

Overview

Analytic Demag

Asymptotics

Tail Sum

Summary

Fast, accurate computation of the demagnetization tensor for periodic boundaries

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Demag tensor

PBC Demag

M.J. Donahue

Overview

Analytic Demag

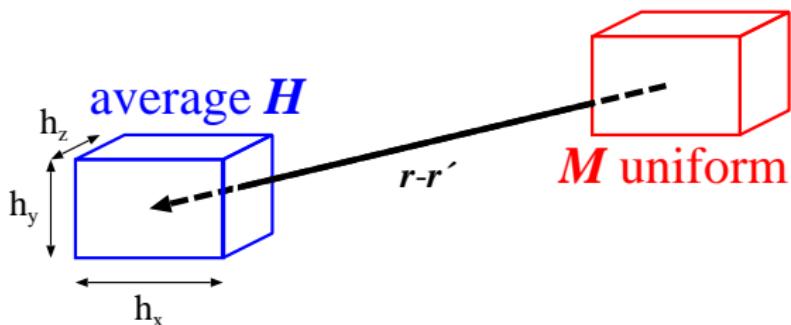
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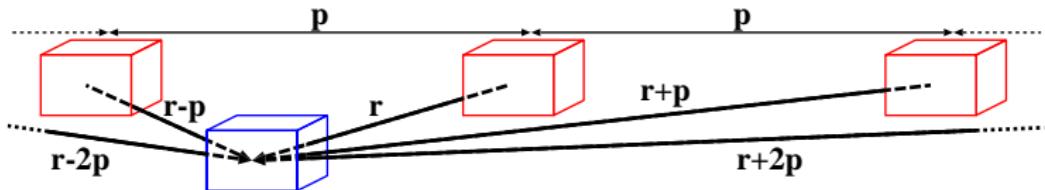
$$\mathbf{H}(\mathbf{r}) = -N(\mathbf{r} - \mathbf{r}'; \mathbf{h})\mathbf{M}(\mathbf{r}'),$$

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



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1D periodic demag field



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

where

\mathbf{p} := offset vector between periods

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- ▶ Analytical form slow to compute, inaccurate for big R
- ▶ Asymptotics fast to compute, inaccurate for small R
- ▶ Asymptotics for high aspect cells inaccurate in midrange
- ▶ Series converges slowly (truncation error $O(1/R^2)$)

Three compute regions

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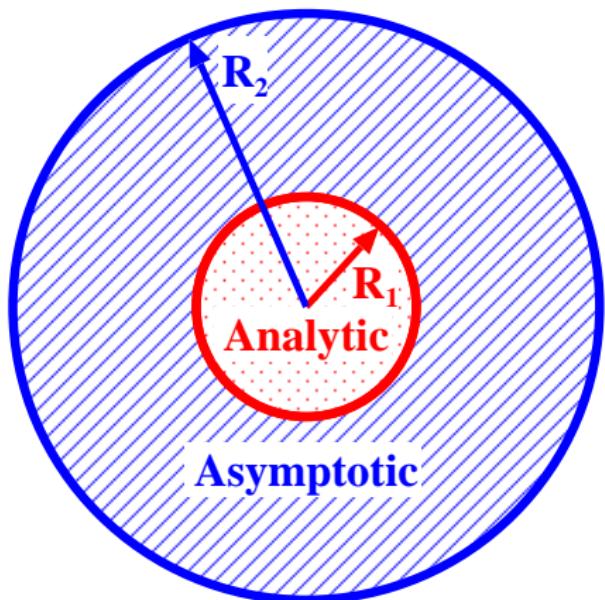
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**$R > R_2$: Integral approximation
to sum of
asymptotics**

Analytic compute error

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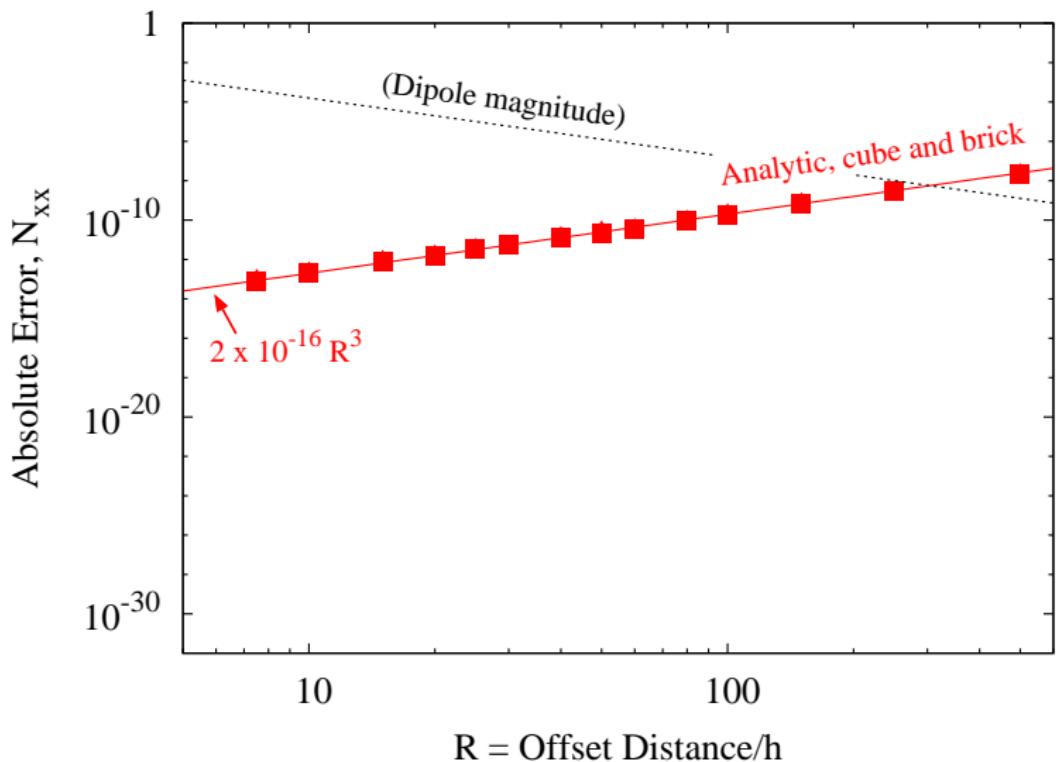
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N_{xx} precursor F

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

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

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

N_{xy} precursor G

$$G(x, y, z) = -(1/3)xyR$$

$$+ (1/2)xyz \log ((R + z)/(R - z))$$

$$+ (1/12)y(3z^2 - y^2) \log ((R + x)/(R - x))$$

$$+ (1/12)x(3z^2 - x^2) \log ((R + y)/(R - y))$$

$$- (1/6)z^3 \arctan (xy/zR)$$

$$- (1/2)y^2z \arctan (xz/yR)$$

$$- (1/2)x^2z \arctan (yz/xR)$$

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

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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

$$L[\phi; \mathbf{h}](x, y, z) = \sum_{\epsilon_1, \epsilon_2, \epsilon_3=-1}^1 \frac{\gamma(\epsilon_1, \epsilon_2, \epsilon_3)}{4\pi h_x h_y h_z} \phi(x + \epsilon_1 h_x, y + \epsilon_2 h_y, z + \epsilon_3 h_z)$$

with

$$\gamma(\epsilon_1, \epsilon_2, \epsilon_3) = 8/(-2)^{(|\epsilon_1|+|\epsilon_2|+|\epsilon_3|)}$$

"L" $3 \times 3 \times 3$ stencil

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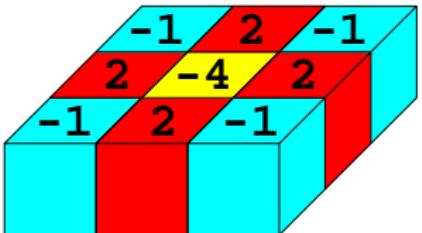
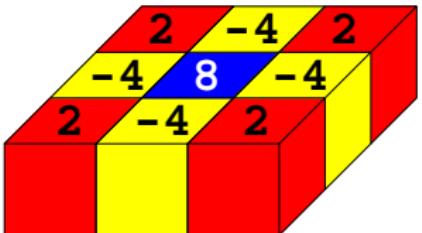
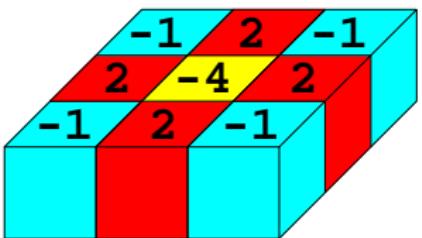
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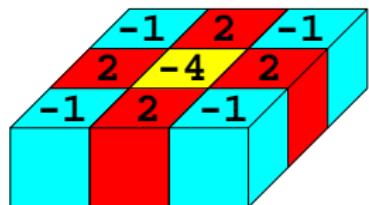
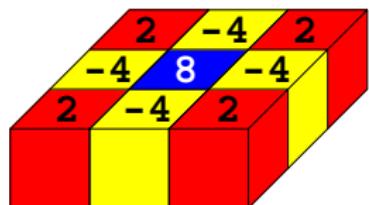
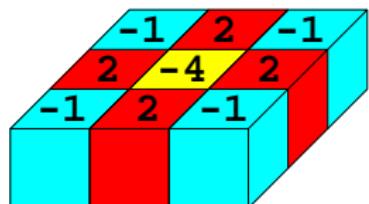
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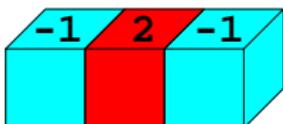
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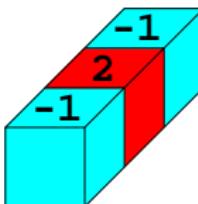
"L" stencil decomposed



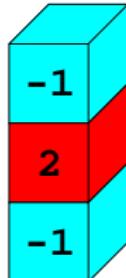
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○



○



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L operator

$$L[\phi; \mathbf{h}](x, y, z) =$$

$$\sum_{\epsilon_1, \epsilon_2, \epsilon_3 = -1}^1 \frac{\gamma(\epsilon_1, \epsilon_2, \epsilon_3)}{4\pi h_x h_y h_z} \phi(x + \epsilon_1 h_x, y + \epsilon_2 h_y, z + \epsilon_3 h_z)$$

Then

$$L[\cdot; \mathbf{h}](x, y, z) = -\delta_x^2 \circ \delta_y^2 \circ \delta_z^2 / 4\pi h_x h_y h_z$$

where

$$\delta_x[\phi](\mathbf{r}) = \phi(x + h/2, y, z) - \phi(x - h/2, y, z), \dots$$

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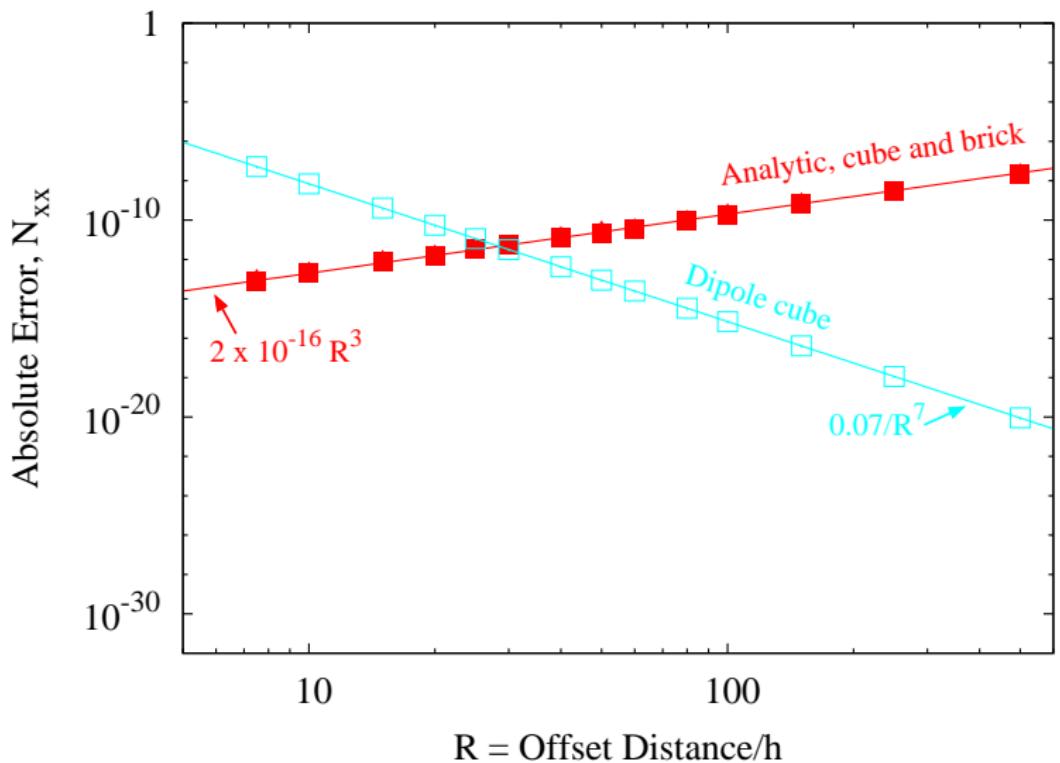
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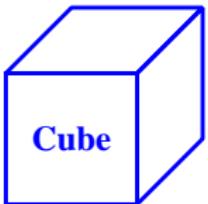
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Analytic vs. asymptotic compute error

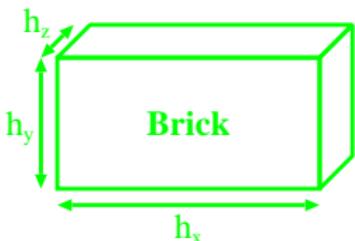


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Sample cell geometries



$h_x = 1 \quad h_y = 1 \quad h_z = 1$
Aspect ratio: 1



$h_x = 2 \quad h_y = 1 \quad h_z = 0.5$
Aspect ratio: 2

where

$$\text{Nominal length } h := \sqrt[3]{h_x h_y h_z}$$

$$\text{Aspect ratio} := \frac{h_{\max}}{\sqrt[3]{h_x h_y h_z}}$$

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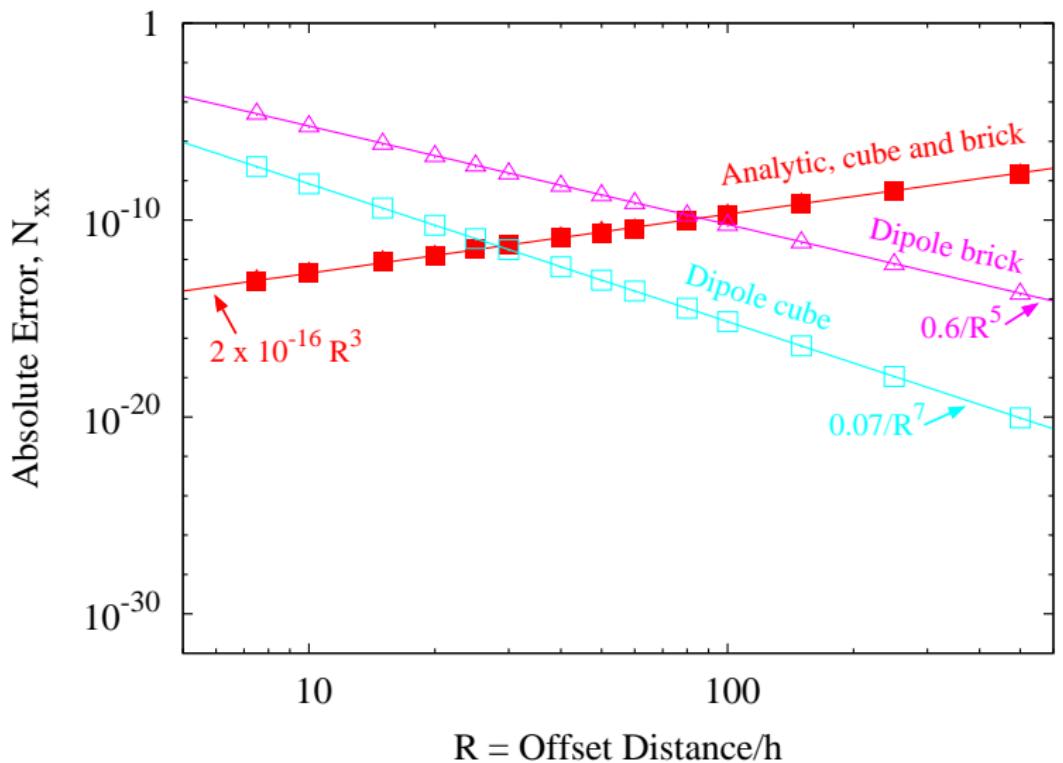
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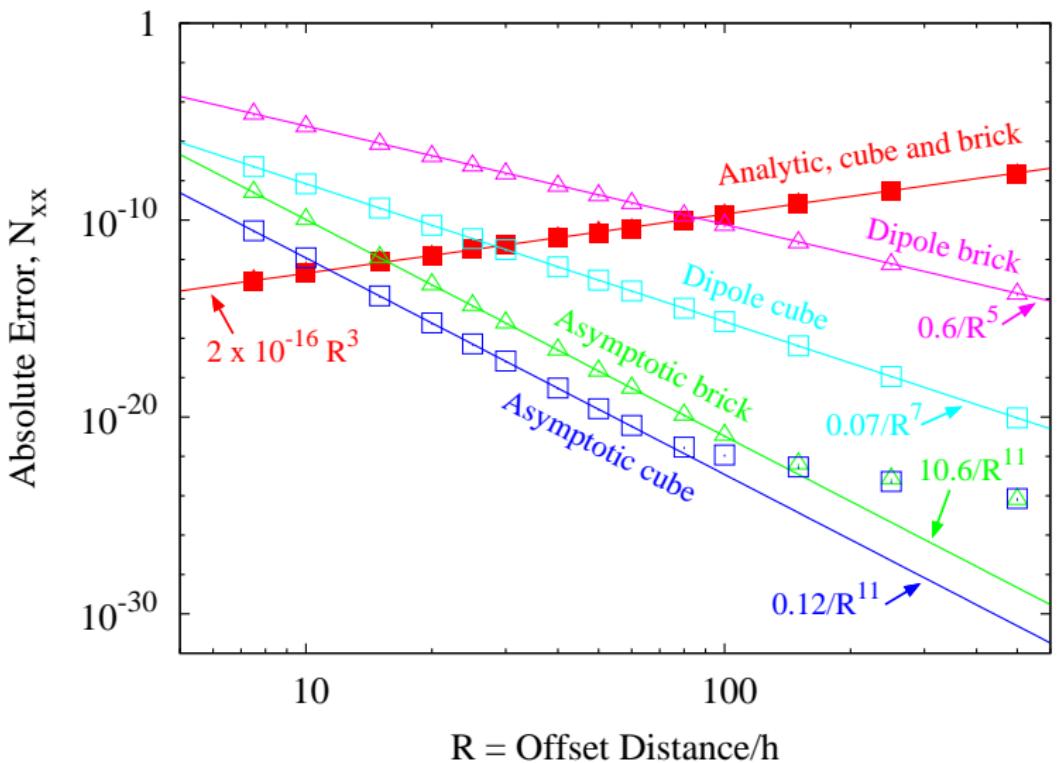
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L operator revisited

$$L[\phi; \mathbf{h}](x, y, z) =$$

$$\sum_{\epsilon_1, \epsilon_2, \epsilon_3 = -1}^1 \frac{\gamma(\epsilon_1, \epsilon_2, \epsilon_3)}{4\pi h_x h_y h_z} \phi(x + \epsilon_1 h_x, y + \epsilon_2 h_y, z + \epsilon_3 h_z)$$

Then

$$L[\cdot; \mathbf{h}](x, y, z) = -\delta_x^2 \circ \delta_y^2 \circ \delta_z^2 / 4\pi h_x h_y h_z$$

where

$$\delta_x[\phi](\mathbf{r}) = \phi(x + h/2, y, z) - \phi(x - h/2, y, z), \dots$$

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$$\frac{\partial}{\partial x} = (1/h_x)\delta_x + \dots$$

$$\frac{1}{2} \delta_x^2 = \frac{h_x^2}{2!} \frac{\partial^2}{\partial x^2} + \frac{h_x^4}{4!} \frac{\partial^4}{\partial x^4} + \frac{h_x^6}{6!} \frac{\partial^6}{\partial x^6} + \dots$$

$$= \cosh\left(h_x \frac{\partial}{\partial x}\right) - 1$$

Asymptotic expansion

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

$$\begin{aligned} &= 8 \left(\frac{\cosh(h_x \frac{\partial}{\partial x}) - 1}{h_x^2 \frac{\partial^2}{\partial x^2}} \right) \circ \left(\frac{\cosh(h_y \frac{\partial}{\partial y}) - 1}{h_y^2 \frac{\partial^2}{\partial y^2}} \right) \\ &\quad \circ \left(\frac{\cosh(h_z \frac{\partial}{\partial z}) - 1}{h_z^2 \frac{\partial^2}{\partial z^2}} \right) \circ \left(h_x^2 h_y^2 h_z^2 \frac{\partial^6}{\partial x^2 \partial y^2 \partial z^2} \right) F(\mathbf{r}) \end{aligned}$$

Surprise! (... or maybe not)

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$$\frac{\partial^6 F}{\partial x^2 \partial y^2 \partial z^2}(\mathbf{r}) = \frac{3x^2 - R^2}{R^5}$$

(dipole field)

$$\frac{\partial^6 G}{\partial x^2 \partial y^2 \partial z^2}(\mathbf{r}) = \frac{3xy}{R^5}$$

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

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

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

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Asymptotics

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

where, for example,

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

Note: For cubes, R^{-5} term is zero.

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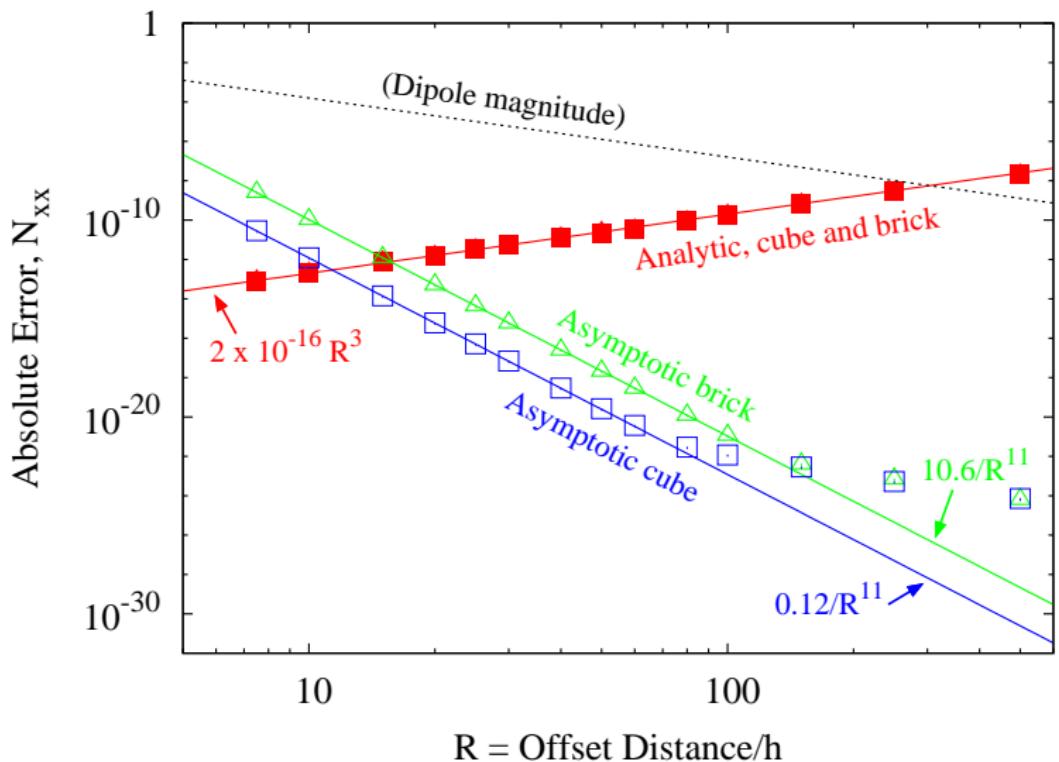
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Asymptotics for high aspect cells

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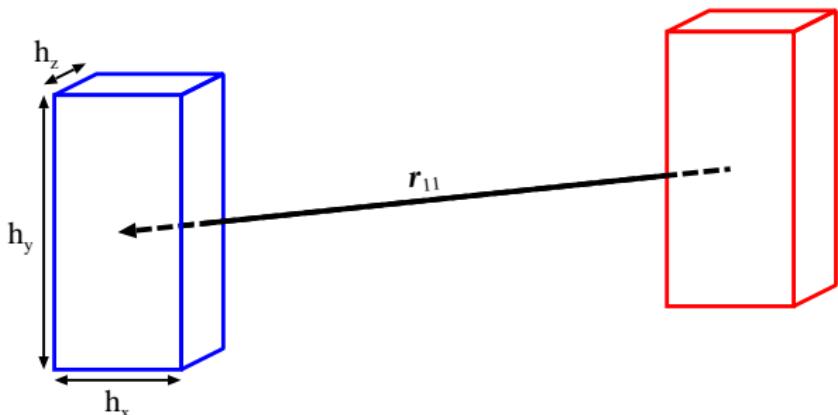
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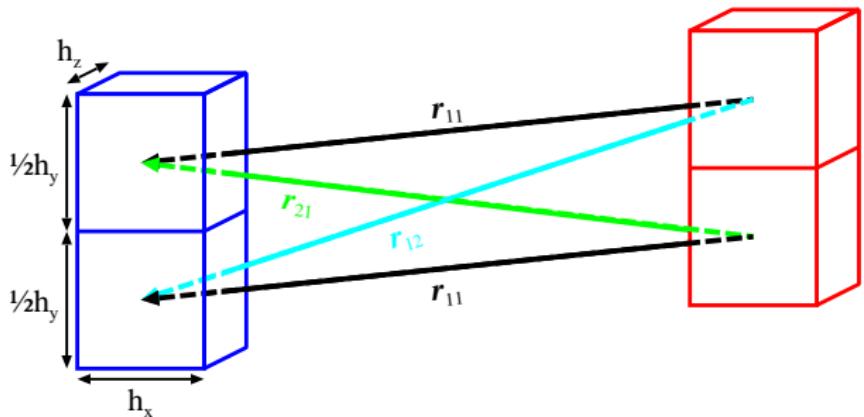
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$$\text{Aspect ratio } A = \frac{h_y}{\sqrt[3]{h_x h_y h_z}}$$

$$\text{Error in asymptotics} \sim \frac{A^8}{|\mathbf{r}/h|^{11}}$$

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$$\text{New aspect ratio } \bar{A} = \frac{h_y}{\sqrt[3]{h_x h_y h_z}} = 2^{-2/3} A$$

$$\text{Error} \sim \frac{2 \bar{A}^8}{|\mathbf{r}/\bar{h}|^{11}} = \frac{(A/2)^8}{|\mathbf{r}/h|^{11}}$$

Tail sum

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$$N_{\text{tail}}(\mathbf{r}) = \sum_{k=K_0}^{\infty} N_{\text{asymp}}(\mathbf{r} + k\mathbf{p}) + N_{\text{asymp}}(\mathbf{r} - k\mathbf{p})$$

$$\sim \sum_{k=K_0}^{\infty} \frac{1}{|k\mathbf{p}|^3}$$

$$\sim \frac{1}{K_o^2 |\mathbf{p}|^3}$$

Extended Simpson's rule

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Set

$$\Delta = \frac{b-a}{n}, \quad f_k = f(a + k\Delta)$$

then

$$\int_a^b f(x) dx$$

$$\approx \Delta \left[\frac{1}{3}f_0 + \frac{4}{3}f_1 + \frac{2}{3}f_2 + \frac{4}{3}f_3 + \frac{2}{3}f_4 + \frac{4}{3}f_5 + \frac{2}{3}f_6 + \dots + \frac{4}{3}f_{n-4} + \frac{17}{24}f_{n-3} + \frac{9}{8}f_{n-2} + \frac{9}{8}f_{n-1} + \frac{3}{8}f_n \right]$$

$$\approx \Delta \left[\frac{3}{8}f_0 + \frac{9}{8}f_1 + \frac{9}{8}f_2 + \frac{17}{24}f_3 + \frac{4}{3}f_4 + \frac{2}{3}f_5 + \frac{4}{3}f_6 + \dots + \frac{2}{3}f_{n-4} + \frac{4}{3}f_{n-3} + \frac{2}{3}f_{n-2} + \frac{4}{3}f_{n-1} + \frac{1}{3}f_n \right]$$

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$$\int_a^b f(x) dx \approx \Delta \left[\frac{17}{48}f_0 + \frac{59}{48}f_1 + \frac{43}{48}f_2 + \frac{49}{48}f_3 + f_4 + f_5 + \dots + f_{n-4} + \frac{49}{48}f_{n-3} + \frac{43}{48}f_{n-2} + \frac{59}{48}f_{n-1} + \frac{17}{48}f_n \right]$$

So

$$\sum_{k=0}^n f_k \approx \frac{1}{\Delta} \int_a^b f(x) dx + \frac{31}{48}f_0 - \frac{11}{48}f_1 + \frac{5}{48}f_2 - \frac{1}{48}f_3 - \frac{1}{48}f_{n-3} + \frac{5}{48}f_{n-2} - \frac{11}{48}f_{n-1} + \frac{31}{48}f_n$$

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$$\begin{aligned} \sum_{k=0}^n f_k &\approx \frac{1}{\Delta} \int_a^b f(x) dx \\ &+ \frac{31}{48} f_0 - \frac{11}{48} f_1 + \frac{5}{48} f_2 - \frac{1}{48} f_3 \\ &- \frac{1}{48} f_{n-3} + \frac{5}{48} f_{n-2} - \frac{11}{48} f_{n-1} + \frac{31}{48} f_n \end{aligned}$$

where

$$|\text{Error}| < C \sum_{k=0}^n \Delta^4 f^{(4)}(\xi_k)$$

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Error in sum approximate

$$|\text{Error}| < C \sum_{k=0}^n \Delta^4 f^{(4)}(\xi_k)$$

In our case

$$f(x) \sim \frac{1}{x^3}, \quad f^{(4)}(x) \sim \frac{1}{x^7}, \quad \Delta = |\mathbf{p}|$$

So

$$\begin{aligned} \sum_{k=K_0}^{\infty} f_k &= \frac{1}{|\mathbf{p}|} \int_{K_0|\mathbf{p}|}^{\infty} f(x) dx \\ &+ \frac{31}{48} f_{K_0} - \frac{11}{48} f_{K_0+1} + \frac{5}{48} f_{K_0+2} - \frac{1}{48} f_{K_0+3} \\ &+ O\left(\sum_{k=K_0}^{\infty} |\mathbf{p}|^4 (k |\mathbf{p}|)^{-7}\right) \end{aligned}$$

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$$|\text{Error}| < C \sum_{k=0}^n \Delta^4 f^{(4)}(\xi_k)$$

In our case

$$f(x) \sim \frac{1}{x^3}, \quad f^{(4)}(x) \sim \frac{1}{x^7}, \quad \Delta = |\mathbf{p}|$$

So

$$\begin{aligned} \sum_{k=K_0}^{\infty} f_k &= \frac{1}{|\mathbf{p}|} \int_{K_0|\mathbf{p}|}^{\infty} f(x) dx \\ &+ \frac{31}{48} f_{K_0} - \frac{11}{48} f_{K_0+1} + \frac{5}{48} f_{K_0+2} - \frac{1}{48} f_{K_0+3} \\ &\quad + O\left(|\mathbf{p}|^{-3} K_0^{-6}\right) \end{aligned}$$

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- ▶ 1D periodic demag tensor $N^{\text{pbc}} = \sum_k N(\mathbf{r} + k\mathbf{p})$.
- ▶ N_{analytic} loses 6 digits/decade in R , and is slow
⇒ Restrict N_{analytic} for $R < R_1 \approx 15\text{--}20h$.
- ▶ Use $\delta \approx \sum \partial$ to derive N_{asymp} ; Error $\sim A^8/R^{11}$
⇒ Subdivide cells to tame big A
⇒ N_{asymp} for $R_1 < R < R_2$
- ▶ $\sum_{R > R_2} N_{\text{asymp}} \approx \int_{R > R_2} N_{\text{asymp}}, \quad R_2 = K_0 |\mathbf{p}|$
- ▶ Tail error $< 5000h^3 |\mathbf{p}|^{-3} K_0^{-12} = 5000h^3 |\mathbf{p}|^9 / R_2^{12}$
- ▶ Single core (initialization) compute time < 1 minute