Hard Simulation Problems in the Modeling of Magnetic Materials: Parallelization and Langevin Micromagnetics

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Abstract. We present recent results on two attempts at understanding and utilizing large-scale simulations of magnetic materials. In the first study we consider massively parallel implementations on a Cray T3E of the \(n\)-fold way algorithm for magnetization switching in kinetic Ising models. We find an intricate relationship between the average time increment and the size of the spin blocks on each processor. This narrows the regime of efficient implementation. The second study concerns incorporating noise into micromagnetic calculations using Langevin methods. This allows measurement of quantities such as the probability that the system has not switched within a given time. Preliminary results are reported for arrays of single-domain nanoscale pillars.

1. Introduction

To model realistic magnetic systems of interest in, for example, the magnetic recording industry requires that a number of difficult simulative problems be addressed. Preliminary results on two such problems are presented here.

Simulating metastable decay involves long characteristic time scales (the metastable lifetime), and several sophisticated algorithms have been developed for serial computers \([1,2,3]\). A common testbed for these algorithms is the kinetic Ising ferromagnet below its critical temperature, \(T_c\), which exhibits slow metastable decay after the reversal of the external magnetic field \([4]\). This model is appropriate for the study of highly anisotropic single-domain nanoparticles and thin films \([5]\). Even with these sophisticated algorithms the computer power required is enormous. Efficient computation requires these algorithms to be scalable and effectively implemented on massively parallel computers. We present an experiment on the parallelization of \(n\)-fold algorithms.

For less anisotropic magnetic materials, continuous-spin models should be simulated. To model metastable decay at finite temperature and measure time dependent quantities of experimental interest requires extensions of normal micromagnetic calculations. We report our first Langevin micromagnetic calculation, designed to model arrays of pillars grown with an STM technique \([6]\).

2. Parallelization of the \(n\)-fold way algorithm

We present and analyze a variation \([7]\) of the \(n\)-fold way algorithm \([1,2]\) for magnetization switching in the kinetic Ising model on a distributed-memory
parallel computer. The implementation of efficient massively parallel algorithms for Monte Carlo simulations is an interesting and challenging problem, which is one of the most complex ones in parallel computing. It belongs to the class of parallel discrete-event simulation (sometimes referred to as distributed simulation) which has numerous applications in engineering, computer science, and economics, as well as in physics [8]. These dynamics, which obviously contain a substantial amount of parallelism, were traditionally simulated on serial computers. Paradoxically, it is difficult to implement an efficient parallel algorithm to simulate them, mainly due to the fact that the discrete events are not synchronized by a global clock.

The kinetic Ising model, either with the standard integer-time updates or with Glauber's continuous-time interpretation, was believed to be inherently serial. Contrary to that belief, Lubachevsky presented a method for parallel simulation of these systems [7] without changing the underlying dynamics. Also, he proposed a way to incorporate the n-fold way algorithm, possibly giving further speedup. We implement his algorithm on the isotropic, square-lattice Ising model with periodic boundary conditions and Hamiltonian $\mathcal{H}= -J\sum_{\langle ij \rangle} s_i s_j - H \sum_i s_i$. Here $J>0$ is the ferromagnetic nearest-neighbor spin-spin interaction and $H$ is the external field. To study metastable decay, all spins are initialized in the +1 state, and we apply a negative magnetic field at constant $T < T_c$. In the corresponding serial algorithm we use the single-spin-flip Metropolis rates, where the probability to flip a spin is $p=\min\{1, \exp(-\Delta \mathcal{H})\}$. In the rejection-free n-fold way update scheme, a flip is always performed, and the time is incremented appropriately. One must then introduce the notion of spin classes which carry the state of the spin itself and its neighbors. In the above model there are ten classes, characterized by the number of spins in class $i$, $n_i$, and the flipping probability of a spin in class $i$, $p_i$. Since the classes are disjoint, $\sum_{i=1}^{10} n_i= L^2$, where $L$ is the linear size of the lattice. To perform an update, first a class is chosen according to the relative weights $\{n_ip_i\}_{i=1}^{10}$, then one of the spins in the class is picked with equal probability, $1/n_i$. Once the class information, in particular the $n_i$'s, have been updated, the time of the next update is determined. The time increment is a random quantity, given by $-\ln(r)L^2/\sum_{i=1}^{10} n_ip_i$, where $r$ is a uniformly distributed random number in $(0, 1]$. For integer-time updates, the only difference is that one must draw the time increments from a discrete geometrical distribution instead of the continuous exponential one [2].

To parallelize the above algorithm, the $L \times L$ lattice is spatially decomposed into $(L/l)^2$ blocks of size $l \times l$. On a parallel computer, each processing element (PE) carries an $l \times l$ block of spins and the number of PEs is $N_{PE}=(L/l)^2$. However, one cannot simply run a copy of the serial n-fold way algorithm on each PE without the possibility of corrupting the history of neighboring PEs. On each PE an additional class is defined which contains the spins on its boundary. The relative weight of this class is the number of spins on the boundary, $N_b=4(l-1)$, which clearly does not change during the simulation. The original tabulation
of spins is only used in the kernel of the block. Hence, \( N_b + \sum_{i=1}^{10} n_i = N \), where \( N = l^2 \) is the total number of spins in a block. The update scheme differs from the original (continuous-time) algorithm in the following steps: (i) if the spin chosen belongs to the boundary, then the updating PE must wait until its local time becomes less or equal than that of its neighboring PEs (at most two in two dimensions). Then the state of this spin may or may not change: its flipping probability is determined by the usual Metropolis rates. (ii) once an update is completed, the time of the next update is determined by the local time increment,

\[
\Delta t = -N \ln(r) \sqrt{\frac{N_b + \sum_{i=1}^{10} n_i p_i}{N_b}}.
\]  

Fig. 1 Speedup measurements for the parallel code as a function of the number of processing elements, \( N_{PE} \). (a) For fixed system size, \( L=512 \), the block size, \( l \), decreases with increasing \( N_{PE} \). (b) For fixed block size, \( l=64 \) and 128, the system size \( L \) is increasing with increasing \( N_{PE} \).

It is clear from the above algorithm that at any given (wall clock) moment different PEs generally have different local simulated times. The “wait until” control structure in (i), however, ensures that the information passed between neighboring PEs does not violate causality [7]. The above asynchronous algorithm is suitable for a continuous-time update scheme, but it can cause inconsistency when integer time is used. Then, to ensure the reproducibility of a simulated path, provided the same set of random seeds are used, explicit barrier synchronization should be incorporated (synchronous algorithm).

We implement the above versions of the \( n \)-fold way algorithm on the Cray T3E parallel computer at NERSC, using the Cray-specific, logically shared, distributed memory access (SHMEM) routines for message passing. The fast SHMEM library supports communication initiated by one PE, together with remote atomic memory operations. Without these features, it would be extremely inconvenient to code an algorithm for stochastic simulation on a distributed memory machine, where the communication pattern is completely un-
predictable. These characteristics outweigh the loss of portability of our code. Details on the implementation will be published elsewhere [9].

We note some inherently weak features, which are not related to the fast communication hardware of the parallel architecture. First, as a general guideline, the fewer communications needed, the better the performance of the parallel code. In our case, the probability to pick a spin on the boundary, which is ultimately followed by some communication, is greater than the surface-to-volume ratio. It is determined by the relative weights in the modified n-fold way algorithm, \( N_b / (N_b + \sum_{i=1}^{10} n_ip_i) \). With very small \( p_i \)'s this ratio can become close to 1, leading to more frequent message passing and idling as required by the “wait until” condition. Second, the average time increment in Eq. (1) is not bounded by \( p_{\text{min}}^{-1} \) as in the serial n-fold way algorithm, but by

\[
\langle \Delta t \rangle_{\text{max}} = \frac{1}{N_b/N + p_{\text{min}}N_k/N} < \frac{l^2}{4(l-1)},
\]

where \( N_k \) is the number of spins in the kernel. Hence, however small the flipping probabilities, the average local time increment is limited by approximately \( l/4 \). Consequently, reasonable performance requires \( lp_{\text{min}} > \sim 1 \).

We tested the scaling of the code (both asynchronous and synchronous versions) up to 256 PEs at \( T=0.7T_c \) and \( |H|/T=0.18 \), in two different ways. First, the system size is kept constant (\( L=512 \)), and we divide it into smaller and smaller blocks (Fig. 1a). Second, we keep the block size fixed (\( l=64, 128 \)), and study larger systems by increasing the number of blocks (Fig. 1b). We determine the efficiency and speedup by comparing with the serial n-fold way performed on one T3E node. The results reflect the features discussed in the previous paragraph. In the first case we observe poor scaling, due to drastically decreasing average time increments and a slightly decreasing utilization ratio. In the second case, the average time increments are not affected while the utilization saturates, leading to reasonably good scaling. The larger the block size, the better the performance. For the continuous time, asynchronous algorithm, with \( l=128 \) and using 256 PEs, the speedup is 100. It can be systematically improved by taking larger \( l \) values. However, the memory of a PE is not unlimited: the largest cell size that we could allocate in a T3E node was \( l=1400 \). The asynchronous algorithm suits this distributed-memory architecture best.

The practical applicability of our implementation is obviously driven to large systems. The narrow regime of efficient implementation is due to the introduction of a special class in the n-fold way algorithm which “shields” the blocks from each other. The algorithm avoids rollbacks, but pays a large price: it looses the most important feature of the serial n-fold way algorithm — the arbitrarily large time increments at arbitrarily low temperature and field. The only way to preserve the advantage of the original n-fold way algorithm is to apply it directly on each block, together with a complex rollback procedure [10]. Work is in progress to incorporate it in our simulations of metastable decay.
Fig. 2 A single snap-shot of a Langevin micromagnetic calculation for magnetization reversal in a square array of Ni pillars that are 200 nm apart, 200 nm tall, and have a diameter of 40 nm. Each pillar is discretized using 5 lattice points. (The vertical scale of this figure is enhanced compared with the horizontal scale for clarity of presentation.) The temperature is 300 K, the spins are initially up, and the applied field is down with a magnitude of 1225 Oe. This is at a time of 14 nsec following the reversal of the field. The integration time step is $\Delta t=1$ psec. Note that this looks very different from a coherent rotation mode of spin reversal.

3. Langevin Micromagnetics

In order to simulate systems for which the Ising model is not a faithful representation, we have programmed a Langevin micromagnetics code similar to that reported in [11]. With a phenomenological damping parameter $\alpha$, and classical spins of constant length given by the bulk saturation magnetization $M_s$, at each lattice site $i$ we have a scaled magnetization $\vec{m} = \vec{M}_s/M_s$. The standard Ginzburg-Landau-Lifshitz micromagnetic equation [12,13] is

$$\frac{d\vec{m}_i}{dt} = -\frac{1}{1 + \alpha^2} \vec{m}_i \times \left( \vec{h}_{i,\text{eff}} + \alpha \vec{m}_i \times \vec{h}_{i,\text{eff}} \right). \quad (3)$$

The scaled field at each site, $\vec{h}_{i,\text{eff}}$, contains contributions from terms including the dipole-dipole interaction, the exchange interaction, the interaction due to crystalline anisotropy, the applied field, and a scaled noise term proportional to the the Langevin fields $\zeta(t)$ [12,13]. In our case the Langevin noise term $\zeta$ and the integration time step $\Delta t$ are related by $\zeta \propto \sqrt{\Delta t}$, which we think is more physical than the $\zeta \propto 1/\sqrt{\Delta t}$ of [11]. Even though the set of equations used in this Langevin micromagnets simulation are approximations to the actual equations [14], the approximation should be reasonable well below the critical temperature. In order to keep the length of the $\vec{m}_i$ constant, we have used
a fourth-order Runge-Kutta algorithm. Fig. 2 shows the type of simulations [15] that can be performed for arrays of magnetic pillars that can be built and measured experimentally [6]. The importance of the finite temperature thermal fluctuations and the rotation mode, which is very different from that of uniform rotation, can be seen in this figure. Note that with standard time-independent micromagnetic calculations there would be no magnetization reversal, since the strength of the applied field is smaller than that of the nucleation field.

Acknowledgements. Special thanks to M. Kolesik for invaluable discussions and to R. Gerber at the NERSC consulting group for helpful hints on debugging the parallel code. This research was supported by NSF Grant No. DMR-9520325, FSU-SCRI (DOE Contract No. DE-FC05-85ER25000), computer time allocated on the NERSC T3E by the DOE, and FSU-MARTECH.

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