Simulation of nano-scale magnetic systems

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Nanoscale magnetism is the key technology in a growing field of applications ranging from magnetic data storage to biomedical application. The design of materials and devices heavily relies on modeling and simulation: (1) Ideas based on intuition or theory can be tested. (2) Devices can be substantially improved by optimization. (3) Virtual design based on computer models reduces the costs. In this talk we will give two examples. One from magnetic data storage and one in cancer therapy. Common to both examples is that traditional finite element simulation for magnetization dynamics is combined with other modern simulation techniques. The underlying concept is the continuum theory of micromagnetism which describes magnetization processes at a length scale ranging from the nanometer scale to several micrometers. The micromagnetic equations describe the magnetization as function of time and space.

Optimization tools for bit patterned recording

Finite element based numerical optimization can help to design nano-magnet devices ranging from storage to sensor and to microwave generators. As an example we will show its application for minimizing the write error rate in magnetic data storage. In magnetic data storage the magnetic units that store single bits reach dimensions below 10 x 10 nm^2. The time to write a single bit is a fraction of a nano-second. Bit patterned magnetic recording, where each bit is stored on a single magnetic island that is predefined on a substrate require a precise engineering of the magnetic elements. The timing and the spatial distribution of the write field has to be optimized so that it the target bit is addressed and successfully written. Numerical optimization techniques are applied to design the optimal head and media structure, so that the bit error rate is minimized [1]. The solution of the micromagnetic equations for the key components of a hard disk give a detailed account of how bits are written onto the magnetic islands. The driving force is the magnetic field created by the current through the coils. This field changes the magnetization in the write head which in turn creates the write field that switches the bits on the data layer. A hybrid/finite element boundary element method is applied for the computation of the interaction between the writer and the data layer. The write field profile can be optimized by changing the shape of the pole tip and the shield geometry. Figure 1 shows the simulation cycle. The writer geometry is parameterized. For a given set of parameters the finite element mesh is generated, the recording process is simulated and an objective function is evaluated. A optimization tool based on a response surface method suggests a new set of geometrical parameters, which describe the pole tip and the shield geometry. These parameters are feed into the mesher for the next step of the optimization cycle.

Design of mircofluidic chips for biomedical applications

In the field of biomedicine magnetic beads are used for drug delivery and to treat hyperthermia. If the surface of the beads a functionalized with antibodies magnetic beads can be used for immuno-magnetic cell capturing and cell sorting. Alternatively, magnetic beads can be used to create well defined structures in a microfluidic chip. If formed by magnetic beads, microposts arrays are tunable: The size, the position, and the shape of the nano-posts can be controlled by an external magnetic field [2]. By changing the distance between the chains it is possbile to switch from immuno-magnetic cell capture to mechanical filtering during in-situ operation of the microfluidic device. On application of microfluidic chip is the isolation of circulating tumor cells from peripheral blood [3]. The proposed tunable chip combines affinity capture and size capture of circulating tumor cells in a single, flexible device. We simulate the arrangement of magnetic beads into nano-post arrays using micromagnetics, discrete particle dynamics and fluid dynamics. The balance between the magnetic force and the drag force leads to the formation of nano-chains as shown in Figure 2. Once the structure has been formed, the Lattice-Boltzmann method with immersed elastic cell models is used, in order to simulate the interaction of cells with the nano-posts. Simulations give design guidelines such as the optimal gap size between the nano-posts for high yield cell enrichment.

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References

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Figures

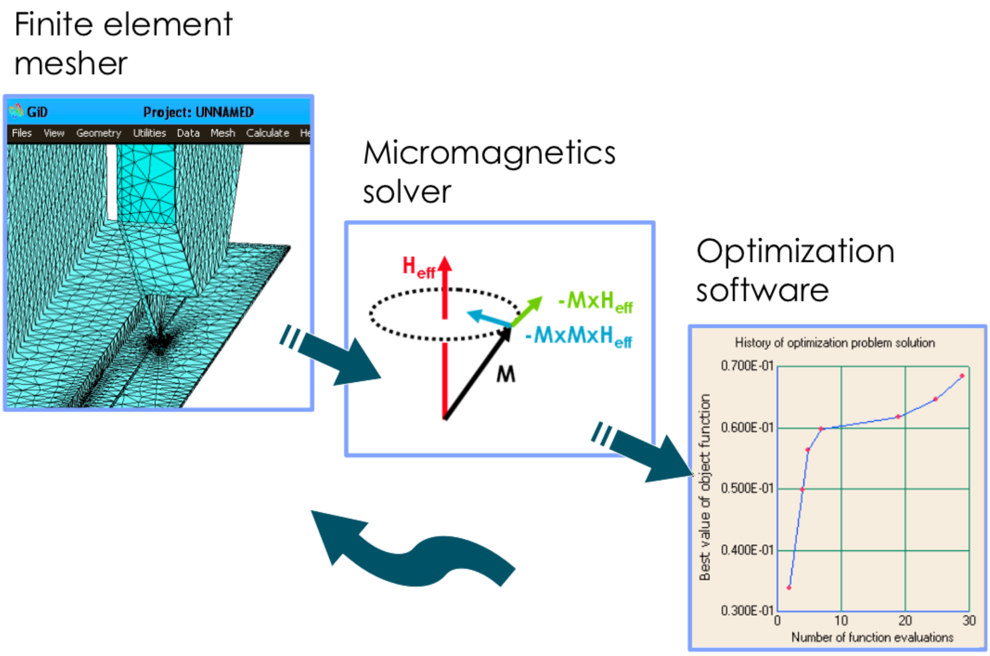

Figure 1. Numerical optimization of the head geometry and media properties for ultra-high density magnetic recording. Finite element micromagnetics together with a global optimization tool provide design guidelines that reduces the bit error rate.

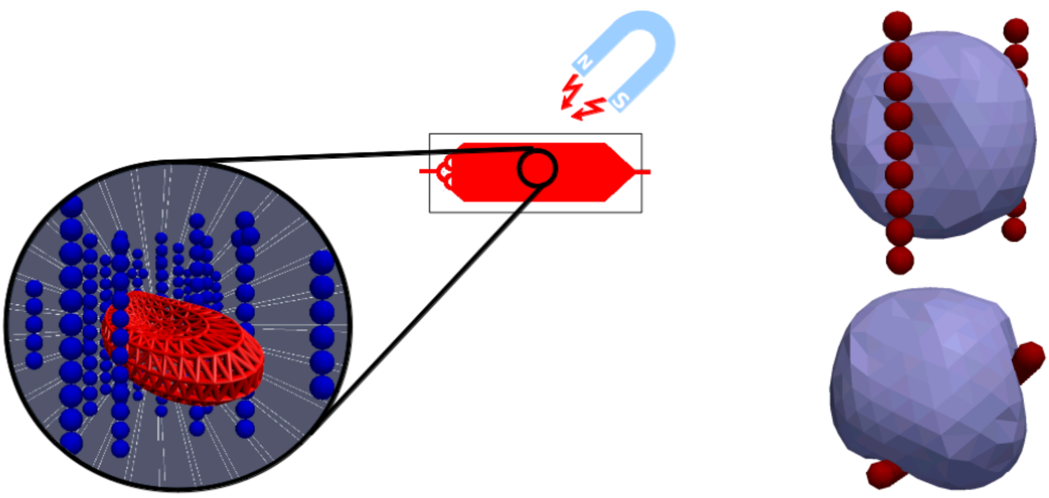

Figure 2. Simulation of magnetic bead arrangement and cell flow in microfluidic chips. Left: Microfluidic chip based on a grid of self-organized magnetic beads. Red blood cells are flexible enough to pass the gap between the nano-posts. Right: Circulating tumor cells are larger and stiffer than blood cells and get trapped in the magnetic bead array.