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Efficient solvers for coupled Brown-Néel Fokker-Planck equations

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Abstract
In magnetic particle imaging (MPI), achieving efficient and accurate solutions to forward models is crucial for solving inverse problems. This work investigates the coupled Brownian and Néel relaxation mechanisms, which leads to a convection-dominated Fokker-Planck equation on a higher-dimensional domain. We propose a joint angular-temporal discretization of this partial differential equation (PDE) combined with a reduced basis method. Preliminary numerical results on simplified models demonstrate the efficacy of our approach, indicating its potential for broader applications in MPI.

I. Introduction

For MPI, there exist various models of different complexities for the forward problem. As described in [1], selecting a physically accurate forward model is crucial to obtain reliable results for the inverse problem in MPI. For this reason, we study the coupled Brown-Néel model of [2]. As in [3], we obtain a Fokker-Planck equation, that is, a convection-dominated PDE given by

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

for the time-dependent probability density f of particle and magnetization directions. This density is a function of time and two variables on the unit sphere $\mathbb{S}^2$. The diffusion tensor $\mathbf{D}$ is diagonal and the convection field $\mathbf{b}$ is determined by the magnetic field, the physical parameters, and the spatial location. In particular, the mean magnetic moment can be computed by integration of f.

In contrast to the classical discretization approaches, e.g., in [4], we propose a simultaneous discretization of f in both directional and temporal variables, which is advantageous for model reduction techniques. The proposed scheme is based on a higher-order method for convection-dominated problems.

We aim to approximate the Fokker-Planck equation across a wide range of combinations of parameters. However, solving the PDE numerically for each combination is highly inefficient. We address this by model reduction using reduced basis methods: at the price of a potentially very expensive precomputation, we obtain a projection of (1) onto a low-dimensional space of functions that can be solved very efficiently for each given $\mathbf{b}$ and $\mathbf{D}$.

II. Methods and materials

We consider a numerical scheme for solving the Fokker-Planck equation that combines an angular-temporal high-order method with a reduced basis approximation.

We adapt the hybrid mixed discontinuous Galerkin

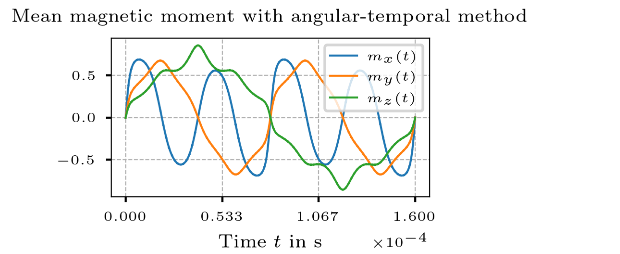

Figure 1: Mean magnetic moment of the Néel Fokker-Planck equation with the magnetic field frequencies f_x, $f_y = f_x/2$ and $f_z = f_x/4$.

finite element method from [5], reformulating (1) as

$$\operatorname{div}_{\mathbb{S}^2\times\mathbb{S}^2\times\mathbb{R}}\left(\begin{pmatrix}\mathbf{b}\\1\end{pmatrix}f-\begin{pmatrix}\mathbf{D}\nabla_{\mathbb{S}^2\times\mathbb{S}^2}f\\0\end{pmatrix}\right)=0.$$

This method combines a (dual) mixed variational formulation for the pure diffusion problem with a discontinuous Galerkin (DG) formulation for the pure convection problem. One major advantage of this method is that it can be used with arbitrary polynomial order to obtain high convergence rates for smooth solutions. The computational complexity caused by the higher-dimensional domain can be reduced by sparse grid combination techniques [6] or low-rank methods [7].

To address the parameter dependence of the PDE, we use reduced basis methods. The main idea is to extract efficient angular-temporal basis functions from solutions of the full problem for different parameter combinations. By projecting onto this reduced basis, we obtain a compressed problem that can be solved very efficiently for new parameter values while maintaining controlled errors with respect to the full solution.

III. Results and discussion

We present preliminary results for the angular-temporal discretization of the pure Néel case [3], considering only a singular angular variable. An example of the computed mean magnetic moments is shown in Fig. 1, where we obtain similar results as in the finite volume scheme [4].

We illustrate the reduced basis approach using a time-dependent model problem in one spatial dimension, where the parameter dependence enters in the scalar convection term $b = \mu$ with $\mu \in [0.1, 5]$, covering weak as well as strong convection. Fig. 2 shows a sample solution of this PDE along with the error decay of the reduced basis method. Here the online phase requires solving reduced linear systems with 16 unknowns for each parameter combination, compared to approximately 10^6 degrees of freedom in the full model, while maintaining an estimated error of 10^{-8} in the mesh norm. The speed-up factor is approximately $4 \cdot 10^5$.

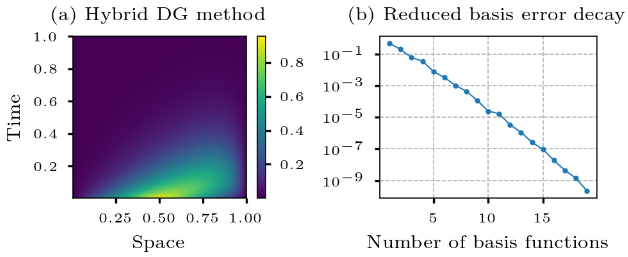

Figure 2: (a): solution for $\mu = 2$ with diffusion $\mathbf{D} = 0.2$; (b): Error decay with respect to number of reduced basis functions.

IV. Conclusion

We demonstrate an efficient high-order numerical scheme for convection-dominated problems with parameter dependence. Preliminary results indicate the potential for developing an efficient solver for the full Brown-Néel model.

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Author statement

No conflicts of interest.

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