Model based reconstruction for magnetic particle imaging in 2D and 3D

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Overview

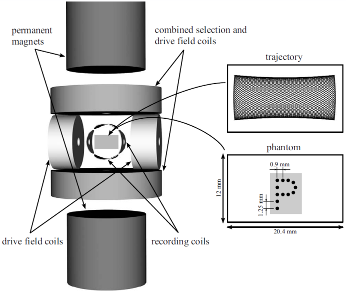
Basic Principles

Data measured in MPI: voltage $\mathbf{u}(t)$ induced in the recording coils.

By Farraday's law of induction,

$$\mathbf{u}(t) = -\frac{d}{dt}\mathbf{\Phi}(t),$$

where the magnetic flux $\mathbf{\Phi}(t)$ is



(courtesy of Knopp et al. 2010)

$$\mathbf{\Phi}(t) = \mu_0 \int_{\mathbb{R}^3} \mathbf{R}(x)(\mathbf{H}(x,t) + \mathbf{M}(x,t))\, dx,$$

μ_0 magnet. permeability.

- The flux $\mathbf{\Phi}(t)$ is caused by the applied field $\mathbf{H}(x,t)$ and the magnetization response $\mathbf{M}(x,t)$.
- $\mathbf{R}(x) \in \mathbb{R}^{3\times3}$ is the sensitivity pattern of the three recording coil pairs.

Basic Principles

Data measured in MPI: voltage $\mathbf{u}(t)$ given by

$$\mathbf{u}(t) = -\frac{d}{dt}\mathbf{\Phi}(t), \qquad \mathbf{\Phi}(t) = \mu_0 \int_{\mathbb{R}^3} \mathbf{R}(x)(\mathbf{H}(x,t) + \mathbf{M}(x,t))\, dx,$$

with magnetic flux $\mathbf{\Phi}(t)$, applied field $\mathbf{H}(x,t)$, magnetization response $\mathbf{M}(x,t)$.

By the Langevin theory of paramagnetism for superparamagnetic nanoparticles,

$$\mathbf{M}(x,t) = \rho(x)\, m\, \mathcal{L}\left(\frac{|\mathbf{H}(x,t)|}{H_{\text{sat}}}\right) \frac{\mathbf{H}(x,t)}{|\mathbf{H}(x,t)|}, \qquad \mathcal{L}(x) = \coth(x) - \frac{1}{x},$$

with $\mathcal{L}$... Langevin function, m... magnetic moment of a single particle, H_{sat}... saturation parameter.

Signal to reconstruct in MPI: concentration of the particles $\rho(x)$.

Simplification

Data: voltage $\mathbf{u}(t)$ given by

$$\mathbf{u}(t) = -\mu_0 \frac{d}{dt} \int_{\mathbb{R}^3} \mathbf{R}(x)(\mathbf{H}(x,t) + \mathbf{M}(x,t))\, dx.$$

Reconstruct the particle density $\rho(x)$ given via

$$\mathbf{M}(x,t) = \rho(x)\; m\; \mathcal{L}\left(\frac{|\mathbf{H}(x,t)|}{H_{\text{sat}}}\right) \frac{\mathbf{H}(x,t)}{|\mathbf{H}(x,t)|}.$$

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Since the applied field $\mathbf{H}$ does not depend on ρ, consider the data

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In the interesting field of view, R is almost constant; hence

$$\mathbf{s}(t) = -\mu_0 \mathbf{R} \frac{d}{dt} \int_{\mathbb{R}^3} \mathbf{M}(x,t)\, dx.$$

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Hence,

$$\mathbf{s}(t) = -\mu_0 m \mathbf{R} \frac{d}{dt} \int_{\mathbb{R}^3} \rho(x)\, \mathcal{L}\left(\frac{|\mathbf{H}(x,t)|}{H_{\text{sat}}}\right) \frac{\mathbf{H}(x,t)}{|\mathbf{H}(x,t)|}\, dx.$$

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Simplified problem: Reconstruct $\rho(x)$ from voltage data $s(t)$ related via

$$\underbrace{\mathbf{s}(t)}_{\text{data}} = \underbrace{-\mu_0 m \mathbf{R}}_{\text{constants}} \frac{d}{dt} \int_{\mathbb{R}^3} \underbrace{\rho(x)}_{\text{signal}} \underbrace{\mathcal{L}\left(\frac{|\mathbf{H}(x,t)|}{H_{\text{sat}}}\right) \frac{\mathbf{H}(x,t)}{|\mathbf{H}(x,t)|}} \, dx.$$

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$$\mathbf{H}(x,t) = \mathbf{H}^S(x) + \mathbf{H}^D(x,t) = \mathbf{G}x + \mathbf{P}\,\mathbf{I}(t)$$

In the interesting region,

$$\mathbf{H}^S(x) = \mathbf{G}x = g\,\mathrm{diag}(-1,-1,2)\,x, \qquad \mathbf{H}^D(x,t) = \mathbf{P}\,\mathbf{I}(t),$$

g ... nominal gradient of the static field, $\mathbf{I}(t)$ ... current in the coils,
$\mathbf{P}$ ... almost constant sensitivity profile of the drive field coils.

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Hence (Goodwill, Connolly),

$$\mathbf{s}(t) = \mu_0\, m\, \mathbf{R} \frac{d}{dt} \int_{\mathbb{R}^3} \rho(x) \mathcal{L}\left(\frac{|\mathbf{G}(r(t)-x)|}{H_{\text{sat}}}\right) \frac{\mathbf{G}(r(t)-x)}{|\mathbf{G}(r(t)-x)|}\, dx.$$

II. The MPI Core Operator

(or, getting rid of particular trajectories)

Decomposing the model

Problem: Reconstruct $\rho(x)$ from voltage data $s(t)$ related via

$$\underbrace{\mathbf{s}(t)}_{\text{data}} = \underbrace{-\mu_0 m \mathbf{R}}_{\text{constants}} \frac{d}{dt} \int_{\mathbb{R}^3} \underbrace{\rho(x)}_{\text{signal}} \underbrace{\mathcal{L}\left(\frac{|\mathbf{G}(r(t)-x)|}{H_{\text{sat}}}\right) \frac{\mathbf{G}(r(t)-x)}{|\mathbf{G}(r(t)-x)|}}_{\text{kernel}} \, dx.$$

From a mathematical viewpoint, by transformation,

$$\bar{\mathbf{s}}(t) = \frac{d}{dt} \int_{\mathbb{R}^3} \bar{\rho}(\widehat{x}) \, \mathcal{L}\left(\frac{|\widehat{r}(t) - \widehat{x}|}{h}\right) \frac{\widehat{r}(t) - \widehat{x}}{|\widehat{r}(t) - \widehat{x}|} \, d\widehat{x},$$

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Or,

$$\mathbf{s}(t) = \nabla_r \mathbf{\Phi}(r) \, \dot{r}(t), \qquad \text{where} \quad \mathbf{\Phi}(r) = \int_{\mathbb{R}^n} \rho(x) \, \mathcal{L}\left(\frac{|r-x|}{h}\right) \frac{r-x}{|r-x|} \, dx.$$

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Problem: Reconstruct $\rho(x)$ from voltage data $s(t)$ related via

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$\Longrightarrow$ The signal **s** only depends on the location r and the velocity $\dot{r}$ of the field free point, and not on the particular trajectory.

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- Mathematically: view MPI as an operator

$$\rho \to A_h[\rho](r, v)$$

where $A_h[\rho]$ is a function on phase space, linear in the velocity v,

$$A_h[\rho](r)v = \nabla_r \mathbf{\Phi}(r) v = \int_{\mathbb{R}^n} \rho(x)\, \nabla_r \left(\mathcal{L}\left(\frac{|r-x|}{h}\right) \frac{r-x}{|r-x|}\right) dx \cdot v.$$

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The MPI core operator A_h is independent of a particular trajectory.

III. Reconstruction in 2D and 3D

Idealization limit $h \to 0$

The MPI core operator A_h is given by

$$A_h[\rho](r)v = \int_{\mathbb{R}^n} \rho(x)\, \nabla_r \left(\mathcal{L}\left(\frac{|r-x|}{h} \right) \frac{r-x}{|r-x|} \right) dx \cdot v.$$

What happens if $h \to 0$?

- Physical meaning: e.g., temperature decreases, or, particle size increases.
- In 1D: kernel tends to Dirac pulse.
- Idealized operator without blurring part.

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Theorem (März, W., IPI, 2016)

Let $\alpha_h[\rho](r) = \mathrm{trace}\, A_h[\rho](r)$ *and let* $\alpha[\rho](r) = \lim_{h\to 0} \alpha_h[\rho](r)$*. Then,*

$$\alpha[\rho](r) = \int_{\mathbb{R}^n} \rho(x)\, \kappa(r-x)\, dx,$$

ρ *in* $BV_0(\Omega)$*. In dimension* $n > 1$*,*

$$\kappa(r-x) := \mathrm{div}_r \left(\frac{r-x}{|r-x|} \right) = \frac{n-1}{|r-x|}.$$

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- In 1D, we have a Dirac-kernel $\kappa(r-x) = 2\,\delta(r-x)$. A peaking property was conjectured for nD which is not true by the theorem.

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- In 1D, we have a Dirac-kernel $\kappa(r-x) = 2\,\delta(r-x)$. A peaking property was conjectured for nD which is not true by the theorem.
- Striking point: the trace $\alpha[\rho]$ already contains all information on ρ. This has not been realized before.

Relation to the Laplace equation

We consider the MPI core operator A_h and its trace

$$\alpha_h[\rho](r) = \mathrm{trace}\, A_h[\rho](r),$$

together with the idealization limit

$$\alpha[\rho](r) = \lim_{h\to 0} \alpha_h[\rho](r), \quad \alpha[\rho](r) = \int_{\mathbb{R}^n} \rho(x)\, \kappa(r-x)\, dx.$$

Corollary (März, W., IPI, 2016)

We have the following dimension-dependent relations of the kernel κ to the fundamental solution $\Phi(r,x)$ of the Laplace equ. $-\Delta_r \Phi = \delta(r-x)$,

$$\text{in 3D,} \qquad \kappa(r-x) = 8\pi\, \Phi(r,x) \quad \text{with} \quad \Phi(r,x) = \frac{1}{4\pi\, |r-x|};$$

$$\text{in 2D,} \qquad \kappa(r-x) = -2\pi\, \nabla_r \Phi(r,x) \cdot \frac{r-x}{|r-x|};$$

$$\text{with} \quad \Phi(r,x) = -\frac{1}{2\pi} \log(|r-x|).$$

$$\text{in 1D,} \qquad \kappa(r-x) = -2\frac{d^2}{dr^2}\Phi(r,x) \quad \text{with} \quad \Phi(r,x) = -|r-x|/2.$$

Reconstruction Formula

Corollary (Reconstruction Formula for the Idealized Case, März, W., IPI, 2016)

Consider the idealized MPI core operator

$$A_0[\rho](r) = \lim_{h \to 0} A_h[\rho](r) \qquad \textit{and}$$

data $F(r) = A_0[\rho](r)$ *at each point* r *given for the idealized scenario. Then,*

$$\rho = \kappa^{-1} \circ \operatorname{trace} A_0[\rho],$$

where κ *is the dimension-dependent convolution kernel from above.*

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That means, we take the pointwise trace and then deconvolve w.r.t. the dimension-dependent κ. In particular, in $3D$,

$$\rho = \frac{1}{8\pi}\Delta \circ \mathrm{trace}\, A_0[\rho],$$

Ill-Posedness

Corollary (Ill-Posedness März, W., IPI, 2016)

Even the idealized MPI problem is ill-posed in 2D and 3D. Depending on the dimension the degree of ill-posedness, i.e., the order of gained Sobolev smoothness of the forward operator, is one in 2D, and two in 3D.

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Remark. This is not the case in 1D where κ is a Dirac distribution.

Non-idealized situation

We consider the non-idealized situation $h > 0$ now.

Theorem (März, W., IPI, 2016)

The trace $\alpha_h[\rho]$ of the MPI core operator $A_h[\rho]$ is given by

$$\alpha_h[\rho](r) = \int_{\mathbb{R}^n} \rho(x)\, \kappa_h(r-x)\, dx,$$

$\rho \in BV_0(\Omega)$, *where the convolution kernel κ_h is given by*

$$\kappa_h(y) = \frac{1}{h} f\left(\frac{|y|}{h}\right), \qquad \text{with} \quad f(z) = \mathcal{L}'(z) + \mathcal{L}(z)\frac{n-1}{z}, \tag{1}$$

$\mathcal{L}$ *the Langevin function;*

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$$\alpha_h[\rho](r) = \int_{\mathbb{R}^n} \rho(x)\, \kappa_h(r - x)\, dx,$$

$\rho \in BV_0(\Omega)$, where the convolution kernel κ_h is given by

$$\kappa_h(y) = \frac{1}{h} f\left(\frac{|y|}{h}\right), \qquad \text{with} \quad f(z) = \mathcal{L}'(z) + \mathcal{L}(z)\frac{n-1}{z}, \tag{1}$$

$\mathcal{L}$ the Langevin function; f is analytic with only purely imaginary singularities; near zero, f has the power series expansion

$$f(z) = \sum_{k=0}^{\infty} \frac{2^{2k+2} B_{2k+2}}{(2k+2)!} (2k+n)\, z^{2k}, \quad B_l \text{ the } l\text{-th Bernoulli number,}$$

with a convergence radius of π. Thus κ_h is analytic.

Reconstruction Formula

Corollary (Reconstruction Formula for the the Non-Idealized Case, März, W., IPI, 2016)

Consider the MPI core operator $A_h[\rho](r)$ and suppose that data $F(r) = A_h[\rho](r)$ at each point r is given. Then,

$$\kappa_h * \rho = \mathrm{trace}\, A_h[\rho],$$

where κ_h is the analytic convolution kernel $\kappa_h(y) = \frac{1}{h} f\left(\frac{|y|}{h}\right)$ with $f(z) = \mathcal{L}'(z) + \mathcal{L}(z)\frac{n-1}{z}$ from the slide before.

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That means, we take the pointwise trace and then deconvolve w.r.t. κ_h.

Ill-Posedness

Corollary (Ill-Posedness März, W., IPI, 2016)

The non-idealized MPI problem is severely ill-posed in the following sense: there are no two spaces H^s, H^t in the (Hilbert-)Sobolev scale, such that the trace α_h of the MPI operator induces an isomorphism $\alpha_h : H^s \to H^t$ between these two spaces.

There is a particularly nice relation between the traces $\alpha[\rho]$ and $\alpha_h[\rho]$ of the idealized and the non-idealized MPI operators in 3D.

Theorem (März, W., IPI, 2016)

In 3D, we have that

$$\alpha_h[\rho] = -\frac{\Delta \kappa_h}{8\pi} * \alpha[\rho].$$

This tells us that in 3D the non-idealized $\alpha_h[\rho]$ is a massively smoothed version of the idealized $\alpha[\rho]$. Recall that

$$\kappa_h(y) = \frac{1}{h} f\left(\frac{|y|}{h}\right), \qquad \text{with} \qquad f(z) = \sum_{k=0}^{\infty} \frac{2^{2k+2} B_{2k+2}}{(2k+2)!} (2k+n)\, z^{2k}.$$

IV. Reconstruction Algorithm

Discretization and Given Data

We use the derived reconstruction formulae to design a reconstruction algorithm for MPI in 2D/3D.

Measured data: Samples $\mathbf{s}_k = \mathbf{s}(t_k)$ of time data $\mathbf{s}(t)$ associated with a scan trajectory $r(t)$.

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- Recall: $r(t)$ is related with the electrical current $\mathbf{I}(t)$ via

$$r(t) = -\mathbf{G}^{-1}\mathbf{P}\,\mathbf{I}(t),$$

$G = g\ diag(-1, -1, 2)$, $g \ldots$ nominal gradient of the static field, $P \ldots$ sensitivity profile of the drive field coils.

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- The measured data are a discrete sampling of the MPI core operator applied to ρ

$$\mathbf{s}_k = \mathbf{s}(t_k) = A_h[\rho](r_k)v_k,$$

  at location $r_k = r(t_k)$, with the trajectory having tangent $v_k = v(t_k)$ at time t_k, for finitely many measurements indexed by k.

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- Note: the presented approach is independent of the particular trajectory type employed.

Major Algorithmic Steps

Measured data are a discrete sampling of the MPI core operator applied to ρ

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Reconstruction formula:

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Our scheme may be subdivided into **two major steps.**

Step 1: Deriving trace data on a spacial grid from the raw input. We obtain a grid function u representing trace data, i.e.,

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in each pixel (grid cell). (Details follow.)

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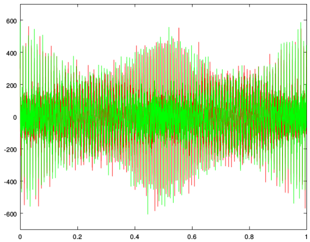
Step 2: Reconstruction of the signal from the derived trace data by deconvolution (ill-posed). Regularized solution of the problem

$$\text{Find} \quad \rho \quad \text{in} \quad \kappa_h * \rho = u,$$

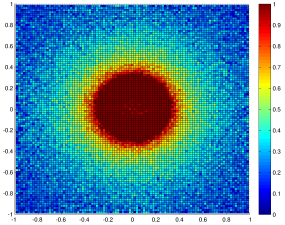
given u.(Details follow.)

Example.

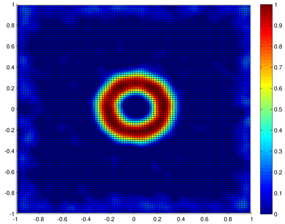


Noisy time signal – cut-out

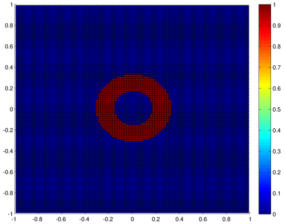
red: component 1, green: component 2



Intermediate: trace after spatial fitting.



Reconstruction using our method.



Original.

Trace Data on a Spacial Grid from the Raw Input

Measured data are samples of the MPI core operator applied to ρ,

$$\mathbf{s}_k = \mathbf{s}(t_k) = A_h[\rho](r_k)v_k,$$

at location $r_k = r(t_k)$, tangent $v_k = v(t_k)$. Reconstruction formula:

$$\kappa_h \circ \rho = \operatorname{trace} A_h[\rho].$$

Step 1: Deriving trace data on a spacial grid from the raw input.
Find a grid function u

$$u \approx \operatorname{trace} A_h[\rho] \text{ defined on a grid of } N_1 \times N_2 \text{ cells.}$$

- On each cell, u is constant; each cell i is represented by its center point x_i.
- A time sample t_k belongs to cell i, if $r(t_k)$ is in this cell; For each cell i, we collect the signal data $\mathbf{s}(t_{k_i})$ from samples t_{k_i} belonging to the cell i and gather them in a matrix S_i. Accordingly, we collect the velocity vectors $\dot{r}(t_{k_i}) = v(t_{k_i})$ and gather them in a matrix V_i.
- We obtain the matrix fitting problem w.r.t. A_i,

$$A_i \; V_i = A_h[\rho](x_i) \; V_i = S_i. \tag{2}$$

which we solve by least squares fitting. Then, $u_i := \operatorname{trace} A_i$.

Signal Reconstruction from the Trace Data by Deconvolution

Reconstruction formula:

$$\kappa_h \circ \rho = \mathrm{trace}\, A_h[\rho].$$

Step 1 yields a grid function u

$$u \approx \mathrm{trace}\, A_h[\rho] \text{ defined on a grid of } N_1 \times N_2 \text{ cells.}$$

Step 2: Reconstruction of the signal from the derived trace data by deconvolution (ill-posed). Regularized solution of the problem

$$\text{Find} \quad \rho \quad \text{in} \quad \kappa_h * \rho = u,$$

given u by classical Tychonov regularization

$$\rho = \arg\min_{\widehat{\rho}} \; \mu \, \|D \, \widehat{\rho}\,\|_2^2 + \|K_h \, \widehat{\rho} - u\|_2^2. \tag{3}$$

We solve the corresponding discrete Euler-Lagrange equation

$$-\mu \, L\rho + K_h \left(K_h\rho - u \right) = 0. \tag{4}$$

Here, $-L = D^T D$ is the five point stencil discretization of the Laplacian with zero Dirichlet boundary and $K_h = K_h^T$ is symmetric.

Reconstruction Algorithm - Summary

input : Time dependent samples $s_k = s(t_k)$ along trajectory $r_k = r(t_k)$ with tangent $v_k = \dot{r}(t_k)$ at times t_k; regularization parameter μ.
output: Reconstructed particle density ρ.

for $k \leftarrow 1$ **to** K **do**
    // Associate time samples with pixel grid.
    if r_k *in cell i* **then**
        $V(i) \leftarrow [V(i),\ v_k]$;   //Append tangent direction.
        $S(i) \leftarrow [S(i),\ s_k]$;   // Append data value.
    end
end
for $i \leftarrow 1$ **to** I **do**
    // For each cell fit trace data using (2).
    $[Q_i, R_i] \leftarrow \mathrm{QR}(V_i^T)$;
    $A_i \leftarrow S_i\ Q_i\ R_i^T$;
    $u_i \leftarrow \mathrm{trace}\ A_i$;
end
// Regularized deconvolution of the trace data using (3) by
// solving (4) with conjugate gradients (CG).
$\rho = CG(-\mu\ L + K_h^2,\ K_h u)$;

Summary

- We have reviewed the MPI model.
- We have extracted the MPI core operator.
- We have analyzed the idealized situation and the non-idealized situation.
- We have obtained reconstruction formulae for both cases based on matrix traces of the MPI core operator.
- We have seen that even the idealized MPI problem is ill-posed in 2D and 3D, which contrasts the 1D situation.
- We have seen that the MPI problem is severly ill-posed.
- We have derived a reconstruction algorithm based on the reconstruction formulae.

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