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Exploiting the Fourier neural operator for parameter identification in MPI

Mirco Grosser [a,b] · Martin Möddel [a,b] · Tobias Knopp [a,b]

[a] Section for Biomedical Imaging, University Medical Center Hamburg-Eppendorf, Hamburg, Germany
[b] Institute for Biomedical Imaging, Hamburg University of Technology, Hamburg, Germany
[*] Corresponding author, email: mirco.grosser@tuhh.de

Abstract

Model-based magnetic particle imaging (MPI) is a challenging task both due to the complicated underlying physical model and the high numerical effort required for the solution of the corresponding equations of motion. A third challenge for practical applications is the identification of model parameters that are consistent with the given experimental setting and produce accurate predictions of the MPI signals. In this work, we show how the parameter identification problem can be addressed using a learned physics simulator based on the Fourier neural operator. As an application, we show how model-based system matrices can be estimated from a small set of calibration measurements, which can also be interpreted as a model-based approach to system matrix recovery. We compared our approach to established compressed sensing and interpolation schemes and found that it outperformed both.

I. Introduction

Accurate knowledge of the magnetic particle imaging (MPI) system matrix (SM) is essential for SM-based MPI reconstruction. Most commonly, the system matrix is acquired in a time-consuming calibration scan. This approach is convenient because of its accuracy and versatility. Drawbacks are the long measurement times and the fact that calibration measurements need to be repeated when the acquisition parameters or the types of magnetic nanoparticles (MNPs) are changed [1].

A promising alternative to the calibration-based approach is a model-based one. Recently, it has shown its ability to provide image reconstruction quality on par with the measurement-based approach [2, 3]. Model-based MPI offers great flexibility and allows to adapt SMs to different physical conditions (e.g. field configurations) once the underlying particle model is specified. However, a drawback are the long computation times required for the solution of the underlying Fokker-Planck or Langevin equations [4]. A breakthrough in this direction was the introduction of learned simulators, based on Fourier neural operators (FNOs) [5]. As shown in [6], these have the potential to speed up Fokker-Planck-simulations by two orders of magnitude.

Another challenge for the model-based approach is the identification of model parameters. This is often done by fitting the model to a number of calibration measurements. For immobilized MNPs, parameter identification is feasible using a set of one-dimensional measurements, as was shown in [2]. However, this approach is not applicable for liquid MNPs where the effective Néel model contains a spatially varying distribution of anisotropy constants and easy axes [3]. A more generic approach is described in [7]. However, this approach becomes impractical for multi-dimensional imaging applications due to its high numerical complexity.

In this work, we show how FNOs can be used for efficient parameter identification in MPI. We exploit the structure of FNOs, which simplifies the computation of gradients with respect to the physical parameters of the magnetization model. Based on this, we propose an optimization scheme to identify the model parameters most consistent with a given set of calibration measurements. Our results indicate that accurate model-based SMs can be obtained from significantly fewer calibration measurements than required for a compressed sensing (CS) or interpolation-based SM estimation.

II. Methods and materials

Particle magnetization model: Our magnetization model is based on the Fokker-Planck equation for the Landau-Lifshitz-Gilbert equation [3, 4]. We consider the Néel relaxation case, which is commonly used for immobilized MNPs [8]. However, we note that it also provides a sufficiently accurate model for MNPs suspended in fluid, when using a spatially varying distribution of anisotropy constants and easy axes [3]. While showing promising results, this effective model also has a large number of parameters, which poses a challenge for parameter identification.

To have an efficient approximation to the Fokker-Planck-model, we follow the FNO-approach described in [6]. In this approach, the solver for the Fokker Planck equation is interpreted as an operator $\mathcal{F}_{\text{Fokker-Plank}} : \boldsymbol{\pi} \mapsto \bar{\boldsymbol{m}}$ that generates the mean magnetic moment $\bar{\boldsymbol{m}} : [0,T] \to \mathbb{R}^3$ from the corresponding acquisition parameter function $\boldsymbol{\pi} : [0,T] \to \mathbb{R}^{N_p}$. Here $\boldsymbol{\pi}$ is a function containing all relevant acquisition parameters, including the applied magnetic fields, particle diameter and the vector $\boldsymbol{K}_{\text{anis}} = K_{\text{anis}}\boldsymbol{n}$. The latter is a combination of the MNPs anisotropy constant K_{anis} and its easy axis $\boldsymbol{n}$. The FNO used in this work has the same architecture as described in [6]. For the model training, we use magnetization dynamics simulated for pseudo-random field sequences. The loss and MNP parameters used for training were chosen as described in [6]. However, instead of keeping the MNP diameter fixed, we sampled it uniformly from the range $[14, 24]$ nm. With this at hand, measured MPI data can be simulated using the forward model

$$s_l(t) \approx \hat{s}_{\pi,l}(t) := -\mu_0 \left(a_l * \boldsymbol{p}_l^T \dot{\mathcal{F}}_{\text{FNO}}\{\boldsymbol{\pi}\} \right)(t), \tag{1}$$

where $\boldsymbol{p}_l$ denotes the receive coil sensitivity of the l^{th}-receive coil and a_l models the high-pass filtering taking place during signal reception.

Parameter identification: To perform parameter identification, we consider a set of time-discrete calibration measurements $\{\boldsymbol{s}_k\}_{k} \in \{1, ..., K\}$ that are performed at varying locations in the field of view (FOV). Each measurement is associated with the MNP parameters $\boldsymbol{\pi}_{\text{MNP},k}$ and sequence parameters $\boldsymbol{\pi}_{\text{S},k}$. The $\boldsymbol{\pi}_{\text{S},k}$ characterize the magnetic field sequence used. These should match for the model and the calibration measurements. To estimate the MNP parameters for each calibration measurement, we exploit the neural network structure of the FNO, which allows an easy computation of gradients with respect to the MNP parameters. Thus, parameter identification can be performed by solving the inverse problem

$$\underset{\boldsymbol{\pi}_{\text{MNP},k}}{\operatorname{argmin}} \left\| \frac{\boldsymbol{s}_k}{\|\boldsymbol{s}_k\|_\infty} - \frac{\hat{\boldsymbol{s}}_{\pi,k}}{\left\|\hat{\boldsymbol{s}}_{\pi,k}\right\|_\infty} \right\|_2^2, \tag{2}$$

where $\hat{\boldsymbol{s}}_{\pi,k}$ denotes the time-discretized form of $\hat{s}_{\pi,k}(t)$. Here, $\hat{\boldsymbol{s}}_{\pi,k}$ combines the information from all receive channels. The minimization objective only considers normalized signals and is thus independent of the tracer concentration used for the calibration measurements. Minimization of the corresponding loss function can be done using standard gradient-descent based solvers. In this work, we used 200 iterations of the Adam optimizer with a learning rate of 100.

System matrix estimation: Using the results from the previous section, model-based SMs can be obtained from a small number of calibration measurements even for the case of liquid MNPs. To achieve this, we note that the spatial distribution of MNP parameters is generally smooth and thus well suited for interpolation. Model-based SMs can thus be obtained by the following procedure

1. Measure SM columns at a small number of calibration positions within the FOV.
2. Estimate MNP parameters based on (2).
3. Estimate the MNP parameters at the remaining positions using interpolation.
4. Simulate high-resolution SMs using the interpolated parameters.

A technical difficulty arises due to the invariance of the magnetization model under inversion of the MNP easy axis. This must be taken into account in the interpolation step. Otherwise, jumps in the parameter maps can cause significant interpolation errors.

Numerical experiments: To evaluate our model, SMs were simulated based on the effective Néel model for fluid MNPs. The imaging sequence used was a two-dimensional Lissajous sequence (frequencies $f_x = 2.5\,\text{MHz}/102$, $f_y = 2.5\,\text{MHz}/96$) with a drive field amplitude of $12\,\text{mT}/\mu_0$ and a selection field gradient of $1\,\text{T/m}/\mu_0$ in both x- and y-direction. The sampling rate was 2.5 MHz. The SM was simulated for MNPs with a core diameter of 20 nm. Following [3], $\boldsymbol{K}_{\text{anis}}$ was assumed to be aligned with the selection field with an anisotropy gradient of $1250\,\text{J}\,\text{m}^{-3}$. The simulated grid had a size of 28×28 and covered a FOV of (30×30) mm. For SM recovery, we estimated the MNP parameters using every third point in each direction as calibration measurements. For the interpolation step we used bicubic interpolation. To simulate measurement noise, we added 5% Gaussian noise to the calibration measurements prior to parameter estimation.

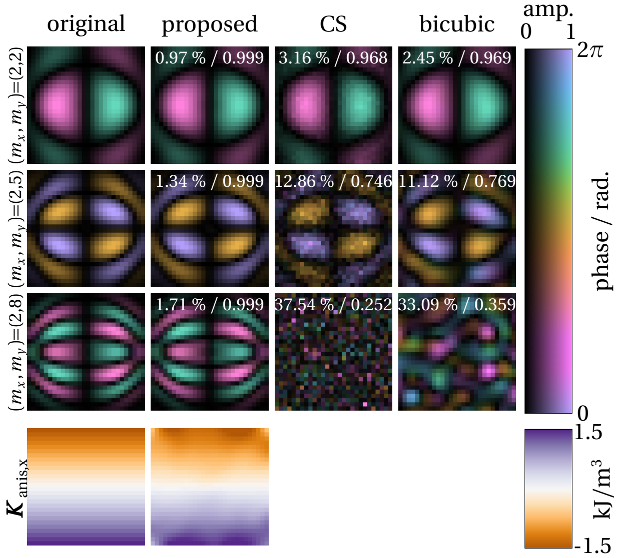

Figure 1: Recovered SM patterns (rows 1-3) and the estimated distribution of $K_{\text{anis,x}}$ (row 4). The superimposed numbers are the NRMSD and structural similarity index (SSIM) of the recovered frequency components.

For comparison, we performed CS-based SM recovery and bicubic interpolation using the same number of calibration measurements. Finally, the recovered SMs were used for image reconstruction. The measured data was simulated for varying phantoms and 3% Gaussian noise was added to the signal. Image reconstruction was performed in frequency space using 100 iterations of the ℓ_2-regularized Kaczmarz algorithm. The regularization parameter was manually optimized for each reconstruction.

III. Results

As illustrated in the bottom row of Figure 1, the distribution of the anisotropy closely matches the underlying ground-truth. Visible differences are only discernible near the boundaries of the FOV. These arise because MNPs near the FOV boundaries are always in saturation. Thus, the induced MNP signal only depends weakly on the underlying MNP parameters. The high quality estimation of the MNP parameters also carries over to the resulting SMs. As illustrated in the upper part of Figure 1, the SM obtained using the proposed method closely matches the ground-truth, whereas the corresponding CS recovery and the bicubic interpolation show clearly visible artifacts. This is also reflected in the mean normalized root mean squared deviation (NRMSD) of all rows of the recovered SMs, which is $2.66 \pm 1.10\%$ for the proposed method, $26.18 \pm 7.24\%$ for the CS recovery and $25.4 \pm 7.36\%$ for the bicubic interpolation.

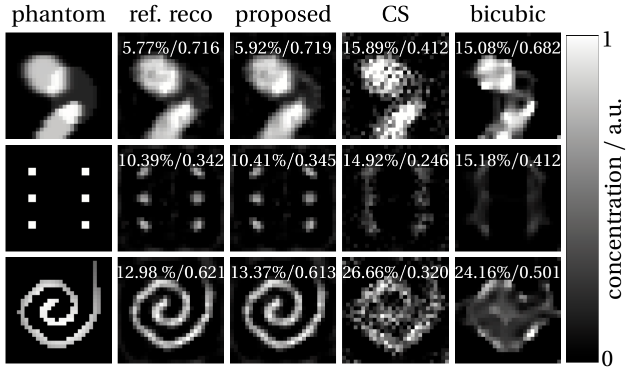

Figure 2: Image reconstruction results for different numerical phantoms. The superimposed numbers are the NRMSD and SSIM with respect to the corresponding phantom.

Similarly, the proposed method results in high-quality image reconstruction results, which are summarized in Figure 2. On the other hand, the SMs obtained using CS and bicubic interpolation show clearly visible artifacts.

IV. Discussion and conclusion

The results obtained in this work show that FNOs are a promising tool to efficiently address the parameter identification problem in MPI. This is an important step to enable a more routine use of model-based MPI in practical MPI applications. We note that our experiments are based on the linear distribution of MNP anisotropies proposed in [3]. In real applications, more complex, but smooth, distributions are likely to occur. In this case, where the larger number of parameters becomes difficult to calibrate, our method can prove invaluable to obtain accurate model-based SMs.

Having estimated the full set of MNP parameters also allows for further interesting applications beyond SM recovery. For instance, it becomes possible to simulate SMs for different patches in the FOV, while taking into account prior knowledge about the inhomogeneities of the applied magnetic fields. We also note that the described method is very generic and could also be used with other, further optimized neural network-based magnetization models.

An important requirement for our method is that the MNP parameters to be estimated influence the magnetization signal sufficiently strongly. As shown in our results this can lead to errors for MNPs near the FOV-boundaries. Moreover, it should be noted that we only considered a mono-dispersed model so far. Generalizing the model to the poly-disperse case is a topic for further research. The next important step, for this project, will be to evaluate the proposed method on measured data.

Author's statement

Conflict of interest: Authors state no conflict of interest.

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