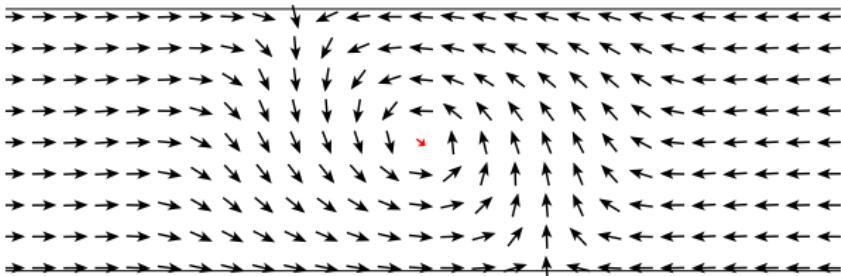
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# Head-to-head domain wall types



Transverse wall



Vortex wall

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# Head-to-head phase diagram

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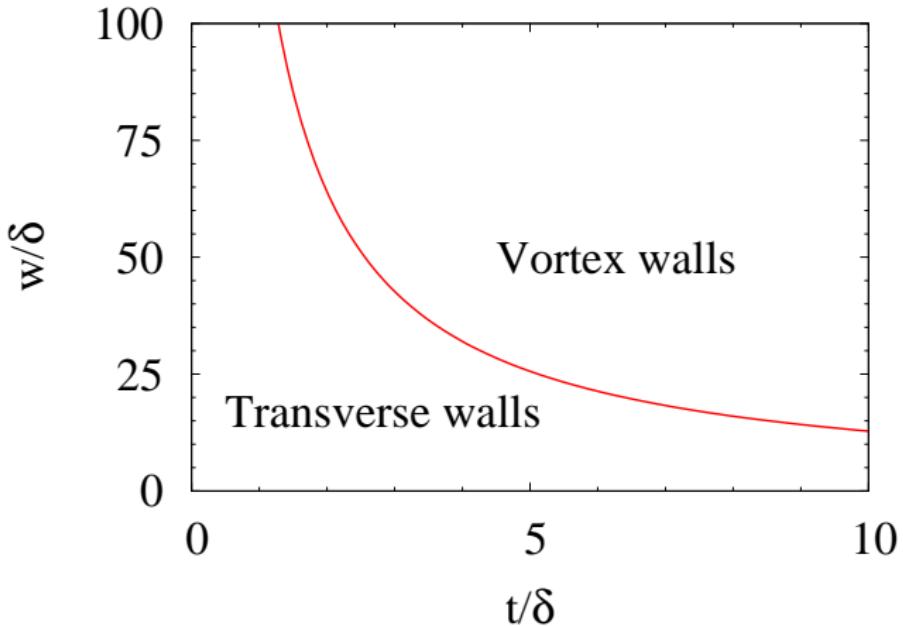
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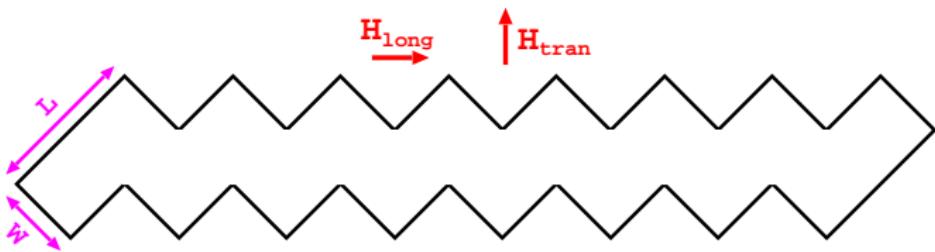
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R.D. McMichael & M.J. Donahue, *IEEE Trans. Magn.*, **33**, 4167 (1997).

# Size effect study



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

$W = 0.5 L$

Thickness = 20 nm

Py material parameters:

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

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

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

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# Size effect study (remanent state)

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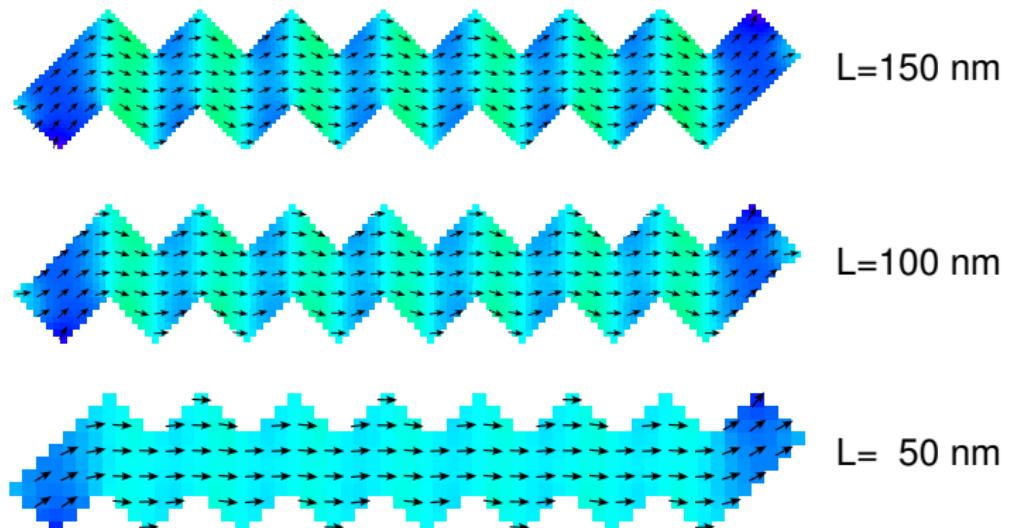
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FCS da Silva, WC Uhlig, AB Kos, S Schima, J Aumentado, J Unguris & DP Pappas, "Zigzag-shaped magnetic sensors," *APL*, **85**, 6025, (2004).

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

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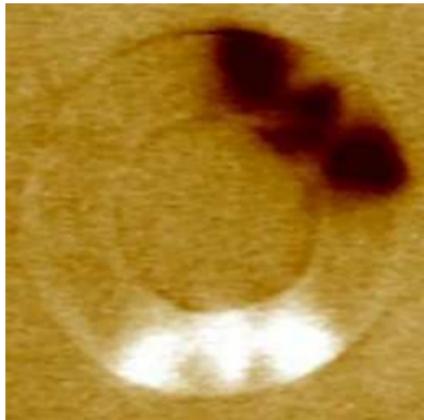
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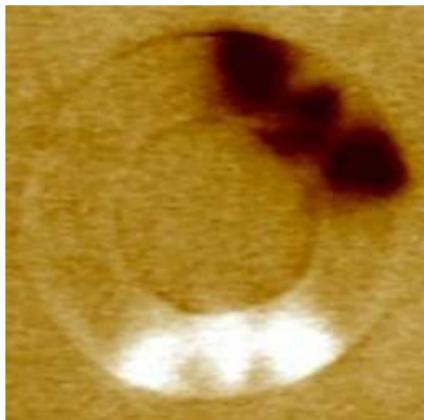


MFM image

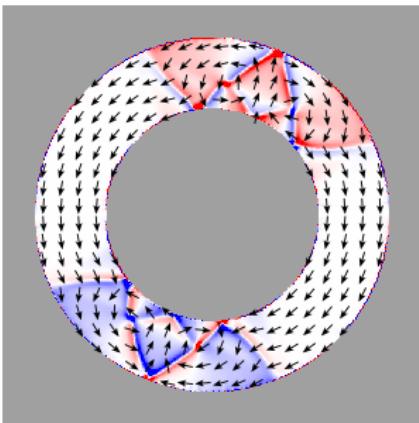
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MH Park, YK Hong, BC Choi, MJ Donahue, H Han & SH Gee, "Vortex head-to-head domain walls and their formation in onion-state ring elements," *Phys. Rev. B*, **73**, 094424 (2006).

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



MFM image



Simulation,  $\nabla \cdot M$

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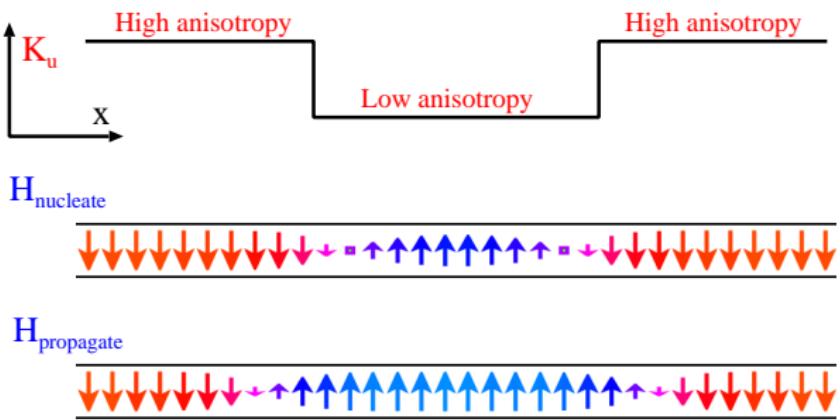
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MH Park, YK Hong, BC Choi, MJ Donahue, H Han & SH Gee, "Vortex head-to-head domain walls and their formation in onion-state ring elements," *Phys. Rev. B*, **73**, 094424 (2006).

## Pinning by simple defect (1D)



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

$$H_{\text{switch}} \geq H_{\text{u,bulk}}/5$$

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

# Brown's equations

## Energies:

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

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

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

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

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# Constraints

$\mathbf{M}$  is smooth

and

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

or equivalently

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

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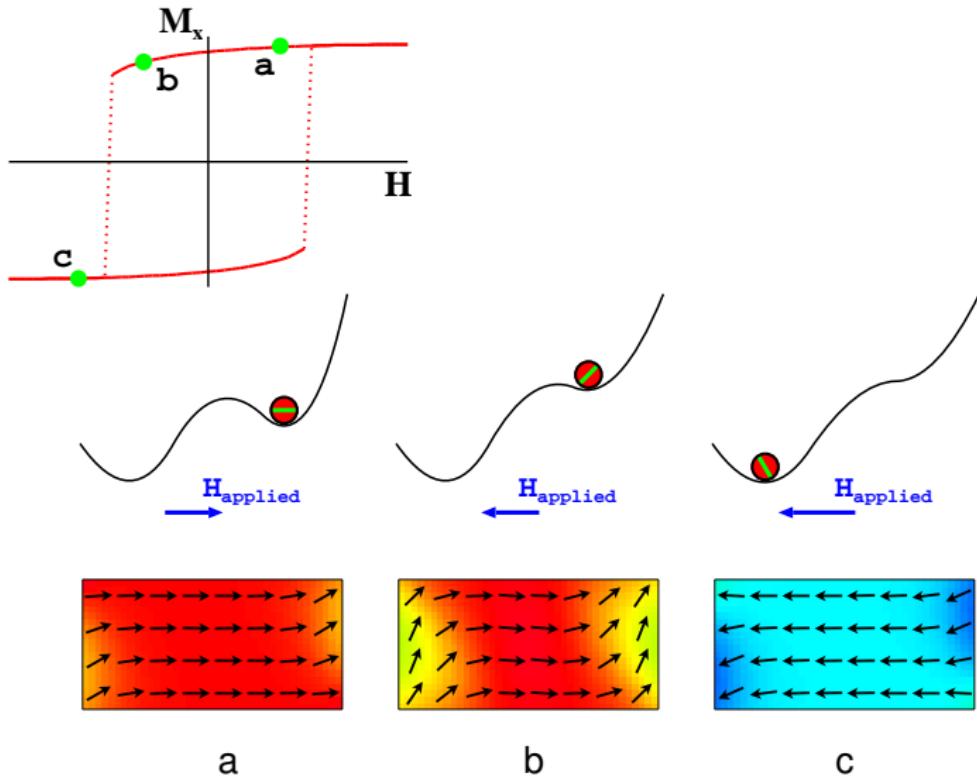
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# Quasi-static micromagnetics



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

where

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

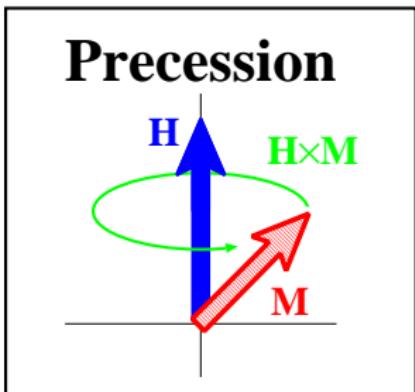
$\gamma_0$  = gyromagnetic ratio

$\alpha$  = damping coefficient

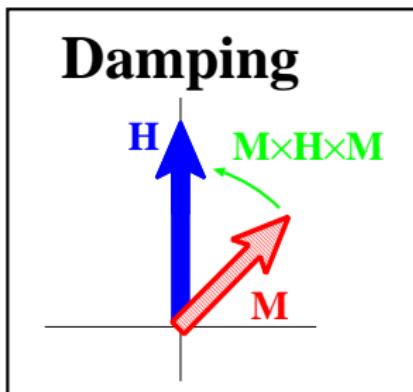
# Magnetization dynamics

## 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

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

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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

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

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

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

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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:

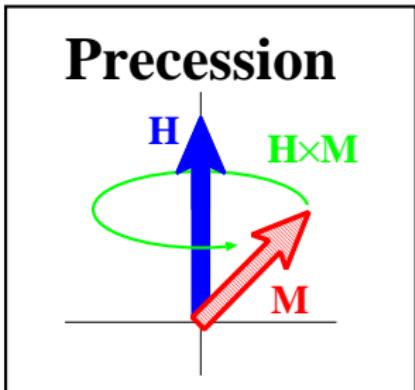
$$\frac{d\mathbf{M}}{dt} = |\gamma_0| \mathbf{H}_{\text{eff}} \times \mathbf{M} + \frac{\alpha}{M_s} \left( \mathbf{M} \times \frac{d\mathbf{M}}{dt} \right)$$

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

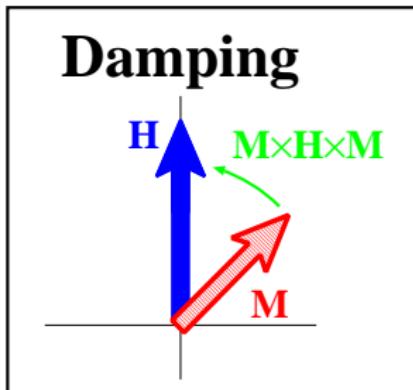
# Magnetization dynamics

## 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

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

as

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

**Discretized form:** If

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

then

$$\frac{\delta E}{\delta \mathbf{M}} \Big|_{x_k} \approx \frac{\partial E}{\partial \mathbf{M}_k} \cdot \frac{1}{\|\phi_k\|_1}$$

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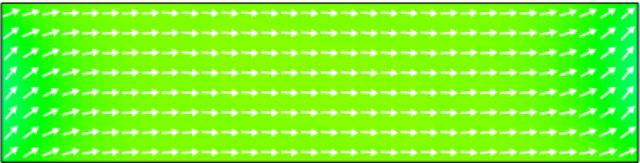
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# Magnetization dynamics

Time

0 ps

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



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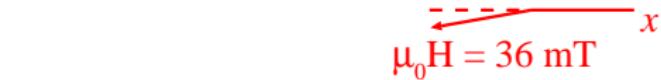
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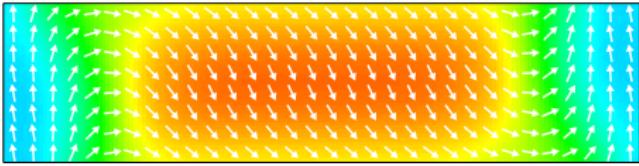
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Time

0 ps



100 ps



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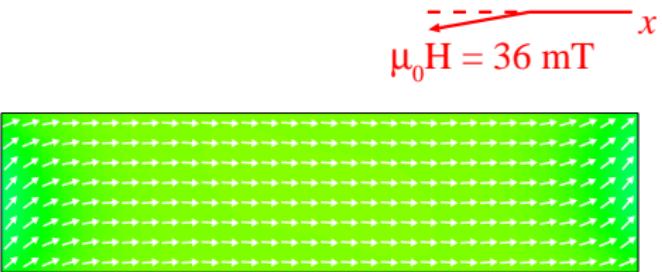
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Micromagnetics

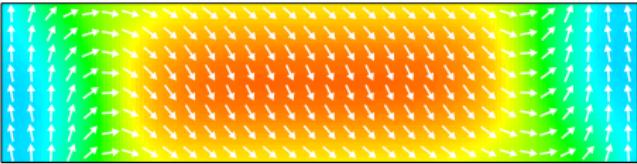
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Time

0 ps



100 ps



150 ps



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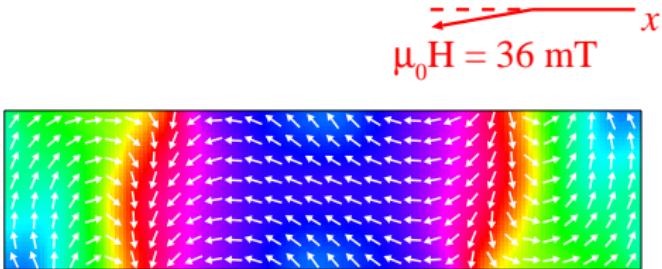
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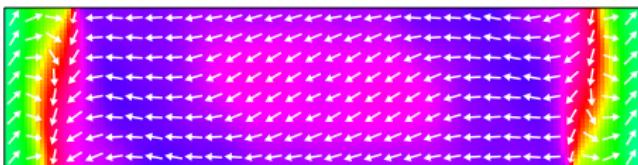
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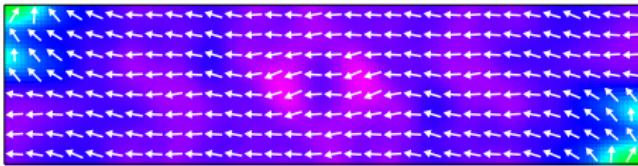
350 ps



450 ps



750 ps



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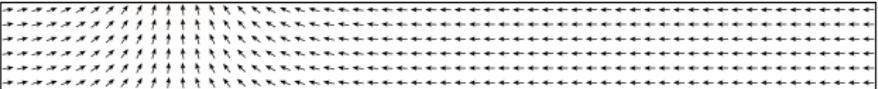
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RD McMichael, MJ Donahue, DG Porter & J Eicke, "Switching dynamics and critical behavior of standard problem no. 4," *JAP*, **89**, 7603 (2001).

# Thin film simulation

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

0 ps

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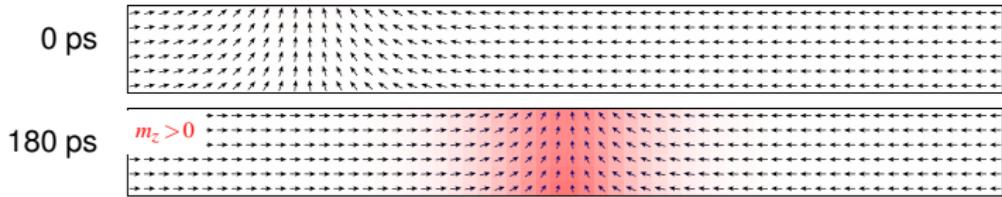
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$$\mu_0 \mathbf{H} = 25 \text{ mT} \rightarrow$$



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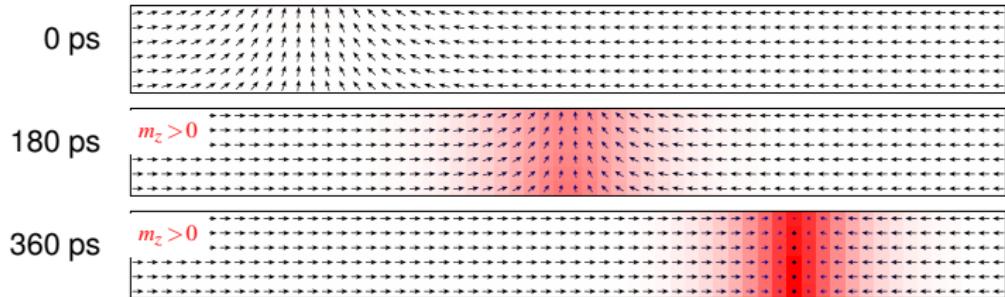
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$$\mu_0 \mathbf{H} = 25 \text{ mT} \rightarrow$$



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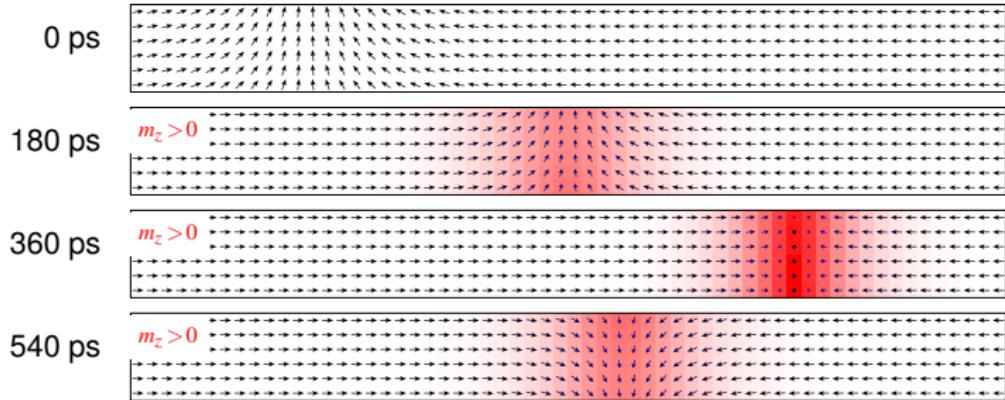
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# Thin film simulation

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



Background

Pitfalls

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

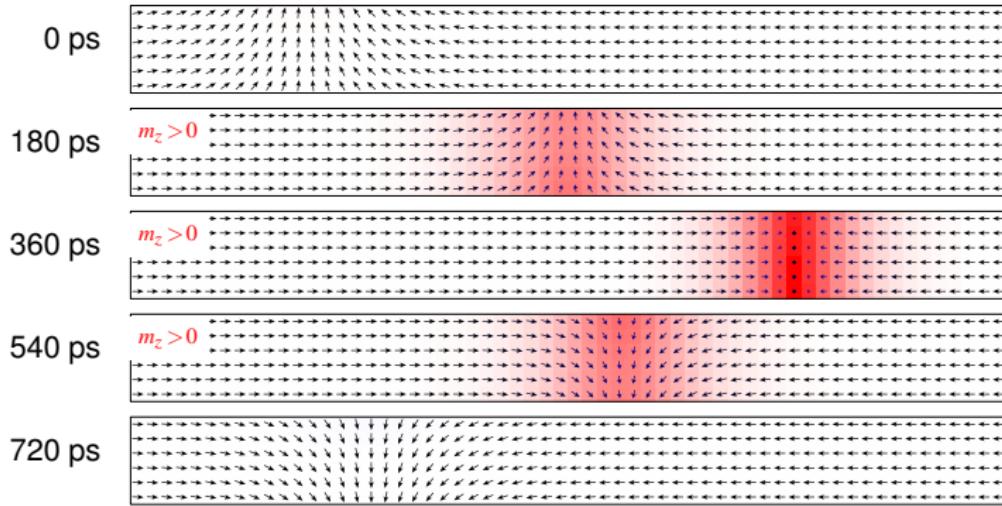
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# Thin film simulation

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



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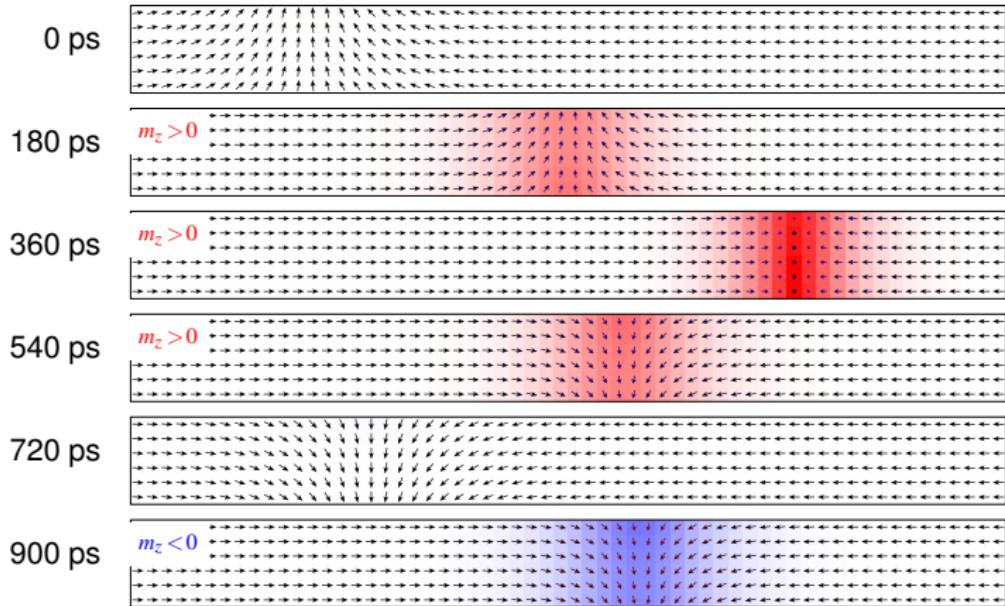
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$$\mu_0 \mathbf{H} = 25 \text{ mT} \rightarrow$$



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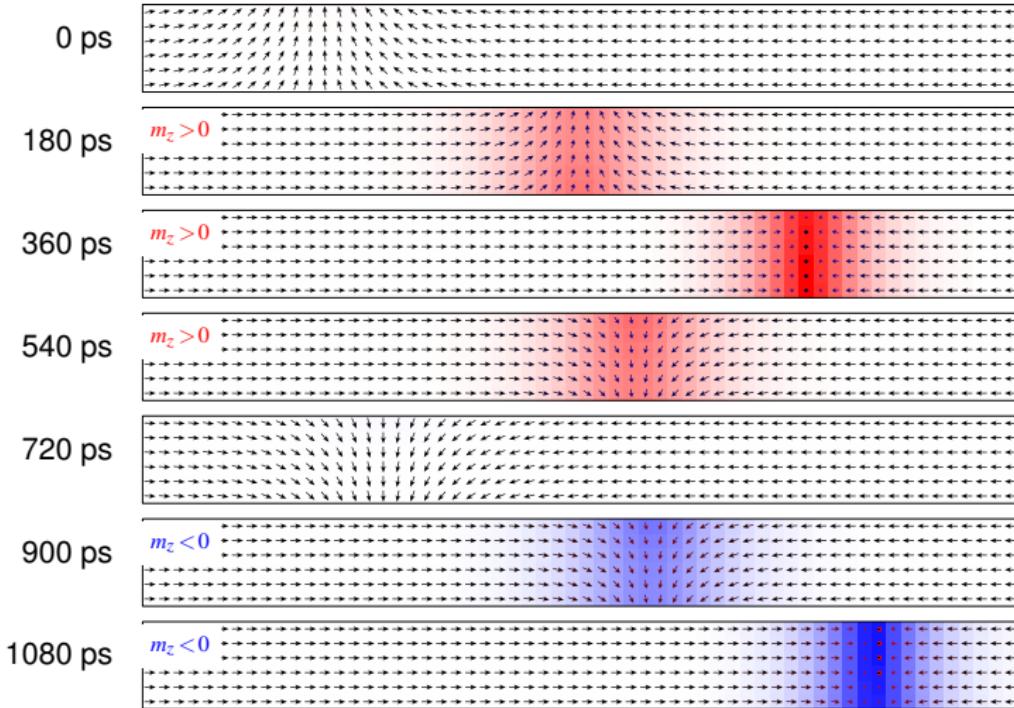
Advanced Topics

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# Thin film simulation

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



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

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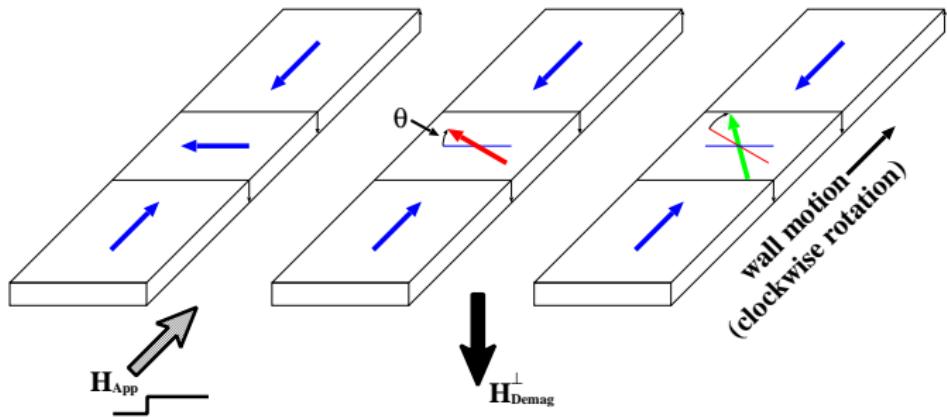
Spin Torque

Fast hardware

OOMMF extensions

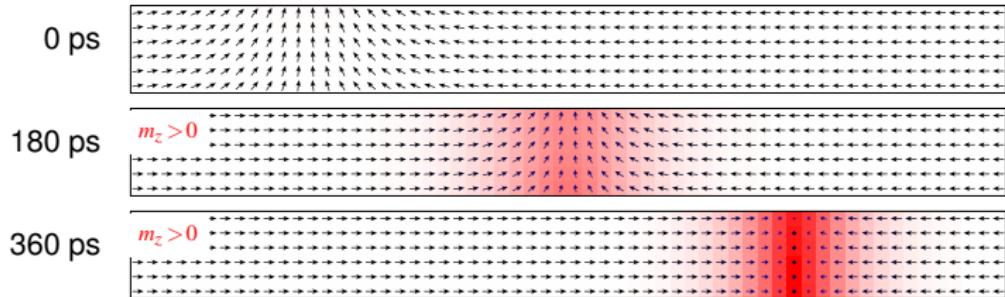
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# Thin film simulation

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



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

Micromagnets

M.J. Donahue

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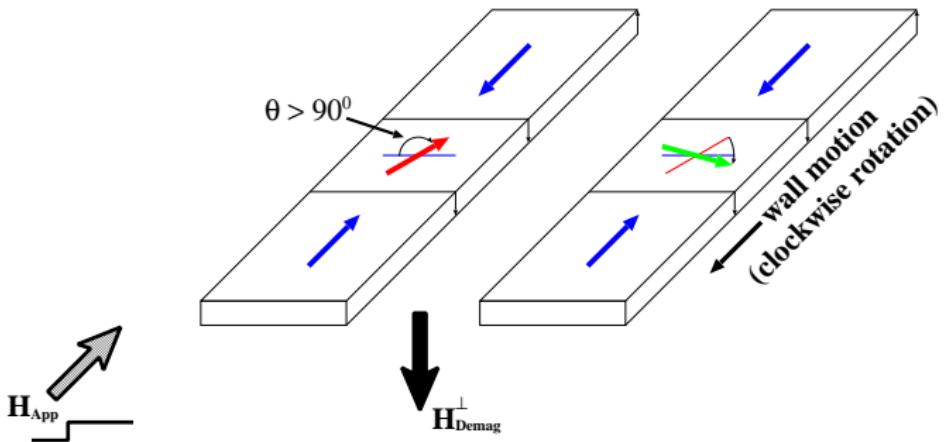
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# Thin film wall dynamics, $m_z \leq 0$

Micromagnets

M.J. Donahue

Background

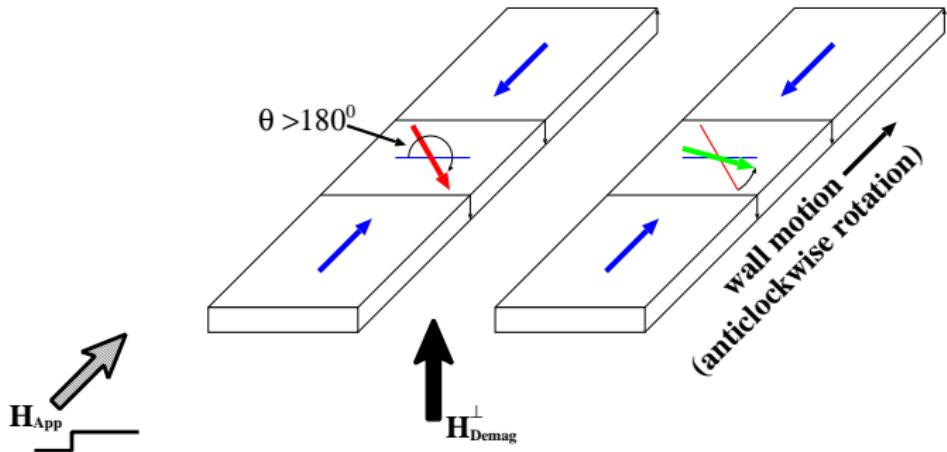
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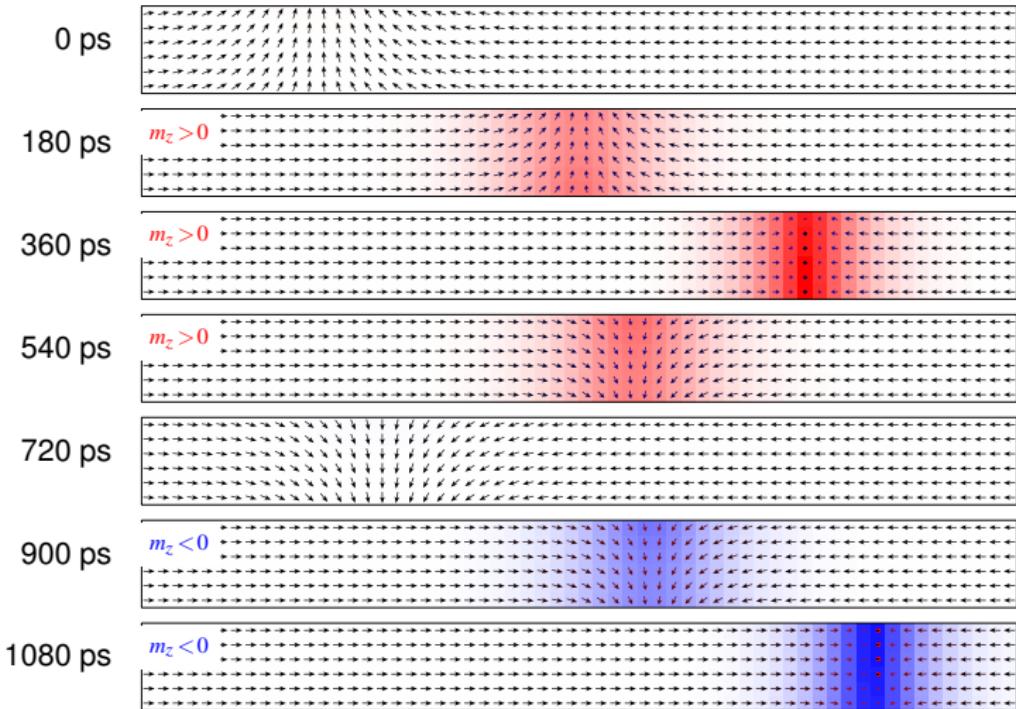
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# Thin film simulation

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



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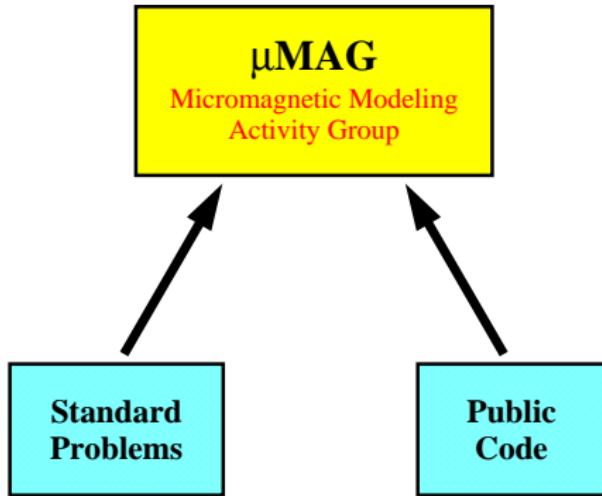
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### Recommendations

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



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Center for Theoretical and Computational Materials Science

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

See also the mailing list and archives!

# $\mu$ MAG standard problems

Micromagnetics

M.J. Donahue

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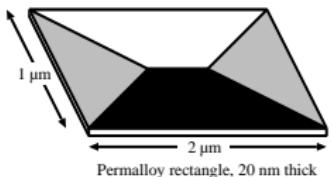
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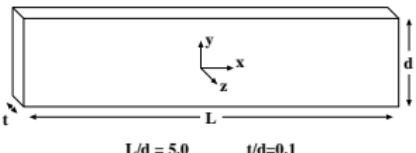
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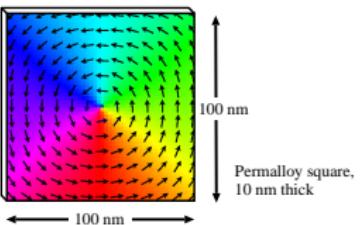
#### Problem 1: Hysteresis



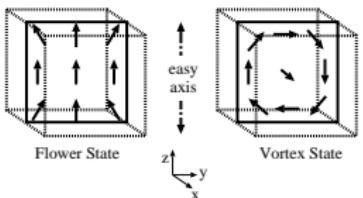
#### Problem 2: Hysteresis



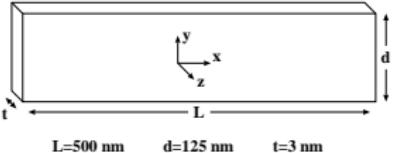
#### Problem 5: CIP Spin Torque



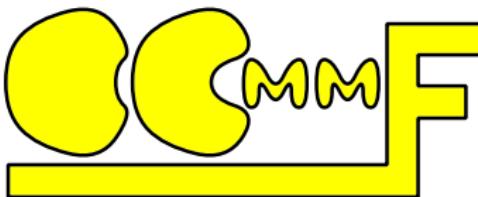
#### Problem 3: Energy Minimization



#### Problem 4: Dynamics



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



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

Primary developers: Don Porter, Mike Donahue (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.

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# 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!

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# Finite Difference

vs.

# Finite Element

Micromagnetics

M.J. Donahue

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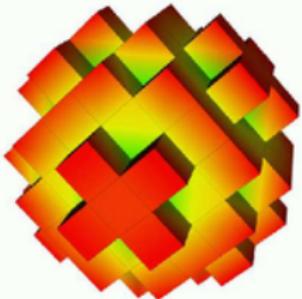
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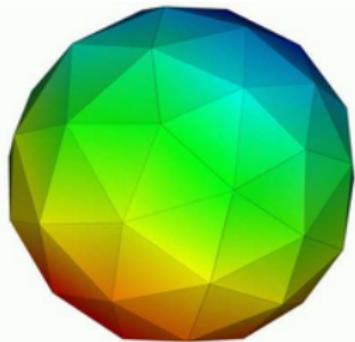
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Recommendations



- ▶ 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).

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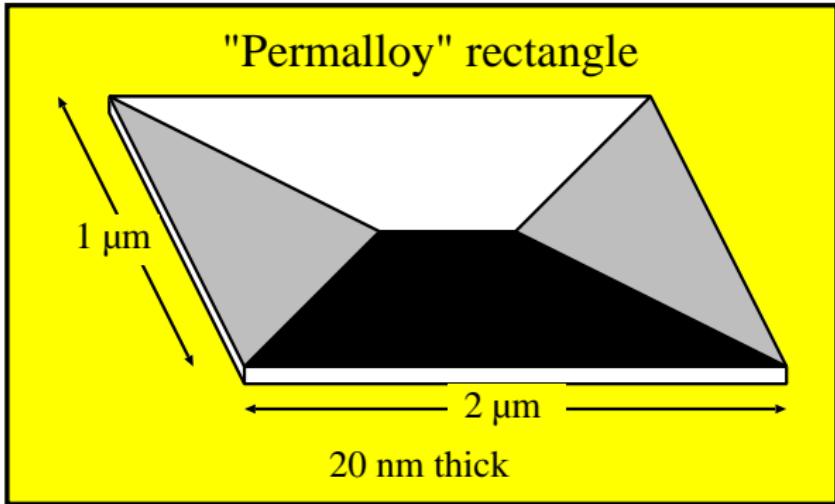
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Task: Run this through a hysteresis loop.

# $\mu$ MAG standard problem 1: results

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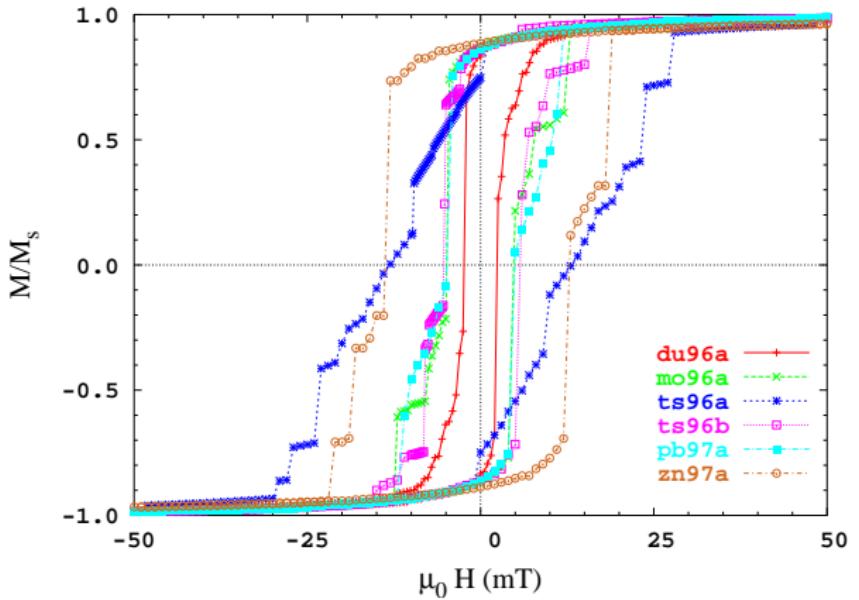
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Problem: ???

# $\mu$ MAG standard problem 1: results

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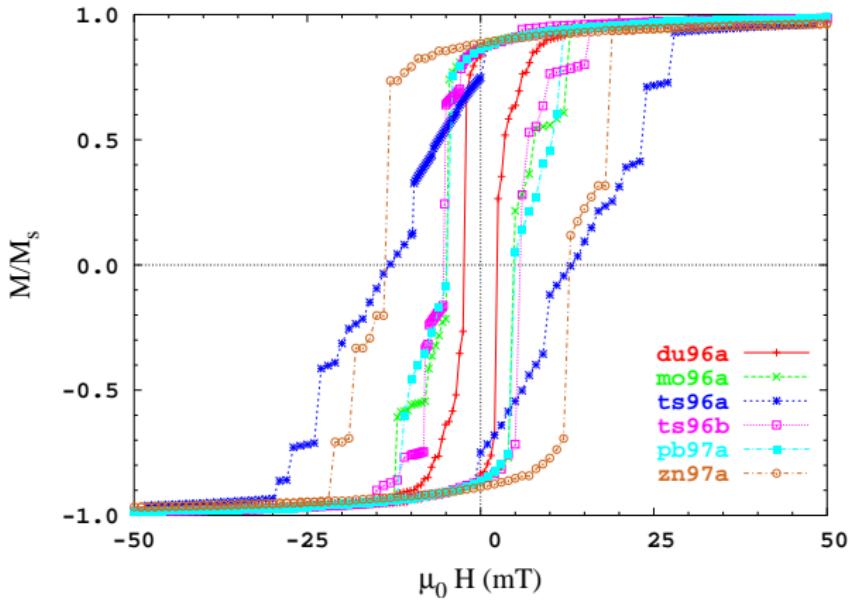
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Problem: Meshes were too coarse!

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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"

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

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

# Example $\ell_{\text{ex}}$ values

Material	$M_s$ (kA/m)	K (kJ/m <sup>3</sup> )	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 <sub>2</sub> Fe <sub>14</sub> B	1280	4500	13	1.7	3.6

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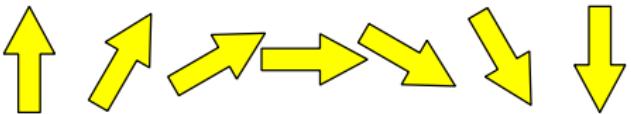
## Recommendations

Bloch wall



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

Néel wall



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

# Bloch wall discretization

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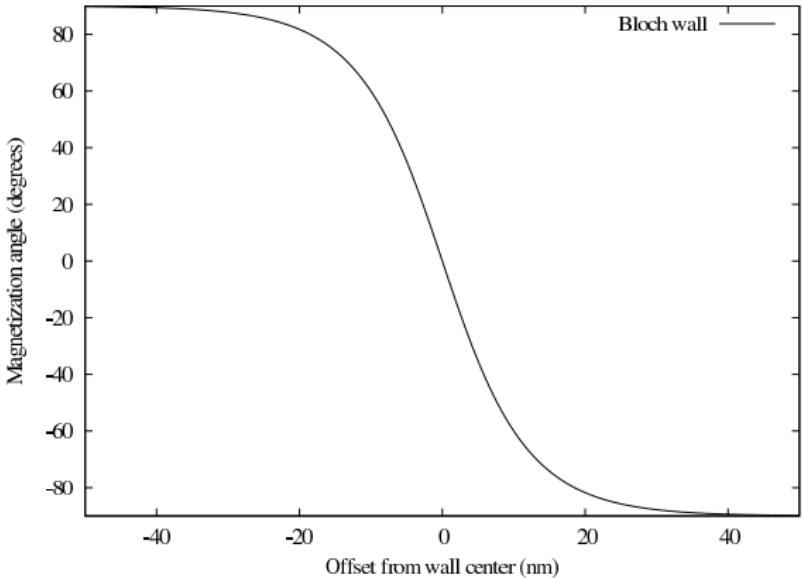
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# Bloch wall discretization

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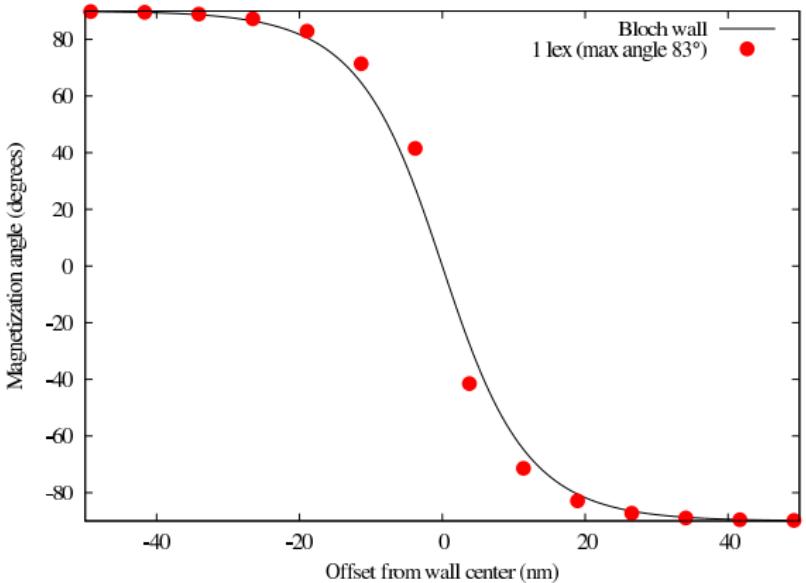
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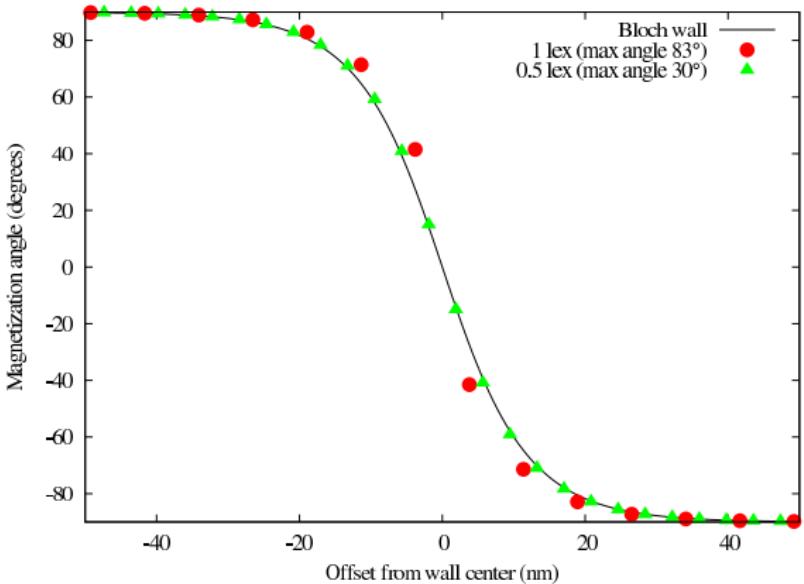
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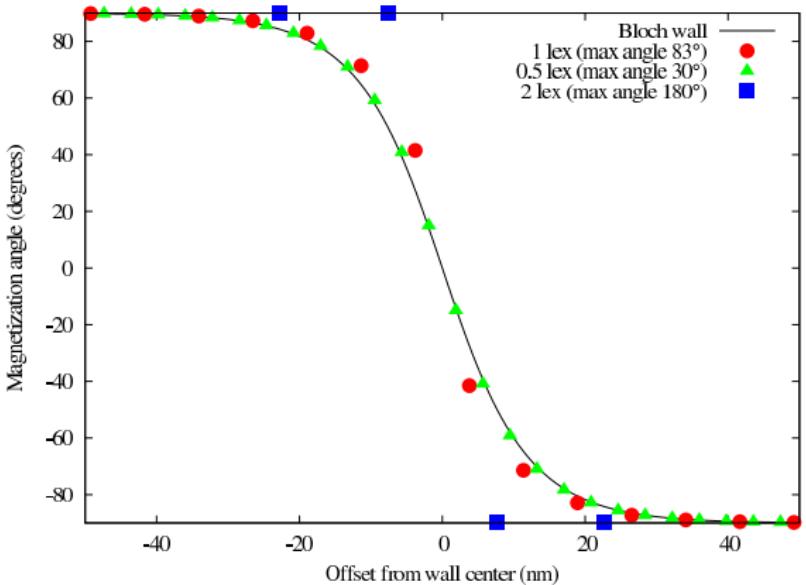
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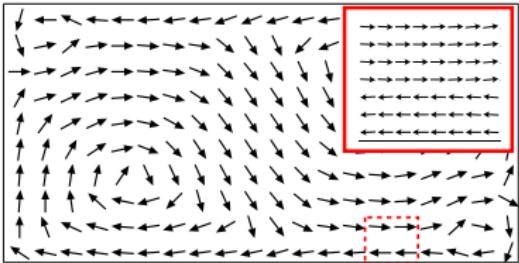
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# Néel wall collapse



25 nm cells

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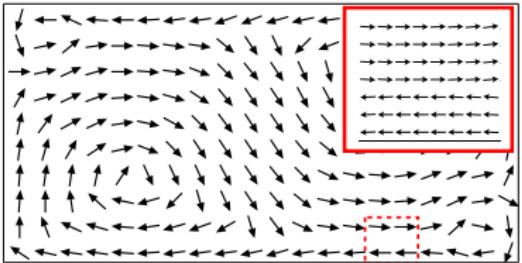
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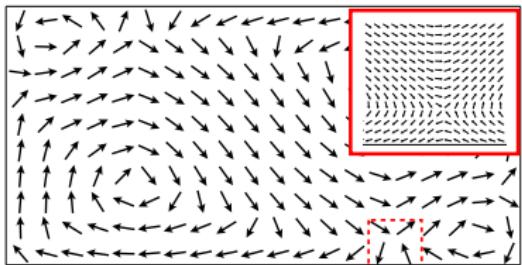
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# Néel wall collapse



25 nm cells



12.5 nm cells

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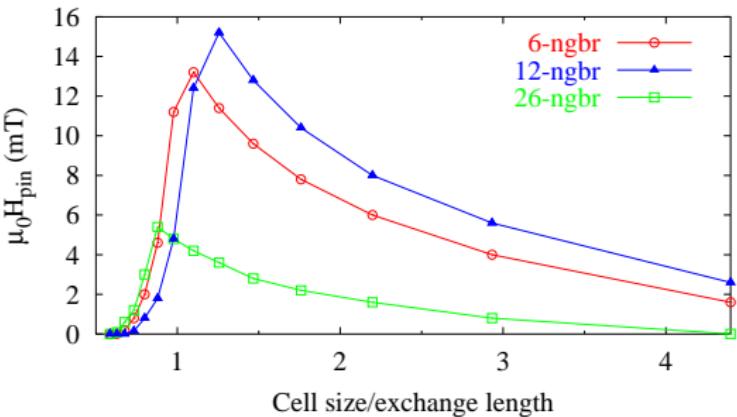
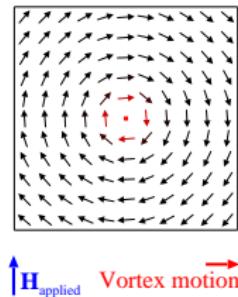
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## Recommendations

## Vortex mobility



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

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

# Cell size recommendations

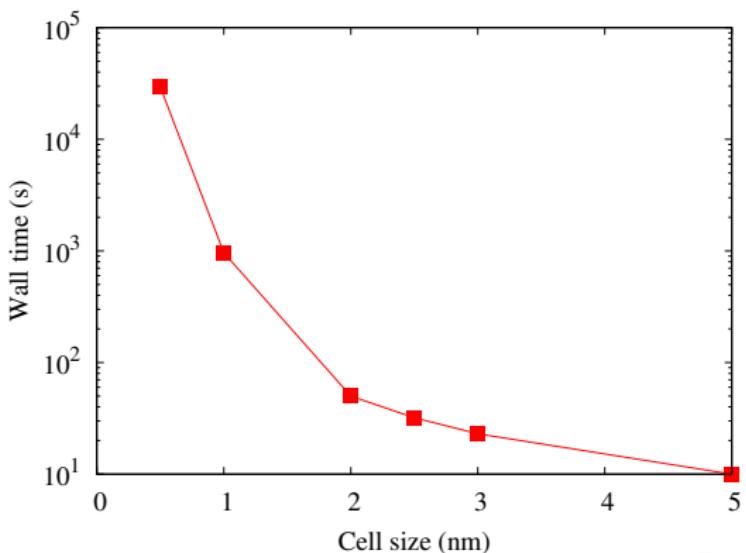
- ▶ Don't mesh coarser than  $\ell_{\text{ex}}$
- ▶ Check max neighbor angle: under  $30^\circ$  is usually reliable, over  $90^\circ$  is questionable,  $180^\circ$  is bogus.
- ▶ Run at multiple discretizations and check for convergence (if possible!)

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# 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



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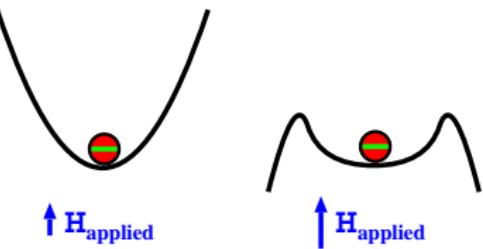
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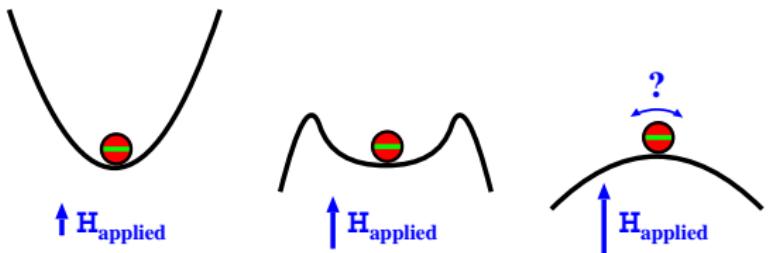
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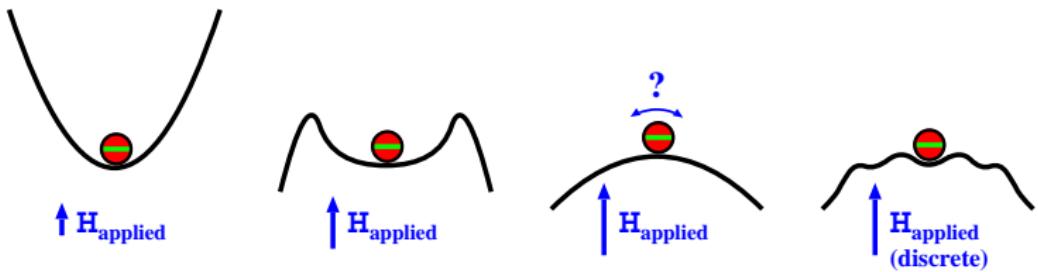
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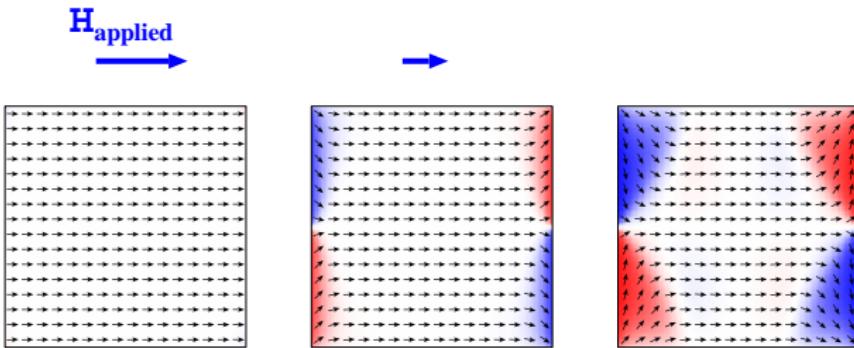
Recommendations



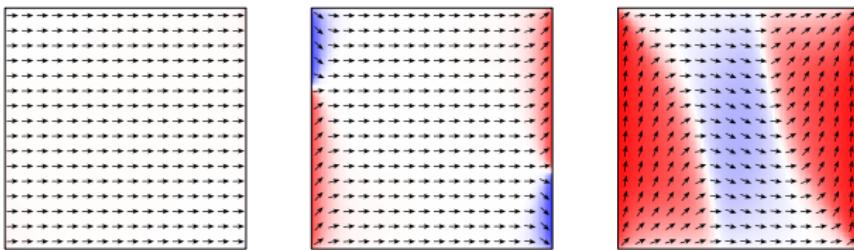
- Discretization introduces (false) divots
- Maximum replaced by saddle in higher dimensions

# Symmetry breaking

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



$H_{\text{applied}}$   
1° off-axis



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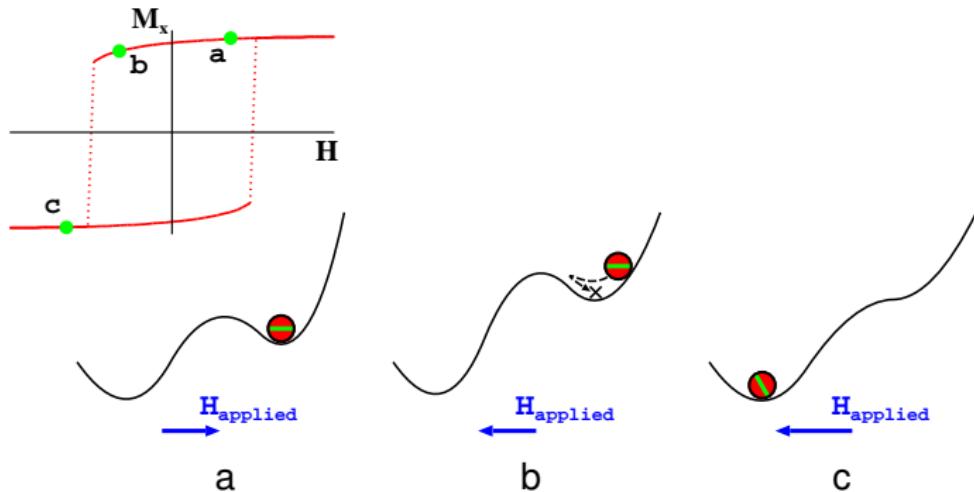
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Big field steps  $\Rightarrow$  premature switching

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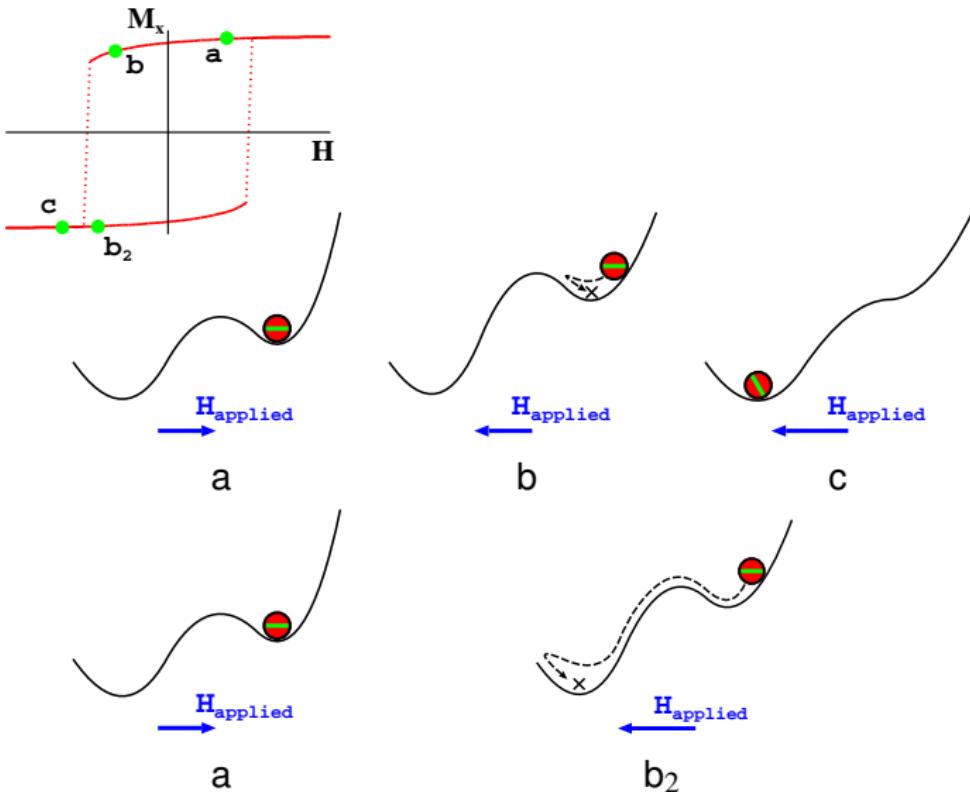
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Big field steps  $\Rightarrow$  premature switching

# Stopping too soon

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



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# Stopping too soon

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



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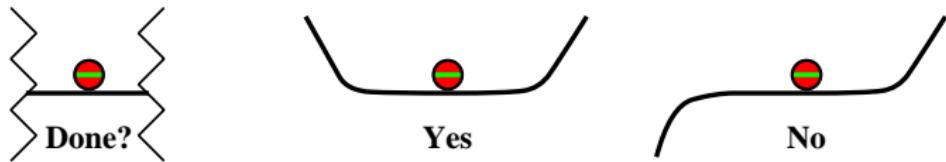
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# Stopping too soon

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



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# LLG vs. Conjugate Gradient

Micromagnets

M.J. Donahue

Standard problem 3 (energy minimization):

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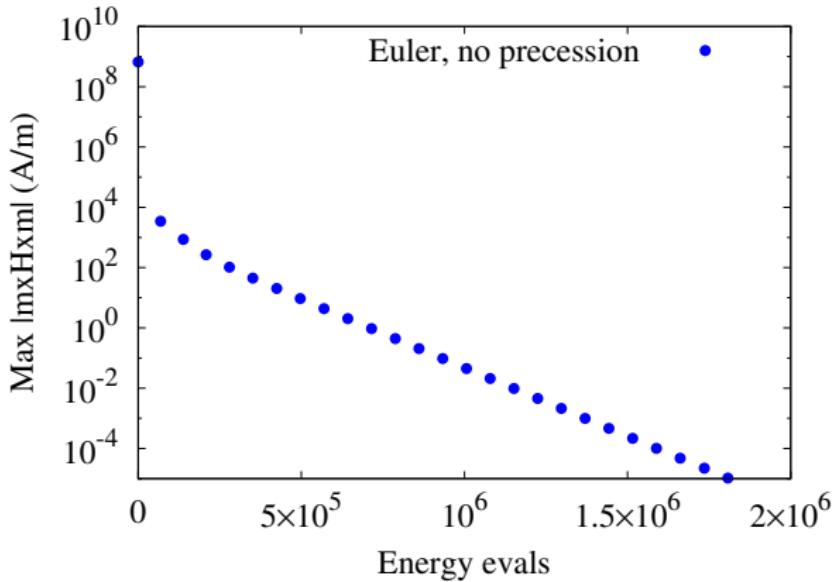
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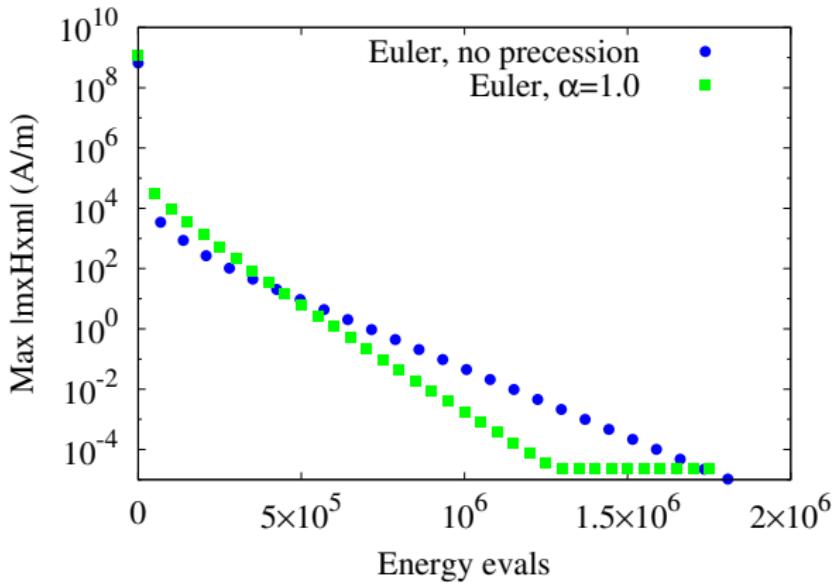
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# LLG vs. Conjugate Gradient

Standard problem 3 (energy minimization):



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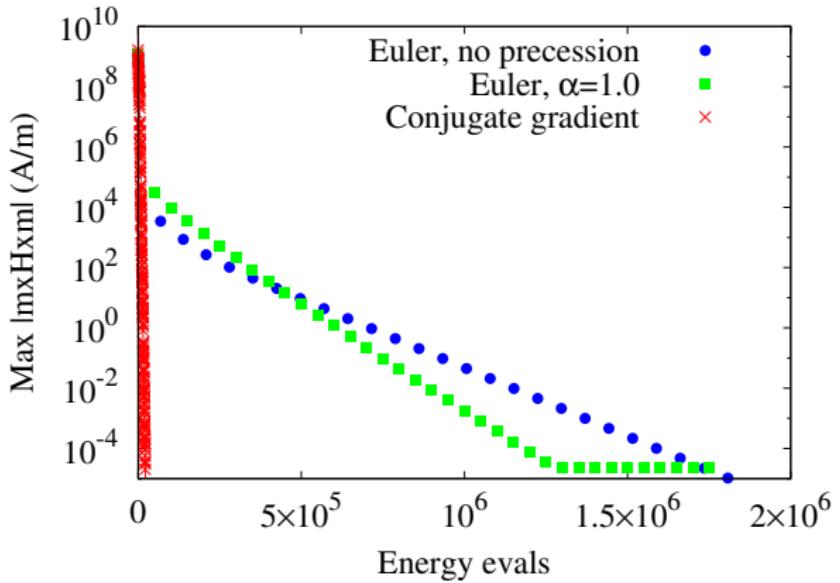
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# LLG vs. Conjugate Gradient

Standard problem 3 (energy minimization):



- ▶ Use the right tool for the job!

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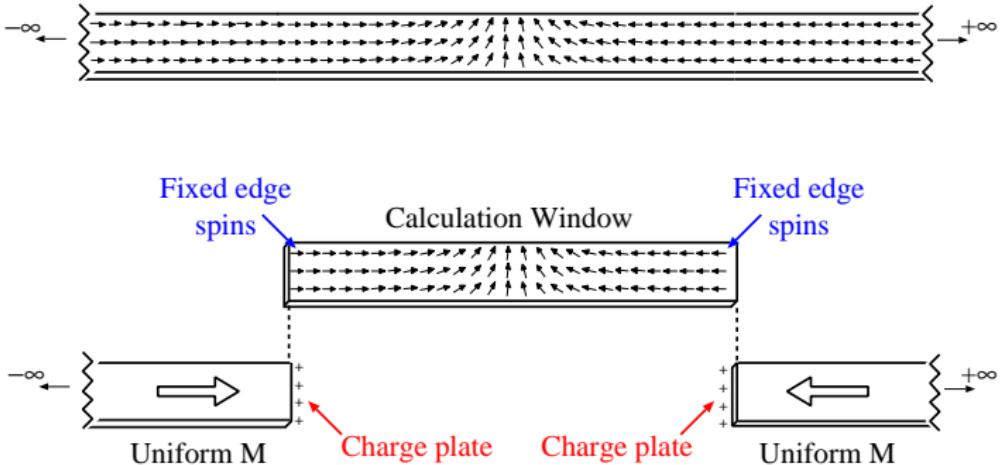
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## Infinite strips

## Extended volumes

## Recommendations



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

## Background

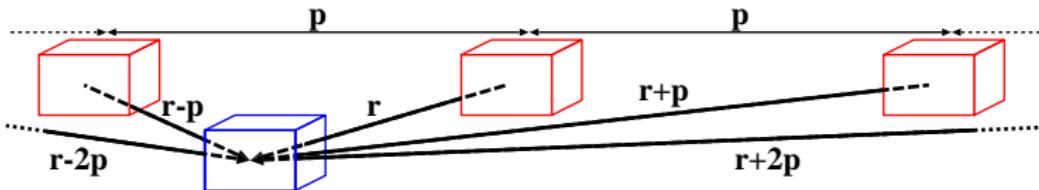
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$$\mathbf{H}_{\text{demag}} = \sum_{k=-\infty}^{\infty} N(\mathbf{r} + k\mathbf{p}) \mathbf{M} = N^{pb} \mathbf{M}$$

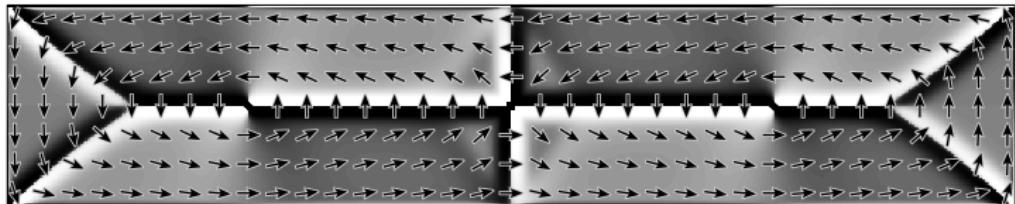
where

$\mathbf{p}$  := 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:  $500 \ell_{\text{ex}} \times 100 \ell_{\text{ex}} \times 6 \ell_{\text{ex}}$

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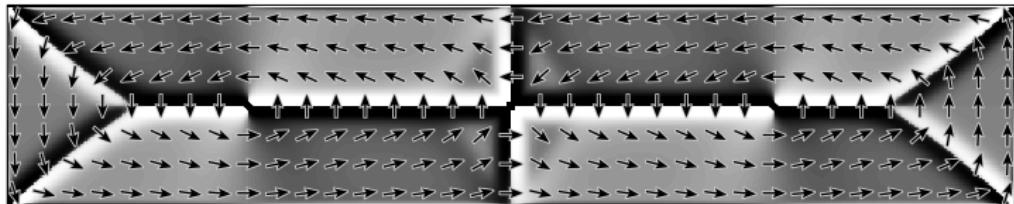
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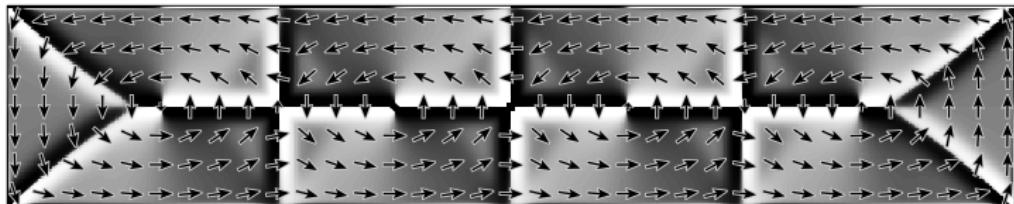
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M J Donahue, "Micromagnetic investigation of periodic cross-tie/vortex wall geometry," *Advances in Condensed Matter Physics*, **2012** (2012).

# Cross-tie walls



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



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### Recommendations

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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.

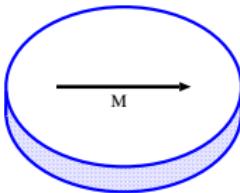
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# Multi-dimension periodic

- ▶ 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.



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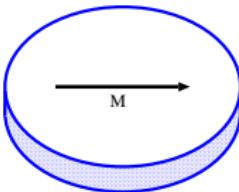
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# Multi-dimension periodic

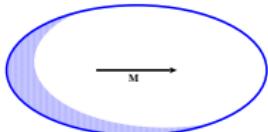
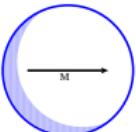
- ▶ 1D periodic: tail sum  $\sim \int_{R_2}^{\infty} 1/x^3 dx < \infty$   
 $\Rightarrow$  boundary doesn't matter.



- ▶ 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.



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# FMR simulations

Micromagnetics

M.J. Donahue

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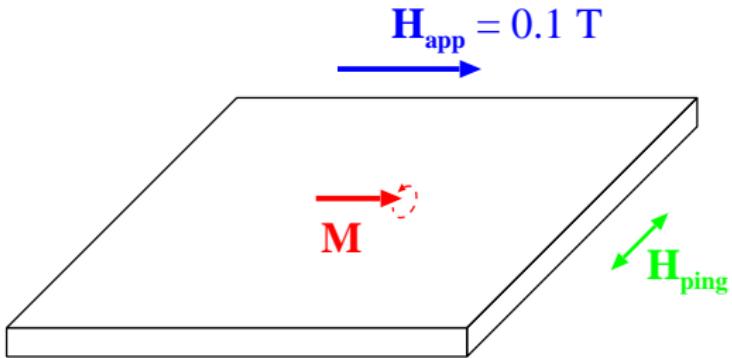
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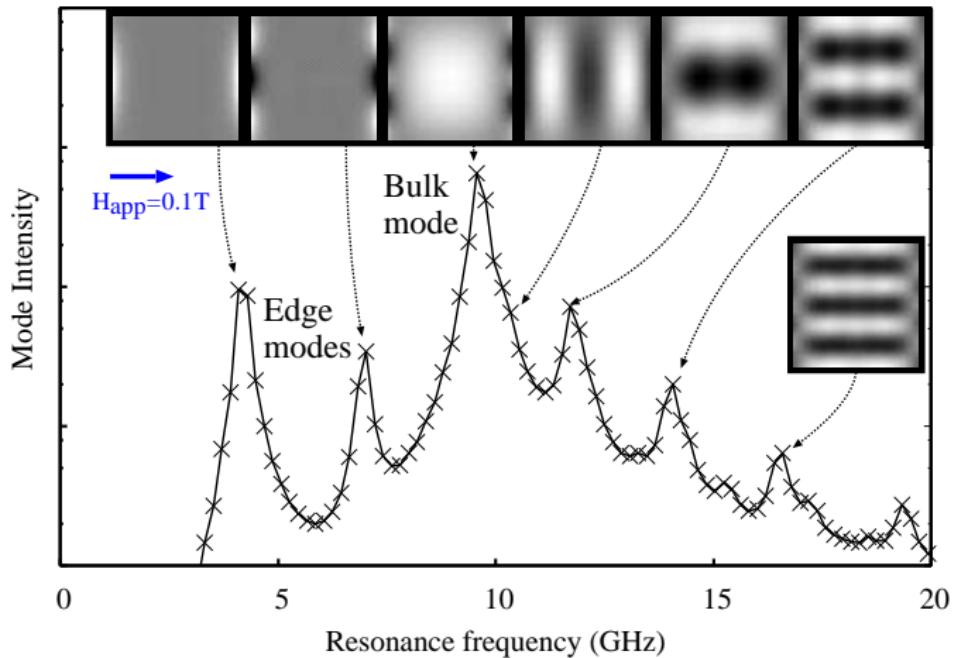
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Small “ping” field induces spinwaves.

# FMR spectra



Background

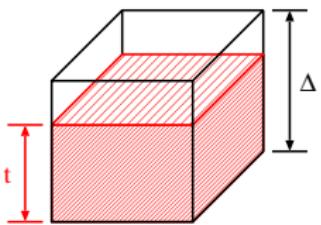
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Partially filled cell,  
height= $t$ ,  $|\mathbf{M}|=M_s$

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

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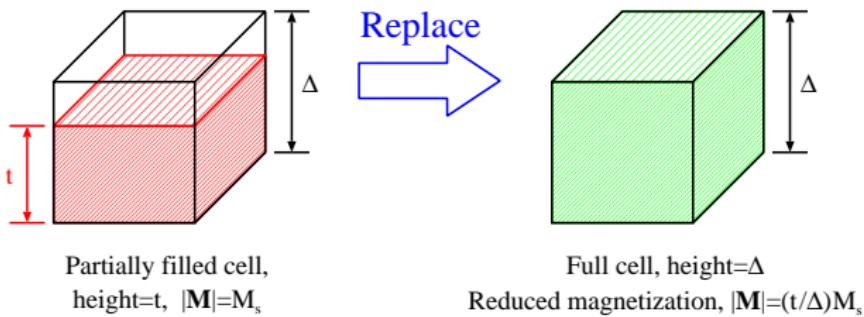
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DG Porter & MJ Donahue, *JAP*, **89**, 7257 (2001).

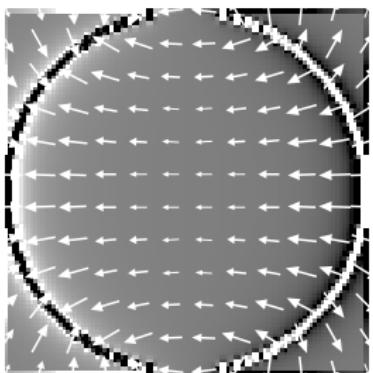
H Min, RD McMichael, MJ Donahue, J Miltat & MD Stiles, *PRL*, **104**, 217201  
(2010).

# Sub-cell thickness variation

Micromagnetics

M.J. Donahue

10x10x1disk



Non-uniform demag field

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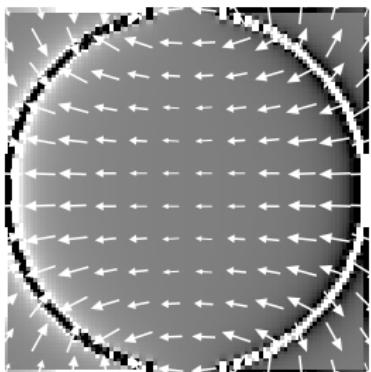
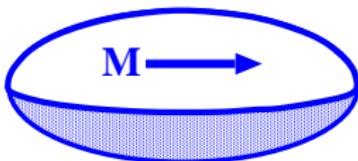
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# Sub-cell thickness variation

10x10x1disk



10x10x1 oblate spheroid



Non-uniform demag field

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# Sub-cell thickness variation

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M.J. Donahue

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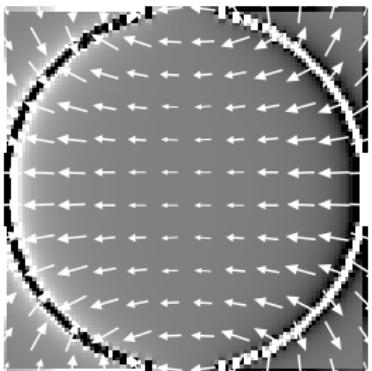
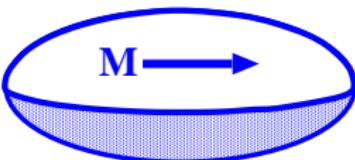
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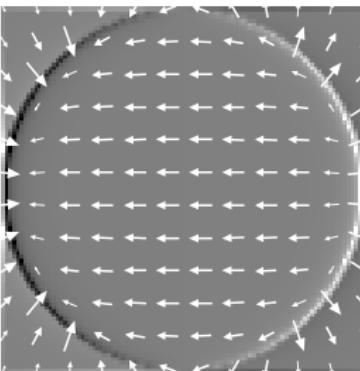
10x10x1disk



10x10x1 oblate spheroid



Non-uniform demag field



Almost uniform demag field

# Edge mode test

Micromagnetics

M.J. Donahue

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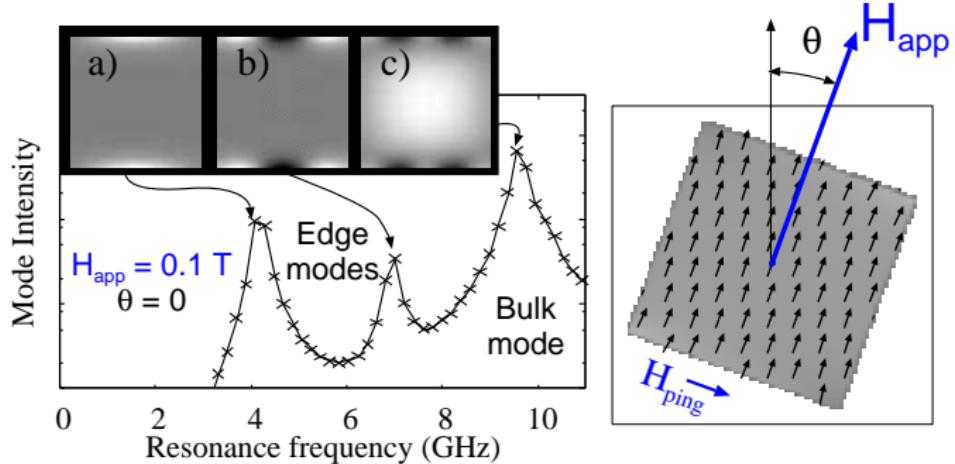
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# Staircase correction

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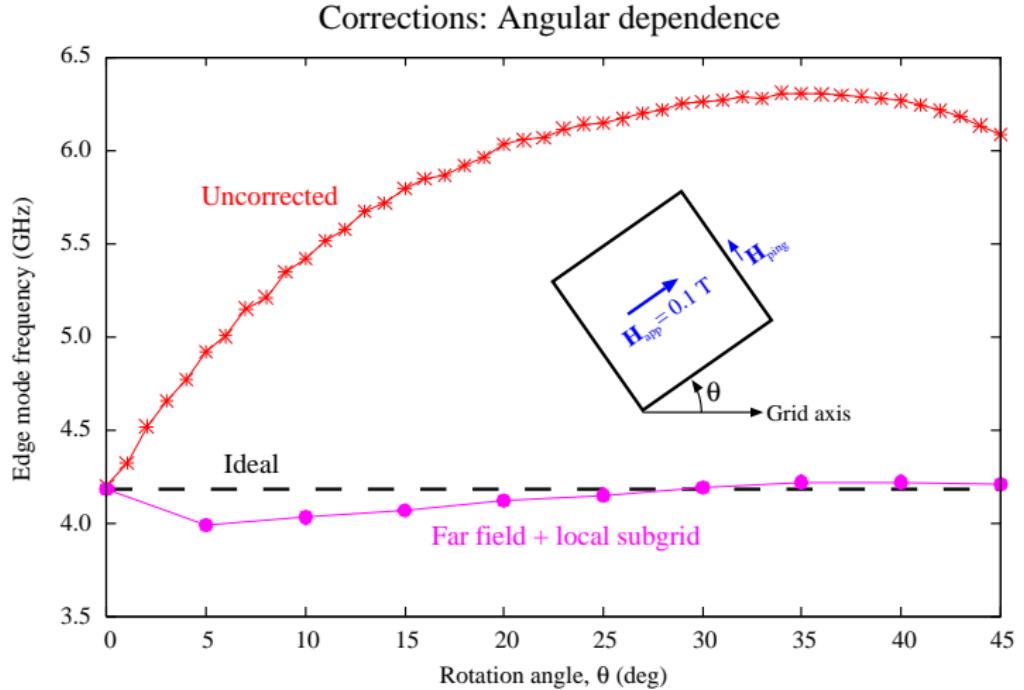
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MJ Donahue & RD McMichael, "Micromagnetics on curved geometries using rectangular cells: error correction and analysis," *IEEE Trans. Magn.*, **43**, 2878 (2007).

# 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  $\mathbf{H}_{\text{th}}$  is Gaussian random process s.t.

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

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

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

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# 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  $\boldsymbol{\eta}^{\perp}, \boldsymbol{\eta}^{\parallel}$ ,  $\langle \boldsymbol{\eta}_i^{\parallel}, \boldsymbol{\eta}_j^{\perp} \rangle = 0$ ,

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

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

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# 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

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# 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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# Nudged elastic band

How to get through the mountains?



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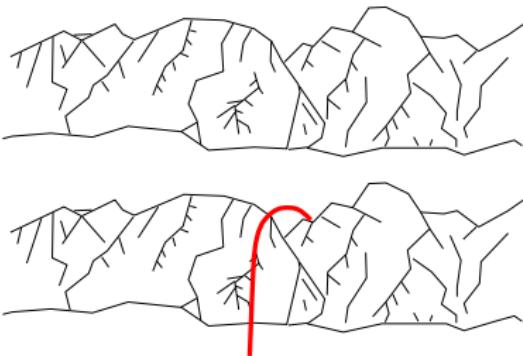
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# Nudged elastic band

How to get through the mountains?

Step 1: Throw a rope.



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# Nudged elastic band

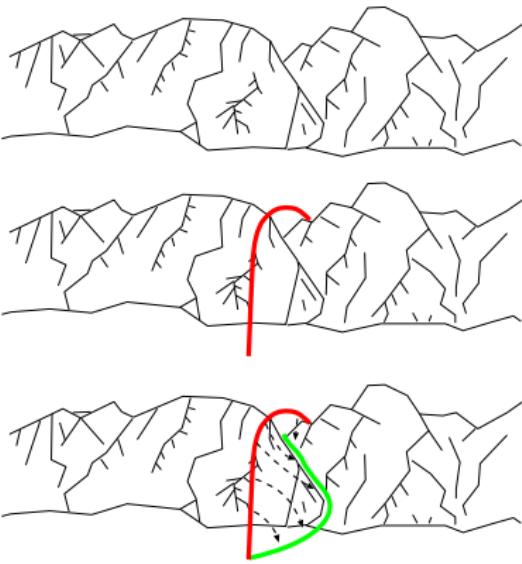
Micromagnetics

M.J. Donahue

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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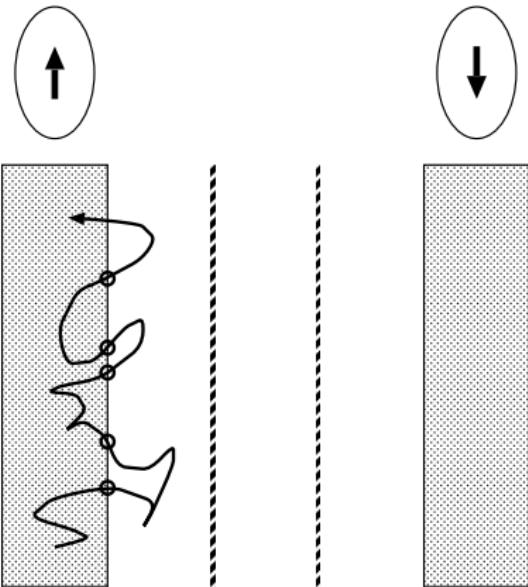
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# Forward flux sampling



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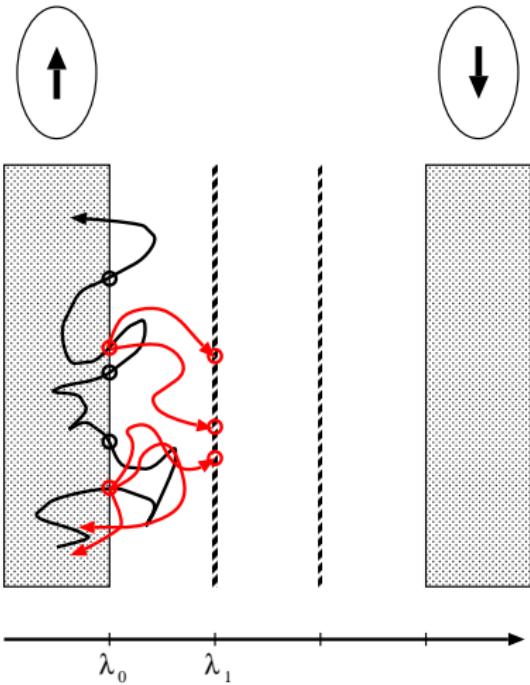
OOMMF extensions

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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).

# Forward flux sampling



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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

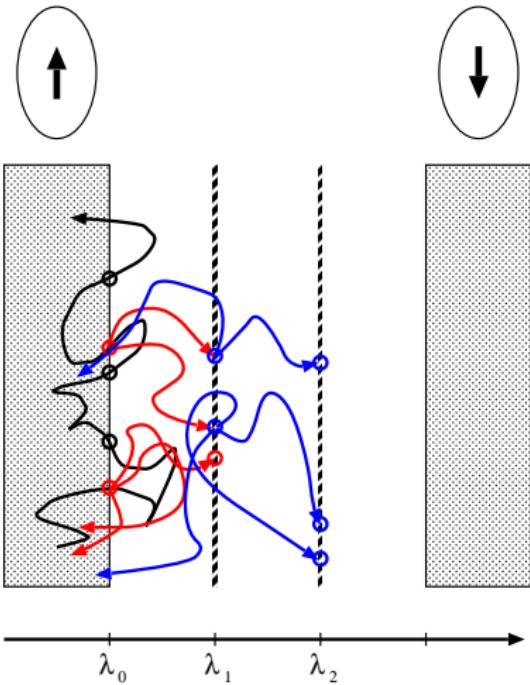
## Pitfalls

- Mesh size
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- Field step size
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- Fast hardware
- OOMMF extensions
- Movies

## Recommendations



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

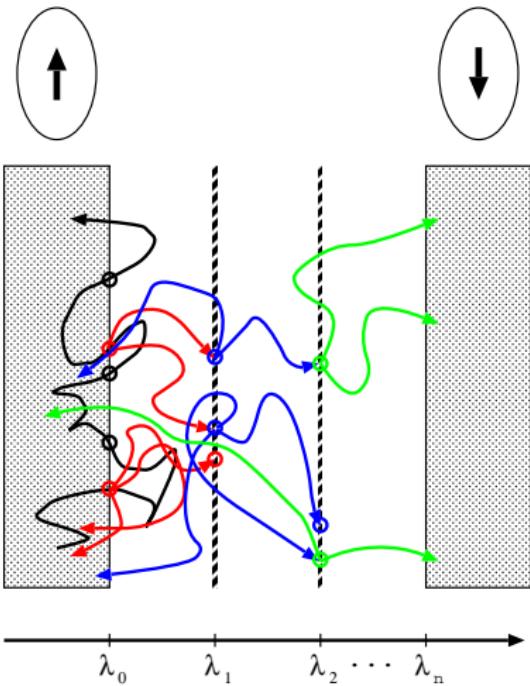
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## Recommendations



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# “Local” spin-torque

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

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  $\tau_{sf}$ , 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. Militat, "Domain wall dynamics under nonlocal spin-transfer torque," *PRL*, **108**, 227208 (2012).

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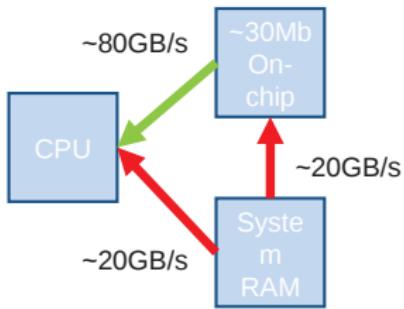
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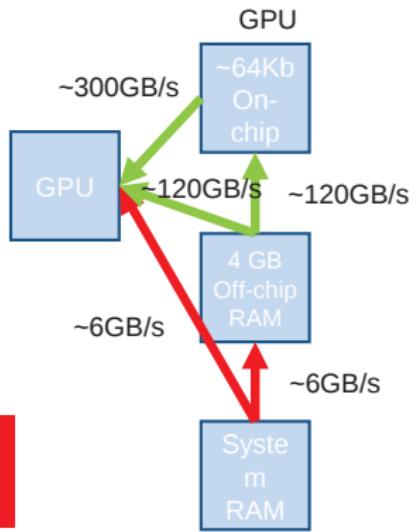


# Why GPU is awesome?

CPU



CPU has much higher chance to be memory throughput limited



GPU can transfer buffers during kernel execution

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Recommendations

Slide courtesy Mykola Dvornik.



# Why GPU is pain?

- 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)

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# 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.

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# Parallelization on CPU: 4 million spins

Micromagnets

M.J. Donahue

## Background

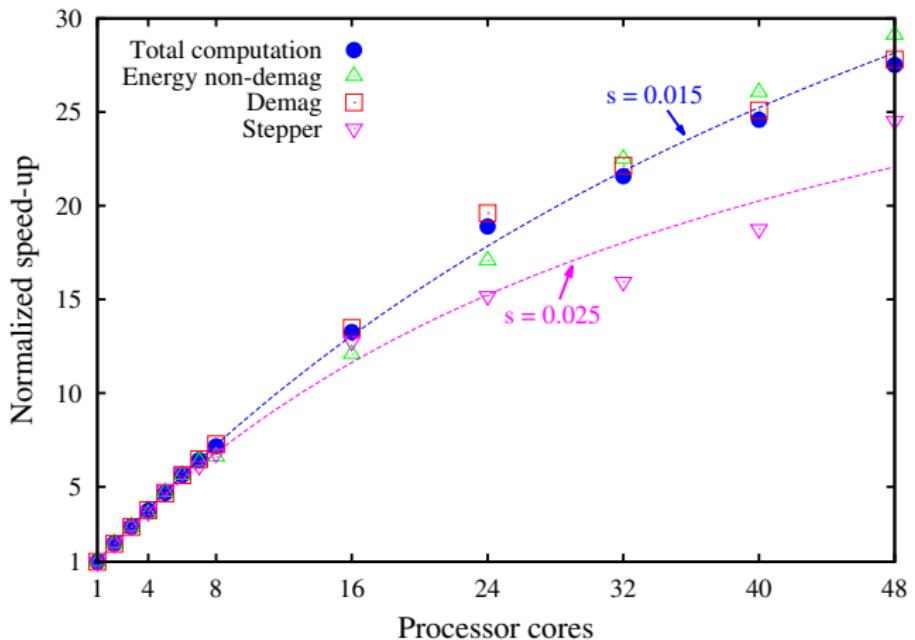
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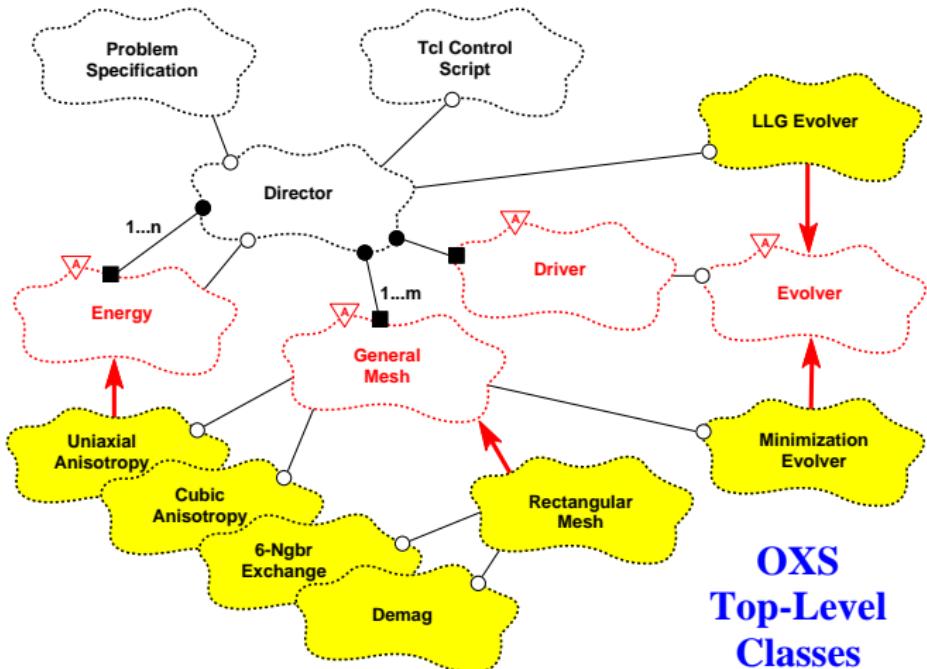
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### Recommendations



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

# OOMMF C++ class structure



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# 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.

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# Example extension: uniaxial anisotropy

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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  $\mathbf{u}$ .

# 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;
};
```

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# 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();  
}
```

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# 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;
        }
    }
}
```

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# Remanent magnetization configuration

Micromagnetics

M.J. Donahue

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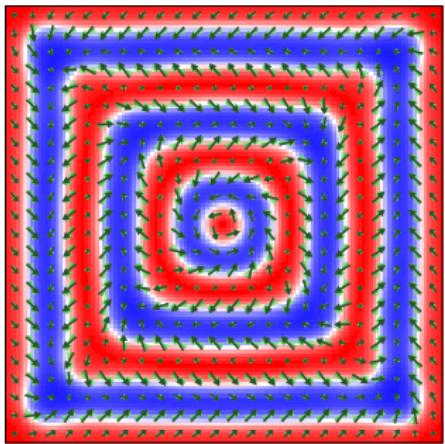
Spin Torque

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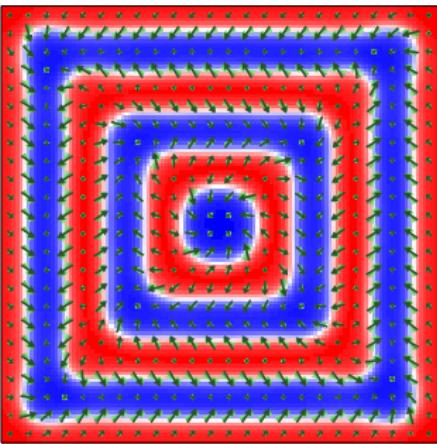
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Simple Anisotropy



Extended Anistropy

# Making movies

See the OOMMF movie page:

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

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# 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.)