An efficient multigrid preconditioner for edge element discretization of Maxwell's equations in micromagnetism.

Ľubomír Baňas

Department of Mathematics Heriot-Watt University, Edinburgh

http://www.ma.hw.ac.uk/~lubomir L.Banas@hw.ac.uk

Joint work with A. Prohl and S. Bartels

Maxwell's equations

$$\begin{aligned} \varepsilon_0 \, \mathbf{E}_t - \nabla \times \mathbf{H} &+ \sigma \mathbf{E} &= -\mathbf{J} & \text{ in } & \Omega_T := (0, T) \times \Omega \,, \\ \mathbf{B}_t + \nabla \times \mathbf{E} &= \mathbf{0} & \text{ in } & \Omega_T \,. \end{aligned}$$

- **H** magnetic field
- **B** magnetic induction $(\nabla \cdot \mathbf{B} = \mathbf{0})$
- ullet **E** electric field
- J electric current, ε_0 permitivity of vacuum, σ conductivity

Constitutive relations B-H

- vacuum $\mathbf{B}=\mu_0\mathbf{H}$
- linear materials ${f B}=\mu {f H}$, $\mu({f x})$ is a 3 imes 3 tensor
- ferromagnetic materials $\mathbf{B} = \mu_0(\mathbf{H} + \mathbf{m})$

Introduction

Landau-Lifshitz-Gilbert (LLG) equation

Landau-Lifshitz formulation

$$\mathbf{m}_t = \mathbf{m} \times \mathbf{H}_{\text{eff}} - \alpha \, \mathbf{m} \times (\mathbf{m} \times \mathbf{H}_{\text{eff}}).$$

Gilbert formulation

$$\mathbf{m}_t + \alpha \, \mathbf{m} \times \mathbf{m}_t = (1 + \alpha^2) \, \mathbf{m} \times \mathbf{H}_{\text{eff}} \, .$$

Both formulations are equivalent for smooth \mathbf{m} .

- \mathbf{m} magnetization vector, $|\mathbf{m}| = 1$
- $\mathbf{H}_{\mathrm{eff}}$ effective field (nonlinear)
- α damping constant

Exact solution

Take $\mathbf{H}_{\mathrm{eff}} = \mathbf{h} = (0, 0, 1)$, then LLG reduces to an ODE.



- $\boldsymbol{m}_t = \boldsymbol{h} \times \boldsymbol{m}$ (precession)
- $\boldsymbol{m}_t = \boldsymbol{m} imes (\boldsymbol{h} imes \boldsymbol{m})$ (phenomenological damping)
- $\boldsymbol{m}_t = \boldsymbol{h} imes \boldsymbol{m} + \boldsymbol{m} imes (\boldsymbol{h} imes \boldsymbol{m})$ (precession and damping)

Effective (total) field

Free energy - magnetic field energy, exchange energy, Zeeman energy, anisotropy energy, magnetomechanical energy. **Effective field**

$$\boldsymbol{H}_{eff} = -\frac{\partial E}{\partial \boldsymbol{m}} = \boldsymbol{H} + \boldsymbol{H}_{ex} + \boldsymbol{H}_{app} + \boldsymbol{H}_{an} + \boldsymbol{H}_{ms}$$

- Magnetic field H coupling with Maxwell's equations
- Exchange $H_{ex} = \Delta m$
- Applied field H_{app} constant in space and time
- Anisotropy $oldsymbol{H}_{an} = (oldsymbol{p} \cdot oldsymbol{m})oldsymbol{p}$
- Magnetostriction field coupling with elastodynamics

Maxwell-LLG system

$$\begin{aligned} \varepsilon_0 \, \mathbf{E}_t - \nabla \times \mathbf{H} + \sigma \, \chi_\omega \mathbf{E} &= -\mathbf{J} & \text{in } \Omega_T \,, \\ \mu_0 \, \mathbf{H}_t + \nabla \times \mathbf{E} &= -\mu_0 \, \chi_\omega \mathbf{m}_t & \text{in } \Omega_T \,, \\ \mathbf{m}_t + \alpha \, \mathbf{m} \times \mathbf{m}_t &= (1 + \alpha^2) \, \mathbf{m} \times \mathbf{H}_{\text{eff}} & \text{in } \omega_T := (0, T) \times \omega. \end{aligned}$$

Boundary conditions

$$\partial_{\mathbf{n}}\mathbf{m} = 0$$
 on $\partial\omega_T$, $\mathbf{E} \times \mathbf{n} = 0$ on $\partial\Omega_T$.

Initial conditions $(\nabla \cdot (\mathbf{H}_0 + \chi_\omega \mathbf{m}_0) = 0 = \nabla \cdot \mathbf{B}$ in $\Omega)$

 $\mathbf{m}(0,\cdot) = \mathbf{m}_0$ in ω , $\mathbf{E}(0,\cdot) = \mathbf{E}_0$, $\mathbf{H}(0,\cdot) = \mathbf{H}_0$ in Ω .

Energy $(\sigma = 0, \mathbf{J} = \mathbf{0})$:

$$\frac{\mu_0}{2} \int_{\omega} |\nabla \mathbf{m}|^2 \, \mathrm{d}\mathbf{x} - \mu_0 \int_{\omega} (\mathbf{m} \cdot \mathbf{H}_{app}) \, \mathrm{d}\mathbf{x} + \int_{\Omega} \left[\frac{\mu_0}{2} |\mathbf{H}|^2 + \frac{\varepsilon_0}{2} |\mathbf{E}|^2\right] \, \mathrm{d}\mathbf{x}.$$

Magnetostaic formulation

Take the stationary Maxwell's equations and $\sigma = 0$, i.e.:

$$\mathbf{E}_t = \mathbf{B}_t = \mathbf{J} = \mathbf{0},$$

we get

$$\begin{array}{rcl} \nabla\times\mathbf{H} &=& \mathbf{0},\\ \nabla\times\mathbf{E} &=& \mathbf{0},\\ \nabla\cdot\mathbf{B} &=& \mathbf{0},\\ \mathbf{B} &=& \mu_0(\mathbf{H}+\mathbf{m}). \end{array} \end{array}$$

We look for $\mathbf{H} = \nabla \phi$ (i.e. $\nabla \times (\nabla \phi) = \mathbf{0}$), then the above reduces to

$$\mu_0 \nabla \cdot (\nabla \phi + \mathbf{m}) = \mathbf{0} \quad \text{in} \quad \Omega,$$

with an interface condition on $\partial\omega$

$$(\nabla \phi + \mathbf{m}) \cdot \mathbf{n} = \mathbf{B} \cdot \mathbf{n} = 0.$$

Notation

- $(\mathbf{f}, \mathbf{g}) = \int_{\Omega} \langle \mathbf{f}, \mathbf{g} \rangle \, \mathrm{d}\mathbf{x}$
- mass lumping $(\boldsymbol{\phi}, \boldsymbol{\beta})_h = \int_{\omega} \mathcal{I}_{\mathbf{V}_{\mathbf{h}}}(\langle \boldsymbol{\phi}, \boldsymbol{\beta} \rangle) \, \mathrm{d}\mathbf{x} = \sum_{\ell \in L} \beta_\ell \langle \boldsymbol{\phi}(\mathbf{x}_\ell), \boldsymbol{\beta}(\mathbf{x}_\ell) \rangle.$
- $d_t \varphi^j := k^{-1} (\varphi^j \varphi^{j-1})$
- $\overline{\varphi}^{j+1/2} := \frac{1}{2} (\varphi^{j+1} + \varphi^j)$
- $\tilde{\Delta}_h : W^{1,2}(\omega; \mathbb{R}^3) \to \mathbf{V}_h$ is a discrete Laplace operator $(-\tilde{\Delta}_h \phi, \chi_h)_h = (\nabla \phi, \nabla \chi_h) \quad \forall \chi_h \in \mathbf{V}_h$.
- projection $\mathbf{P}_{\mathbf{V}_h}: L^2(\omega, \mathbb{R}^3) \to \mathbf{V}_h$ is defined as $(\mathbf{P}_{\mathbf{V}_h}\mathbf{u}, \boldsymbol{\varphi}_h)_h = (\mathbf{u}, \boldsymbol{\varphi}_h)$

Implicit finite element approximation

Fully discrete system nonlinear and coupled [LB, Bartels, Prohl (2008)]

$$\begin{aligned} &(d_{t}\mathbf{m}_{h}^{j+1},\boldsymbol{\phi}_{h})_{h} + \alpha \left(\mathbf{m}_{h}^{j} \times d_{t}\mathbf{m}_{h}^{j+1},\boldsymbol{\phi}_{h}\right)_{h} \\ &= (1+\alpha^{2}) \left(\overline{\mathbf{m}}_{h}^{j+1/2} \times (\tilde{\Delta}_{h}\overline{\mathbf{m}}_{h}^{j+1/2} + \mathbf{P}_{\mathbf{V}_{h}}\overline{\mathbf{H}}_{h}^{j+1/2}), \boldsymbol{\phi}_{h}\right)_{h} \quad \forall \boldsymbol{\phi}_{h} \in \mathbf{V}_{h} \,, \\ &\varepsilon_{0} \left(d_{t}\mathbf{E}_{h}^{j+1}, \boldsymbol{\varphi}_{h}\right) - (\overline{\mathbf{H}}_{h}^{j+1/2}, \nabla \times \boldsymbol{\varphi}_{h}) + \sigma \left(\chi_{\omega}\overline{\mathbf{E}}_{h}^{j+1/2}, \boldsymbol{\varphi}_{h}\right) = \mathbf{0} \quad \forall \boldsymbol{\varphi}_{h} \in \mathbf{X}_{h} \,, \\ &\mu_{0} \left(d_{t}\mathbf{H}_{h}^{j+1}, \mathbf{3}_{h}\right) + \left(\nabla \times \overline{\mathbf{E}}_{h}^{j+1/2}, \mathbf{3}_{h}\right) = -\mu_{0} \left(\chi_{\omega}d_{t}\mathbf{m}_{h}^{j+1}, \mathbf{3}_{h}\right) \quad \forall \mathbf{3}_{h} \in \mathbf{Y}_{h} \,. \end{aligned}$$

Finite element spaces

•
$$\mathbf{V}_h = \left\{ \boldsymbol{\phi}_h \in C(\overline{\omega}; \mathbb{R}^3) : \boldsymbol{\phi}_h |_K \in \mathcal{P}_1(K; \mathbb{R}^3) \quad \forall K \in \mathcal{T}_h |_{\omega} \right\},$$

- $\mathbf{X}_h = \left\{ \boldsymbol{\varphi}_h \in \mathbf{H}_0(\mathbf{curl}; \Omega) : \boldsymbol{\varphi}_h |_K \in \mathcal{P}_1(K; \mathbb{R}^3) \quad \forall K \in \mathcal{T}_h \right\},$
- $\mathbf{Y}_h = \{\mathbf{\mathfrak{Z}}_h \in L^2(\Omega; \mathbb{R}^3) : \mathbf{\mathfrak{Z}}_h |_K \in \mathcal{P}_0(K; \mathbb{R}^3) \quad \forall K \in \mathcal{T}_h\}.$

Stability

Lemma 1. Suppose that $|\mathbf{m}_h^0(\mathbf{x}_\ell)| = 1$ for all $\ell \in L$. Then the sequence $\{(\mathbf{m}_h^j, \mathbf{E}_h^j, \mathbf{H}_h^j)\}_{j\geq 0}$ satisfies for all $j \geq 0$

(i)
$$|\mathbf{m}_h^{j+1}(\mathbf{x}_\ell)| = 1 \quad \forall \ell \in L,$$

(ii)
$$\mathcal{E}_{h}\left(\{\mathbf{m}_{h}^{j+1}, \mathbf{H}_{h}^{j+1}, \mathbf{E}_{h}^{j+1}\}\right) + k \sum_{\ell=0}^{j} \frac{\alpha \mu_{0}}{1 + \alpha^{2}} \|d_{t}\mathbf{m}_{h}^{\ell+1}\|_{h}^{2} + \sigma \|\overline{\mathbf{E}}_{h}^{\ell+1/2}\|_{L^{2}(\omega)}^{2}$$
$$= \mathcal{E}_{h}\left(\{\mathbf{m}_{h}^{0}, \mathbf{H}_{h}^{0}, \mathbf{E}_{h}^{0}\}\right) - k \sum_{\ell=0}^{j} (\overline{\mathbf{J}}_{h}^{\ell+1/2}, \overline{\mathbf{E}}_{h}^{\ell+1/2}),$$

where

$$\mathcal{E}_h\big(\{\mathbf{m}_h^j, \mathbf{H}_h^j, \mathbf{E}_h^j\}\big) = \frac{\mu_0}{2} \int_{\omega} |\nabla \mathbf{m}_h^j|^2 - 2(\mathbf{m}_h^j \cdot \mathbf{H}_{app}) \,\mathrm{d}\mathbf{x} + \int_{\Omega} \Big[\frac{\mu_0}{2} |\mathbf{H}_h^j|^2 + \frac{\varepsilon_0}{2} |\mathbf{E}_h^j|^2\Big] \,\mathrm{d}\mathbf{x}$$

Convergence

Theorem 1. [LB, Bartels, Prohl (2008)] Suppose that we have $|\mathbf{m}_h^0(\mathbf{x}_\ell)| = 1$ for all $\ell \in L$ and let $\{(\mathbf{m}_h^j, \mathbf{E}_h^j, \mathbf{H}_h^j)\}_{j\geq 0}$ be the finite element solution. Assume that $\mathbf{m}_h^0 \to \mathbf{m}_0$ in $W^{1,2}(\omega)$ and $(\tilde{\mathbf{H}}_h^0, \tilde{\mathbf{E}}_h^0) \to (\mathbf{H}_0, \mathbf{E}_0)$ in $L^2(\Omega, \mathbb{R}^3)$ as $h \to 0$ and let T > 0 be a fixed constant. As $k, h \to 0$, a subsequence of $(\tilde{\mathbf{m}}, \tilde{\mathbf{H}}, \tilde{\mathbf{E}})$ converges weakly to $(\mathbf{m}, \mathbf{H}, \mathbf{E})$ in $[L^{\infty}(0, T; W^{1,2}(\omega, \mathbb{S}^2)) \cap W^{1,2}(\omega_T, \mathbb{R}^3)] \times [L^{\infty}((0, T); L^2(\Omega, \mathbb{R}^3))]^2$, and $(\mathbf{m}, \mathbf{H}, \mathbf{E})$ is a weak solution.

Where $(\, {\tilde{\mathbf{m}}}, {\tilde{\mathbf{H}}}, {\tilde{\mathbf{E}}}\,)$ are defined as

$$\tilde{\boldsymbol{\xi}}(t,\mathbf{x}) := \frac{t-t_j}{k} \boldsymbol{\xi}_h^{j+1}(\mathbf{x}) + \frac{t_{j+1}-t}{k} \boldsymbol{\xi}_h^j(\mathbf{x}).$$

Solution of the nonlinear system

Fixed-point iterations

$$\begin{aligned} \frac{2}{k} (\mathbf{w}_{h}^{\ell+1}, \boldsymbol{\phi}_{h})_{h} &- \frac{2\alpha}{k} (\mathbf{w}_{h}^{\ell+1} \times \tilde{\mathbf{m}}_{h}^{j}, \boldsymbol{\phi}_{h})_{h} \\ &- (1+\alpha^{2}) \big(\mathbf{w}_{h}^{\ell+1} \times (\tilde{\Delta}_{h} \mathbf{w}_{h}^{\ell} + \mathbf{P}_{\mathbf{V}^{h}} \mathbf{G}_{h}^{\ell}), \boldsymbol{\phi}_{h} \big)_{h} &= \frac{2}{k} (\tilde{\mathbf{m}}_{h}^{j}, \boldsymbol{\phi}_{h})_{h}, \\ \frac{2\varepsilon_{0}}{k} (\mathbf{F}_{h}^{\ell+1}, \boldsymbol{\varphi}_{h}) &- (\mathbf{G}_{h}^{\ell+1}, \nabla \times \boldsymbol{\varphi}_{h}) + \sigma(\chi_{\omega} \mathbf{F}_{h}^{\ell+1}, \boldsymbol{\varphi}_{h}) &= \frac{2\varepsilon_{0}}{k} (\tilde{\mathbf{E}}_{h}^{j}, \boldsymbol{\varphi}_{h}) - (\overline{\mathbf{J}}_{h}^{j+1/2}, \boldsymbol{\varphi}_{h}), \\ \frac{2\mu_{0}}{k} (\mathbf{G}_{h}^{\ell+1}, \mathbf{J}_{h}) &+ (\nabla \times \mathbf{F}_{h}^{\ell+1}, \mathbf{J}_{h}) + \frac{2\mu_{0}}{k} (\mathbf{w}_{h}^{\ell+1}, \mathbf{J}_{h}) &= \frac{2\mu_{0}}{k} (\tilde{\mathbf{H}}_{h}^{j}, \mathbf{J}_{h}) + \frac{2\mu_{0}}{k} (\tilde{\mathbf{m}}_{h}^{j}, \mathbf{J}_{h}), \end{aligned}$$

where $\mathbf{w}_h := \overline{\mathbf{m}}_h^{j+1/2}$, $\mathbf{F}_h := \overline{\mathbf{E}}_h^{j+1/2}$ and $\mathbf{G}_h := \overline{\mathbf{H}}_h^{j+1/2}$. Stopping criterion

$$||\tilde{\Delta}_h(\mathbf{w}_h^{\ell+1} - \mathbf{w}_h^{\ell})||_h + ||\mathbf{G}_h^{\ell+1} - \mathbf{G}_h^{\ell}||_{L^2} \le \varepsilon.$$

Time step restriction $k = \mathcal{O}(h^2)$.

Solution of the discrete Maxwell system

Matrix notation

$$\left(egin{array}{cc} \mathbf{A} & -\mathbf{C}^T \ \mathbf{C} & \mathbf{B} \end{array}
ight) \left(egin{array}{cc} \overline{\mathbf{e}} \ \overline{\mathbf{h}} \end{array}
ight) = \left(egin{array}{cc} \overline{\mathbf{f}} \ \overline{\mathbf{g}} \end{array}
ight),$$

 $\overline{\mathbf{e}}$, $\overline{\mathbf{h}}$ vectors of unknown finite element coefficients. Matrix definitions

$$\mathbf{A}_{ij} = \frac{2\varepsilon_0}{k} (\boldsymbol{\varphi}_h^i, \boldsymbol{\varphi}_h^j) , \quad \mathbf{B}_{ij} = \frac{2\mu_0}{k} (\mathbf{\mathfrak{Z}}_h^i, \mathbf{\mathfrak{Z}}_h^j) , \quad \mathbf{C}_{ij} = (\nabla \times \boldsymbol{\varphi}_h^j, \mathbf{\mathfrak{Z}}_h^i) ,$$

Preconditioned Uzawa algorithm solves Schur complement formulation

$$\left(\mathbf{C}^T \mathbf{B}^{-1} \mathbf{C} + \mathbf{A}\right) \overline{\mathbf{e}} = \overline{\mathbf{f}} + \mathbf{C}^T \mathbf{B}^{-1} \overline{\mathbf{g}}.$$

Two sub-steps:

1. $\overline{\mathbf{h}}^n = \mathbf{B}^{-1}(\overline{\mathbf{g}} - \mathbf{C}\overline{\mathbf{e}}^n)$

2.
$$\overline{\mathbf{e}}^{n+1} = \overline{\mathbf{e}}^n + \rho \mathbf{S}^{-1} (\overline{\mathbf{f}} + \mathbf{C}^T \overline{\mathbf{h}}^n - \mathbf{A} \overline{\mathbf{e}}^n)$$

Preconditioner

Preconditioning dramatically reduces the number of Uzawa iterations. We need:

$$\mathbf{S}^{-1} \approx [\mathbf{C}^T \mathbf{B}^{-1} \mathbf{C} + \mathbf{A}]^{-1}$$

Auxiliary problem edge elements $\mathbf{X}_h \subset \mathbf{H}_0(\mathbf{curl}; \Omega)$

$$\frac{2\varepsilon_0}{k}(\mathbf{F}_h^*,\boldsymbol{\varphi}_h) + \frac{k}{2\mu_0}(\nabla \times \mathbf{F}_h^*,\nabla \times \boldsymbol{\varphi}_h) = (\mathbf{f}_h,\boldsymbol{\varphi}_h) + \frac{k}{2\mu_0}(\nabla \times \mathbf{g}_h,\boldsymbol{\varphi}_h) \qquad \forall \boldsymbol{\varphi}_h \in \mathbf{X}_h.$$

with $\mathbf{g}_h = \sum_i \{ \overline{\mathbf{g}} \}_i oldsymbol{arphi}_{h,i}$.

In matrix notation $\mathbf{S} = \mathbf{M} + \mathbf{R}$, with

$$\mathbf{M}_{ij} = \frac{2\varepsilon_0}{k} (\boldsymbol{\varphi}_h^i, \boldsymbol{\varphi}_h^j), \quad \mathbf{R}_{ij} = \frac{k}{2\mu_0} (\nabla \times \boldsymbol{\varphi}_h^i, \nabla \times \boldsymbol{\varphi}_h^j).$$

 \mathbf{S}^{-1} needs to be approximated effectively, e.g., by multigrid.

Multigrid algorithm

Multigrid components

- grid hierarchy
- prolongation \mathbf{I}_{k-1}^k [eg. Bossavit, Rapetti 2005],
- restriction $\mathbf{I}_k^{k-1} = (\mathbf{I}_{k-1}^k)^T$,
- smoother (Gauss-Seidel type iterative scheme)

Two-grid scheme

- **pre smoothing** *m* smoothing iterations
- coarse grid correction solve the coarse problem exactly
- **post smoothing** *m* smoothing iterations

Smoothers for edge elements

Hybrid smoother one smoothing steps consists of one loop over all edges followed by one loop over all vertices [Hiptmair (1998)]

Patch smoother smooth several edges simultaneously [Arnold, Falk, Winther (2000)]



Figure 1: Local smoothing patch

Blow-up of MLLG



Figure 2: Plot of $t \mapsto \|\nabla \mathbf{m}_h(t, \cdot)\|_{\infty}$ and $t \mapsto \|\nabla \mathbf{m}_h(t, \cdot)\|_2$

Blow-up of MLLG



Figure 3: Magnetization at times t = 0, 0.01, 0.015, 0.020, 0.030, 0.214 for $h = 1/2^4$

Blow-up of MLLG



Figure 4: Details of the magnetization near the singularity times t=0,0.01,0.015,0.020,0.030,0.214 for $h=1/2^4$.

 $\begin{array}{l} \mu \text{-mag standard problem 4: } \mu_0 \mathbf{H}_{app} = (-24.6, 4.3, 0), \ \omega = 500 \times 125 \times 3 \ \text{nm}, \\ h = 3.90625 \times 10^{-9}, \ \tau = 1.13 \times 10^{-13} \ ([\text{d'Aquino, Serpico, Miano (2005)}] \ \text{used} \\ \tau = 2.5 \times 10^{-12}). \end{array}$

Initial condition S-state



Figure 5: Initial condition \mathbf{m}^0 .

Unstructured grid



Figure 6: Mesh for the domain Ω at $x_3 = 0$ (left) and zoom at the mesh for the domain ω at $x_3 = 0$ (right).



Figure 7: MLLG: solution at $|\omega|^{-1} \int_{\omega} \mathbf{m}_x = 0$.



Figure 8: Magnetostatic formulation: solution at $|\omega|^{-1} \int_{\omega} \mathbf{m}_x = 0$.



Figure 9: Evolution of $|\omega|^{-1} \int_{\omega} \mathbf{m}_{x(y)}$.



Figure 10: Evolution of $|\omega|^{-1} \int_{\omega} \mathbf{m}_{x(y)}$.

End

Thank you for your attention!