

Micromagnetics on curved geometries using rectangular cells: error correction and analysis

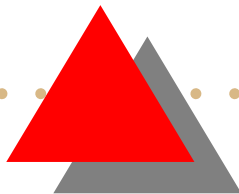
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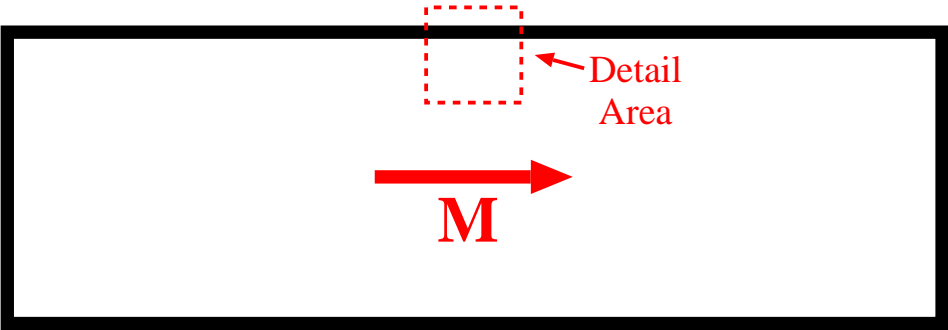


Outline

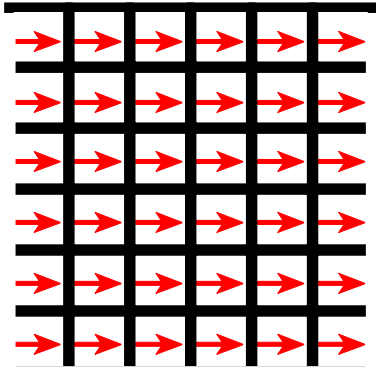
- Staircase artifact
- 1D correction
- General case
 - Local subgrid
- Correction tests
 - Edge mode resonance
 - Vortex expulsion
- Analytic model



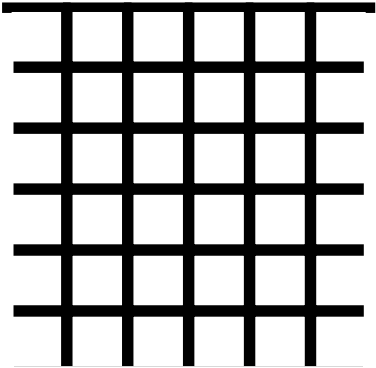
Uniformly Magnetized Strip



Detail

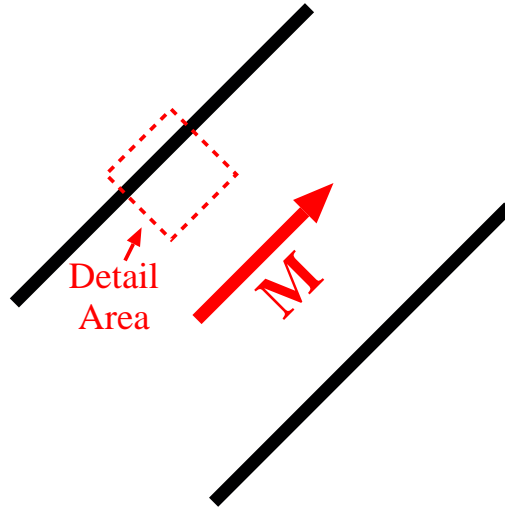


Magnetization

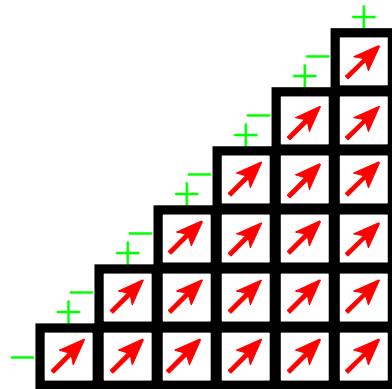


Demag Field

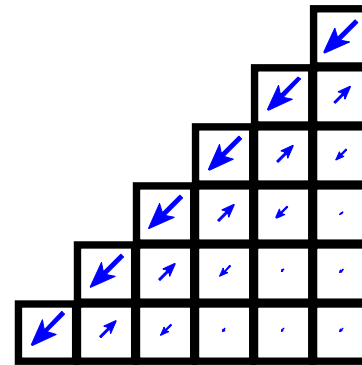
Uniformly Magnetized Strip, Rotated



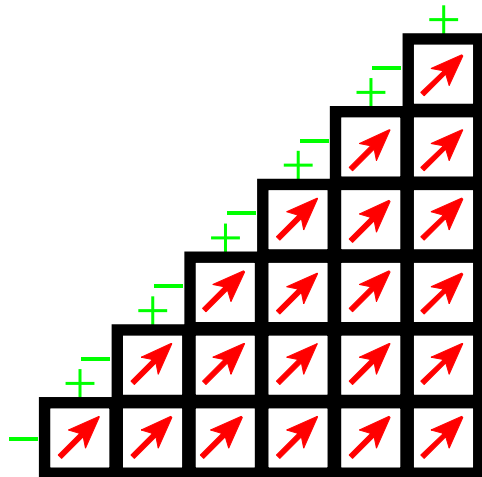
Detail



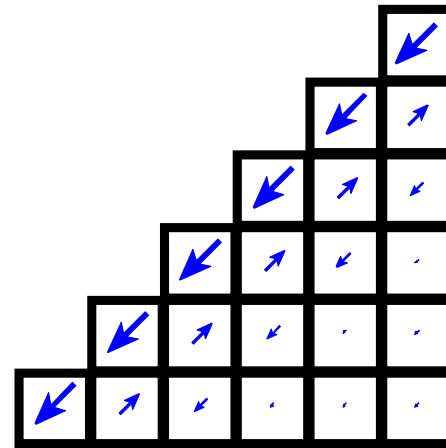
Magnetization



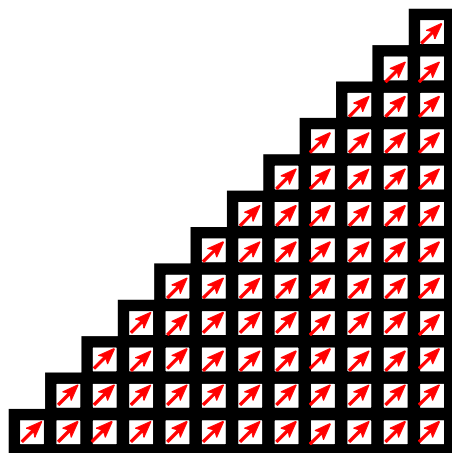
Demag Field



Magnetization

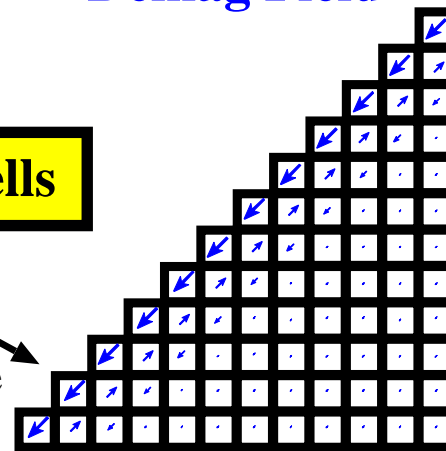


Demag Field



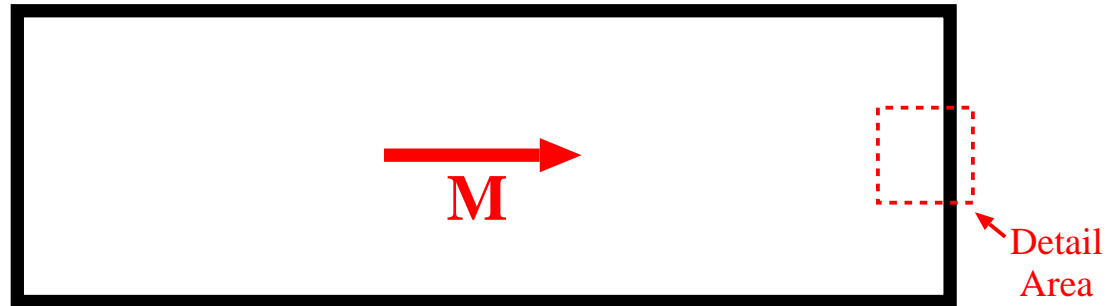
Half-size cells

H_D increases slightly on edge

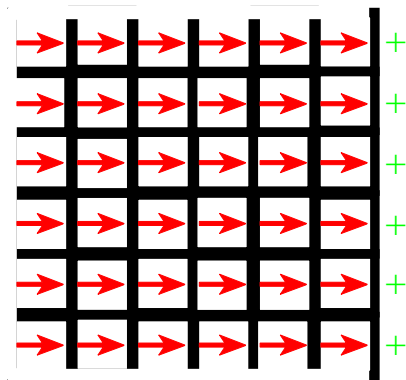


H_D decreases inside

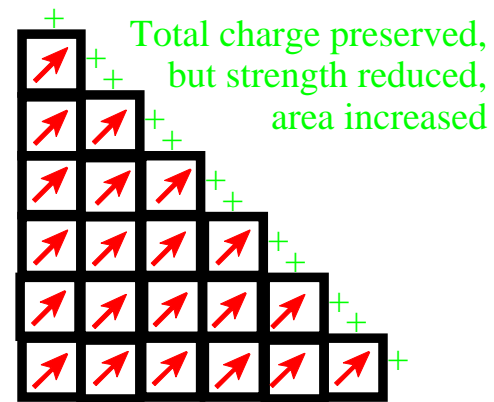
Uniformly Magnetized Strip



Magnetization Detail

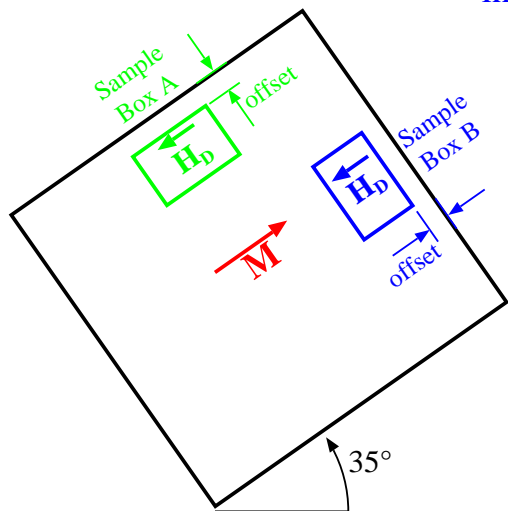


Grid Aligned

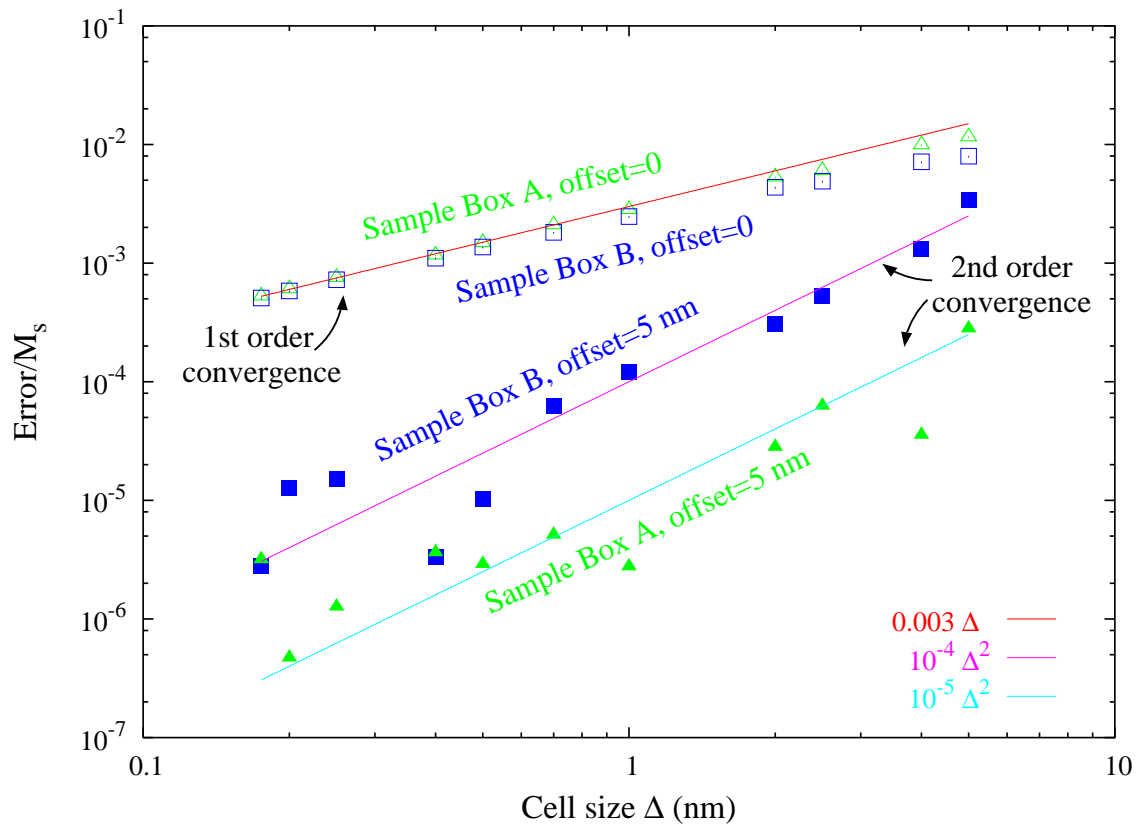


Rotated

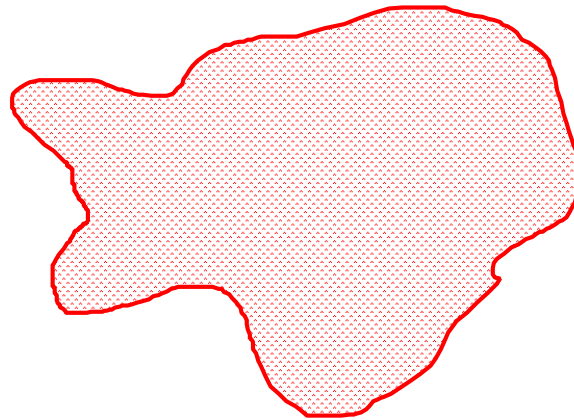
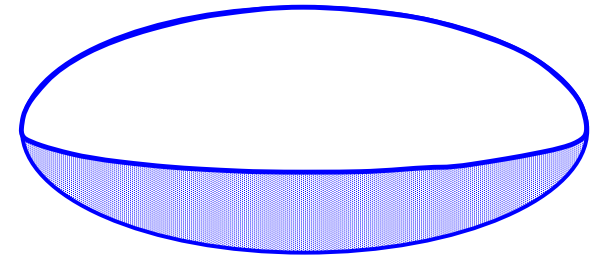
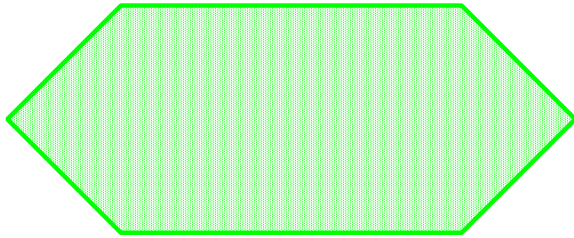
Average $\mathbf{H}_{\text{Demag}} \cdot \mathbf{M}$ computed
in each sample box



Py squares
350 nm x 350 nm x 5 nm
Uniform Magnetization



General Geometries



Demag field

$$\mathbf{H}_{\text{demag}}(\mathbf{r}) = -\frac{1}{4\pi} \int_V \nabla \cdot \mathbf{M}(\mathbf{r}') \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} d^3 r' + \frac{1}{4\pi} \int_S \hat{\mathbf{n}}(\mathbf{r}') \cdot \mathbf{M}(\mathbf{r}') \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} d^2 r'.$$

Assume \mathbf{M} uniform in each cell gives

$$\langle \mathbf{H}_{\text{demag},i} \rangle = - \sum_j N_{i,j} \mathbf{M}_j.$$

where formulae for $N_{i,j}$ are given in

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

Demag field (cont.)

If cells are identical on a uniform grid, then

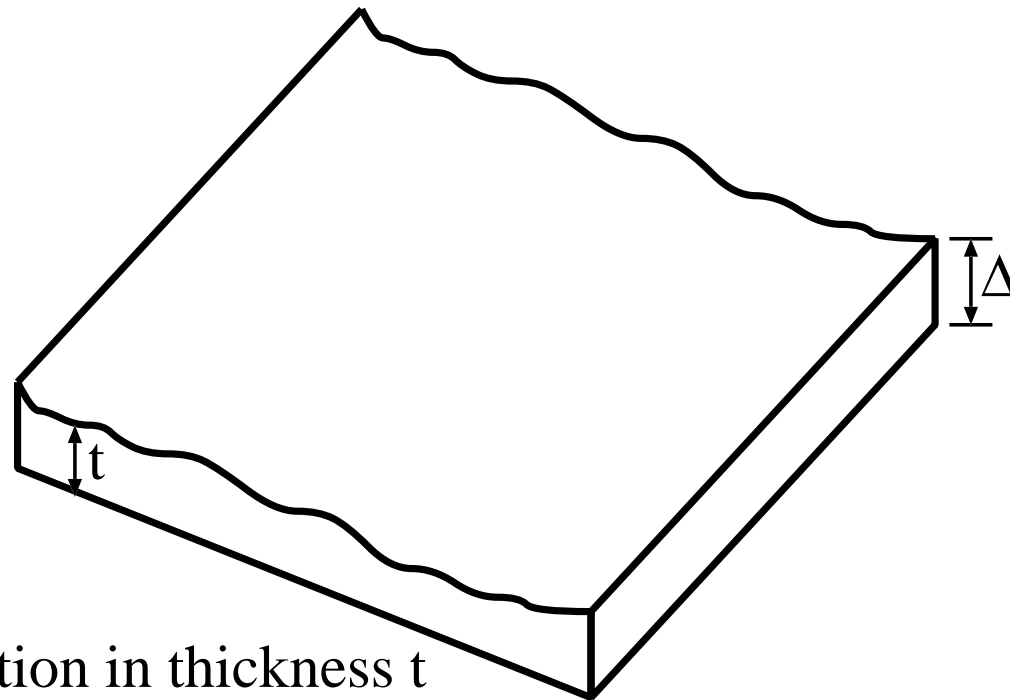
$$\langle \mathbf{H}_{\text{demag},i} \rangle = - \sum_j N_{i,j} \mathbf{M}_j$$

becomes

$$\langle \mathbf{H}_{\text{demag},i} \rangle = - \sum_j N_{i-j} \mathbf{M}_j$$

where FFT can be used to evaluate $\mathbf{H}_{\text{demag},i}$.

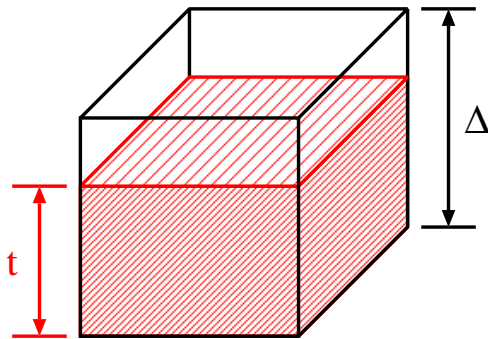
(Note: Uniform **grid**; $|M_i|$'s can vary cell-to-cell.)



Variation in thickness t
smaller than cell height Δ

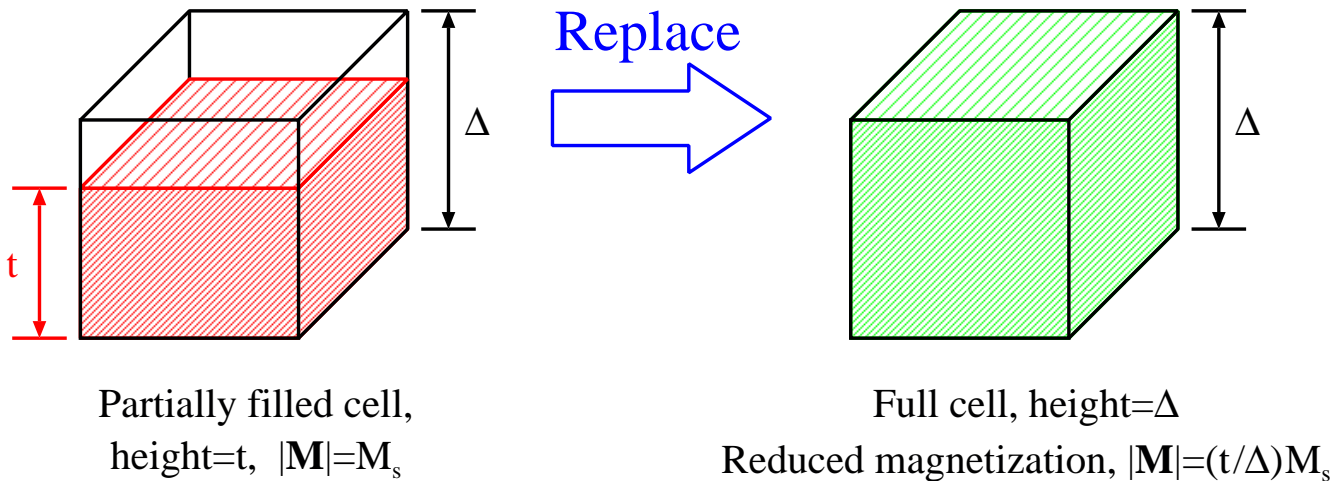
Porter & Donahue, "Generalization of a two-dimensional micromagnetic model to non-uniform thickness," *JAP*, **89**, 7257 (2001).

PROBLEM: Partially filled cell has different geometry,
so FFT can't be used to compute demag field.

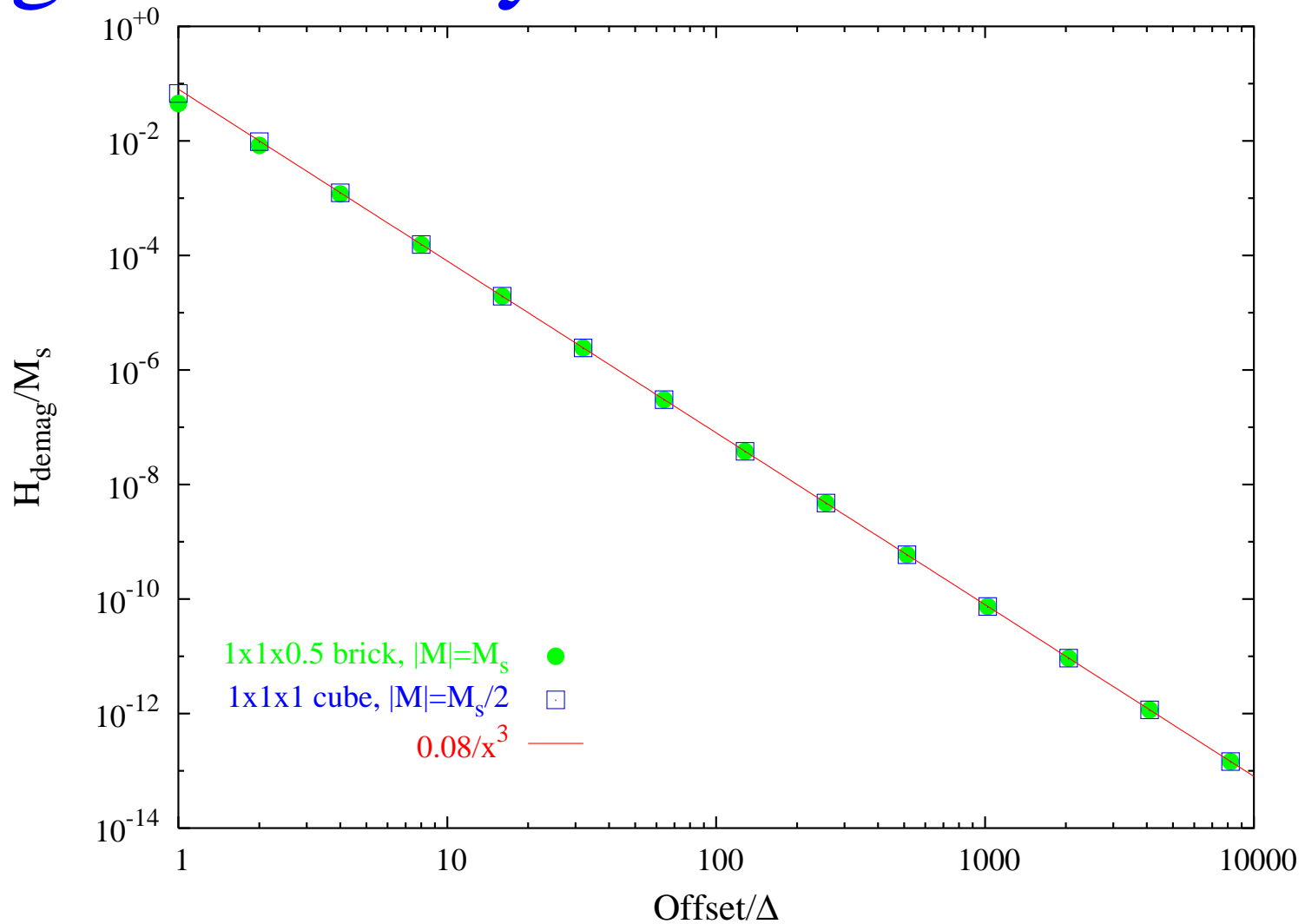


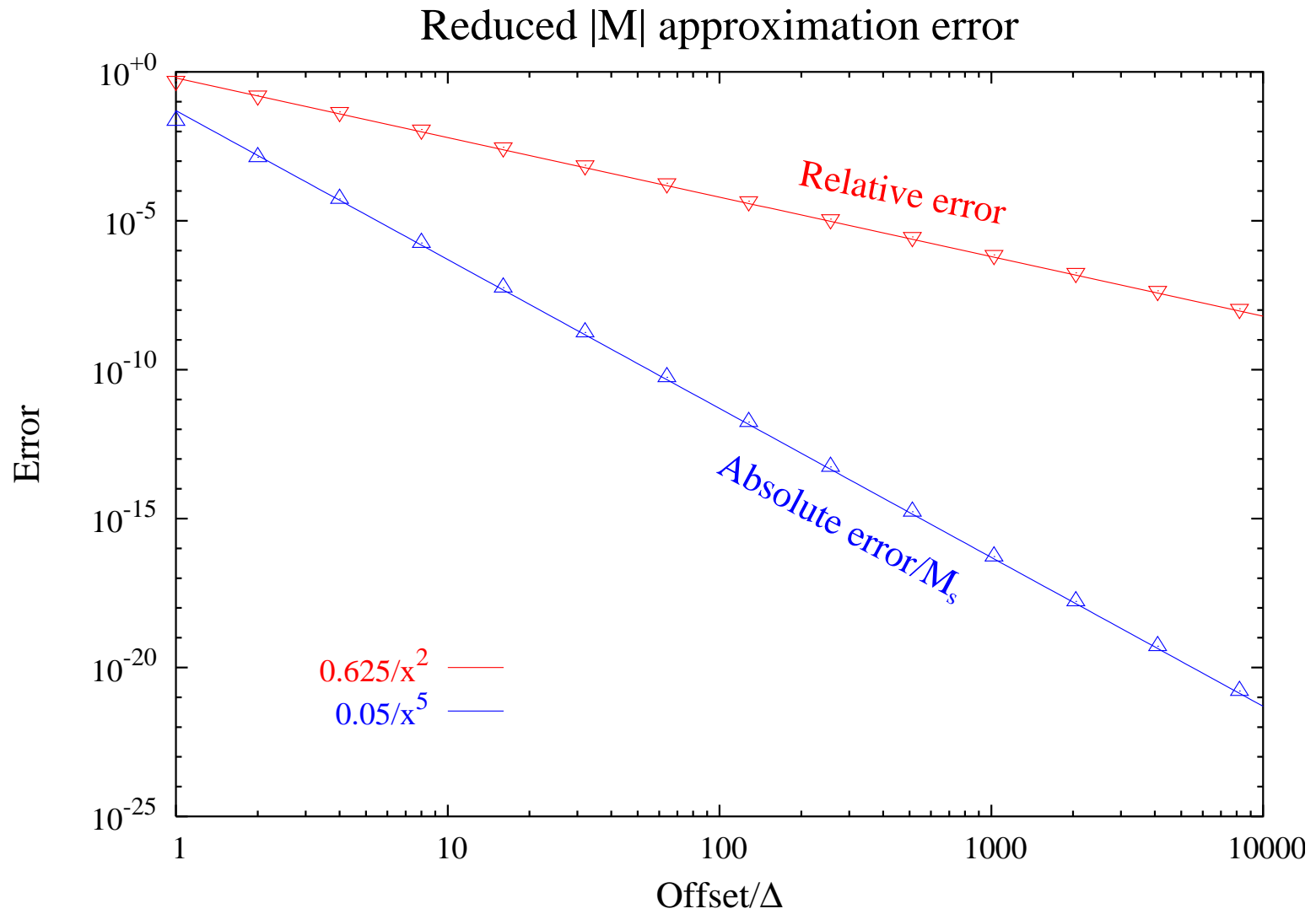
Partially filled cell,
height=t, $|\mathbf{M}|=M_s$

SOLUTION: Use full cell so all cells have same geometry,
but reduce M_s so far-field demag is correct.

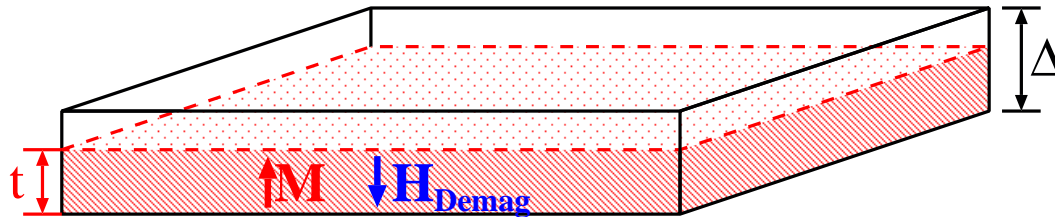


Single cell stray field

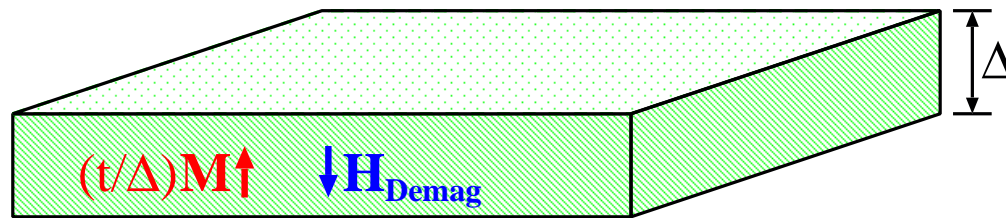




Infinite plate



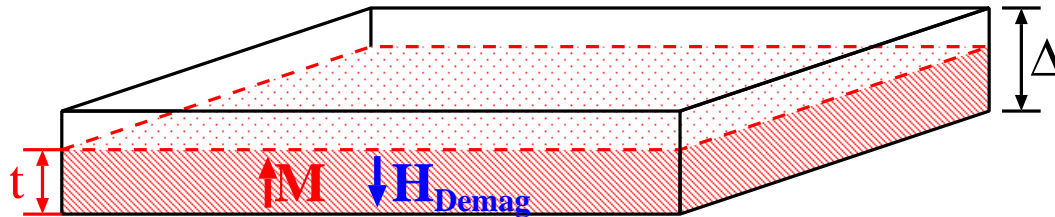
$$\mathbf{H}_{\text{Demag}} = -\mathbf{M} \text{ independent of } t$$



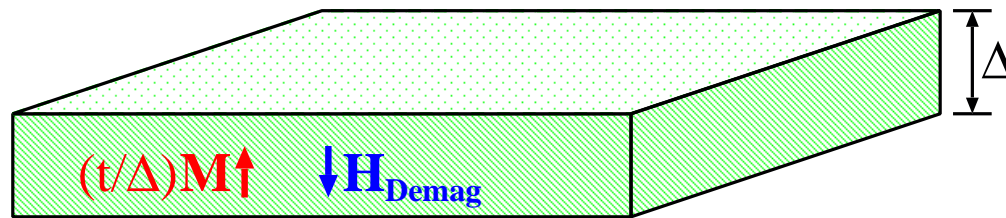
Problem: For reduced magnetization $|\mathbf{M}| = (t/\Delta)\mathbf{M}_s$ model

$$|\mathbf{H}_{\text{Demag}}| = (t/\Delta)\mathbf{M}_s$$

Infinite plate



$$\mathbf{H}_{\text{Demag}} = -\mathbf{M} \text{ independent of } t$$



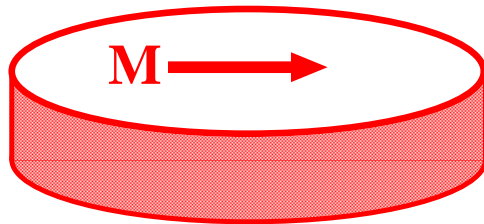
Problem: For reduced magnetization $|\mathbf{M}| = (t/\Delta)M_s$ model

$$|\mathbf{H}_{\text{Demag}}| = (t/\Delta)M_s$$

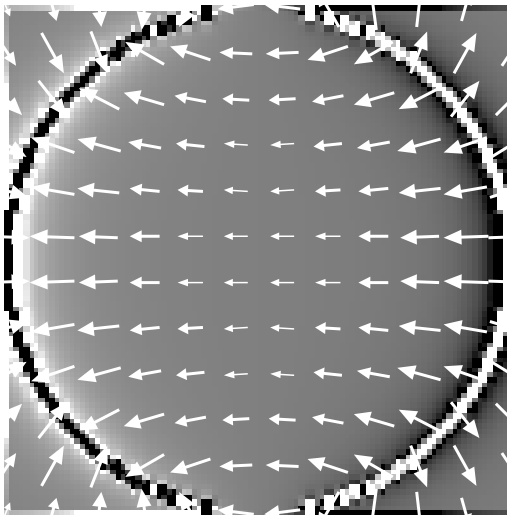
Solution: Add local anisotropy field to correct deficit:

$$\mathbf{H}_{\text{anis}} = -(1-t/\Delta)M_s(\mathbf{m} \cdot \mathbf{e}_z)\mathbf{e}_z$$

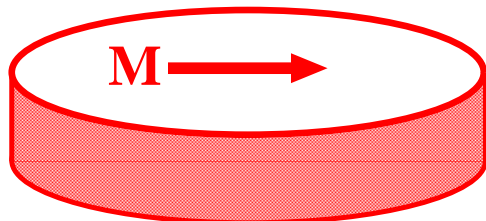
10x10x1 disk



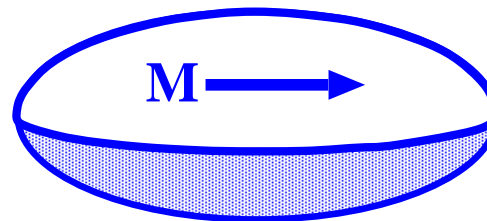
Demag Field



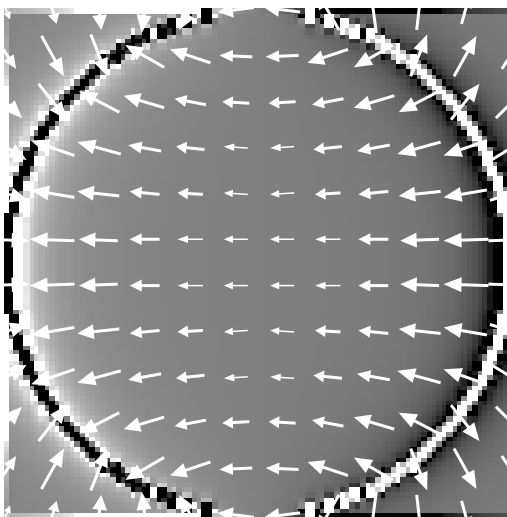
10x10x1 disk



10x10x1 oblate spheroid

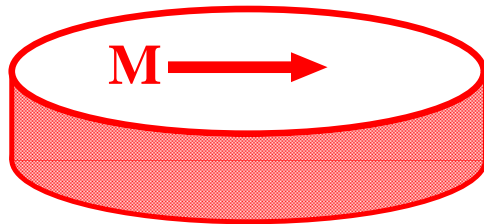


Demag Field

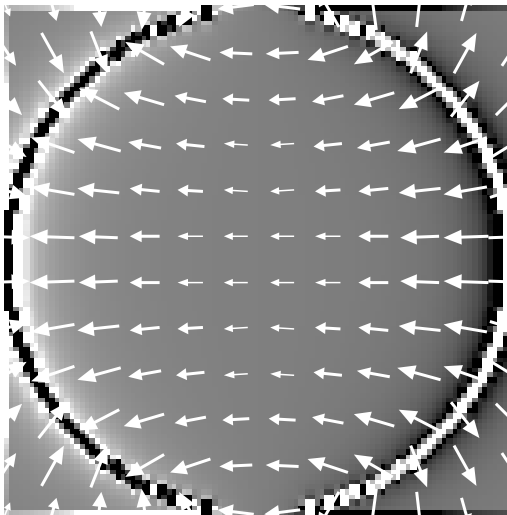


RMS error = 118%

10x10x1 disk

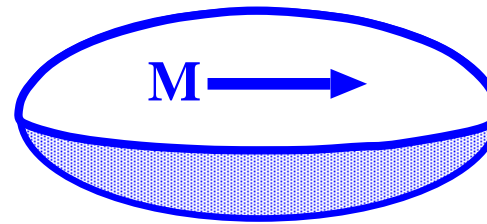


Demag Field

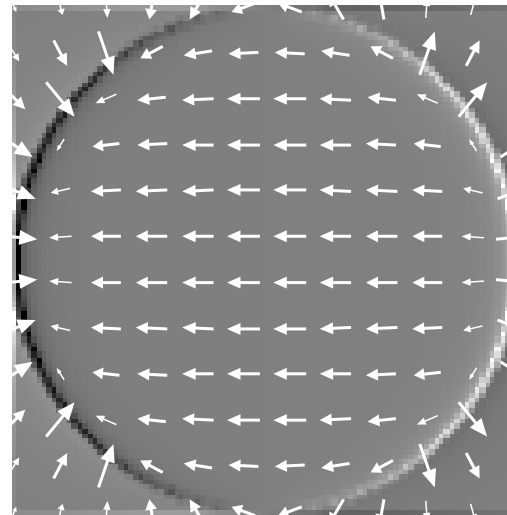


RMS error = 118%

10x10x1 oblate spheroid



Demag Field with
Thickness Corrections



RMS error = 29%

General case

Decompose

$$\mathbf{H}_{\text{demag},i} = - \sum_j N_{i,j} \mathbf{M}_j$$

into

$$\mathbf{H}_{\text{demag},i} = - \sum_{j \in \Omega_{\text{local}}} N_{i,j} \mathbf{M}_j - \sum_{j \in \Omega_{\text{far}}} N_{i,j} \mathbf{M}_j$$

Handle Ω_{far} via modified M_s and FFT, Ω_{local} some other way.

General case (cont.)

Concept:

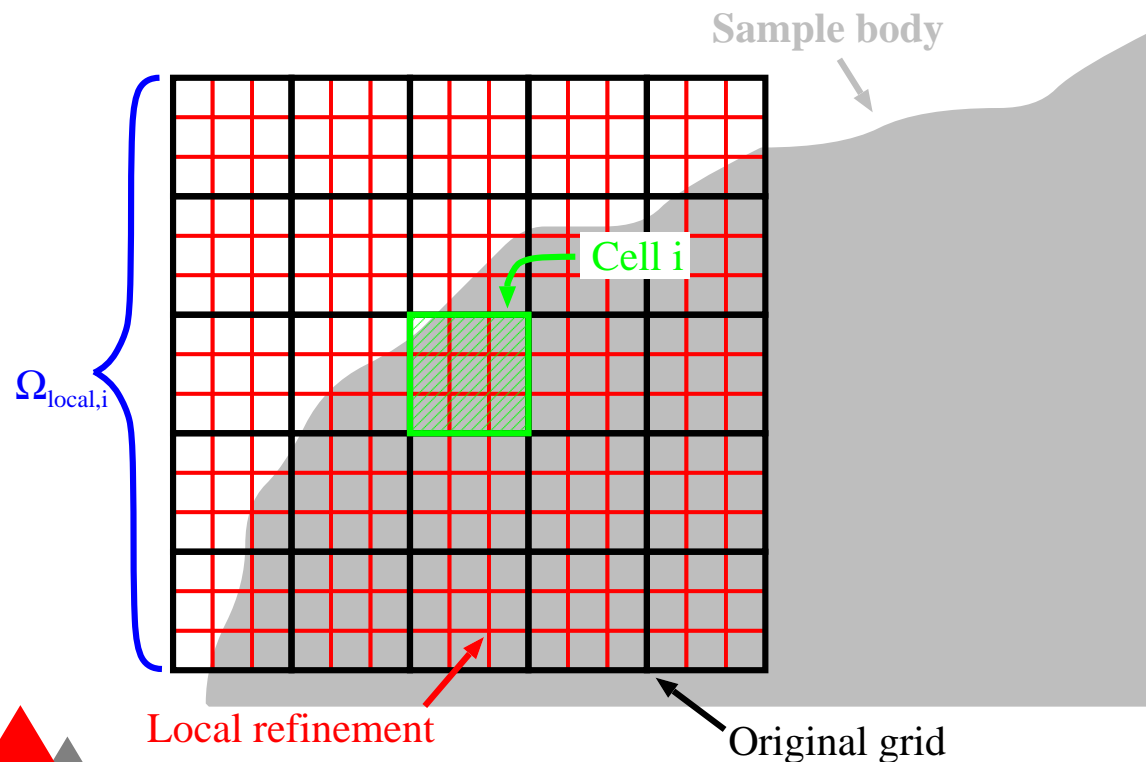
- Far field computed efficiently via FFT.
- Near field computed accurately.
- Restricted size keeps $\Omega_{\text{local}} O(N)$.

García-Cervera, Gimbutas, & E, “Accurate numerical methods for micromagnetics simulations with general geometries,” *J. Comp. Physics*, **184**, 37 (2003).

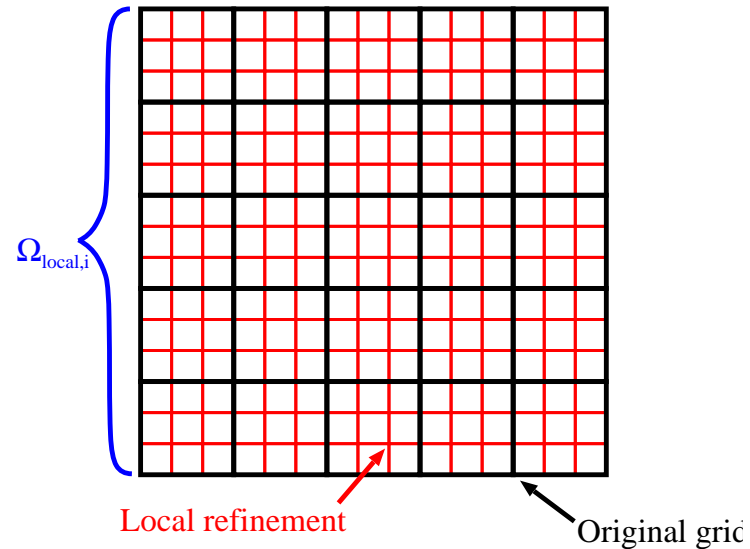
Local field computation

Problem: Implementing Ω_{local} not so simple.

Idea: Use existing demag code to compute Ω_{local} , but on a local, refined grid.

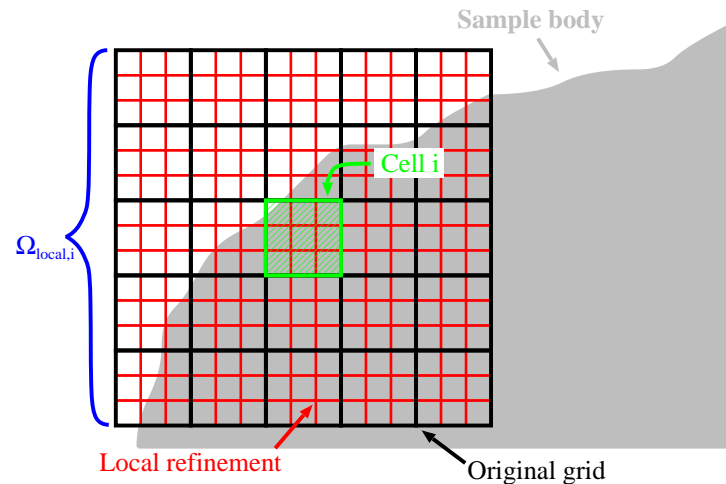


Local field computation



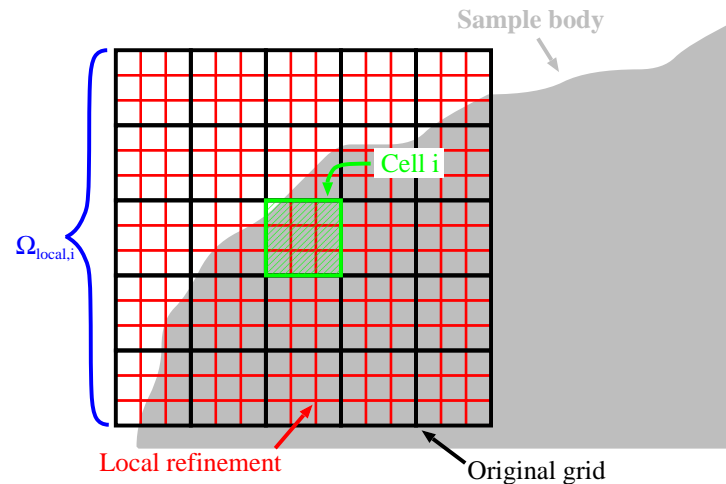
- Compute $N_{i'-j'}^{\text{fine}}$ for fine mesh on Ω_{local} (once)

Local field computation



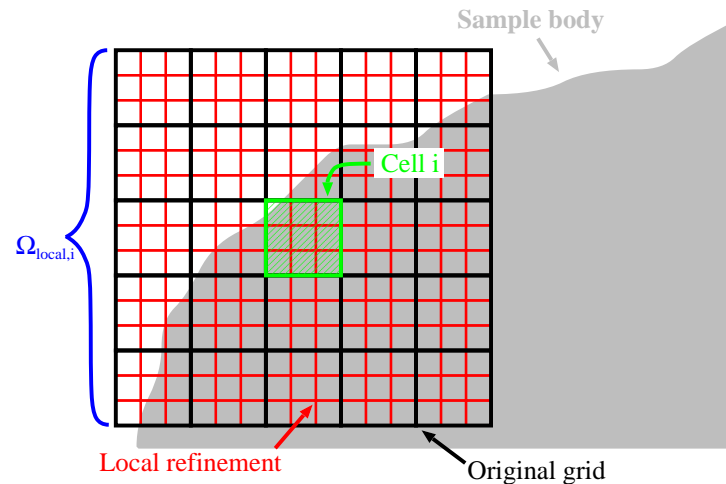
- Compute $N_{i'-j'}^{fine}$ for fine mesh on Ω_{local} (once)
- For i, j near boundary, compute $\langle \mathbf{H}_{demag}^{fine} \rangle_{i,j}$

Local field computation



- Compute $N_{i'-j'}^{\text{fine}}$ for fine mesh on Ω_{local} (once)
- For i, j near boundary, compute $\langle \mathbf{H}_{\text{demag}}^{\text{fine}} \rangle_{i,j}$
- $\mathbf{H}_{\text{demag}}^{\text{fine}} - \mathbf{H}_{\text{demag}}^{\text{coarse}}$ define correction factors $K_{i,j}$

Local field computation



- Compute $N_{i'-j'}^{\text{fine}}$ for fine mesh on Ω_{local} (once)
- For i, j near boundary, compute $\langle \mathbf{H}_{\text{demag}}^{\text{fine}} \rangle_{i,j}$
- $\mathbf{H}_{\text{demag}}^{\text{fine}} - \mathbf{H}_{\text{demag}}^{\text{coarse}}$ define correction factors $K_{i,j}$
- NOTE: Done once during initialization!

Local field computation

During simulation run:

- Compute $\mathbf{H}_{\text{demag}}$ as usual, with volume-modified $|M|$.
- For cells near boundary, include local corrections

$$\mathbf{H}_{\text{corr},i} = - \sum_{j \in \Omega_{\text{local}_i}} K_{i,j} \mathbf{M}_j$$

- Correction is $O(N_{\text{boundary}})$

Local correction, pushed

Energy of correction is

$$\begin{aligned} E_{i,j} &\propto \mathbf{m}_i^T K_{i,j} \mathbf{m}_j \\ &= \mathbf{m}_i^T K_{i,j} (\mathbf{m}_j - \mathbf{m}_i) + \mathbf{m}_i^T K_{i,j} \mathbf{m}_i. \end{aligned}$$

If $|\mathbf{m}_j - \mathbf{m}_i|$ is small (exchange), then

$$E_{i,j} \tilde{\propto} \mathbf{m}_i^T K_{i,j} \mathbf{m}_i$$

which is a local anisotropy.

Local correction, pushed

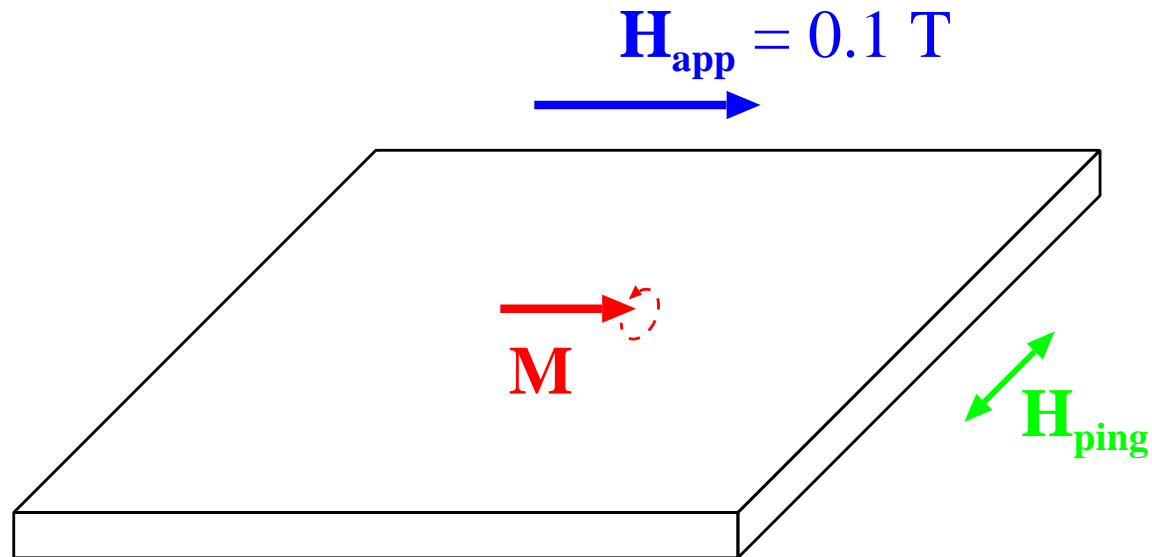
So

$$\mathbf{H}_{\text{demag},i} \approx - \sum_j N_{i-j} \mathbf{M}_j - K_i \mathbf{M}_i$$

where

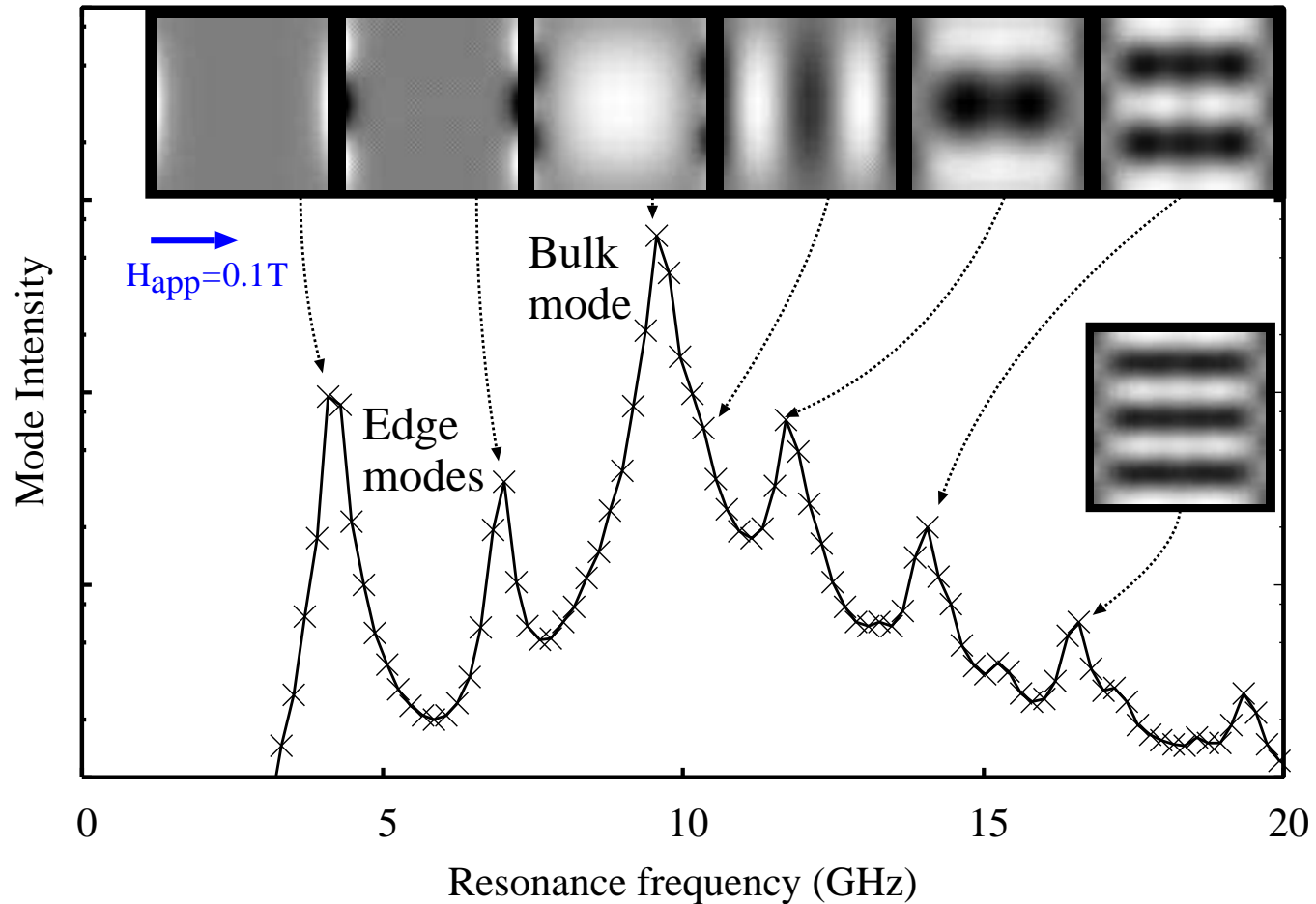
$$K_i = \sum_{j \in \Omega_{\text{local}}} K_{i,j}$$

FMR simulations

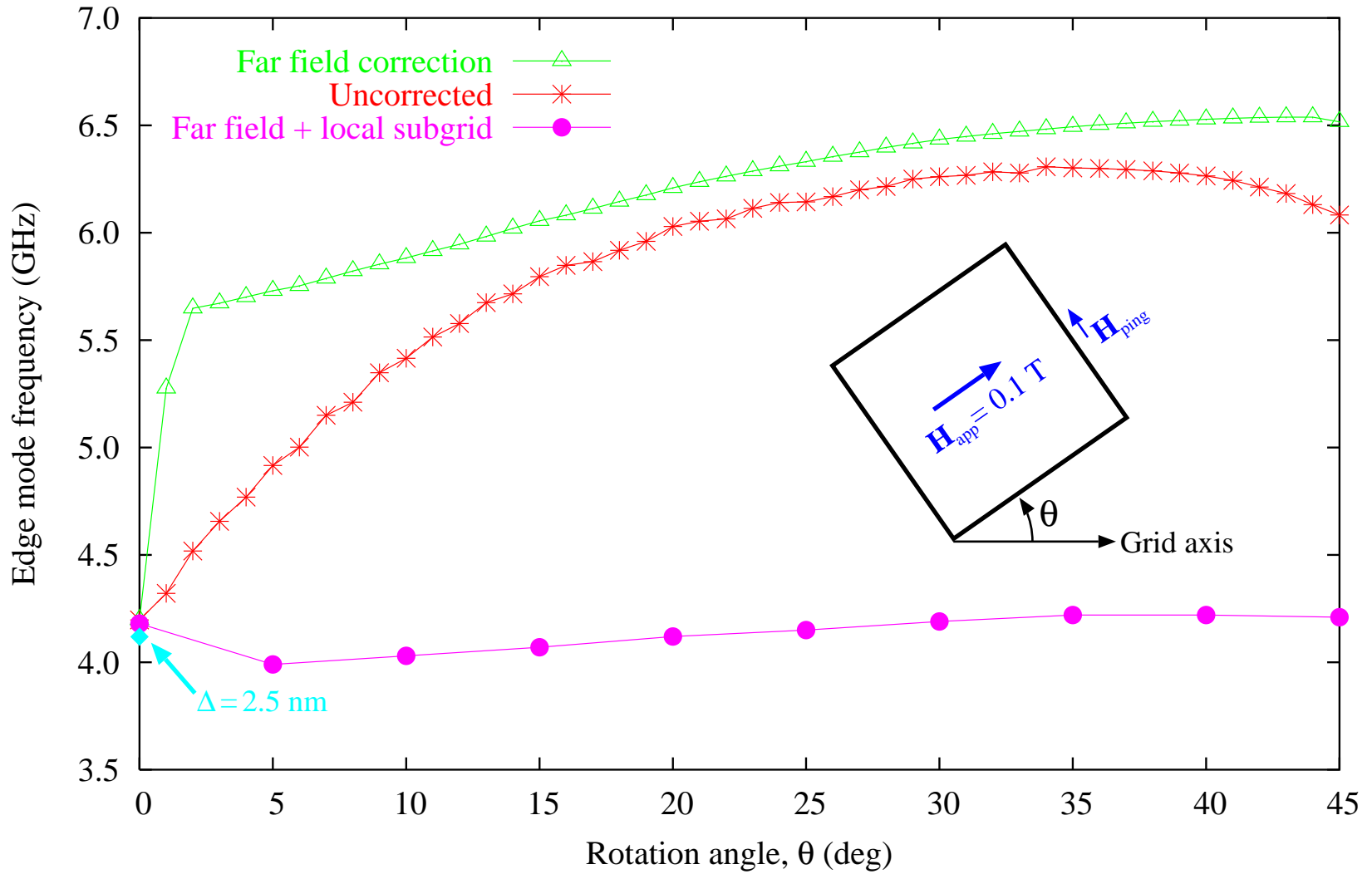


Small "ping" field
induces spinwaves.

FMR spectrum



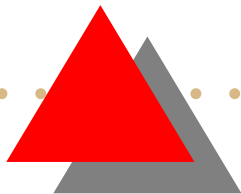
Corrections: Angular dependence



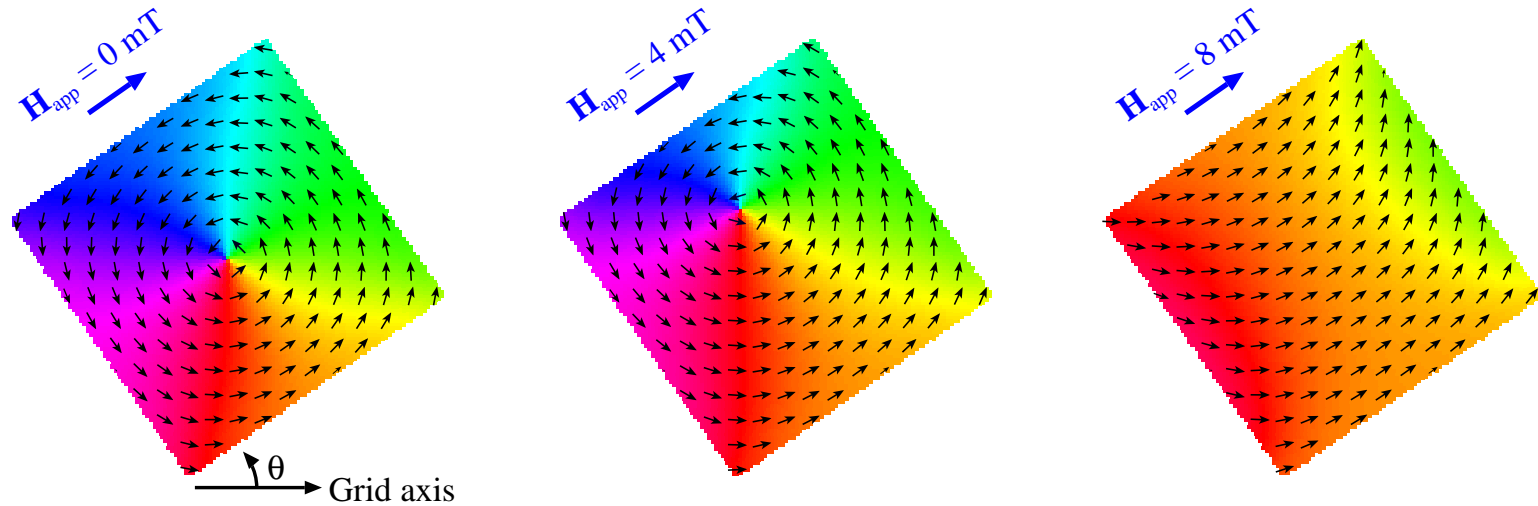


Key points

- Edge mode sensitive only to edge effects
- Quantitative
- Robust quantity, does not involve critical field
- Experimentally relevant



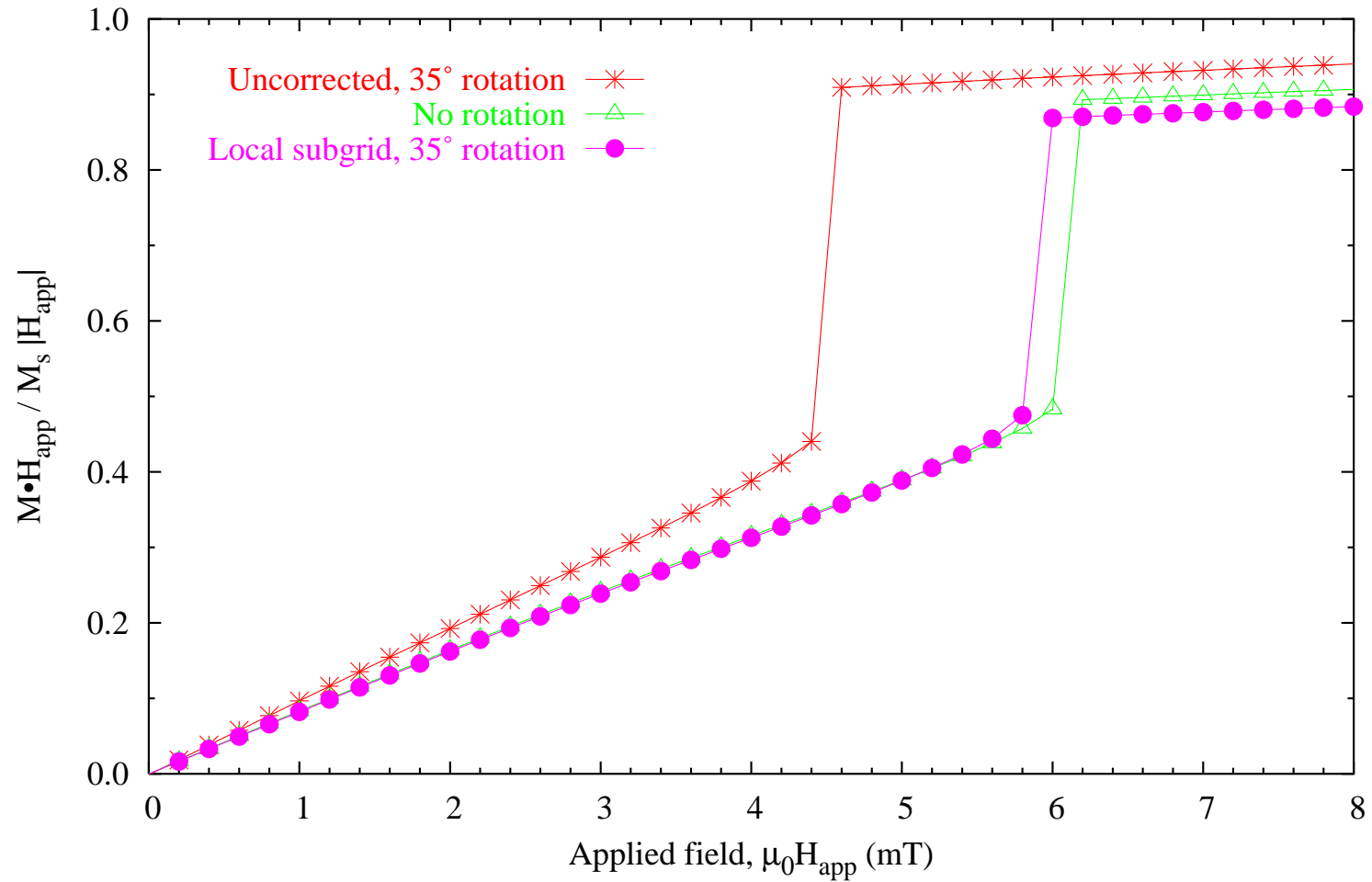
Vortex Expulsion Test



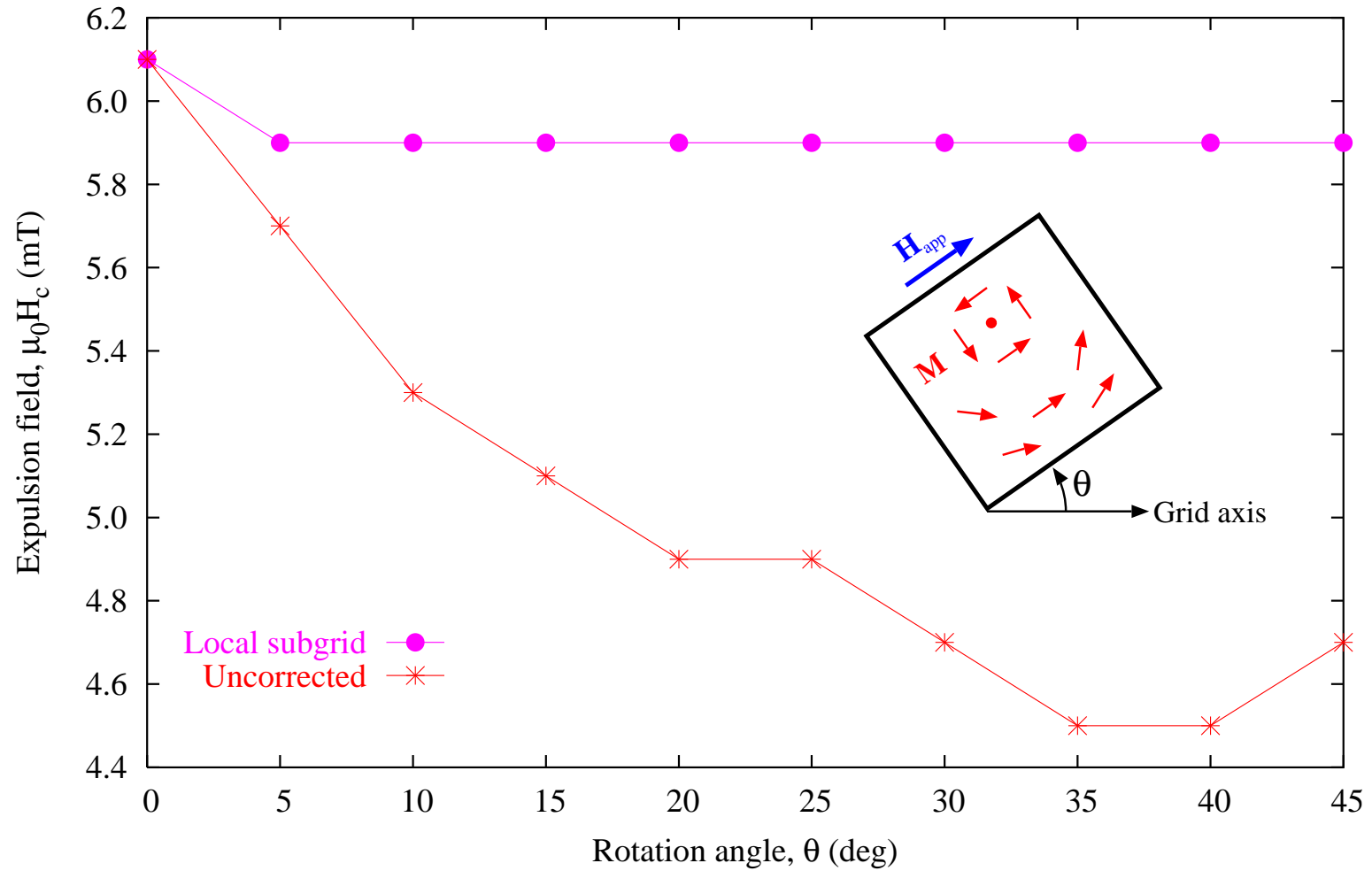
220 nm x 220 nm x 2.5 nm Py square
Cellsize $\Delta = 2.5 \text{ nm}$ (cubes)

- Compute M vs. H_{app}
- Compute expulsion field H_c vs. grid angle θ

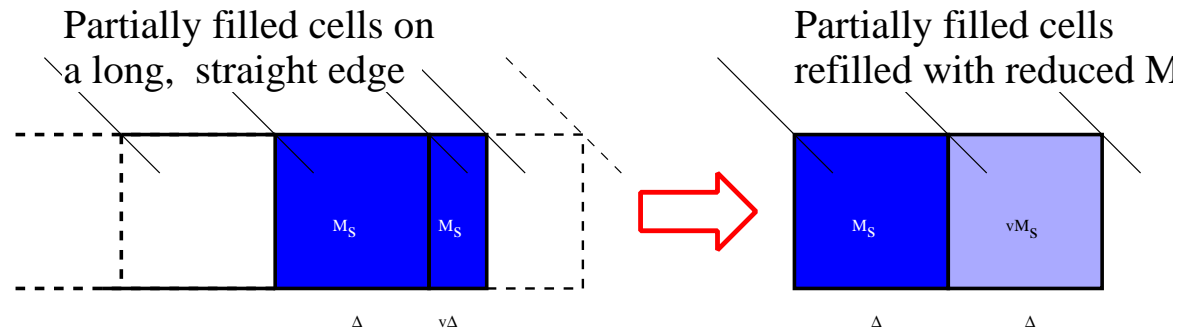
Vortex Expulsion: Field dependence



Vortex Expulsion: Angular dependence



Edge cell adjustment



Additional demag energy of strip of partial cells

$$E_{\text{partial}} = \frac{1}{2} \mu_0 M_s^2 m_z^2 v \Delta \cdot t$$

Same energy as embedding a strip far away from the edge.

Additional demag energy of strip of diluted cells, for $\Delta=t$

$$E_{\text{diluted}} = \left\{ \frac{1}{4} \mu_0 (v M_s)^2 (m_x^2 + m_z^2) + \frac{1}{4} \mu_0 M_s v M_s (m_z^2 - m_x^2) \right\} \Delta \cdot t$$

Self demag of diluted edge cells. *Interaction with the bulk of the film.*

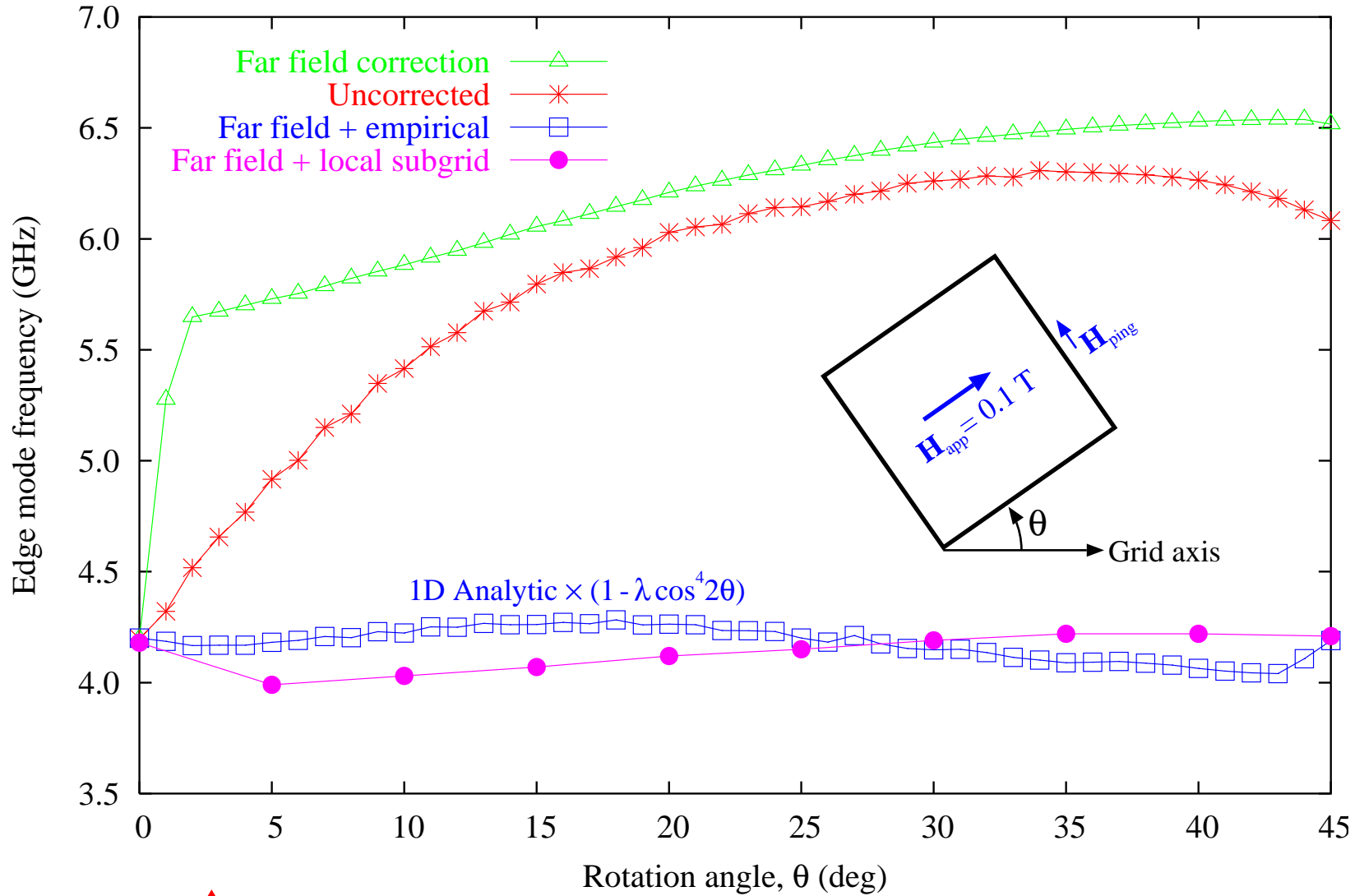
$$E_{\text{correction}} = E_{\text{partial}} - E_{\text{diluted}}$$

$$E_{\text{correction}} = \frac{1}{4} \mu_0 M_s^2 v (1 - v) (m_x^2 + m_z^2) \Delta \cdot t$$

No correction for empty cells ($v = 0$).

No correction for filled cells ($v = 1$).

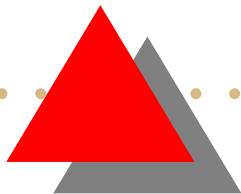
Corrections: Angular dependence



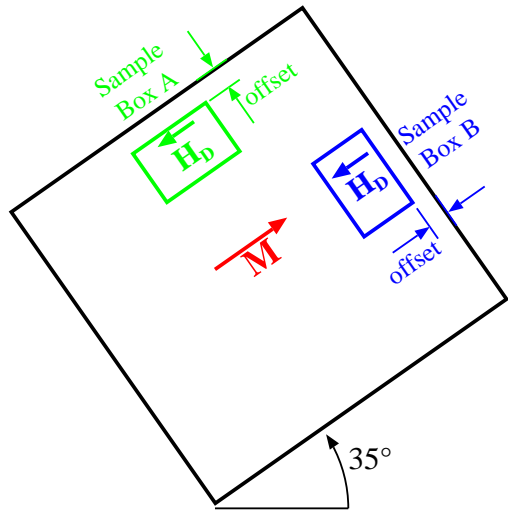


Summary

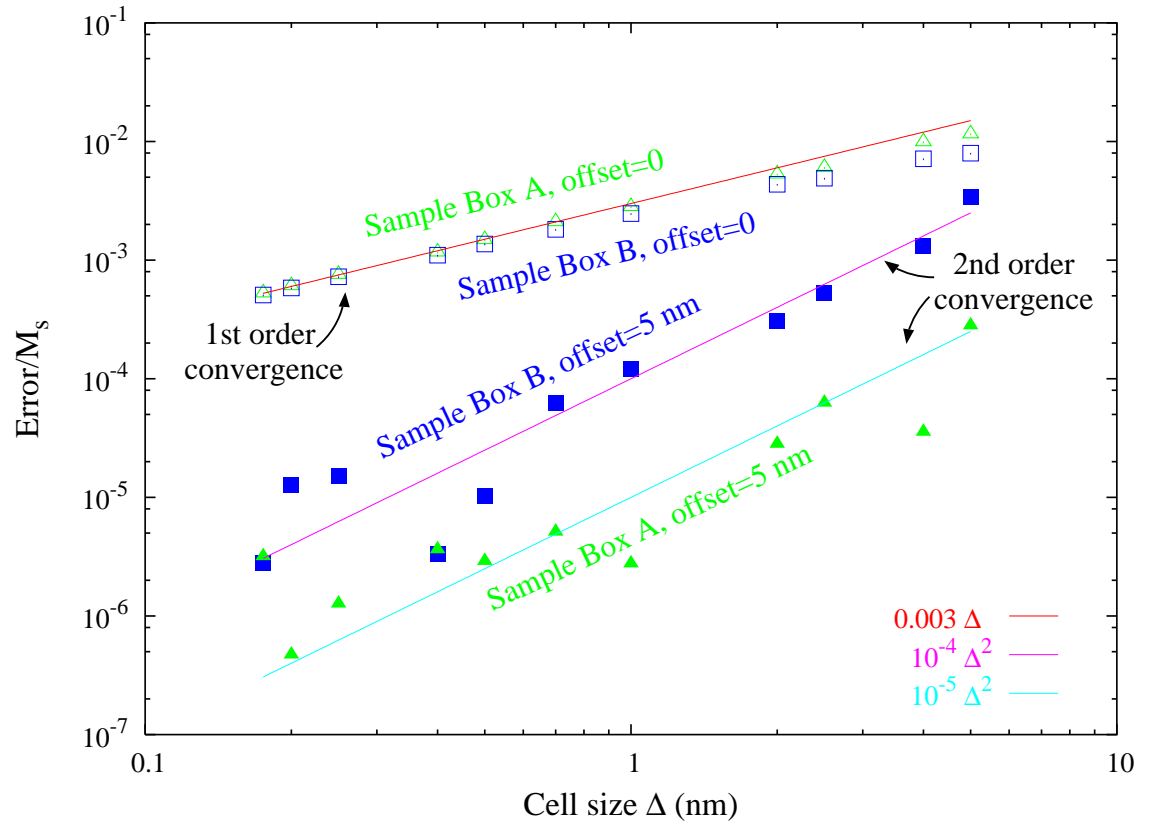
- Staircase demag artifact effectively corrected.
- Efficient far-field computation via FFT.
- Local correction coefficients computed using usual demag code.
- Local corrections have minimal run-time cost.
- Edge resonance test examined.
- Simple analytic + empirical edge anisotropy correction introduced.



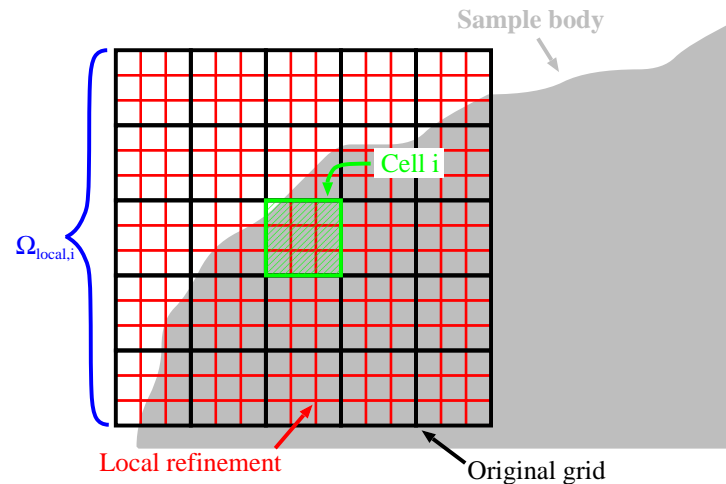
Average $\mathbf{H}_{\text{Demag}} \cdot \mathbf{M}$ computed
in each sample box



Py squares
350 nm x 350 nm x 5 nm
Uniform Magnetization



Local field computation



- Compute $N_{i'-j'}^{\text{fine}}$ for fine mesh on Ω_{local} (once)
- For i, j near boundary, compute $\langle \mathbf{H}_{\text{demag}}^{\text{fine}} \rangle_{i,j}$
- $\mathbf{H}_{\text{demag}}^{\text{fine}} - \mathbf{H}_{\text{demag}}^{\text{coarse}}$ define correction factors $K_{i,j}$
- NOTE: Done once during initialization!

Exchange (uniform ℓ_{ex})

Usual exchange expression:

$$\mathbf{H}_{ij} = \frac{2A}{\mu_0 \Delta_{ij}^2 M_s} (\mathbf{m}_j - \mathbf{m}_i)$$

Volume-modified M_s causes trouble if $M_s \approx 0$.

Instead, define

$$\ell_{\text{ex}} = \sqrt{\frac{2A}{\mu_0 M_s^2}} \quad (\text{fixed})$$

and

$$\mathbf{H}_{ij} = \ell_{\text{ex}}^2 M_s (\mathbf{m}_j - \mathbf{m}_i) / \Delta_{ij}^2.$$

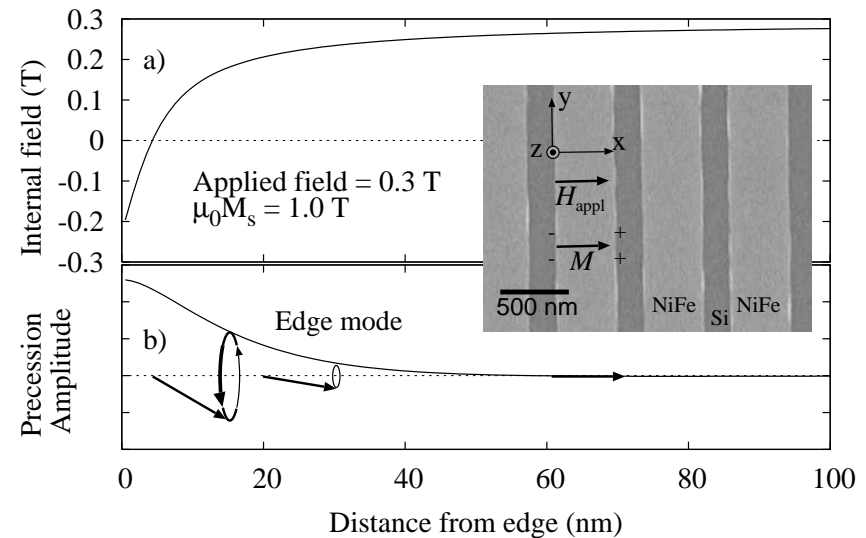
Edge mode refinement

Thin films magnetized in plane,
perpendicular to edge.

Precession is localized at the edge
by low fields

J. Jorzick et al., Phys. Rev. Lett. 88, 047204 (2002)

J. P. Park et al., Phys. Rev. Lett. 89, 277201 (2002)



Edge mode frequencies fit Kittel expression with 2 parameters:

$$f(H_{\text{appl}}) = \frac{\mu_0 \gamma}{2\pi} [(H_{\text{appl}} - H_x)(H_{\text{appl}} + H_z)]^{1/2}$$

*Effective EDGE-normal
anisotropy field*

*Effective FILM-normal
anisotropy field*

B. B. Maranville et al., J. Appl. Phys 99, 08C703 (2006).

R. D. McMichael and B. B. Maranville, Phys. Rev. B, 74, 024424 (2006).

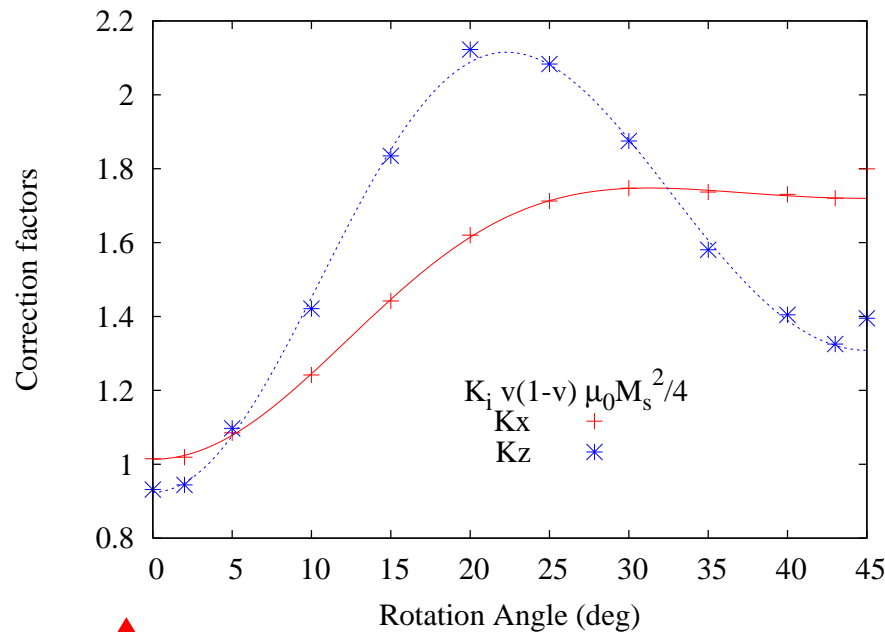
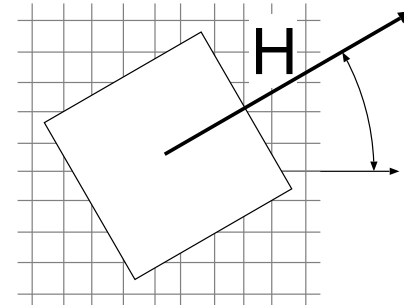
Edge mode refinement

$$E_{\text{correction}} = \frac{1}{4} \mu_0 M_s^2 \cdot v(1-v) \cdot [K_x(\phi)m_x^2 + K_z(\phi)m_z^2]$$

"Correct" edge mode frequencies at $\phi = 0$; no partial cells.

For each angle ϕ , find $K_x(\phi)$ and $K_z(\phi)$ such that

$$f(\phi, 0.1\text{T}) = f(0, 0.1\text{T}) \quad f(\phi, 0.5\text{T}) = f(0, 0.5\text{T})$$



Calculated for 350 nm square x 5 nm thick Py with 5 nm cubic cells.

Spinwaves

