Exchange Energy Formulations for Micromagnetics

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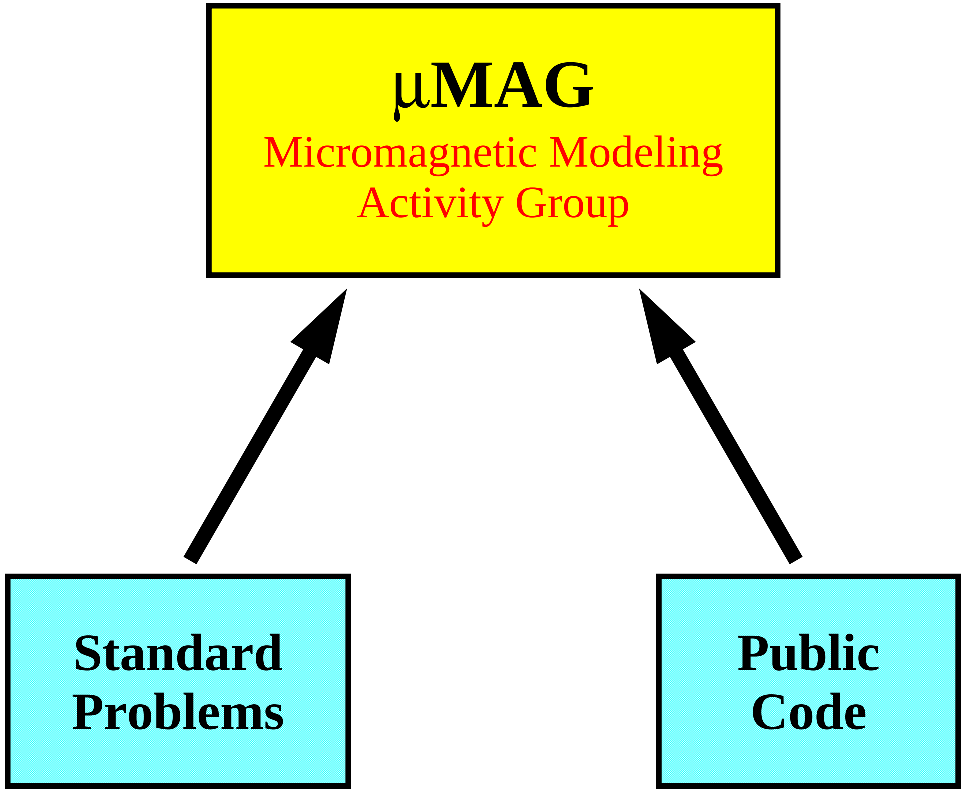
Outline

- Background
  - Quasi-static vs. Dynamic
- Exchange energy formulations
  - 6-ngbr, 12-ngbr, 26-ngbr
  - Numerical integration
  - Integrand representation
  - Boundary conditions



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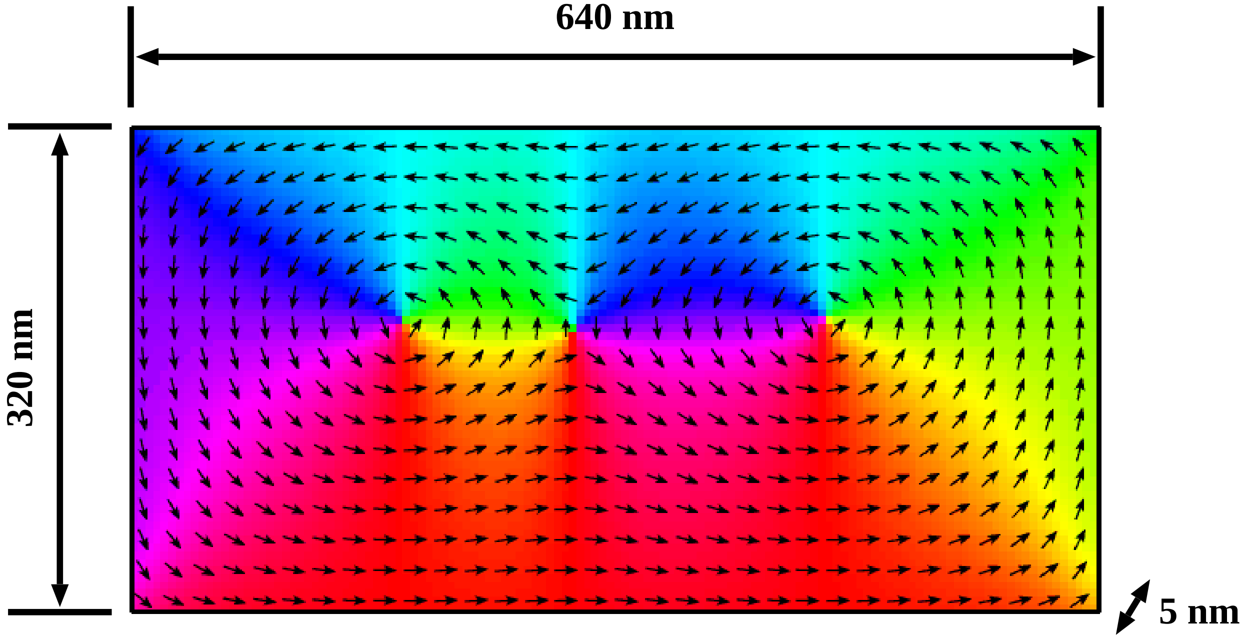
Micromagnetics



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

Brown's equations

Energies:

$$
\begin{aligned}
E_{\text{exchange}} &= \int_V \frac{A}{M_s^2}\left(|\nabla M_x|^2 + |\nabla M_y|^2 + |\nabla M_z|^2\right)\, d^3r \\
E_{\text{anisotropy}} &= \int_V \frac{K_1}{M_s^2}(\mathbf{M}\cdot\mathbf{u})^2\, d^3r \\
E_{\text{demag}} &= \frac{\mu_0}{8\pi}\int_V \mathbf{M}(r)\cdot\left[\int_V \nabla\cdot\mathbf{M}(\mathbf{r}')\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}\, d^3r' \right. \\
&\qquad \left. - \int_S \hat{\mathbf{n}}\cdot\mathbf{M}(\mathbf{r}')\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}\, d^2r'\right]\, d^3r \\
E_{\text{Zeeman}} &= -\mu_0\int_V \mathbf{M}\cdot\mathbf{H}_{\text{ext}}\, d^3r
\end{aligned}
$$

Constraints

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

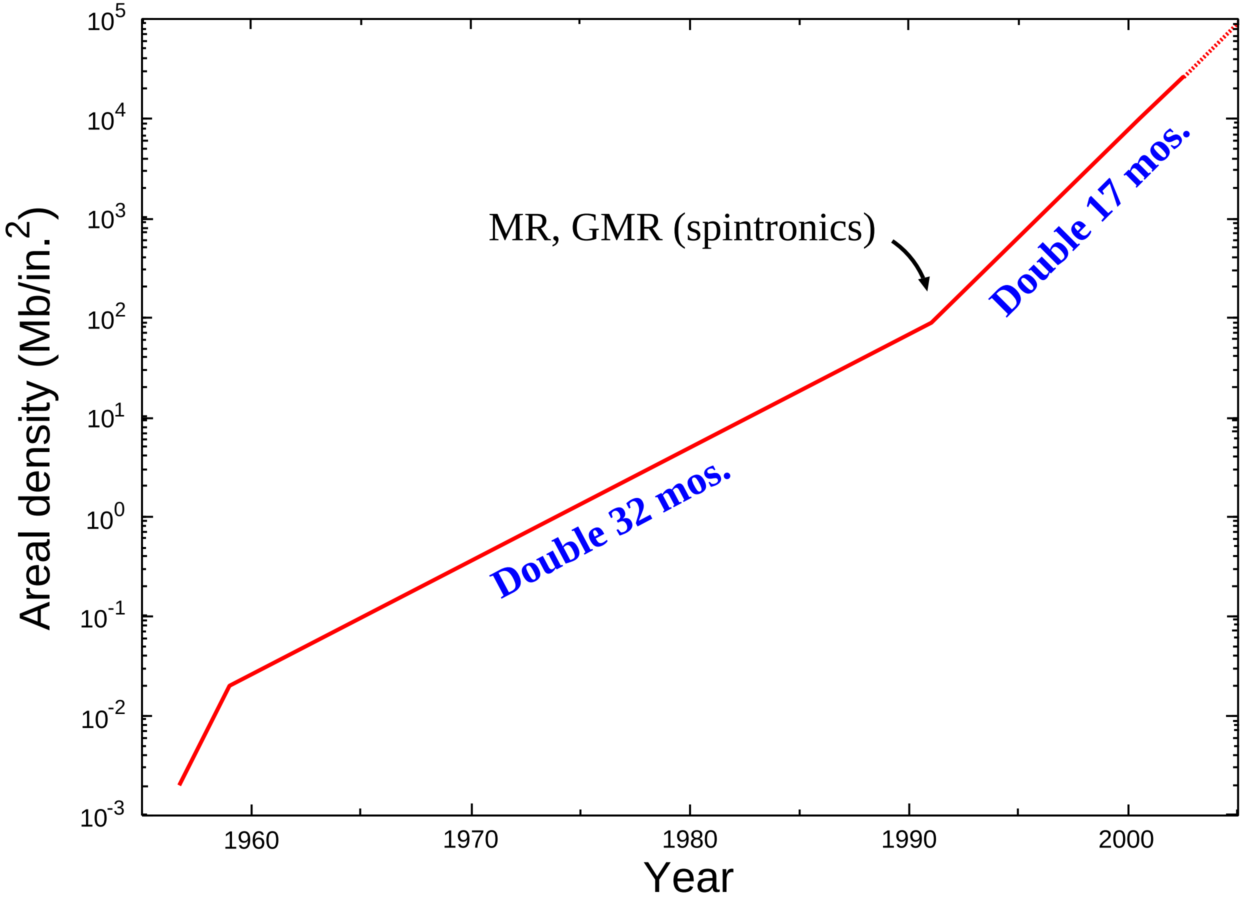
and

$$\|\mathbf{M}(t)\| = \|\mathbf{M}\| = M_\mathrm{s}$$

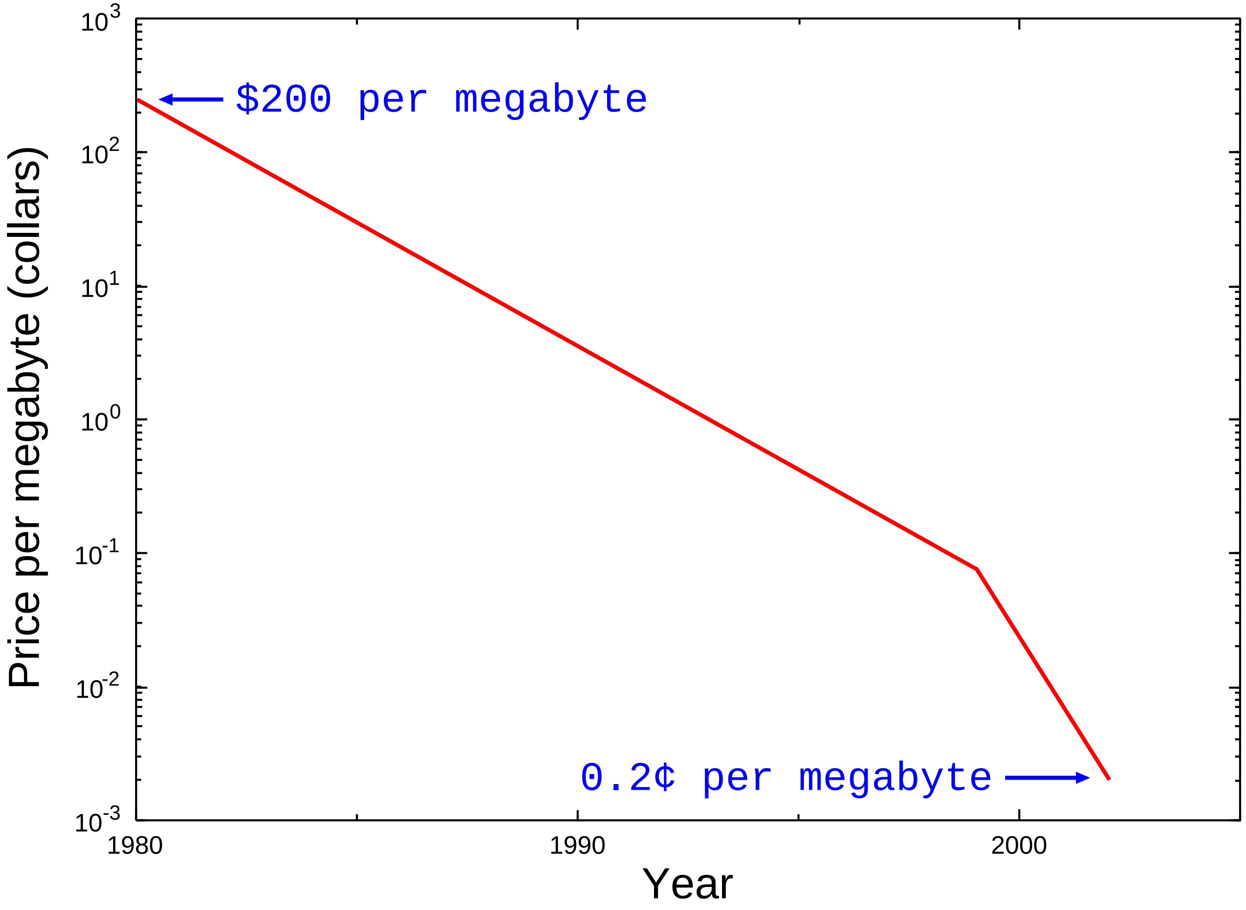
or equivalently

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

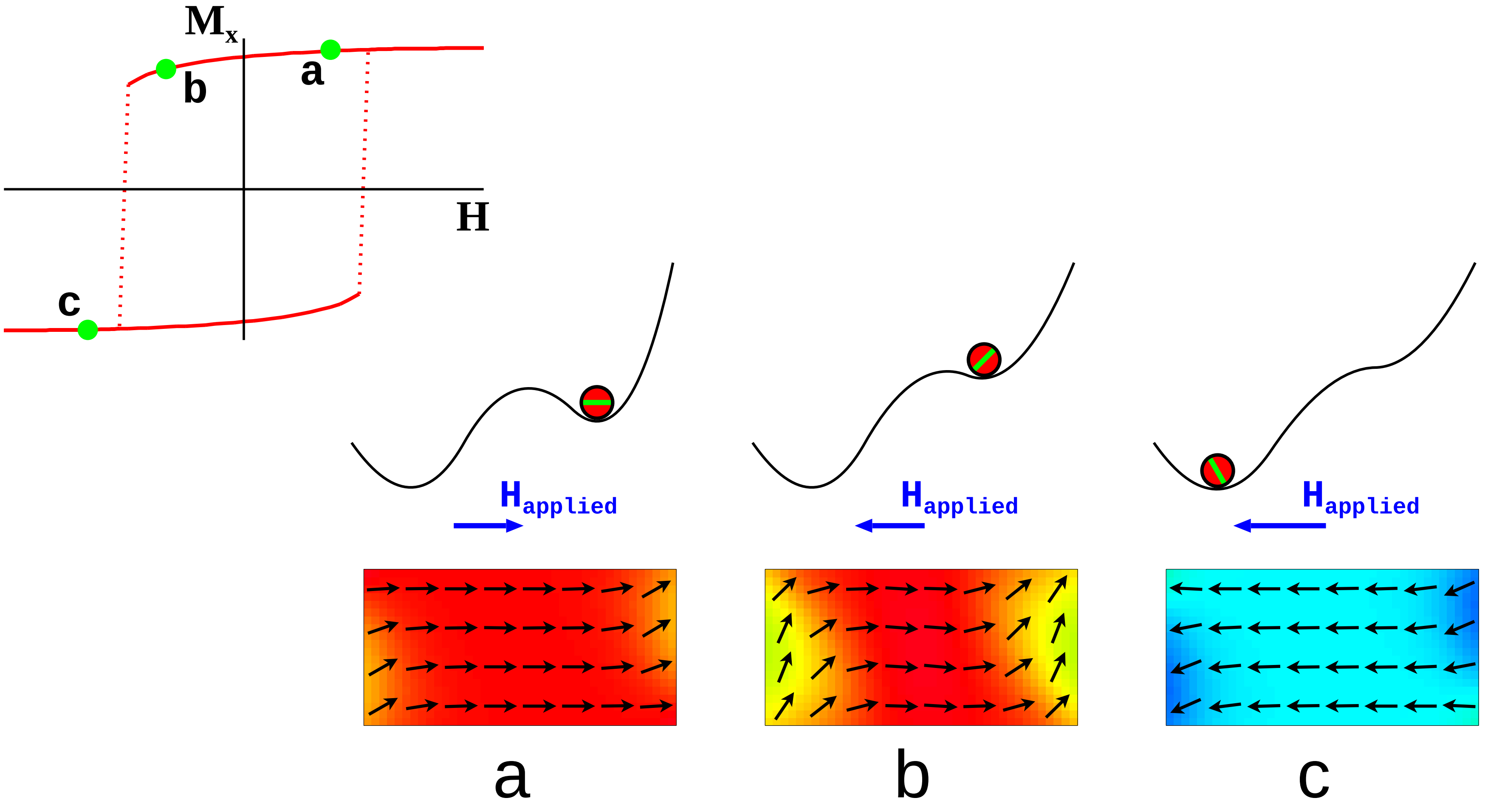
Magnetic disk storage



Magnetic disk storage



Quasi-static micromagnetics



Magnetization dynamics

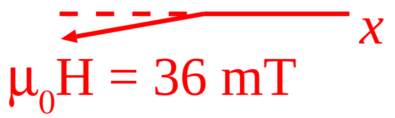
Landau-Lifshitz-Gilbert:

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

where

$$\begin{aligned} \mathbf{H}_{\mathrm{eff}} &= -\frac{1}{\mu_0}\frac{\partial E}{\partial \mathrm{M}} \\ \omega &= \text{gyromagnetic ratio} \\ \alpha &= \text{damping coefficient} \end{aligned}$$

Magnetization dynamics

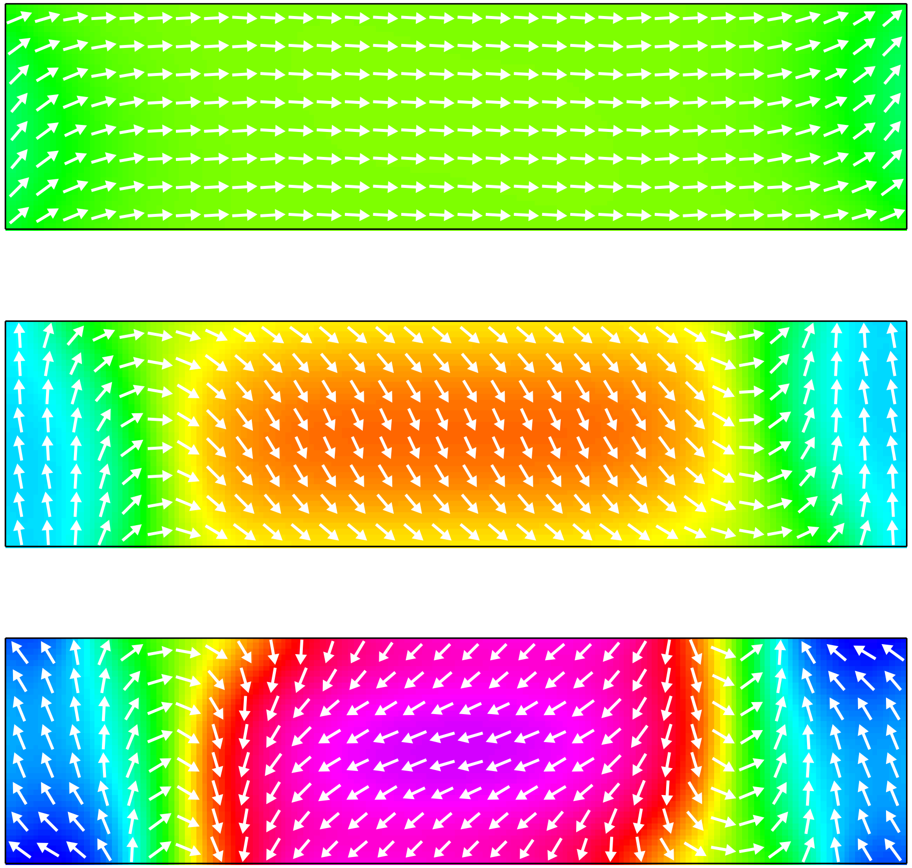


Time

0 ps

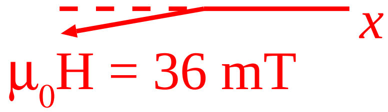
100 ps

150 ps



Magnetization dynamics

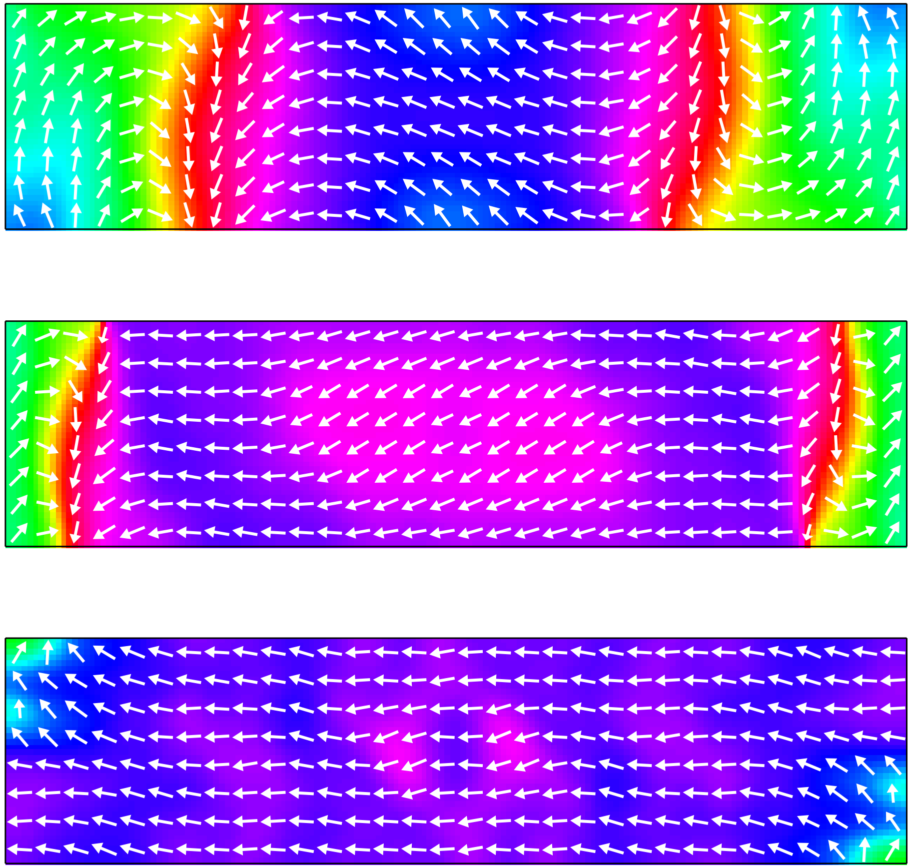
Time



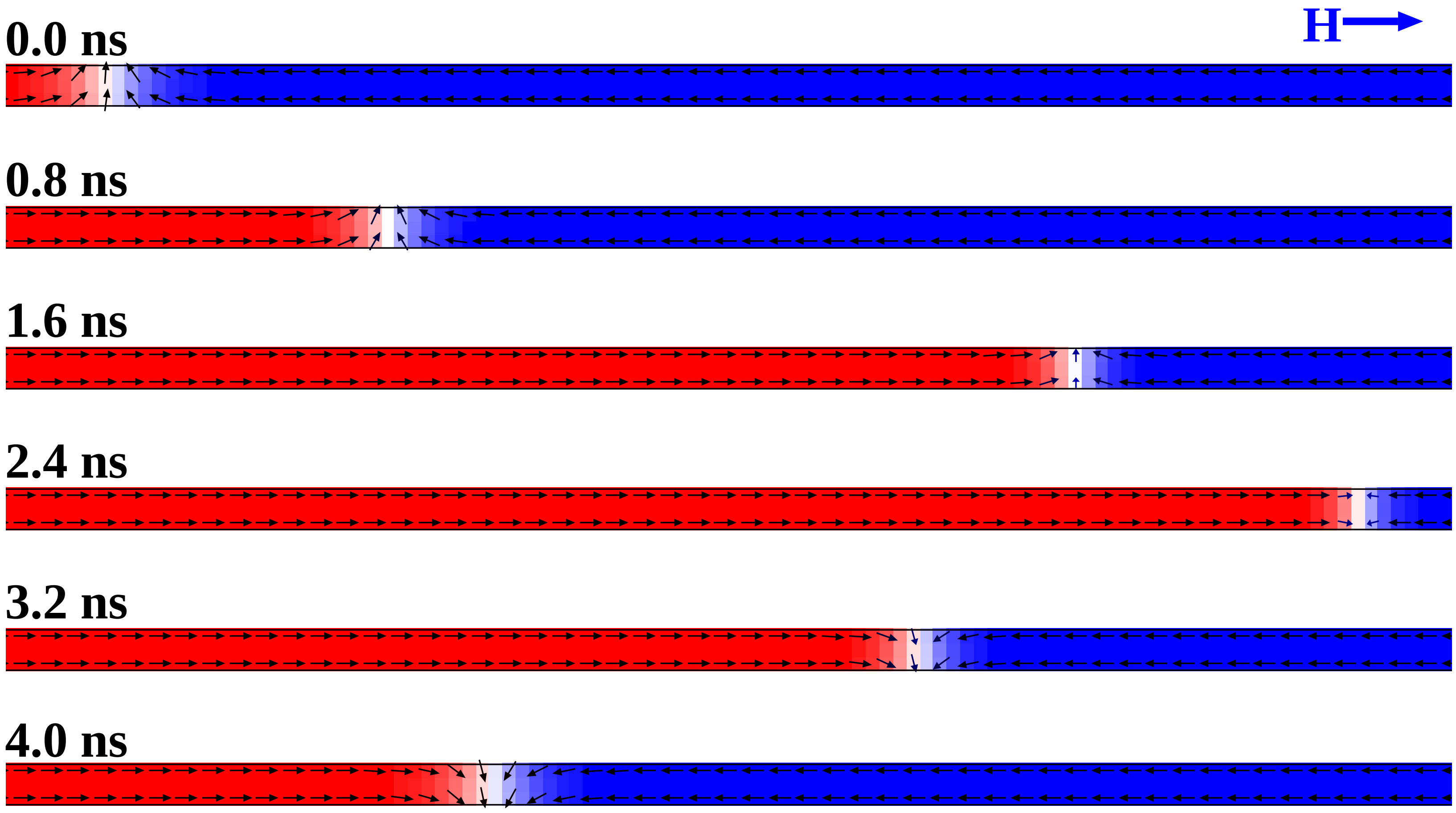
350 ps

450 ps

750 ps



Magnetization yoyo



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

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

Brown's equations

Energies:

$$
\begin{aligned}
E_{\text{exchange}} &= \int_V \frac{A}{M_s^2}\left(|\nabla M_x|^2 + |\nabla M_y|^2 + |\nabla M_z|^2\right)\, d^3r \\
E_{\text{anisotropy}} &= \int_V \frac{K_1}{M_s^2}(\mathbf{M}\cdot\mathbf{u})^2\, d^3r \\
E_{\text{demag}} &= \frac{\mu_0}{8\pi}\int_V \mathbf{M}(r)\cdot\left[\int_V \nabla\cdot\mathbf{M}(\mathbf{r}')\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}\, d^3r'\right. \\
&\qquad\qquad \left. - \int_S \hat{\mathbf{n}}\cdot\mathbf{M}(\mathbf{r}')\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}\, d^2r'\right]\, d^3r \\
E_{\text{Zeeman}} &= -\mu_0\int_V \mathbf{M}\cdot\mathbf{H}_{\text{ext}}\, d^3r
\end{aligned}
$$

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 cell size
k is approximation order

Discrete approximation

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

- Numerical integration
- Integrand representation
- Boundary conditions

Numerical integration

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

Closed intervals, $x_k = a + kh$,

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

Numerical integration

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

Open intervals, $x_k = a + (k - 1/2)h$,

$$\begin{aligned} O(h^2) \text{ error: } (w_k) &= [1 \;\; 1 \;\; 1 \;\; \ldots \;\; 1] \\ O(h^4) \text{ error: } (w_k) &= \left[\tfrac{13}{12} \;\; \tfrac{7}{8} \;\; \tfrac{25}{24} \;\; 1 \;\; 1 \;\; \ldots \;\; 1 \;\; \tfrac{25}{24} \;\; \tfrac{7}{8} \;\; \tfrac{13}{12}\right] \end{aligned}$$

Integrand representation

$$E_{\text{exchange}} = \int_V A\left(|\nabla m_x|^2 + |\nabla m_y|^2 + |\nabla m_z|^2\right) d^3r$$
$$= -\int_V A\,\mathbf{m}\cdot\left(\frac{\partial^2 \mathbf{m}}{\partial x^2} + \frac{\partial^2 \mathbf{m}}{\partial y^2} + \frac{\partial^2 \mathbf{m}}{\partial z^2}\right) d^3r$$

Since

$$|\nabla f|^2 = \nabla \cdot (f \nabla f) - f \nabla^2 f$$

and

$$\|\mathbf{m}\| = 1.$$

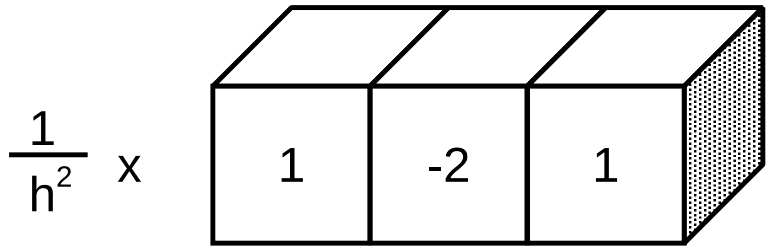
Discretized energy

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

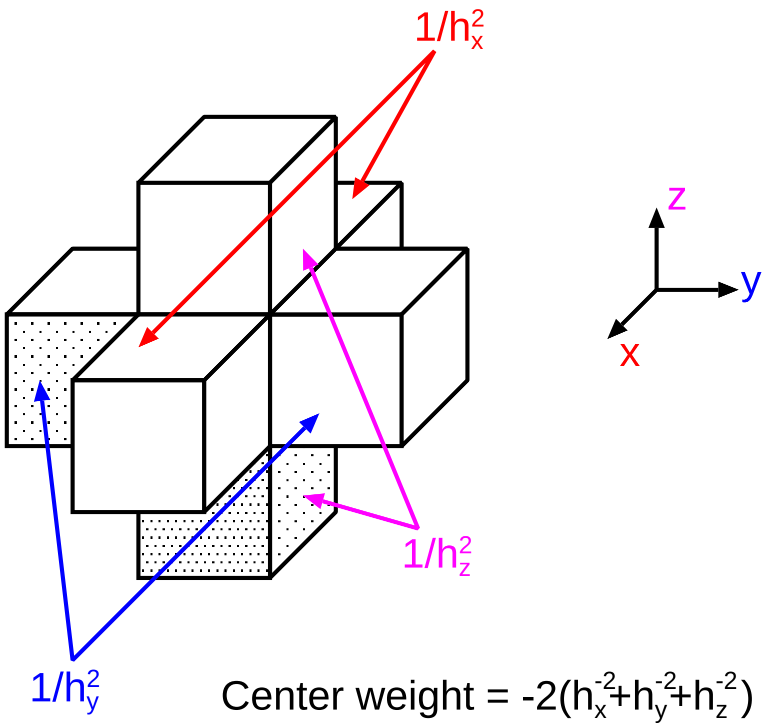
$$\approx\;\; -h_x h_y h_z \sum_{kjii'} w_k^z w_j^y w_i^x A_{ijk} d_{ii'}\,\mathbf{m}_{ijk}\cdot\mathbf{m}_{i'jk}$$

3-pt stencil

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



3-pt stencil

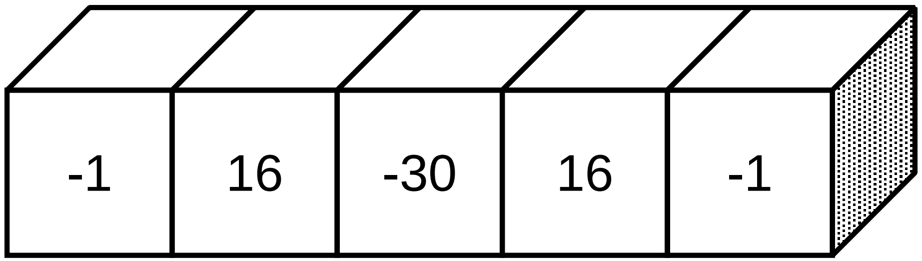


"6-neighbor exchange"

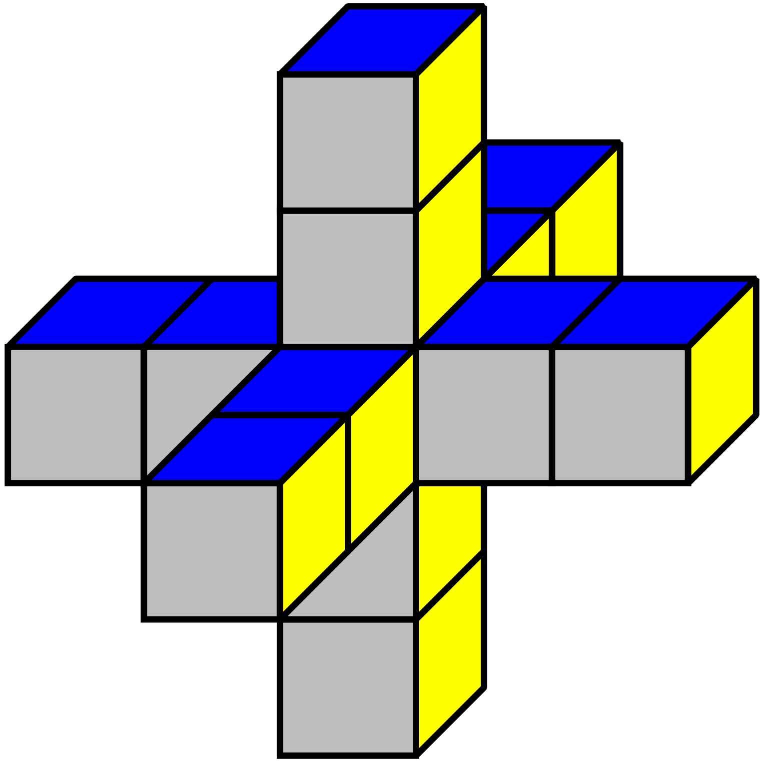
5-pt stencil

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

$\frac{1}{12h^2}$ x

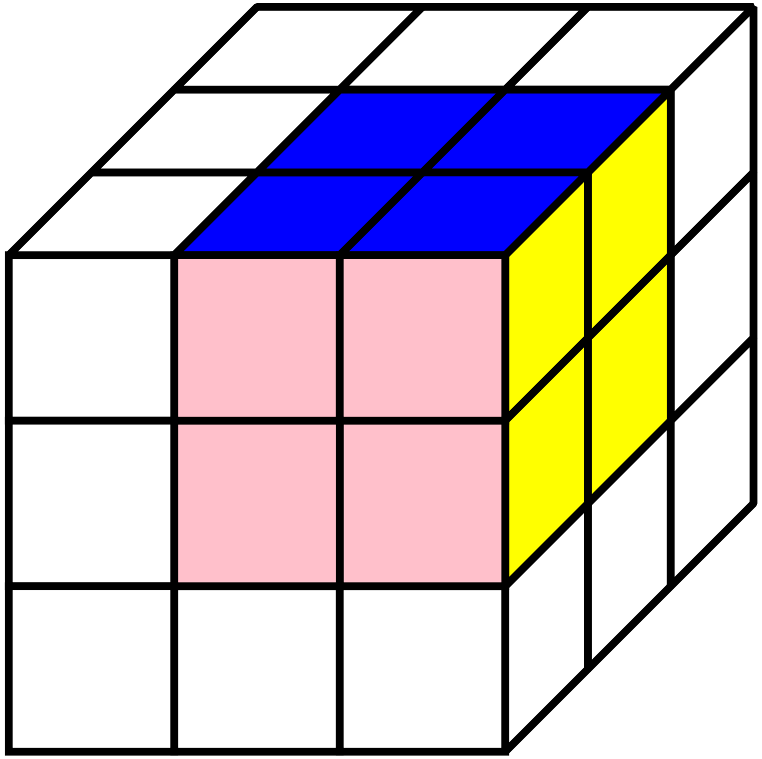


5-pt stencil



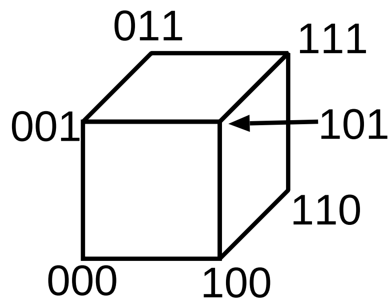
“12-neighbor exchange”

Trilinear interpolation



“26-neighbor exchange”

Trilinear interpolation



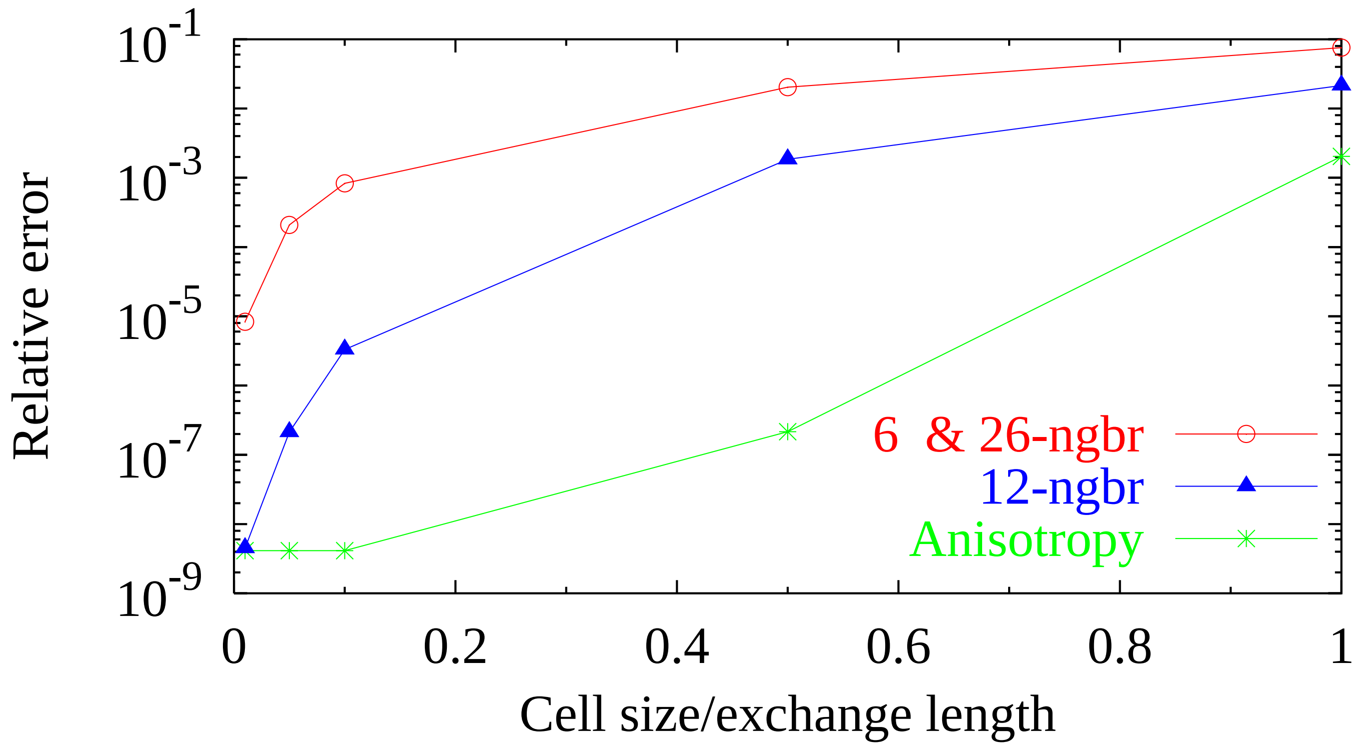
Given $\mathbf{m}_{000}, \mathbf{m}_{100}, \ldots,$ solve for

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

Then use

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

Analytic 1D domain wall



Relative energy error vs. discretization cell size

Exchange lengths

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

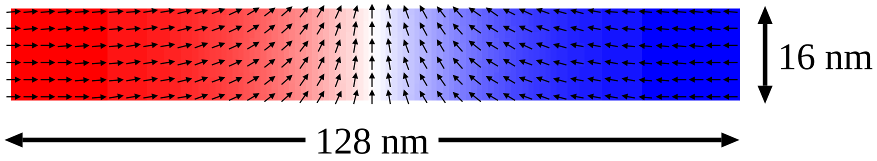
$$\text{Magnetocrystalline-exchange length} = \sqrt{\frac{A}{|K|}}$$

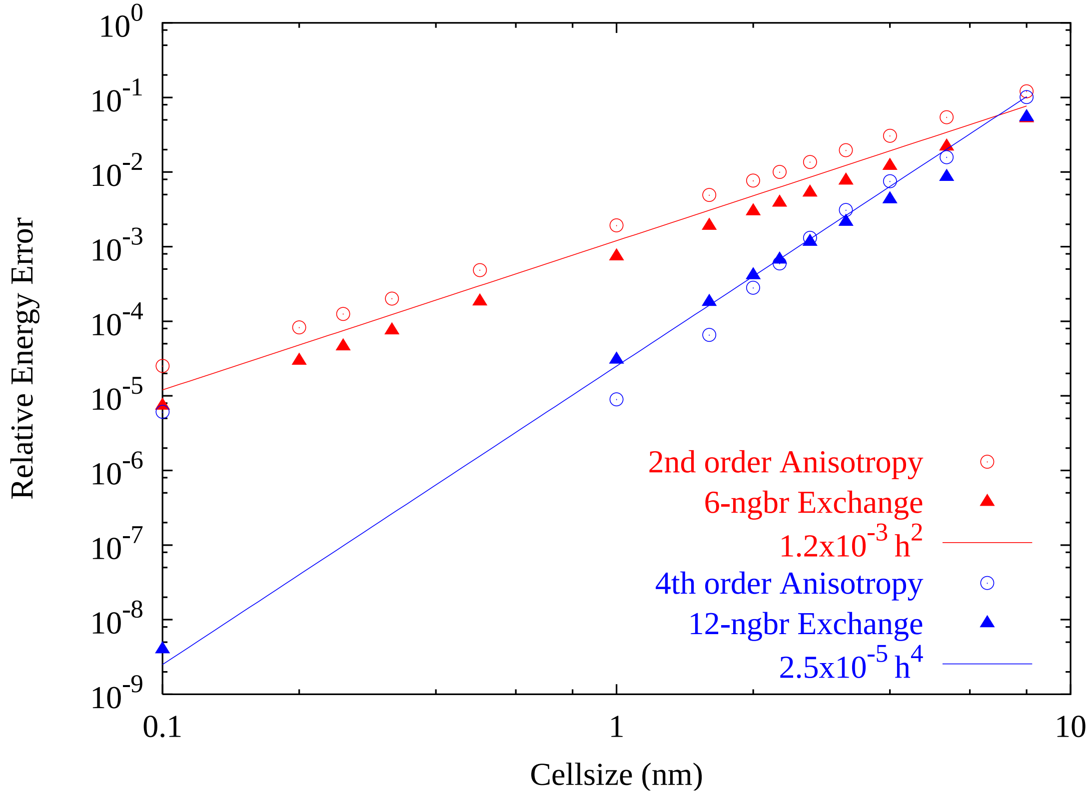
Convergence of equilibrium

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

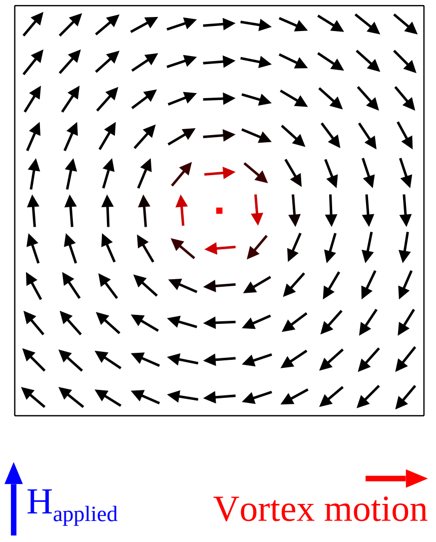
$K_u = (4.6 \times 10^5) r^2/(1+r^2)$ J/m^3

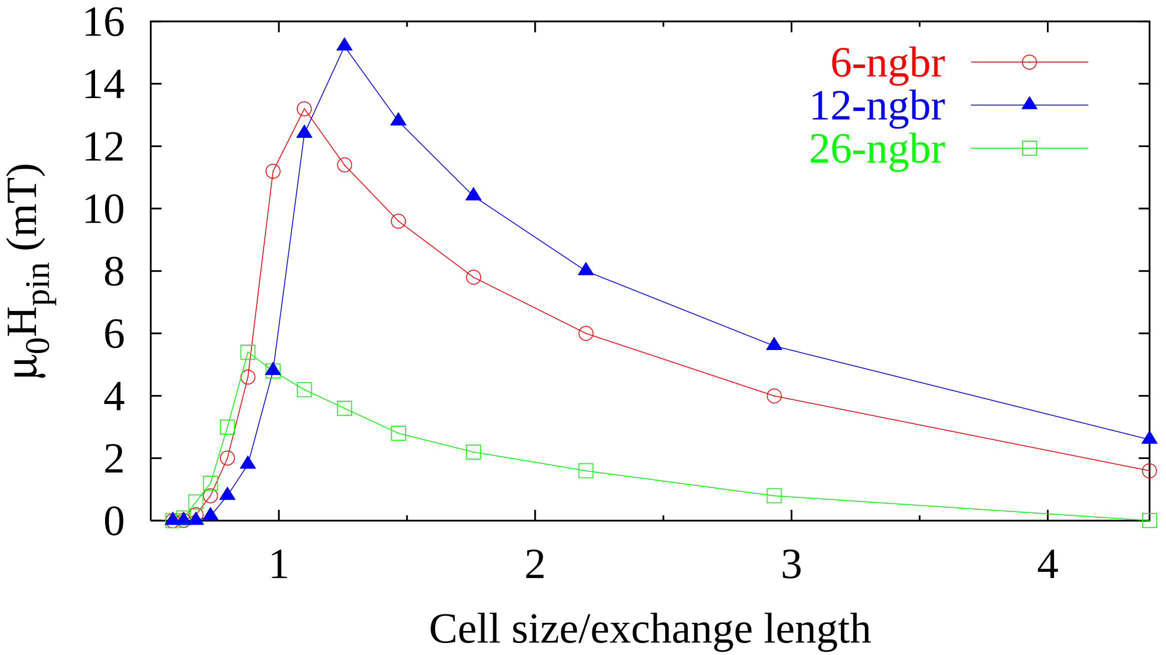
10 nm thick





Vortex mobility





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

Discretized energy

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

$$\approx\;\; -h_x h_y h_z \sum_{kjii'} w_k^z w_j^y w_i^x A_{ijk} d_{ii'}\,\mathbf{m}_{ijk}\cdot\mathbf{m}_{i'jk}$$

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

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

Boundary?

$$\frac{1}{h^2} \times \begin{bmatrix} \boxed{?} & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & 1 & -2 & 1 & \\ & & & 1 & -2 & 1 \\ & & & & & \ddots \end{bmatrix}$$

Boundary conditions, 6-ngbr

Neumann boundary:

$$\left.\frac{\partial^2 \mathbf{m}}{\partial x^2}\right|_{x_1} = \frac{\mathbf{m}_2 - \mathbf{m}_1}{h^2} - \frac{1}{h}\left.\frac{\partial \mathbf{m}}{\partial x}\right|_a + O(h).$$

Dirichlet boundary:

$$\left.\frac{\partial^2 \mathbf{m}}{\partial x^2}\right|_{x_1} = \frac{4\mathbf{m}_2 - 12\mathbf{m}_1}{3h^2} + \frac{8}{3h^2}\mathbf{m}(a) + O(h).$$

6-ngbr, Neumann

$$(d_{ii'}) = \frac{1}{h^2} \begin{bmatrix} -1 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & 1 & -2 & 1 \\ & & & & \ddots \end{bmatrix}$$

+ boundary derivative field (if any).

6-ngbr, Dirichlet

$$(d_{ii'}) = \frac{1}{h^2} \begin{bmatrix} -4 & 4/3 & & & & \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & 1 & -2 & 1 & \\ & & & & \ddots & \end{bmatrix}$$

+ boundary value field.

Discretized representation

$$
\begin{aligned}
& -\iiint A\,\mathbf{m}\cdot\frac{\partial^2\mathbf{m}}{\partial x^2}\;d^3r \\
\approx\;\; & -h_x h_y h_z \sum_{jk} w_k^z w_j^y \sum_{ii'} A_{ijk} w_i^x d_{ii'}\,\mathbf{m}_{ijk}\cdot\mathbf{m}_{i'jk} \\
\stackrel{\text{def}}{=}\;\; & \Phi
\end{aligned}
$$

Discretized representation

$$\frac{\partial \Phi}{\partial \mathbf{m}_{ijk}} = -2h_x h_y h_z \sum_{jk} w_k^z w_j^y \sum_{ii'} c_{ii'jk} \mathbf{m}_{i'jk}$$

where

$$c_{ii'jk} = \left(A_{ijk} w_i^x d_{ii'} + A_{i'jk} w_{i'}^x d_{i'i}\right) /2$$

or

$$c_{ii'} = A \left(w_i^x d_{ii'} + w_{i'}^x d_{i'i}\right) /2$$

if A is constant.

6-ngbr, Dirichlet

Clean up representation:

- Include w_i^x terms
- Symmetrize
- Adjust diagonal so row sums = 0

6-ngbr, Dirichlet

$$C = \frac{A}{h^2} \begin{bmatrix} -7/6 & 7/6 & & & \\ 7/6 & -13/6 & 1 & & \\ & 1 & -2 & 1 & \\ & & 1 & -2 & 1 \\ & & & & \ddots \end{bmatrix}$$

+ boundary value field.

12-ngbr, Neumann boundary

$$\left.\frac{\partial^2 \mathbf{m}}{\partial x^2}\right|_{x_1} = \frac{-59\mathbf{m}_1 + 64\mathbf{m}_2 - 5\mathbf{m}_3}{38h^2}$$

$$-\frac{16}{19h}\left.\frac{\partial \mathbf{m}}{\partial x}\right|_a - \frac{11}{19h}\left.\frac{\partial \mathbf{m}}{\partial x}\right|_{x_1} + O(h^3)$$

Norm constraint $\Rightarrow \mathbf{m}_1 \cdot \partial \mathbf{m}/\partial x|_{x_1} = 0$.

12-ngbr, Neumann boundary

$$\left.\frac{\partial^2 \mathbf{m}}{\partial x^2}\right|_{x_2} = \frac{335\mathbf{m}_1 - 669\mathbf{m}_2 + 357\mathbf{m}_3 - 23\mathbf{m}_4}{264h^2}$$

$$+\frac{1}{11h}\left.\frac{\partial \mathbf{m}}{\partial x}\right|_a + O(h^3)$$

12-ngbr, Neumann boundary

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

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

12-ngbr, Dirichlet boundary

$$\left.\frac{\partial^2 \mathbf{m}}{\partial x^2}\right|_{x_1} = \frac{-165\mathbf{m}_1 + 40\mathbf{m}_2 - 3\mathbf{m}_3}{30h^2}$$

$$+\frac{64}{15h}\mathbf{m}(a) + \frac{1}{h}\left.\frac{\partial \mathbf{m}}{\partial x}\right|_{x_1} + O(h^3)$$

Norm constraint $\Rightarrow \mathbf{m}_1 \cdot \partial\mathbf{m}/\partial x|_{x_1} = 0$.

12-ngbr, Dirichlet boundary

$$\left.\frac{\partial^2 \mathbf{m}}{\partial x^2}\right|_{x_2} = \frac{4\mathbf{m}_1 - 15\mathbf{m}_2 + 12\mathbf{m}_3 - 4\mathbf{m}_4}{6h^2}$$

$$-\frac{1}{h}\left.\frac{\partial \mathbf{m}}{\partial x}\right|_{x_2} + O(h^3)$$

Norm constraint $\Rightarrow \mathbf{m}_2 \cdot \partial \mathbf{m}/\partial x|_{x_2} = 0$.

12-ngbr, Dirichlet boundary

$$C = \frac{A}{12h^2}\begin{bmatrix} -11.0 & 12.2 & -1.2 & & & & \\ 12.2 & -29.6 & 18.8 & -1.4 & & & \\ -1.2 & 18.8 & -33.0 & 16.3 & -1 & & \\ & -1.4 & 16.3 & -30.0 & 16 & -1 & \\ & & -1 & 16 & -30 & 16 & -1 \\ & & & & & \ddots & \end{bmatrix}$$

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

Eigenvalue analysis

For 6-ngbr methods:

$$\text{Eigenvalues of } -C \subset [0, 4)$$

For 12-ngbr methods:

$$\text{Eigenvalues of } -C \subset [0, 5\tfrac{1}{3})$$

$\Rightarrow$ Good iterative convergence!

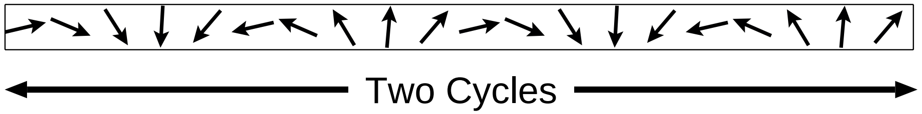
12-ngbr exchange

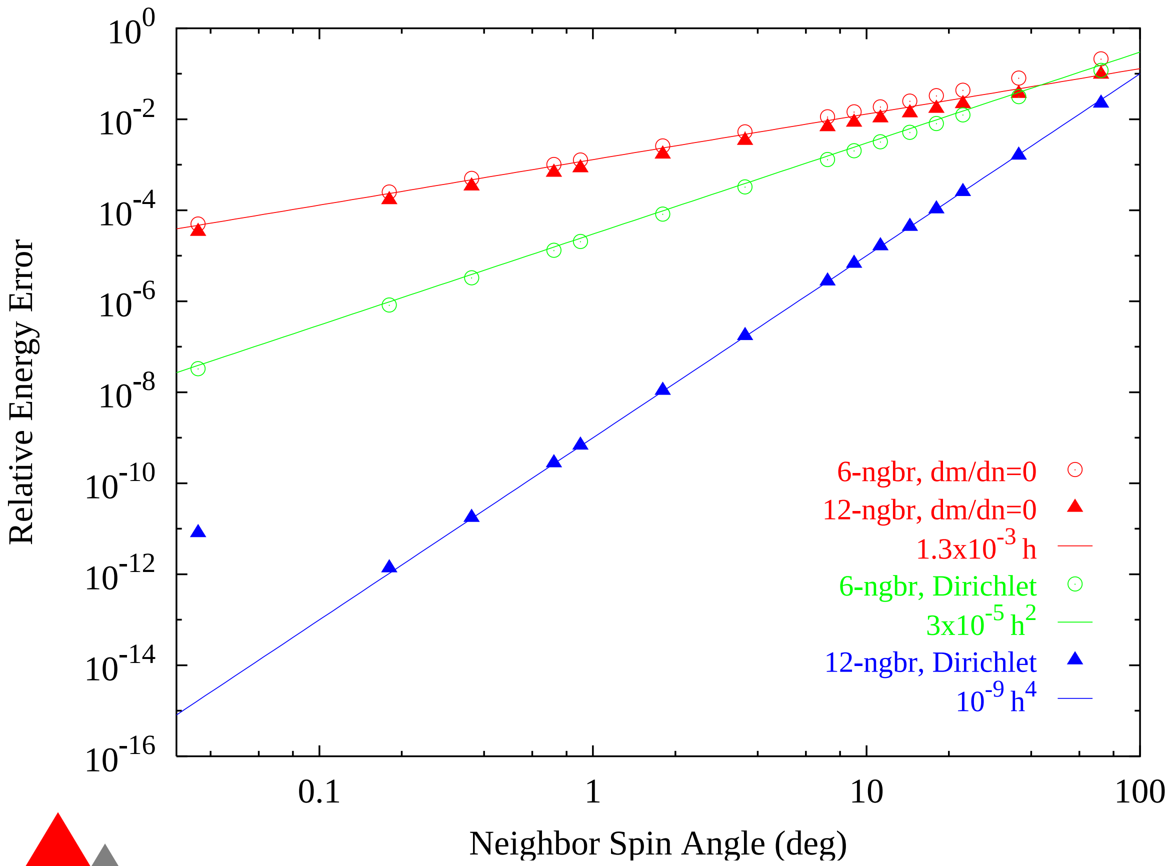
Assume $\partial \mathbf{m} / \partial \hat{\mathbf{n}} = 0$:

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

$\Rightarrow$ Bad eigenvalues!

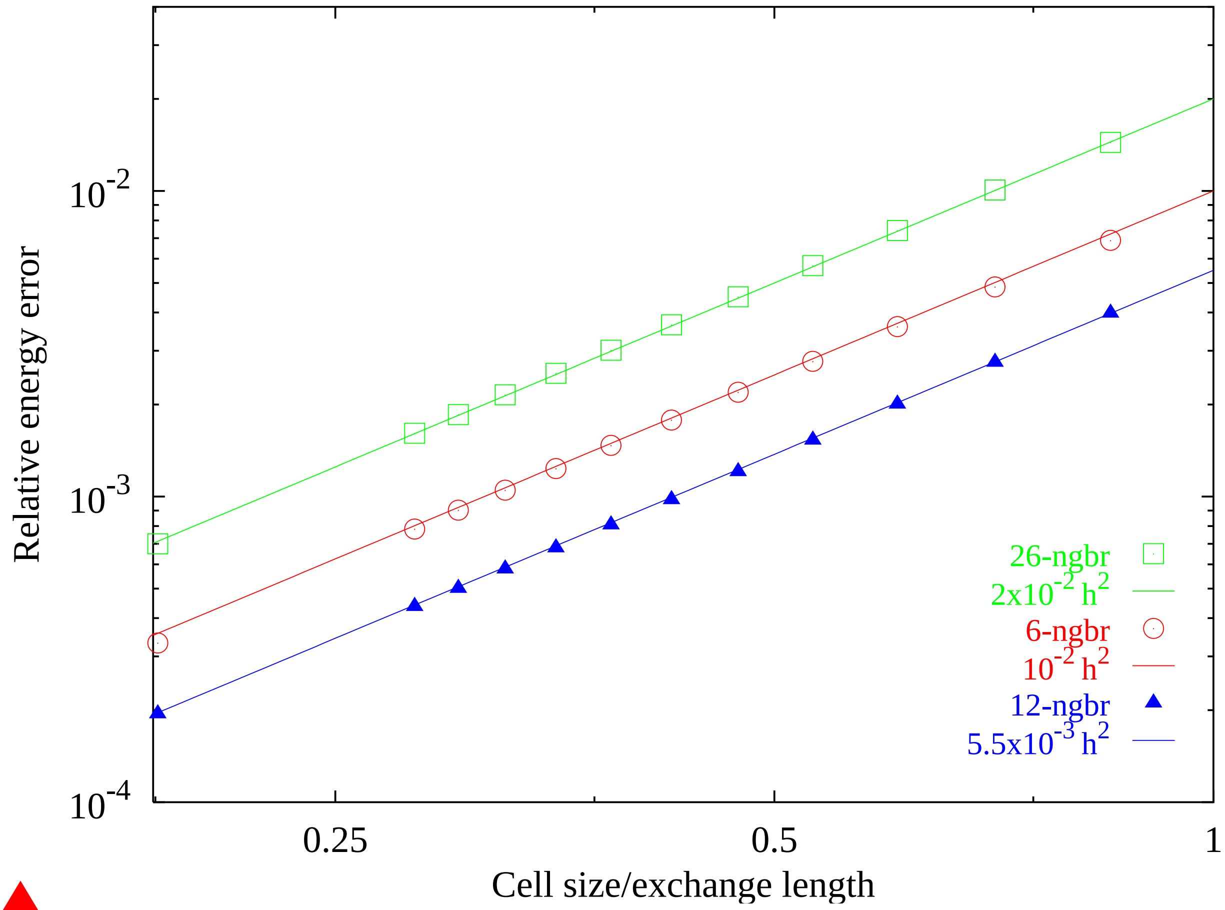
Magnetization spiral





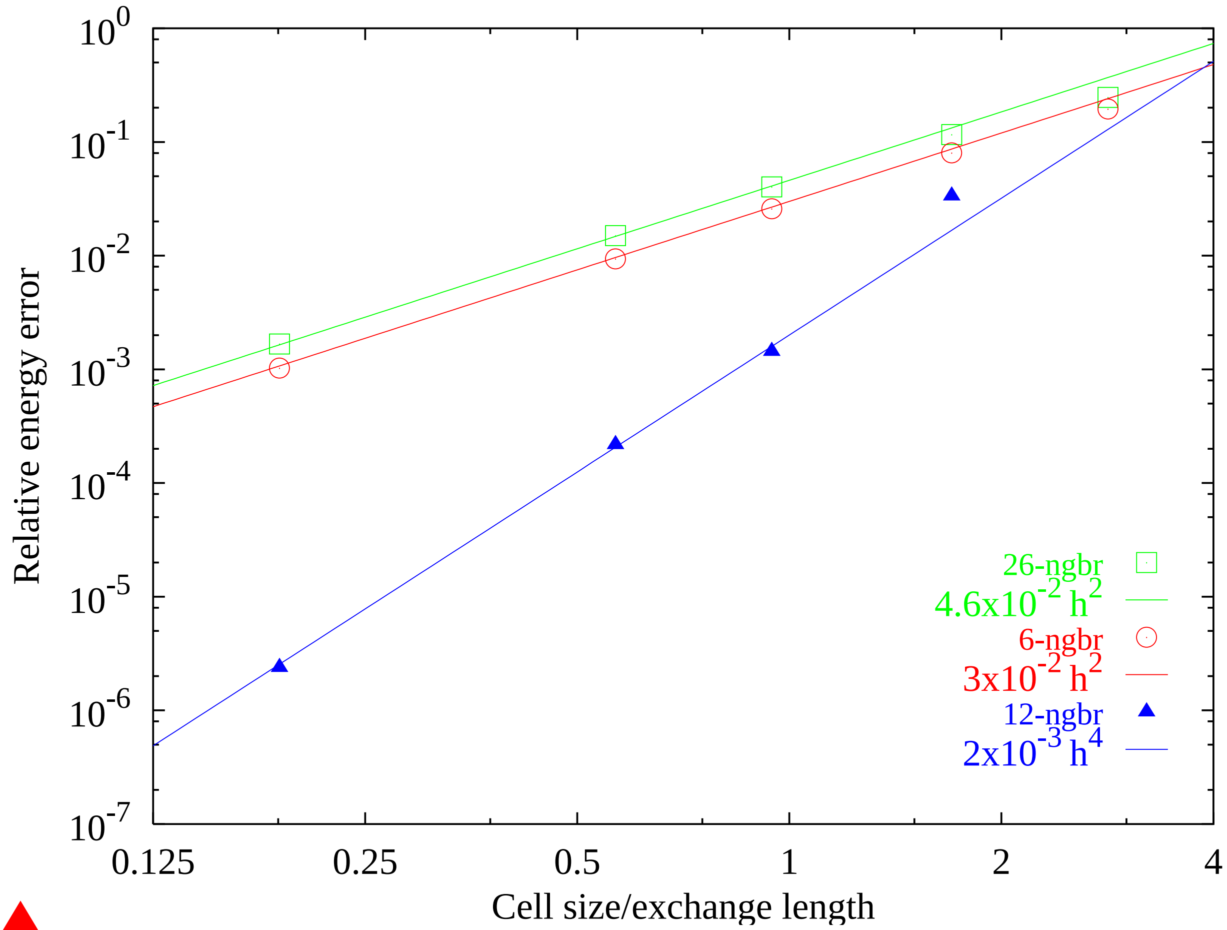
muMAG Standard Problem 3

Equilibria convergence:



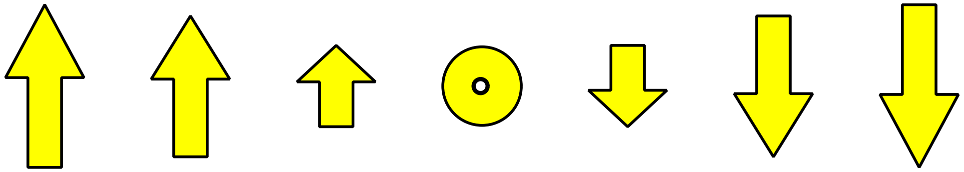
muMAG Standard Problem 3

Subsample convergence:



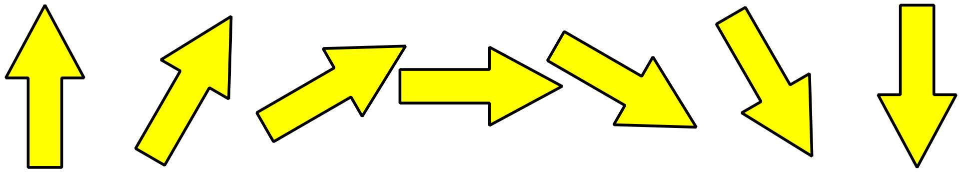
Wall types

Bloch wall



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

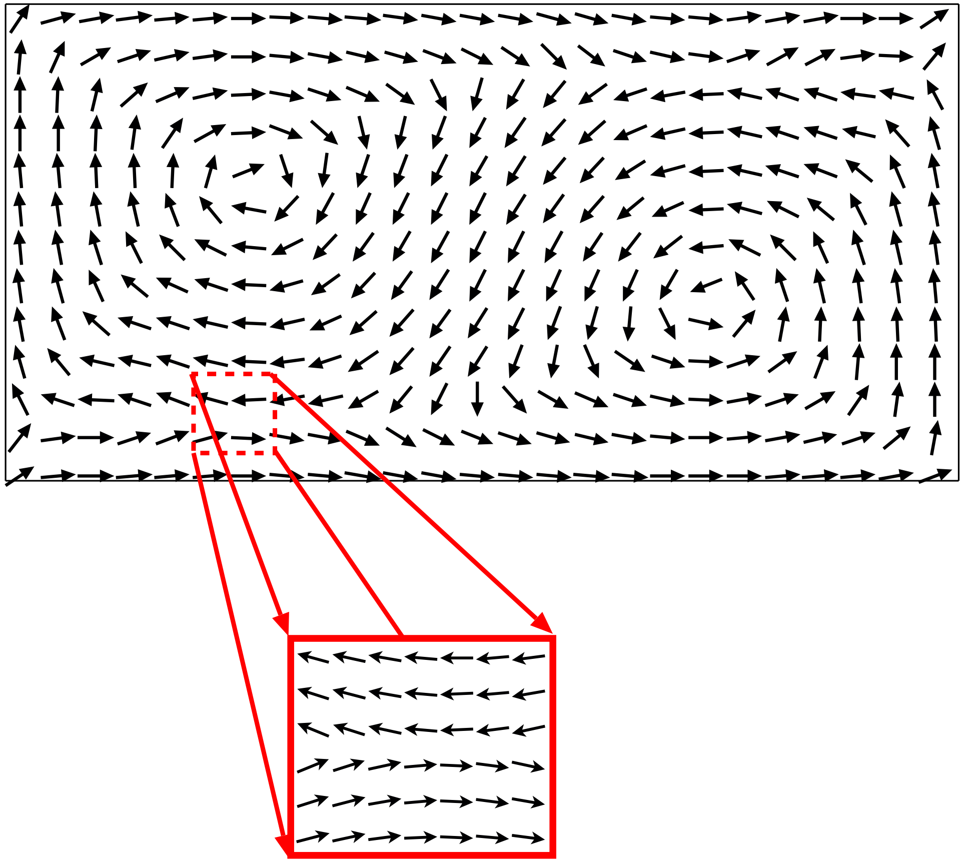
Néel wall



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

Néel-wall collapse

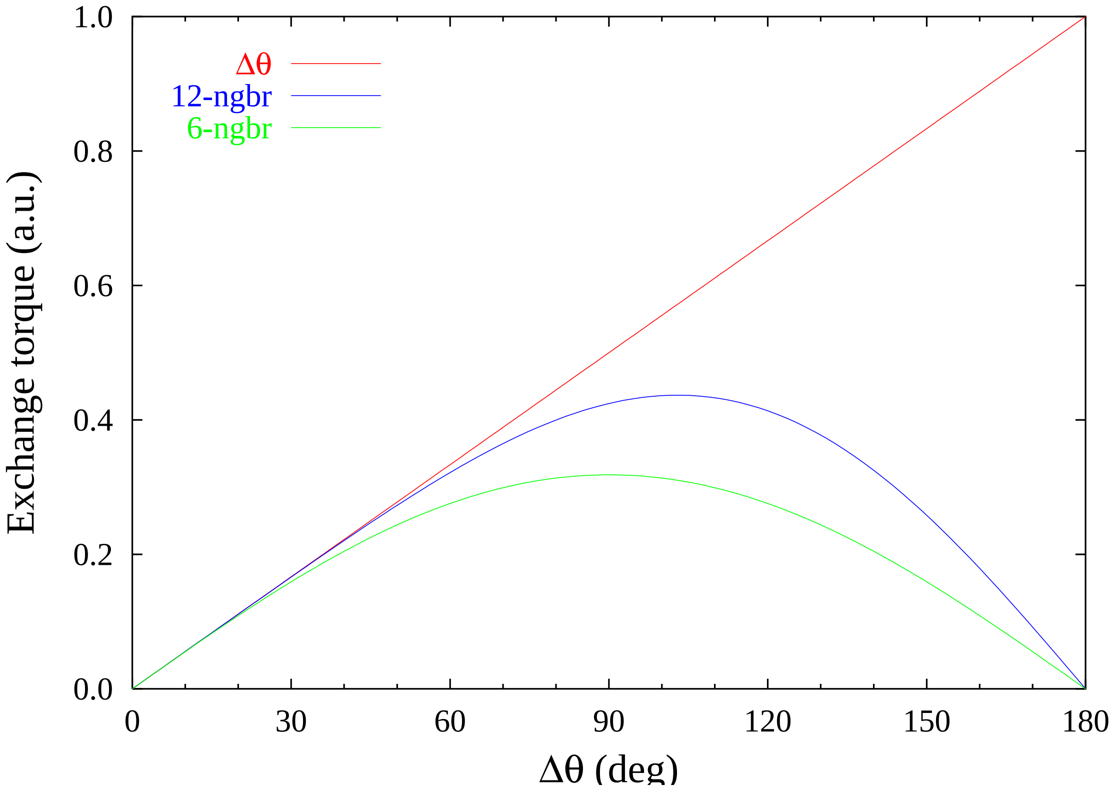
6-pt exchange, $\mu_0 H = 5$ mT, $h = 20$ nm



Magnetization spiral

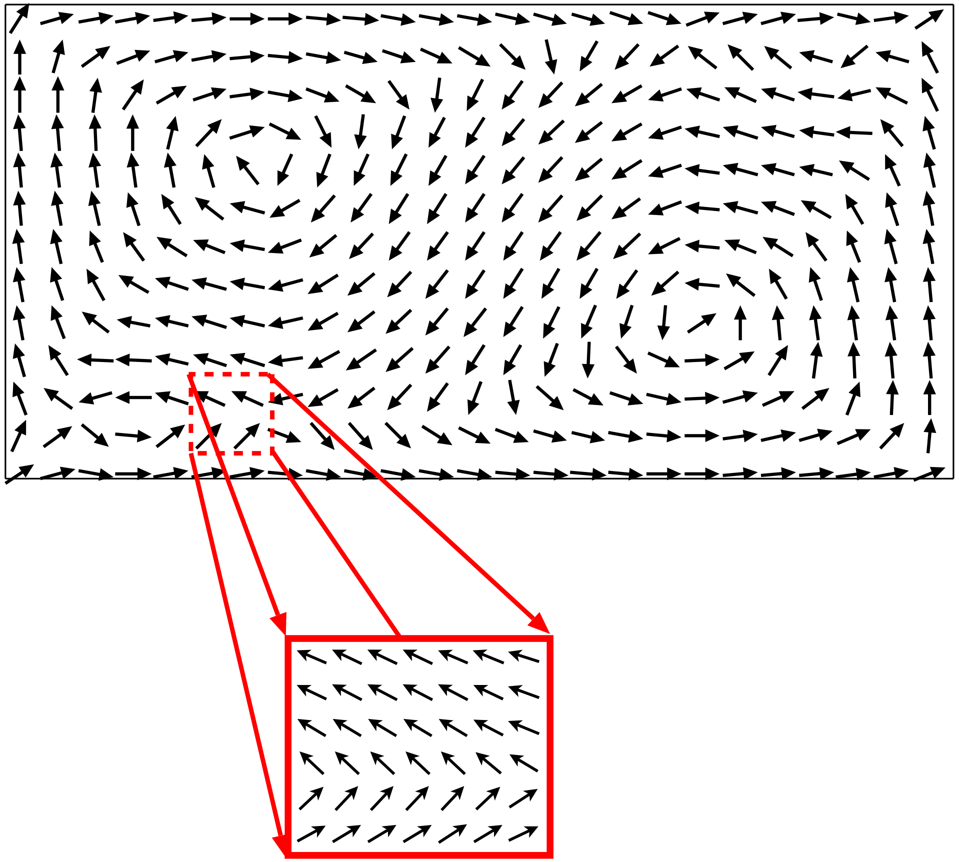
$$\mathbf{m} = (\cos \omega x, \sin \omega x)$$

Exchange torque vs. ω



Néel-wall non-collapse

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



Conclusions

- 6-ngbr and 26-ngbr are 2nd order.
- 12-ngbr is 4th order.
- Proper boundary conditions must be applied.
- Eigenvalues determine iterative behavior.
- 26-ngbr has less pinning for large cells, 12-ngbr dominates for $h < l_{\mathrm{ex}}$.
- 12-ngbr helps against Néel wall collapse.

References

- μMAG:

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

- OOMMF:

  http://math.nist.gov/oommf

- In press:

  M.J. Donahue and D.G. Porter, “Exchange Energy Formulations for 3D Micromagnetics,” *Physica B*