Maxwell parallel imaging

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Purpose: To develop a general framework for parallel imaging (PI) with the use of Maxwell regularization for the estimation of the sensitivity maps (SMs) and constrained optimization for the parameter-free image reconstruction.

Theory and Methods: Certain characteristics of both the SMs and the images are routinely used to regularize the otherwise ill-posed optimization-based joint reconstruction from highly accelerated PI data. In this paper, we rely on a fundamental property of SMs—they are solutions of Maxwell equations—we construct the subspace of all possible SM distributions supported in a given field-of-view, and we promote solutions of SMs that belong in this subspace. In addition, we propose a constrained optimization scheme for the image reconstruction, as a second step, once an accurate estimation of the SMs is available. The resulting method, dubbed Maxwell parallel imaging (MPI), works for both 2D and 3D, with Cartesian and radial trajectories, and minimal calibration signals.

Results: The effectiveness of MPI is illustrated for various undersampling schemes, including radial, variable-density Poisson-disc, and Cartesian, and is compared against the state-of-the-art PI methods. Finally, we include some numerical experiments that demonstrate the memory footprint reduction of the constructed Maxwell basis with the help of tensor decomposition, thus allowing the use of MPI for full 3D image reconstructions.

Conclusion: The MPI framework provides a physics-inspired optimization method for the accurate and efficient image reconstruction from arbitrary accelerated scans.

KEYWORDS
constrained optimization, electromagnetic basis, Maxwell regularization, parallel imaging, tensor decomposition

1 | INTRODUCTION

Parallel imaging (PI) is admittedly one of the most disruptive technologies in modern magnetic resonance imaging (MRI) and probably the best example of a successful transition from academic research to widespread usage in clinic. Essentially, PI exploits the multi-physic nature of MRI and the ubiquitous use of sophisticated spatially distributed receiving coils in order to significantly reduce the scan time. Indeed, the interplay of electrodynamics and spin-dynamics in the spatiotemporal encoding, as evinced by the bilinear form of the MR signal equation, suggests that the spatial selectivity of the receivers could be harnessed in order to reduce the time-consuming gradient encoding.

There is a plethora of PI reconstruction methods that could be roughly categorized into 2 main approaches: the
image-space (or spatial-domain) and the k-space (or spectral-domain). As main representatives of the former approach, which calls for the a-priori knowledge of the associated sensitivity maps (SMs), one can mention the pioneering works of SMASH\textsuperscript{1} and SENSE.\textsuperscript{2} The k-space methods followed a few years later aiming exactly at breaking the dependence of separate precalibration scans, which increase the overall acquisition time and are more susceptible to motion artifacts. The beginning of those so-called autocalibrating methods can be identified with the emergence of GRAPPA,\textsuperscript{3} which makes use of some extra autocalibration signals (ACS) in order to fit the kernels for approximating the missing k-space lines. A more detailed description of all the methods developed in the early days of PI can be found in the review paper.\textsuperscript{4}

The first PI techniques, both image-space and k-space, were geared to fast reconstruction times, allowing certain simplifications at the expense of extra precalibration scans or ACSs in order to transform the inherently nonlinear problem into a linear one. Naturally, more sophisticated PI methods followed that consider the original bilinear form of the inverse problem at hand, incorporating the estimation of the coil SMs. The common point of the most notable among them (JSENSE\textsuperscript{5} and NLINV\textsuperscript{6}) is the use of appropriate regularization, necessary for the otherwise ill-posed inverse problem. More specifically, in both methods, the authors exploit the smoothness of the SMs by making use of a polynomial expansion for constraining the subspace of the possible solutions of the SMs in the former while applying a smoothness-enforcing regularization term in the later. Recently, NLINV was further generalized to a method dubbed ENLIVE with the addition of extra bilinear forms in order to account for the violation of the standard model in case of limited field-of-view (FOV).\textsuperscript{7} Another aspect of the smoothness and the spatial selectivity of the SMs is that they also favor purely algebraic techniques based on modern numerical linear algebra algorithms that promote low-rank and subspace-specific solutions.\textsuperscript{8-11}

As the above-mentioned iterative PI reconstruction approaches started gaining more traction, the interest shifted toward the use of more expressive regularizers, ranging from ones readily available in the mathematical optimization literature\textsuperscript{12-14} to more modern data-driven variational models.\textsuperscript{15} Again, it became clear that although the joint reconstruction of both the SMs and the images was offering certain advantages, there was a strong argument for considering the SMs estimation first and then using those SMs in the solution of the linear image reconstruction. This justifies the further proliferation of numerical methods that are tailored to the accurate estimation of the SMs\textsuperscript{16-20}; among them, ESPIRiT\textsuperscript{19} deserves a special mention as it appears to be a true workhorse and the method of choice for most of the recent studies, including the benchmark challenge for the deep-learning PI reconstruction techniques.\textsuperscript{21,22} More specifically, ESPIRiT is based on an eigenvalue decomposition of an image-domain operator, and essentially exploits the smoothness of the SMs and the rank-deficient properties of the calibration matrix.

Evidently, the modern PI reconstruction techniques have gone a long way from the first days of accelerated MR scans and today it is quite common to use more sophisticated methods of linear and bilinear numerical optimization as well as deep learning for reconstructing both the SMs and the images. Nevertheless, even the most effective PI methods available today are based on regularizers that are oversimplified and/or require case-dependent fine-tuning of the penalty parameters. In this work, we develop a general PI framework that relies on physics-inspired regularization for the estimation of the SMs and parameter-free constrained optimization for the image reconstruction. More specifically, we note that smoothness is only one of the characteristics of SMs that depends, among other, on the scanner’s main field strength. Foremost, SMs are solutions of Maxwell equations; they correspond to the magnetic fields collected by the receiving coils in the presence of the patient. Hence we choose to generate the subspace of the associated SMs (ie, a complete numerical basis of magnetic fields in the FOV) in a patient-agnostic fashion and we proceed to the solution of the regularized bilinear optimization problem, where the SMs are expressed as arbitrary linear combinations of the elements of the Maxwell basis. In addition, we make use of a tensor compression scheme for reducing the memory footprint of the Maxwell basis in the case of 3D reconstruction. Finally, we appreciate the need for more expressive regularizers and we propose a parameter-free, constrained optimization scheme for improving the image quality when SMs are available. The effectiveness of the proposed general PI framework, dubbed Maxwell parallel imaging (MPI), is demonstrated for a wide range of typical sequences (both 2D and 3D) with various reduction factors (R) and ACSs.

2 | THEORY

We consider the discretized form of the PI problem, which can be described by the forward model

$$y = FSp + n,$$

where $p$ is an N-dimensional vector that contains in rasterized form the samples of the unknown density to be reconstructed (eg, a 2D MRI slice, a 3D MRI volume, or a 4D MRI multicontact tensor), and $y, n \in \mathbb{C}^N$ are column vectors corresponding to the k-space samples obtained from the C receiver coils and i.i.d complex Gaussian noise, respectively. Furthermore, $S \in \mathbb{C}^{NC \times N}$ is a matrix composed as $S = [S_1^H \ldots S_N^H]^H$, where $S_k \in \mathbb{C}^{NC \times N}$ is a diagonal matrix constructed by the SM $s_k \in \mathbb{C}^N$ of the kth coil, $k = 1, \ldots, C$, $(\cdot)^H$ denotes the Hermittian
transpose, and \( \mathbf{F} \in \mathbb{C}^{K \times N} \) is a block diagonal matrix obtained as \( \mathbf{I}_c \otimes \mathbf{F}_i \), where \( \mathbf{I}_c \in \mathbb{R}^{C \times C} \) is the identity matrix, \( \otimes \) denotes the Kronecker product, and \( \mathbf{F}_i \in \mathbb{C}^{K \times N} \) is the undersampled operator that provides a mapping from image space to \( k \)-space, with \( K \leq N \). The nominal \( R \) is defined as \( \frac{N}{K} \) and corresponds to the undersampling rate of the \( k \)-space.

The recovery of the underlying density \( \mathbf{p} \) from the acquired \( k \)-space data \( \mathbf{y} \) belongs to the category of inverse problems. Due to the presence of noise \( \mathbf{n} \), whose exact realization is unknown, and since the operator \( \mathbf{F} \) is singular, it is an ill-posed problem. This implies that in order to obtain a statistically or physically meaningful solution, we need to exploit any prior knowledge we might have about the solution. Another complicating factor that makes the recovery of \( \mathbf{p} \) even more challenging, is that the SMs embedded in \( \mathbf{S} \) are typically unknown and need to be also recovered. This results in an observation model that is not anymore linear w.r.t. the unknown quantities, but instead has the following bilinear form:

\[
\mathbf{y} = \mathcal{G}(\mathbf{p}, \mathbf{s}_1, \ldots, \mathbf{s}_C) + \mathbf{n},
\]

where

\[
\mathcal{G}(\mathbf{p}, \mathbf{s}_1, \ldots, \mathbf{s}_C) = \begin{bmatrix}
\mathbf{F}_j(\mathbf{s}_1 \odot \mathbf{p}) \\
\vdots \\
\mathbf{F}_j(\mathbf{s}_C \odot \mathbf{p})
\end{bmatrix}
\]

and \( \odot \) indicates element-wise multiplication of vectors.

### 2.1 Regularized nonlinear inversion

One popular way to tackle the joint recovery problem of \( \mathbf{p} \) and \( \{\mathbf{s}_j\}_{j=1}^C \) is to employ the iteratively regularized Gauss–Newton (IRGN) method that was introduced in \( \cite{Knoll2013} \) and was later used for PI reconstruction in Uecker et al. \( \cite{Uecker2015} \). The underlying idea of this approach consists of (a) considering the linearized approximation of the nonlinear operator \( \mathcal{G}(\mathbf{x}) \) around some current estimate of the solution, \( \mathcal{G}(\mathbf{x}^n + \Delta \mathbf{x}) \approx \mathcal{G}(\mathbf{x}^n) + \mathbf{J}_\mathcal{G}(\mathbf{x}^n) \Delta \mathbf{x} \), where \( \mathbf{J}_\mathcal{G}(\mathbf{x}^n) \) is the Jacobian of \( \mathcal{G} \) evaluated at \( \mathbf{x}^n \), (b) minimizing an objective function of the form:

\[
\Delta \mathbf{x}^* = \arg \min_{\Delta \mathbf{x}} \frac{1}{2} \| \mathbf{y} - \mathcal{G}(\mathbf{x}^n) \|_2^2 + \mathcal{R}(\mathbf{x}^n + \Delta \mathbf{x}),
\]

where \( \mathcal{R}(\cdot) \) is a regularization functional and (c) updating the current estimate as \( \mathbf{x}^{n+1} = \mathbf{x}^n + \gamma \Delta \mathbf{x}^* \), where \( \gamma \) can be computed using a line-search strategy.

Initially, in Uecker et al. \( \cite{Uecker2015} \), the authors considered using the regularizer \( \mathcal{R}(\mathbf{x}^n) = \alpha_n \| \mathbf{p}^n \|_2^2 + \beta_n \sum_{k=1}^C \| \mathbf{W} \mathbf{F} \mathcal{S}_{k}^\star \|_2^2 \), where \( \mathbf{F} \in \mathbb{C}^{N \times N} \) is the DFT matrix, \( \mathbf{W} \in \mathbb{R}^{N \times N} \) is a weighting diagonal matrix and \( \alpha_n, \beta_n \geq 0 \). Note that, given that the SMs are expected to be smooth, the second term of this regularizer penalizes their high-frequency content. Later, in Knoll et al. \( \cite{Knoll2015} \) the authors replaced the Tikhonov regularizer on the density, \( \| \mathbf{p}^n \|_2^2 \), with non-quadratic regularizers that can better model certain properties of the underlying density, at the cost of a more involved minimization strategy; the minimizer of Equation (4) cannot be derived anymore as the solution of a system of linear equations and more advanced convex optimization techniques must be employed.

In this work, we also rely on the IRGN method as an initial step that provides an estimate of the unknown SMs. Then in a second step, as we describe later, we use the estimated SMs in order to recover a high-quality estimate of the underlying density by solving the linear inverse problem of Equation (1). We note that such a 2-step strategy has been regularly followed in other image processing applications, such as blind deconvolution, \( \cite{Selesnick2011} \) where aside from the underlying image the degradation operator is also unknown. Similar to Ref. [5] and unlike to, \( \cite{Knoll2015} \), where an analysis-based regularization approach is pursued both for the density and the SMs, we consider a modified version of the objective function in (4), which leads to a synthesis-based regularization strategy for the SMs, by penalizing their expansion coefficients \( \mathbf{a} \) on a predefined subset of basis vectors \( \mathbf{U}_h \in \mathbb{R}^{N \times q} \). A thorough discussion about the analysis- and synthesis-based regularization and their difference can be found in Selesnick and Figueiredo, \( \cite{Selesnick2005} \) while details on the construction of an appropriate physics-inspired basis are provided in the following Sections.

In particular, we express each SM as \( \mathbf{s}_k \approx \mathbf{U}_h \mathbf{a}_k \) and thus, our observation model takes the form:

\[
\mathbf{y} = \mathcal{G}(\mathbf{p}, \mathbf{a}_1, \ldots, \mathbf{a}_C) + \mathbf{n},
\]

where

\[
\mathcal{G}(\hat{\mathbf{x}} \equiv [\mathbf{p}^h, \mathbf{a}_1^h, \ldots, \mathbf{a}_C^h]^H) = \begin{bmatrix}
\mathbf{F}_j(\mathbf{U}_h \mathbf{a}_1 \odot \mathbf{p}) \\
\vdots \\
\mathbf{F}_j(\mathbf{U}_h \mathbf{a}_C \odot \mathbf{p})
\end{bmatrix}.
\]

Then, we seek the solution of the following minimization problem:

\[
\Delta \hat{\mathbf{x}}^* = \arg \min_{\Delta \mathbf{x}} \frac{1}{2} \| \mathbf{y} - \mathcal{G}(\hat{\mathbf{x}}^n) \|_2^2 + \mathcal{R}(\mathbf{x}^n + \Delta \mathbf{x}),
\]

where we impose an \( \ell_2^2 \)-squared penalty both on the density and the expansion coefficients of the SMs. It is worth noticing that by estimating the expansion coefficients \( \mathbf{a} \) instead of the SMs themselves and since the coils are represented in a reduced order model, that is, \( N >> q \), the solution of Equation (6) corresponds to that of an overdetermined problem. Due to the quadratic form of the objective function to be minimized in Equation (6), the solution can be derived by solving the relevant
normal equations using the conjugate gradient method. This requires the ability to compute the matrix-vector products of the Jacobian of $\mathcal{G}$ and its adjoint, with a vector. These products are computed as follows:

$$
\mathbf{J}_\mathcal{G} (\mathbf{x}) = \begin{bmatrix}
\Delta \mathbf{p} \\
\Delta \alpha_1 \\
\vdots \\
\Delta \alpha_c
\end{bmatrix} = \mathcal{G} \left( [\Delta \mathbf{p}^1, \Delta \mathbf{a}_1^1, \ldots, \Delta \mathbf{a}_c^1]^H \right) + \mathcal{G} \left( [\mathbf{p}^1, \Delta \mathbf{a}_1^1, \ldots, \Delta \mathbf{a}_c^1]^H \right)
$$

$$
= \begin{bmatrix}
\mathbf{F} \left( \mathbf{U}_1 \mathbf{a}_1 \circ \Delta \mathbf{p} + \mathbf{p} \odot \mathbf{U}_1 \Delta \alpha_1 \right) \\
\vdots \\
\mathbf{F} \left( \mathbf{U}_c \mathbf{a}_c \circ \Delta \mathbf{p} + \mathbf{p} \odot \mathbf{U}_c \Delta \alpha_c \right)
\end{bmatrix}
$$

(7)

and

$$
\mathbf{J}_\mathcal{G}^H (\mathbf{x}) \begin{bmatrix}
\mathbf{y}_1 \\
\vdots \\
\mathbf{y}_c
\end{bmatrix} = \begin{bmatrix}
\sum_{k=1}^C \left( \mathbf{U}_k \mathbf{a}_k \right)^H \mathbf{F}_k^H \mathbf{y}_k \\
\mathbf{U}_1^H \left( \mathbf{p} \odot \mathbf{F}_1^H \mathbf{y}_1 \right) \\
\vdots \\
\mathbf{U}_c^H \left( \mathbf{p} \odot \mathbf{F}_c^H \mathbf{y}_c \right)
\end{bmatrix}
$$

Finally, it is worth noting that the same procedure can be followed in the case of dynamic or multicontrast PI data, expecting that the associated artifacts will be captured by the density while the estimation of the (constrained) SMs will remain unaffected, especially when using some average of the $k$-space data.

### 2.2 Regularized density reconstruction via constrained optimization

While the regularization applied on $\mathbf{p}$ in Equation (6) is rather plain and thus not capable of modeling complex properties of the underlying density, it allows us to perform a joint reconstruction of the sensitivities and the density without having to rely upon a computationally heavy and time consuming minimization scheme. Furthermore, due to the implicit regularization of the SMs, by expressing them in terms of a proper basis expansion, and the explicit Tikhonov regularization of the corresponding expansion coefficients, we expect that most of the reconstruction errors will be accumulated in the recovered density, while the unknown SMs will be more accurately restored.

Having this in mind, we use the estimated SMs, discard the estimated density and solve the linear inverse problem described in Equation (1). Hence, we obtain the final density estimate as the minimizer of the following constrained optimization problem:

$$
\mathbf{p}^* = \arg \min_{\mathbf{p} \in \mathbb{C}^N} \mathcal{R} (\mathbf{p}),
$$

$$
\| \mathbf{y}_k - \mathbf{F}_k \mathbf{S}_k \mathbf{p} \|_2 \leq \varepsilon_k, \forall k
$$

(8)

where $\varepsilon_k$ is a scalar that is proportional to the standard deviation of the complex Gaussian noise realization that degrades the $k$-space measurements acquired from the $k$th coil, that is, $\varepsilon_k = \sqrt{K - 1} \sigma_k$. While for the experiments that we report in this work, we have considered Total Variation as the regularization functional $\mathcal{R} (\mathbf{p})$ of choice, the minimization strategy that we outline next can be also used without modifications when different and more expressive regularizers are considered, such as the structure tensor total variation (STV) and it is nonlocal extension or the Hessian–Schatten norm regularizers of Lefkimmiatis.31 We also note that one particular advantage of the above constrained problem formulation, compared with the unconstrained minimization approach that is typically pursued in PI reconstruction, is that in this case there is no need of fine-tuning any regularization penalty parameter, which in practice is not a straightforward task and requires a certain level of experience from the user. The only parameters involved in the above formulation, are the scalars $\varepsilon_k$ which can be directly estimated from the $k$-space measurements. A related constrained formulation for parameter-free PI reconstruction has also been studied in Tamir et al.32 However, differently than our approach, in Tamir et al the authors consider a single norm-constraint for the standard deviation of the noise present in the coil measurements, while their minimization strategy is focused only on $\ell_1$-type of regularizers.

Now, let us first note that the constrained formulation of Equation (7) can be equivalently expressed in the unconstrained form

$$
\mathbf{p}^* = \arg \min_{\mathbf{p} \in \mathbb{C}^N} \mathcal{R} (\mathbf{p}) + \sum_{k=1}^C t_{\mathcal{G}(y_k, x_k)} (\mathbf{F}_k \mathbf{S}_k \mathbf{p}),
$$

(9)

where

$$
t_{\mathcal{G}(y_k, x_k)} (\mathbf{z}) = \begin{cases}
0, & \text{if } \| \mathbf{y}_k - \mathbf{z} \|_2 \leq \varepsilon_k \\
\infty, & \text{otherwise}
\end{cases}
$$

is an indicator function which ensures that the imposed constraints are satisfied by the solution. Next, since the transformed problem is still hard to solve directly, we rely on the alternating direction method of multipliers (ADMM).33,34 The strategy of ADMM is to split the original problem in smaller and easier ones to solve, by decoupling the different terms of the objective function. Based on this idea and following a similar splitting strategy as in,35 we instead consider the problem
where \( A = [I_N \ (F_S S_I)^T, \ldots \ (F_S S_C)^T]^T \), \( B = -I_{(N+K)C} \) and 
\( z = [z_0^N \ldots z_C^N]^T \in \mathbb{C}^{N+KC} \). Then, using the scaled form of ADMM\(^{34}\) we obtain the solution to our original problem of Equation (8) in an iterative way, where each iteration involves the following update steps:

\[
\begin{align*}
    z_k^{n+1} &= \text{prox}_{\frac{1}{\rho} \mathcal{R}} \left( z_k^n - \frac{\rho}{2} (p^n + u_k^n) \right),
    \\
    p_k^{n+1} &= \Pi_{\psi(y_{s_k}, s)} \left( F_S S_k p^n_k + u_k^n \right), \quad \forall k = 1, \ldots, C,
    \\
    u_k^{n+1} &= u_k^n + \frac{\rho}{2} \left( z_k^{n+1} - u_k^n \right) + \sum_{k=1}^{C} S_k^T F_S (z_k^{n+1} - u_k^n),
    \\
    y_k^{n+1} &= y_k^n + \frac{\rho}{2} \left( z_k^{n+1} - y_k^n \right).
\end{align*}
\]  

(11)

In Equation (11), we have that \( \Pi_{\psi(y_{s_k}, s)} (z) = y + \frac{\psi(y, s)}{\max(|y-z|^2, \gamma)} (y-z) \) is the proximal operator\(^{36}\) of the regularizer \( \mathcal{R} (\cdot) / \rho \). In particular, the steps described in Equation (11) can also be applied when multicontrast or dynamic MRI are considered, with some minor required modifications, which we discuss in the Supporting Information.

2.3 | Maxwell regularization

A key ingredient of the proposed nonlinear inversion scheme is the physics inspired regularization of the coil model. Because SMs \( s_k \) are solutions to Maxwell equations, we propose to constrain the solution space of the imaging problem to a subspace where SMs are indeed solutions to Maxwell equations, and conjecture that it is possible to express each SM as \( s_k \approx U_h a_k \), where \( a_k \in \mathbb{C}^q \) is a column vector collecting the expansion coefficients of the \( k \)th coil, and \( U_h \in \mathbb{C}^{N \times q} \) is a proper change of basis matrix, referred to as Maxwell basis in the following. The dimension \( q \) of the basis will play an important role in controlling the accuracy of the representation and the regularization properties.

Because the basis \( U_h \) collects solutions of Maxwell equations, a scheme for solving Maxwell equations within the FOV is a prerequisite. One approach is based on Lové’s form of the field equivalence theorem\(^{38,39}\); fields inside a source-free volume are fully determined if the tangential electromagnetic (EM) fields on the boundary of the volume are known. Following this idea, the problem of finding volumetric fields inside the source-free FOV is conveniently addressed as a 2-step procedure: first, solve for equivalent electric (\( j \)) and magnetic (\( m \)) currents on the boundary. Subsequently, EM fields \( e \) and \( h \) inside the FOV are expanded as

\[
\begin{align*}
    e &= [\nabla \times \mathcal{H} \times] \left( \mathcal{H} \times \mathcal{H} \right) \left( \begin{array}{c} j \\ m \end{array} \right),
    \\
    h &= [\nabla \times \mathcal{E} \times] \left( \mathcal{E} \times \mathcal{E} \right) \left( \begin{array}{c} j \\ m \end{array} \right),
\end{align*}
\]  

(12)

and \( \mathcal{G}^{\beta} \) is the dyadic Green function, mapping \( \beta \)-kind currents to \( \alpha \)-kind fields. Note that \( j \) and \( m \) are only proxies for computing \( h \); we are interested in finding a basis to represent a basis for all possible realizations of \( h \). This reflects into the need of spanning the range of the integral operators \( \mathcal{H}^{\beta, j} \) and \( \mathcal{H}^{\beta, m} \), and not in a particular solution of Equation (12).

Unfortunately, evaluation of the dyadic Green functions in Equation (12) requires knowledge of the object to be imaged: this implies that \( U_h \) is acquisition dependent, which would clearly be a major limitation. However, in view of the investigations documented in\(^{40}\) and references therein, at MRI frequencies and for short TE sequences the magnetic field is only slightly perturbed by the biological tissue, due to its weakly magnetic properties and the relatively small (in terms of electric length) FOV. We then conjecture that, in the absence of fast spatial variations in the magnetic field, the problem can be simplified by a homogeneous medium problem, and one can rewrite the field equation for \( h \) in Equation (12) in terms of the free-space scalar Green function \( g (r, r') = e^{jkr'/(4\pi r')} \) with \( k = \omega \sqrt{\varepsilon_0 \mu_0} \) the wavenumber in vacuum:

\[
\begin{align*}
    \mathcal{G}^{\beta, j} (r, r') &= \nabla \times \mathcal{G} (r, r') \times \mathcal{J},
    \\
    \mathcal{G}^{\beta, m} (r, r') &= \frac{1}{j \omega \mu} \left( \nabla \times \mathcal{E} \right) \times \mathcal{G} (r, r').
\end{align*}
\]  

(14)

(15)

This is crucial for the practical applicability of the method: because the basis is computed in the absence of the biological tissue, it is applicable to imaging problems sharing the same FOV. In other words, the basis is precomputed offline for a few FOVs of interest, given only the dimensions of the FOV and the target resolution. In practice, this is achieved via a numerical discretization of Equation (12). Finally, because the detected MRI signal is a circular polarization of the magnetic field \( h \), the subspace is further restricted to span only circularly polarized fields.
3  |  METHODS

The EM basis is numerically computed by sampling the range of Equation (12) via a technique known as randomized matrix decomposition. This method allows to sample the left subspace of $K$ without actually building it, and to extract an orthogonal basis up to any prescribed accuracy. The process to numerically generate the EM basis is described in previous relevant works, which make use of the scripts found in the open-source software MARIE. The difference in this work is that we generate a basis only for circularly polarized magnetic fields in the absence of a realistic human body model. The proposed method is valid for fully 3D FOVs or can be reduced to 2D problems by restricting the support of the basis to a single slice. On the other hand, when the problem is fully 3D, storage requirements for the basis itself can be a limitation. To overcome this potential issue, we represent the basis in a compressed form, as described in the Supporting Information.

The series of experiments described below was selected as a representative subset often found in various PI-related investigations, mainly because they are of significant clinical interest while posing challenges to traditional reconstruction techniques. Data used in the preparation of this article were obtained from the NYU fastMRI Initiative database (fastmri.med.nyu.edu). As such, NYU fastMRI investigators provided data but did not participate in analysis or writing of this report. A listing of NYU fastMRI investigators, subject to updates, can be found at: fastmri.med.nyu.edu. The dataset from the fastMRI database corresponds to a fully sampled FLASH acquisition (TR/TE = 250/3.4 ms, matrix size: 320 × 320, slice thickness: 5 mm) with a FOV of 220 × 220 mm², acquired at 3T using a 16-channel head coil. The dataset used for generating Figures 6 and 9 is a fully undersampled Ultrafast GRE acquisition (TR/TE = 153.6 ms, matrix size: 192 × 192 × 170, slice thickness: 1.2 mm) with a FOV of 240 × 240 × 204 mm³, acquired with a 1.5T GE Optima 450 W scanner using a 12-channel head coil. The dataset used for comparisons with other methods is a synthetic 8 channels 2D acquisition of a human brain acquired with 3D FLASH at 3T (TR/TE = 114.9 ms) using a 32-channel head coil. Except for the demonstration of 3D capabilities, the frequency encoding is resolved and all further reconstruction and processing is done on a single axial slice. In the following, densities and SMs obtained via regularized nonlinear inversion are labeled as “MPI-BL” (MPI BiLinear), while densities obtained via Regularized Density Reconstruction via Constrained Optimization as “MPI-L” (MPI Linear).

4  |  RESULTS

Figure 1 exemplifies the elements of a typical Maxwell basis over square and circular supports. The randomized SVD-based approach guarantees that the basis vectors possess a spatial frequency content growing with the index of the basis vector: increasing the dimension of the basis increases the high-frequency (spatial) components of the SM that can be captured by $U_p$. Consequently, the low-pass filtering properties help also with the regularization of the inverse problem. The representation properties of the basis are demonstrated in Figure 2, where the capability to expand known synthetic 2D SMs via the basis is analyzed. The convergence of the error of the expansion of a known SM is shown as a function of the basis dimension $q$, proving that by increasing the dimension of the basis it is possible to control the accuracy of the representation.

Figures 3 and 4 depict the extracted SMs and density of an MPI reconstructed axial slice from a Cartesian acquisition of a human brain obtained from the fastMRI database. The stability of the recovered SMs for different combination of R and ACS regions proves the effectiveness of the physics-based regularization scheme. Aliasing artifacts are visible in the final reconstructed image for acceleration factors $R \geq 4$, and substantial stability of the image is observed for ACS lines ≥ 4. The above conclusion is also supported by the error maps provided as Supporting Information Figure S2, showing 5 × pixel-wise errors of MPI reconstructions with respect to the fully sampled solution. Computation time on an Intel Xeon CPU E5-2650 with NVIDIA Tesla K80 GPU is 346 and 36 seconds for SMs and image reconstruction ($R = 2, ACS = 16$), respectively. Figure 5 demonstrates the performance of MPI for simultaneous Cartesian accelerations along phase and slice directions. Different Cartesian downsampling schemes are retrospectively applied, with fixed number of ACS lines (16) and Maxwell basis with $q = 50$. The reconstructed image is free from artifacts for combined $R \leq 6$.

Figure 6 shows the capability of MPI to address non-Cartesian acquisitions. Provided that the operator $F$ of Equation (1) is available, the described formulation is directly applicable. A synthetic 8 channels 2D acquisition of 402 spokes (readout length 256) with golden angle radial sampling is generated from a Shepp–Logan model of size 256 × 256 and a set of 8 artificial SMs computed via the open-source Python package SigPy, corresponding to a
fully sampled k-space according to Nyquist–Shannon theory. The dataset has been retrospectively downsampled, and white Gaussian noise added independently to each coil. Figure 7 explores variable-density Poisson-disc undersampled reconstructions of a knee, comparing MPI with ENLIVE and SAKE. All methods provide artifact-free reconstructions up to acceleration \( R = 3 \), with the denoising step performed by MPI-L providing a generally cleaner image. For higher accelerations \( R = 5 \) SAKE misses signal from the center of the image, ENLIVE and MPI-BL both provide a rather noisy image, while the MPI-L reconstructed image has significantly better quality.

A single slice in readout direction of a fully sampled dataset, from a human brain acquired with 3D FLASH at 3T (TR/TE = 11/4.9 ms) using a 32-channel head coil, has been retrospectively undersampled with CAIPIRINHA patterns, with different acceleration factors and 24 ACS lines, as described in51. Results obtained with MPI reconstruction are compared with ESPIRiT and ENLIVE reconstructions in Figure 8. All images appear free from artifacts even at \( R = 16 \) (see also error maps in Supporting Information Figure S3, and the robustness of MPI with respect to the number of acquired low-frequency k-space lines in Supporting Information Figure S4).

Finally, Figure 9 shows the results of a full 3D reconstruction of the same dataset of Figure 5, undersampled with a combined acceleration factor 4 and 16 ACS lines, and reconstructed with MPI-BL with a variable dimension
of the Maxwell basis. The results show the flexibility of MPI in addressing seamlessly 3D $k$-spaces with the same formulation. When using a small number of basis elements ($q = 50$), aliasing artifacts are visible, as highlighted by the green arrow, which disappear as we add more basis elements. Additionally, Tucker compression reduces the memory footprint of the Maxwell basis from 19.1 GB to 31 MB when $q = 200$, in turn enabling accelerated computations on GPU (see also Table S1 in Supporting Information). Computation time on an Intel Xeon E5-2686 CPU with NVIDIA Tesla V100 GPU is 73 minutes for 9 iterations of MPI-BL and $q = 200$.

5 | DISCUSSION

There are cases where the bilinear form of the MR signal fails to capture accurately the underlying physics. More specifically, it is well documented that the image-domain methods, with the exception of ENLIVE,\(^7\) produce erroneous results...
when the chosen FOV does not include entirely the object under study. As mentioned above, the SMs are essentially the circularly polarized magnetic fields received by the coils, and due to the nature of Maxwell equations their values depend strongly on the EM properties of the entire object, not only the portion inside the FOV. Hence the estimation of the actual SMs for small FOVs is an ill-posed problem. Fortunately, MPI allows the extension of the original signal

**FIGURE 5**  A 1.5T fully sampled Cartesian acquisition of a human head is retrospectively downsampled, with different Cartesian undersampling factors along the phase encoding (Rp) and slice encoding (Rs) dimensions, and a fixed number of 16 ACSs. The frequency encoding is resolved and one single axial slice is reconstructed as a 2D problem. The reconstructed MPI-L density is shown, with SMs extracted via MPI- BL and basis dimension \( q = 50 \)

**FIGURE 6**  A 256 \times 256 \ pixels  
Shepp–Logan phantom and a set of 8 synthetic SMs with the same size are used to simulate a synthetic golden angle acquisition with readout length 256. Independent white Gaussian noise is then added to the simulated k-space signal of each coil, yielding decreasing SNR values [\( \infty, 25\text{dB}, 20\text{dB}, 15\text{dB} \)] (left to right). The solution of MPI-L is shown for different numbers of acquired spokes \( N \in [200, 100, 50, 25] \), corresponding to acceleration factors \( R \in [2, 4, 8, 16] \) (top to bottom). The basis dimension is set to \( q = 100 \) for all cases
equation, much like ENLIVE, with the addition of extra bilinear terms, resulting in a fairly accurate approximation of the governing physics, though in this case the estimated SMs do not correspond anymore to the true magnetic field distributions and should be considered as merely dummy variables. Nevertheless, the image reconstruction is devoid of artifacts, as evinced by the Supporting Information Figure S5, where MPI with 2 sets of maps is applied on a dataset from Ref. [7].

While in this work we focused on an optimization-based reconstruction approach, a promising future research direction, which could lead to additional improvements in the reconstruction quality, is the design of physics-constrained deep reconstruction networks. The motivation is that by constraining the solution space of a neural network, we can gain more control on the outcome and reduce the risk of introducing erroneous reconstruction artifacts, which are highly undesirable in medical applications. Following the discussion on the construction of the Maxwell basis, one possible way to enforce such physics-based constraints is to combine the implicit Maxwell regularization approach with a variational-inspired deep network such as those introduced in our prior work.53-55 This way, it is possible to learn more meaningful...
and accurate representations for the SMs, which in turn can lead to better and more robust reconstruction results. At the same time, it is expected that by providing more information to the network about the space of solutions, we can avoid its overfitting during training and further require less training data.

6 | CONCLUSIONS

In this work, we described a novel general framework for the joint reconstruction of PI data. The proposed framework introduces an expressive, physics-based regularizer for the estimation of the SMs and a constrained optimization scheme for the subsequent parameter-free density reconstruction, for improved image quality. In addition, the use of a Maxwell basis for the expansion of the SMs reduces dramatically the overall number of the unknowns in the inverse problem. Finally, we utilized some relatively modern tensor decomposition methods in order to reduce the memory footprint of the Maxwell basis, which can become prohibitively large for high-resolution 3D scans. We expect this framework to allow MRI scientists and practitioners to obtain images of higher quality from datasets with even more aggressive acceleration.

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CONFLICT OF INTEREST

Authors are employees of Q Bio, Inc.

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SUPPORTING INFORMATION
Additional Supporting Information may be found online in the Supporting Information section.

**TABLE S1** Time and memory requirements for the basis stored as a dense matrix and in compressed form with accuracy $\epsilon = 10^{-4}$. The FOV has size $192 \times 192 \times 170$ voxels, with corresponding matrix size $k$. MVP: Matrix Vector Multiplication time (*): computed on CUDA-enabled pyTorch code (CUDA Version: 10.1, GPU NVIDIA Tesla V100). –: the data does not fit on GPU.

**FIGURE S1** Pictorial representation of the Tucker decomposition of a 3D tensor $\mathcal{T} = \mathcal{G} \times_1 U_1 \times_2 U_2 \times_3 U_3$. For a better understanding of the $k$-mode product $x_k$, it is useful to realize that it amounts to multiplying each mode-$k$ fiber of the core tensor $\mathcal{G}$ by the matrix $U_k$, that is, it is a convolution along the $k$th axis of $\mathcal{G}$. If the tensor $\mathcal{T}$ is rank deficient, we have that $r_k < n_k$ and the decomposition results in a compression. When $\mathcal{T}$ is full rank we can introduce an approximated decomposition of $\mathcal{T}$ up to an arbitrary accuracy $\epsilon$, by truncating the ranks $r_k$ such that $\| \mathcal{T} - \mathcal{G} \times_1 \hat{U}_1 \times_2 \hat{U}_2 \times_3 \hat{U}_3 \|_2 < \epsilon \| \mathcal{T} \|_2$. 

**FIGURE S2** Error maps displayed with enhanced brightness ($5 \times$) corresponding to Figure 4. The largest percentage error is reported in the inset of each figure. Up to acceleration factors $R = 3$ MPI reconstructions are virtually independent from the number of low-frequency k-space lines (ACS).

**FIGURE S3** Error maps displayed with enhanced brightness ($5 \times$) corresponding to Figure 8. The largest percentage error is reported in the inset of each figure. All methods provide similar error distributions with noise-like patterns.

**FIGURE S4** MPI reconstruction of the same dataset of Figure 8, undersampled with Cartesian CAIPIRINHA pattern with undersampling factor $R = 9$ and variable number of ACS lines. The results of MPI-BL (with basis dimension $q = 200$) and with MPI-L demonstrate the flexibility of MPI, which does not explicitly depend on the sampling pattern, allowing to reduce the size of the low-frequency portion of k-space without abruptly breaking up.

**FIGURE S5** MPI reconstruction of the dataset from. This is a retrospectively 2-fold undersampled 2D spin-echo dataset (TR/TE = 550/14 ms, FA = 90°, BW = 19 KHz, matrix size: $320 \times 168$, slice thickness: 3 mm) with a FOV of $200 \times 150 \text{mm}^2$, acquired at 1.5T using a 8-channel head coil. Nineteen iterations of the MPI-BL solver with basis dimension $q = 50$ are used to generate solutions with 1 and 2 maps: the solution allowing 2 maps (right) is free from artifacts, which are clearly visible in the center of the single map solution (left).

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