Comparison of Exchange Energy Formulations for 3D Numerical Micromagnetics

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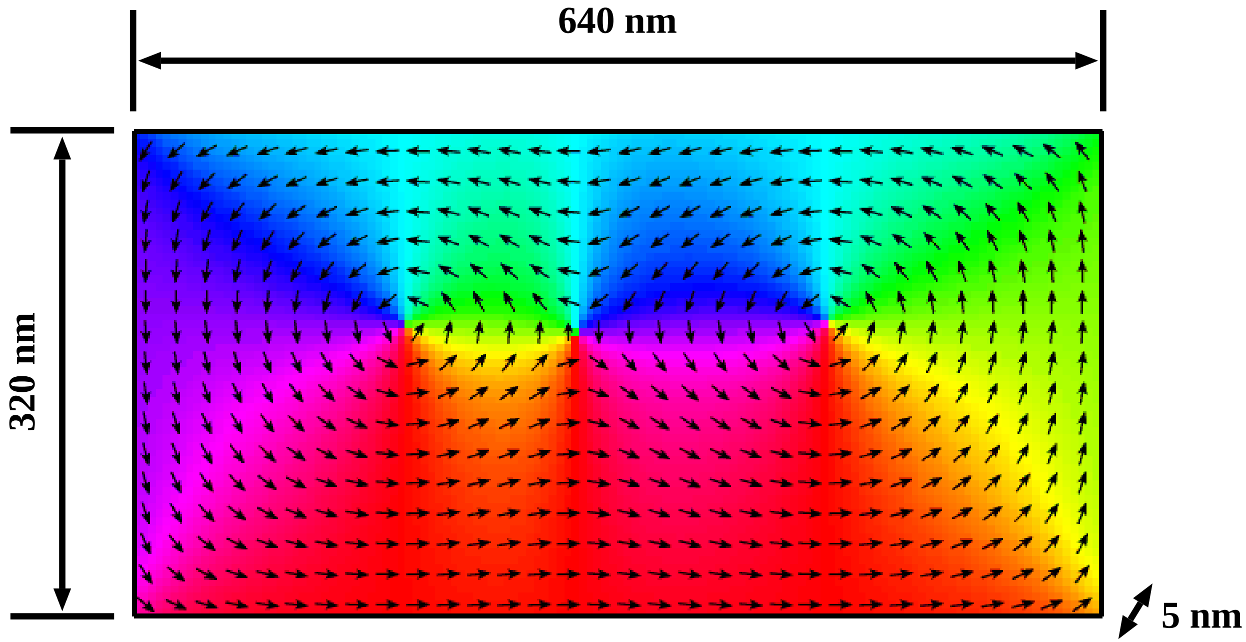
Outline

- Background
- μMAG
- Exchange energy
  - Numerical integration
  - Integrand representation
  - Boundary conditions

Micromagnetics



The study, modeling and simulation
of magnetic materials and their behavior
at the nanometer scale.

Brown's equations

Energies:

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

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

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

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

Constraints

$$\mathbf{M} \quad \text{is smooth}$$

and

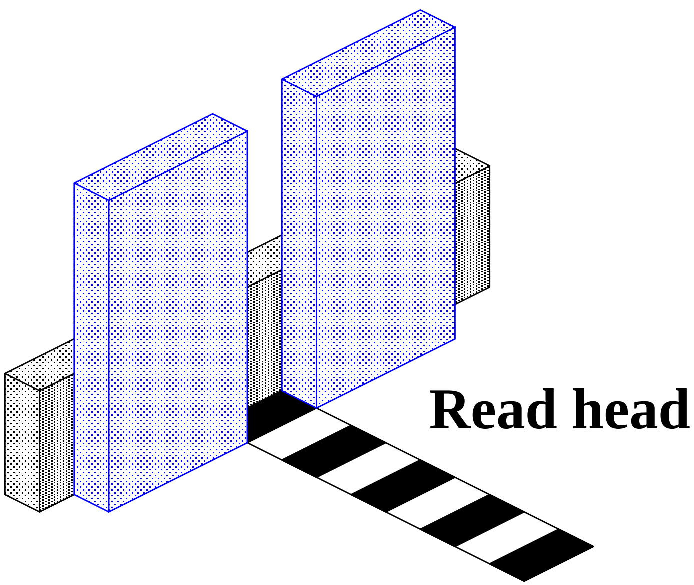
$$\|\mathbf{M}\| = M_{\mathrm{s}}$$

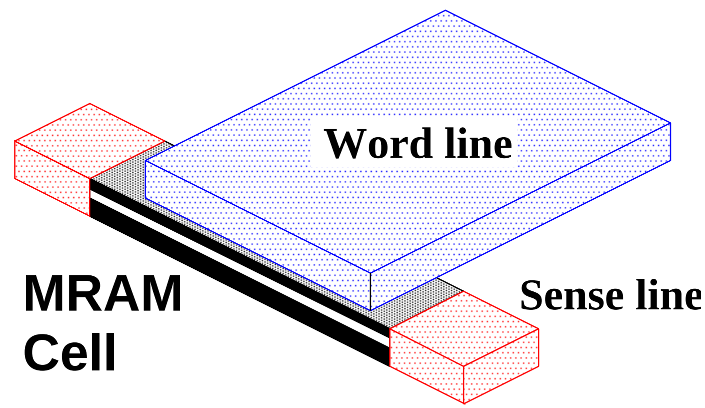
or equivalently

$$\|\mathbf{m}\| = \mathbf{M}/M_{\mathrm{s}} = 1.$$

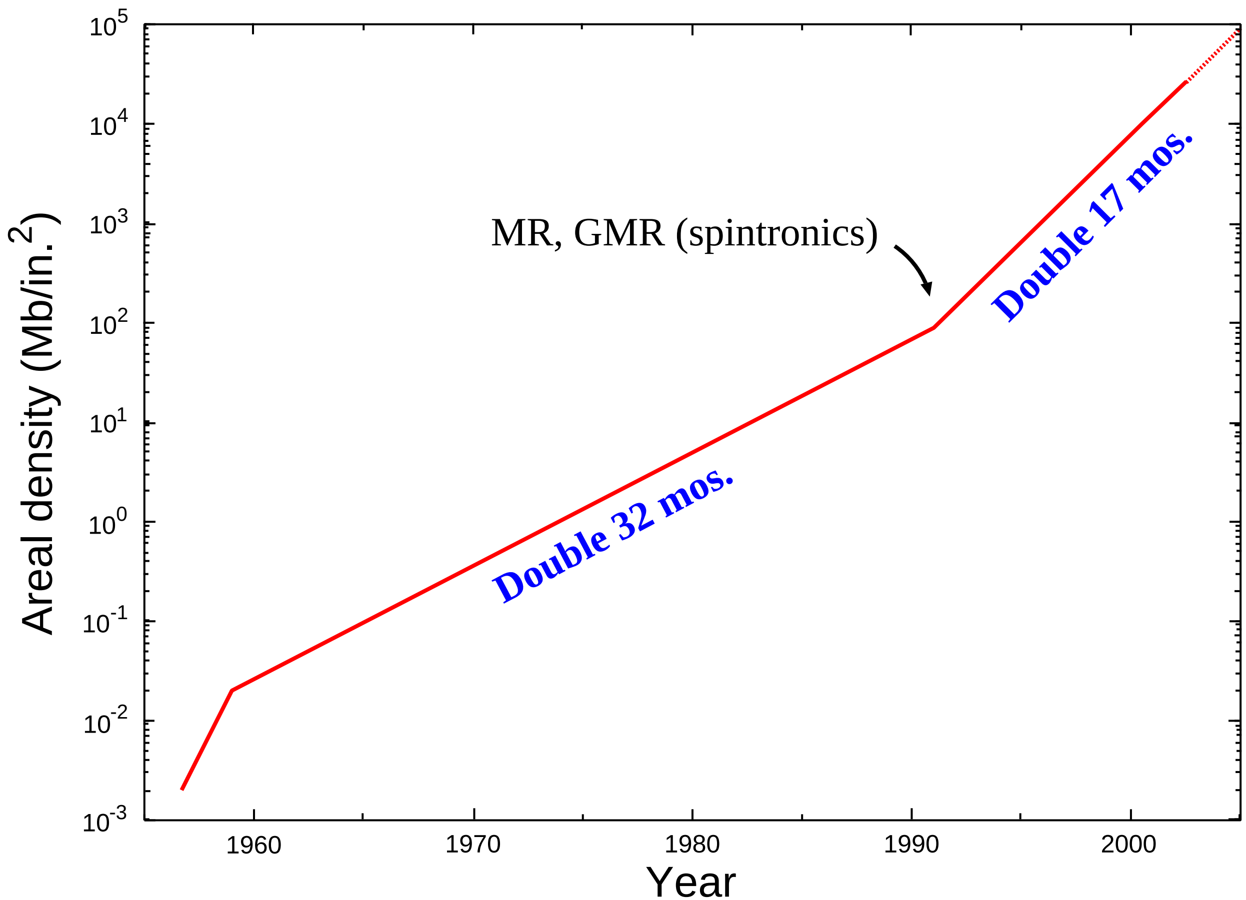
Why computational micromagnetics?

- Disk Drives
- Sensors
- Nonvolatile Memory
- Spintronics

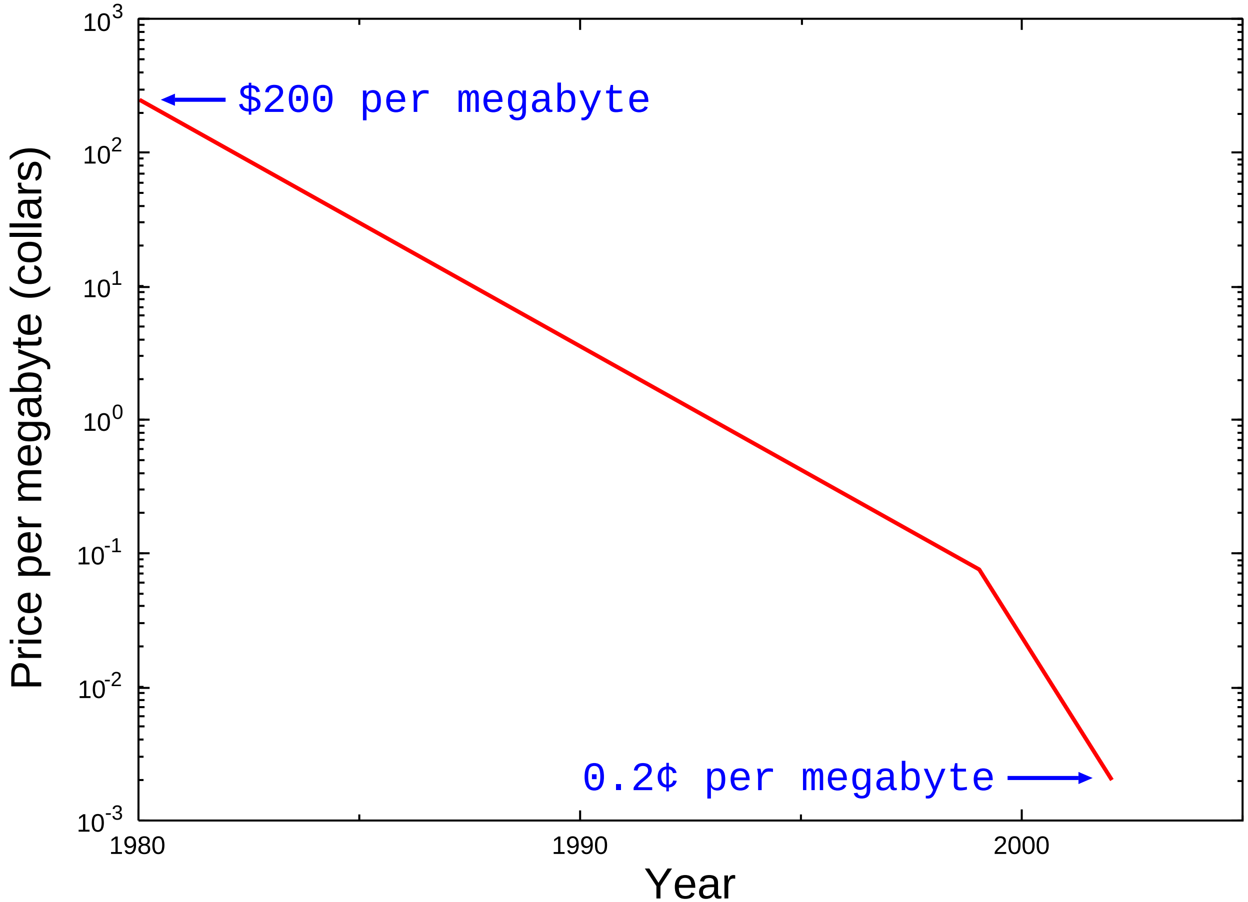




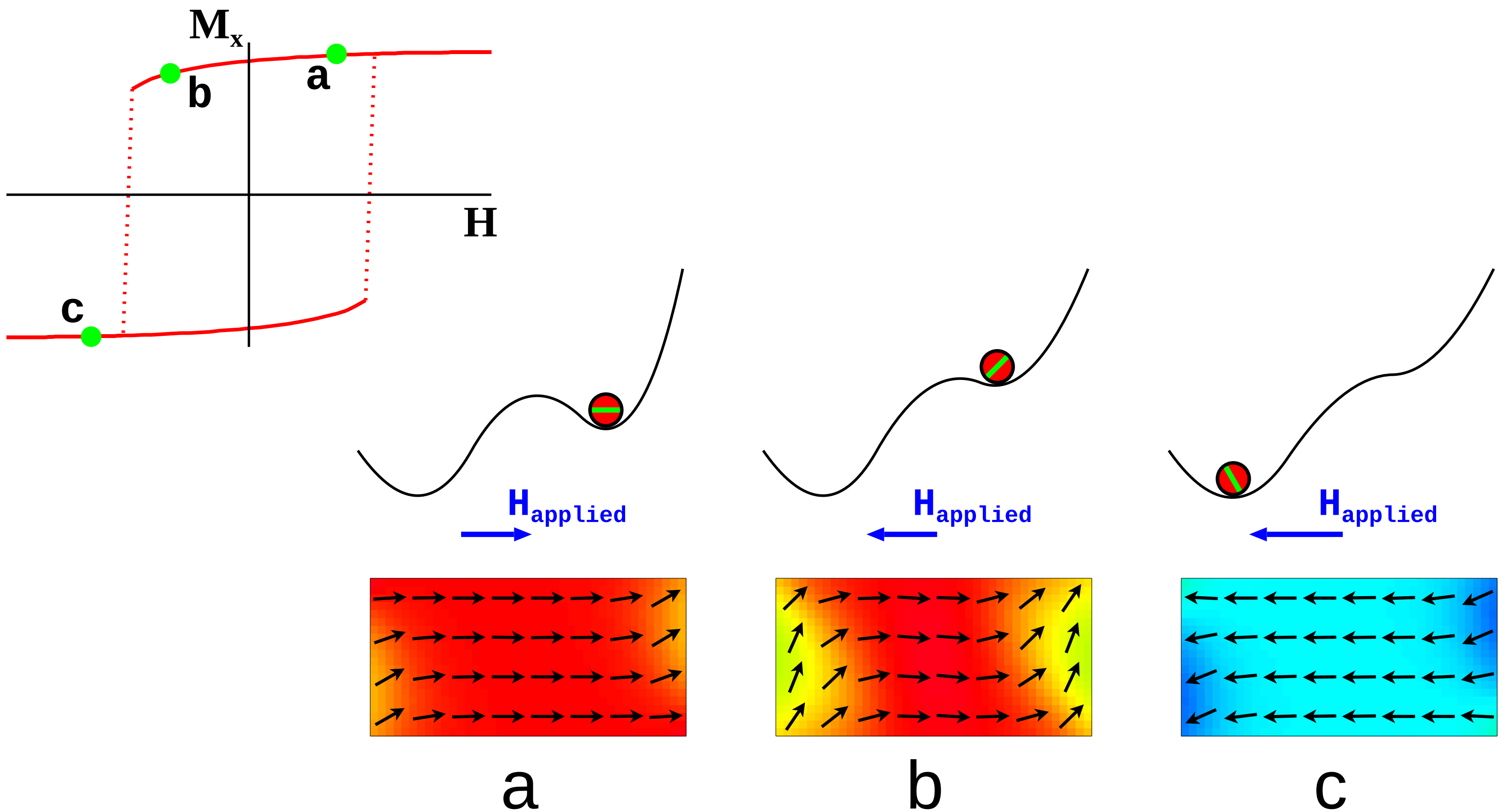
Magnetic disk storage



Magnetic disk storage



Quasi-static micromagnetics



Magnetization dynamics

Landau-Lifshitz-Gilbert:

$$\frac{d\mathbf{M}}{dt} = \frac{-\omega}{1+\alpha^2}\mathbf{M}\times\mathbf{H}_{\text{eff}} - \frac{\alpha\,\omega}{(1+\alpha^2)M_{\text{s}}}\mathbf{M}\times(\mathbf{M}\times\mathbf{H}_{\text{eff}})$$

where

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

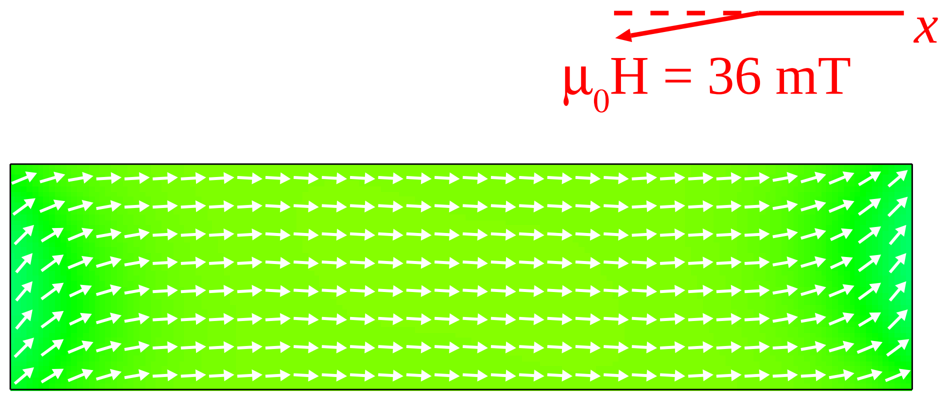
ω = gyromagnetic ratio

α = damping coefficient

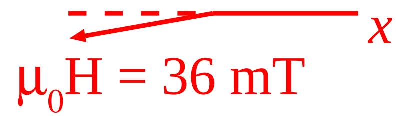
Magnetization dynamics

Time

0 ps

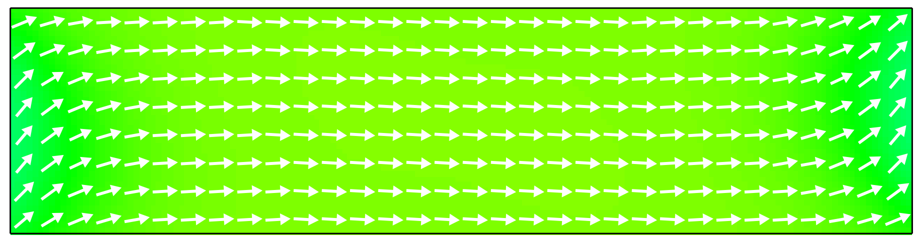


Magnetization dynamics

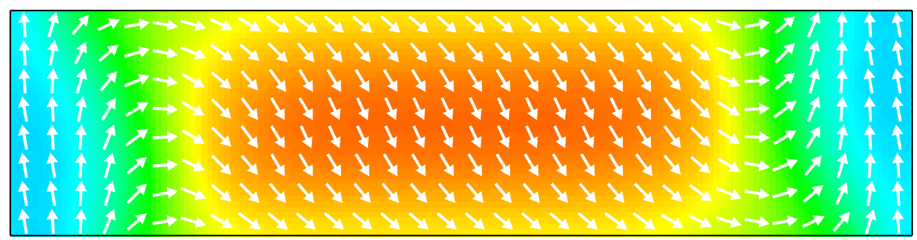


Time

0 ps



100 ps



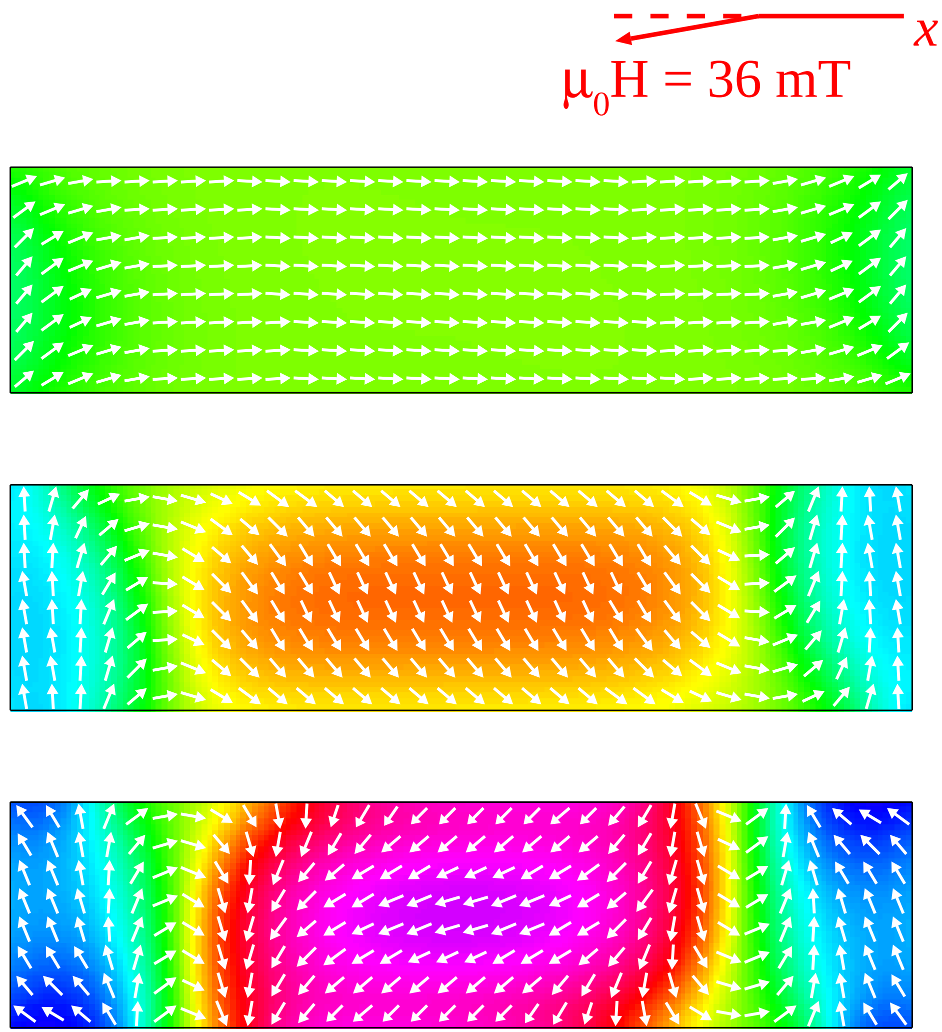
Magnetization dynamics

Time

0 ps

100 ps

150 ps



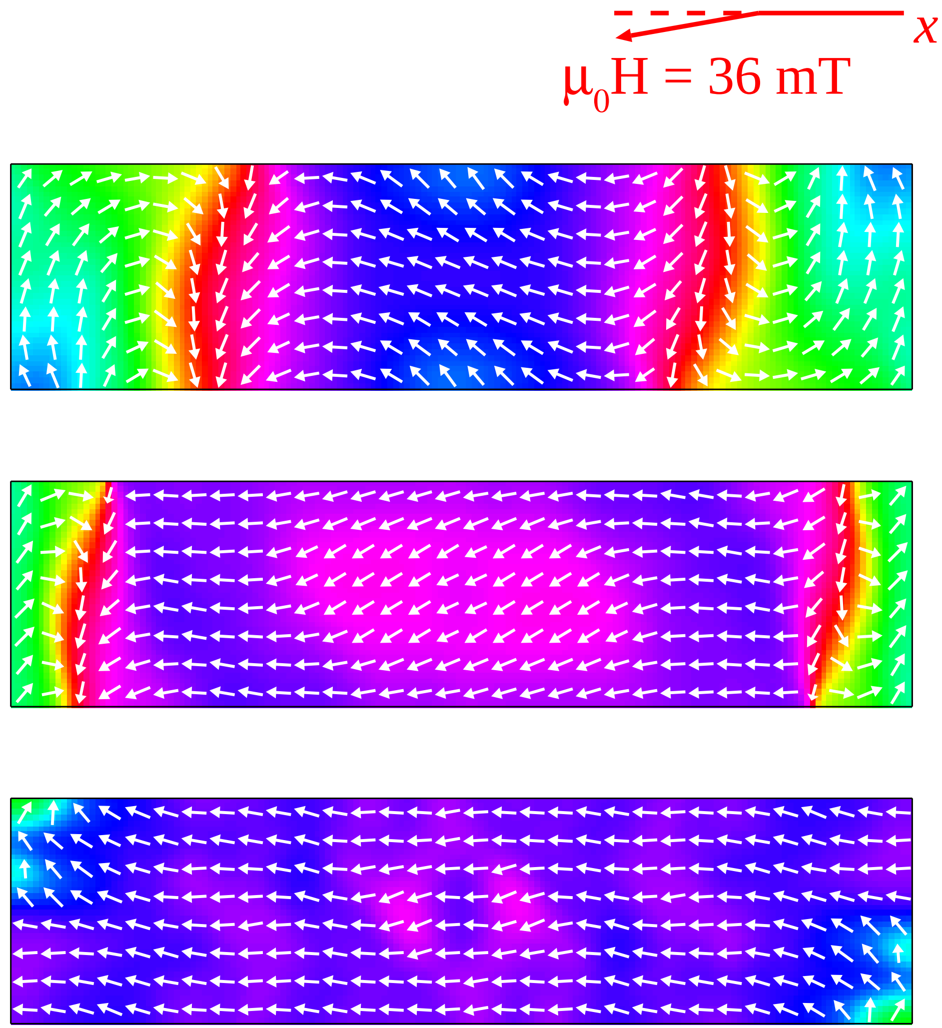
Magnetization dynamics

Time

350 ps

450 ps

750 ps



Variational derivatives

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

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

$$\epsilon \to 0, \quad \|\Delta\mathbf{M}\|_\infty \to 0.$$

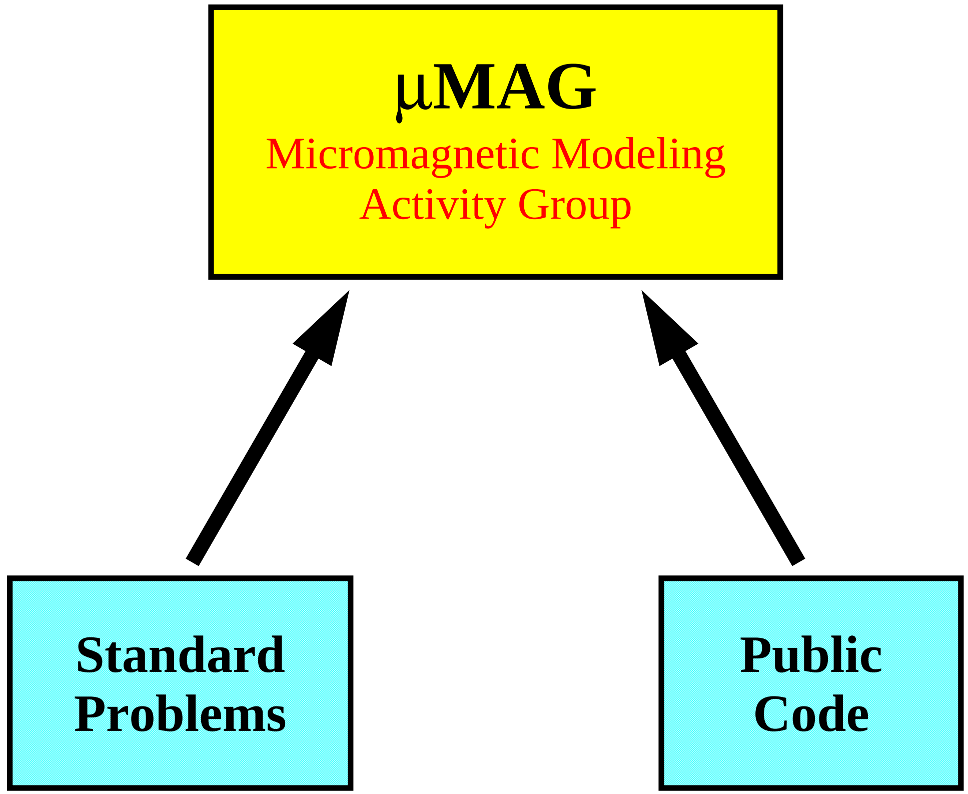
Variational derivatives

In particular, if

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

then

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



Center for Theoretical and Computational Materials Science

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

Standard problems

μMAG

Micromagnetic Modeling Activity Group

Four Standard Problems for micromagnetics

`http://www.ctcms.nist.gov/~rdm/mumag.html`

Check computed outputs against contributed solutions:

- Verify algorithms
- Compare methods
- Optimize parameters

Standard problems

μMAG

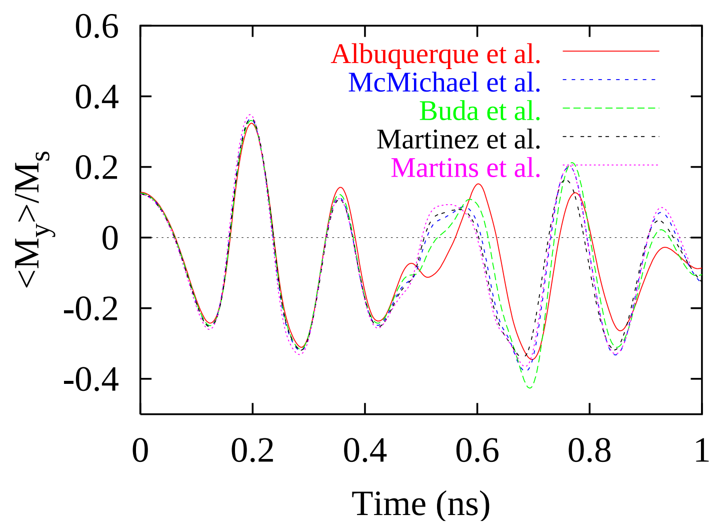
Micromagnetic Modeling Activity Group

Four Standard Problems for micromagnetics

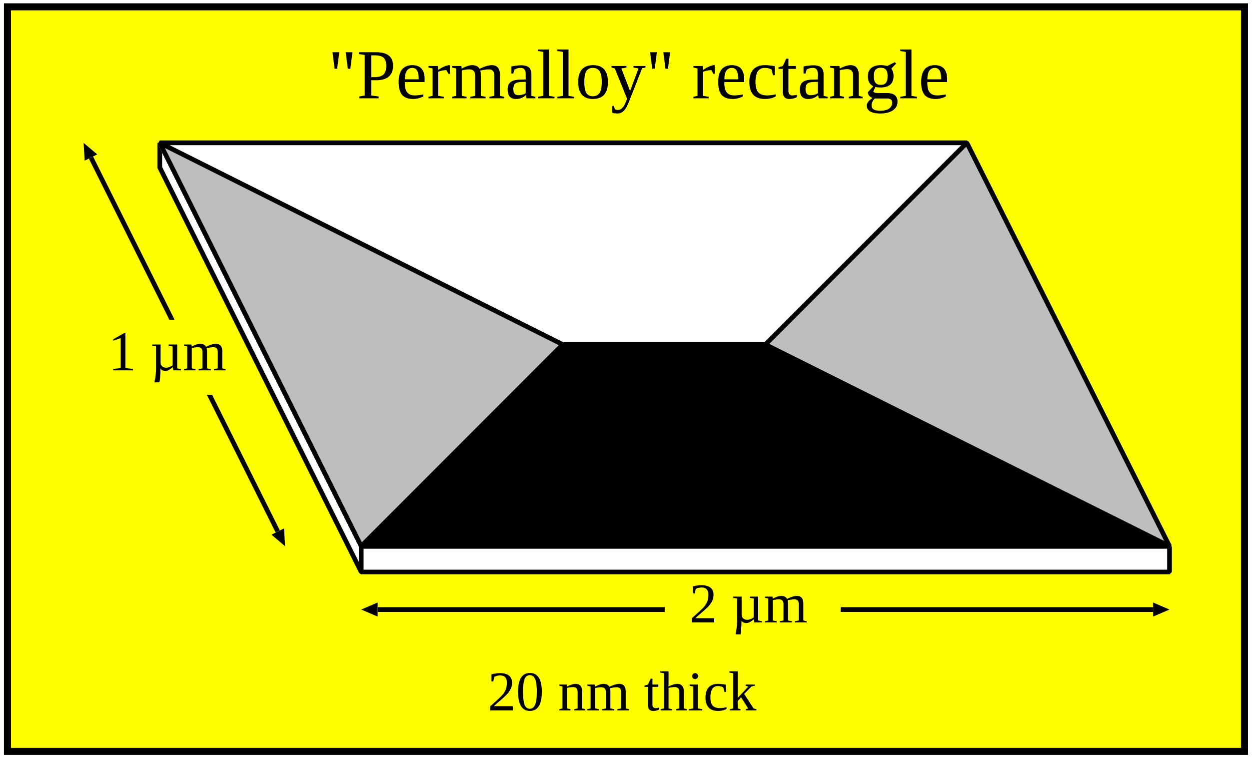
http://www.ctcms.nist.gov/~rdm/mumag.html

Example #4,

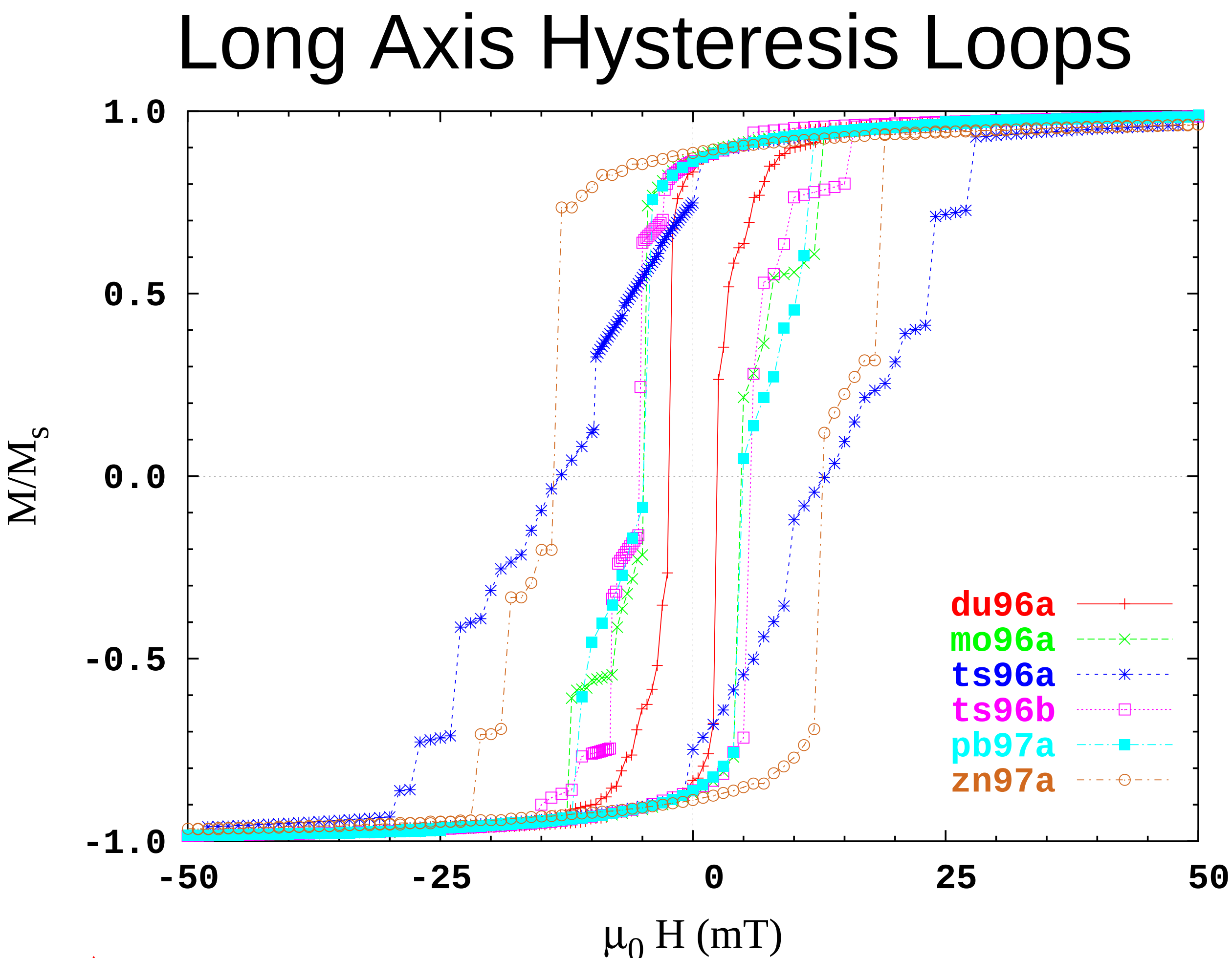
Switching dynamics:



μMAG standard problem #1



μMAG standard problem #1



Public code

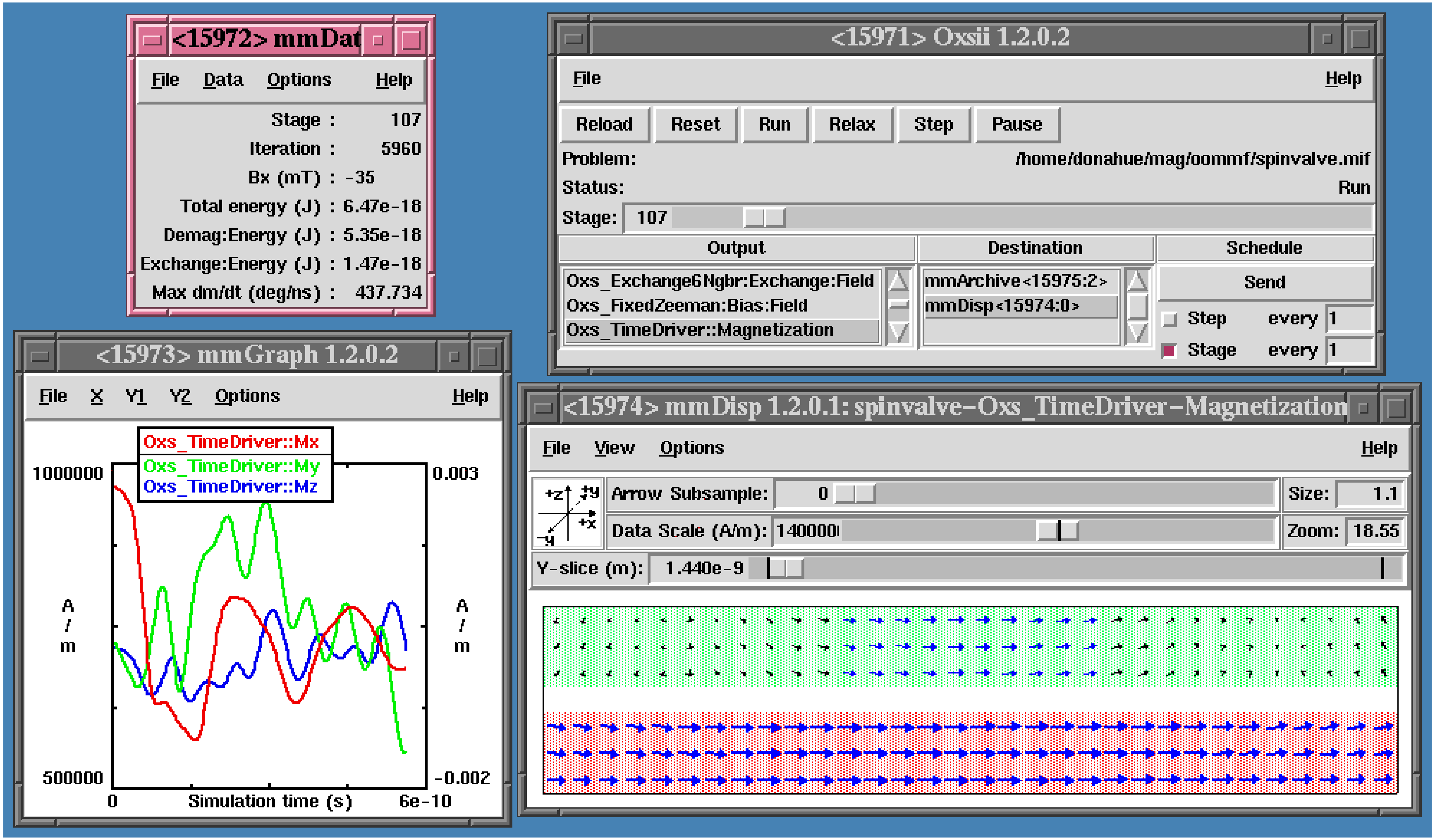
Portable, extensible,
public domain
programs & tools
for micromagnetics

`http://math.nist.gov/oommf`

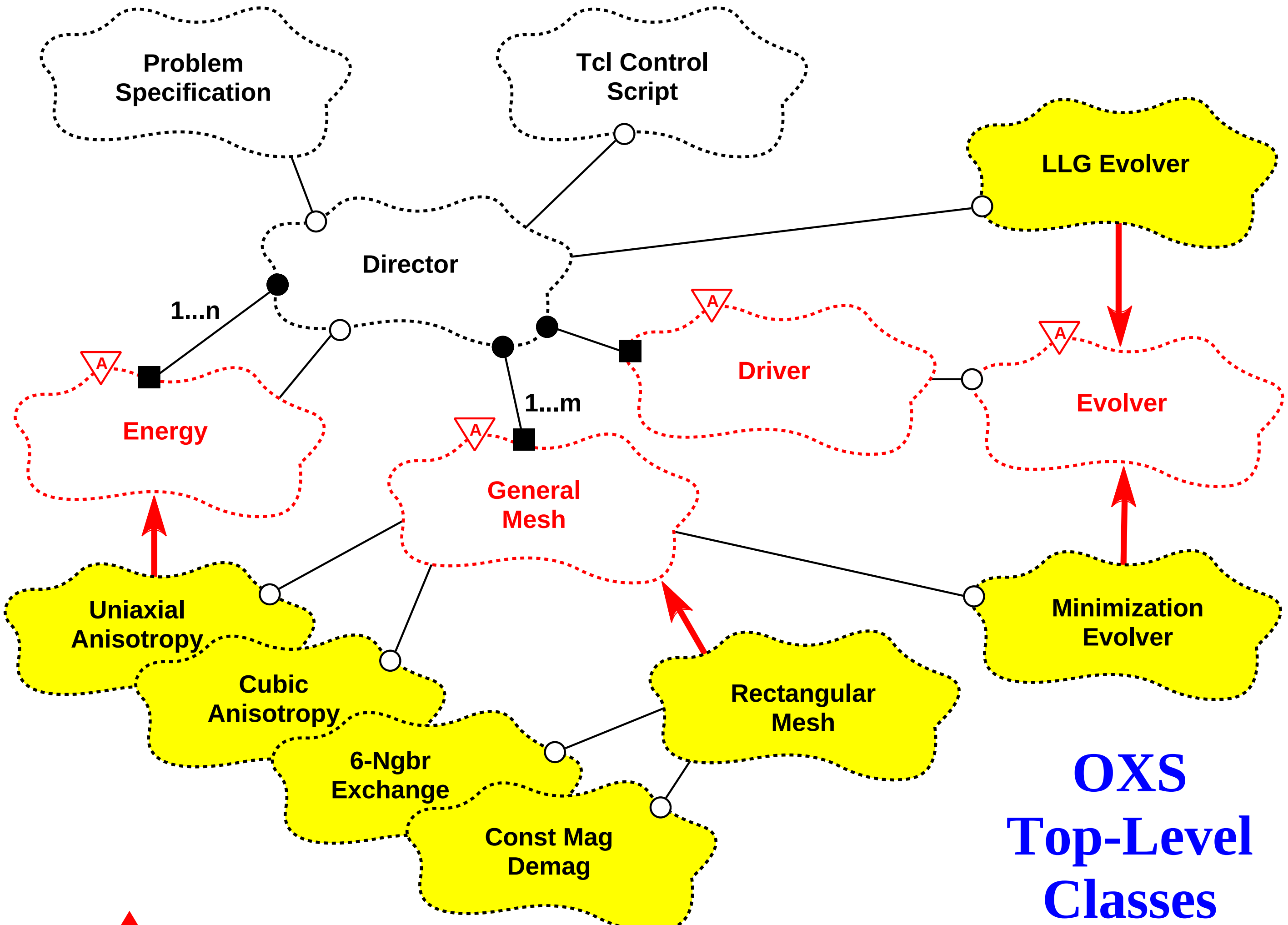
- Graphical User Interface
- Windows and Unix
- 150 page user’s manual

- Binaries and source code
- Tcl/Tk and C++ based modular architecture
- 1000+ downloads in 2002

Public code


<15972> mmDat
File Data Options Help
Stage : 107
Iteration : 5960
Bx (mT) : -35
Total energy (J) : 6.47e-18
Demag:Energy (J) : 5.35e-18
Exchange:Energy (J) : 1.47e-18
Max dm/dt (deg/ns) : 437.734
<15971> Oxsii 1.2.0.2
File Help
Reload Reset Run Relax Step Pause
Problem: /home/donahue/mag/oommf/spinvalve.mif
Status: Run
Stage: 107
Output
Destination
Schedule
Oxs_Exchange6Ngbr:Exchange:Field
Oxs_FixedZeeman:Bias:Field
Oxs_TimeDriver::Magnetization
mmArchive<15975:2>
mmDisp<15974:0>
Send
Step every 1
Stage every 1
<15973> mmGraph 1.2.0.2
File X Y1 Y2 Options Help
Oxs_TimeDriver::Mx
Oxs_TimeDriver::My
Oxs_TimeDriver::Mz
1000000
500000
0.003
-0.002
A/m
0
Simulation time (s)
6e-10
<15974> mmDisp 1.2.0.1: spinvalve-Oxs_TimeDriver-Magnetization
File View Options Help
Arrow Subsample: 0
Size: 1.1
Data Scale (A/m): 1400000
Zoom: 18.55
Y-slice (m): 1.440e-9

OOMMF eXtensible Solver



OXS Top-Level Classes

Brown's equations

Energies:

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

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

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

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

Discrete approximation

$$
\begin{aligned}
E_{\text{exchange}} &= \int_V A\left(|\nabla m_x|^2 + |\nabla m_y|^2 + |\nabla m_z|^2\right)\, d^3r \\
&= \Phi[\mathbf{m}(\mathbf{x}_1), \mathbf{m}(\mathbf{x}_2), \ldots, \mathbf{m}(\mathbf{x}_n)] + O(h^k)
\end{aligned}
$$

where

h is step size
k is approximation order

Discrete approximation

$$E_{\text{exchange}} = \int_V A\left(|\nabla m_x|^2 + |\nabla m_y|^2 + |\nabla m_z|^2\right)\, d^3r$$

- Numerical integration
- Integrand representation
- Boundary conditions

Numerical integration

$$\int_a^b f \approx h \sum c_k f_k$$

Closed intervals, $x_k = a + kh$,

$$
\begin{aligned}
O(h^2) \text{ error: } (c_k) &= \left[\tfrac{1}{2} \;\; 1 \;\; 1 \;\; \ldots \;\; 1 \;\; \tfrac{1}{2}\right] \\
O(h^4) \text{ error: } (c_k) &= \tfrac{1}{3}\left[1 \;\; 4 \;\; 2 \;\; 4 \;\; \ldots \;\; 2 \;\; 4 \;\; 1\right] \\
O(h^4) \text{ error: } (c_k) &= \left[\tfrac{3}{8} \;\; \tfrac{7}{6} \;\; \tfrac{23}{24} \;\; 1 \;\; 1 \;\; \ldots \;\; 1 \;\; \tfrac{23}{24} \;\; \tfrac{7}{6} \;\; \tfrac{3}{8}\right]
\end{aligned}
$$

Numerical integration

$$\int_a^b f \approx h \sum c_k f_k$$

Open intervals, $x_k = a + kh + h/2$,

$O(h^2)$ error: $(c_k) \; = \; [1 \;\; 1 \;\; 1 \;\; \ldots \;\; 1]$

$O(h^4)$ error: $(c_k) \; = \; \left[\frac{13}{12} \;\; \frac{7}{8} \;\; \frac{25}{24} \;\; 1 \;\; 1 \;\; \ldots \;\; 1 \;\; \frac{25}{24} \;\; \frac{7}{8} \;\; \frac{13}{12}\right]$

Integrand representation

$$
\begin{aligned}
E_{\mathrm{exchange}} &= A \iiint |\nabla m_x|^2 + |\nabla m_y|^2 + |\nabla m_z|^2 \, dV \\
&= -A \iiint \mathbf{m} \cdot \nabla^2 \mathbf{m} \, dV \\
&\quad + A \iint (m_x \nabla m_x + m_y \nabla m_y + m_z \nabla m_z) \cdot \hat{\mathbf{n}} \, dS.
\end{aligned}
$$

The norm constraint, $\|\mathbf{m}\| = 1$, implies

$$
m_x \nabla m_x + m_y \nabla m_y + m_z \nabla m_z = \mathbf{0}.
$$

Discretized energy

$$E_{\mathrm{exchange}} = -A \iiint \mathbf{m} \cdot \nabla^2 \mathbf{m} \; d^3 r$$

$$= \quad -A \iiint \mathbf{m} \cdot \frac{\partial^2 \mathbf{m}}{\partial x^2} + \mathbf{m} \cdot \frac{\partial^2 \mathbf{m}}{\partial y^2} + \mathbf{m} \cdot \frac{\partial^2 \mathbf{m}}{\partial z^2} \; d^3 r$$

Discretized energy

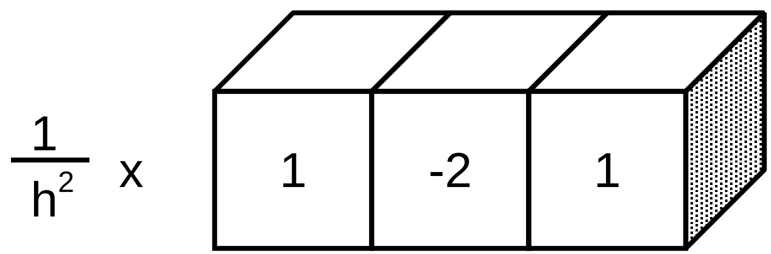
$$\iiint \mathbf{m} \cdot \frac{\partial^2 \mathbf{m}}{\partial x^2}\; d^3 r$$

$$\approx \; \sum_k c_k^z \sum_j c_j^y \sum_i c_i^x \, \mathbf{m}_{ijk} \cdot \left(\sum_{i'} D_{ii'} \mathbf{m}_{i'jk} \right)$$

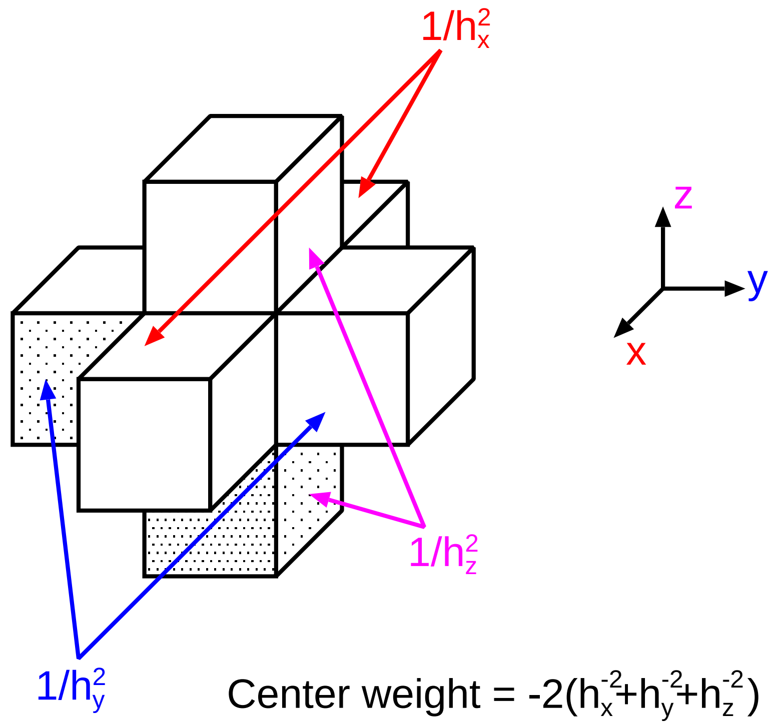
$$= \; c_k^z \, c_j^y \, m_{ijk}^{\nu} \, c_i^x \, D_{ii'} \, m_{i'jk}^{\nu}$$ (summation convention)

3-pt stencil

$$\frac{\partial^2 f(x)}{\partial x^2} = \frac{1}{h^2}\left[f(x-h) - 2f(x) + f(x+h)\right] + O(h^2)$$



3-pt stencil

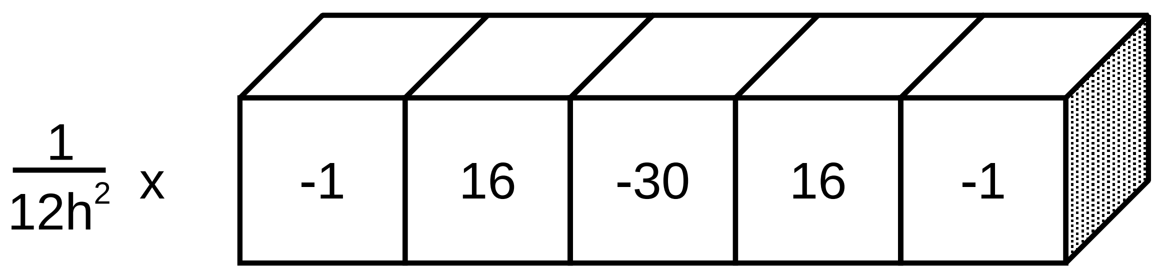


Center weight = $-2(h_x^{-2}+h_y^{-2}+h_z^{-2})$

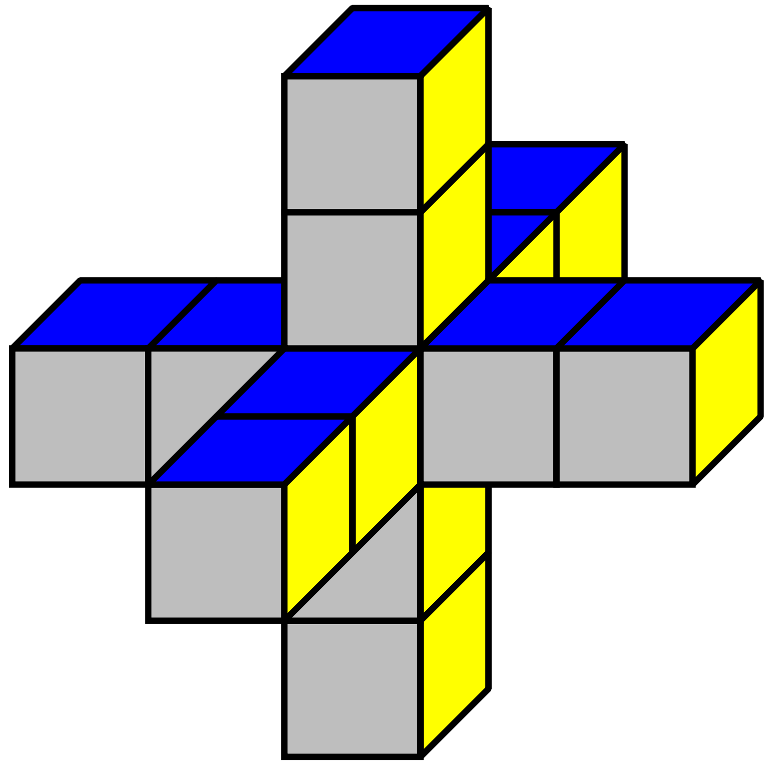
“6-neighbor exchange”

5-pt stencil

$$\frac{\partial^2 f(x)}{\partial x^2} = \frac{1}{12h^2}\left[-f(x-2h) + 16f(x-h) - 30f(x)\right.$$
$$\left. + 16f(x+h) - f(x+2h)\right] + O(h^4)$$

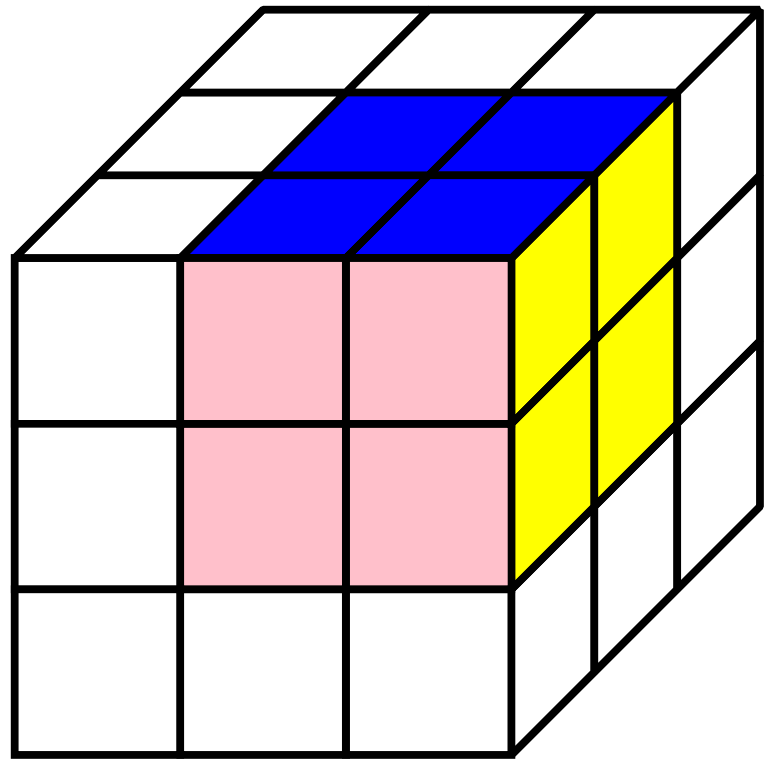


5-pt stencil



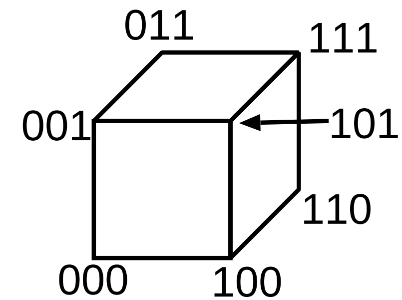
“12-neighbor exchange”

Trilinear interpolation



"26-neighbor exchange"

Trilinear interpolation



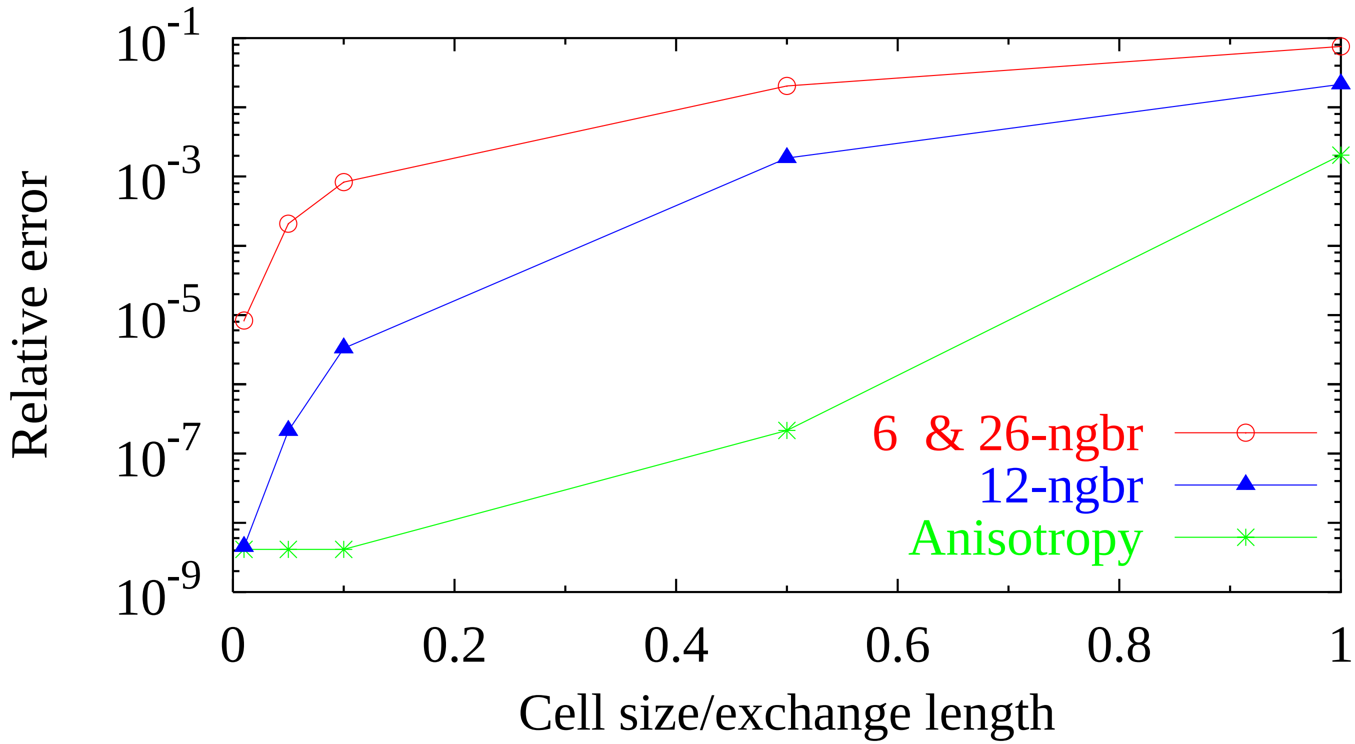
Given $\mathbf{m}_{000}, \mathbf{m}_{100}, \ldots,$ solve for

$$\begin{aligned}\mathbf{m}(x) \;&=\; \mathbf{a}_0 + \mathbf{a}_{100}x + \mathbf{a}_{010}y + \mathbf{a}_{001}z \\ &\quad +\mathbf{a}_{110}xy + \mathbf{a}_{101}xz + \mathbf{a}_{011}yz + \mathbf{a}_{111}xyz.\end{aligned}$$

Then use

$$E_{\mathrm{exchange}} = \int_V A\left(|\nabla m_x|^2 + |\nabla m_y|^2 + |\nabla m_z|^2\right)\, d^3r$$

Analytic 1D domain wall



Relative energy error vs. discretization cell size

Exchange lengths

$$\text{Magnetostatic-exchange length} = \sqrt{\frac{2A}{\mu_0 M_s^2}}$$

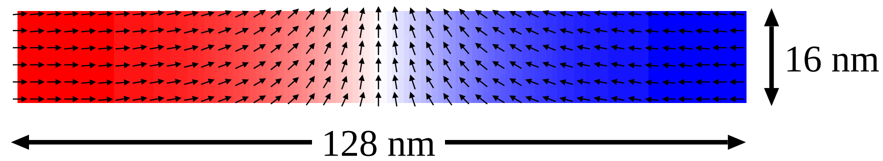
$$\text{Magnetocrystalline-exchange length} = \sqrt{\frac{A}{|K|}}$$

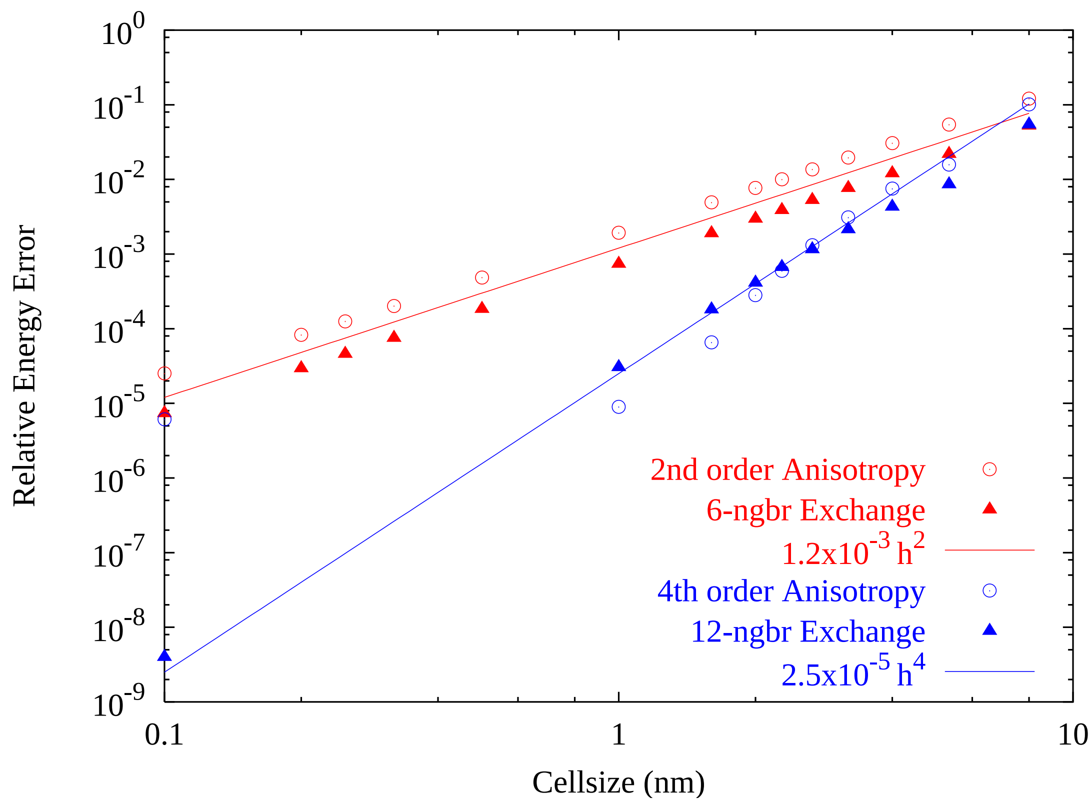
Iterative convergence

$A = 13 \times 10^{-12}$ J/m

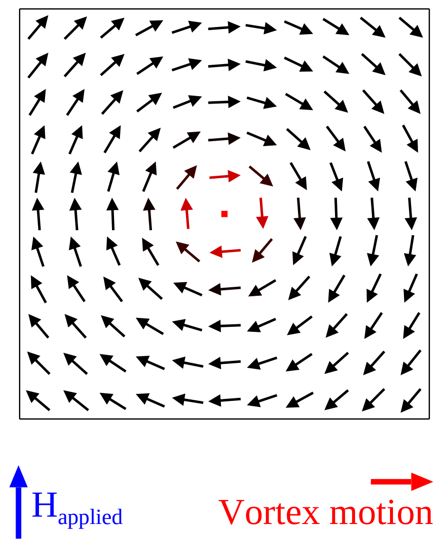
$K_u = (4.6 \times 10^{5}) r^2/(1+r^2)$ J/m^3

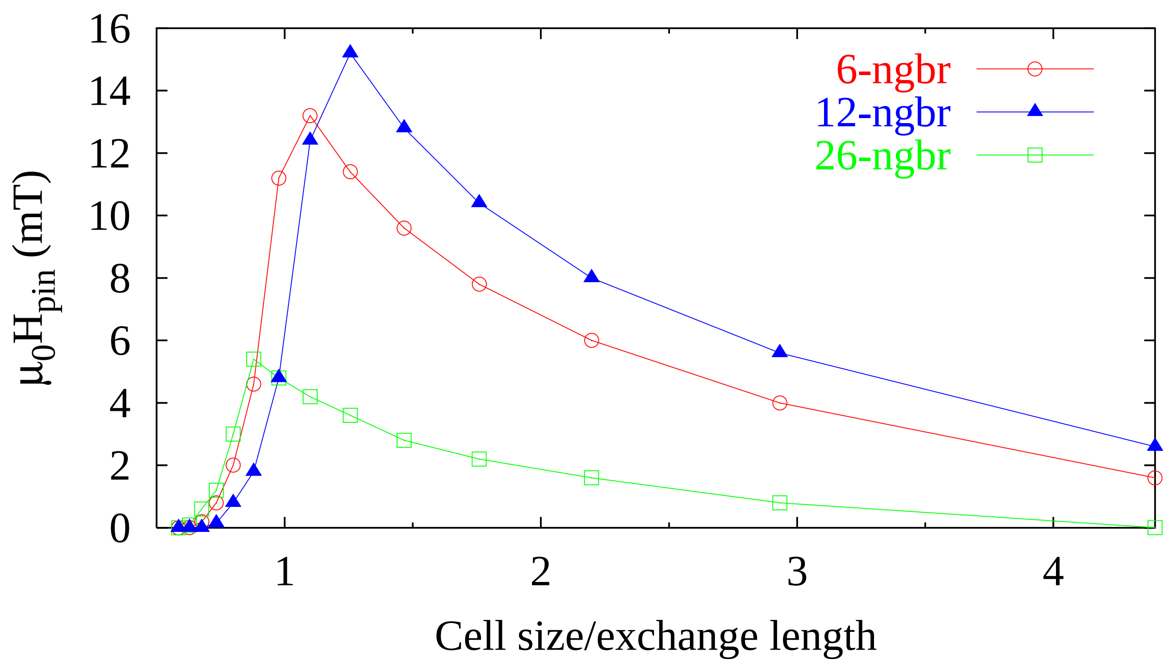
10 nm thick





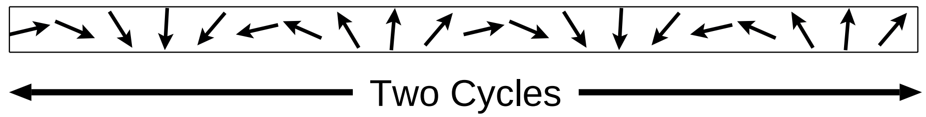
Vortex mobility

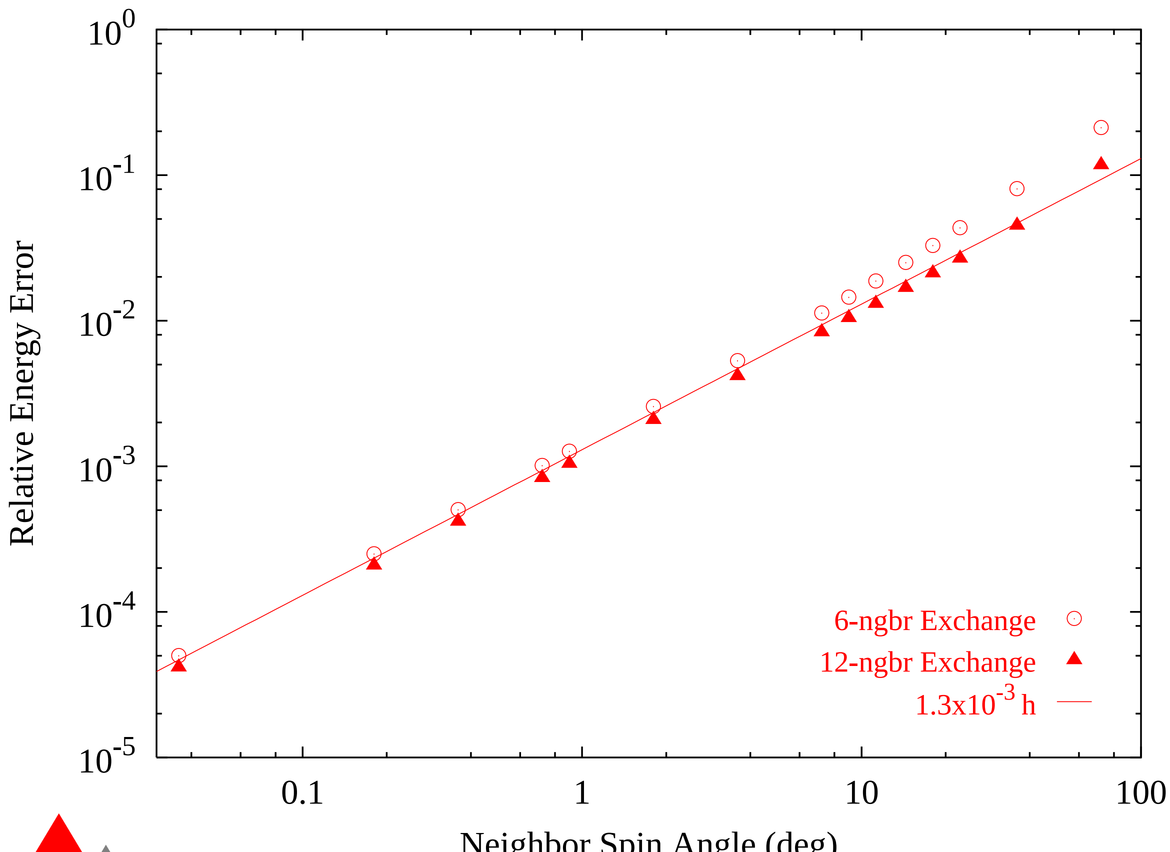




(Compare to Donahue & McMichael, Physica B, **233**, 272 (1997).)

Magnetization spiral





Discretized energy

$$\iiint \mathbf{m} \cdot \frac{\partial^2 \mathbf{m}}{\partial x^2} \; d^3 r$$

$$\approx \; \sum_k c_k^z \sum_j c_j^y \sum_i c_i^x \, \mathbf{m}_{ijk} \cdot \left(\sum_{i'} D_{ii'} \mathbf{m}_{i'jk} \right)$$

$$= \; c_k^z \, c_j^y \, m_{ijk}^\nu \, c_i^x \, D_{ii'} \, m_{i'jk}^\nu$$ (summation convention)

Boundary?

$$\frac{1}{12h^2} \times \begin{array}{cc} \boxed{?} & \boxed{?} \\ & \boxed{?} \\ & \\ & \\ & \end{array} \begin{bmatrix} -30 & 16 & -1 & & & \\ 16 & -30 & 16 & -1 & & \\ -1 & 16 & -30 & 16 & -1 & \\ & -1 & 16 & -30 & 16 & -1 \\ & & & & \ddots & \end{bmatrix}$$

Variational calculus

Let

$$E[m] = \int_a^b f(x, m, m')\, dx$$

Then

$$E[m+h] - E[m] = \int_a^b \left(f_m - \frac{d}{dx} f_{m'} \right) h\, dx$$

$$+h(b) f_{m'}(b, m(b), m'(b)) - h(a) f_{m'}(a, m(a), m'(a))$$

$$+O\left(h^2 + h'^{\,2}\right).$$

Euler-Lagrange eqn

If m is extremal, then

$$f_m - \frac{d}{dx} f_{m'} = 0 \qquad \text{(Euler-Lagrange)}$$

Boundary conditions

Since

$$h(a)f_{m'}(a, m(a), m'(a)) = 0,$$

if $m(a)$ is free, then

$$f_{m'}(a, m(a), m'(a)) = 0.$$

But

$$f(x, m, m') = Am'^{\,2} + g(x, m)$$

and

$$f_{m'} = 2Am' \quad \Rightarrow \quad m'(a) = 0.$$

12-ngbr exchange

Assume $\partial\mathbf{m}/\partial\hat{\mathbf{n}} = 0$:

$$\frac{1}{12h^2} \times \begin{bmatrix} * & * & * & * & & \\ * & * & * & * & & \\ -1 & 16 & -30 & 16 & -1 & \\ & -1 & 16 & -30 & 16 & -1 \\ & & & & \ddots & \end{bmatrix}$$

$\Rightarrow$ Not positive semi-definite!

12-ngbr exchange

Recall

$$
\begin{aligned}
E_{\text{exchange}} &= A \iiint |\nabla m_x|^2 + |\nabla m_y|^2 + |\nabla m_z|^2 \, dV \\
&= -A \iiint \mathbf{m} \cdot \nabla^2 \mathbf{m} \, dV \\
&\quad + A \iint (m_x \nabla m_x + m_y \nabla m_y + m_z \nabla m_z) \cdot \hat{\mathbf{n}} \, dS.
\end{aligned}
$$

12-ngbr exchange

Include $\frac{\partial}{\partial x}$ at boundary:

$$\frac{1}{12h^2} \times \begin{bmatrix} \star & \star & \star & \star & & & \\ * & * & * & * & & & \\ -1 & 16 & -30 & 16 & -1 & & \\ & -1 & 16 & -30 & 16 & -1 & \\ & & & & \ddots & & \end{bmatrix}$$

Positive semi-definite, but slow convergence

12-ngbr exchange

Add in more $\frac{\partial}{\partial x}$ at boundary:

$$\frac{1}{12h^2} \times \begin{bmatrix} \diamond & \diamond & \diamond & & & & \\ * & * & * & * & & & \\ -1 & 16 & -30 & 16 & -1 & & \\ & -1 & 16 & -30 & 16 & -1 & \\ & & & & \ddots & & \end{bmatrix}$$

12-ngbr exchange

Clean up:

- Include c_i^x terms
- Symmetrize

$$E = \mathbf{m}^T D \mathbf{m} = \mathbf{m}^T \left(\frac{D + D^T}{2} \right) \mathbf{m}$$

12-ngbr exchange

Assuming $\partial \mathbf{m}/\partial \hat{\mathbf{n}} = 0$:

$$\frac{\partial^2}{\partial x^2} = \frac{1}{12h^2} \begin{bmatrix} -16.2 & 17.6 & -1.4 & & & & \\ 17.6 & -32.1 & 15.4 & -1.0 & & & \\ -1.4 & 15.4 & -29.4 & 16.3 & -1 & & \\ & -1.0 & 16.3 & -30.4 & 16 & -1 & \\ & & -1 & 16 & -30 & 16 & -1 \\ & & & & & \ddots & \end{bmatrix}$$

$$+O(h^4).$$

12-ngbr exchange

Eigenvalues $\subset [0, 5\frac{1}{3})$

$\Rightarrow$ Good convergence!

12-ngbr exchange

No boundary assumptions:

$$\frac{\partial^2}{\partial x^2} = \frac{1}{1152h^2} \times \begin{bmatrix} -6125 & 11959 & -8864 & 3613 & -583 & & & \\ 11959 & -25725 & 20078 & -7425 & 1113 & & & \\ -8864 & 20078 & -17175 & 6752 & -791 & & & \\ 3613 & -7425 & 6752 & -4545 & 1701 & -96 & & \\ -583 & 1113 & -791 & 1701 & -2880 & 1536 & -96 & \\ & & & -96 & 1536 & -2880 & 1536 & -96 \\ & & & & & & \ddots & \end{bmatrix} + O(h^4).$$

12-ngbr exchange

Eigenvalues $\subset [0, 45)$

$\Rightarrow$ Slow convergence

6-ngbr exchange

Assume $\partial \mathbf{m}/\partial \hat{\mathbf{n}} = 0$:

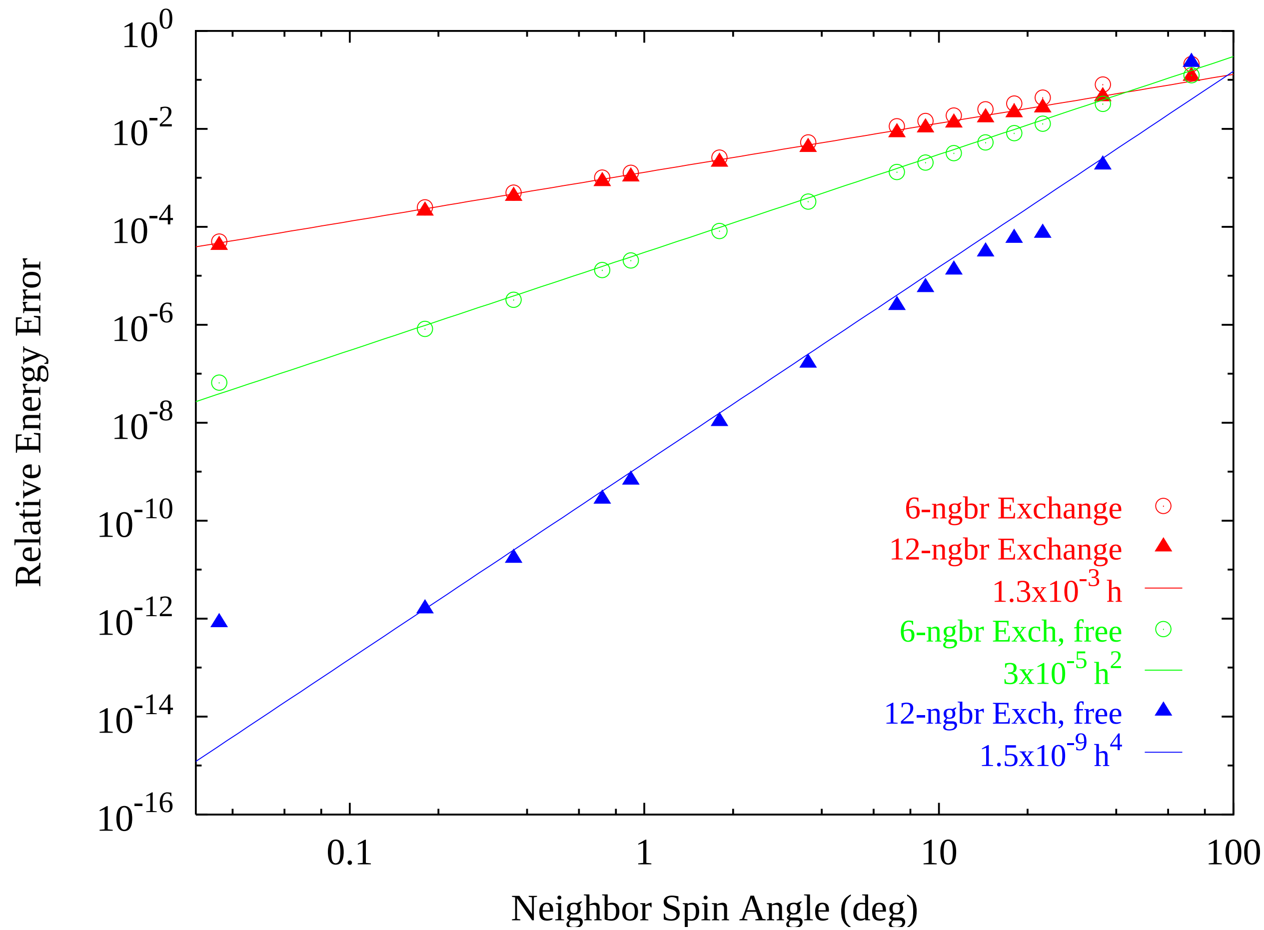
$$\frac{\partial^2}{\partial x^2} = \frac{1}{h^2}\begin{bmatrix} -1 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & 1 & -2 & 1 & \\ & & & & \ddots & \end{bmatrix} + O(h^2).$$

6-ngbr exchange

No boundary assumptions:

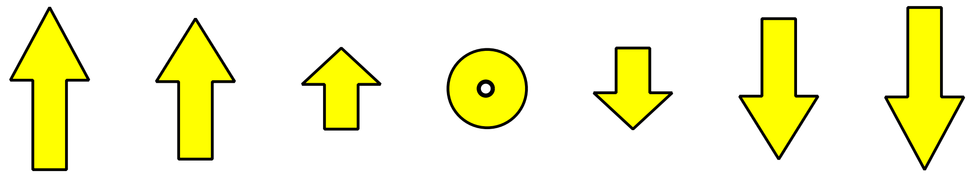
$$\frac{\partial^2}{\partial x^2} = \frac{1}{h^2} \begin{bmatrix} -1.5 & 1.5 & & & \\ 1.5 & -2.5 & 1 & & \\ & 1 & -2 & 1 & \\ & & 1 & -2 & 1 \\ & & & & \ddots \end{bmatrix} + O(h^2).$$

Magnetization spiral



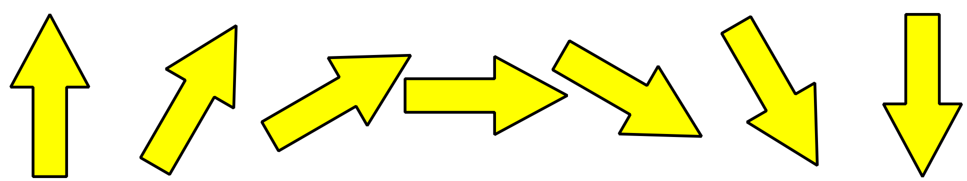
Wall types

Bloch wall



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

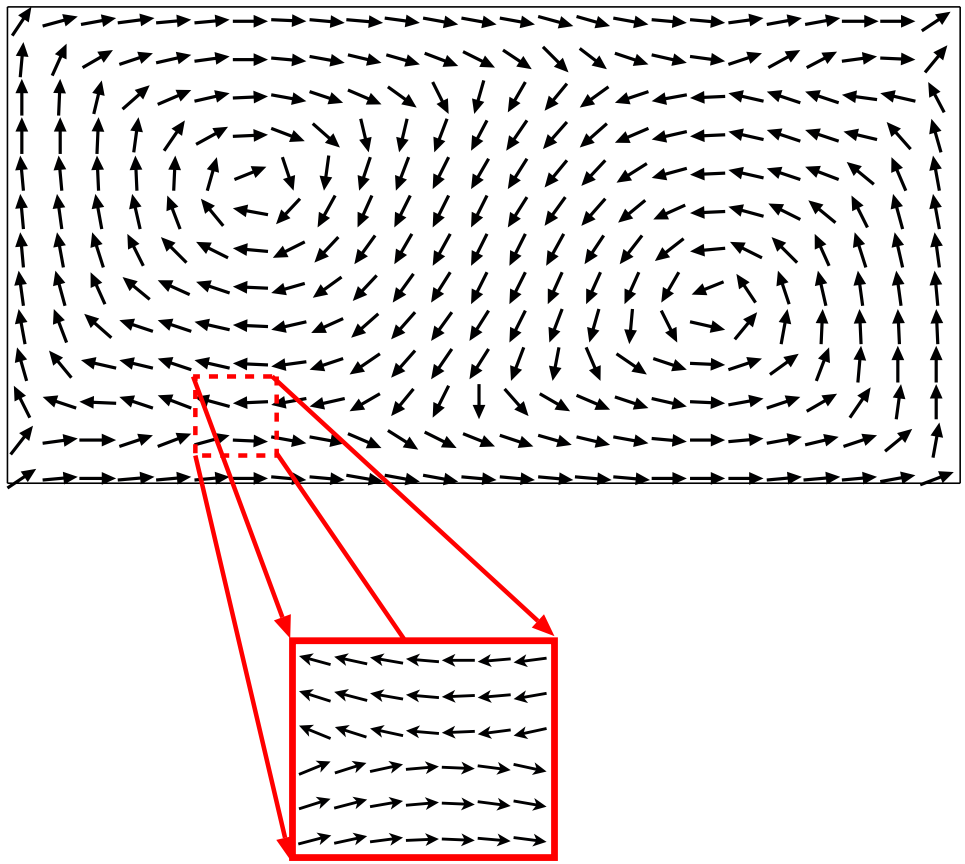
Néel wall



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

Néel-wall collapse

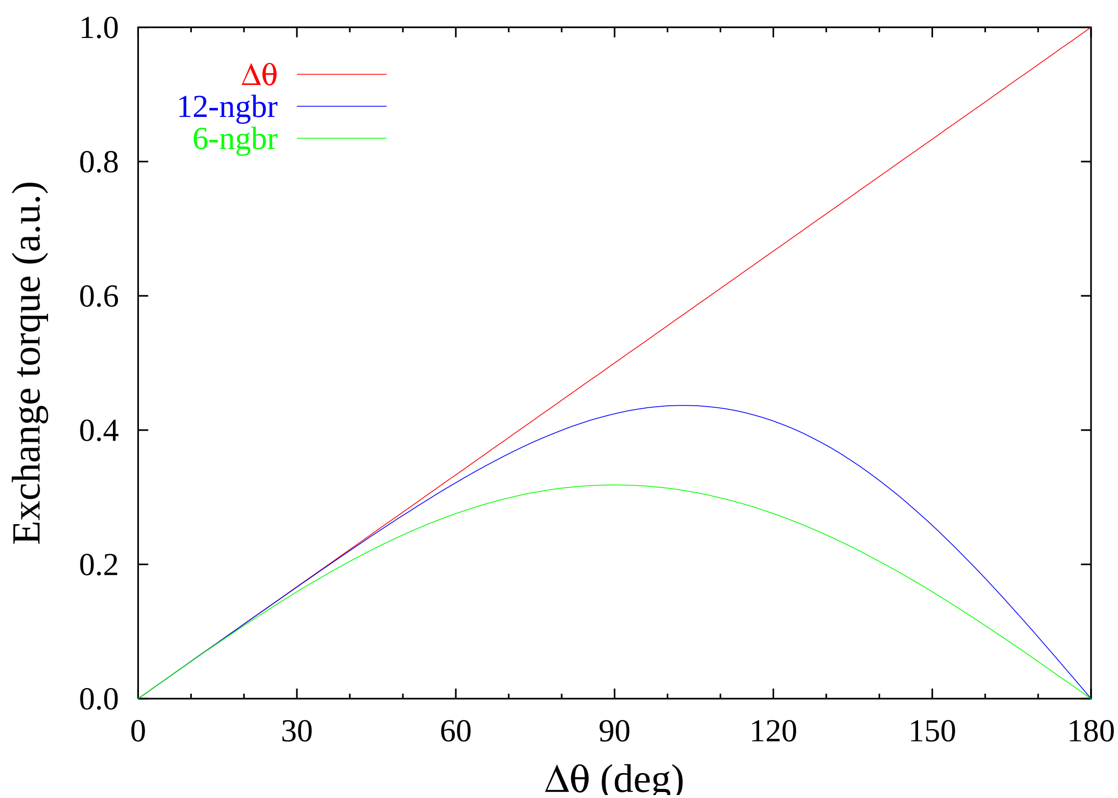
6-pt exchange, $\mu_0 H = 5$ mT, $h = 20$ nm



Magnetization spiral

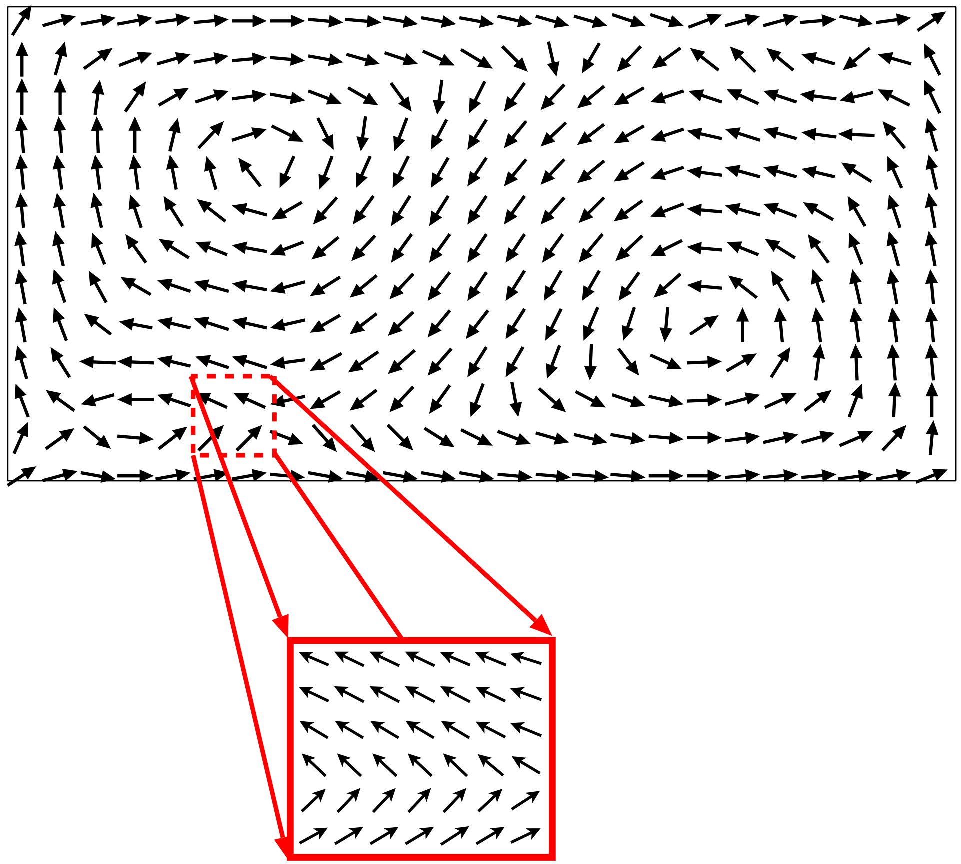
$$\mathbf{m} = (\cos \omega x, \sin \omega x)$$

Exchange torque vs. ω

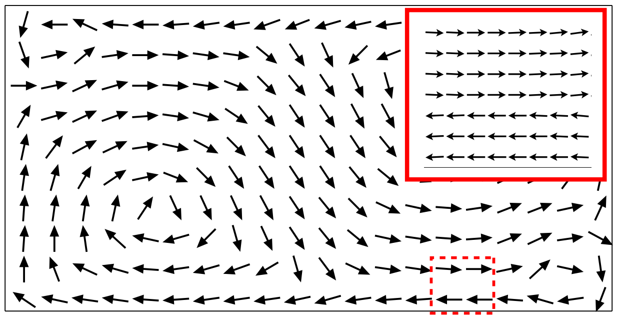


Néel-wall non-collapse

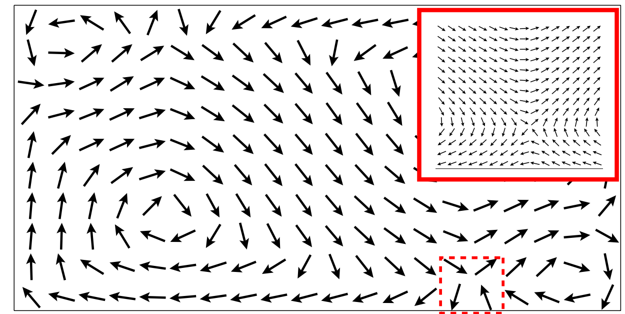
12-pt exchange, $\mu_0 H = 6$ mT, $h = 20$ nm



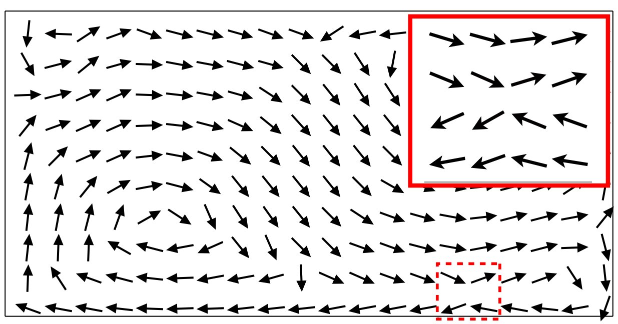
More Néel-walls



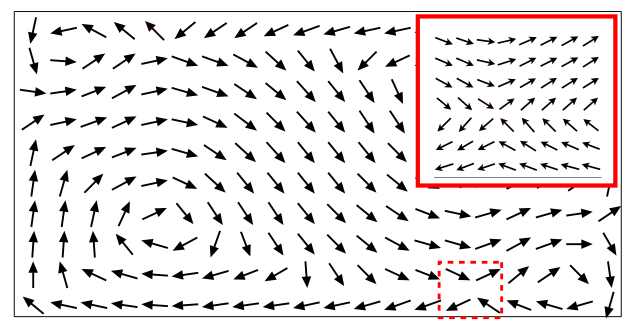
Standard Exchange, 25 nm cells



Standard Exchange, 12.5 nm cells



Variational Exchange, 50 nm cells



Variational Exchange, 25 nm cells

Conclusions

- 6-ngbr and 26-ngbr are 2nd order.
- 12-ngbr is 4th order.
- 26-ngbr has less pinning for large cells, 12-ngbr dominates for $h < l_{\mathrm{ex}}$.
- 12-ngbr helps against Néel wall collapse.
- $\partial\mathbf{m}/\partial\hat{\mathbf{n}} = 0$ good BC for equilibrium states with no surface pinning. Free BC possible.

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