Comparison of Exchange Energy Formulations for 3D Numerical Micromagnetics

Michael J. Donahue
Donald G. Porter

NIST, Gaithersburg, Maryland, USA

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

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

- Numerical integration
- Integrand representation
- Boundary conditions

Numerical integration

$$\int f \approx h \sum a_k f_k$$

For open intervals,

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

Integrand representation

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

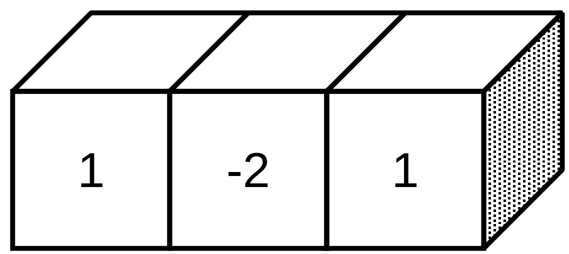
The norm constraint, $\|\mathbf{m}\| = 1$, implies

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

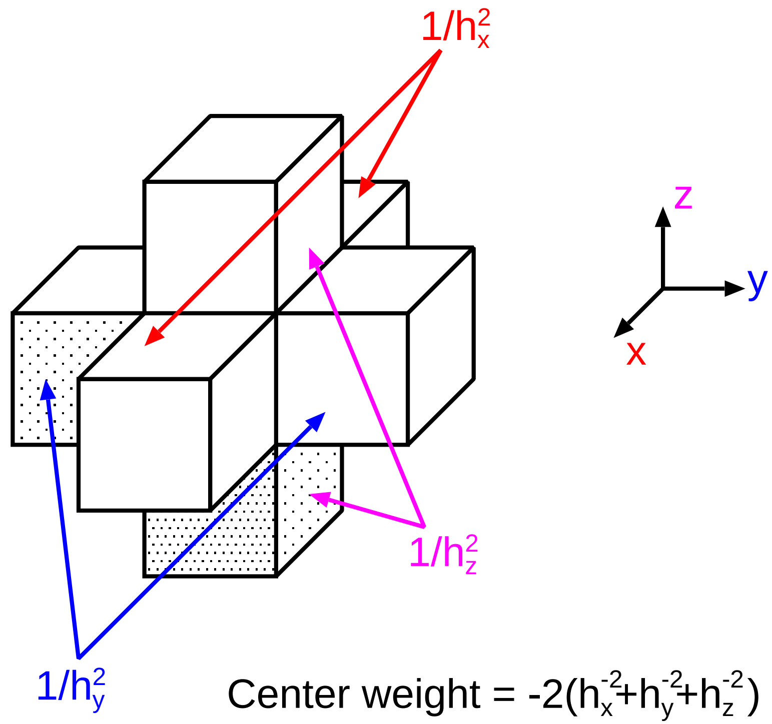
3-pt stencil

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

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



3-pt stencil



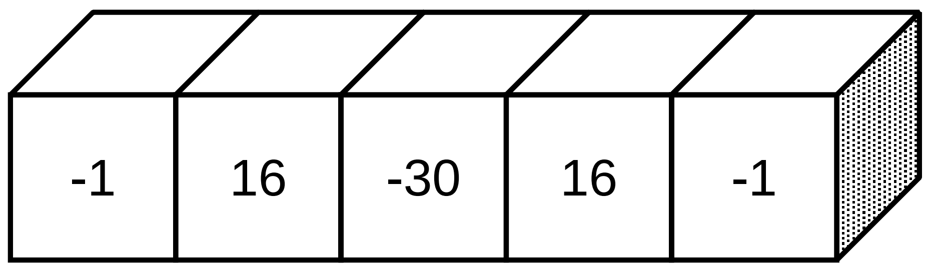
Center weight = $-2(h_x^{-2}+h_y^{-2}+h_z^{-2})$

“6-neighbor exchange”

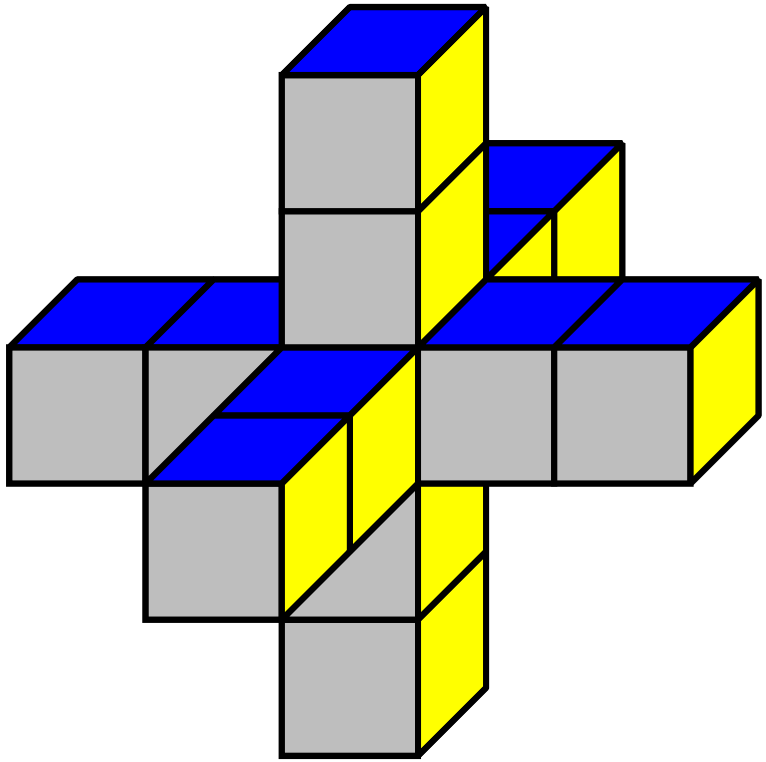
5-pt stencil

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

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

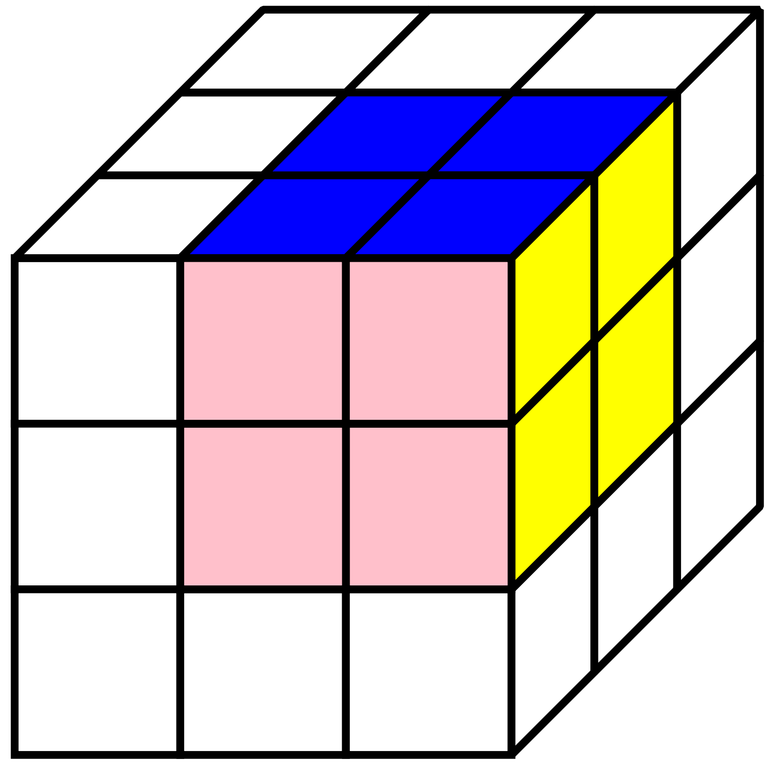


5-pt stencil



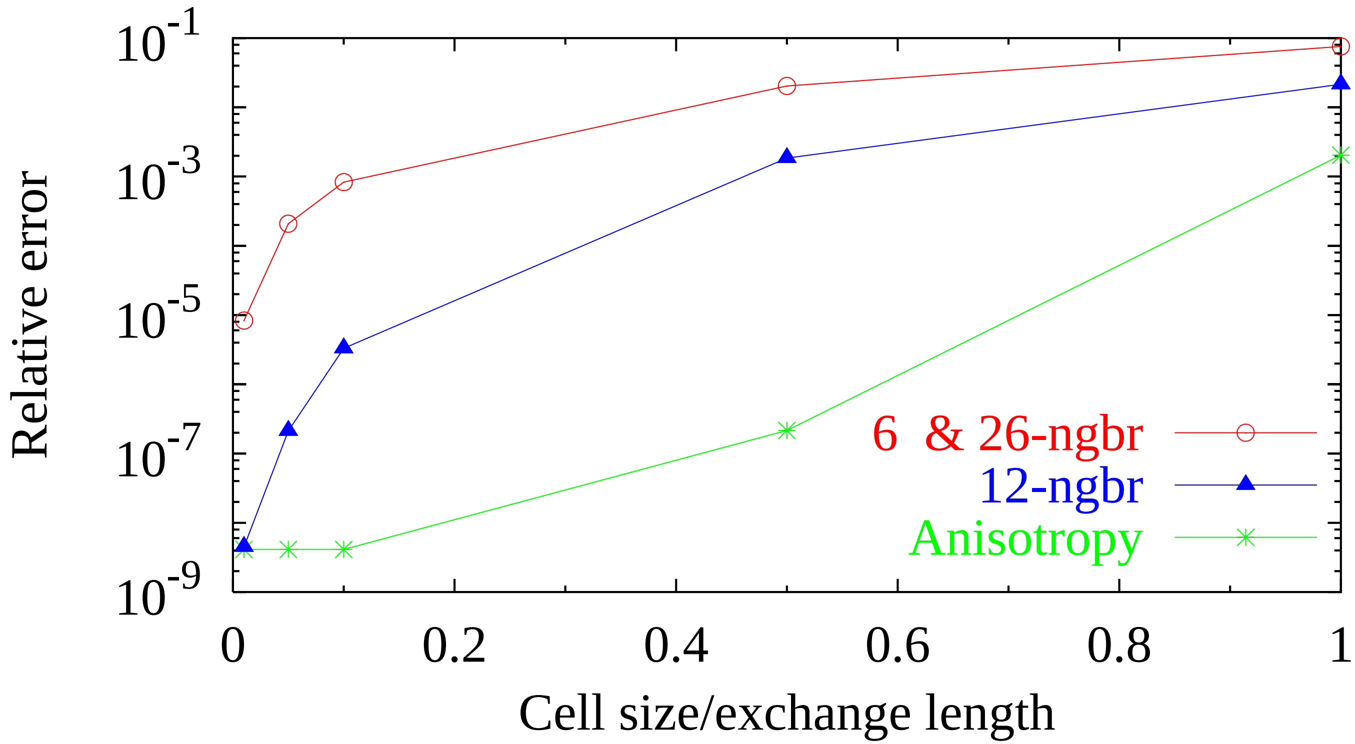
“12-neighbor exchange”

Trilinear interpolation



“26-neighbor exchange”

Analytic 1D Domain Wall



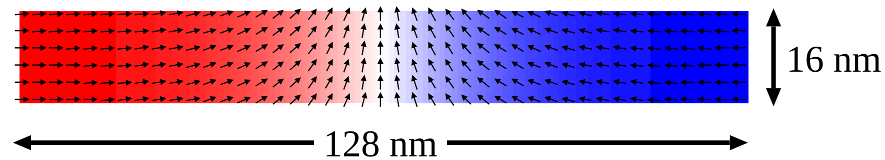
Relative energy error vs. discretization cell size

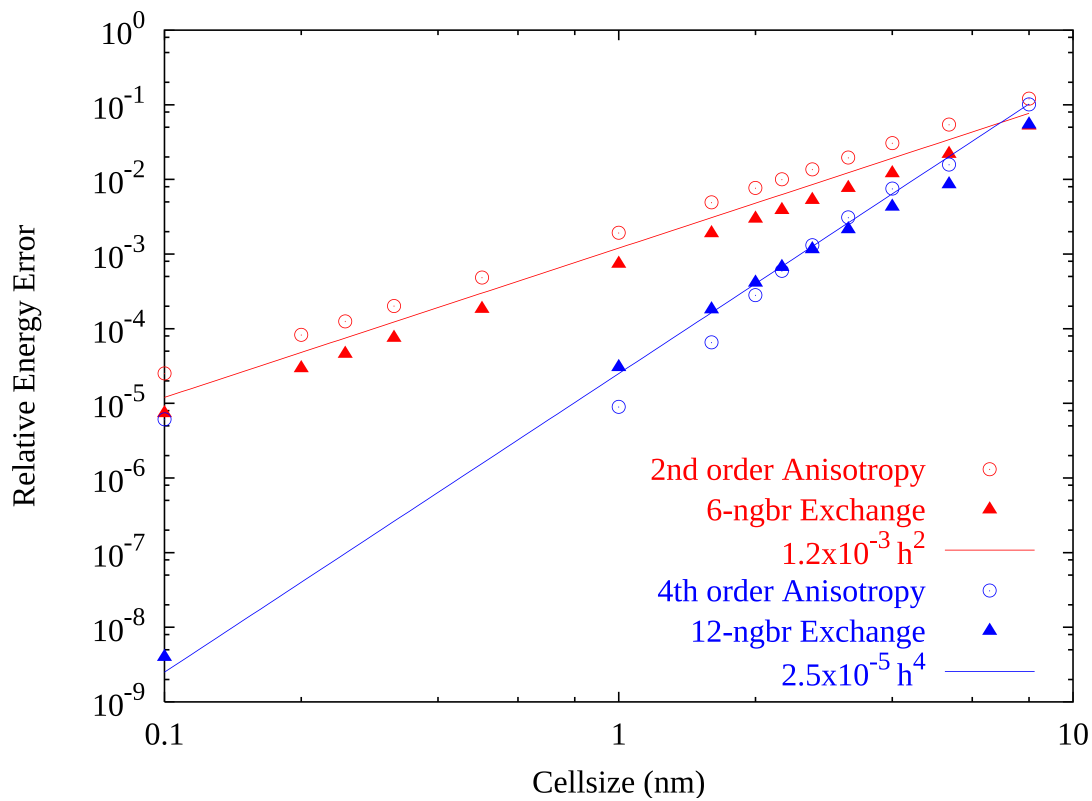
Iterative Convergence

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

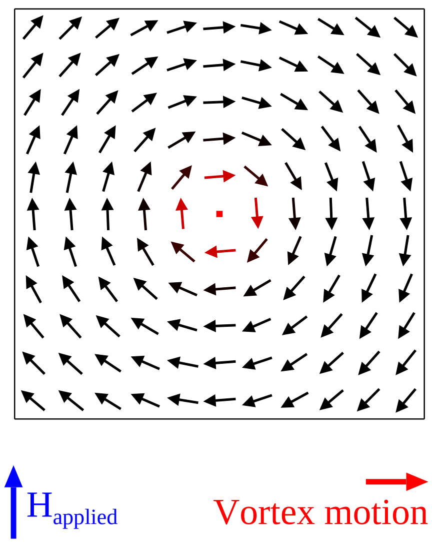
$K_u = (4.6 \times 10^5) r^2/(1+r^2)$ J/m^3

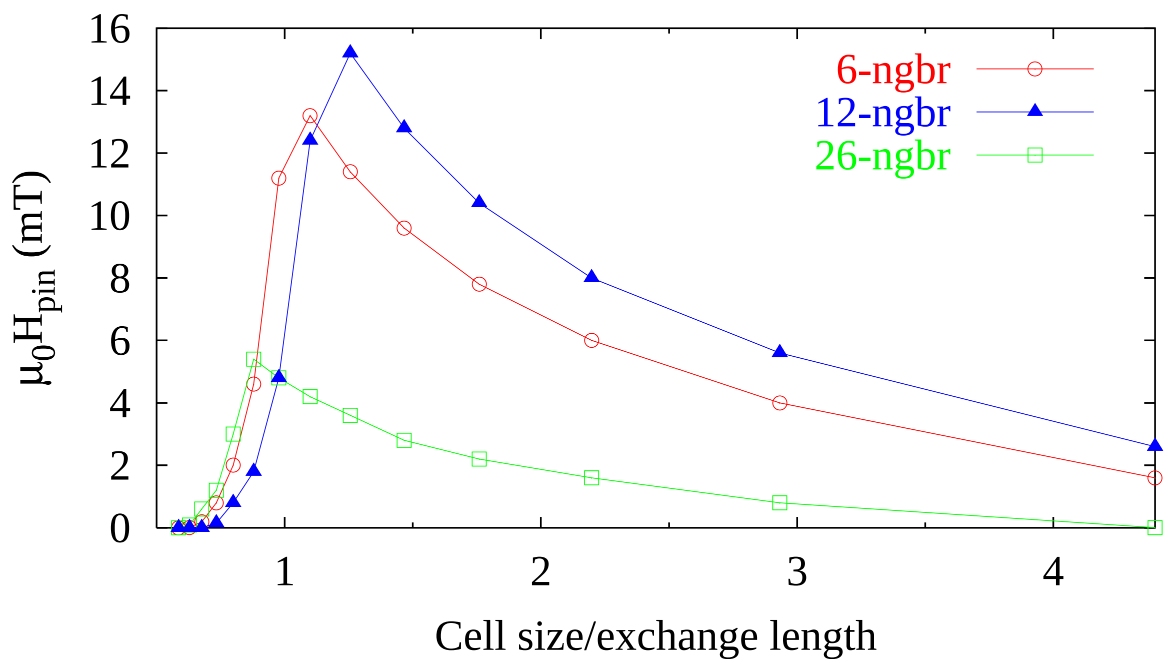
10 nm thick





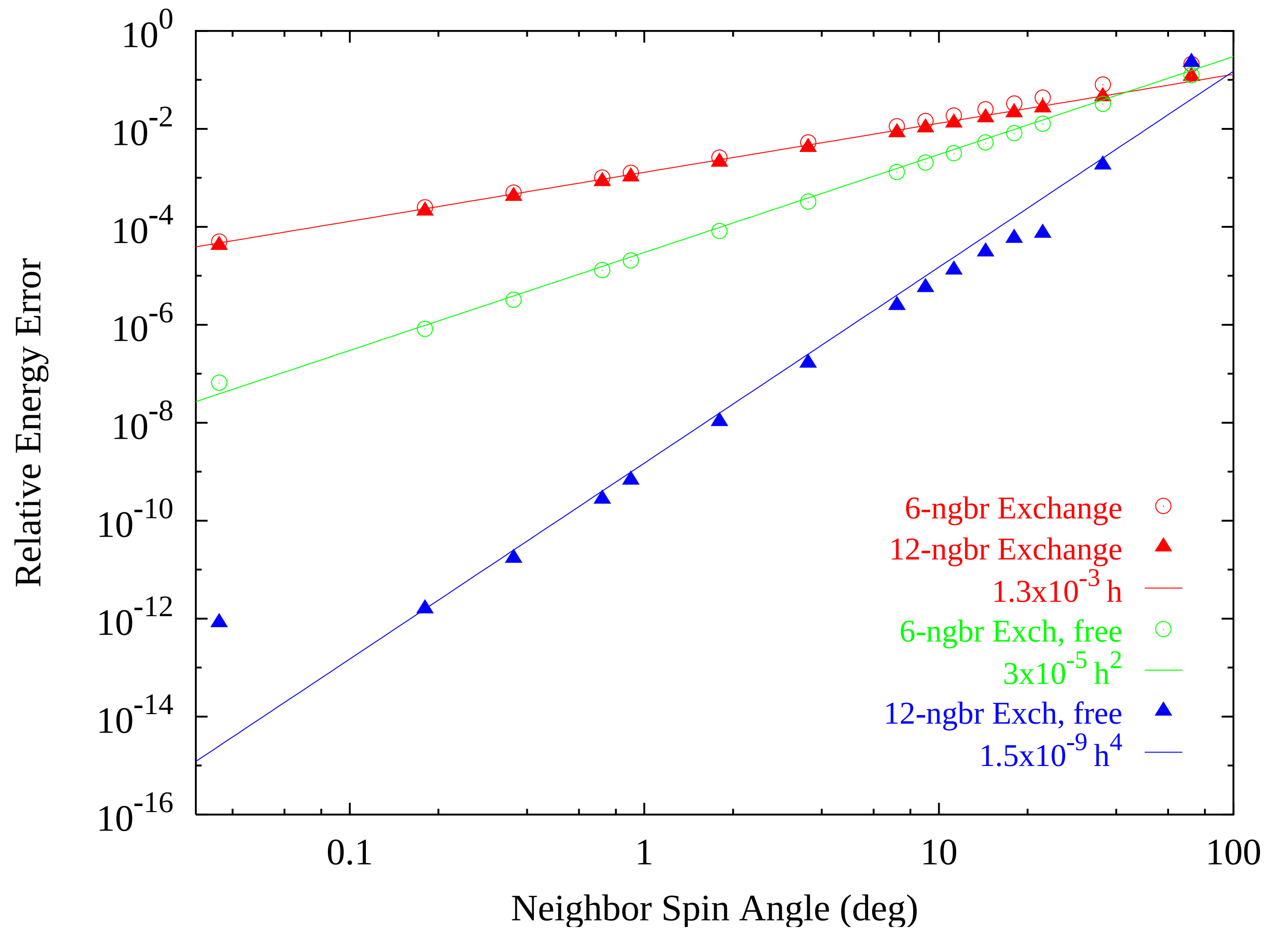
Vortex Mobility





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

Magnetization spiral



Conclusions

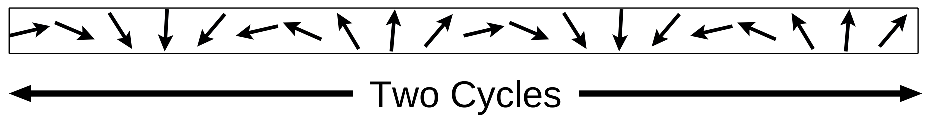
- 6-ngbr and 26-ngbr are 2nd order.
- 12-ngbr is 4th order.
- 26-ngbr has less pinning for large cells, 12-ngbr dominates for $h < l_{\mathrm{ex}}$.
- $\partial\mathbf{m}/\partial\hat{\mathbf{n}} = 0$ good BC for equilibrium states with no surface pinning; otherwise free BC should be considered.

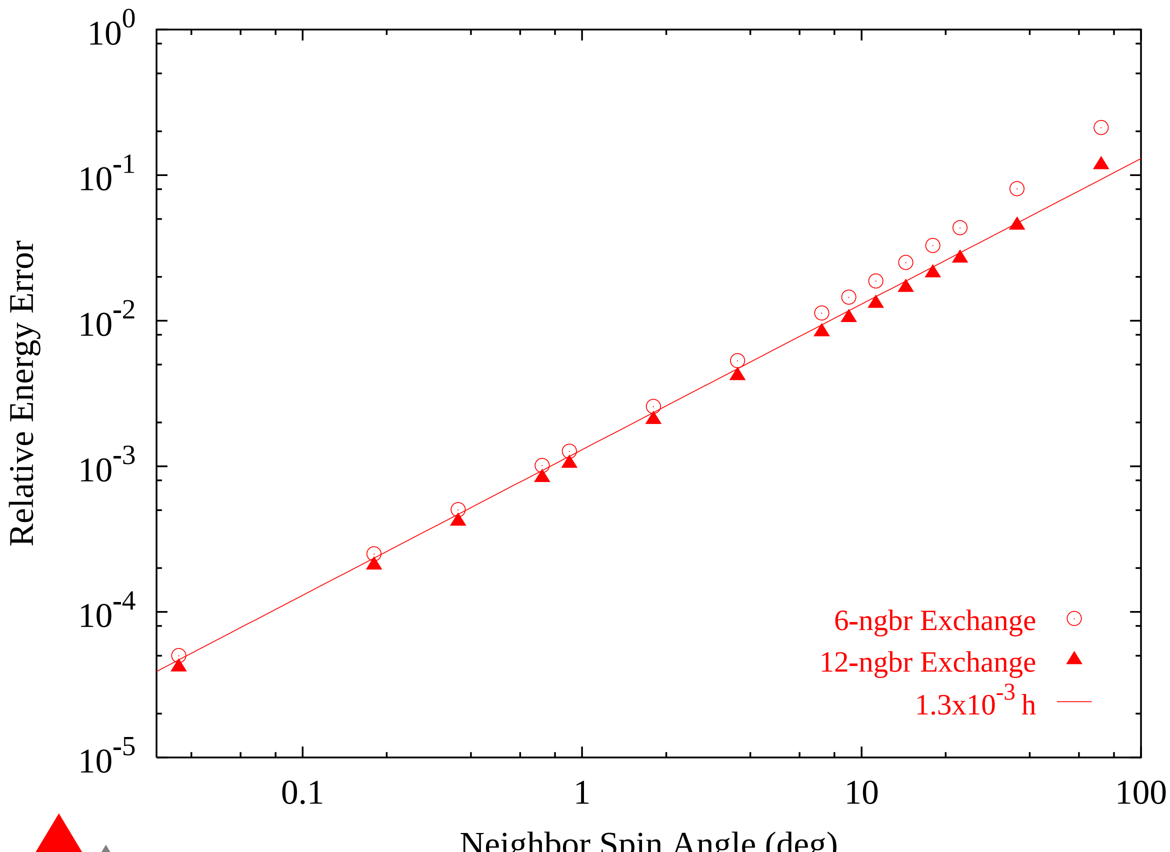
Brown's Equations

Energies:

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

Magnetization spiral





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:

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

12-ngbr Exchange

Assume $\partial \mathbf{m}/\partial \hat{\mathbf{n}} = 0$, $\partial^3 \mathbf{m}/\partial \hat{\mathbf{n}}^3 = 0$:

$$\frac{\partial^2}{\partial x^2} = \frac{1}{12h^2} \begin{bmatrix} -14 & 15 & -1 & & & & \\ 15 & -30 & 16 & -1 & & & \\ -1 & 16 & -30 & 16 & -1 & & \\ & -1 & 16 & -30 & 16 & -1 & \\ & & & & \ddots & & \end{bmatrix} + O(h^4).$$

12-ngbr Exchange

No boundary assumptions:

$$\frac{\partial^2}{\partial x^2} = \frac{1}{1152h^2} \times$$

$$\begin{bmatrix} -6125 & 11959 & -8864 & 3613 & -583 & & & \\ 11959 & -25725 & 20078 & -7425 & 1113 & & & \\ -8864 & 20078 & -17175 & 6752 & -791 & & & \\ 3613 & -7425 & 6752 & -4545 & 1701 & -96 & & \\ -583 & 1113 & -791 & 1701 & -2880 & 1536 & -96 & \\ & & & -96 & 1536 & -2880 & 1536 & -96 \\ & & & & & & \ddots & \end{bmatrix}$$

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