Compression of boundary element matrix in micromagnetic simulations

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Motivation

The electrodeposition from lead salt solutions onto graphite substrates allows for the fabrication of Pb mesostructures with few defects and smoothly faceted faces [1]. Another striking feature is that many different morphologies can be grown just by adjusting the potential between the electrodes (see Figure 1) . The dimensions of those mesostructures (100 – 1000 nm) lie in the range of different characteristic length scales for ferromagnets (e. g. the ferromagnetic domain size). As a consequence one expects the physical properties of ferromagnetic mesostructures to be very sensitive to their size and shape. Therefore the extension of the method to the growth of ferromagnetic metals and alloys seems to be a very promising research direction. Finite element simulations based on the theory of micromagnetism are a standard tool for a theoretical description of ferromagnetic nanostructures. In order to be able to do corresponding simulations on the relatively large mesostructures one needs to modify this approach.

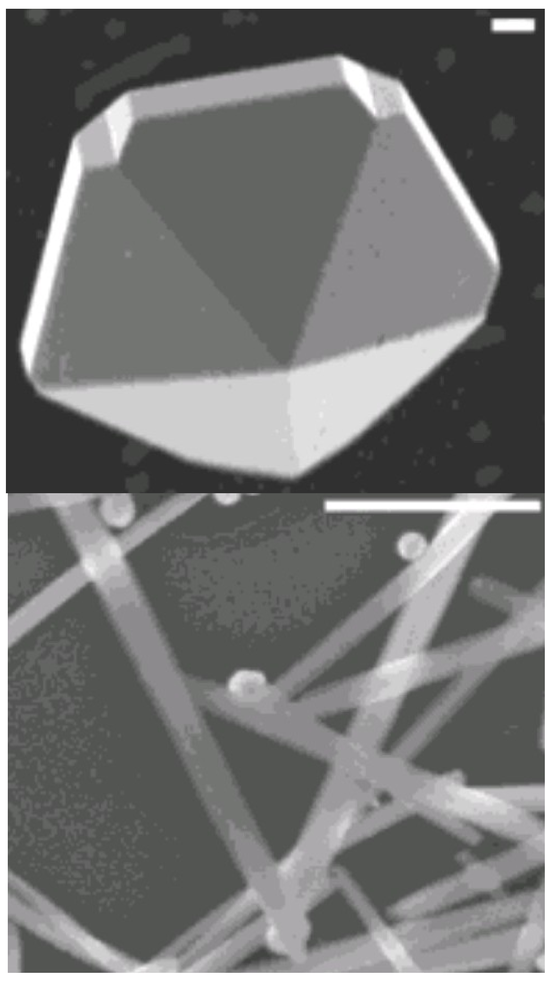


Figure 1: Novel Pb mesostructures produced with the electrodeposition method. The length of the scale bar is 500 nm. Top: decahedron, Bottom: nanowires

Numerical Approach

In micromagnetism the scalar magnetic potential Φ needs to be regular at infinity, so that $\Phi(\vec{r}) \to \frac{1}{|\vec{r}|}$ *for* $|\vec{r}| \to \infty$ applies. Consequently a pure finite element solution requires a mesh over a region which goes far beyond the magnetic domain. This can be avoided by using the hybrid finite element-boundary element method [2]. The main trick of the method is to split Φ into a sum of two auxiliary potentials Φ_1 and Φ_2, which can be solved on a finite element mesh within the magnetic region. However, in order to obtain the boundary conditions for Φ_2 one needs to calculate a surface integral of the form

$$\Phi_2(\vec{r}) = \oint_{\partial V} \Phi_1(\vec{r}\,') \nabla \frac{1}{|\vec{r} - \vec{r}\,'|} \vec{n}(r')\, dS \qquad (1)$$

$\Phi_2(\vec{r})$ is equal to the surface integral over the product of $\Phi_1(\vec{r}\,')$ and the normal derivative of the Green's function. The discretization on a surface mesh yields:

$$\vec{\Phi}_2 = \underline{\underline{B}}\, \vec{\Phi}_1 \qquad (2)$$

The boundary element matrix $\underline{\underline{B}}$ is generally dense and just depends on the geometry of the problem.

Hierarchical matrices

The size of the boundary element matrix $\underline{\underline{B}}$ is of the order $O(m^2)$, where m is the number of surface nodes. In order to investigate mesostructures with a large surface, one needs to compress $\underline{\underline{B}}$. For this compression we use the library hlib [3], which is based on hierarchical matrices. A hierarchical matrix is usually represented in a quad tree structure, i.e. each matrix block is subdivided into four sons until the block itself is a leaf. The set of all leaves represents the approximation of our matrix. There are admissible and non-admissible leaves.

Admissible leaves are the white-green blocks of Figure 2. They can be stored in the data-sparse representation of Figure 3. Non-admissible leaves are the red blocks of Figure 2. They are stored in the full matrix format. Whether a block is admissible or not is determined by geometrical arguments. The row and column indices of a certain block of $\underline{\underline{B}}$ represent the interaction between Φ_1 and Φ_2 for two regions in the integration regime of equation (1). In case the regions are well separated the kernel in equation (1) will be sufficiently smooth, so that one can expand it. Such an expansion makes the approximation of matrix blocks by a data-sparse format of Figure 3 possible.

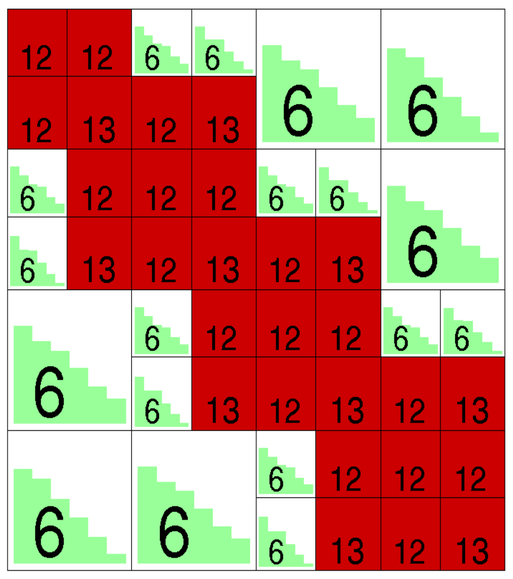
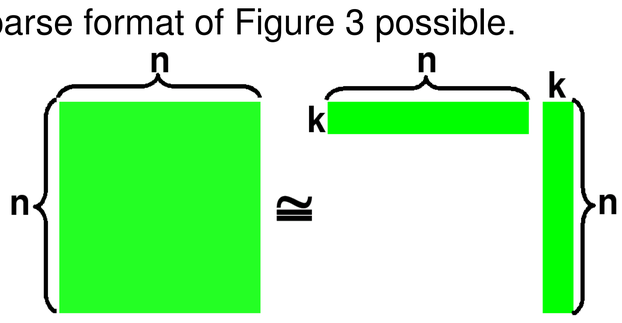


Figure 2: Simple example of an hierarchical matrix taken from the 1D standard example of the hlib tutorial [3]. The red blocks are uncompressed. The green-white blocks are compressed in the way shown in Figure 3. The numbers denote the rank of each block.

Figure 3: Low rank approximation of an admissible block. Since k << m and k <<n applies, the amount of storage is significantly reduced.



Example: Sphere

A simple way of constructing spherical surface grids of varying coarseness is to start from an octahedron and recursively add nodes to the middle of the edges. The new nodes have to be rescaled to the correct radius of the sphere. This technique has been used to compare the storage requirements between the full boundary element matrix and its hierarchical matrix approximation with an increasing number of surface nodes. The results are shown in Figure 5. While the amount of memory of the full matrix scales quadratically, the behavior of the approximation is nearly linear. In theory [3] it should behave according to $m \cdot \log(m)$.

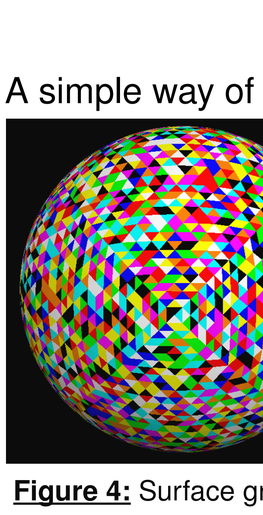
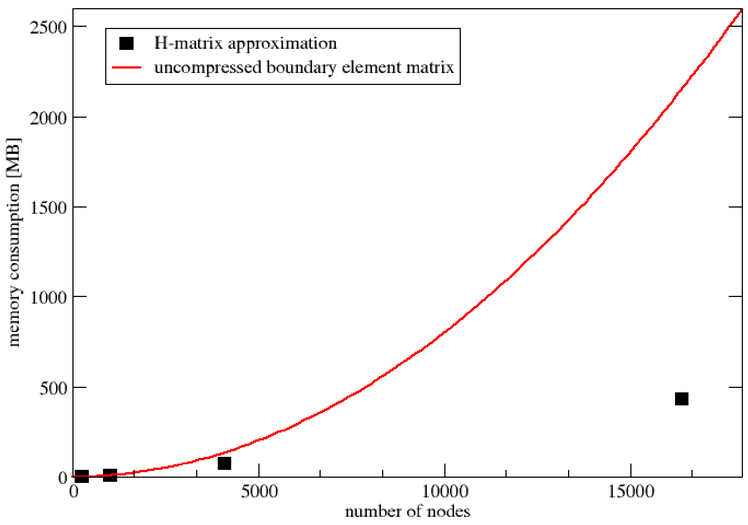


Figure 4: Surface grid of a sphere with 4098 nodes

Figure 5: Comparison between the storage requirements for the boundary element matrix of different spherical surface grids andits hierarchical matrix approximation. The radius of the sphere is 200 nm. For the approximation of admissible blocks the so called hybrid cross approximation has been used (see the hlib tutorial [3]). (internal hlib parameters: p=3, q=4, η=2.0, eps=0.0001)



As a conclusion we can state that hierarchical matrices seem to be an appropriate mean for the study of mesostructures in micromagnetics. A next step in the project will be to use the library hlib in connection with the micromagnetic simulation package nmag [4] for the simulation on corresponding structures.

[1] Xiao et al., J. Am. Chem. Soc.
[2] DR Fredkin and TR Koehler, IEEE Trans. Magn. 26, (1990), 415
[3] http://www.hlib.org
[4] http://nmag.soton.ac.uk