P3-02: High Order Methods for Computing the Demagnetization Tensor for Periodic Boundaries

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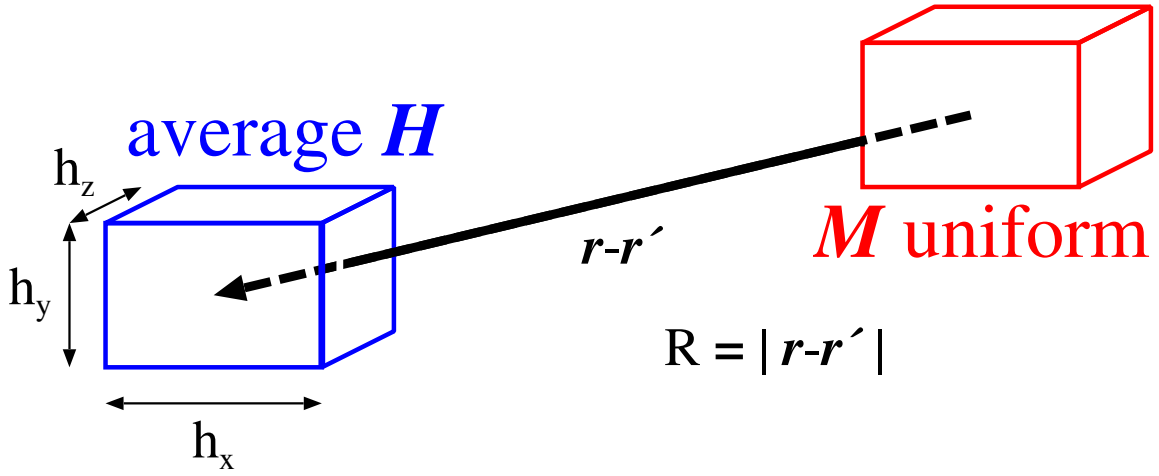
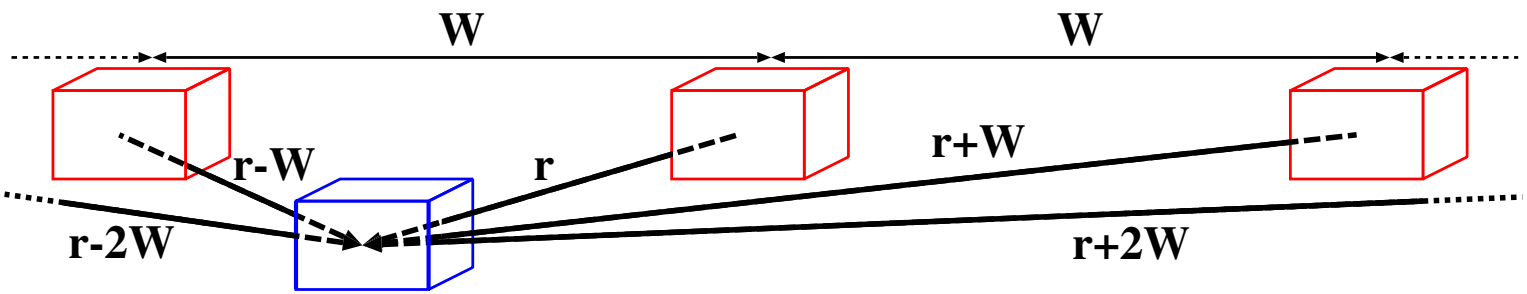
Demag tensor

$$\mathbf{H}(\mathbf{r}) = -N(\mathbf{r}-\mathbf{r}';\mathbf{h})\mathbf{M}(\mathbf{r}'),$$

$$N := \begin{pmatrix} N_{xx} & N_{xy} & N_{xz} \\ N_{xy} & N_{yy} & N_{yz} \\ N_{xz} & N_{yz} & N_{zz} \end{pmatrix}$$



1D periodic demag field

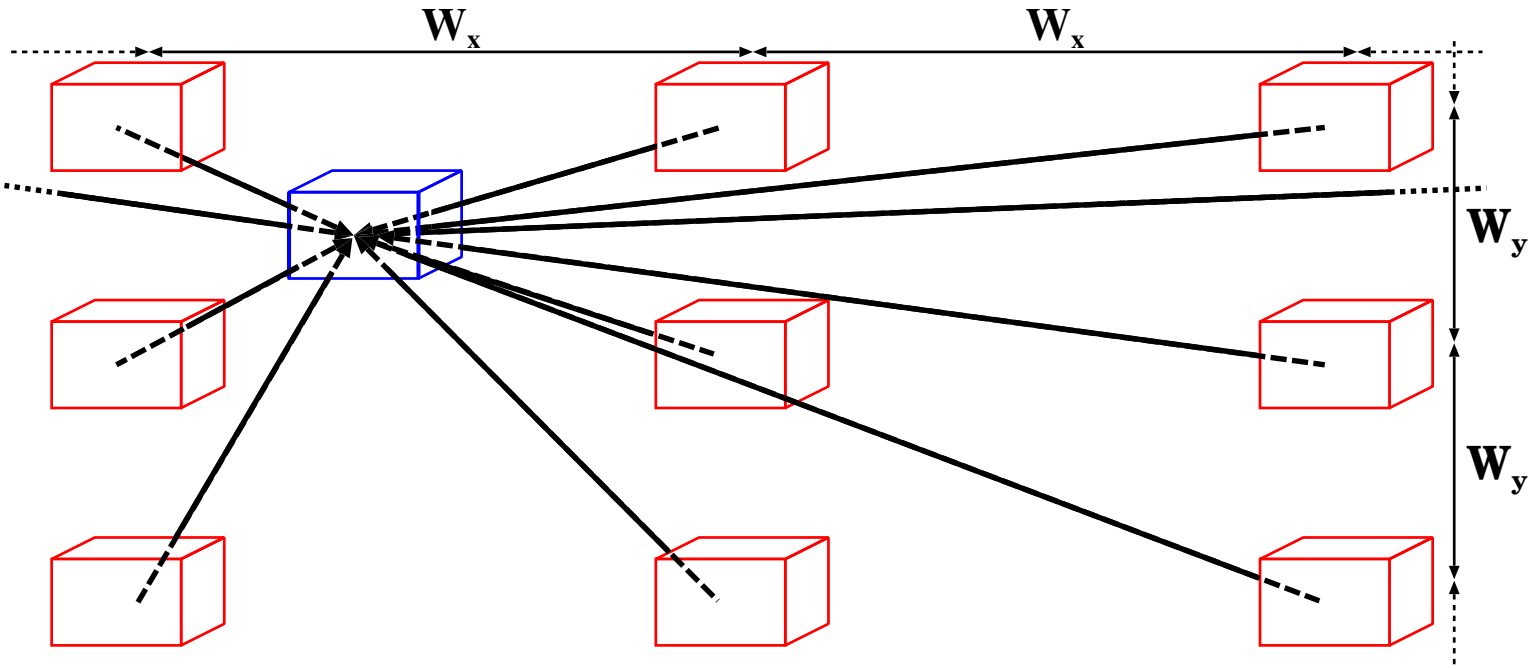


$$\boldsymbol{H} = \sum_{k=-\infty}^{\infty} N(\boldsymbol{r} + k\boldsymbol{W})\boldsymbol{M} = N^{pbc}\boldsymbol{M}$$

where

$\boldsymbol{W} :=$ offset vector between periods

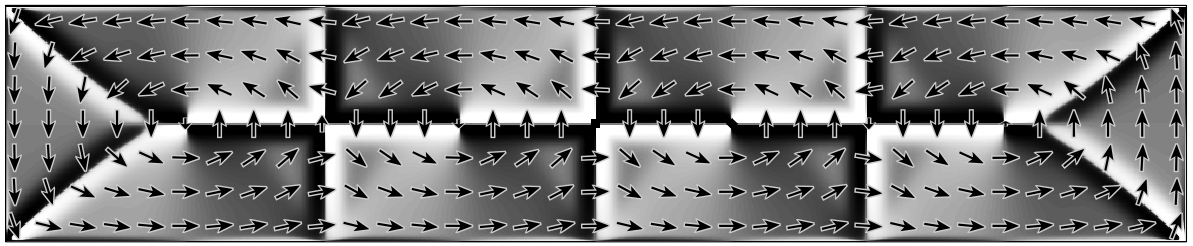
2D periodic demag field



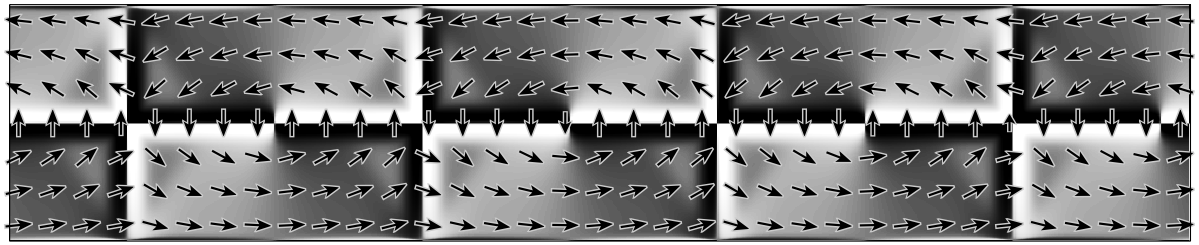
$$\boldsymbol{H} = \sum_{j=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} N(x + jW_x, y + kW_y, z)\boldsymbol{M} = N^{pbc}\boldsymbol{M}$$

Aperiodic vs. periodic simulations

Permalloy strip, 2500 nm $\times$ 500 nm $\times$ 30 nm



Non-periodic simulation



Simulation periodic in x direction

N_{xx} precursor F

$$
\begin{aligned}
F(x,y,z) &= (1/6)(2x^2 - y^2 - z^2)R \\
&\quad + (1/4)y(z^2 - x^2)\log((R+y)/(R-y)) \\
&\quad + (1/4)z(y^2 - x^2)\log((R+z)/(R-z)) \\
&\quad - xyz\arctan(yz/xR)
\end{aligned}
$$

Here $R = \sqrt{x^2 + y^2 + z^2}$.

$$\boxed{\text{Note: } F(\alpha x, \alpha y, \alpha z) = \alpha^3 F(x,y,z)}$$

N_{xy} precursor G

$$
\begin{aligned}
G(x,y,z) = &-(1/3)xyR \\
&+(1/2)xyz\log((R+z)/(R-z)) \\
&+(1/12)y(3z^2-y^2)\log((R+x)/(R-x)) \\
&+(1/12)x(3z^2-x^2)\log((R+y)/(R-y)) \\
&-(1/6)z^3\arctan(xy/zR) \\
&-(1/2)y^2z\arctan(xz/yR) \\
&-(1/2)x^2z\arctan(yz/xR)
\end{aligned}
$$

Note: $G(\alpha x, \alpha y, \alpha z) = \alpha^3 G(x,y,z)$

Demag tensor formulae

$$
\begin{aligned}
N_{xx}(\mathbf{r}) &= L[F;\mathbf{h}](\mathbf{r}) \\
N_{xy}(\mathbf{r}) &= L[G;\mathbf{h}](\mathbf{r})
\end{aligned}
$$

where

$$
L[\phi;\mathbf{h}](x,y,z) = \sum_{\varepsilon_1,\varepsilon_2,\varepsilon_3=-1}^{1} \frac{\gamma(\varepsilon_1,\varepsilon_2,\varepsilon_3)}{4\pi h_x h_y h_z} \phi(x+\varepsilon_1 h_x, y+\varepsilon_2 h_y, z+\varepsilon_3 h_z)
$$

with

$$
\gamma(\varepsilon_1,\varepsilon_2,\varepsilon_3) = 8/(-2)^{(|\varepsilon_1|+|\varepsilon_2|+|\varepsilon_3|)}
$$

Analytical formulae

For cubes:

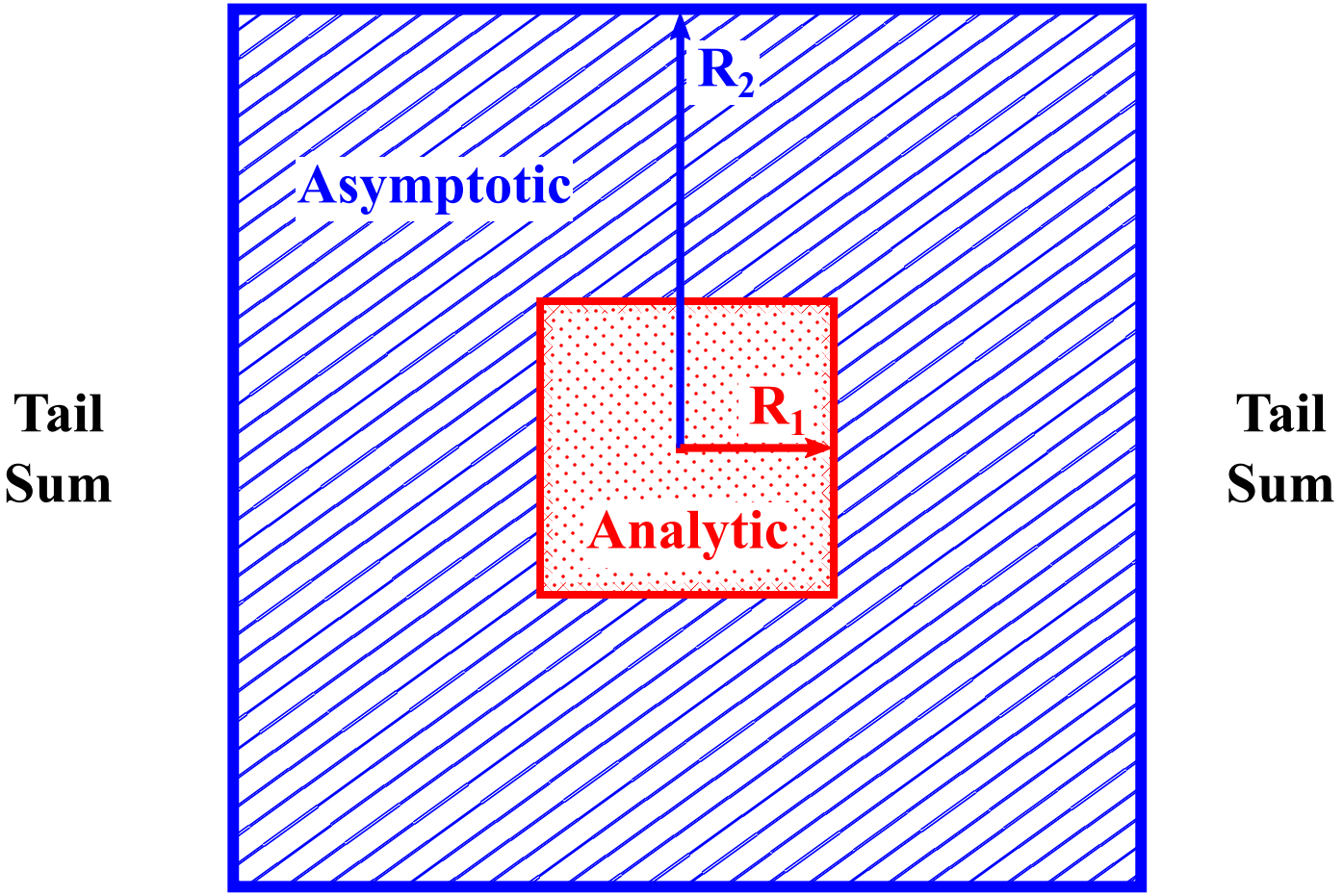
M.E. Schabes and A. Aharoni, “Magnetostatic interaction fields for a 3-dimensional array of ferromagnetic cubes,” *IEEE Trans. Magn.*, **23**, 3882–3888 (1987).

For rectangular prisms:

A.J. Newell, W. Williams, and D.J. Dunlop, “A generalization of the demagnetizing tensor for nonuniform magnetization,” *J. Geophysical Research-Solid Earth*, **98**, 9551–9555 (1993).

H. Fukushima, Y. Nakatani, and N. Hayashi, “Volume average demagnetizing tensor of rectangular prisms,” *IEEE Trans. Magn.*, **34**, 193–198 (1998).

Three compute regimes



K.M. Lebecki, M.J. Donahue, M.W. Gutowski, J. Phys. D Appl. Phys., **41**, 175005 (2008).

Asymptotic expansion

$$\frac{-4\pi}{h_x h_y h_z} N_{xx}(\mathbf{r}) =$$

$$\left(\frac{\cosh\left(h_x \frac{\partial}{\partial x}\right) - 1}{h_x^2 \frac{\partial^2}{\partial x^2}} \right) \circ \left(\frac{\cosh\left(h_y \frac{\partial}{\partial y}\right) - 1}{h_y^2 \frac{\partial^2}{\partial y^2}} \right)$$

$$\circ \left(\frac{\cosh\left(h_z \frac{\partial}{\partial z}\right) - 1}{h_z^2 \frac{\partial^2}{\partial z^2}} \right) \circ \left(\frac{2x^2 - y^2 - z^2}{R^5} \right)$$

Asymptotic expansion

$$\frac{\left(\cosh\left(h_x \frac{\partial}{\partial x}\right) - 1\right)\left(\cosh\left(h_y \frac{\partial}{\partial y}\right) - 1\right)\left(\cosh\left(h_z \frac{\partial}{\partial z}\right) - 1\right)}{h_x^2 h_y^2 h_z^2 \frac{\partial^2}{\partial x^2}\frac{\partial^2}{\partial y^2}\frac{\partial^2}{\partial z^2}}$$

$$= \left(\frac{1}{2} + \frac{h_x^2}{4!}\frac{\partial^2}{\partial x^2} + \frac{h_x^4}{6!}\frac{\partial^4}{\partial x^4} + \cdots\right) \cdot \left(\frac{1}{2} + \frac{h_y^2}{4!}\frac{\partial^2}{\partial y^2} + \frac{h_y^4}{6!}\frac{\partial^4}{\partial y^4} + \cdots\right) \cdot \left(\frac{1}{2} + \frac{h_z^2}{4!}\frac{\partial^2}{\partial z^2} + \frac{h_z^4}{6!}\frac{\partial^4}{\partial z^4} + \cdots\right)$$

$$= \frac{1}{8} + \frac{1}{4 \cdot 4!}\left(h_x^2 \frac{\partial^2}{\partial x^2} + h_y^2 \frac{\partial^2}{\partial y^2} + h_z^2 \frac{\partial^2}{\partial z^2}\right) + \text{4th order terms} + \cdots$$

Asymptotics

$$N_{xx} = \frac{h_x h_y h_z}{-4\pi}\left[\frac{\left(3x^2/R^2\right)-1}{R^3} + \frac{\mathbf{h}_2^T A_5 \mathbf{r}_4}{R^5} + \frac{\mathbf{h}_4^T A_7 \mathbf{r}_6}{R^7}\right] + O(1/R^9)$$

where, for example,

$$\mathbf{h}_2^T A_5 \mathbf{r}_4 = \begin{pmatrix} h_x^2 \\ h_y^2 \\ h_z^2 \end{pmatrix}^T \begin{pmatrix} -8 & -3 & -3 & 24 & 24 & -6 \\ 4 & 4 & -1 & -27 & 3 & 3 \\ 4 & -1 & 4 & 3 & -27 & 3 \end{pmatrix} \begin{pmatrix} x^4 \\ y^4 \\ z^4 \\ x^2y^2 \\ x^2z^2 \\ y^2z^2 \end{pmatrix} \cdot \frac{1}{R^4}$$

$$\#A_3 = 3, \quad \#A_5 = 18, \quad \#A_7 = 60, \quad \#A_9 = 150, \quad \#A_{11} = 315$$

Derivatives of P_m/R^k

Consider the N_{xx} dipole component:

$$\frac{2x^2 - y^2 - z^2}{(x^2+y^2+z^2)^{5/2}} \xrightarrow{\frac{\partial}{\partial x}} \frac{-6x^3 + 9xy^2 + 9xz^2}{(x^2+y^2+z^2)^{7/2}}$$

Derivatives of P_m/R^k

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More generally,

$$\frac{P_m}{R^k} \xrightarrow{\frac{\partial}{\partial x}} \frac{\left(\frac{\partial}{\partial x}P_m\right)R^2 - kxP_m}{R^{k+2}} = \frac{P_{m+1}}{R^{k+2}}$$

Where P_m is a homogeneous polynomial of degree m. Expressions of this type form a subset of algebraic fractions closed under addition and differentiation.

Representation of P_m/R^k in computer code

The N_{xy} dipole component:

$$\frac{3x^1y^1}{(x^2+y^2+z^2)^{5/2}} \xrightarrow{\frac{\partial}{\partial y}} \frac{3x^3-12xy^2+3xz^2}{(x^2+y^2+z^2)^{7/2}}$$

maps to the 5-tuple

$$(3,1,1,0;5) \xrightarrow{\frac{\partial}{\partial y}} (3,3,0,0;7)\,,\ (-12,1,2,0;7)\,,\ (3,1,0,2;7)$$

Representation of P_m/R^k in computer code

The N_{xy} dipole component:

$$\frac{3x^1y^1z^0}{(x^2+y^2+z^2)^{5/2}} \xrightarrow{\frac{\partial}{\partial y}} \frac{3x^3-12xy^2+3xz^2}{(x^2+y^2+z^2)^{7/2}}$$

maps to

$$\text{coef} \rightarrow (3,1,1,0;5) \xrightarrow{\frac{\partial}{\partial y}} (3,3,0,0;7)\,,\ (-12,1,2,0;7)\,,\ (3,1,0,2;7)$$

x power, y power, z power, R power

Representation of P_m/R^k in computer code

The N_{xy} dipole component:

$$\frac{3x^1y^1z^0}{(x^2+y^2+z^2)^{5/2}} \xrightarrow{\frac{\partial}{\partial y}} \frac{3x^3-12xy^2+3xz^2}{(x^2+y^2+z^2)^{7/2}}$$

maps to

$$(3,1,1,0;5) \xrightarrow{\frac{\partial}{\partial y}} (3,3,0,0;7)\,,\ (-12,1,2,0;7)\,,\ (3,1,0,2;7)$$

coef

x power

y power

z power

R power

Derivatives and point evaluations are implemented as operations on lists of 5-tuples.

Tail series convergence

In the far field, $N \approx 1/R^3$, so

$$\left(\sum_{j=-\infty}^{-m} + \sum_{j=m}^{\infty}\right) N(x+jW_x, y, z) = O\left(\frac{1}{m^2}\right) \qquad \text{1D PBC}$$

for interior sum cost $\sim m$, and

$$\sum\sum_{|jW_x+kW_y|>R_0} N(x+jW_x, y+kW_y, z) = O\left(\frac{1}{R_0}\right) \qquad \text{2D PBC}$$

with interior sum cost $\sim R_0^2$.

Note: The 3D version is not absolutely convergent.

Tail sum estimation with Euler-Maclaurin

$$\sum_{j=m}^{\infty} N_{\text{asymp}}(x+jW,y,z) =$$

$$\frac{1}{W}\int_{mW}^{\infty} N_{\text{asymp}}(x+sW,y,z)\,ds$$

$$+\frac{1}{2}N_{\text{asymp}}(x+mW,y,z)$$

$$-\sum_{k=1}^{\lfloor p/2 \rfloor} W^{2k-1}\left(\frac{B_{2k}}{(2k)!}\right) D_x^{2k-1} N_{\text{asymp}}(x+mW,y,z)$$

$$+\,\text{Remainder}\,[N_{\text{asymp}},p,mW]$$

where B_k are Bernoulli numbers, D_x^k is the kth derivative wrt x.
(NB: N and all derivatives $\to 0$ at ∞.)

Integrals of P_m/R^k

$$\begin{tikzcd}
 & \int N_{\text{asymptotic}} \\
\text{Dipole} \arrow[r, "\text{derivative}", "\text{series (cosh)}"'] & N_{\text{asymptotic}} \arrow[u, "\text{integrate in}", "\text{periodic direction}"']
\end{tikzcd}$$

Integrals of P_m/R^k

$$\begin{tikzcd}
\int \text{Dipole} \arrow[r, "\text{derivative}", "\text{series (cosh)}"'] & \int \mathrm{N}_{\text{asymptotic}} \\
\text{Dipole} \arrow[u, "\text{integrate in}", "\text{periodic direction}"'] \arrow[r, "\text{derivative}", "\text{series (cosh)}"'] & \mathrm{N}_{\text{asymptotic}} \arrow[u, "\text{integrate in}", "\text{periodic direction}"']
\end{tikzcd}$$

Integrals of dipoles (1D)

$$\int \frac{3xy}{R^5}\,dx = \frac{-y}{R^3}$$

Integrals of dipoles (1D)

$$\int \frac{3xy}{R^5}\,dx = \frac{-y}{R^3}$$

$$\int \frac{3yz}{R^5}\,dx = \frac{2x^3yz + 3xyz^3 + 3xy^3z}{\left(y^2+z^2\right)^2 R^3}$$

For the latter we need the more general form

$$\frac{P_m}{\left(x^2+y^2\right)^a \left(x^2+z^2\right)^b \left(y^2+z^2\right)^c R^k}$$

represented as a list of 7-tuples. But derivatives and evaluation can be implemented in a manner analogous to 5-tuples.

Integrals of dipoles (2D)

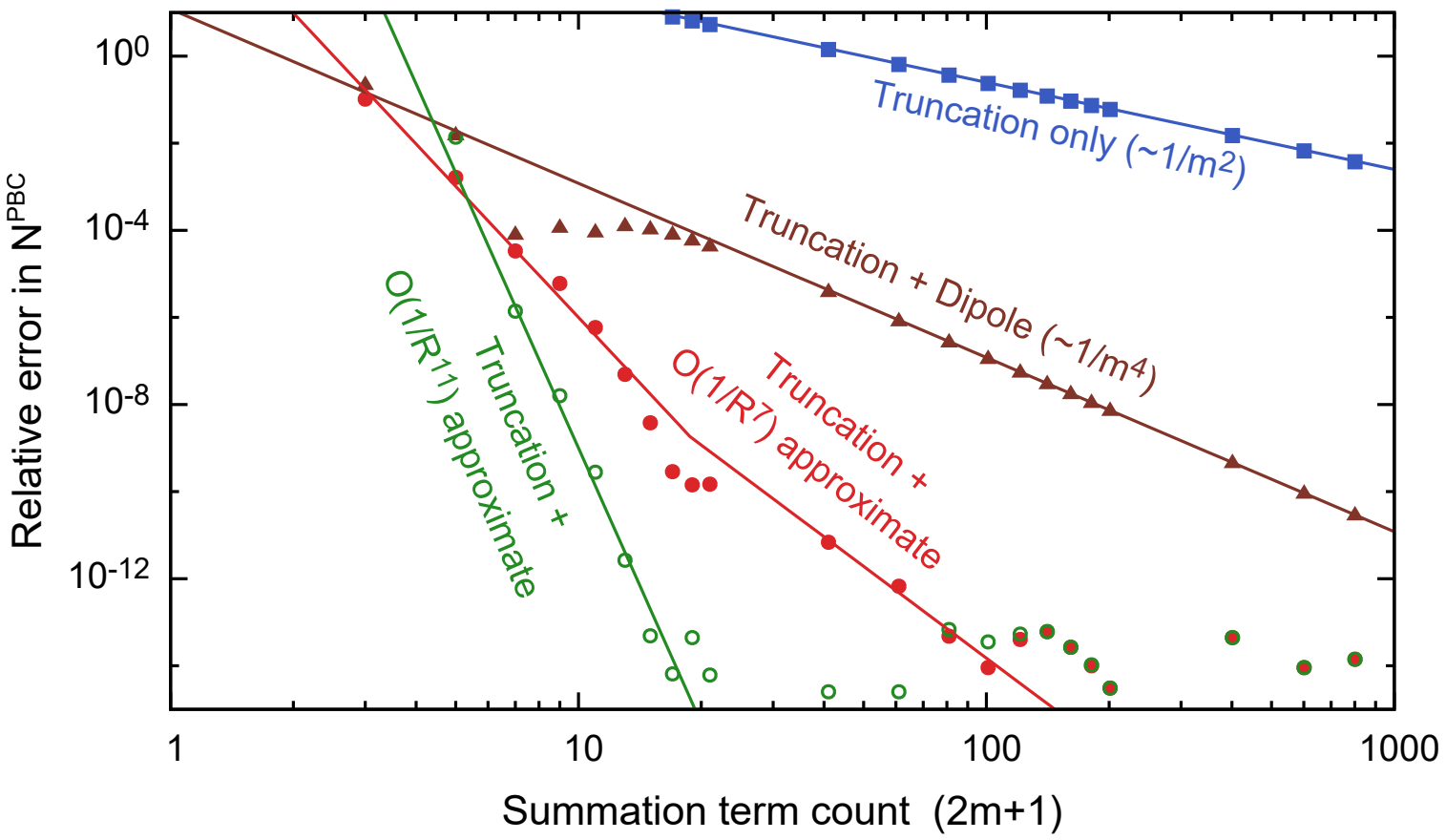
$$\iint \frac{3xy}{R^5}\,dx\,dy = \frac{1}{R}$$

$$\iint \frac{2x^2 - y^2 - z^2}{R^5}\,dy\,dz = \frac{2x^2yz + y^3z + yz^3}{(x^2+y^2)(x^2+z^2)R}$$

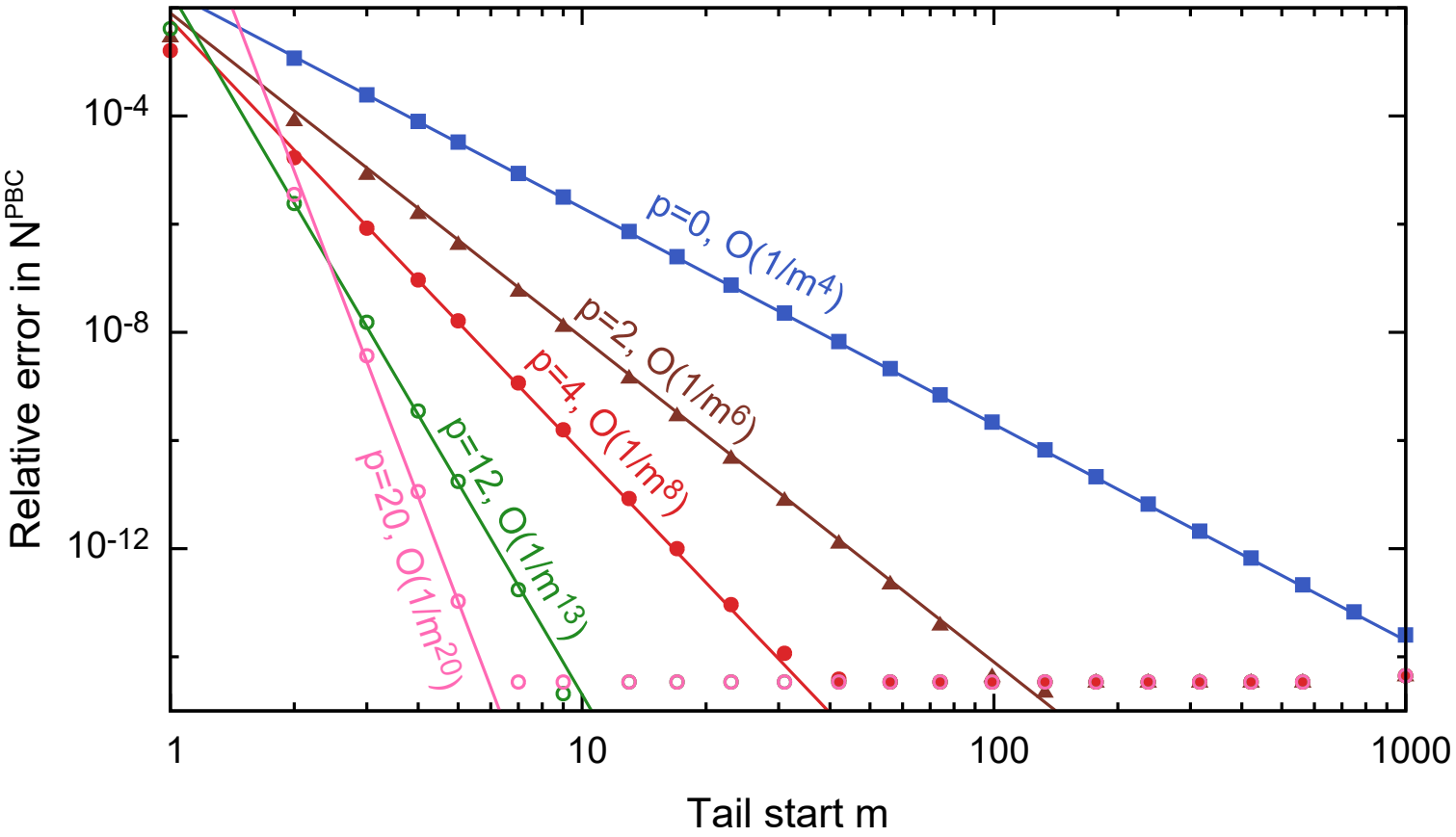
These use the same 7-tuple general form as 1D PBC:

$$\frac{P_m}{(x^2+y^2)^a (x^2+z^2)^b (y^2+z^2)^c R^k}$$

1D PBC convergence by N_{asymp} order



Convergence by Euler-Maclaurin derivatives ($N_{\text{asymp}} = O\left(1/R^{11}\right)$)



Full N tensor Euler-Maclaurin term count

N_{asymp} order k	N_{asymp}	$\int N_{\text{asymp}}$	$\sum_{k=1}^{\lfloor p/2 \rfloor} D_x^{2k-1} N_{\text{asymp}}$			
			p=2	p=4	p=12	p=20
3	12	16	16	49	471	1645
5	39	74	49	135	1131	3727
7	87	201	103	274	2020	6310
9	162	425	188	479	3175	9455
11	270	771	308	760	4630	13220

Summary

- Micromagnetics w/ PBC requires periodic demag tensor.
- Accurate $N^{\text{pbc}} = \sum_{-\infty}^{+\infty} N$ or $\sum\sum_{-\infty}^{+\infty} N$ not possible with truncation.
- Instead, decompose N^{pbc} computation into three parts: near-field finite sum with analytic N, mid-field finite sum with asymptotic N, and tail sum approximation.
- Euler-Maclaurin provides a flexible, highly accurate tail approximation for N^{pbc}.
- N^{pbc} + E-M can be implemented in a straightforward manner as operations on 5- and 7-tuples.