# *Exchange Energy Formulations for 3D Micromagnetics*

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# Exchange energy

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

$$= -\int_V A \, \mathbf{m} \cdot \left( \frac{\partial^2 \mathbf{m}}{\partial x^2} + \frac{\partial^2 \mathbf{m}}{\partial y^2} + \frac{\partial^2 \mathbf{m}}{\partial z^2} \right) \, d^3r$$

Since

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

and

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

# Discrete approximation

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

- Numerical integration
- Integrand representation
- Boundary conditions

# *Numerical integration*

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

Closed intervals, $x_k = a + kh$,

$O(h^2)$ error: $(w_k) \;=\; \left[\frac{1}{2} \;\; 1 \;\; 1 \;\; \ldots \;\; 1 \;\; \frac{1}{2}\right]$

$O(h^4)$ error: $(w_k) \;=\; \frac{1}{3}\left[1 \;\; 4 \;\; 2 \;\; 4 \;\; \ldots \;\; 2 \;\; 4 \;\; 1\right]$

$O(h^4)$ error: $(w_k) \;=\; \left[\frac{3}{8} \;\; \frac{7}{6} \;\; \frac{23}{24} \;\; 1 \;\; 1 \;\; \ldots \;\; 1 \;\; \frac{23}{24} \;\; \frac{7}{6} \;\; \frac{3}{8}\right]$

# Numerical integration

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

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

$$\begin{aligned} O(h^2) \text{ error: } (w_k) &= \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \end{bmatrix} \\ O(h^4) \text{ error: } (w_k) &= \begin{bmatrix} \frac{13}{12} & \frac{7}{8} & \frac{25}{24} & 1 & 1 & \dots & 1 & \frac{25}{24} & \frac{7}{8} & \frac{13}{12} \end{bmatrix} \end{aligned}$$

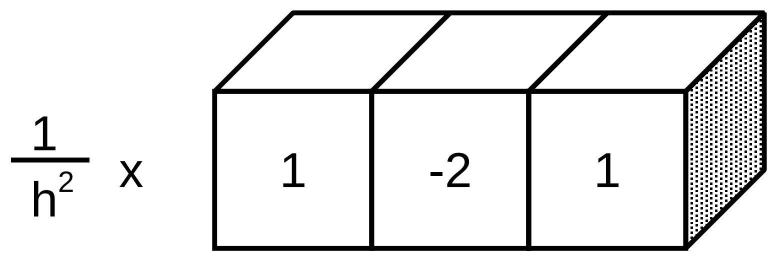
# Discretized energy

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

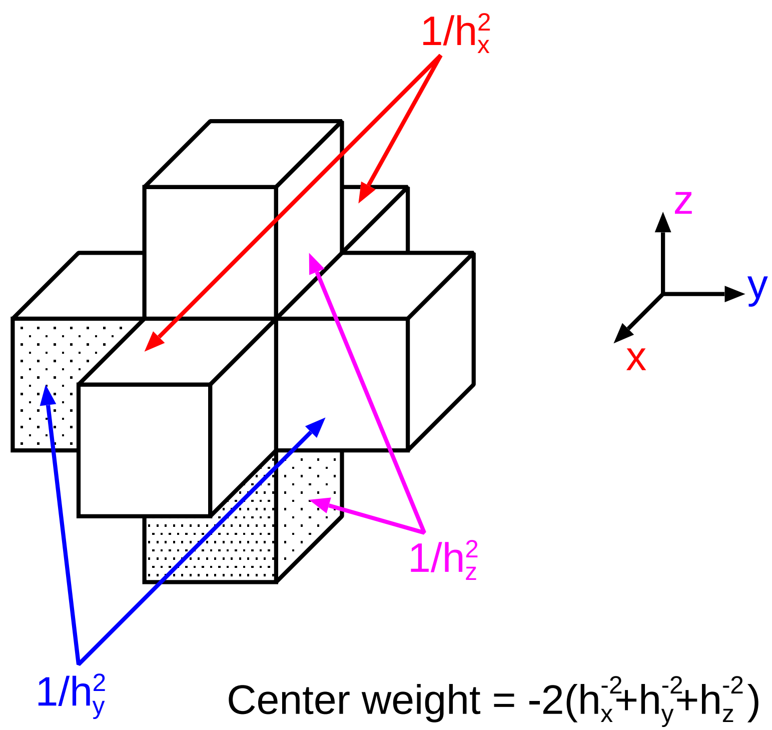
$$\approx\;-h_x h_y h_z\sum_{kjii'} w_k^z w_j^y w_i^x A_{ijk} d_{ii'}\,\mathbf{m}_{ijk}\cdot\mathbf{m}_{i'jk}$$

# 3-pt stencil

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



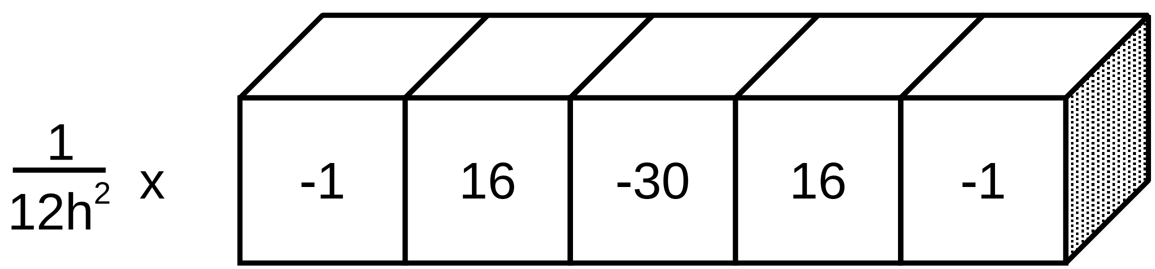
# *3-pt stencil*



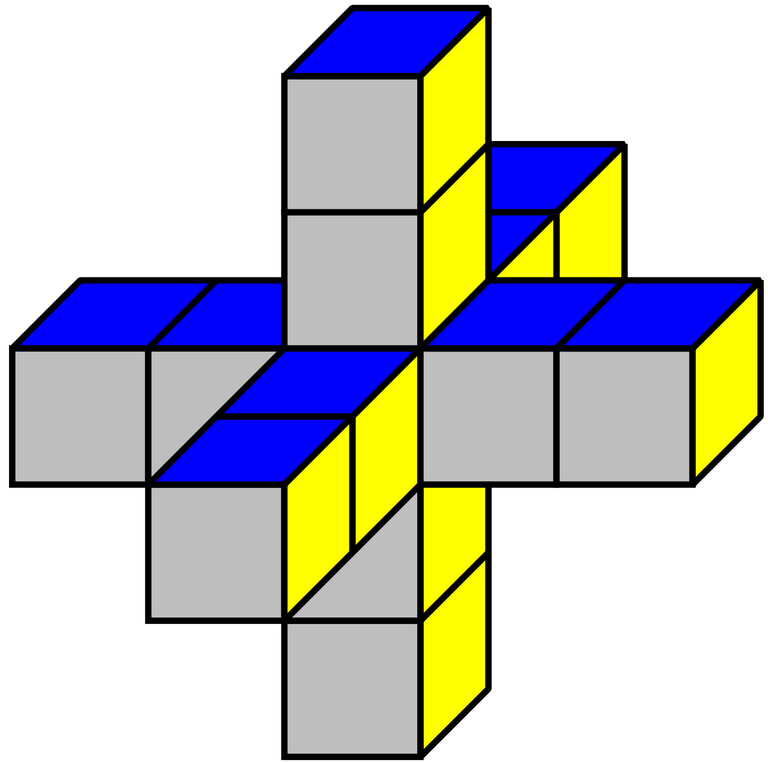

"6-neighbor exchange"

# 5-pt stencil

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

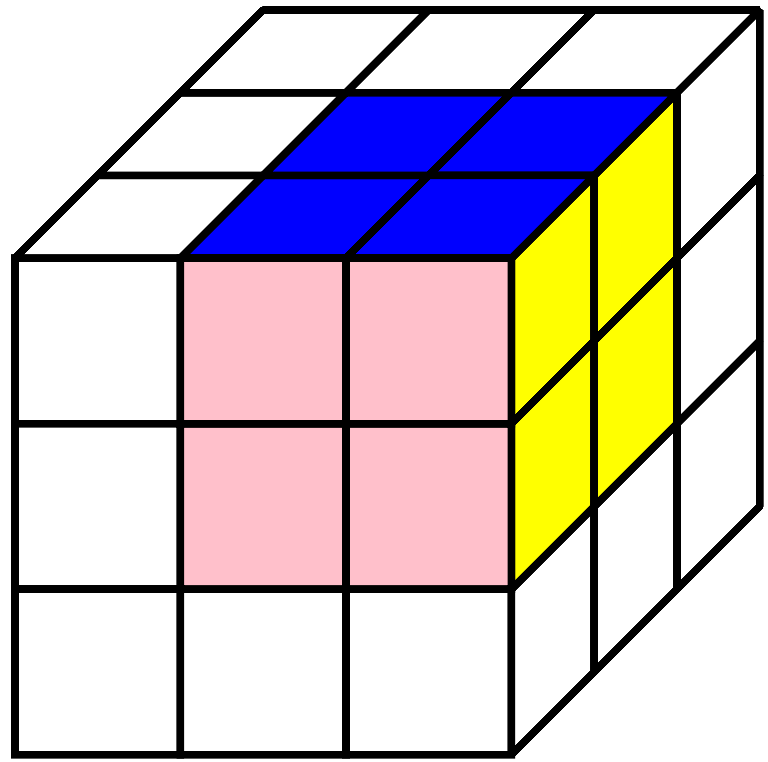


# *5-pt stencil*



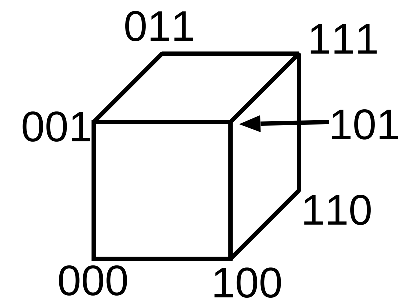
“12-neighbor exchange”

# *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

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

# *Boundary?*

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

# 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*

$$C = \frac{1}{h^2}\begin{bmatrix} -1 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & 1 & -2 & 1 & \\ & & & & \ddots & \end{bmatrix}$$

+ boundary derivative field (if any).

# *6-ngbr, Dirichlet*

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

+ boundary value field.

# Discretized representation

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

# 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, Neumann 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 method:

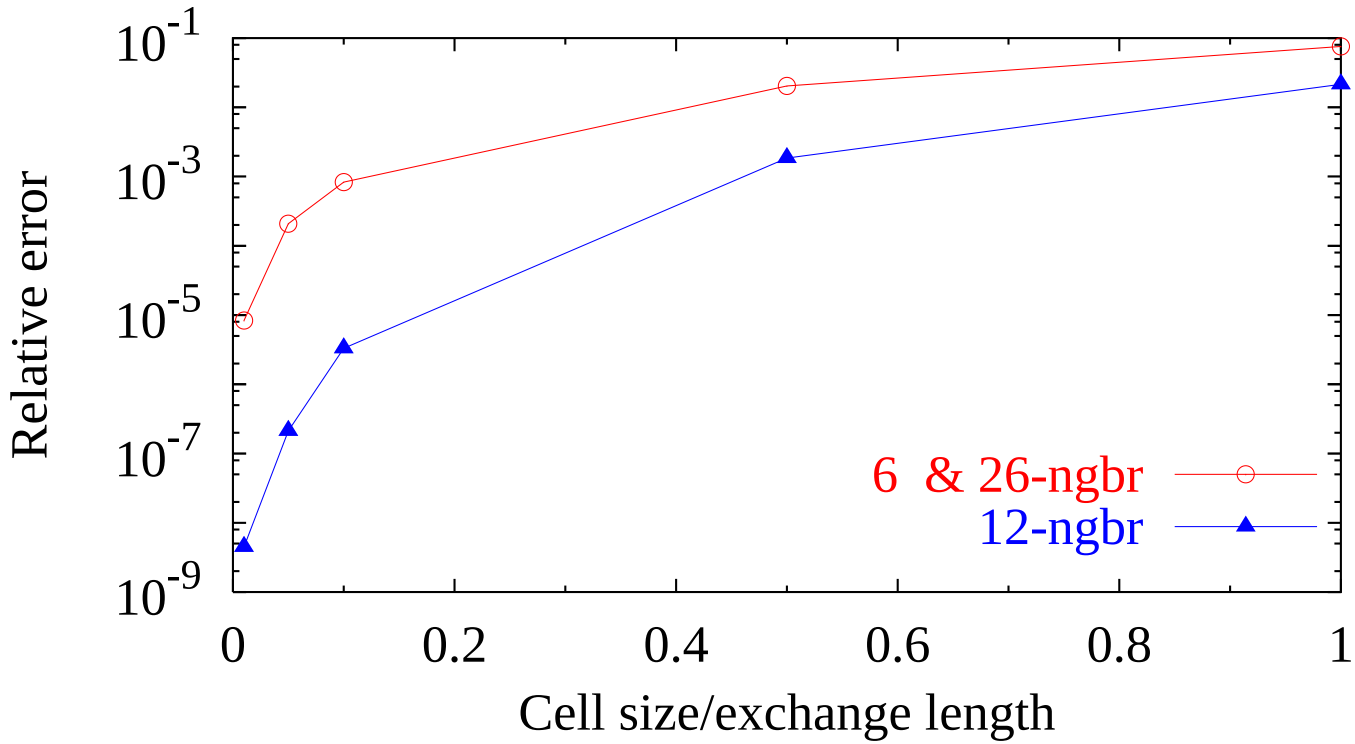
Eigenvalues of $-C \subset [0, 4)$

For 12-ngbr method:

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

$\Rightarrow$ Good iterative convergence!

# *Analytic 1D domain wall*



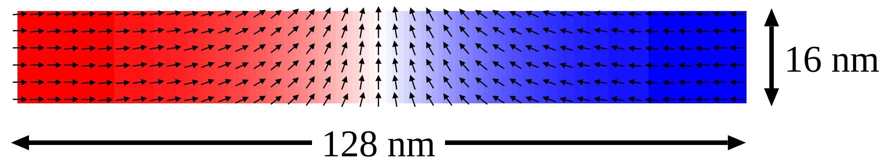

Relative energy error vs. discretization cell size

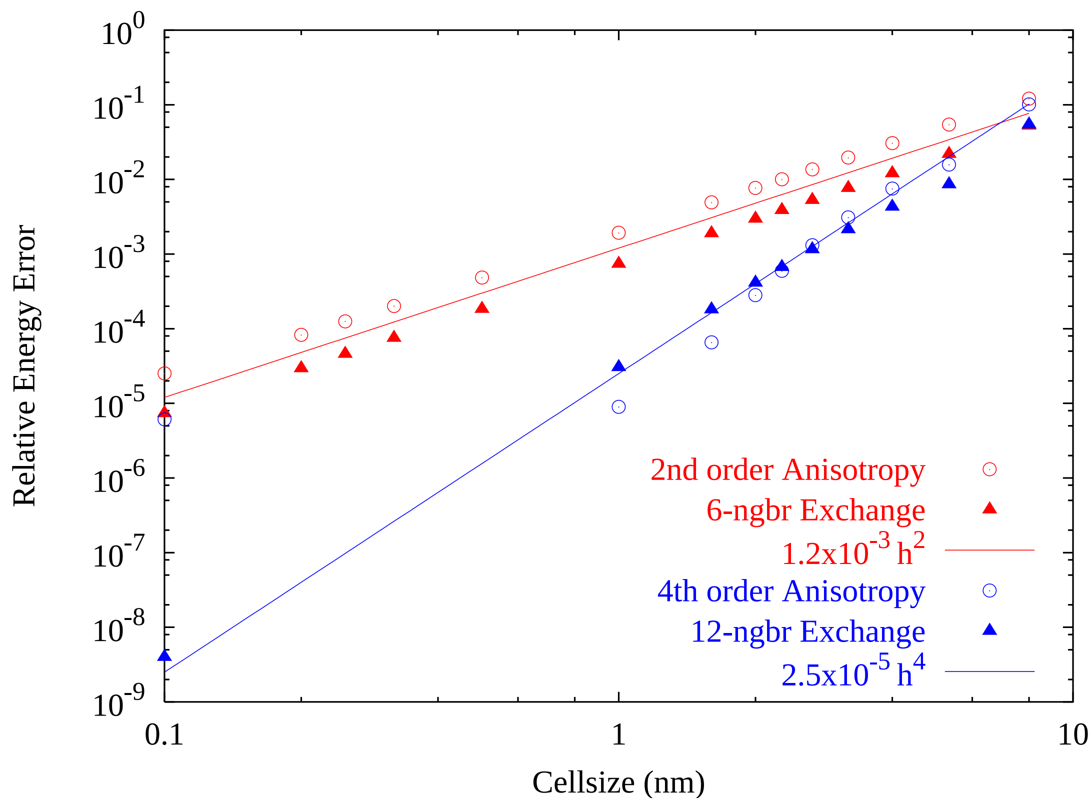
# *Equilibria convergence*

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

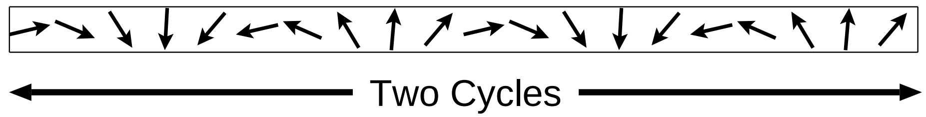
$K_u = (4.6 \times 10^{5}) r^2/(1+r^2)$ J/m$^3$

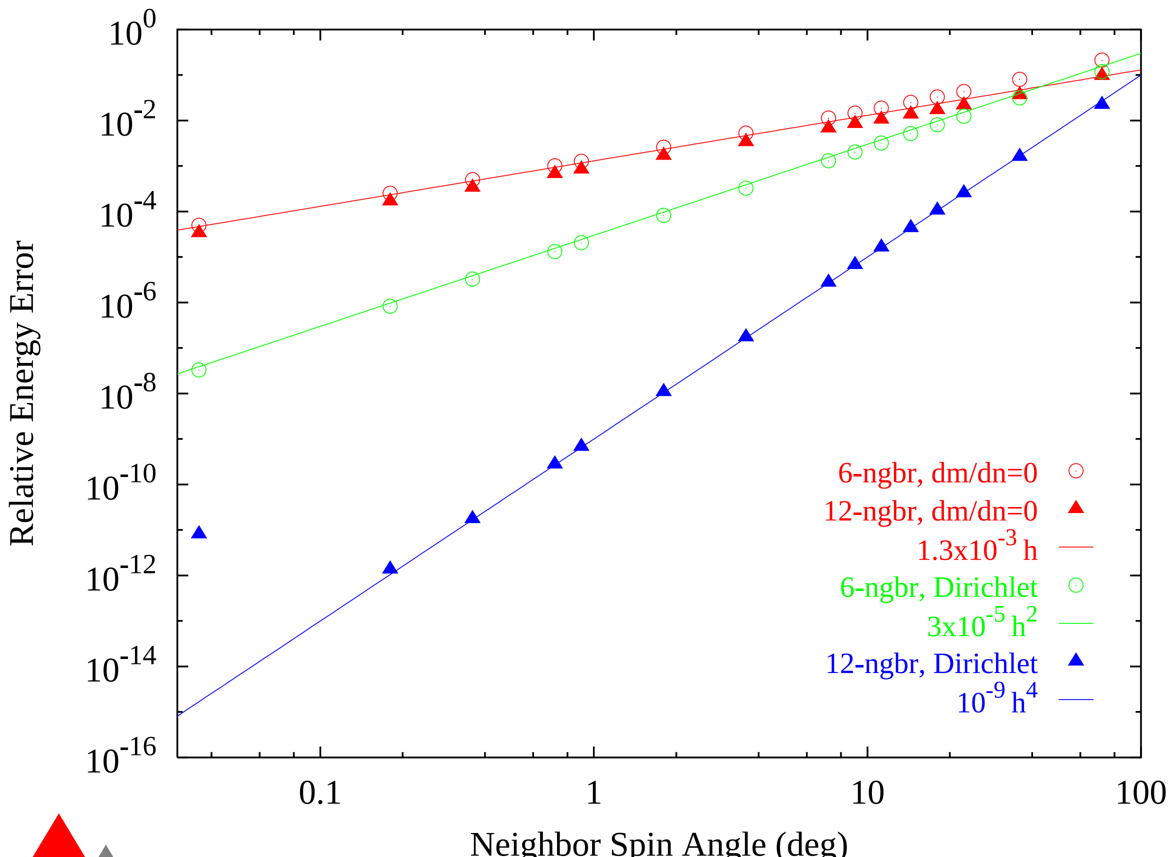
10 nm thick



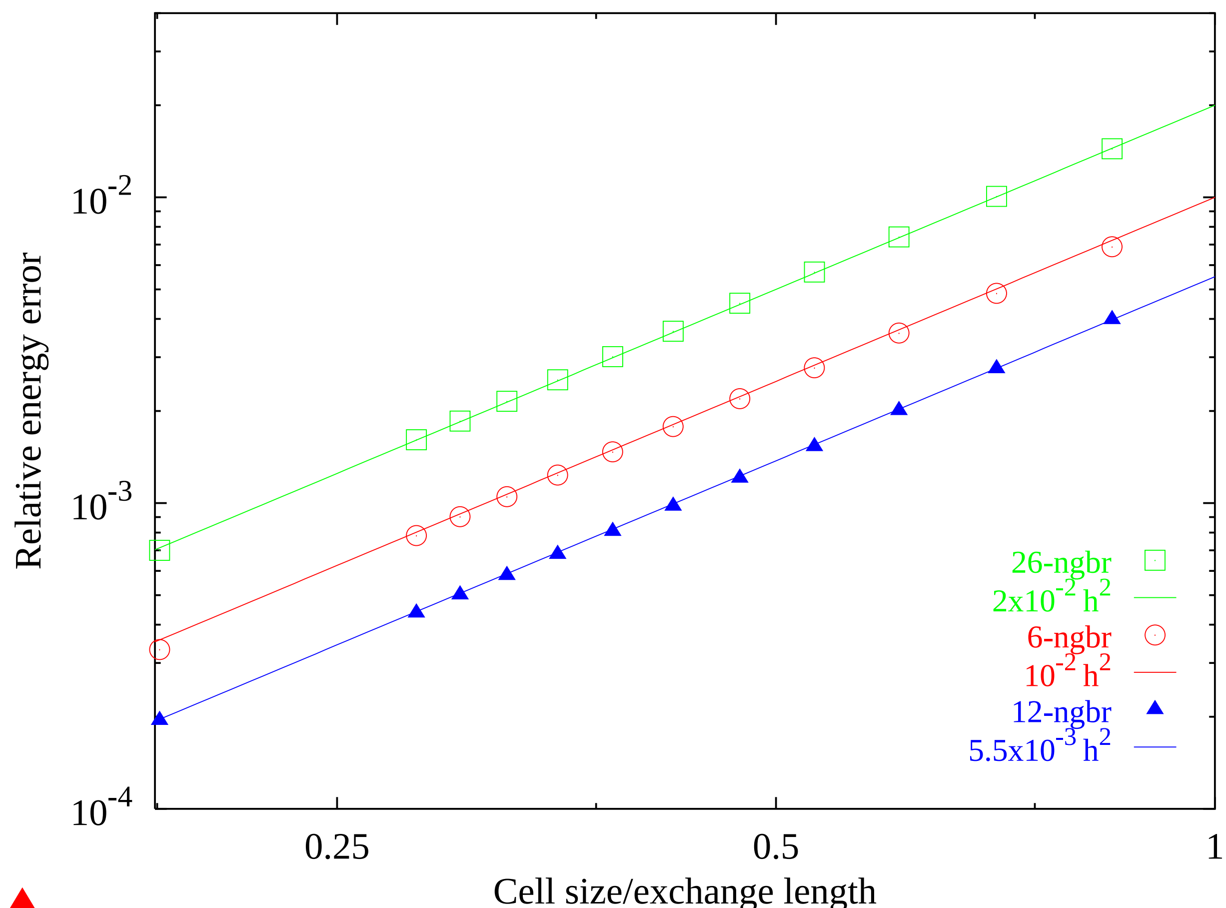
# *Magnetization spiral*



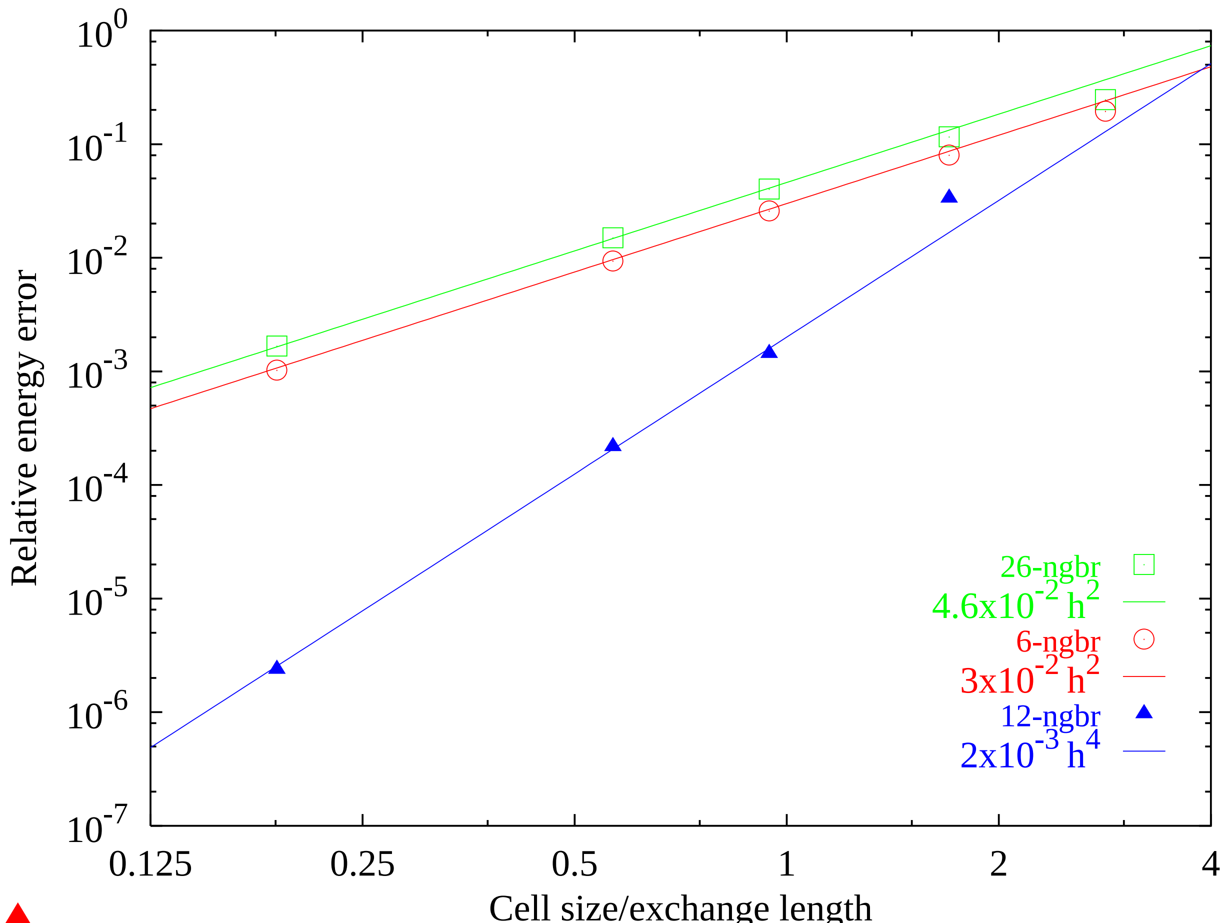
# *muMAG Standard Problem 3*

Equilibria convergence:

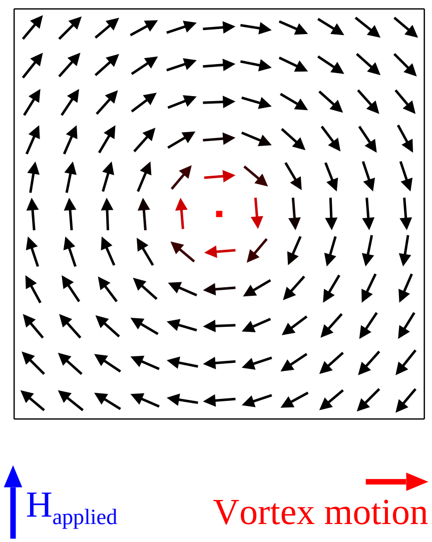


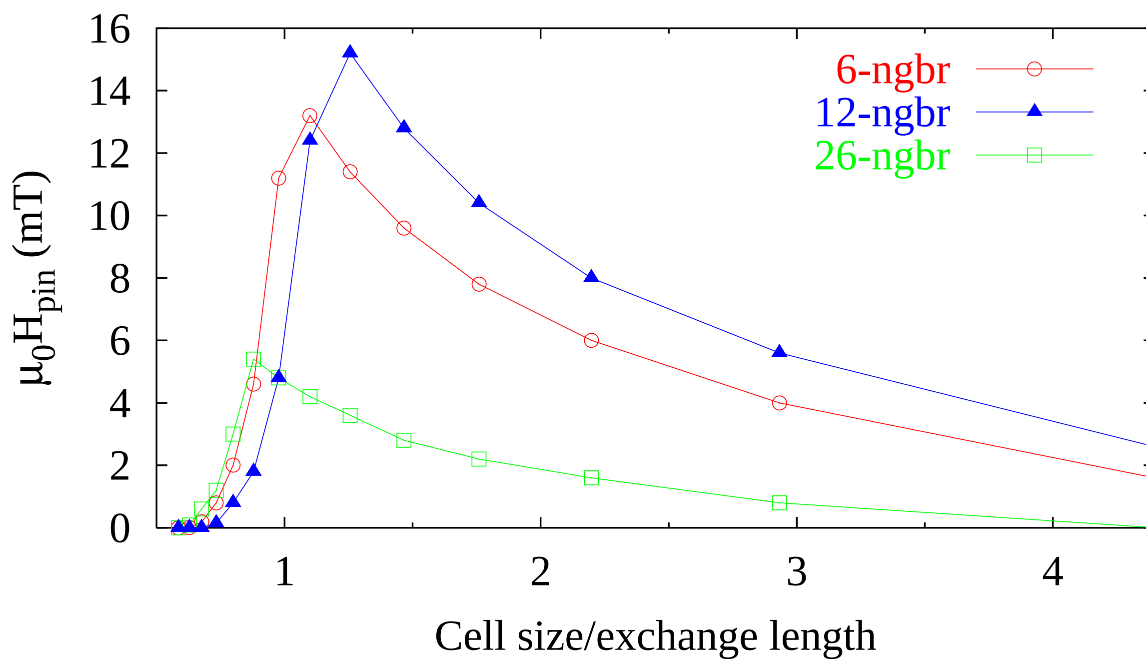
# *muMAG Standard Problem 3*

Subsample convergence:



# *Vortex mobility*

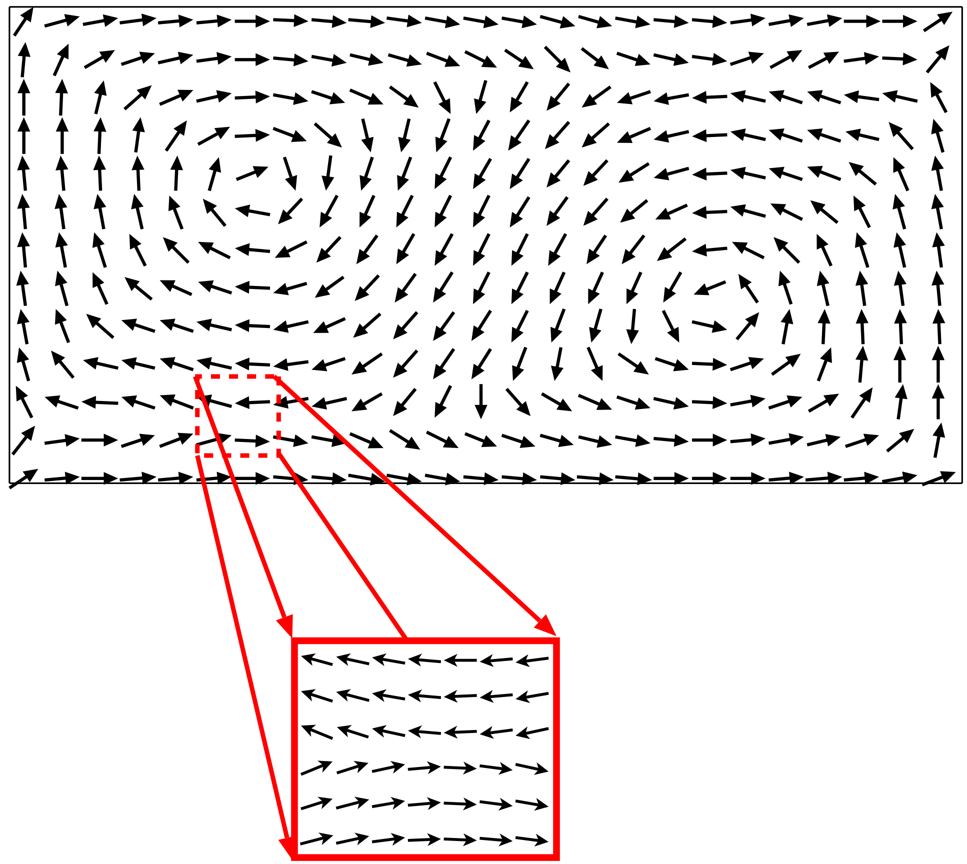



(Compare to Donahue & McMichael, Physica B, **233**, 272 (1997).)

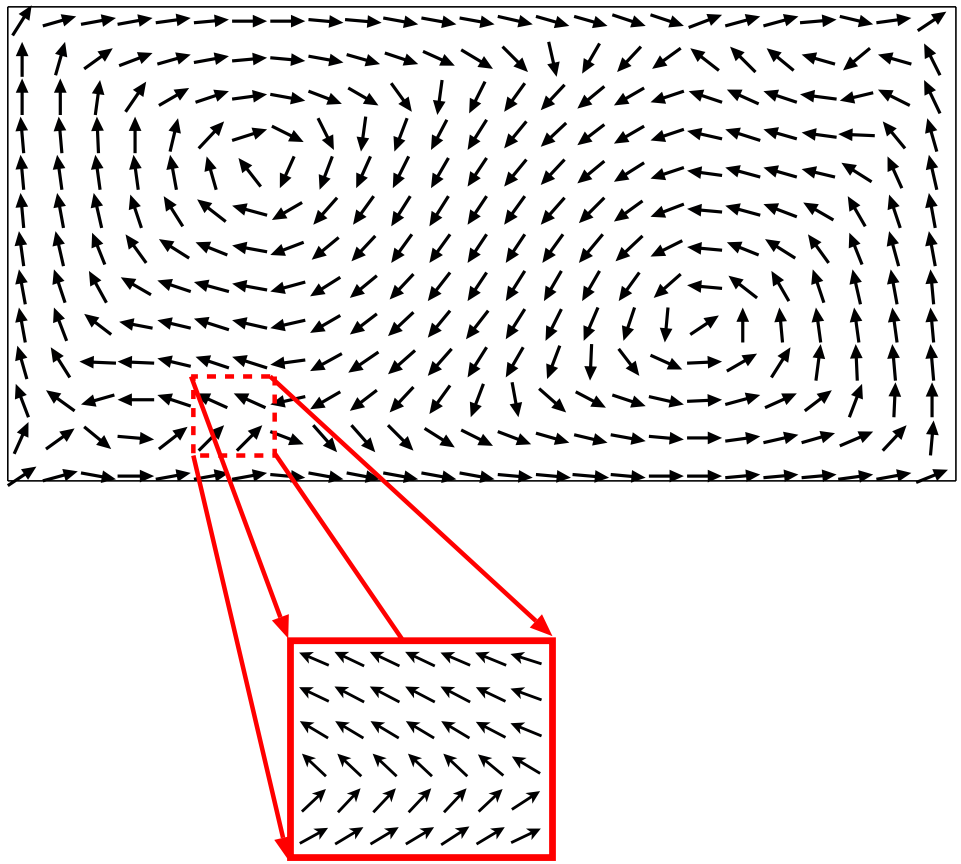
# *Néel-wall collapse*

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



# *Néel-wall non-collapse*

## 12-ngbr 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.
- 26-ngbr has less pinning for large cells, 12-ngbr dominates for $h < l_{\mathrm{ex}}$.
- 12-ngbr helps against Néel wall collapse.