Discretisation induced stiffness in micromagnetic simulations

David Shepherd[*] (david.shepherd-2@man.ac.uk), Jim Miles[*], Matthias Heil[†] and Milan Mihajlović[*]

∗ NEST Group, School of Computer Science, The University of Manchester, Manchester, M13 9PL, UK
† School of Mathematics, The University of Manchester, Manchester, M13 9PL, UK

EPSRC Engineering and Physical Sciences Research Council

The University of Manchester

NEST Nano Engineering & Storage Technology

Abstract

- *Micromagnetic models are sometimes stiff (explicit time integration is slow) but when and why?*
- *Find that it can occur due to spatial discretisation alone.*
- *Find that FEM/BEM magnetostatic calculations increases stiffness.*
- *Find that decreasing damping parameter increases stiffness.*

1. The Landau-Lifshitz-Gilbert equation

- Dynamic micromagnetic models centre around solving the Landau-Lifshitz-Gilbert equation (LLG).
- Partial differential equations for behaviour of magnetisation in a ferromagnetic material over time.
- The non-dimensional Landau-Lifshitz-Gilbert equation is:

$$\frac{\partial \mathbf{m}}{\partial t} = \underbrace{-\mathbf{m} \times \mathbf{h}[\mathbf{m}]}_{\text{precession}} + \underbrace{\alpha \mathbf{m} \times \frac{\partial \mathbf{m}}{\partial t}}_{\text{damping}} \tag{1}$$

where the field terms are

$$\mathbf{h}[\mathbf{m}] = \underbrace{\mathbf{h}_{\text{ap}}}_{\text{applied}} + \underbrace{\mathbf{h}_{\text{ms}}[\mathbf{m}]}_{\text{magnetostatic}} + \underbrace{\nabla^2 \mathbf{m}}_{\text{exchange}} . \tag{2}$$

2. Approaches to numerical solution of the LLG

- Discretise LLG in space (*e.g.* macrospin, finite difference, finite element).
- Calculate magnetostatic effects (*e.g.* Fourier transform, FEM/BEM).
- Discretise in time (*e.g.* Runge-Kutta, BDF2, implicit midpoint rule). Ideally sufficiently *stable*: don't need high time refinement to stop the solution exploding.

3. Implicit vs explicit methods

- Explicit methods (*e.g.* most Runge-Kutta methods, Predictor-Corrector methods):
  - Calculate values at next time step in terms of values at previous steps: *each step is cheap*.
  - Unstable for some problems: many extra steps needed for stability.
- Implicit methods (*e.g.* BDF2, implicit midpoint rule):
  - Include value at the next step in the calculation: requires solution of a system of equations.
  - More expensive but *always stable*.
- "Stiff problem"
  - When explicit methods require so many additional steps that they become inefficient.
  - Can occur due to physics, *e.g.* models of chemical reactions.
  - Can also occur due to fine spatial discretisations.

4. The experiment

- Examine stiffness of a simple micromagnetic problem: coherent reversal of a small spherical nanoparticle[3], as shown in figure.
- Try with single macrospin and with various finite element meshes.
- Try with and without magnetostatics (using FEM/BEM method[2]).
- Try various time integration methods
  - Explicit 2nd order Runge-Kutta (RK2).
  - Implicit midpoint rule (IMR)[1].
  - Semi-implicit midpoint rule (SIMR): implicit LLG with explicit magnetostatics[4].
- Examine maximum stable time steps for each while varying parameters.

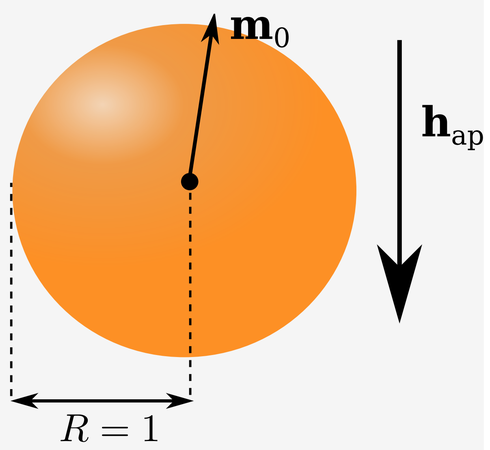

Figure 1 : Spherical nanoparticle of radius 1 exchange length in an applied field $\mathbf{h}_{\text{ap}} = [0, 0, -1.1]$. Initial magnetisation is slightly off the z-axis.

5. Macrospin results

- Maximum time step tested is stable for all time integration methods.
- Same with/without magnetostatics and with $\alpha = 1.0, 0.1$ or 0.01.
- Therefore problem is not physically stiff.

6. FEM results without magnetostatics

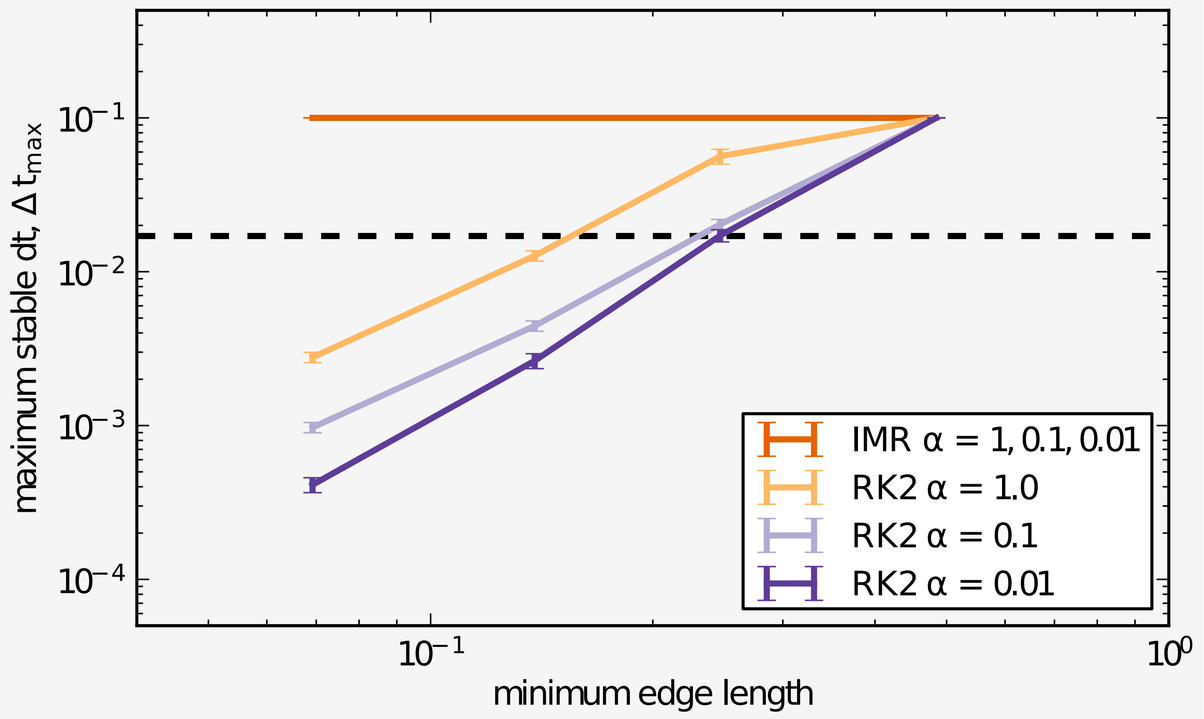

Figure 2 : Maximum stable steps vs mesh fineness without magnetostatics. Dashed line shows RK2 time step needed for equal efficiency of IMR and RK2 method.

- Stiffer as spatial discretisation is improved.
- Stiffer as damping decreases.

7. FEM results with magnetostatics

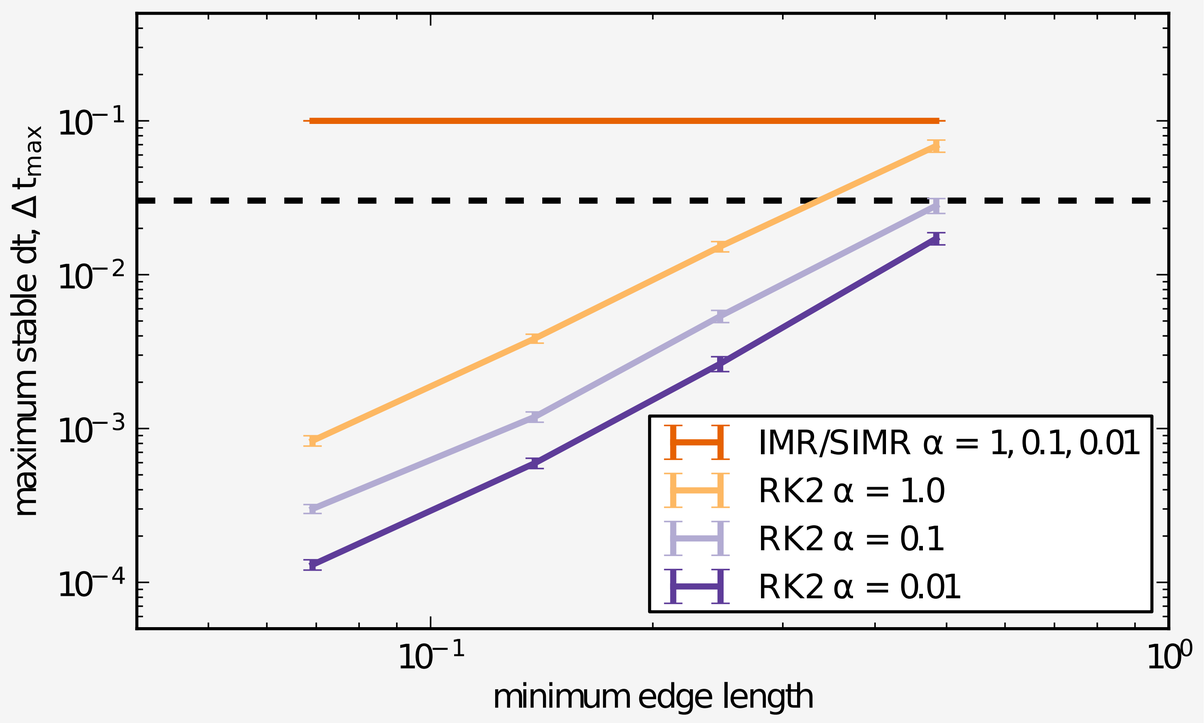

Figure 3 : Maximum stable steps vs mesh fineness with FEM/BEM magnetostatics.

- Qualitatively the same as above, but more stiff.
- Semi-implicit method (implicit LLG, explicit magnetostatics) does not show any stability issues.

8. Conclusions

- Stiffness in micromagnetic simulations can arise purely from a fine spatial discretisation.
- For realistic dynamic models (magnetostatics, $\alpha = 0.01$) the problem we examined is always stiff.
- The semi-implicit method tested here shows no stability issues.

9. Acknowledgements

This project is funded by the Engineering and Physical Sciences Research Council (EPSRC) through the NoWNano Doctoral Training Centre on grant number EP/G01705/1.

10. References

[1] M. d'Aquino, C. Serpico, and G. Miano. "Geometrical integration of Landau–Lifshitz–Gilbert equation based on the mid-point rule". In: *Journal of Computational Physics* 209.2 (2005), pp. 730–753.

[2] A. Knittel. "Micromagnetic simulations of three dimensional core-shell nanostructures". PhD thesis. University of Southampton, 2011.

[3] J. C. Mallinson. "Damped gyromagnetic switching". In: *IEEE Transactions on Magnetics* 36.4 (2000), pp. 1976–1981.

[4] D. Shepherd et al. "Discretisation induced stiffness in micromagnetic simulations". In: *In publication* (2014).