Spreadsheet analysis of stability and meta-stability of low-dimensional magnetic particles using Ising approach – accepted version

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Modeling hysteresis behavior, as it can be found in a broad variety of dynamical systems, can be performed in different ways. An elementary approach, applied for a set of elementary cells, which uses only two possible states per cell, is the Ising model. While such Ising models allow for a simulation of many systems with sufficient accuracy, they nevertheless depict some typical features which must be taken into account with proper care, such as meta-stability or the externally applied field sweeping speed. The article gives a general overview of recent results from Ising models from the perspective of a didactic model, based on a 2D spreadsheet analysis, which can be used also for solving general scientific problems where direct next-neighbor interactions take place.

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Introduction

Random number generators and utilization of Monte Carlo methods for solving scientific problems are known for many decades [1]. In physics of magnetism, this type of methodology is represented mainly by Ising models, and the main characteristic is revealed via hysteretic behavior. However, hysteresis loops occur in various problems in science and technology, from the magnetic field dependent behavior of a ferromagnet to physical phase transitions or economics. Importantly, an easy theoretical description of such hysteresis loops can be based on the Ising model [2], in which each variable can vary between two values +1 and -1, with the variables interacting with their (nearest) neighbors. For the special case of the external field $H = 0$, the two-dimensional Ising model has been solved by Onsager [3], while for other cases, analytical solutions are not yet known. Computational solutions of Ising models are described in several books, describing modeling principles and Monte Carlo algorithms, often with sample codes in C++, Java, True Basic and / or Fortran code [4-7]. For readers without programming knowledge, however, these examples may be difficult to apply and modify. Oppositely, the Java applets dealing with Ising systems which are available in the internet (e.g. [8-10]) have normally less degrees of freedom and do not necessarily allow examining (or even changing) the source code, so that students do not have the chances to understand the simulated systems in detail.

Thus our model tries to combine the advantages of both approaches, being simple with respect to programming and allowing students to change all parameters used in the model. In this way, the article aims at serving as an introduction for undergraduate students, showing the possibilities and limits of such a simple model by testing one of the crucial features of Ising models, i.e. stable and meta-stable states.

Principally, the following effects can be expected to be found in an Ising model, described frequently in terms of magnetism, always intended to work for intense interactions

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between the magnetic moments, leading at sufficiently low temperatures to a spontaneous macroscopic cumulative order. For high temperatures an unordered metastable phase with vanishing macroscopic order can occur. Both phases are separated by a critical temperature, i.e. the Curie temperature.

However, for low intensity external fields, the Ising model is known to produce meta-stable states even at low temperatures. Such metastable phases are related to the energy state, which does not reach a global minimum, but it can persist for times which are many orders of magnitude longer than the system's characteristic timescales [11]. Cirillo and Lebowitz found such a meta-stable phase using Monte-Carlo simulations after switching on a small positive magnetic field after negative saturation – this meta-stable state occurred by nucleation of a critical droplet in one corner of the system [12]. Similar results have been found by Schonmann for the case of vanishing temperature, calculated by Metropolis dynamics for a two-dimensional ferromagnet with nearest-neighbor interaction [13]. Rikvold *et al.* used Monte-Carlo simulations to examine the escape processes from such a meta-stable state in dependence on the system size and the applied field intensity. Depending on these parameters, the transitional decay was dominated either by a single droplet or by several droplets at nucleation sites [14]. Numerical calculation of meta-stable free energies in a two-dimensional Ising ferromagnet by the so-called Constrained-Transfer-Matrix method has been used by Günther *et al.* to prove the agreement between the imaginary parts of the free energies with a field-theoretical droplet model [15]. Godrèche and Luck have found differences between single-spin-flip dynamics of ferromagnetic Ising models at zero temperature, leading either to phase ordering by domain growth or to dynamical systems with many attractors [16]. For a rapid cooling process from infinitely high temperatures to zero temperature, Spirin *et al.* found that small systems most often reached the (ferromagnetic) ground state, but with a certain probability could evolve into frozen, static stripe-domain state. Larger systems,

however, reached a set of meta-stable states instead which was not left on very large timescales [17]. Similar results were found by Lipowski before who attributes phase ordering anomalies in two and three dimensions to scaling behavior [18]. In a one-dimensional Ising model with short-ranges three-spin interactions, Kisker *et al.* found a glass-like state of a large number of meta-stable configurations which are stable against singular spin-flips [19].

Additional to theses examinations of the escape from a meta-stable configuration, calculations and Monte-Carlo simulations have been used to investigate the dependence of the hysteresis loop area and the coercive fields on the switching speed / frequency of the external magnetic field. While Monte-Carlo simulations have shown a power law correlation between the hysteresis loop area and the frequency [20,21], classical nucleation theory resulted in a logarithmic dependence of the hysteresis loop area on the frequency [22]. These findings depend strongly on the lattice dimensions as well as on the frequency range [23]. Detcheverry *et al.* calculated the number of meta-stable states inside a hysteresis loop, finding very complex results, depending on several parameters [24]. For the case of a zero-temperature random-field Ising model, in three or more dimensions, Sethna *et al.* found a transition between a continuous hysteresis loop and a discontinuous loop with a jump, depending on the disorder in the system [25].

While the above mentioned examinations are based either on pure theoretical calculations or on Monte-Carlo simulations, this article examines meta-stability and hysteresis loops in a simple Ising model [26,27] which is implemented by a spreadsheet analysis program, such as Microsoft Excel®, providing imaging of cells under evolution. This model enables test of the influence of different parameters on the hysteresis shape and coercive field, additionally allowing for static observations. In order to avoid the restriction on ferromagnetic hysteresis, the model avoids magnetic terms strictly and instead uses generalized variables and parameters.

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Since even the sophisticated approaches mentioned above give several answers, but also leave some questions open, it is important to test whether the simple spreadsheet program gives similar answers, according to meta-stability and hysteresis loop area, or if any new problems occur which are not known from established calculation models and simulation systems.

Experimental

In the Microsoft Excel® based spreadsheet analysis program "MagCalc", an elementary system consisting of 16 x 16 cells (the dimension can be enlarged or reduced) contains two possible discrete states +1 or -1 (up or down) per cell. Interactions are restricted to the four nearest neighbors as in usual Ising models. The overall "magnetization" is calculated by averaging over several, for example 10, elementary systems, with the saturated magnetization normalized to values of ± 1.

The main quantity guiding a given system under study is the total energy. Looking at the energy state of a given local cell, it is assumed that its local energy depends on four factors of interaction with the surrounding cells, similar to the Random Field Ising Model [28-31]. Namely, these are: energy resulting from the cell interaction with the four nearest neighbors (1), the random energy of thermal origin (2), and the energy of an externally applied magnetic field (3). Additionally, the recent state of cells depends dynamically on the speed of changes of the externally imposed magnetic field (4). To express the parameters above quantitatively, we can introduce the following respective parameters:

1) the single cell interaction strength w_{cr}, which can be taken from the <0, 1> range. The maximum value of 1 describes capability of switching independently from neighbors, while values smaller than 1 mean increased influence of the four neighbors;

2) the thermal probability or "temperature" P_{wm}, with the value 0 for the temperature factor completely excluded, with (0 - 0.5) period for a ferromagnetic-like particle, 0.5 for the transient, paramagnetic case, and the higher values defining an antiferromagnetic behavior of the elementary system, for example the 16 x 16 one, possessing a chessboard-like structure as lowest-energy state;

3) the external field intensity H_{ext}, having ± 1 maximum values. The maximum values provides an energy which is stronger than any other interaction energy in the system itself;

4) and the field sweeping speed v_s.

This approach follows the classical Metropolis method (described in detail in [7]). Each new configuration is created from a previous step by calculating a transition probability which is dependent on the energy difference between original and new state. Thus, in a so-called Markov chain of states, each state follows from the preceding state. One Monte Carlo step consists of choosing an initial state and an initial site, deciding – based on the cell interaction strength and a random number generated in each step – whether a cell content should be flipped or not, and going on to the next site in the same line (after the end of the line, going on to the next line) until all places in the system have been considered. Afterwards, the same process is performed for the next Monte Carlo step.

Fig. 1 shows a reversal sequence for $w_{cr} = 0.1$ and $P_{wm} = 0.1$, starting from negative saturation (all cells red), after switching on a small positive external field $H_{ext} = 0.001$. Snapshots are taken after 1 step, 10, 50, 100, and 1000 steps. The reversal process occurs via nucleation and growth of domains. It should be mentioned that due to the relatively large "temperature" P_{wm}, the reversed areas change during all states, opposite to the above mentioned descriptions of the process for $T = 0$.
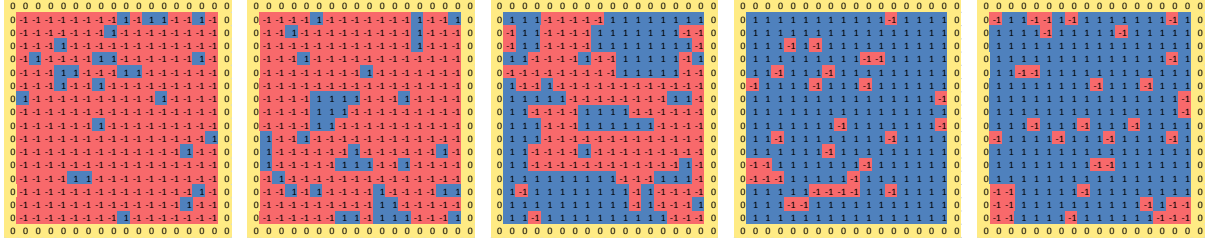
Fig. 1: Reversal for $w_{cr} = 0.1$ and $P_{wm} = 0.1$ from negative saturation (all cells red) due to a small positive external field $H_{ext} = 0.001$ for 1 step, 10, 50, 100, and 1000 steps.

This process is depicted in Fig. 2 for different values of w_{cr} and P_{wm} in terms of the overall "magnetization" understood as algebraic sum carried out over all single cells states. For relatively large reverse fields of $H_{ext} = 0.1$, the reversal process occurs in all cases in a few steps only. For middle reverse fields of $H_{ext} = 0.01$ or 0.001, this statement is also true; for the higher "temperature" ($P_{wm} = 0.1$, upper panels), however, positive saturation is not reached. The "magnetization" stays on a lower level than 1, the value of which depends also on the influence of the neighbor cells w_{cr}. For even smaller external fields of $H_{ext} = 0.0001$ or $H_{ext} = 0.00001$, the reversal is only possible on the timescales (measured by numbers of simulation steps) under examination for a high weight w_{cr} of the switching energy, i.e. a small influence of the neighbor cells. For small w_{cr}, i.e. strong "ferromagnetic" interaction between neighboring cells, and low "temperatures" P_{wm}, the original state of negative saturation is frozen and can only be reversed by relatively large external fields. Another interesting finding is that strong fluctuations occur for relatively high "temperature" and relatively low coupling between neighboring cells (Fig. 2, upper left panel), depicting an instable state.
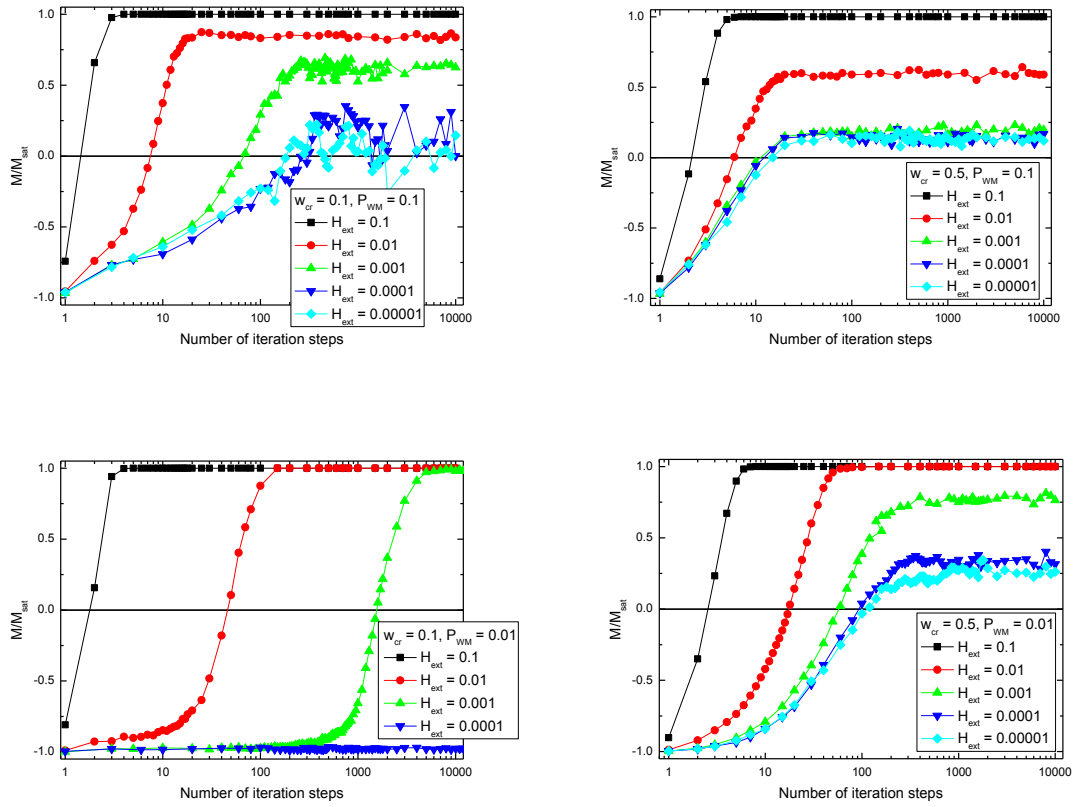
Fig. 2. Time-dependent "magnetization" for diverse external fields H_{ext} after negative saturation, calculated in a 2D elementary system of 16 x 16 cells for different values of the weight w_{cr} of the switching energy of a cell and the "temperature" P_{wm}.

While these findings agree with experimental experience, the same tests have been performed for larger and smaller 2-dimensional systems. Fig. 3 shows the results for an elementary system consisting of 64 x 64 cells. Principally, the results agree with those from the smaller system. It can be recognized that the larger particles show more stable results. Additionally, the number of steps necessary for the magnetization reversal is slightly changed, without the possibility to define a precise trend.

For the smaller 4 x 4 cell system (the elementary particle) depicted in Fig. 4, the particles become correspondingly less stable. While for smaller external fields the systems start fluctuating around zero "magnetization", the "frozen" state for small w_{cr} and low P_{wm} can

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here also be forced to leave the saturated state by very small external fields (Fig. 4, lower left panel).
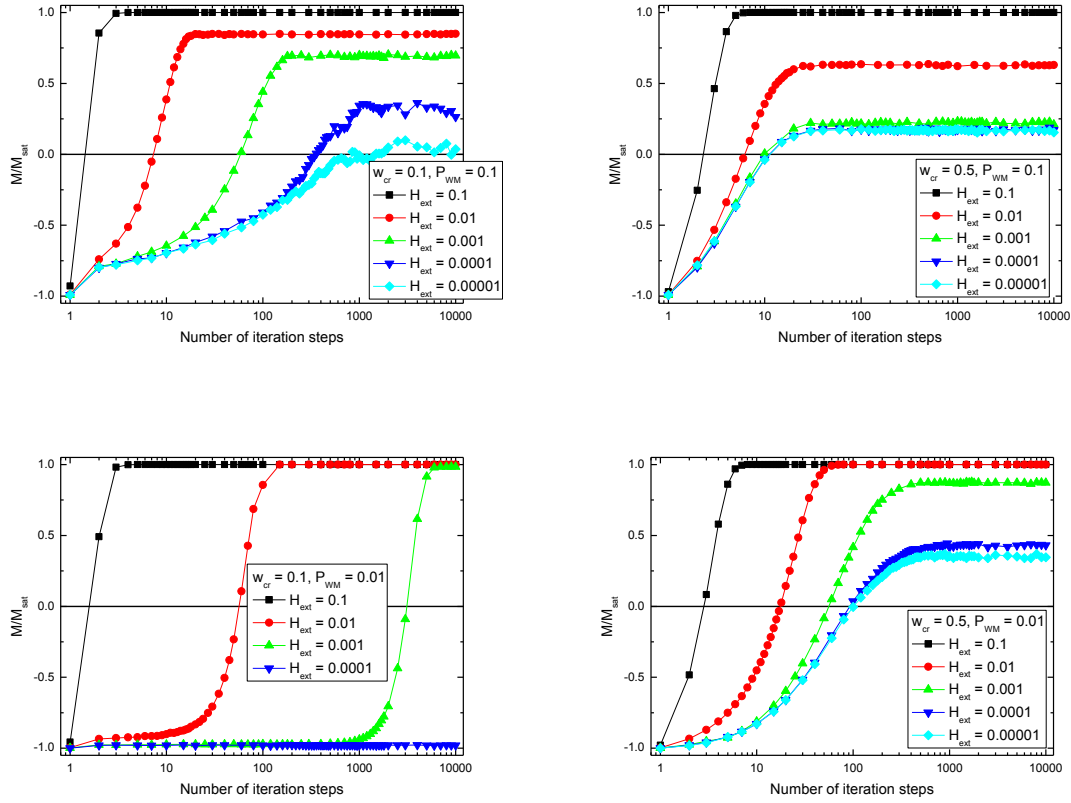

Fig. 3: Time-dependent "magnetization" for diverse external fields H_{ext} after negative saturation, calculated in a 2D elementary system of 64 x 64 cells for different values of the weight w_{cr} of the switching energy of a cell and the "temperature" P_{wm}.

In order to test whether these findings can be transferred into 3-dimensional systems, Fig. 5 shows the results for Ising particles of dimensions 16 x 16 cells x 5 layers. Opposite to the 2D systems, the higher value of w_{cr}, i.e. the lower coupling between neighboring cells, results in an increased possibility to "de-magnetize" the system, i.e. to result not in a (nearly) saturated state but behave more like a "paramagnetic" particle. This can be explained by the increased number of nearest neighbors in the 3D system which modifies the influence of the

parameter w_{cr} on the time-dependent behavior of the system. Nevertheless, the 2D and the 3D particles behave quite similarly.
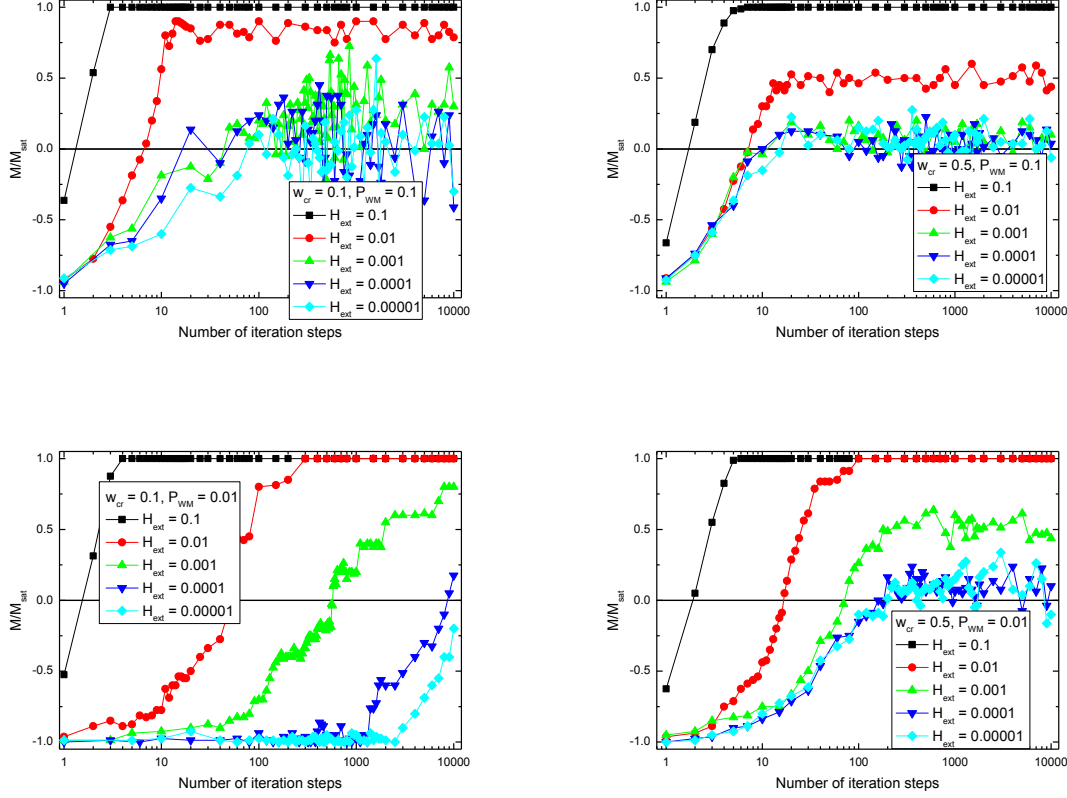

Fig. 4: Time-dependent "magnetization" for diverse external fields H_{ext} after negative saturation, calculated in a 2D elementary system of 4 x 4 cells for different values of the weight w_{cr} of the switching energy of a cell and the "temperature" P_{wm}.

Another interesting question, taking into account that the Ising calculation should be able to model the behavior of real systems, deals with the calculated coercive field and hysteresis loop area, dependent on the field sweeping speed. Fig. 6 depicts the results of calculations for a 2D and a 3D particle, performed with different field sweeping speeds, i.e. different field step width. Obviously, the hysteresis loop area and coercive field depend strongly on the field sweeping speed, with more significant modifications in the 2D system. As described above, this behavior is typical for Ising systems. However, it must be taken into

account that students working with such a program cannot be expected to know about these effects – and that they should be informed about this special property of the system under investigation.
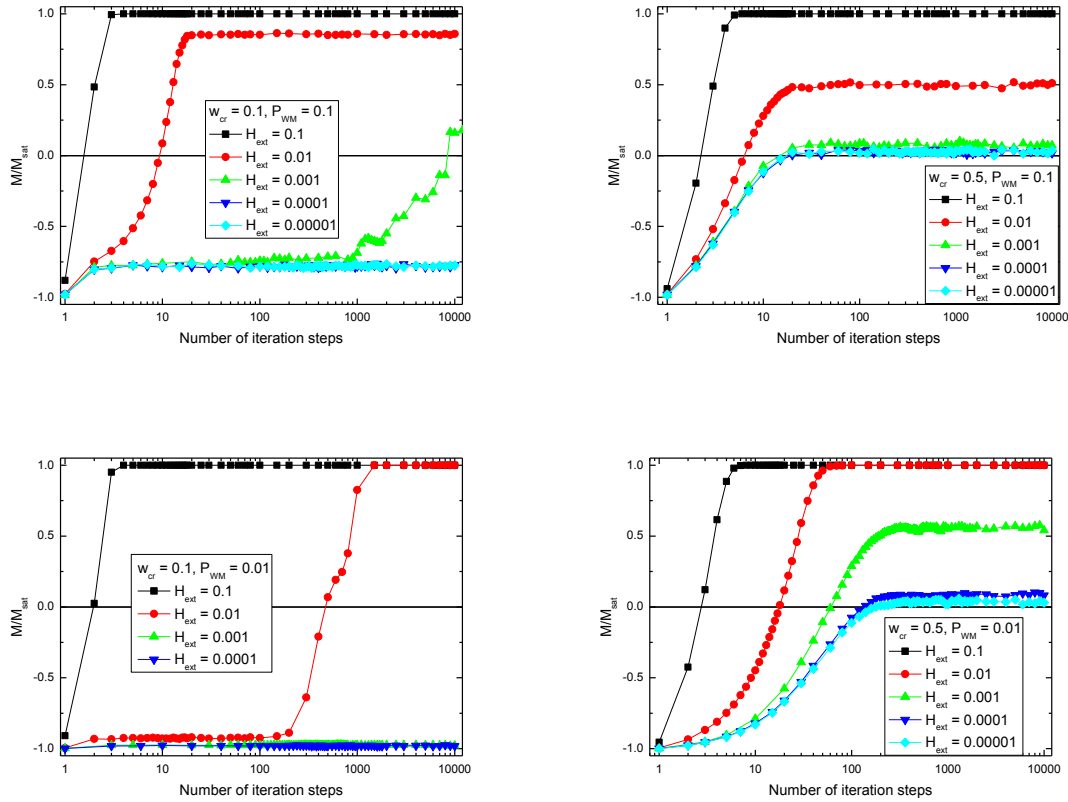

Fig. 5: Time-dependent "magnetization" for diverse external fields H_{ext} after negative saturation, calculated in a 3D elementary system of 16 x 16 cells x 5 layers for different values of the weight w_{cr} of the switching energy of a cell and the "temperature" P_{wm}.

In spite of these typical Ising simulation problems, the simple spreadsheet based simulation program offers the possibility to examine reversal processes in dependence on the coupling between neighboring cells, temperature, system size and external field, to observe in the step-by-step mode the interactions between all influences on each single cell, and thus to gain a certain feel for the microscopic processes in systems which show a hysteretic behavior on a macroscopic scale. Opposite to more sophisticated theoretical models and Monte-Carlo

simulations, the simple "MagCalc" can be easily understood and used by students – and allow researchers to model systems without more complicated interactions in a fast way.
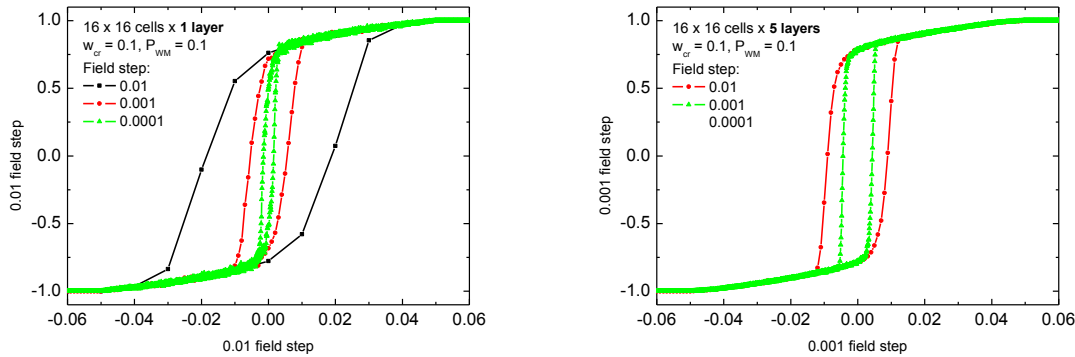

Fig. 6: Hysteresis curves, calculated in a 2D and a 3D systems for different field sweeping speeds, depicted by different field step widths.

Conclusion

The article gives an overview of the recent research results with respect to simple and more sophisticated Ising systems, using different parameters and dynamical effects in a newly developed simple Ising spreadsheet model. Thank to this it was possible to examine characteristic features of systems, such as meta-stability and field sweeping speed dependent hysteresis loops. The model has been found to reproduce the proper physical features. While these special features must be communicated to students using the program to gain an insight into Ising systems, the simulations can easily be employed in self-learning and research efforts to study scientific problems related to next-neighbor interactions.

Acknowledgements

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