Stiffness in Micromagnetic Simulations

V.D. Tsiantos[*] J.J. Miles[+] B.K. Middleton[**]

Abstract

In this paper we investigate stiffness in micromagnetic simulations in the ODE context. We introduce some pragmatic measures of stiffness based on the total number of time steps taken by a non stiff and a stiff method to solve the LLG equation, and the cost of each method per time step. We present a family of micromagnetic calculations that simulates materials with strong exchange coupling between grains, and varying crystalline anisotropy. The simulations show a high degree of stiffness.

Key words: micromagnetics, stiffness, ordinary differential equations, initial value problems, exchange coupling.

AMS subject classifications: 37C10, 62P30.

1 Introduction

In this paper some comments on the issue of stiffness in micromagnetics using numerical methods for systems of ODEs are presented. Furthermore, some pragmatic measures of stiffness in micromagnetics are introduced. In addition to this, a set of micromagnetic simulations investigating the effect of crystalline anisotropy and exchange scale on stiffness is presented. Finally, an attempt to provide a possible physical explanation of the phenomenon of stiffness in micromagnetics has been made, although we anticipate the difficulty of the issue.

More specifically, Section 2 presents some comments on stiffness in micromagnetic simulations using numerical methods for systems of ODEs. Moreover, Section 3 presents the pragmatic measures of stiffness in micromagnetics. Furthermore, in Section 4 a set of micromagnetic simulations is presented, investigating cases with strong exchange coupling between grains. Finally, Section 5 points out some very useful remarks on the appropriateness of numerical methods for systems of ODEs in micromagnetics, as well as a possible explanation for the cause of stiffness.

2 Stiffness In Micromagnetics

As it has been mentioned by J.D Lambert there are many definitions of stiffness [1]. A detailed theoretical description of stiffness can be found in numerous textbooks [1, 2, 3, 4]. We point out here that the use of non stiff methods when the problem is stiff is inappropriate because the solution needs extremely small time steps and so it is very expensive to use them even with recent advances in computer power. So it has to be anticipated by the micromagnetic modellers the immense importance of using an ODE solver which is well suited to the characteristics of the system.

Moreover, although in literature in micromagnetics stiffness is widely acknowledged [5-13], there is no rigorous investigation of the question of stiffness in micromagnetics in the ODE context. The abovementioned papers can be split in three groups. The first group contains the work mainly done by Hayashi *et al* [5] and Nakatani *et al* [6]. Both papers concentrate on stability issues using finite difference method and the authors correctly identify the cause of instability. Moreover, they suggest a possible solution of the instability problem in the solution of the LLG equation with a finite difference method. This solution is the use of implicit finite difference methods, such as the backward difference method, which have better stability properties than the corresponding explicit ones. Moreover, they connect the problem of stiffness with the stability problem of the numerical solution of the LLG equation. So, their work can be considered as pioneering

[*] University of Manchester, Department of Computer Science, Electronic & Information Storage Systems Research Group, Oxford Road, IT Building, Room IT102, Manchester, M13 9PL, UK, v.tsiantos@stud.man.ac.uk

[+] University of Manchester, Department of Computer Science, Electronic & Information Storage Systems Research Group, Oxford Road, Manchester, M13 9PL, UK, j.j.miles@man.ac.uk

[**] University of Manchester, Department of Computer Science, Electronic & Information Storage Systems Research Group, Oxford Road, Manchester, M13 9PL, UK, mbgesbm1@fs1.eng.man.ac.uk

because they address correctly the question of stiffness in micromagnetics solving the LLG equation with finite difference methods. The second group [7-10] concentrates on the problem of stiff modes in the solution of the linear systems involved in energy minimisation techniques. The physical explanation of the cause of stiff modes using energy minimisation techniques, that is the co-operative rotation of magnetisation, is a pioneering work of Edward Della Torre and co-workers [7-10].

Finally, the last group mentions stiffness in the ODE context [11, 12, 13]. However, they did not investigate thoroughly the subject of stiffness solving the LLG equation by a numerical method for systems of ODEs and they rather used their experience from using different solvers to conclude that stiffness is present when the time steps used by their methods were extremely small.

3 Pragmatic measures of stiffness

In this Section a more pragmatic way of measuring stiffness in the context of ODEs is given. A rough guide to stiffness is based on the total number of time steps taken by a non stiff method (for example Adams) and a stiff one (for example BDF). Then, if

$$\frac{\text{nst (Adams)}}{\text{nst (BDF)}} > 1, \tag{1}$$

we can theoretically consider the case as stiff [14]. However, this is rather academic definition because it doesn't consider the cost per time step of the two methods. Thus, since BDF has an extra cost per step for the linear algebra involved then the total cost for the BDF (stiff) can be bigger than the total cost of the Adams (non stiff) method. So, if BDF needs fewer time steps than the Adams method we can theoretically say that it is stability considerations that constrain the time steps chosen and not accuracy and so the problem is stiff [14].

However, if we look more carefully at the cost of each method, Cost(method), then we can say more accurately if the case is stiff, or not. The Cost(method) is given by,

$$\text{Cost}(\text{method}) = \frac{\text{cost (BDF)}}{\text{cost (Adams)}}. \tag{2}$$

So, then the cost per time step for the Adams methods, that is cost(Adams), is,

$$\text{cost}(\text{Adams}) = \frac{\text{NFE (Adams)}}{\text{nst (Adams)}}, \tag{3}$$

and similarly the cost of the BDF methods, that is cost(BDF), is,

$$\text{cost}(\text{BDF}) = \frac{\text{NFE (BDF)}}{\text{nst (BDF)}}. \tag{4}$$

If now we have that,

$$\frac{\text{cost}(\text{BDF})}{\text{cost}(\text{Adams})} < \frac{\text{nst (Adams)}}{\text{nst (BDF)}}, \tag{5}$$

then the case is stiff, but if this is not the case then the problem is not stiff. However, we can relax these criteria and accept a time step ratio bigger than 5 to consider the case stiff, a ratio between 1 to 5 as mildly stiff, and the rest cases not stiff.

Finally, an ultimate measure of the stiffness is the actual run time of the simulation with the two methods, non stiff and stiff ones. If the stiff method takes much less time than the non stiff one then the problem is definitely stiff. However, in this paper we did not consider the run time of the simulation mainly due to the fact that the other two measures give enough information for the stiffness of the calculations. The approach defined in this Section is going to be employed for the measure of stiffness in micromagnetic simulations in Section 4, since it is very difficult to calculate the eigenvalues of the problem matrix when we have a very large number of grains. Moreover, things are more complicated with the dynamic calculation of magnetisation in micromagnetics because the system of LLG equations can become stiff at a certain point in the calculation.

4 Measuring Stiffness in Micromagnetic Simulations

In this section we use a family of simulations from an extensive number of simulations run by the authors to show that stiffness in the ODE context is an important phenomenon in micromagnetics which requires much attention. In addition to this, the problems called "stiff" are too important to ignore, and are too expensive to overpower [16]. They are very important in micromagnetics as well, because micromagnetic simulations can take an enormous amount of time to run with inappropriate solvers and this limits the opportunity to use micromagnetics in industry. The phenomenon of stiffness appears in

micromagnetics probably in situations where there is co-operative rotation of grains [8]. They are too expensive to overpower because of their size and the inherent difficulty they present to classical methods [15].

4.1 Simulation Results

In this Section a set of simulations is presented. The main parameters of this set of simulations are: exchange constant (A) = 2.0e-11, crystalline anisotropy = [4.0e2, 4.0e5], and magnetisation saturation (M_s) = 9.5×10^5. The exchange scale parameter for this particular set of simulations is equal to 1.0, which means high exchange interactions between grains. These interactions will probably cause high degree of stiffness of the systems. The damping constant is equal to 1.0 and the easy axes are randomly distributed in plane.

The error criterion used is the mixed one with absolute and relative error tolerance equal to 10^{-3}. We used the LSODKR code, written by P.N. Brown and A.C. Hindmarsh, with parameter mf =10 to run only with the Adams methods option, and also LSODKR with the option mf = 22 to run the simulations with the backward differentiation formulae (BDF) methods and the scaled GMRES method. In Table 1 the specific values for the crystalline anisotropy and maximum applied field parameters, as well as the measures of the performance of the two methods for the simulations are presented. More specifically, the number of function evaluations (NFEs) and total number of time steps (nst) for the simulations are given. The micromagnetic model used was the model developed by M. Jones and J.J. Miles [16].

Table 1: Values of crystalline anisotropy and maximum applied field parameters, and NFEs and time steps (nst) for the simulations taken by the two different solvers.

	Crystalline Anisotropy	***Maximum Applied Field***	**LSODKR(Adams)**		**LSODKR(BDF)**	
			NFE	*nst*	*NFE*	*nst*
Cryst_Anisotr_1	4.0×10^2	2.0×10^5	522121	197269	708	145
Cryst_Anisotr_2	4.0×10^3	2.0×10^5	508667	198491	1496	549
Cryst_Anisotr_3	4.0×10^4	2.0×10^5	248048	95348	3862	2245
Cryst_Anisotr_4	7.0×10^4	2.0×10^5	247472	95062	5575	3441
Cryst_Anisotr_5	1.0×10^5	5.0×10^5	259857	99485	6541	3401
Cryst_Anisotr_6	2.0×10^5	6.0×10^5	265587	103207	20202	8182
Cryst_Anisotr_7	4.0×10^5	7.0×10^5	253642	98762	25600	11484

The hysteresis loops were produced by the two methods, LSODKR(Adams) and LSODKR(BDF), for all cases (Table 2). Note that the value of the maximum applied field was 2.0×10^5 for Cryst_Anisotr_1/2/3/4 and 5.0×10^5, 6.0×10^5, and 7.0×10^5 for Cryst_Anisotr_5, Cryst_Anisotr_6, and Cryst_Anisotr_7 (Table 1). The results for NFEs with LSODKR(Adams) vary with the various values of the crystalline anisotropy. More specifically, for the case Cryst_Anisotr_1 we have a large number of function evaluations (NFEs=522121), and then a very small decrease to 508667 for crystalline anisotropy equal to 4.0×10^3. Then the number of NFEs decreases dramatically to 248048 (crystalline anisotropy = 4.0×10^4), and then decreases further to 247472 (crystalline anisotropy = 7.0×10^4). With crystalline anisotropy equal to 1.0×10^5, we have a very small increase to 259857 and then a small increase again (NFEs=265587, crystalline anisotropy = 2.0×10^5) followed by a small decrease (NFEs=253642) for the case of crystalline anisotropy equal to 4.0×10^5. The last three cases are possibly affected by the change in the value of the maximum applied field. From Table 1 we can observe that the NFEs for the LSODKR(Adams) is extremely large for Cryst_Anisotr_1. Moreover, in comparison with the low value of the NFEs for the LSODKR(BDF) we can assume that this should be a very stiff case. We will return to this point when we will discuss the ratios of time steps and the ratio of the cost of each method per time step. The value of NFEs using the LSODKR(BDF) method is monotonically increasing for Cryst_Anisotr_1 to Cryst_Anisotr_7 from 708 to 25600. The behaviour of the parameter nst for LSODKR(Adams) and LSODKR(BDF) is similar to that of the corresponding NFEs (Table 1).

In Table 2 the ratios for the time steps taken by LSODKR(Adams) and LSODKR(BDF) methods are given. These values are plotted in Figure 1 in red. For the first two cases, that is Cryst_Anisotr_1/2, we can conclude even observing only the ratios of the time steps that they are extremely stiff cases. It is impossible for the cost per step of the LSODKR(BDF) method to be as high as it requires to compensate this very large ratio of the time steps. In fact, from Table 3 which gives the values of the measures cost(method) for LSODKR(Adams) and LSODKR(BDF), we can see a very small increase into the cost per step for the BDF method to 4.88 for the case Cryst_Anisotr_1. However, this increase is very small to compensate the high ratio of the time steps, and so the BDF method is the more efficient method.

Table 2: Ratio of time steps, and values of cost(method) for LSODKR(Adams) and LSODKR(BDF) methods.

	$\frac{\text{nst (Adams)}}{\text{nst (BDF)}}$	$\text{cost (Adams)} = \frac{\text{NFE (Adams)}}{\text{nst (Adams)}}$	$\text{cost (BDF)} = \frac{\text{NFE (BDF)}}{\text{nst (BDF)}}$
Cryst_Anisotr_1	*197269 / 145 = 1360.48*	*522121 / 197269 = 2.65*	*708 / 145 = 4.88*
Cryst_Anisotr_2	*198491 / 549 = 361.55*	*508667 / 198491 = 2.56*	*1496 / 549 = 2.72*
Cryst_Anisotr_3	*95348 / 2245 = 42.47*	*248048 / 95348 = 2.60*	*3862 / 2245 = 1.72*
Cryst_Anisotr_4	*95062 / 3441 = 27.63*	*247472 / 95062 = 2.60*	*5575 / 3441 = 1.62*
Cryst_Anisotr_5	*99485 / 3401 = 29.25*	*259857 / 99485 = 2.61*	*6541 / 3401 = 1.92*
Cryst_Anisotr_6	*103207 / 8182 = 12.61*	*265587 / 103207 = 2.57*	*20202 / 8182 = 2.47*
Cryst_Anisotr_7	*98762 / 11484 = 8.60*	*253642 / 98762 = 2.57*	*25600 / 11484 = 2.23*

Moreover, in Table 3 the values of the cost of method parameter, Cost(method), as it is defined in Section 3 is presented. The values of Cost(method) are plotted in Figure 1 in colour against the corresponding value of crystalline anisotropy. From Table 3 we can see that except for the first two cases the cost per step is higher for the Adams (non stiff) method. For the first case the value of Cost(method) is 1.84 which is very small to cover the difference in the number of the time steps between the two methods. In the second case (Cryst_Anisotr_2) is just 1.06, which means that the two methods have the same almost cost per time step.

Table 3: Cost of method, Cost(method), as a fraction of the cost per step of LSODKR(BDF) and LSODKR(Adams) methods.

	$\text{Cost (method)} = \frac{\text{cost (BDF)}}{\text{cost (Adams)}}$
Cryst_Anisotr_1	*4.88 / 2.65 = 1.84*
Cryst_Anisotr_2	*2.72 / 2.56 = 1.06*
Cryst_Anisotr_3	*1.72 / 2.60 = 0.66*
Cryst_Anisotr_4	*1.62 / 2.60 = 0.62*
Cryst_Anisotr_5	*1.92 / 2.61 = 0.74*
Cryst_Anisotr_6	*2.47 / 2.57 = 0.96*
Cryst_Anisotr_7	*2.23 / 2.57 = 0.87*

In Figure 1 the time step ratios, as well as the Cost(method) ratios are plotted for the simulations against the values of crystalline anisotropy used. We can see in Figure 1 that for all the values of crystalline anisotropy the cases are stiff, since the ratio of time steps is larger than the value of Cost(method). This means that the non stiff method takes much more time steps than the stiff method (Table 1). Moreover, the cost of the stiff method is not higher than the cost of the non stiff method, so stiff methods (like BDF) should be used in such cases. Furthermore, it is not advisable to use a non stiff method in cases such as this set of micromagnetic simulations because the speed of the simulation will be extremely slow and the performance of the micromagnetic calculation very inefficient.

The hysteresis loops for the case of Cryst_Anisotr_1 (extremely stiff) can be seen in Figure 2 produced by the two methods. The hysteresis loops are so similar that it is very difficult to distinguish them. This family of simulations simulates relatively low coercivity materials with high remanence.

5 Conclusions

To summarise the results of this paper we can say that measuring the stiffness of the system of equations representing the dynamic behaviour of the motion of magnetisation is of immense importance in micromagnetics as has already been explained in Section 2. For measuring the stiffness in micromagnetics we suggest to use a non stiff method, such as Adams, to run the micromagnetic calculations and then to use a stiff method, such as BDF, to do so [17]. Then using the measures that we introduced in Section 3 it can be decided if the case is stiff, mildly stiff, or non-stiff. This approach ensures that the appropriate method will be used. We believe that the simulations presented in this paper provide the necessary justification of the need for

stiff methods when the system of equations is stiff. Otherwise, employing non stiff methods in such cases causes the speed of the simulation to be extremely slow.

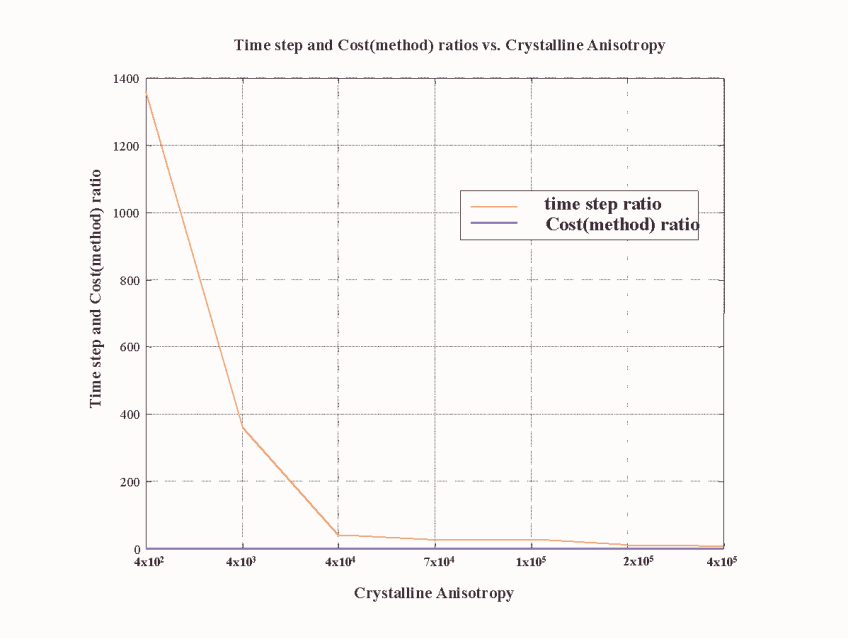

Figure 1: Stiffness ratios vs. Crystalline Anisotropy.

An important question is what causes stiffness in micromagnetics. In Section 2 we mentioned that E. Della Torre and co-workers explain the cause of stiff modes in micromagnetics during the energy minimisation techniques and the relationship between these methods and dynamic methods was shown in [7-10]. E. Della Tore mentions that the mode of magnetisation change where all the magnetisations of grains rotate by an equal amount is referred to as a *stiff mode* [8]. Moreover, he adds that the stiff modes in micromagnetics are the ones that involve the co-operative rotation of the magnetisation of many grains [8]. In addition to this, we can conclude that micromagnetic calculations for materials with no or weak exchange interactions lead to a lower degree of stiffness [19]. In fact, when the exchange scale is zero only the particular case with crystalline anisotropy equal to 4.0×10^3 is stiff [19]. This particular case has zero exchange field and low crystalline anisotropy, so maybe magnetostatic interactions dominate the behaviour of the system and thus we have probably a higher degree of co-operative rotation of the magnetisation of grains for this particular case.

Simulations with higher value of the exchange scale parameter (=0.5), which means higher value for the exchange field and so stronger exchange interactions between grains were investigated also in [19]. These strong interactions between neighbour grains maybe determine the rate of the magnetisation rotation. It has been shown in [19] that low values of crystalline anisotropy lead to very stiff systems, then values of crystalline anisotropy equal to 2.0×10^3, 4.0×10^3 and 2.0×10^4 to cases that are not stiff, and finally higher values of the crystalline anisotropy also give rise to stiff systems.

Finally, the simulations presented in this paper illustrate a very stiff case, especially for Cryst_Anisotr_1 and Cryst_Anisotr_2. The value of the exchange scale is equal to 1.0, which means that the exchange field has high value, and thus strong exchange interactions exist between grains. The curve of the ratio of time steps is a smooth one for these simulations. As we increase the value of the crystalline anisotropy the degree of stiffness decreases. So it seems that here we have a reverse proportional relationship of the ratio of time steps and the value of the crystalline anisotropy. These simulations can validate the claim that systems with strong exchange coupling are stiff because they have a higher degree of co-operative rotation of the magnetisation of the grains [17, 8].

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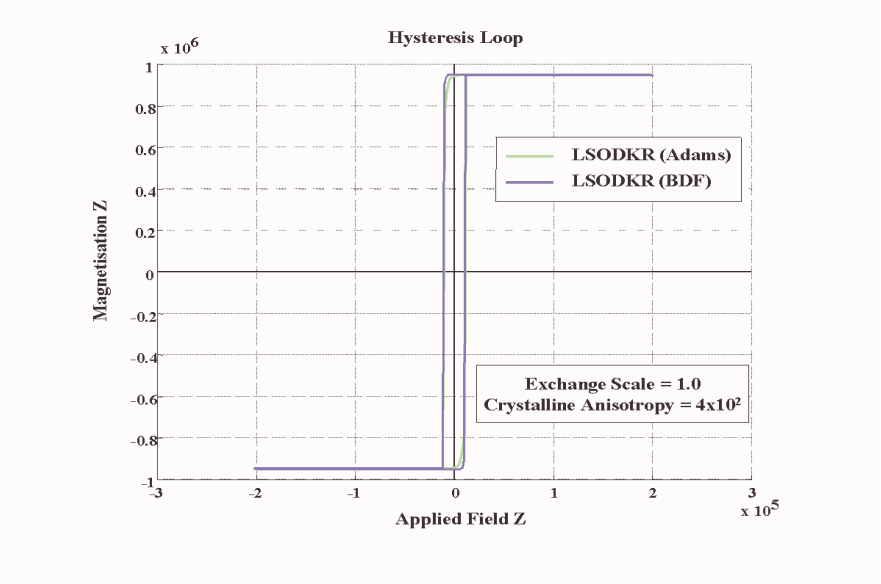

Figure 2: Hysteresis loops produced by the three methods.

References

[1] J.D. Lambert, *Numerical methods for ordinary differential systems - The initial value problem*, John Wiley & Sons, Chichester, 1995.

[2] E. Hairer, and G. Warner, *Solving ordinary differential equations II: Stiff and differential-algebraic problems*, second revised edition, Springer, Berlin, 1996.

[3] L.F. Shampine, *Numerical solution of ordinary differential equations*, Chapman & Hall, New York, 1994.

[4] G. Hall, and J.M. Watt, *Modern numerical methods for ordinary differential equations*, Clarendon Press, Oxford, 1976.

[5] N. Hayashi, Y. Nakatani, and T. Inoue, *Numerical solution of the Landau-Lifshitz-Gilbert equation with two space variables for vertical bloch lines*, Japanese J. Appl. Phys., 27(3), 1988, pp. 366-378.

[6] Y. Nakatani, Y. Uesaka, and N. Hayashi, *Direct solution of the Landau-Lifshitz-Gilbert equation for micromagnetics*, Jap. J. Appl. Phys., 28(12), 1989, pp. 2485-2507.

[7] M. Torfeh-Isfahani, and E. Della Torre, *Mode pushing and stiff convergent problems*, IEEE Trans. Magnetics, Vol. MAG-19(6), 1983, pp. 2527-2530.

[8] E. Della Torre, S*tiff modes in numerical micromagnetic problems*, IEEE Trans. Magn., 29(6), 1993, pp. 2371-2373.

[9] Z. Guo, and E. Della Torre, *Micromagnetic analysis of domain variations in thin films*, IEEE Trans. Magn., 29(6), 1993, pp. 2521-2523.

[10] D. Lewis, and E. Della Torre, *Migrating mesh micromagnetic model*, IEEE Trans. Magn., 33(5), 1997, pp. 1141-1143.

[11] Yang, B. and Fredkin, D.R., *Dynamical micromagnetics by the finite element method*, IEEE Trans. Magn., 34(6), 1998, pp. 3842-3852.

[12] T. Schrefl, J. Fidler, K.J. Kirk, and J.N. Chapman, *A higher order FEM-BEM method for the calculation of domain processes in magnetic nano-elements*, IEEE Trans. Magn., 33(5), 1997, pp. 4182-4184.

[13] T. Schrefl, and J. Fidler, Reversal *modes and reversal times in submicron sized elements for mram applications*, at *the European Materials Conference Spring Meeting*, paper no. C-VII.02, Strasbourg, France, 1-3 June 1999.

[14] A.C. Hindmarsh, private communication, 1999.

[15] L.F. Shampine, and C.W. Gear, *A user's view of solving stiff ordinary differential equations*, SIAM Review, 21(1), 1979, pp. 1-17.

[16] M. Jones, and J.J. Miles, *An accurate and efficient 3-D micromagnetic simulation of metal evaporated tape*, JMMM, 171,1997, pp. 190-208.

[17] G.D. Byrne, and A.C. Hindmarsh, *Stiff ODE solvers: A review of current and coming attractions*, J. Comp. Phys., 70(1), 1987, pp. 1-62.

[18] G.E. Kay, A. Hart, D.A. Parker, and P.R. Bissel, *A model of an isolated column of metal evaporated tape*, IEEE Trans. Magn., 33, 1997, pp. 3058-3060.

[19] V.D. Tsiantos, *Numerical methods for ordinary differential equations in micromagnetic simulations*, PhD thesis, University of Manchester, Department of Computer Science, June 2000.