

Accurate computation of the demagnetization tensor

Michael J. Donahue

NIST, Gaithersburg, Maryland, USA

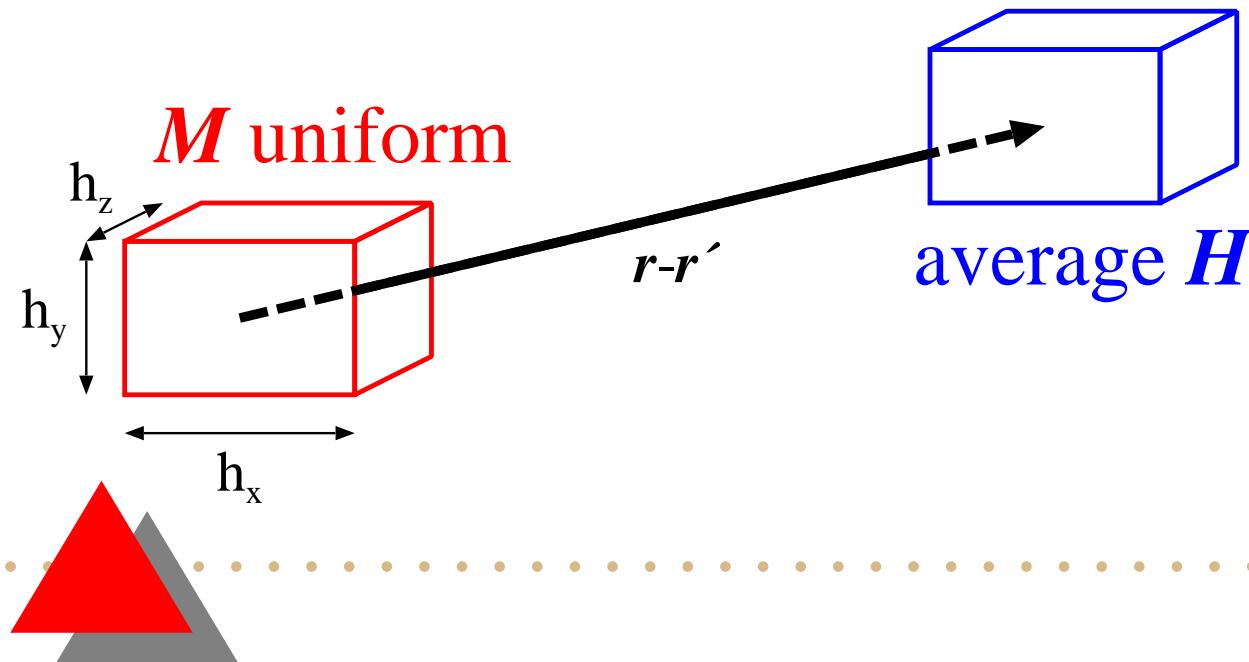
HMM-2007, Naples, Italy

4-Jun-2007

Demag tensor

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

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



Formulae

$$N_{xx}(\mathbf{r}) = L[F; \mathbf{h}](\mathbf{r})$$

$$N_{xy}(\mathbf{r}) = L[G; \mathbf{h}](\mathbf{r})$$

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

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

N_{xx} precursor F

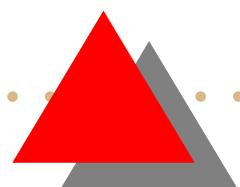
$$\begin{aligned} F(x, y, z) = & (1/6)(2x^2 - y^2 - z^2)R \\ & + (1/2)y(z^2 - x^2) \log(y + R) \\ & + (1/2)z(y^2 - x^2) \log(z + R) \\ & - xyz \arctan(yz/xR) \end{aligned}$$

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



N_{xy} precursor G

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

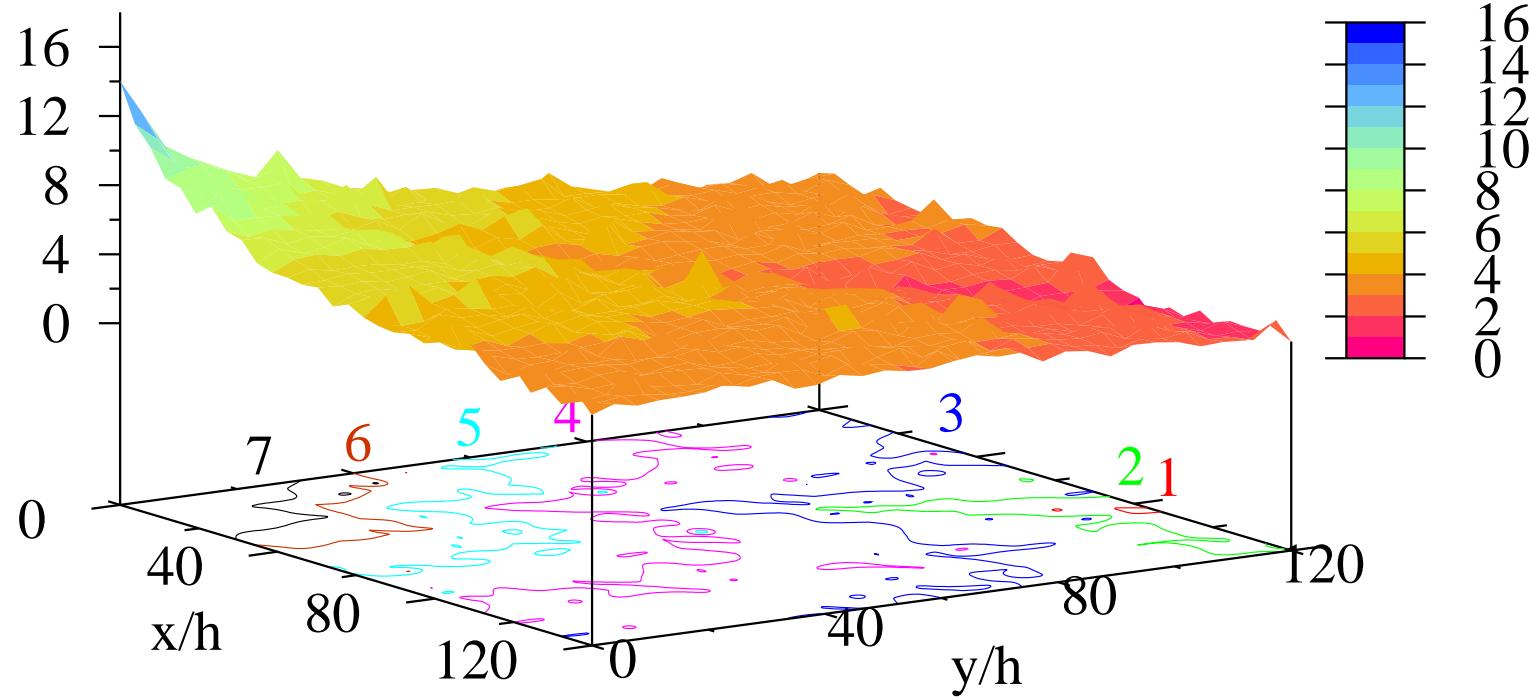


References

- [1] M.E. Schabes and A. Aharoni, “Magnetostatic interaction fields for a 3-dimensional array of ferromagnetic cubes,” *IEEE Trans. Magn.*, **23**, 3882–3888 (1987).
- [2] 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).

Relative Error: N_{xx}

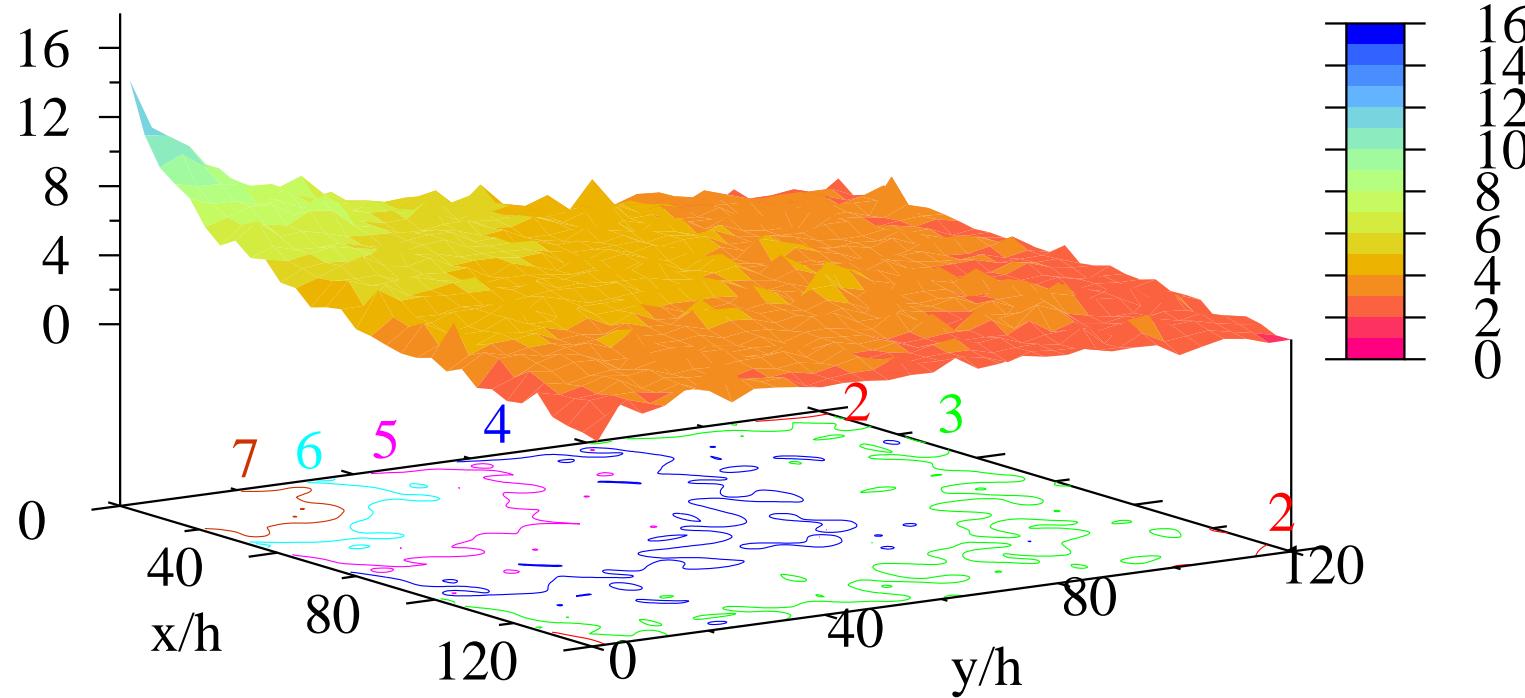
Sig. Figs.
($-\log_{10}(\text{Rel. Err.})$)



Direct numeric implementation,
cubic cells, $z=0$.

Relative Error: N_{xy}

Sig. Figs.
($-\log_{10}(\text{Rel. Err.})$)



Direct numeric implementation,
cubic cells, $z=0$

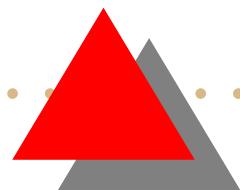


Who cares?



Who cares?

- Refining grid increases errors



Who cares?

- Refining grid increases errors
- Wrong physics (worse than cutoff)



So, why so bad?

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

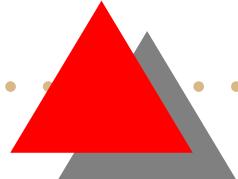
$$\sum_{\epsilon_1, \epsilon_2, \epsilon_3 = -1}^1 \frac{\gamma(\epsilon_1, \epsilon_2, \epsilon_3)}{4\pi h_x h_y h_z} \phi(x + \epsilon_1 h_x, y + \epsilon_2 h_y, z + \epsilon_3 h_z)$$

Then

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

where

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





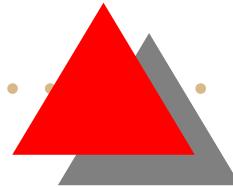
Catastrophic cancellation

$$f(x+h) = a_0 + a_1 h + a_2 h^2 + \dots$$

For $h=1/10$:

$$\begin{array}{r} a_0 \quad \boxed{6 \quad 5 \quad 4 \quad 3 \quad 2 \quad 1} \\ + a_1 h \quad \boxed{6 \quad 5 \quad 4 \quad 3 \quad 2 \quad 1} \\ \hline f(x+h) \quad \boxed{7 \quad 1 \quad 9 \quad 7 \quad 5 \quad 3} \\ - f(x) \quad \boxed{6 \quad 5 \quad 4 \quad 3 \quad 2 \quad 1} \\ \hline \quad \quad \quad \boxed{ \quad 6 \quad 5 \quad 4 \quad 3 \quad 2} \end{array}$$

← 1 digit lost





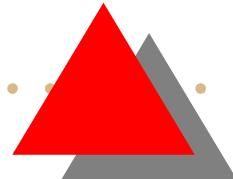
Catastrophic cancellation

$$f(x+h) = a_0 + a_1 h + a_2 h^2 + \dots$$

For $h=1/100$:

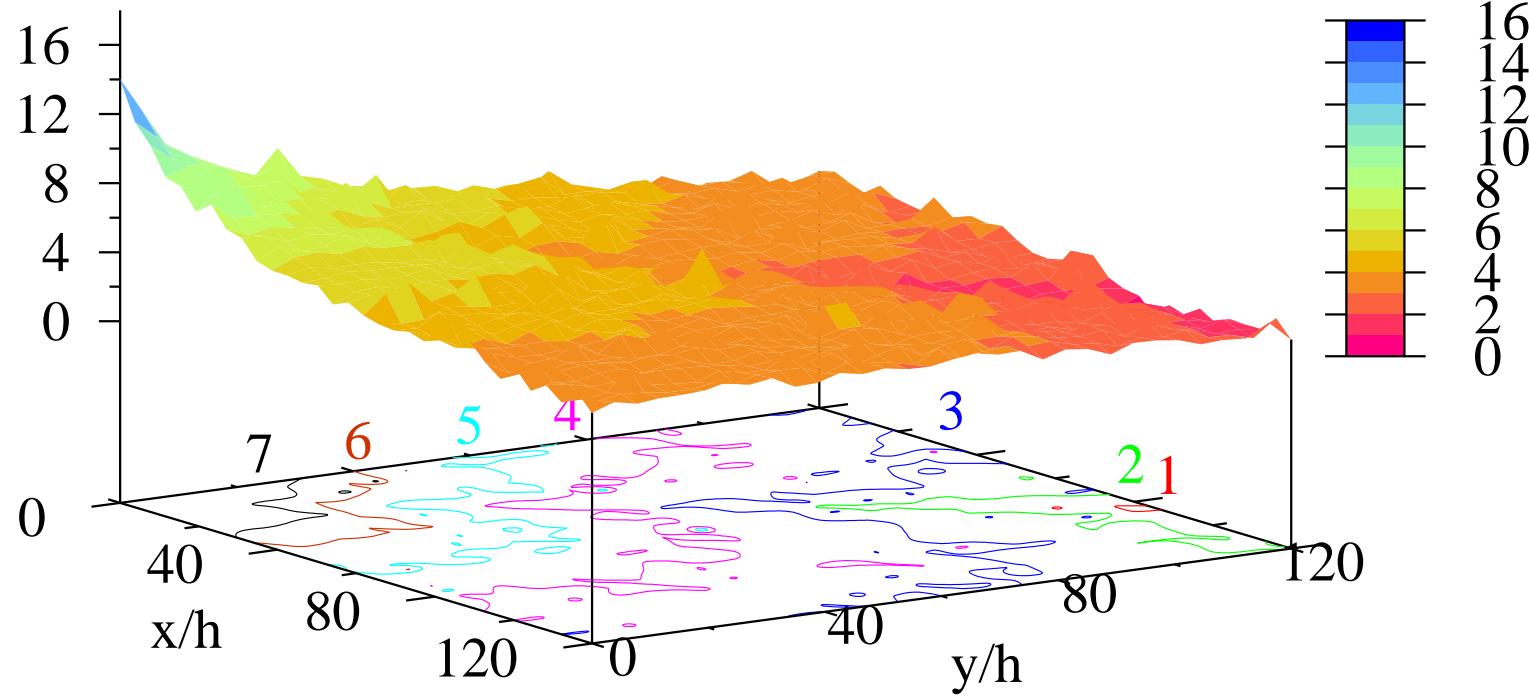
$$\begin{array}{r} a_0 \quad \boxed{6 \ 5 \ 4 \ 3 \ 2 \ 1} \\ + a_1 h \quad \boxed{6 \ 5 \ 4 \ 3 \ 2 \ 1} \\ \hline f(x+h) \quad \boxed{6 \ 6 \ 0 \ 8 \ 6 \ 4} \\ - f(x) \quad \boxed{6 \ 5 \ 4 \ 3 \ 2 \ 1} \\ \hline \quad \quad \quad \boxed{ \ 6 \ 5 \ 4 \ 3} \end{array}$$

← 2 digits lost



Relative Error: N_{xx}

Sig. Figs.
($-\log_{10}(\text{Rel. Err.})$)



Direct numeric implementation,
cubic cells, $z=0$.

What to do?

- Multiprecision library

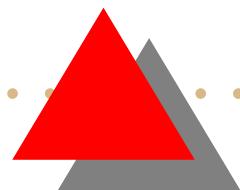
What to do?

- Multiprecision library
→ slow



What to do?

- Multiprecision library
→ slow
- Use “long double” (19 digits)



What to do?

- Multiprecision library
→ slow
- Use “long double” (19 digits)
→ helpful, but not enough

What to do?

- Multiprecision library
→ slow
- Use “long double” (19 digits)
→ helpful, but not enough
- Algebraic manipulations

Algebraic manipulations

$$R(x + h) - R(x) = \sqrt{(x + h)^2 + a^2} - \sqrt{x^2 + a^2}$$

$$= \frac{((x + h)^2 + a^2) - (x^2 + a^2)}{\sqrt{(x + h)^2 + a^2} + \sqrt{x^2 + a^2}}$$

$$= \frac{2xh + h^2}{\sqrt{(x + h)^2 + a^2} + \sqrt{x^2 + a^2}}$$

What to do?

- Multiprecision library
→ slow
- Use “long double” (19 digits)
→ helpful, but not enough
- Algebraic manipulations
→ too complicated

What to do?

- Multiprecision library
→ slow
- Use “long double” (19 digits)
→ helpful, but not enough
- Algebraic manipulations
→ too complicated
- Dipole approximation for far field

What to do?

- Multiprecision library
→ slow
- Use “long double” (19 digits)
→ helpful, but not enough
- Algebraic manipulations
→ too complicated
- Dipole approximation for far field
→ general case, only $O(1/R^2)$

What to do?

- Multiprecision library
→ slow
- Use “long double” (19 digits)
→ helpful, but not enough
- Algebraic manipulations
→ too complicated
- Dipole approximation for far field
→ general case, only $O(1/R^2)$
- **Solution:** Some algebraic + higher order asymptotics

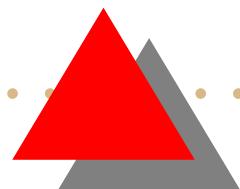


Tools and tricks

$$\log(A) - \log(B) = \log(A/B)$$

$$= \log(1 + (A - B)/B)$$

$$= \log(1 + \epsilon)$$



Tools and tricks

Arctan differences:

$$\arctan(A) - \arctan(B) = \arctan\left(\frac{A - B}{1 + AB}\right)$$

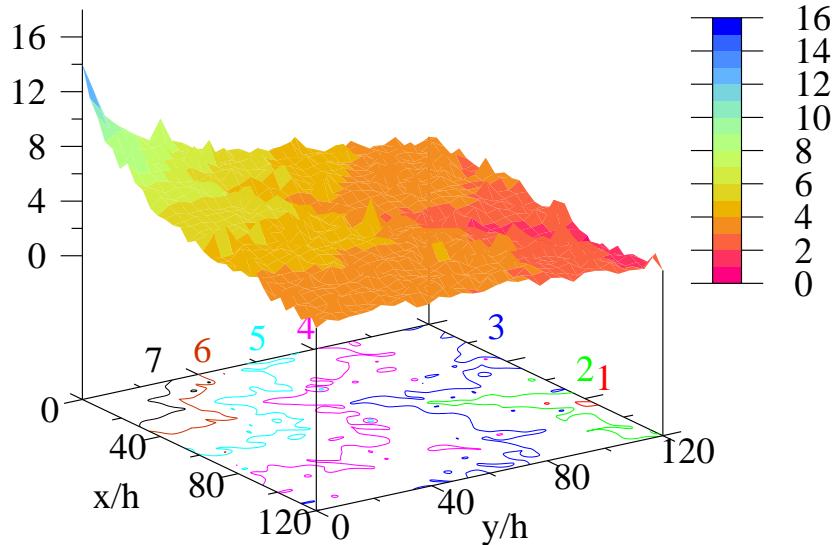
Difference of products:

$$\delta^2(fg) = f\delta^2g + g\delta^2f + \Delta f\Delta g + \nabla f\nabla g$$

where Δ and ∇ are the forward and backward difference operators, respectively.

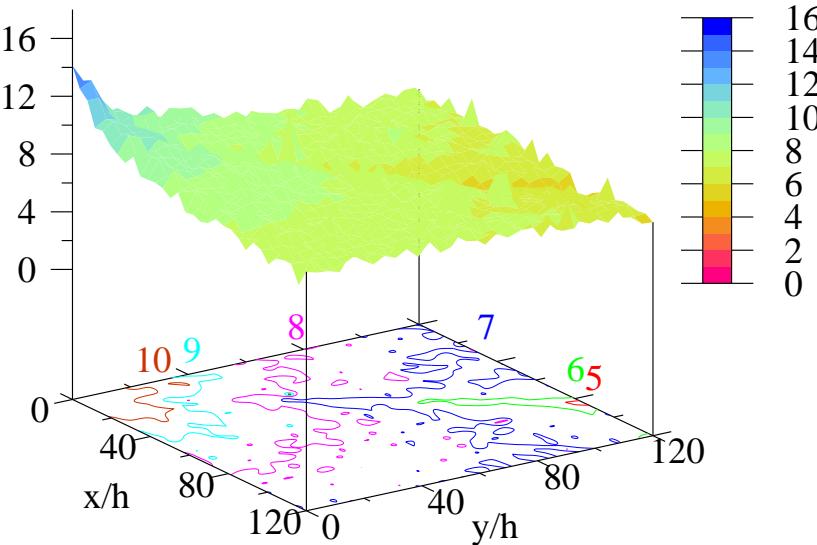
Algebraic recast (N_{xx})

Sig. Figs.
(-Log₁₀(Rel. Err.))



Direct

Sig. Figs.
(-Log₁₀(Rel. Err.))



Modified

Differences vs. Derivatives

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

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

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

Asymptotic expansion

$$(-4\pi h_x h_y h_z) N_{xx}(\mathbf{r}) = (-4\pi h_x h_y h_z) L[F; \mathbf{h}] (\mathbf{r})$$

$$= \delta_x^2 \circ \delta_y^2 \circ \delta_z^2 [F] (\mathbf{r})$$

$$= 8 (\cosh(h_x \partial/\partial x) - 1) \circ (\cosh(h_y \partial/\partial y) - 1) \\ \circ (\cosh(h_z \partial/\partial z) - 1) F(\mathbf{r})$$

Asymptotic expansion

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

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

Surprise!

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

(dipole field)

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

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,

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

Alternative asymptotics

$$N_{xx}(\mathbf{r}) = -1/(4\pi h_x h_y h_z) \delta_x^2 \circ \delta_y^2 \circ \delta_z^2 [F](\mathbf{r})$$

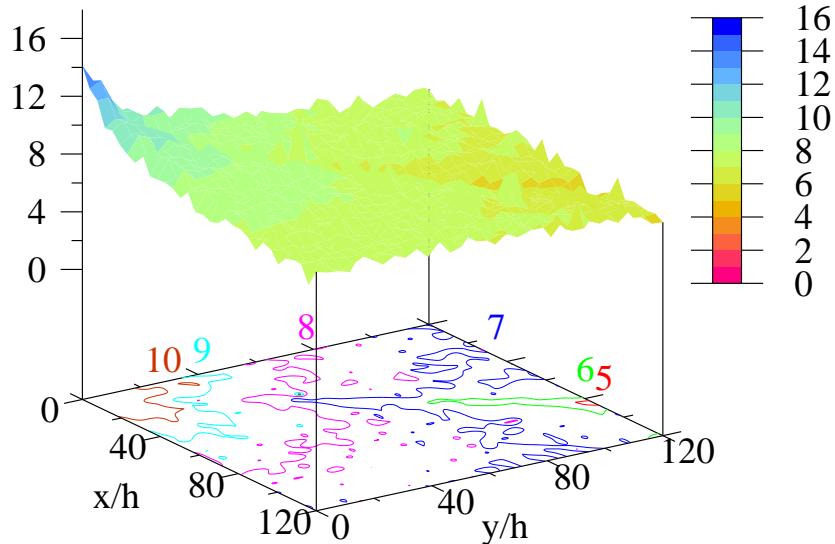
$$= -1/(\pi h_x h_y h_z) \cdot \delta_x^2 \\ \circ (\cosh(h_y \partial/\partial y) - 1) \circ (\cosh(h_z \partial/\partial z) - 1) F(\mathbf{r})$$

$$= -\frac{h_y h_z}{\pi h_x} \cdot \delta_x^2 \left[\frac{1}{R} + \frac{\mathbf{h}_{yz,2}^T B_3 \mathbf{r}_2}{R^3} + \frac{\mathbf{h}_{yz,4}^T B_5 \mathbf{r}_4}{R^5} + \frac{\mathbf{h}_{yz,6}^T B_7 \mathbf{r}_6}{R^7} \right]$$

$$+ O(1/R^{11})$$

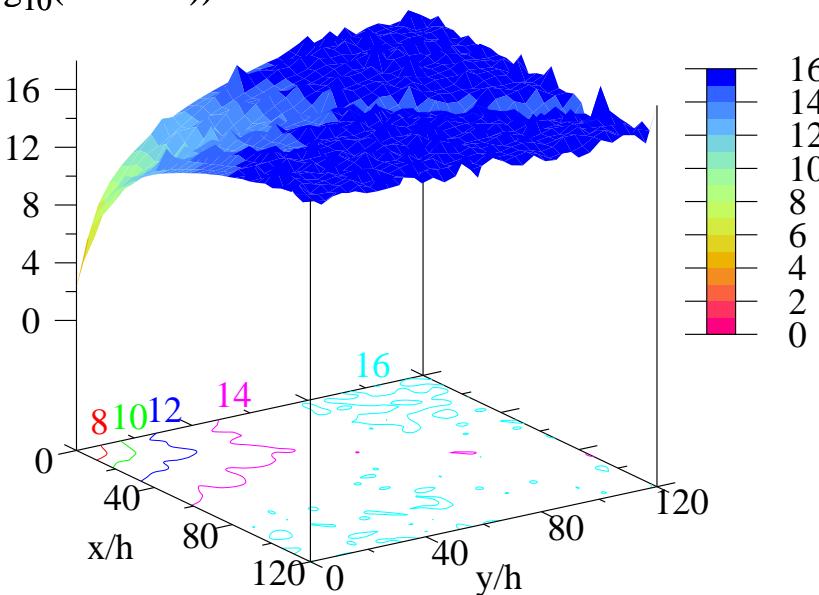
N_{xx} : Near and far

Sig. Figs.
($-\log_{10}(\text{Rel. Err.})$)



Algebraic

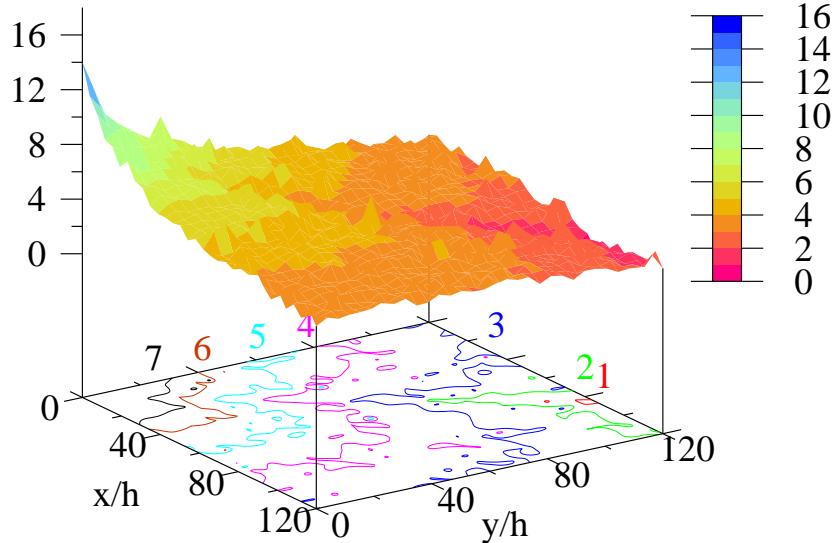
Sig. Figs.
($-\log_{10}(\text{Rel. Err.})$)



Asymptotic, $O(1/R^8)$

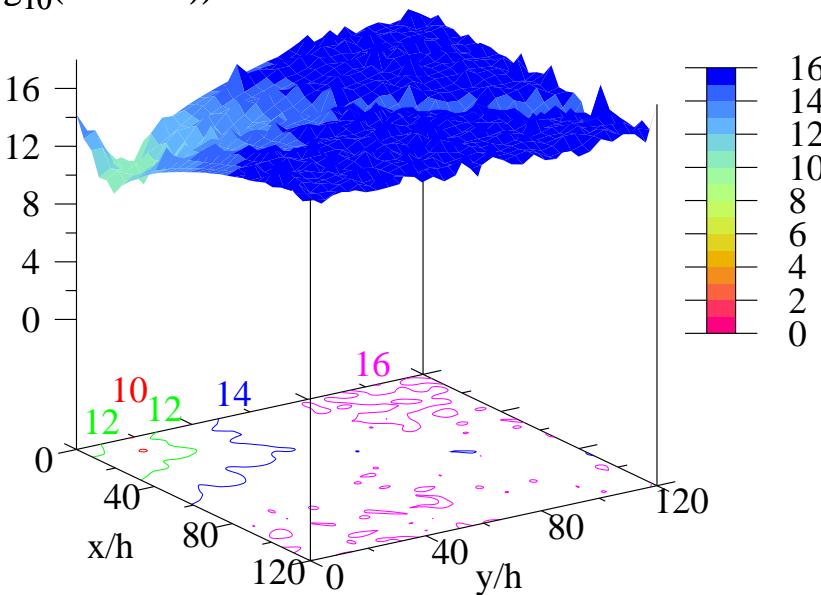
Results: N_{xx}

Sig. Figs.
(-Log₁₀(Rel. Err.))



Original

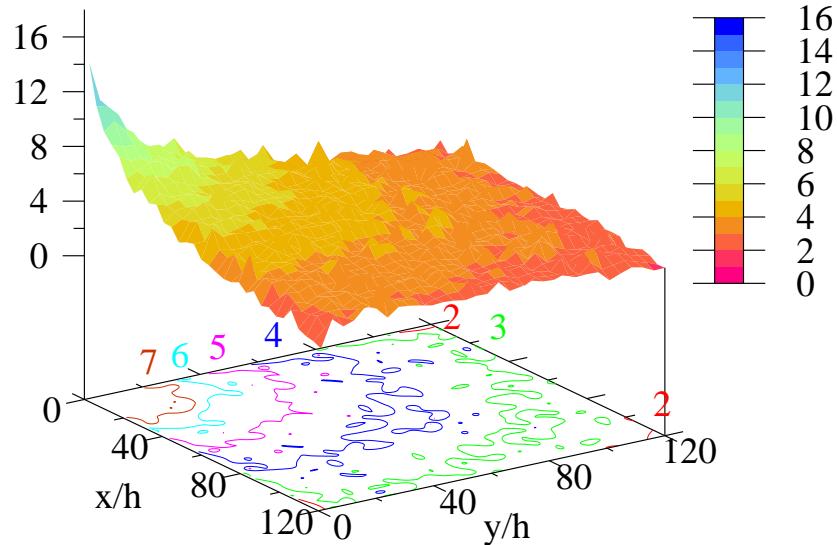
Sig. Figs.
(-Log₁₀(Rel. Err.))



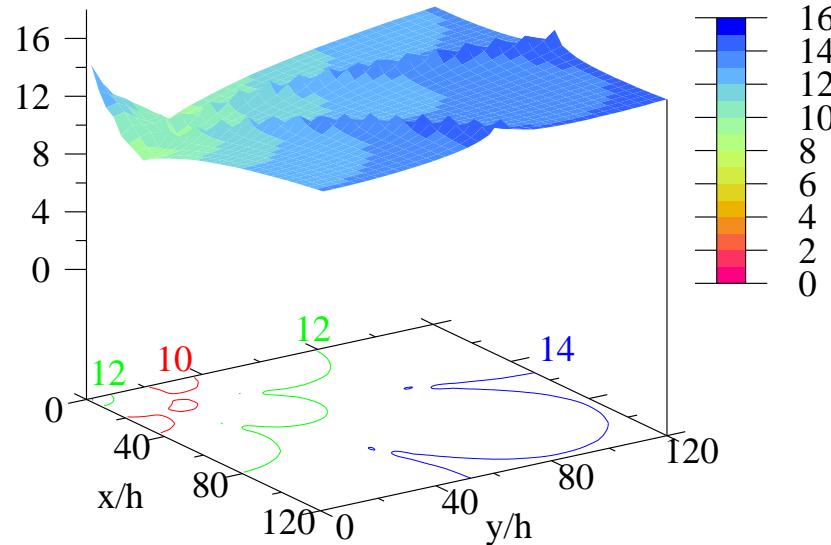
Algebraic+Asymptotic,
crossover at $R/h = 20$.

Results: N_{xy}

Sig. Figs.
($-\log_{10}(\text{Rel. Err.})$)

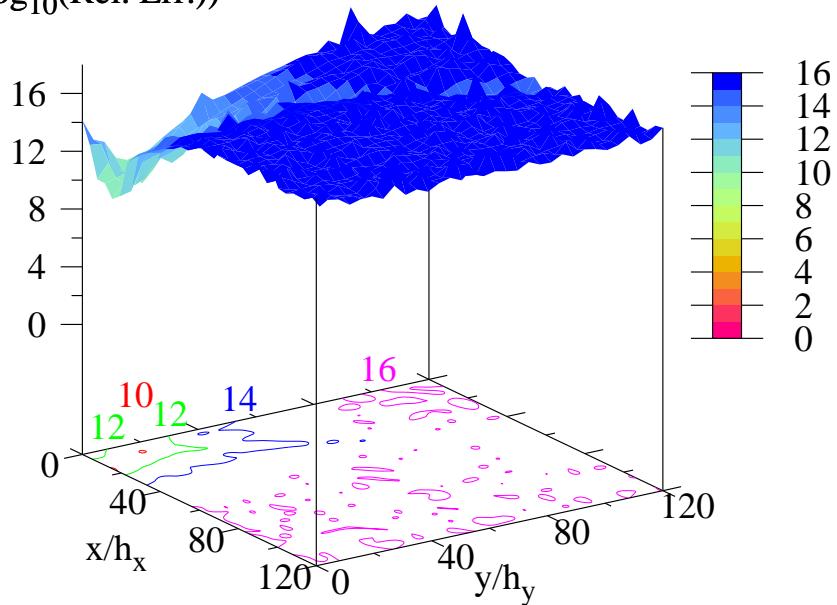


Sig. Figs.
($-\log_{10}(\text{Rel. Err.})$)



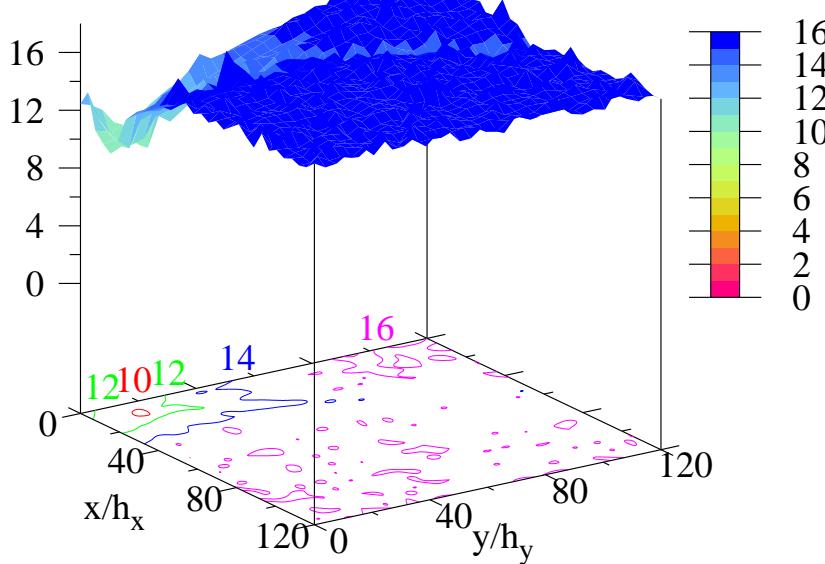
N_{xx} , 3:2:1 cell geometry

Sig. Figs.
(-Log₁₀(Rel. Err.))



Offset $z/h_z = 0$

Sig. Figs.
(-Log₁₀(Rel. Err.))



Offset $z/h_z = 10$

Conclusions

- Algebraic + asymptotics \Rightarrow 10 digits
- Worse accuracy at mid-field transition ($20h$)
- + “long double” >12 digits?
- High order asymptotics allow MP library use restricted to near field
- Valid for arbitrary rectangular prisms