

Time Integration Methods in Micromagnetic Simulations: Stiffness on Granular Media and μ MAG standard problem #4 – Speed up of Simulations in Granular Recording Media

Vassilios D. Tsiantos, *Member, IEEE*, Thomas Schrefl, *Member, IEEE*, Dieter Suess, Werner Scholz, *Student Member, IEEE*, Hermann Forster and Josef Fidler, *Member, IEEE*

Abstract--In this paper an investigation of the stiffness of granular media of CoCrPtTa structure (type a) and micromagnetic standard problem #4 has been done. Moreover, an investigation of the effect of the maximum dimension of the Krylov subspace projection methods, within the Ordinary Differential Equations (ODEs) context, on the speed of micromagnetic simulations on granular media of Co structure (type b) has been done. The stiffness of the problems has been investigated using two different solvers, a non-stiff (Adams) and a stiff one (backward differentiation formulae, BDF) for the solution of the large system of ODEs. The results show that granular media (type a) micromagnetic simulations are stiff, whereas μ MAG standard problem #4 is not. Furthermore, it has been found that increasing the maximum dimension of the Krylov subspace to 20 (default value =5) a considerable increase to the speed of the granular media simulations occurs in the order of approximately 90%.

Index terms-- Micromagnetics, ordinary differential equations, stiffness, Landau-Lifshitz-Gilbert equation, Krylov methods, granular media.

I. INTRODUCTION

The basic structural units of modern magnetic materials are nanocrystalline grains [1-3]. Moreover, as the magnetic devices are miniaturized by the magnetic recording industry understanding of the connection between the structural properties and the domain formation is of immense importance. Micromagnetic modelling is an effective tool to analyze the domain configurations during magnetization reversal. However, micromagnetic calculations are time consuming and efficient ways to speed up the simulations have to be employed. In this paper micromagnetic simulations for granular media, as

well as on μ MAG standard problem #4 have been run in order to investigate the stiffness of the simulations. Moreover, the effect of the maximum dimension of the Krylov subspace on the speed of the simulations on granular media (type b) has been investigated in order to define an optimum value.

II. MODEL AND SIMULATION METHOD

In micromagnetics the magnetic polarization is assumed to be a continuous function of space. The time evolution of the magnetization follows the Gilbert equation of motion.

$$\frac{d\mathbf{J}}{dt} = -|\gamma_0| \mathbf{J} \times \mathbf{H}_{\text{eff}} + \frac{\alpha}{J_s} \mathbf{J} \times \frac{\partial \mathbf{J}}{\partial t} \quad (1)$$

which describes the physical path of the magnetic polarization \mathbf{J} towards equilibrium. The effective field \mathbf{H}_{eff} is the negative functional derivative of the total magnetic Gibb's free energy, which can be expressed as the sum of the exchange energy, the magneto-crystalline anisotropy energy, the magnetostatic energy, and the Zeeman energy [4]. γ_0 is the gyromagnetic ratio of the free electron spin and α is the damping constant. To solve the Gilbert equation numerically the magnetic particle is divided into finite elements. A hybrid finite element boundary element method [5], is used to calculate the scalar potential u on every node point of the finite element mesh. The demagnetizing field, which contributes to the effective field, is the negative derivative of the scalar potential u . The effective field $\mathbf{H}_{\text{eff}}^i$ at the node point i of an irregular finite element mesh can be approximated using the box scheme

The authors are adjuncts to Institute of Technical and Applied Physics, Vienna University of Technology, Wiedner Hauptstrasse 8-10/137, A-1040, Vienna, Austria. Email: v.tsiantos@computer.org

$$\mathbf{H}_{\text{eff}}^i = - \left(\frac{\delta E_t}{\delta \mathbf{J}} \right)_i = - \frac{1}{V_i} \frac{\partial E_t}{\partial \mathbf{J}_i}, \text{ for } V_i \rightarrow 0, \quad (2)$$

where V_i is the volume of the surrounding node i , such that

$$\sum_i V_i = V, \text{ and } V_i \cap V_j = 0 \text{ for } i \neq j, \quad (3)$$

The discretization of the Gilbert equation leads to an ordinary differential equation for every node for each component. In the case of a non-stiff problem it is advisable to use an appropriate method, such as Adams [6], whereas in stiff problems a backward differentiation formula (BDF) method could be an option for the time integration. BDF method is implicit, so at each time step a non-linear algebraic system must be solved. For the solution of the non-linear system a method, such as Newton, has to be used which leads usually to a very large system of linear equations. In this paper the latter is solved using the scaled preconditioned incomplete generalised minimum residual method (SPIGMR) [7], based on GMRES (generalized minimum residual method) proposed by Youcef Saad [8]. SPIGMR belongs to the family of Krylov subspace methods, which are iterative methods for solving systems of linear equations. SPIGMR has been explored in micromagnetics by Vassilios D. Tsiantos *et al* [9,10], and also used by Bo Yang and Donald Fredkin [11].

III. STIFFNESS

The stiffness of the problems has been investigated solving the system of ordinary differential equations with two different solvers. A non-stiff method (Adams) and a stiff one (backward differentiation formulae, BDF) have been used to measure the stiffness of the problem. For the latter the ratio of the total number of time steps (nst) taken by the two solvers, that is $\text{nst(Adams)}/\text{nst(BDF)}$, has been used. Note that the simulation time has to be the same in order to have a fair comparison. The abovementioned method has been proposed to approximate numerically the stiffness of a system of ordinary differential equations (ODEs) in micromagnetics by Vassilios Tsiantos and James Miles [12]. Another factor that has to be considered is the cost of each method per time step. This cost per time step is important in cases that the ratio $\text{nst(Adams)}/\text{nst(BDF)}$ is larger than 1. If the ratio of time steps is smaller than 1 then the case is nonstiff. For the Adams the main cost per time step is the function evaluation. However, for the case of BDF there is some extra cost for the linear algebra involved. This extra cost is due to linear and nonlinear iterations. To solve the nonlinear equation arisen using BDF method a Newton-like scheme can be used which leads to a large system of linear equations. The linear system is in general nonsymmetric, so to solve it we use

GMRES method. GMRES has been reported to work better with some kind of preconditioning [7]. In general, the preconditioned case gives faster results in terms of the nonlinear and linear iterations. However, the preconditioned method roughly doubles the average cost per nonlinear iteration because it computes and processes the preconditioner [7]. In this paper the unpreconditioned SPIGMR method has been considered [7]. Finally, the ultimate measure of stiffness is the total CPU time that is needed to solve the problem with the Adams and the BDF method.

III.A. μ MAG problem #4

The magnetic material defined by μ MAG standard problem no. #4 is a rectangle NiFe film, with thickness $t=3\text{nm}$, width $d=500\text{nm}$, and length $L=125\text{nm}$. The initial state is an equilibrium s-state. The s-state is obtained after applying and slowly reducing a saturating field along the [1,1,1] direction to zero. Standard problem no. #4 is focused on the dynamic aspects of micromagnetic computations [13]. The problem has been studied using a 3D-finite element simulation based on the solution of the Gilbert equation. The problem runs for two different applied fields, one at 170 degrees (field 1) and the other at 190 degrees (field 2) counterclockwise from the positive x axis.

The total number of nodes for the finite element analysis is 5252, so the total number of equations is 15756. The ratio of the total number of time steps taken by the two solvers, that is $\text{nst(Adams)}/\text{nst(BDF)}$, is 0.784 for field 1 and 0.614 for field 2, which means that the non-stiff method (Adams) uses larger time steps than the stiff method (BDF) and consequently the systems are not stiff. The total number of the time steps taken by each method for field 1 is 11473 (Adams) and 14628 (BDF). For field 2 we have that $\text{nst(Adams)}=11342$ and $\text{nst(BDF)}=18479$. The simulation time considered for field 1 is 2.15ns and for field 2 is 2.23ns. The average time step for the Adams method was 0.2 ps for both fields.

μ MAG problem no. #4 can be misleading with regards to its stiffness because the Adams method takes too many time steps. Thus, it can be thought as a stiff case if it will not be compared to a stiff method. The possible explanation for the large number of time steps is the low value of the damping constant used, $\alpha=0.02$. The low value of α causes the magnetization to move around the effective field so the time integrator needs very small time steps to follow the path of the magnetization. For the ODE solver we used mixed error criterion with absolute and relative tolerance equal to 10^{-4} . Moreover, after 2.42 ns for field 1 and 2.23 ns for field 2 the amplitude of the oscillations of

the magnetization obtains the requested numerical accuracy.

III.B. CoCrPtTa granular media

Micromagnetic simulations for granular media (type b) have been run in order to examine the stiffness of the systems. The number of nodes used in the finite element method was 494, 946, 1681, 4426, and 12882. The ratio of the total number of time steps taken by the Adams and the BDF method with the default value of the maximum dimension of Krylov subspace, $l_{\max}=5$, that is $nst(\text{Adams})/nst(\text{BDF})$, is 13.19, 16.56, 18.06, 23.24, and 31.80, for the systems with 494, 946, 1681, 4426, and 12882 nodes, respectively. These ratios mean that the systems are stiff. However, the cost of Adams and BDF methods is different and this should be taken into account. So, the ultimate measure is the CPU time run with the two solvers for the same simulation time. Table 1 presents the CPU time for Adams and BDF for the given simulation time (in nsec).

Table 1. Total CPU times for the same simulation time.

Nodes	BDF	Adams	Sim. Times
494	321.0167	1083.1152	0.14580
946	1159.8037	4664.4670	0.17128
1681	1823.4912	7935.7000	0.13613
4426	7469.1875	39947.4000	0.17715
12882	59294.2890	171977.0000	0.30975

The results show that BDF method is approximately three times faster than the Adams method and this means that the systems are stiff. So, BDF is a better option for the solution of the large system of ODEs than Adams.

IV. EFFECT OF MAXIMUM DIMENSION OF KRYLOV SUBSPACE ON Co GRANULAR MEDIA

The Co granular media material (type a) is uniformly magnetised and perpendicular to the plane of the film. The geometry of the sample can be shown in Fig. 1. This is a test case used for the calculation of the effect of the maximum dimension of the Krylov subspace on the micromagnetic simulations of Co granular media. So, the magnetisation arrangement at zero field was of our interest. Due to random in plane anisotropy an

inhomogeneous magnetisation distribution has been expected.

The intrinsic parameters of the Co nano-particles used for the simulations were, crystalline anisotropy $K_1 = 4.5 \times 10^6 \text{ J/m}^3$, saturation magnetisation $J_s = 1.76 \text{ T}$, and exchange constant $A = 1.3 \times 10^{-11} \text{ J/m}$. The damping constant used was $\alpha=0.1$, the error criterion was the mixed one and the tolerance 10^{-5} .

Table 2 shows the CPU times and the total number of time steps taken by BDF for simulation time approximately 3.185 ns. The values of maximum dimension of the Krylov subspace, l_{\max} , were 5 (default value), 10 and 20. The gain in CPU time is 62.09% for $l_{\max}=10$, and 83.5% for $l_{\max}=20$. With regards to the total number of time steps for $l_{\max}=10$ we have 82.96% less time steps, and for $l_{\max}=20$ we have 91.96% less. Thus, we can see that we get considerable speed up with increasing the value of l_{\max} .

Table 2. Total CPU times for the same simulation time, for different value of maximum dimension of the Krylov subspace, l_{\max} .

l_{\max}	CPU Time	nst	Sim. Times
5	3.473618e5	37082	3.184953
10	9.695233e4	6319	3.187996
20	5.739658e4	2984	3.184879

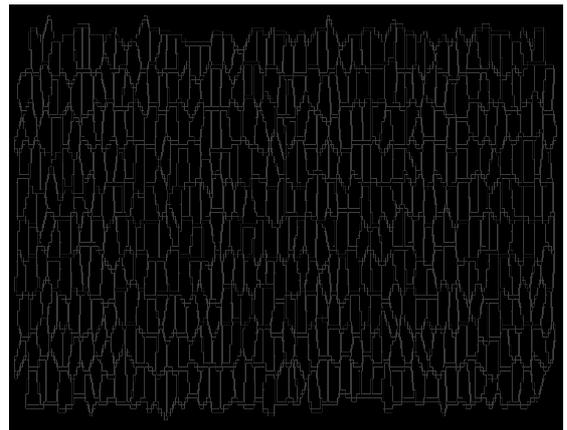


Fig. 1. Plot of the geometry of the sample.

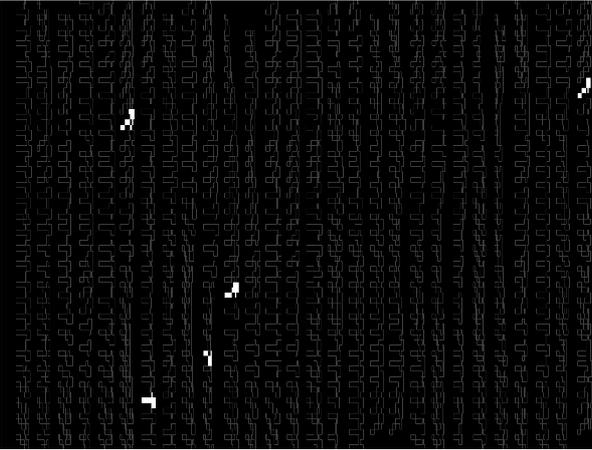


Fig. 2. The magnetisation distribution of the sample ($l_{\max}=10$).

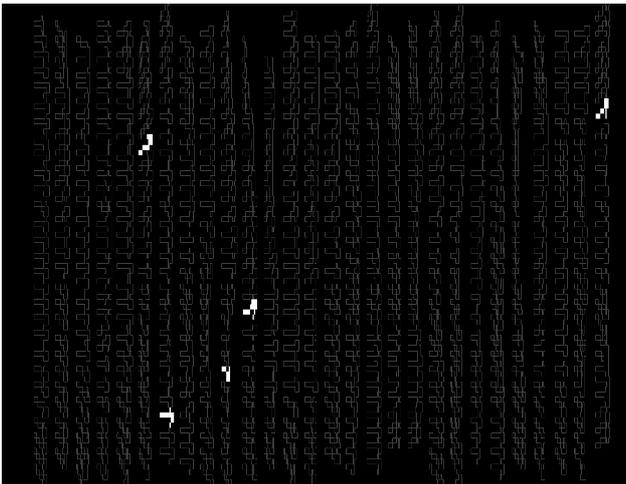


Fig. 3. The magnetisation distribution of the sample ($l_{\max}=10$).

Figures 2 and 3 show the magnetization distribution at two different points of the simulation.

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