Stiff modes in spinvalve simulations with OOMMF

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Abstract

Micromagnetic simulations are an important tool for the investigation of magnetic materials. Micromagnetic software uses various techniques to solve differential equations, partial or ordinary, involved in the dynamic simulations. Euler, Runge-Kutta, Adams, and BDF (Backward Differentiation Formulae) are some of the methods used for this purpose. In this paper, spinvalve simulations are investigated. Evidence is presented showing that these systems have stiff modes, and that implicit methods such as BDF are more effective than explicit methods in such cases.

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1 Introduction

There are many micromagnetic codes that simulate magnetic materials. Some of the codes are freeware, such as magpar [1], OOMMF [2], PC Micromagnetic Simulator (SimulMag), General Dynamic Micromagnetics (GDM2) [3], NMag [4]; some, like FastMag [5], are designed for ultra-complex systems; and some are commercial products, such as LLG [6], MicroMagus [7], FEMME [8], etc. These codes use different ODE solvers, either explicit or implicit. Explicit methods are suitable for nonstiff problems, whereas implicit methods are more efficient for stiff problems.

Stiffness is an important issue in the solution of Ordinary Differential Equations (ODEs) and much attention has been paid to this subject. Hundreds of theoretical papers have been written about stiffness and also on constructing appropriate methods to overcome this problem. There is not yet a rigorous definition of stiffness that is accepted by all authors. However, there are various proposed definitions and criteria about stiffness [9]. One criterion to consider is that an ordinary differential equation problem is stiff if the solution being sought is varying slowly, but there are nearby solutions that vary rapidly, so the numerical method must take small steps to obtain satisfactory results. Moreover, stiffness is an efficiency issue—if the computation time was not a concern we perhaps wouldn't be concerned about stiffness [10]. Nonstiff methods can (generally) solve stiff problems; they just take a long time to do it. Stiff methods, such as BDF, use larger time steps due to larger regions of stability [11-13], whereas explicit methods have to depress the step size to avoid instability. In the context of micromagnetics, stiffness has been studied by Della Torre and co-workers [14,15], and Tsiantos [16,17]. According to Della Torre in many magnetic structures strong exchange coupling leads to numerical problem stiffness. The stiffness manifests itself in that the time step becomes very small and the linear solver part of implicit time integration methods becomes slowly convergent. Therefore, there are codes, such as FastMag, that use implicit schemes including BDF [18]. The BDF method requires the evaluation of the numerical system Jacobian to enhance the time integration. FastMag implements a technique that allows evaluating the product of the numerical system Jacobian with the magnetization vector exactly without a need to create any matrices, and it does it so at the speed of a conventional effective field evaluation. This allows the use of the BDF method without a linear solver preconditioner, which is important for running on GPUs with limited memory [5].

2 Micromagnetic simulations

We used the 3D OOMMF (Object-Oriented MicroMagnetic Framework) software [2] for the spinvalve hysteresis simulations. This software uses a finite difference grid with rectangular cells. The calculations in this study are based on the Landau-Lifshitz (LL) equation, where the effective field includes the anisotropy, applied, exchange, and self magnetostatic fields. With regards to the ODE solver we used one of the Runge-Kutta methods that OOMMF provides (RKF54) and we also incorporated into OOMMF the CVODE code from the SUNDIALS package for the analysis of stiffness [17].

A spin valve is a device that consists of two or more layers of conducting magnetic material in which the electrical resistance changes between two values depending on the relative alignment of the magnetisation in the layers. The magnetisation in the layers of the device aligns either "up" or "down", and the alignment can be controlled by an external magnetic field. In the simple case, a spin valve consists of a non-magnetic material sandwiched between two ferromagnets, one of which has its magnetisation fixed (pinned) by an antiferromagnet, raising its magnetic coercivity so that it behaves as a "hard" layer, while the other ferromagnet is free (unpinned) and behaves as a "soft" layer [20]. Due to the difference in coercivity, the soft layer changes polarity at a lower applied magnetic field strength than the hard layer. Upon application of a magnetic field of appropriate strength, the soft layer switches polarity, producing two distinct states: a parallel, low-resistance state, and an antiparallel, high-resistance state (Fig. 1).

In the micromagnetic simulations the form for the equation of motion of the moment due to Landau and Lifshitz has been used,

$$\frac{d\mathbf{m}}{dt} = \gamma_L(\mathbf{m}\times\mathbf{h}) - \alpha_L \mathbf{m}\times(\mathbf{m}\times\mathbf{h}), \qquad (1)$$

where $\mathbf{m}$ is the pointwise magnetization and $\mathbf{h}$ is the total effective field, γ_L is the gyromagnetic ratio and α_L is the damping factor. The so-called effective field is the sum of the demagnetising field, the anisotropy field, the exchange field, and the external (Zeeman) field. Solving this equation (or an equivalent formulation by Gilbert, known collectively as the LLG equation) allows the equilibrium state to be found using standard ODE solvers, which are inherently designed to accurately follow a trajectory defined by a gradient.

We assume that the system of ODEs (initial value problem, IVP)

$$\dot{\boldsymbol{m}} = \boldsymbol{f}(\mathrm{t}, \boldsymbol{m}), \quad \boldsymbol{m}(\mathrm{t}_0) = \boldsymbol{m}_0 \qquad (2)$$

is stiff, meaning that one or more strongly damped modes are present.

The general form of the BDF method is

$$\boldsymbol{m}_{\mathrm{n}} = \sum_{\mathrm{j=1}}^{\mathrm{q}} \alpha_{\mathrm{j}}\, \boldsymbol{m}_{\mathrm{n-j}} + \mathrm{h}\,\beta_0\, \dot{\boldsymbol{m}}_{\mathrm{n}}, \qquad \dot{\boldsymbol{m}}_{\mathrm{n}} = \boldsymbol{f}(\mathrm{t}_{\mathrm{n}}, \boldsymbol{m}_{\mathrm{n}}), \qquad (3)$$

where q is the method order, h is the time step, α_j and β_0 are constants for the multistep methods, in which family belong BDF methods. The BDF methods are implicit, so at each time step n an algebraic system must be solved,

$$\boldsymbol{m}_{\mathrm{n}} - \mathrm{h}\,\beta_0\, \boldsymbol{f}(\mathrm{t}_{\mathrm{n}}, \boldsymbol{m}_{\mathrm{n}}) - \alpha_{\mathrm{n}} = 0, \qquad (4)$$

where $\alpha_{\mathrm{n}} = \sum_{\mathrm{j=1}}^{\mathrm{q}} \alpha_{\mathrm{j}}\, \boldsymbol{m}_{\mathrm{n-j}}$, $\beta_0 > 0$, for $\boldsymbol{m}_{\mathrm{n}}$.

In practice we solve an equivalent system, namely

$$\boldsymbol{F}_{\mathrm{n}}(\boldsymbol{x}_{\mathrm{n}}) \equiv \boldsymbol{x}_{\mathrm{n}} - \mathrm{h}\, \boldsymbol{f}(\mathrm{t}_{\mathrm{n}}, \alpha_{\mathrm{n}} + \beta_0 \boldsymbol{x}_{\mathrm{n}}) = 0, \qquad (5)$$

where $\boldsymbol{x}_{\mathrm{n}}$ is defined by

$$\boldsymbol{x}_n = h\,\dot{\boldsymbol{m}}_n = \frac{\boldsymbol{m}_n - \alpha_n}{\beta_0}. \qquad (6)$$

Newton's method is used by most ODE solvers to solve equation (5). Variations of Newton's method that could be used can be found in [16].

3 Results

Two variants of the simple structure in Fig. 1 were considered: one where the two layers were ferromagnetically coupled (FM) and one where the layers were anti-ferromagnetically coupled (AF). Material parameters similar to Co were used, namely exchange coupling constant $A=30.0\times10^{-12}$ J/m, saturation magnetization $Ms=1400\times10^{3}$ A/m, but crystalline anisotropy $K=0$ J/m^3. To enable a not too-sluggish convergence to minima, the damping constant alpha was set to 0.5. The particle size was 400 nm x 200 nm x 9 nm, or 400 nm x 200 nm x 3 nm for each layer, and the cell size was 5 nm x 5 nm x 3 nm in x, y, and z-directions, respectively. The exchange field was computed using the six nearest cell neighbors.

To compare the speed of different methods, we look at the number of function (i.e. effective field) evaluations (NFEs). The field computation tends to dominate micromagnetic simulations and so NFEs provides a good first criterion for method speed ([16], [17]). Our simulations showed that for the FM spinvalve case the NFEs taken by the RKF54 Runge-Kutta method are almost double the number of the iterations taken by the implicit BDF solver from the CVODE package, 2.968913e6 and 1.66961e6 evaluations, respectively, for the same simulation time of 5.83160e-7 seconds (Table 1). The initial configuration of the magnetization was random. The external field strength in the simulations was varied, from 500 mT to 50 mT. In the simulations presented in this paper two values of the external field were used (500 mT and 250 mT). We used 500 field steps for the 500 mT range of the external field (the values of external field were from -500 mT to 500 mT and back again to get the hysteresis loop, and similarly 250 fields for the 250 mT case). For the AF spinvalve case with antiferromagnetic coupling the NFEs are 3.296803e6 for the RKF54 and 1.98188e6 for the CVODE cases, for the same simulation time of 6.46313e-7 seconds. So, considering NFEs as a measure of stiffness we conclude that both the FM and AF spinvalve simulations are stiff problems and implicit methods, such as BDF, should be employed. It should be mentioned that fewer time steps (iterations) means larger dt (time step), on average. Slight variations to the cell size or the size of the layers did not yield any significant differences in this comparison. Moreover, the maximum spin angle between neighboring cells was within the accepted limits, that is, less than 30 degrees (Fig. 2-3). Spin angle is referred to the difference of the magnetization vector of one cell to the next one [21]. For example, a spin angle of 180 degrees means that the magnetization at neighboring cells (in finite difference methods) points in exactly opposite directions.

	NFEs		Simulation Time
	CVODE	**RK**	
Spinvalve	1.66961e6	2.968913e6	5.83160e-7 s
Spinvalve AF	1.98188e6	3.296803e6	6.46313e-7 s

Table 1. The number of function evaluations for the two cases (spinvalve FM and spinvalve AF)

The error criterion used for step size control was a mixed one with (reduced) absolute error tolerance equal to 10^{-8} and relative error tolerance equal to 10^{-5} in both cases for both methods (CVODE and RKF54), so the comparison is fair. The stopping criterion, which determines when an applied field stage should be considered complete, was to require the maximum value of $|d\mathbf{m}/dt|$ across all spins to be below 0.01 degrees per nanosecond. The applied field was aligned at a small angle to the x axis, with maximum value 500 mT. Simulations with smaller values of the field (Fig. 2, Hmax=250 mT) were also run, but no differences in the behavior of the system were observed. The plots of the hysteresis loops were identical in both cases (CVODE and RKF54).

Simulations were also run for many of the example problems included with the OOMMF distribution, and none showed indications of stiffness. For example, in a run of muMAG standard problem 4a, the NFE count was 91045 for RKF54, which was significantly smaller than the CVODE NFE count of 370530 (simulation time 6.96755e-9 seconds). Moreover, the maximum value for the spin angle in both cases, RKF54 and CVODE, was 14.9866 degrees. A thorough investigation of many cases where nonstiff solvers showed better performance on nonstiff problems can be found in [16, 22]. However, this issue warrants further examination.

Conclusions

The spinvalve is a technologically important structure of much current interest. Accurate and efficient modeling of this structure is an important aspect of device design. In the present work we have examined two spinvalve structures, one having ferromagnetic and the other antiferromagnetic exchange coupling between the layers. In both cases we found that solving the Landau-Lifshitz-Gilbert equation of motion using a stiff (implicit) ODE solver required much less time than using an explicit solver. This leads us to the conclusion that strong stiffness appears in the studied systems, and we expect this to be the case in spinvalve structures generally. One obvious difference between spinvalve structures and the numerous other non-stiff systems that we have examined is that in spinvalves there are two magnetic domains (i.e., the two layers) that are in close proximity and yet are only relatively weakly exchange coupled, that is, the exchange coupling inside each layer is much stronger that the exchange coupling between the layers. Although more work is needed, we suspect that the stiffness in spinvalves originates from the weak coupling between the layers, in contrast to earlier work on other magnetic systems where numerical stiffness was found to arise from strong exchange coupling.

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List of figures

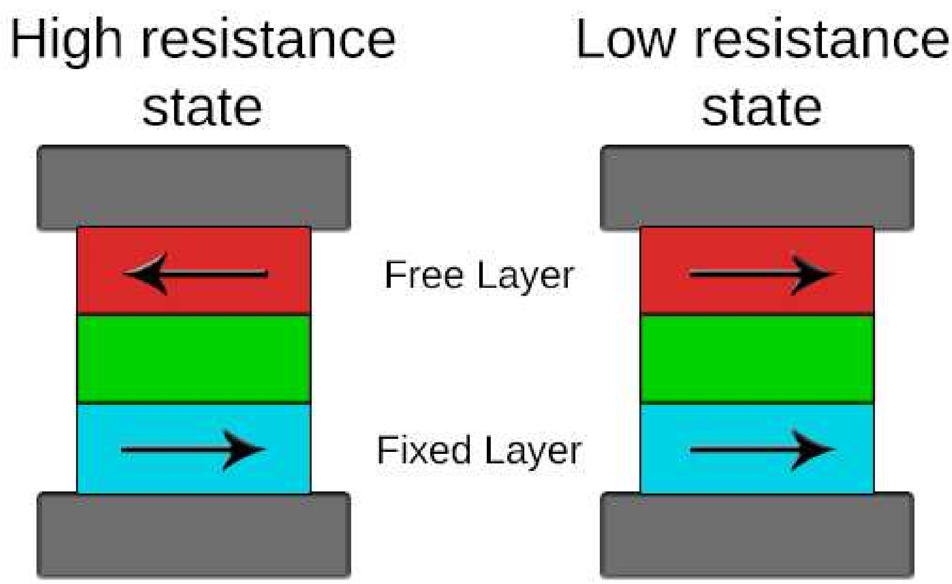

Fig. 1. A schematic diagram of a pseudo spin valve. The free layer is magnetically soft and the fixed layer is magnetically hard. When the magnetic layers are antiparallel the electrical resistance is higher than when they are aligned.

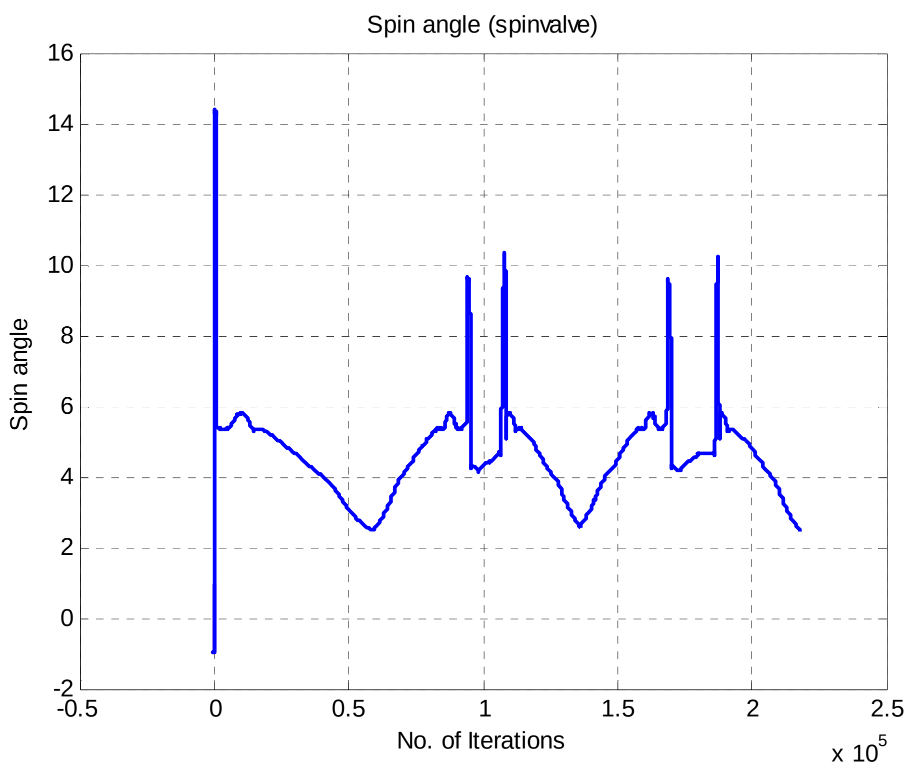

Fig. 2. The maximum spin angle for the spinvalve FM simulation with OOMMF/CVODE (Hmax=500 mT).

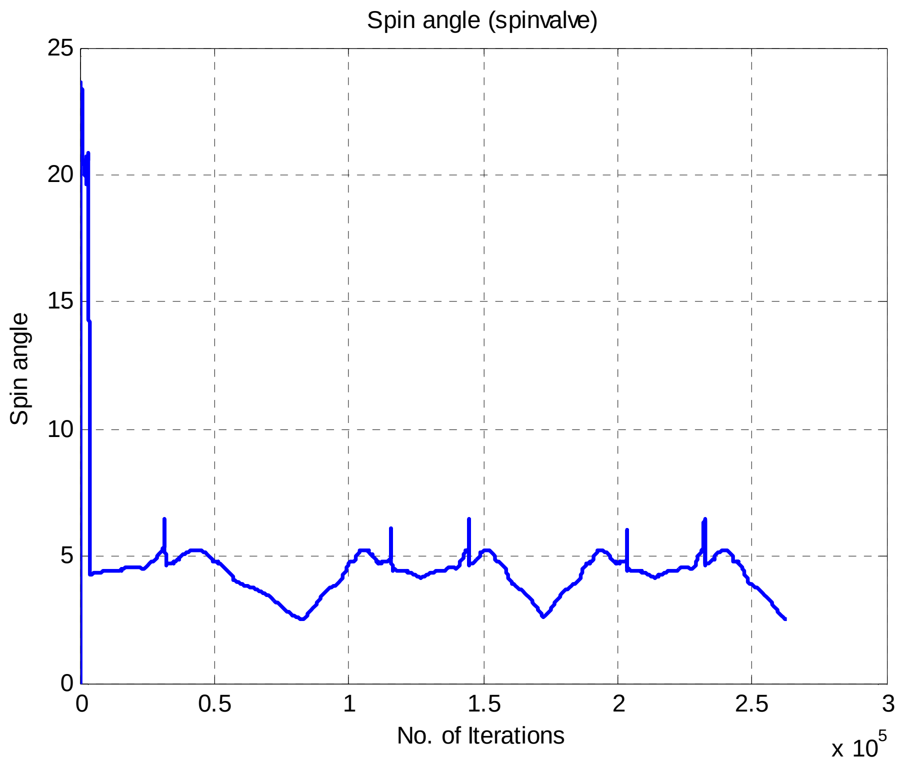

Fig. 3. The maximum spin angle for the spinvalve AF simulation with OOMMF/CVODE (Hmax=500 mT).

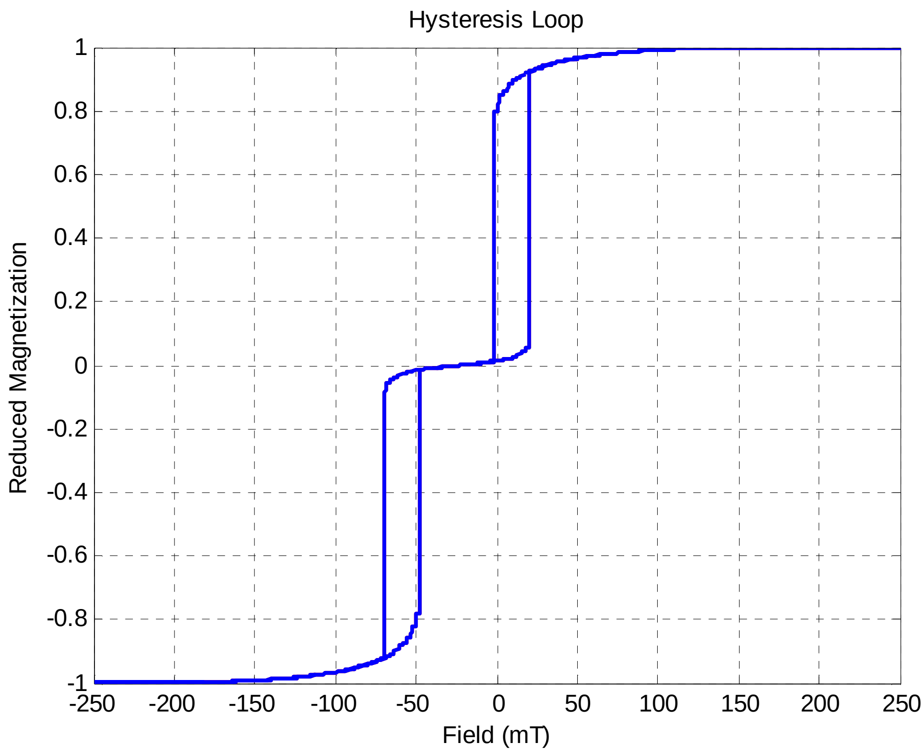

Fig. 4. Hysteresis Loop for Spinvalve Simulation FM with OOMMF/CVODE and OOMMF/RKF54 (Hmax=250 mT). The two curves overlap.

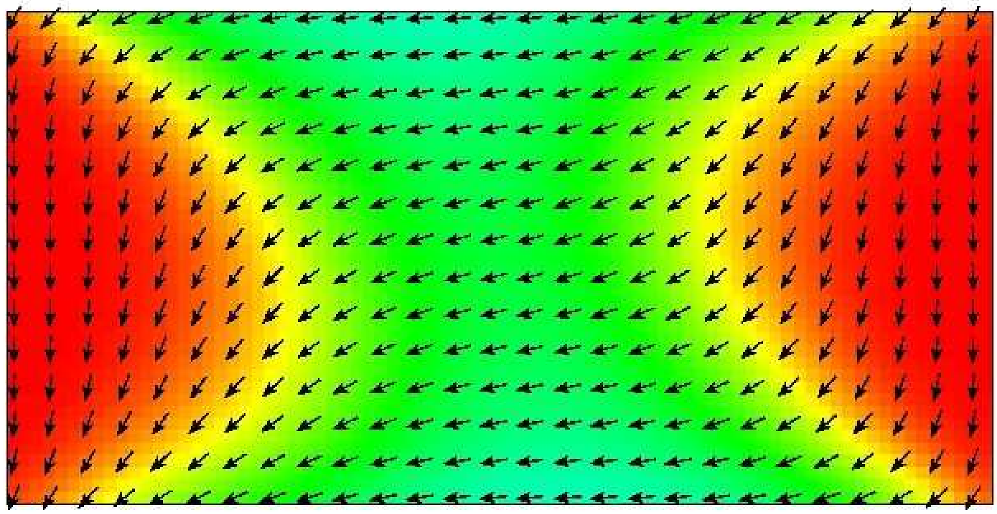

Fig. 5. A snapshot of the spinvalve FM simulation with OOMMF/CVODE (Hmax=250 mT).