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Efficient solvers for coupled Brown-Néel Fokker-Planck equations II

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Abstract

Solving the inverse problem in magnetic particle imaging (MPI) relies on efficient and accurate solutions to the forward model. In a previous work we proposed a numerical method for solving the convection-dominated Fokker-Planck equation arising from coupled Brownian and Néel relaxation mechanisms. Furthermore, this method tackles the parameter dependence coming from the potentially large number of physical parameter combinations. In this work, we present numerical results for the coupled problem using the joint angular-temporal discretization of this partial differential equation (PDE) and a reduced basis (RB) method for the parameter dependence.

I. Introduction

Using a physically accurate forward model is crucial to obtain reliable results for the inverse problem in magnetic particle imaging (MPI). Therefore, in the previous work [1] we investigate the coupled Brown-Néel model [2]. Here we obtain a Fokker-Planck equation

$$\partial_t f = -\mathrm{div}_{\mathbb{S}^2\times\mathbb{S}^2}(\mathbf{b}f - \mathbf{D}\nabla_{\mathbb{S}^2\times\mathbb{S}^2} f) \tag{1}$$

on two copies of the unit sphere $\mathbb{S}^2$ for the time-dependent probability density f of particle and magnetization directions with diffusion matrix $\mathbf{D}$. The convection field $\mathbf{b}$ depends on different physical parameters, the magnetic field and the spatial location. The dynamic magnetization of the nanoparticles is determined by this probability density; therefore, our focus is on efficiently computing this solution across the relevant range of physical parameter combinations.

In [1], we proposed a method to calculate an accurate approximation of the solution of this Fokker-Planck equation efficiently for a large number of parameter combinations. In this work, we present first numerical results for the proposed method for the coupled Brown–Néel model.

II. Methods and materials

For solving the Fokker-Planck equation for a fixed set of parameters we use a slightly modified version of the hybrid mixed discontinuous Galerkin finite element method from [3]. This method can be used with arbitrary polynomial order, which results in high convergence rates for smooth solutions. Additionally, this method allows for discretizations simultaneously in the temporal and the angular variables.

To address the parameter dependence, we use the reduced basis (RB) method. In the offline phase of the RB method we compute highly accurate solutions of the Fokker-Planck equation (1) for different parameter combinations, which are called snapshots. To do this, we use the joint angular-temporal method described above. In the online phase, we can calculate the numerical solution for new parameters by expressing the RB solution in

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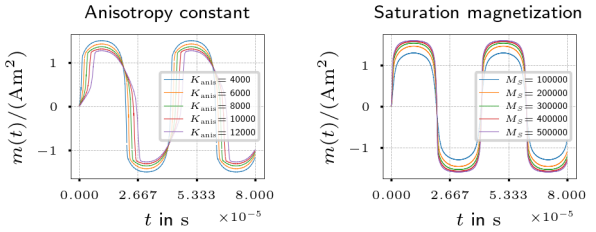


Figure 1: Mean magnetic moment m with varying anisotropy constant K_{anis} left and saturation magnetization M_S right.

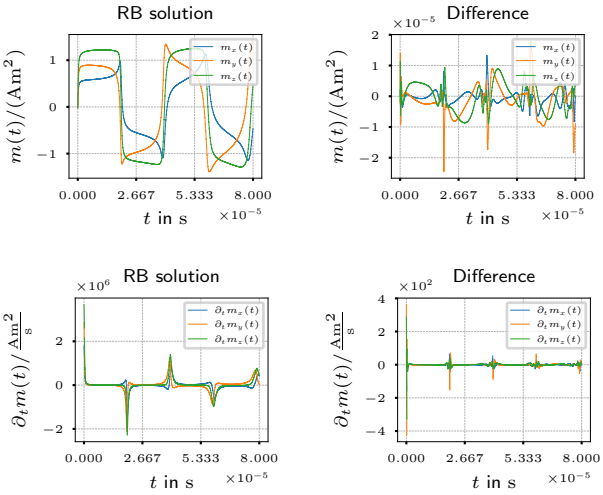


Figure 2: RB solution and difference to full numerical solution with relative error $5.6{\cdot}10^{-6}$ in L_2-norm and $5.1{\cdot}10^{-5}$ in H^1-norm.

terms of the previously computed snapshots. The major advantage is that the runtime of the online phase only depends on the number of snapshots, which results in a potentially tremendous speed-up.

III. Results and discussion

Fig. 1 illustrates results of the mean magnetic moment m with transient excitation only in x-direction calculated by our numerical method for the Fokker-Planck equation (1) corresponding to the coupled Brown-Néel model, where all physical parameters except one are fixed (left: anisotropy constant, right: saturation magnetization). The choice of the fixed parameters is based on [4].

As an example for the RB approach we use the Fokker-Planck equation (1) with three varying parameters, the three drive field amplitudes in a range of $[8\,\mathrm{mT}, 16\,\mathrm{mT}]$ with $F_D = 25\,\mathrm{kHz}$. The remaining parameters are fixed in this experiment. Fig. 2 shows the RB solution using 50 snapshots for a specific parameter combination and the difference to the full numerical solution. The reconstruction has a small relative error, both in L_2 and H^1 norm. The runtime of the online phase to generate the RB solution is 0.5 ms, a significant reduction to 6 min for the full numerical solution. Fig. 3 shows the corresponding RB residual decay with respect to the number of snapshots used in the offline phase, indicating exponential convergence of RB approximations.

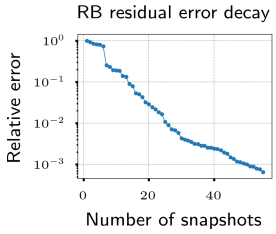


Figure 3: RB error decay with respect to the number of snapshots.

IV. Conclusion

The proposed high-order joint angular-temporal numerical method provides first promising results for the coupled Brown-Néel model for fixed physical parameters. Furthermore, preliminary results with several varying parameters demonstrate a highly efficient RB surrogate model.

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Author statement

No conflicts of interest.

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