Inference of Boundary Data from Magnetic Measurements of Accelerator Magnets

Inferenz von Randdaten aus Magnetfeldmessungen von Beschleunigermagneten

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Zusammenfassung

In dieser Forschungsarbeit wird die mathematische Modellierung genutzt, um den Messprozess für das magneto-statische Feld innerhalb eines Beschleunigermagneten zu beschreiben, und Verfahren zur Erschließung von Modellvariablen, basierend auf Messdaten werden präsentiert. Die physikalischen Grundgleichungen des magnetischen Feldes sind impliziert, durch die Felddarstellung als Lösung einer partiellen Differentialgleichung. Durch die Formulierung als Randwertproblem reicht es aus, Feldmessungen am Rand des Problemgebietes durchzuführen. Somit kann der Aufwand für die vollständige Kartografierung des Feldes in drei Dimensionen von $O(1/h^3)$ auf $O(1/h^2)$ reduziert werden, wobei h die Messauflösung darstellt.

Eine iso-geometrische Randelementmethode höherer Ordnung wird für die Felddarstellung verwendet, was Vorteile für die Berechnung von Teilchenbahnen mit sich bringt, da hinreichend glatte Feldableitungen beliebiger Ordnung zugänglich sind. Zudem wird eine indirekte Formulierung der Integralgleichung präsentiert, welche einen linearen Zusammenhang zwischen Feld und Randdaten bereitstellt, ohne die Notwendigkeit der Lösung eines Gleichungssystems, um zwischen Dirichlet und Neumann Daten zu transformieren. Dies ist für die Erschließung von Randdaten, basierend auf Messdaten vorteilhaft.

Die Magnetfeldmessung liefert Spannungen, oder deren Integrale über kurze Zeitfenster, welche oftmals nicht direkt proportional zu den Feld-, beziehungsweise Modellvariablen sind. Das Bayes'sche Paradigma bietet einen Rahmen zur Erschließung von Modellvariablen aus abhängigen Beobachtungen, die unter dem Einfluss von Messfehlern stehen. Auf diese Weise können Unsicherheiten effektiv quantifiziert werden, da lediglich eine einzige Realisierung des Messvorgangs erforderlich ist, ohne dass Wiederholungen durchgeführt werden müssen. Zudem wird ein aktiver Lernalgorithmus entwickelt, welcher genutzt wird, um das Problemgebiet in Orten mit großer Unsicherheit zu erkunden.

Im Rahmen dieser Doktorarbeit wurde ein neues Messsystem bestückt, in Betrieb genommen und messtechnisch charakterisiert. Es handelt sich um ein Messsystem zur Kartografierung des Magnetfeldes mit Hilfe eines drei-Achsen Hall-Sensors und einer Positionierplatform. Aus diesem Grund liegt der Fokus für die Anwendung der theoretischen Aspekte, in der Kartografierung von dreidimensionalen Feldverteilungen basierend auf Messungen mit Hall-Sensoren. Dies umfasst die Kalibrierung von Hall-Effekten in drei Dimensionen, der Lösung des absoluten Positions- und Orientierungsproblems, sowie der Herleitung eines magnetomechanischen Modells, für die Quantifizierung vom Messunsicherheiten auf Grund von Vibrationen und Positionierfehlern.

Für die modellbasierte Messdatenauswertung unter der Verwendung der Bayes'schen Schlussfolgerung, wird ein generelles Konzept ausgearbeitet, welches auf drei verschiedene Problemstellungen im Zusammenhang mit der Magnetfeldmessung angewendet wird.

Abstract

In this research, mathematical modeling is used to express the measurement process for the magneto-static field in an accelerator magnet and approaches to infer model variables from on magnetic measurements are presented. The physical relations are implied by solving a partial differential equation, for the field evaluation. With the formulation by means of a boundary value problem, measurements can be restricted to the domain boundary, reducing the effort to provide field maps in three dimensions from $O(1/h^3)$ to $O(1/h^2)$, where h is the measurement resolution.

A higher order, iso-geometric boundary element method is used for the field model, which comes with benefits for the extraction of Taylor maps used for particle tracking applications, because sufficiently smooth derivatives of arbitrary order can be determined. Moreover, an indirect boundary element formulation is presented, establishing a linear relation between field and boundary data, without the need to map between Dirichlet and Neumann data, or the solution of a similar linear equation system for field evaluation. This is of advantage for the inference of boundary data from measurements.

Magnetic measurements are providing voltages, or their integrals over small time windows, which are often not directly proportional to the field, or model variables. The Bayesian paradigm provides a framework to infer model variables from dependent observations, under the influence of measurement errors. In this way, uncertainty quantification is achieved effectively, as only a single realization of the measurement process is needed, without the need to execute repetitions. Moreover, an active learning algorithm is developed, used to explore the physical domain in regions with large uncertainty.

In the scope of this doctoral thesis, a new three-axes Hall-probe mapper system has been commissioned and metrologically characterized. For this reason, the focus is on the application of Hall probe field mapping, for the practical realization of the above mentioned theoretical aspects. This includes the calibration of Hall effects in three dimensions, the solution of the absolute sensor position and orientation problem, as well as the derivation of a magneto-mechanical model for the quantification of measurement uncertainties due to mechanical vibrations and positioning errors.

The model-based post processing using Bayesian inference is put into a general framework, which is applied to three different problems, appearing in the context of magnetic measurements.

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1 Introduction

Magnetic fields generated by electromagnets are widely used in physical experiments to guide and focus particle trajectories. This enables the control, the storage and hence the experiments with ions, isotopes and subatomic particles. The interaction between the particle motion and the electromagnetic field is governed by the Lorentz force

$$\boldsymbol{F} = q\left(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}\right),\tag{1.1}$$

where q is the particle's charge, and v its velocity vector. The Lorentz force is the sum of an accelerating force, proportional to the electric field E and a deflecting force, the velocity v and the magnetic flux density B. As B generates a force perpendicular to the particle velocity v, no net energy is gained for a passage through the magnetic field. This is why acceleration in particle physics is realized by strong electric fields, generated in radio-frequency (RF) cavities [1]. The interaction by means of the magnetic flux density B is used to steer the particle motion in a desired direction. For this purpose, electromagnets (normal or superconducting), permanent magnets or combinations of these technologies are used for bending and focusing the beam, and for the correction of abberations in beam related quantities, which are important for the beam quality and stability.

1.1 The mandate of the testing and magnetic measurement section

This thesis summarizes the work carried out during a doctoral student placement at the European Organization for Nuclear Research (CERN), in the section for testing and measurement of normal and superconducting magnets (TE-MSC-TM). The mandate of the test and measurement section is closely linked to the life cycle of an accelerator magnet as summarized in the flow-chart in Fig. 1.1.

It all begins with the specification of a list of field requirements for the physical experiment. This may include the magnet's bending strength, field gradient, field homogeneity, and the specification of budgets for field and alignment errors when the magnet is installed in the accelerator complex. The magnet design must consider the requirements stated before, as well as additional constraints that affect the choice of magnet technology, materials, and the available budget. At this stage, the magnet prototype relies on numerical tools in order to solve the multi-physics problem and to predict the behavior of the physical object that will later be installed in the accelerator.

Especially for superconducting accelerator magnets, the routine for the optimization of magnet X-sections, inverse field calculation and coil end design, short *ROXIE*, has been developed [2]. In ROXIE, a finite element solver for the computation of iron magnetization is coupled with boundary element formulations for the computation of coil fields and the evaluation of field distributions in the air gap. In this way, the domain discretization in the vicinity of the particle beam can be avoided and the evaluation of the integral equation for field evaluation enjoys a smoothing property of the approximation errors in the iron domain.



Figure 1.1: Tests and measurements are required at different stages of the life cycle of an accelerator magnet.

The required tolerance for errors in the prediction of field integrals in accelerator magnets is often in the range of 1 unit in 10 000. Predictions of modern-day numerical field simulation, such as the ones provided by ROXIE, are capable to provide the required accuracy in the case of linear, isotropic and homogeneous material properties. This is the case for the evaluation of Biot-Savart integrals, establishing the relation between field and current. However, most of the material laws rely on macroscopic models, which are often empirically determined and based on measurements rather than first-principle physical relations. This is the case for all material laws involved in iron saturation and hysteresis modeling, as well as for hysteresis effects occurring in superconducting cables.

Elaborate measurement campaigns (cf. Fig. 1.1 (1)) have therefore been performed over the years in order to validate the predictions of numerical field computation. In some cases, such validated numerical codes achieve the required accuracy. This is the case for the computation of field transients in superconducting magnets affected by superconductor magnetization, or transient effects due to eddy currents in coil dominated magnets. However, the interdependence of iron saturation, hysteresis, eddy currents, and temperature effects, involving empirical material properties, is still too complex to expect the same performance in case of iron dominated magnets.

With a prototype fully validated, the production of the series magnets can be launched. In the this phase, electric, geometric and magnetic measurements are performed at different stages to follow up the manufacturing process and to intercept production errors (cf. Fig. 1.1 (2)). To give some examples: cables and coils, are tested at room or cryogenic temperatures, samples of the iron yoke are characterized by permeability measurements, and collars supporting the assembly are tested to resist physical stress.

To emphasize the difference to the numerical prototype, the real magnet, which is the result of the manufacturing process, is marked in green. Even with the most careful production follow-up, one cannot exclude all possible errors affecting the magnet performance. Mechanical tolerances and uncertainties in the production process may sum up and lead to field errors exceeding the specifications. But even without such manufacturing errors, the presence of modeling errors and uncertainties in the design phase might have a non-negligible impact on the magnetic field quality. As a result, a third measurement campaign is necessary in order to characterize the magnet, as built, in almost all cases (cf. Fig. 1.1 (3)). Depending on the application, the magnet's transient behavious, current versus field transfer function, field quality, or fringe fields might be of interest.

Even though the magnets true physical state, after an arbitrary excitation history, might not be predictable to the required accuracy, it is reproducible after a well defined current cycles. For this reason the static magnetic field is characterized on plateaus of the excitation current, after well defined demagnetization and precylcing. Measurements of this kind have a long history as they have been adopted to assess the field quality in normal conducting magnets for more than half of a century [3]. Most established approaches make use of rotating induction coils and express the integrated field quality in a cylindrical magnet bore by means of multipolar fields, also known as *field harmonics*.

Another mandate of the TE-MSC-TM section, are real-time magnetic field measurements (cf. Fig. 1.1 (4)). Such measurements are required to give direct feedback during the operation of the accelerator complex. Here, the measurement equipment is installed inside the magnet, either at a position not occupied by the particle beam or inside a separate reference magnet powered in the same circuit as the magnets in the accelerator. Monitoring the magnetic field during the magnet cycling is required for all iron dominated magnets in particle accelerators, as iron hysteresis and saturation effects in the magnet end-plates are difficult to predictable.

1.2 The field model

Field harmonics may be regarded as a mathematical model for the integrated field in an accelerator magnet. Characterizing the field in this way has several benefits:

- 1. Link to beam dynamics: The effects of multi-polar fields on beam related quantities are well understood and thus can be seen as a direct link between magnet production and particle physics. As an example, the measured multipole errors of the LHC bending dipole magnets have been used for particle tracking simulations, in order to find optimal magnet arrangements with respect to beam quality and stability. Moreover, corrector magnets have been designed particularly to counteract the impacts of measured multipole errors in the main dipole and qaudrupole magnets.
- 2. **Scaling laws:** Knowing the field at a given radius inside the magnet bore, allows one to scale the results to different radii, by means of scaling laws derived from multipole theory. In this way, the field can be fully characterized by the measured quantities at a reference radius.
- 3. Exact magneto-static solution: Field harmonics are solutions to Maxwell's equations. Extracting field harmonics from the measurement data filters out non-physical solutions, which might stem from random or systematic measurement errors.

Field harmonics are most convenient for integrated fields in cylindrical magnets. As an extension to arbitrarily shaped, two dimensional domains, formulations by means of boundary element methods have been adopted in [4] and [5], and the stretched wire technique was used to measure the magnetic flux through the boundary of the domain of interest. This technique is capable to provide field-quality maps considerably faster than sampling on a two-dimensional grid. Moreover, measurement errors are restricted to the domain boundary

and evaluating the integral equation yields an exact magneto-static solution. In this way a smoothing property for random and systematic measurement errors is accomplished.

Field integrals alone may not provide all the required insight for particle tracking, as the magnetic field strays non-linearly in the magnet extremities. This is true for spectrometer magnets [6], strongly curved bending magnets [7] and focusing lenses exhibiting large diameters [8]. The benefit of relying on field models, such as multipoles or boundary element methods, rather than direct measurements, increases drastically when three dimensional field distributions are required. The number of measurements M needed to sample the field in a three dimensional grid of resolution h scales like $M \propto O(1/h^3)$, whereas sampling the domain boundary only requires $M \propto O(1/h^2)$ measurements. This might reduce the overall measurement duration from several days to a few hours. The idea of using measured boundary data to characterize the three dimensional field distribution in an arbitrarily shaped domain may be seen as the trigger of this research [5].

Particle tracking codes require *a good interpolation method that interpolates both the field values and the derivatives accurately* ([9] p. 254). Special finite-element and boundary-element approaches have been developed in order to express the magnetic field in the vicinity of the reference orbit and to use these formulations for particle tracking [10] [11]. This thesis ties in with the approaches presented in [5], [7] and [12], as a field model derived from boundary-integral equations will be presented.

1.3 The generic inverse problem

Although the physical background and a more detailed mathematical description will be the subject of chapter 3, a generic problem statement is now formulated.

Consider a domain Ω in the air gap of a particle accelerator magnet. The field is expressed by means of a scalar function, i.e., the *magnetic scalar potential* $\phi_m : \Omega \to \mathbb{R}$. The physical relations of the magneto-static field in Ω are implied if a partial differential equation holds for ϕ_m ; the *Laplace* equation $\Delta \phi_m = 0$. The function ϕ_m , and therefore the physical state of the magneto-static field, is uniquely determined if a boundary condition is given for ϕ_m . This means explicitly that ϕ_m , or its outward directed normal derivative¹ $\partial_n \phi_m$ is given by means of a function ν on the boundary $\partial \Omega$. A domain Ω , its boundary $\partial \Omega$ and the potential ϕ_m , are shown in Fig. 1.2 in two dimensions. The challenge lies in the determination of the *boundary data* ν , from magnetic measurements.

A measurement provides a vector of M measurement data $y = y_{det} + \epsilon \in \mathbb{R}^M$. Here, it is beneficial to differ between the deterministic part y_{det} and the error term ϵ . The latter accounts for microscopic and macroscopic effects such as the electronic noise of a sensor and errors due to perturbations of the measurement position.

From the physical properties of the magneto-static field, as well as the sensor, a mathematical model for the measurement process can be derived. This yields a comparable quantity to the deterministic part y_{det} , which will be denoted as *predicted measurement* \tilde{y} . The result of the mathematical modeling is an *observation operator* $H : (\nu, \theta) \mapsto \tilde{y}$ which maps the boundary data to \tilde{y} .

As it will be useful in later discussions, the observation operator is formulated in terms of *sensor parameters* θ , which can express the sensor orientation and positioning perturbations.

¹It will be discussed in chapter 3, how to restrict the function space for a unique formulation in case of the latter boundary condition.



Figure 1.2: Problem domain Ω (gray), in the air gap of an electromagnet. Its boundary is denoted by $\partial \Omega$. The magnetic scalar potential ϕ_m , and therefore the field, is uniquely determined by means of the boundary data ν on $\partial \Omega$.

Due to the error term ϵ , an exact solution of the inverse problem usually does not exist, nor is it desired, as it would fit to the error term ϵ , an effect known as *over-fitting*. The number of measurements M is finite, whereas the boundary data ν are generally in an infinite dimensional function space. To obtain a unique solution of the inverse problem, ν must be approximated in finite dimensions. Therefore the predicted measurements \tilde{y} might differ from the deterministic part y_{det} due to the approximation of ν . In the end, the equivalence between y and \tilde{y} must be established by minimizing the error expressed in some error metric $\|\cdot\|_*$, such as the sum of the squared differences between y and \tilde{y} scaled with the measurement accuracy.

Combining all these aspects yields a generic inverse problem:

Definition 1 (The generic inverse problem)			
For a given	$oldsymbol{y} \in \mathbb{R}^M$,		
find:	the boundary data $ u$,		
such that:	$\ oldsymbol{y}-(oldsymbol{H}(oldsymbol{ heta}) u)\ _*\stackrel{!}{=}\min$,		
subject to:	$\Delta \phi_{ m m}(m{r})=0,$	$oldsymbol{r}\in\Omega$,	
where:	$ u$ is a boundary condition for $\phi_{ m m}(r')$,	${m r}'\in\partial\Omega.$	

The first applications of using measurements to determine ν , were based in direct measurements along the domain boundary [4] [5]. In this case the observation function can give a direct relation to ν , without the need to solve $\Delta \phi_m = 0$. It was found early in this research, that direct boundary measurements are difficult to realize. The boundary of the domain of interest usually matches with the magnet poles or the vacuum chamber, while particle beams might occupy all the available space. Bringing the sensor close to this boundary is a non-trivial task, and particular measurement equipment needs to be designed [13].

Fig. 1.3 shows images of standard measurement equipment, developed in the TE-MSC-TM section at CERN. Some aspects of these systems concerning the direct measurement of boundary data are:

- Rotating-coil measurement system use arrays of induction coils, mounted on different radii, in order to improve their sensitivity for certain multipole components [14].
- Translating induction coils need to be supported by rails on a sledge, limiting the minimal distance between the coils and yoke to some centimeters [15].
- Hall-probe measurements use bulky sensor heads, covering the Hall sensors for thermal stabilization. Cross sensitivity errors due to probe misalignment affect the sampling of the three components of the magnetic flux density. Moreover, the offsets between the Hall elements in three-axes measurements are often not negligible.

In this thesis, the assumption for boundary measurements is relaxed, which enables the use of standardized measurement equipment. All that is needed is a more comprehensive mathematical model for the observation operator H, including the influence of three dimensional magneto-static fields.

The alternative approach to definition 1, which is usually followed when field maps in accelerator magnets are required, is to distribute measurements on a grid in Ω and interpolate between the measurement positions. Reconstructing the field by means of definition 1, has the following advantages:

- 1. A magnetic potential is obtained from measured voltages.
- 2. The magneto-static solution is implied in the field reconstruction.
- 3. Only the domain boundary needs to be sampled with measurements.

1.4 The blueprint

Throughout this work, field models and sensor systems will be considered for different kinds of application. This will yield different versions of the generic inverse problem. The solution, however, will follow the same pattern. This pattern is denoted as the *blueprint*, shown in Fig. 1.4. It may also be considered as a guide through the chapters of this thesis.

In the center of all considerations are the quantities of interest, which comprise the magnetic flux density B, as well as the magnetic scalar and the magnetic vector vector potentials, ϕ_m and A. Whereas all quantities are equally well suited for the reconstruction of the magnetic field, the magnetic vector potential A is often the basis for particle tracking algorithms. Chapter 2 therefore starts by introducing the requirements for particle beam dynamics.

The numerical field model has the capability to predict the quantities of interest within the magnet bore from given boundary data ν . To this end, physical relations are exploited to derive prediction operations, similar to the scaling laws used for multipole fields. The mathematical modeling used to derive the field model is described in chapter 3.

Sensors used for magnetic measurements do not provide direct observations of the magnetic field. For instance, induction coils provide a voltage proportional to the rate of change of flux linked with the coil area. Hall sensors are generating voltages with a non-linear dependency on the components of the flux density. The magnetic flux density B can therefore never be measured directly, and needs to be *inferred*, based on a mathematical model.



Figure 1.3: Various sensor systems used for magnetic measurements. Top left: Rotating radial coil array. Top right: Translating induction coil system using a sledge to move induction coils through the magnetic field. Bottom: Three-axes, Hall cube embedded in a sensor head for thermal stabilization.



Figure 1.4: Blueprint for the treatment of inverse problems in the context of magnetic measurements. The aim is to reconstruct the magnetic field inside an accelerator magnet from measurement data y_i , affected by measurement errors. The magnetic field may be expressed by means of the magnetic flux density B, the magnetic scalar potential ϕ_m , or the magnetic vector potential A. These are the quantities of interest. The physical relations of the magnetic field are implied when deriving the quantities of interest by the solution of a partial differential equation; $\Delta \phi_{\rm m} = 0$. Moreover, expressing the field as the solution of a boundary value problem, only the boundary data ν is needed to uniquely determine the field. In order to derive a quantity comparable to y_i , a numerical model for the sensor system is derived. This model may comprise sensor parameters θ , and provides a sensitivity function $s: (B, \theta) \mapsto U \in \mathbb{R}$. Linking the field model with the sensor model yields the observation operator H which maps ν and θ to the comparable quantity \tilde{y} . The challenge lies in the inference of ν from measurements y. The Bayesian framework provides the means to blend data with physical relations and prior knowledge in the inference process. This not only allows to quantify uncertainties in ν , but also establishes the framework for active learning algorithms, which are exploring the physical space based on uncertainties in the quantities of interest.

This model must comprise the field and the sensor in order to derive a quantity that is comparable with the measurement data. Deriving a numerical model for the sensor system requires the investigation of all physical effects on the measurement data; a *metrological characterization*. To this end, chapter 4 describes all the steps necessary at the example of a new three-axes Hall-probe mapper, which has been fully commissioned and characterized within the scope of this doctoral thesis. The result is a *sensitivity function* $s : (B, \theta) \mapsto U \in \mathbb{R}$, mapping the magnetic flux density B and sensor parameters θ to the voltage $U \in \mathbb{R}$. The observation operator can be derived by linking the sensor and field models.

There is a fundamental difference between the sensor parameters θ and the boundary data ν , as only ν is needed for the prediction of the quantities of interest. Explicitly, θ will comprise perturbations in sensor positioning and orientation, but it might also include other physical quantities affecting the measurement outcome, such as the temperature and Hall current.

All downstream arrows in the blueprint relate to *forward calculations*, which are the basis for sensitivity analyses in the design phase of a measurement system. The observation operator H is designed in a way that the predicted measurement \tilde{y} is uniquely determined by the boundary data ν , given the sensor parameters θ . This, however, is not true for the *inverse problem* inferring from y to ν .

This leads to one of the core ideas of this work, namely to the use of statistical inference, not only to combine measurement data with physical modeling, but also to include *prior knowledge*. The concepts followed in this thesis are closely related to *data assimilation*, which *has recently reached the rank of a discipline per se* [16]. It developed from numerical weather forecasting, *but its application is becoming widespread in many other areas of climate, atmosphere, ocean and environment modeling* [16]. A good overview on data assimilation in the geosciences is found in [16].

In data assimilation, the state of a dynamical system is considered as an often discrete stochastic-dynamical system. In this way, model errors are represented as stochastic perturbations of the system dynamics. *Observations* of the real process are available from measurement data. Because of measurement errors and noise, these observations are naturally affected by randomness. Therefore also the observations are considered as a stochastic process. The two models are then fused by using the *Bayes rule of probability*, which yields update rules for the physical state whenever new data becomes available (see [17, Section 1.2]).

The assumption of Gaussian distributions for the dynamical and the observation model leads to the *Kálmán filter* [18], which is widely used in real time tracking applications, such as the guidance, navigation, and control of aircrafts [19]. In the framework of Gaussian distributions, the stochastic physical state of the system can be described by its first two statistical moments, namely the mean and the covariance matrix. In Kálmán filtering, the mean and the covariance matrix are propagated in time by means of prediction and update rules, involving only the solution of a set of linear equation systems.

Particularly in the context of the geosciences, the propagation of the full covariance matrix becomes infeasible, due to the high dimension of the state space. For this reason, the *ensemble Kálmán* filter has been developed [20], which approximates the full covariance matrix by means of a smaller-dimensional *ensemble* of state vectors. The ensemble Kálmán filter may therefore be regarded as a special type of particle filter, where a set of samples, called "particles", is representing the statistics of the state variables [21].

In addition to the reduced computational complexity, the ensemble Kálmán filter allows for an observationmatrix free implementation (see [22, Section 3]). This is of advantage, because the observation operator might require the solution of a linear equation system in order to imply $\Delta \phi_m = 0$, or might not be available in matrix format because of the high memory requirements. In [23], for instance, it is shown how to efficiently use conjugate gradient iterations for data assimilation problems involving the solution of sparse linear equation systems. In [24] a Kálmán filter powered by hierarchical (H2) matrices is presented and applied to the tracking of fluid movement based on measurement data. Hierarchical matrices enjoy great popularity also in computational electromagnetics, as they allow to drastically reduce the complexity of matrix multiplications and memory requirements [25].

The ensemble Kálmán filter has also been successfully applied to nonlinear, and non-Gaussian data-assimilation applications [26]. Even though the optimality of the state estimation requires a linear observation operator and Gaussian stochastic models, the ensemble may be computed from a nonlinear observation operator [20]. Although this is affected by errors, as the statistics are approximated by Gaussian distributions, in complex high-dimensional systems the ensemble Kálmán filter *is essentially the only way to do approximate inference, while alternative exact inference techniques can only be applied to highly simplified versions of the problem* [26].

At CERN, data assimilation and Kálmán filtering is applied for the reconstruction of charged particle trajectories and particle-beam related quantities, based on detector plane or beam profile measurements. Recent advances are reported in [27] [28] and [29].

The idea of using Bayesian inference for the blueprint problem in the context of magnetic measurement data was first formulated in [11] and applied to the analysis of rotating coil measurements in [10]. These approaches are conceptually related to data-assimilation, whereas in the magneto-static scenario, the dynamic state propagation is an identity transformation.

One of the key results of this thesis is the development of an *active learning algorithm*, which uses an ensemble Kálmán filter to update field estimates by taking new measurements at locations with large uncertainty [30]. In this way, the physical space is explored dependent on the uncertainties in the quantities of interest. This principle is illustrated in Fig. 1.5 and it will be described in chapter 5.

Theory is put into practice in chapter 6, where three inference problems will be presented. All three problems will require different sensor and field modelling. Even if the boundary data ν , sensor parameters θ and measurements y might change widely in their physical nature, the post-processing will always follow the blueprint, which is why the same notation for ν , θ and y will be adopted. Remarks about the physical nature of all variables will be given at the beginning of each subsection of chapter 6.



Figure 1.5: Active learning applied to three dimensional field mapping. The principle is illustrated for measurements in a curved dipole magnet (1). The measurement system provides measurements in the left fringe field (2). In block (3), a Kálmán update is performed. This update combines the measurement data with prior knowledge for the mean and the covariance of the boundary data. The mean and variance are illustrated for prior and posterior. The update improves the variance in the left side of the domain. In block (4), the uncertainties are propagated to the quantity of interest. Here the uncertainty in the field along a reference trajectory is shown. Based on the local uncertainties, new measurement positions are identified and transferred to the system (5). The updated mean and covariance are considered as prior knowledge for the next Kálmán update (6).

2 Particle Beam Dynamics

The motion of a charged particle through the electromagnetic field can be expressed as the solution of a first order differential equations system

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{z} = \boldsymbol{f}(t, \boldsymbol{z}), \tag{2.1}$$

subject to initial conditions for t = 0. The particles *state vector* z(t) may comprise positions, momenta, velocities, or any other beam related quantity, such as a particle spin, mass or charge [31]. The fact that the system in Eq. (2.1) is of first order is not a restriction, since higher order systems can be reduced by introducing new variables of type $x = d^n z/dt^n$ [31]. The computation of the state vector z for a passage through an electromagnetic field, is frequently referred to as *particle tracking*.

In principle, one could derive the right-hand-side f from Newton's second law [32]

$$\frac{\mathrm{d}\boldsymbol{p}^{\mathrm{mech}}}{\mathrm{d}t} = \boldsymbol{F},\tag{2.2}$$

where p^{mech} is the particle momentum vector and F is the Lorenz force according to Eq. (1.1). However, this is not the approach generally taken in accelerator beam dynamics. The main reason is that solving Newton's second law involves integrating the equation of motion with respect to time, whereas in an accelerator beam line the electric and magnetic fields are usually specified as functions of position [32].

The path that is more often taken is to start with the *Hamiltonian equations of motion*, providing a way to reparameterize and obtain a more elegant formulation using the path length as independent variable rather than time. Moreover the Hamiltonian formalism provides a powerful tool to analyze the beam stability for repetitive systems, especially due to the conservation of certain invariants of motion.

The following subsections give a result-orientated overview of Hamiltonian mechanics and the Hamiltonian formulation used for particle tracking. The main objective of this thesis is to derive of a field model from measured data, which is capable of providing the required input data for particle tracking applications. The approach presented in chapter 3 is powerful as it is not tailored to one specific implementation and allows to compute field components, potentials, and their derivatives, as well as local field expansions in the vicinity of the particle trajectory.

2.1 Hamiltonian motion

The statement of Hamilton's principle is that the trajectory of a mechanical system is found in the minimum of a functional, frequently denoted as *action* S [33]. Considering the coordinate vector $\boldsymbol{q} = (x, y, z)^T$, which

describes the particle trajectory in three dimensions, the action between the two instants t_0 and t_1 is denoted by $S : q(t) \to \mathbb{R}$ and defined by

$$S(t_0, t_1, \boldsymbol{q}(t_0), \boldsymbol{q}(t_1)) = \int_{t_0}^{t_1} L(t, \boldsymbol{q}(t), \dot{\boldsymbol{q}}(t)) \,\mathrm{d}t.$$
(2.3)

 $L(t, q, \dot{q})$ is the *Lagrange function*, a smooth, real-valued function that is equal to the *difference* of kinetic and potential energies in a mechanical system. In the above equation and in what follows the dot denotes the time derivative d/dt. In a conservative system, where no energy is gained or lost, the Lagrangian *L* is an *invariant* of motion

$$\frac{\mathrm{d}L}{\mathrm{d}t} = 0. \tag{2.4}$$

In particle accelerators the motion is invariant in the case of static magnetic fields, when neglecting the effects of synchrotron radiation. This is known as the *principle of least action* [34]; the observed trajectory q(t) minimizes the action S and is computed by solving the *Euler-Lagrange* equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}} = \frac{\partial L}{\partial x}, \qquad \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{y}} = \frac{\partial L}{\partial y}, \qquad \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{z}} = \frac{\partial L}{\partial z}, \tag{2.5}$$

which one may summarize in the vector notation

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{\boldsymbol{q}}} := \frac{\mathrm{d}}{\mathrm{d}t} \begin{pmatrix} \frac{\partial L}{\partial \dot{x}} \\ \frac{\partial L}{\partial \dot{y}} \\ \frac{\partial L}{\partial \dot{z}} \end{pmatrix} = \begin{pmatrix} \frac{\partial L}{\partial x} \\ \frac{\partial L}{\partial y} \\ \frac{\partial L}{\partial z} \end{pmatrix} =: \frac{\partial L}{\partial \boldsymbol{q}}.$$
(2.6)

The same notation is adopted in the following for partial derivatives with respect to vectors in \mathbb{R}^3 : $\partial f/\partial x = (\partial f/\partial x_1, \partial f/\partial x_2, \partial f/\partial x_3)^T$.

Hamiltonian mechanics is a results of the Legendre transformation, defined as the map $(q, \dot{q}) \mapsto (p, q)$ [35]. p is the *canonical momentum*

$$\boldsymbol{p} = \frac{\partial L}{\partial \dot{\boldsymbol{q}}},\tag{2.7}$$

which is **not** the momentum variable $p^{\text{mech}} = m\dot{q}$, used in classical mechanics. The variables p and q describe the particle motion in an abstract phase space and are therefore denoted as *phase-space coordinates*. Taking the derivative of L with respect to time

$$\frac{\mathrm{d}L}{\mathrm{d}t} = \frac{\partial L}{\partial q} \cdot \dot{q} + \frac{\partial L}{\partial \dot{q}} \cdot \ddot{q}, \qquad (2.8)$$

and using equations Eq. (2.6) and (2.7), it yields [33]

$$\frac{\mathrm{d}}{\mathrm{d}t}\underbrace{(\boldsymbol{p}\cdot\dot{\boldsymbol{q}}-L)}_{:=H} = \frac{\mathrm{d}}{\mathrm{d}t}H = 0,$$
(2.9)

if the motion is conservative. Here the Hamiltonian H is defined as the transformed invariant of motion

$$H(\boldsymbol{p},\boldsymbol{q}) = \boldsymbol{p} \cdot \dot{\boldsymbol{q}} - L(\boldsymbol{q}, \dot{\boldsymbol{q}}). \tag{2.10}$$

The Hamiltonian has the physical meaning of the *sum* of kinetic and potential energy. From the Euler-Lagrange equations in phase space coordinates it yields *Hamilton's equations*

$$\frac{\mathrm{d}\boldsymbol{q}}{\mathrm{d}t} = \frac{\partial H}{\partial \boldsymbol{p}}, \qquad \frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = \frac{\partial H}{\partial \boldsymbol{q}}.$$
(2.11)

Defining $z := (x, p_x, y, p_y, z, p_z)^T$, one can derive a system of differential equations of type Eq. 2.1 describing the particle trajectory in phase space.

The explicit formulation of H is often derived from energy considerations [33]. The motion of a relativistic particle in a static electromagnetic field is governed by the Hamiltonian [32]

$$H = c\sqrt{(p - qA)^2 + m^2c^2} + q\phi.$$
 (2.12)

A is the magnetic vector potential ϕ is the electric scalar potential, q and m are the particle charge and mass, and c is the speed of light.

2.2 Accelerator Hamiltonian

A formulation based on the Hamiltonian given in Eq. (2.12) is inelegant, as it is formulated in terms of t as its independent variable. Moreover, it is beneficial to work with scaled variables and approximate power-series expressions. Therefore, transformations of variables are necessary. The new variables should also evolve according to Hamilton's equations. Such variables are known as *canonical variables* and a transformation between such is known as a *canonical transformation*. Details about deriving canonical transformations and how to transform Hamiltonians can be found in [32].

Of special interest in particle beam dynamics is the Hamiltonian in a curved coordinate system following the the design orbit of the beam. This Hamiltonian is frequently denoted as the accelerator Hamiltonian. The underlying coordinate system is shown in Fig. 2.1. Denoting a cartesian frame by capital letters (X, Y, Z) the curved coordinates x, y, s are defined as

$$X = (x + \rho) \cos\left(\frac{s}{\rho}\right) - \rho$$

$$Y = y$$

$$Z = (x + \rho) \sin\left(\frac{s}{\rho}\right)$$
(2.13)

and the reference curvature is given by $h = 1/\rho$. The components of the magnetic vector potential in the curved co-ordinates are given by

$$A_{x} = A_{X} \cos\left(\frac{s}{\rho}\right) - A_{Z} \sin\left(\frac{s}{\rho}\right)$$

$$A_{y} = A_{Y}$$

$$A_{s} = A_{Z} \cos\left(\frac{s}{\rho}\right) + A_{X} \sin\left(\frac{s}{\rho}\right),$$
(2.14)

where $A = (A_X, A_Y, A_Z)$ is the magnetic vector potential in the cartesian frame.

As the following result is well known in the community of particle beam dynamics, a derivation is omitted and the resulting Hamiltonian as well as the corresponding variables of motion are summarized in definition 2.



Figure 2.1: Curved coordinate system based on a circular reference trajectory (dashed). The x, y, scoordinates are shifted by ρ such that they are matching the X, Y, Z frame for s = 0.

Quantity	Meaning	Equation
c	speed of light	
s	path length	
P_0	reference momentum, often chosen as the longitudinal mo-	
	mentum of an ideal particle	
E	total particle energy	$E = \gamma mc^2 + q\phi$
eta_0	velocity of the reference particle, scaled by the speed of light	$\beta_0 = v_0/c$
γ_0	Lorentz factor of the reference particle	$\gamma_0 = \frac{1}{\sqrt{1 - \beta_0^2}}$
a_x	scaled horizontal magnetic vector potential	$a_x = qA_x/P_0^0$
a_y	scaled vertical magnetic vector potential	$a_y = qA_y/P_0$
a_s	scaled longitudinal magnetic vector potential	$a_s = qA_s/P_0$
ϕ	electric scalar potential	

Table 2.1: Quantities related to the relativistic Hamiltonian in scaled coordinates to compute the evolution of the variables of motion. The ideal particle travels with the designed longitudinal momentum.

Definition 2 The accelerator Hamiltonian for the motion of a relativistic particle traveling in a curved reference system of curvature h is given by [32]

$$H = \frac{\delta}{\beta_0} - (1+hx)\sqrt{\left(\delta + \frac{1}{\beta_0} - \frac{q\phi}{cP_0}\right)^2 - (p_x - a_x)^2 - (p_y - a_y)^2 - \frac{1}{\beta_0^2\gamma_0^2} - (1+hx)a_s.}$$
 (2.15)

The variables of motion are $z = (x, p_x, y, p_y, z, \delta)^T$. Their meanings and definitions are found in table 2.2. Definitions of other Hamiltonian related quantities are found in table 2.1.

Variable	Meaning	Equation
x	horizontal co-ordinate (Fig. 2.1)	
y	vertical co-ordinate (Fig. 2.1)	
z	longitudinal co-ordinate	$z = \frac{s}{\beta_0} - ct$
p_x	scaled horizontal momentum	$\frac{\beta_x \gamma mc + qA_x}{P_0}$
p_y	scaled vertical momentum	$\frac{\beta_y \gamma mc + qA_y}{P_0}$
δ	energy deviation	$\frac{E}{cP_0} - \frac{1}{\beta_0}$

Table 2.2: Summary of the variables of particle motion. These quantities are commonly used to describe the physical state of a particle and are related to a reference particle, traveling with velocity $c\beta_0$ and momentum P_0 . See table 2.1, for other motion related quantities.

2.3 Equations of motion

Equations of motion according to Eq. (2.1) can be derived from Hamiltons equations in the transformed variables

$$\frac{dx}{ds} = \frac{\partial H}{\partial p_x}, \qquad \frac{dp_x}{ds} = -\frac{\partial H}{\partial x},$$
(2.16)

$$\frac{dy}{ds} = \frac{\partial H}{\partial p_y}, \qquad \frac{dp_y}{ds} = -\frac{\partial H}{\partial y},$$
(2.17)

$$\frac{dz}{ds} = \frac{\partial H}{\partial \delta}, \qquad \frac{dp_z}{ds} = -\frac{\partial H}{\partial z},$$
(2.18)

imposing that [36]

$$\frac{d\boldsymbol{z}}{ds} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \end{pmatrix} \begin{pmatrix} \partial/\partial x \\ \partial/\partial p_x \\ \partial/\partial y \\ \partial/\partial p_y \\ \partial/\partial z \\ \partial/\partial \delta \end{pmatrix} H = \boldsymbol{f}(s, \boldsymbol{z}).$$
(2.19)

To derive explicit formulas, a suitable field representation by means of a magnetic vector potential A is substituted in the Hamiltonian and the partial derivatives are built. Computing the state of a particle at a position z_1 , with an initial condition at z_0 , involves the integration of the resulting expressions in s. There are two sources of approximation errors that need to be distinguished in this procedure: First, the approximation errors related to the expression for the magnetic vector potential A and second, errors accompanied with the numerical integration in s. Approaches to express A in the vicinity of the particle beam will be discussed in chapter 3.

2.4 Field-model requirements

To close this chapter it should be summarized that several approaches for the treatment of three dimensional fields in tracking codes have been developed, all tailored to slightly different applications [7] [37] [38] [39] [40] [41]. The goal of this thesis is to provide a general framework for the metrological determination of a field model, providing the data for any of the above implementations. This will prevail itself as a standard post-processing tool in the portfolio of the testing and magnetic measurement section at CERN. Five requirements for the field model can be formulated:

- 1. **Potential formulation:** The field shall be described by means of a magnetic scalar or vector potential, in a way that the three components of the magnetic flux density are accessible.
- 2. **Magneto-static solution:** Evaluating the field description shall always provide an exact local magnetostatic solution, obeying Maxwell's equations.
- 3. **Smooth solution:** Field derivatives [38] and local multipole expansions [7] of arbitrary order have to be accessible.
- 4. **Convergence:** Errors accompanied with numerical approximations should converge when increasing the complexity of the field solution.
- 5. **Uncertainty quantification:** Measurement uncertainties should be propagated to the potentials, field, and derivatives.

Field models meeting these requirements will be presented in chapter 3.

3 Magnetic Fields in Accelerator Magnets

Consider a simply connected, open domain Ω , free of currents and magnetic material, with sufficiently smooth boundaries. In the magneto-static case, the magnetic flux density *B* is governed by the equations:

$$\boldsymbol{r} \in \Omega \qquad \begin{cases} \operatorname{div} \boldsymbol{B}(\boldsymbol{r}) = 0, \\ \operatorname{curl} \boldsymbol{H}(\boldsymbol{r}) = \boldsymbol{0}. \end{cases}$$
 (3.1)

H is the magnetic field strength that relates to *B* via $H = 1/\mu_0 B$ in Ω. μ_0 is the vacuum permeability $\mu_0 = 4\pi 10^{-7} \text{Vs A}^{-1} \text{m}^{-1}$.

Physical relations can be simplified using potential formulations. Since curl grad f = 0, curl H(r) = 0 holds in Ω for gradient fields:

$$\boldsymbol{B} = -\mu_0 \operatorname{grad} \phi_{\mathrm{m}}.\tag{3.2}$$

Thus the magnetic field is equally well described by means of the *magnetic scalar potential* ϕ_m . Similarly, one can imply div B(r) = 0 by

$$B = \operatorname{curl} A, \tag{3.3}$$

where A is referred to as *magnetic vector potential*. The requirements for the existence of ϕ_m , and A are discussed in [42, Chapter 3.14]. Throughout this work, trivial domains Ω are considered for which all requirements are met.

The definitions for ϕ_m and A by means of the differential operators grad and curl are not unique. Obviously, any magnetic scalar potential $\phi_m^* = \phi_m + c$, with $c \neq f(r)$ yields the same B. The same applies for $A^* = A + \text{grad } f$. The gauge functions c and f can be exploited to simplify the solutions of partial differential equations, or to save on computational demands in particle tracking [40].

Working with potential formulations allows to derive compact notations for the electromagnetism in Ω by means of partial differential equations. Substituting Eq. (3.2) in div B(r) = 0 yields

$$-\operatorname{div}\mu_0\operatorname{grad}\phi_{\mathrm{m}}=0. \tag{3.4}$$

Since μ_0 is constant,

$$\operatorname{div}\operatorname{grad}\phi_{\mathrm{m}} = \Delta\phi_{\mathrm{m}} = 0, \tag{3.5}$$

with the Laplace operator $\Delta f := \operatorname{div} \operatorname{grad} f$.

A similar equation for A is derived from Eq. (3.3) and curl H(r) = 0

$$\operatorname{curl} \frac{1}{\mu_0} \operatorname{curl} \boldsymbol{A} = \boldsymbol{0}, \tag{3.6}$$

which is known as the *curl-curl equation*.

In principle, both ϕ_m and A are equally suitable to express the magnetic field in the bore of an accelerator magnet. However, A is a vector field, whereas ϕ_m is a scalar field, associated with reduced computational

complexity. For this reason it is beneficial to first derive a closed solution for ϕ_m and then identify the components of A via the equivalence

$$\boldsymbol{B} = \operatorname{curl} \boldsymbol{A} = -\mu_0 \operatorname{grad} \phi_{\mathrm{m}}.$$
 (3.7)

Of particular importance for the field reconstruction from measurement data are cases where the potential $\phi_{\rm m}$ or its normal derivative $\partial_n \phi_{\rm m}$ are known at the boundary $\partial \Omega$. A partial differential equation, endowed with such a boundary condition is known as *boundary value problem*. The *Dirichlet problem* reads:

Find
$$\phi_{\mathbf{m}} \in \mathcal{V}$$
,
such that $\Delta \phi_{\mathbf{m}}(\mathbf{r}) = 0$, $\mathbf{r} \in \Omega$, (3.8)
subject to $\phi_{\mathbf{m}}(\mathbf{r}) = u(\mathbf{r})$, $\mathbf{r} \in \partial \Omega$,
with $u \in \mathcal{V}_{u}$.

The Neumann problem reads:

Find
$$\phi_{\rm m} \in \mathcal{V}$$
,
such that $\Delta \phi_{\rm m}(\mathbf{r}) = 0$, $\mathbf{r} \in \Omega$, (3.9)
subject to $\partial_{\mathbf{n}} \phi_{\rm m}(\mathbf{r}) = g(\mathbf{r})$, $\mathbf{r} \in \partial \Omega$
with $g \in \mathcal{V}_g^*$,
and $\int_{\partial \Omega} \phi_{\rm m}(\mathbf{r}') \, \mathrm{d}\mathbf{r}' = 0$

The gauge condition $\int_{\partial\Omega} \phi_{\rm m}(\mathbf{r}') d\mathbf{r}' = 0$, is needed for a unique formulation of the Neumann problem¹. The space of all functions $\phi_{\rm m} \in \mathcal{V}$ with $\int_{\partial\Omega} \phi_{\rm m}(\mathbf{r}') d\mathbf{r}' = 0$ will be denoted as $\mathcal{V}^* \subset \mathcal{V}$. The functions g with $\int_{\partial\Omega} g(\mathbf{r}') d\mathbf{r}' \neq 0$ must be excluded in case of the Neumann problem, otherwise the source free condition for the magnetic field according to Eq. (3.1) would be violated. One therefore defines \mathcal{V}_g^* such that $\forall g \in \mathcal{V}_g^* : \int_{\partial\Omega} g d\mathbf{r}' = 0$.

In the above boundary-value problems, the function spaces \mathcal{V} , \mathcal{V}_u and \mathcal{V}_g have been introduced for ϕ_m , u and g, without elaborating further on their properties. Details about the structure and mathematical properties of \mathcal{V} , \mathcal{V}_u and \mathcal{V}_g are found in [43, Chapter 4]. It will be seen in the following sections, that the approaches to solve boundary-value problems differ by means of the function spaces in which the solutions are sought for.

3.1 The problem statement

Representing the field by means of a Dirichlet or Neumann boundary condition, u or g and using Eq. (3.8) or (3.9) for the reconstruction of the field within Ω implies the physical relations for the magneto-static field. This is one of the core ideas followed in this thesis. The generic inverse problem (see definition 1) is now rewritten for the Dirichlet and Neumann problems:

¹The gauge function is implied with the boundary condition in case of the Dirichlet problem.

Definit	Definition 3 (The inverse problems for the magnetic scalar potential)			
		Dirichlet problem	Neumann problem	
For a g	given	$oldsymbol{y}\in \mathcal{Y}$	\mathbb{R}^{M} ,	
	find	$u \in \mathcal{V}_u$	$g\in\mathcal{V}_g^*$	
such	that	$\ \boldsymbol{y} - (\boldsymbol{H}(\boldsymbol{\theta})u)\ _* \stackrel{!}{=} \min$	$\ \boldsymbol{y} - (\boldsymbol{H}(\boldsymbol{\theta})g)\ _* \stackrel{!}{=} \min$	
subje	ect to	$\Delta \phi_{ m m}$ ($(oldsymbol{r})=0,$	$oldsymbol{r}\in\Omega$
	with	$\phi_{\mathbf{m}} \in \mathcal{V}$	$\phi_{\mathrm{m}} \in \mathcal{V}^{*}$	
	and	$\phi_{\mathbf{m}}(\boldsymbol{r}) = u(\boldsymbol{r}),$	$\partial_{\boldsymbol{n}}\phi_{\boldsymbol{m}}(\boldsymbol{r}) = g(\boldsymbol{r}),$	$r \in \partial \Omega.$

In accordance with the discussion in section 1.3, the measurement data are assumed to be distributed in Ω , and not on the boundary $\partial\Omega$. As it is central to the definition 1, some approaches to solve $\Delta\phi_m(\mathbf{r}) = 0$ in Ω are presented in the following sections. Depending on the approach, the problem statement may be reformulated.

3.2 The separation of variables method

Interpreting the left and right-hand side of the boundary-value problems, Eq. (3.8) and Eq. (3.9), as continuous functions, the minimum requirement for ϕ_m is its twice continuous differentiability, $\phi_m \in C^2$. Such a solution is called *strong solution* to the underlying problem. The separation of variables method leads to such a solution by choosing the formulation $\phi_m = A(\zeta)B(\xi)C(\chi)$. Here ζ , ξ and χ denote the coordinates of an orthogonal system. One then tries to separate the partial differential equation into a set of ordinary differential equations in $A(\zeta)$, $B(\xi)$ and $C(\chi)$. From the eigensolutions of these ordinary differential equations, one can construct homogeneous solutions for the Laplace equation by linear combination. The coefficients of this linear combination are identified to match a given boundary condition.

In three dimensions, there are eleven orthogonal coordinate systems based on surfaces of first and second degree [44]. It is shown in [45], that all of these coordinate systems allow for the separation of the Laplace equation. Some popular examples are cartesian, cylindrical, and spherical coordinates. To express the boundary conditions in a simple way, one must have iso-surfaces that fit the physical boundaries of the problem [46]. This limits the applicability of the approach to basic geometries such as the ones listed in [44].

Of particular interest for the field representation in accelerator magnets is the case of repetitive cylindrical systems, for instance in multipole magnets. For this reason, one may express ϕ_m in cylindrical coordinates with a periodic boundary condition along z; see [32, Section 1.3.2] for the field representation in such geometries. On the other hand, spherical geometries will also be important throughout this thesis. Table 3.1 gives the homogeneous solution of the Laplace equation in spherical coordinates, a figure of the iso-surfaces, and the relevant boundary conditions. The definitions of the associated Legendre polynomials P_l^m are found in [47] and [48].

The benefit from expanding the field into eigenfunctions is that $\Delta \phi_m = 0$ is intrinsically implied by the ansatz. Let us denote by $\boldsymbol{\nu} = \{\nu_{l,n}\}$ the *state vector of the magnetic field*, containing the coefficients of a truncated harmonic expansion, for instance, according to table 3.1, and by $\psi_l^n(\boldsymbol{r})$ the corresponding eigenfunctions. The inverse problem can be approximated in span (ψ_l^n) for the index sets $\{l\}, \{n\} \subset \mathbb{Z}$. The resulting problem is



Table 3.1: Series expansion of the homogeneous solution of the Laplace equation in spherical coordinates.

given in definition 4. In this case, the observation operator can be formulated in terms of the state vector ν and the sensor parameters θ .

Definition 4 (The inverse problem using separation of variables)				
For a given	$oldsymbol{y} \in \mathbb{R}^M$,			
find	$oldsymbol{ u} = \{ u_{l,n}\} \in \mathbb{C}^K$			
such that	$\ oldsymbol{y}-oldsymbol{H}(oldsymbol{ heta},oldsymbol{ u})\ _* \stackrel{!}{=} \min$			
with	$K = \operatorname{card}(\{l\} \times \{n\})$			

The total number of expansion coefficients K depends on truncating the l and n sums, which introduces approximation errors. Nevertheless, since eigenfunctions are used, $\Delta \psi_l^n(\mathbf{r}) = 0$, and the truncation is still a "Maxwellian" solution of the magneto-static problem.

3.3 Boundary element methods

The separation of variables method is limited to simple geometries in which the boundaries of the computational domain match the iso-surfaces of an underlying orthogonal coordinate system. In boundary element methods (BEM), this assumption is relaxed and the partial differential equation in Ω is transformed into an integral equation at the boundary $\partial\Omega$ that can describe more complex geometries. To cope with the dimensionality of the problem, only the boundary data is approximated on a boundary mesh, using locally supported basis functions. This has the following benefits over finite element methods (FEM), where the entire volume in Ω is discretized and approximated with local basis functions:

- 1. Boundary element methods possess a smoothing property to approximation errors in the solution domain.
- 2. Only the domain boundary needs to be discretized. This yields a reduced complexity with respect to finite element approximations.
- 3. High convergence rates for the evaluation inside the domain are achieved, not only for the potentials, but also for the spatial derivatives of arbitrary order.

3.3.1 The representation formula

The boundary integral equation can be derived from Gauss' integral theorem:

Theorem 3.3.1 (Gauss' integral theorem) Let $\Omega \subset \mathbb{R}^d$ be a compact (closed and bounded) domain with a piecewise smooth boundary $\partial\Omega$, and F be a continuously differentiable vector field $\mathbb{R}^d \mapsto \mathbb{R}^d$, then

$$\int_{\Omega} \operatorname{div} \boldsymbol{F}(\boldsymbol{r}') \, \mathrm{d} \boldsymbol{r}' = \int_{\partial \Omega} \boldsymbol{n}(\boldsymbol{r}') \cdot \boldsymbol{F}(\boldsymbol{r}') \, \mathrm{d} \boldsymbol{r}',$$

where n is an outward directed normal field at $\partial \Omega$.

Substituting F(r') = v(r')grad $\phi_m(r') - \phi_m(r')$ grad v(r') in Gauss' integral theorem yields Green's second identity

$$\int_{\Omega} v(\mathbf{r}') \Delta \phi_{\mathrm{m}}(\mathbf{r}') - \phi_{\mathrm{m}}(\mathbf{r}') \Delta v(\mathbf{r}') \,\mathrm{d}\mathbf{r}'$$

$$= \int_{\partial \Omega} v(\mathbf{r}') \,\partial_{\mathbf{n}} \phi_{\mathrm{m}}(\mathbf{r}') \,\mathrm{d}\mathbf{r}' - \int_{\partial \Omega} \phi_{\mathrm{m}}(\mathbf{r}') \,\partial_{\mathbf{n}} v(\mathbf{r}') \,\mathrm{d}\mathbf{r}',$$
(3.11)

with the normal derivative $\partial_n f(\mathbf{r}) = \mathbf{n}(\mathbf{r}) \cdot \operatorname{grad} f(\mathbf{r})$. One then chooses $v(\mathbf{r}') = u^*(\mathbf{r}, \mathbf{r}')$ with $u^*(\mathbf{r}, \mathbf{r}')$ satisfying the sampling property

$$-\int_{\Omega}\phi_{\rm m}(\boldsymbol{r}')\Delta_{\boldsymbol{r}'}u^{*}(\boldsymbol{r},\boldsymbol{r}')\,\mathrm{d}\boldsymbol{r}'=\phi_{\rm m}(\boldsymbol{r}),\tag{3.12}$$

such that $\Delta_{{\pmb r}'} u^*({\pmb r},{\pmb r}')$ can be identified with the Dirac delta distribution

$$\Delta_{\mathbf{r}'}u^*(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'). \tag{3.13}$$

Functions satisfying Eq. (3.13) in the distributional sense are called *fundamental solutions*. The fundamental solutions of the Laplace equation in two and three dimensions are given by

$$u^{*}(\boldsymbol{r},\boldsymbol{r}') = \begin{cases} -\frac{1}{2\pi} \log \frac{|\boldsymbol{r}-\boldsymbol{r}'|}{R}, & \boldsymbol{r} \in \mathbb{R}^{2} \\ \frac{1}{4\pi} \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|}, & \boldsymbol{r} \in \mathbb{R}^{3} \end{cases}$$
(3.14)

Scaling the argument in $\log |\cdot|$ with $R \in \mathbb{R}$, for the two dimensional case, has the advantage that the ellipticity of a certain integral operator may be achieved by choosing $R > \operatorname{diam}(\Omega)$ (see [43], Theorem 6.23). In the three dimensional case, this scaling is not necessary.

With $v(\mathbf{r}') = u^*(\mathbf{r}, \mathbf{r}')$ and $\Delta \phi_m(\mathbf{r}) = 0$ one then finds the *representation formula* for the Laplace equation

$$\phi_{\mathrm{m}}(\boldsymbol{r}) = \int_{\partial\Omega} u^{*}(\boldsymbol{r}, \boldsymbol{r}') \,\partial_{\boldsymbol{n}} \phi_{\mathrm{m}}(\boldsymbol{r}') \,\mathrm{d}\boldsymbol{r}' - \int_{\partial\Omega} \phi_{\mathrm{m}}(\boldsymbol{r}') \,\partial_{\boldsymbol{n}} u^{*}(\boldsymbol{r}, \boldsymbol{r}') \,\mathrm{d}\boldsymbol{r}' \\ = \underbrace{(\widetilde{V}\partial_{\boldsymbol{n}}\phi_{\mathrm{m}})(\boldsymbol{r})}_{\text{single layer potential}} - \underbrace{(W\phi_{\mathrm{m}})(\boldsymbol{r}),}_{\text{double layer potential}} \qquad \boldsymbol{r} \in \Omega,$$
(3.15)

in terms of the single layer- and double layer potentials \tilde{V} and W.

The appearance of single- and double-layer potentials can be understood as placing fictitious magnetic monopoles and dipoles at $\partial\Omega$ in order to represent the field in the interior domain. Evaluating the right-hand-side in the *exterior domain* $\Omega_c := \mathbb{R} \setminus \Omega$, yields zero,

$$0 = (\tilde{V}\partial_{\boldsymbol{n}}\phi_{\mathrm{m}})(\boldsymbol{r}) - (W\phi_{\mathrm{m}})(\boldsymbol{r}), \qquad \boldsymbol{r} \in \Omega_{\mathrm{c}}, \tag{3.16}$$

which is known as *null property*.

3.3.2 Indirect formulations

The null property can be exploited to reduce one of the integrals in the representation formula. The fact that the exterior domain is masked out by the combination of single and double layer potentials, motivates the definition of an artificial exterior problem:

$$\Delta \phi_{\rm m}^{\rm ext}(\boldsymbol{r}) = 0, \qquad \boldsymbol{r} \in \Omega_{\rm c}, \tag{3.17}$$

subject to either a Dirichlet- or Neumann-type boundary condition. For Eq. (3.17) holds the representation formula

$$\begin{cases} 0\\ \phi_{\rm m}^{\rm ext}(\boldsymbol{r}) \end{cases} = -(\widetilde{V}\partial_{\boldsymbol{n}}\phi_{\rm m}^{\rm ext})(\boldsymbol{r}) + (W\phi_{\rm m}^{\rm ext})(\boldsymbol{r}) \begin{cases} \boldsymbol{r} \in \Omega\\ \boldsymbol{r} \in \Omega_{\rm c} \end{cases}$$
(3.18)

Taking the sum of Eq. (3.15) and Eq. (3.18) yields

$$\phi_{\mathbf{m}}(\mathbf{r}) \\ \phi_{\mathbf{m}}^{\mathsf{ext}}(\mathbf{r}) \\ \right\} = (\widetilde{V} \llbracket \partial_{\mathbf{n}} \phi_{\mathbf{m}} \rrbracket)(\mathbf{r}) - (W \llbracket \phi_{\mathbf{m}} \rrbracket)(\mathbf{r}) \begin{cases} \mathbf{r} \in \Omega \\ \mathbf{r} \in \Omega_{\mathsf{c}} \end{cases}$$
(3.19)

where

$$\llbracket \phi_{\mathbf{m}} \rrbracket = \phi_{\mathbf{m}} - \phi_{\mathbf{m}}^{\mathsf{ext}}, \quad \llbracket \partial_{\mathbf{n}} \phi_{\mathbf{m}} \rrbracket = \partial_{\mathbf{n}} \phi_{\mathbf{m}} - \partial_{\mathbf{n}} \phi_{\mathbf{m}}^{\mathsf{ext}}, \tag{3.20}$$

are the jump discontinuitites in the Dirichlet and Neumann data, from the interior to the exterior domain. One can enforce the single or double layer potential to vanish, by imposing a Dirichlet or Neumann condition to the exterior problem (see definition 5).

Definition 5 (Indirect Formulations) For the Dirichlet condition $\llbracket \phi_m \rrbracket = 0$, the representation by means of the SINGLE LAYER POTENTIAL is

$$\phi_{\mathbf{m}}(\boldsymbol{r}) = (V[\![\partial_{\boldsymbol{n}}\phi_{\mathbf{m}}]\!])(\boldsymbol{r}) \quad \boldsymbol{r} \in \Omega.$$
(3.21)

For the Neumann condition $[\![\partial_n \phi_m]\!] = 0$, the representation by means of the DOUBLE LAYER POTENTIAL yields

$$\phi_{\mathbf{m}}(\boldsymbol{r}) = -(W[\![\phi_{\mathbf{m}}]\!])(\boldsymbol{r}) \quad \boldsymbol{r} \in \Omega.$$
(3.22)

3.3.3 The stream function

The densities $[\![\partial_n \phi_m]\!]$ and $[\![\phi_m]\!]$ do not coincide with the original Dirichlet and Neumann data ϕ_m and $\partial_n \phi_m$. The jump density $[\![\partial_n \phi_m]\!]$ can be interpreted as an artificial single layer of magnetic charges, while $[\![\phi_m]\!]$ has the meaning of a *stream function* generating surface currents on the boundary. This can be seen by reformulating the evaluation of the double layer potential.

Consider a stream function ν and the double layer potential formulation

$$\phi_{\mathrm{m}}(\boldsymbol{r}) = -(W\nu)(\boldsymbol{r}) = -\int_{\partial\Omega} (\boldsymbol{n}(\boldsymbol{r}') \cdot \operatorname{grad}_{\boldsymbol{r}'} u^*(\boldsymbol{r}, \boldsymbol{r}'))\nu(\boldsymbol{r}') \,\mathrm{d}\boldsymbol{r}'.$$
(3.23)

Here and in the following the subscripts in $grad_{(.)}$ and $curl_{(.)}$ denote the variables to which the operation is applied. Computing the magnetic field $B = -\mu_0 \operatorname{grad} \phi_m$ yields

$$\boldsymbol{B}(\boldsymbol{r}) = \mu_0 \operatorname{grad}_{\boldsymbol{r}} \int_{\partial \Omega} (\boldsymbol{n}(\boldsymbol{r}') \cdot \operatorname{grad}_{\boldsymbol{r}'} u^*(\boldsymbol{r}, \boldsymbol{r}')) \nu(\boldsymbol{r}') \, \mathrm{d}\boldsymbol{r}'.$$
(3.24)
At this stage one can make use of the equivalence of a double layer and an eddy ring [49]:

$$\begin{aligned} \operatorname{grad}_{\boldsymbol{r}} & \int_{\partial\Omega} (\boldsymbol{n}(\boldsymbol{r}') \cdot \operatorname{grad}_{\boldsymbol{r}'} u^*(\boldsymbol{r}, \boldsymbol{r}')) \nu(\boldsymbol{r}') \, \mathrm{d}\boldsymbol{r}' \\ &= -\operatorname{curl}_{\boldsymbol{r}} \int_{\partial\Omega} (\boldsymbol{n}(\boldsymbol{r}') \times \operatorname{grad}_{\boldsymbol{r}'} u^*(\boldsymbol{r}, \boldsymbol{r}')) \nu(\boldsymbol{r}') \, \mathrm{d}\boldsymbol{r}' \\ &= -\operatorname{curl}_{\boldsymbol{r}} \int_{\partial\Omega} u^*(\boldsymbol{r}, \boldsymbol{r}') (\boldsymbol{n}(\boldsymbol{r}') \times \operatorname{grad}_{\boldsymbol{r}'} \nu(\boldsymbol{r}')) \, \mathrm{d}\boldsymbol{r}', \end{aligned}$$
(3.25)

where in the last operation, an integration by parts was used. As a result,

$$\boldsymbol{B} = -\mu_0 \operatorname{curl}_{\boldsymbol{r}} \int_{\partial\Omega} u^*(\boldsymbol{r}, \boldsymbol{r}')(\boldsymbol{n}(\boldsymbol{r}') \times \operatorname{grad}_{\boldsymbol{r}'} \nu(\boldsymbol{r}')) \, \mathrm{d}\boldsymbol{r}', \qquad (3.26)$$

which is equal to

$$\boldsymbol{B}(\boldsymbol{r}) = \operatorname{curl}_{\boldsymbol{r}} \boldsymbol{A}(\boldsymbol{r}), \qquad (3.27)$$

with the magnetic vector potential

$$\boldsymbol{A}(\boldsymbol{r}) = -\mu_0 \int_{\partial\Omega} u^*(\boldsymbol{r}, \boldsymbol{r}')(\boldsymbol{n}(\boldsymbol{r}') \times \operatorname{grad}_{\boldsymbol{r}'} \nu(\boldsymbol{r}')) \, \mathrm{d}\boldsymbol{r}'.$$
(3.28)

As the integral ([50], 5.28)

$$\boldsymbol{A}(\boldsymbol{r}) = \mu_0 \int_{\partial\Omega} u^*(\boldsymbol{r}, \boldsymbol{r}') \boldsymbol{s}(\boldsymbol{r}') \,\mathrm{d}\boldsymbol{r}'$$
(3.29)

has the physical meaning of a vector potential, generated by the *surface current density* s on $\partial\Omega$, one can define the *vectorial surface curl*

$$\operatorname{curl}_{\partial\Omega}\nu(\boldsymbol{r}') := -\boldsymbol{n} \times \operatorname{grad}_{\boldsymbol{r}'}\nu(\boldsymbol{r}'), \tag{3.30}$$

and interpret $\nu(\mathbf{r}')$ as a stream function, generating the surface current density² $s = \operatorname{curl}_{\partial\Omega} \nu$. A stream function and its resulting surface current density are illustrated in Fig. 3.1.

Eq. (3.23) and Eq. (3.28) provide the magnetic scalar and vector potentials ϕ_m and A by means of integral equations based on the boundary data ν . These results are summarized in definition 6.

Definition 6 (Dual boundary integral formulation for the magneto-static field) The magnetic scalar potential ϕ_m and the magnetic vector potential A can be traced back to the same density function ν . Whereas ϕ_m is defined by applying the double layer operator

$$\phi_{\rm m}(\boldsymbol{r}) = -(W\nu)(\boldsymbol{r}),\tag{3.31}$$

 $m{A}$ results from applying a single layer operator on the surface current density ${
m curl}_{\partial\Omega}
u$

$$\mathbf{A}(\mathbf{r}) = (\tilde{V}\operatorname{curl}_{\partial\Omega}\nu(\mathbf{r}')). \tag{3.32}$$

Here $\operatorname{curl}_{\partial\Omega}$ is the vectorial surface curl:

$$\operatorname{curl}_{\partial\Omega}\nu(\boldsymbol{r}') = -\boldsymbol{n} \times \operatorname{grad}_{\boldsymbol{r}'}\nu(\boldsymbol{r}'). \tag{3.33}$$

As the stream function ν describes the jump discontinuity in the Dirichlet data, it lies in the same function space as the Dirichlet data $u, \nu \in \mathcal{V}_u$.

²To be precise, ν needs to be interpreted as a smooth extension in the neighborhood of the domain boundary [51].



Figure 3.1: A stream function ν as contour plot generating a surface current density s. The stream function ν is constructed by tensor product cubic basis splines on a regular grid (black).

Remark 1 The forces which are acting on charges in the magneto-static field relate to the gradient of the magnetic scalar potential. Constant potentials do not affect the particle motion, nor can they be observed by measurements. As a consequence, the measurement operator \boldsymbol{H} has a non-trivial kernel, which means that $(\boldsymbol{H}(\boldsymbol{\theta})c) = 0$ for all constants $c \in \mathbb{R}$. In order to obtain a unique formulation for the inverse problem, the function space $\mathcal{V}_u^* \subset \mathcal{V}_u$ is used for the boundary data ν , containing all functions $\nu \in \mathcal{V}_u$ with $\int_{\partial\Omega} \nu(\boldsymbol{r}') d\boldsymbol{r}' = 0$.

The problem statement can now be formulated in terms of the stream function ν .

Definition 7 (The inverse problem using the indirect double layer formulation)For a given: $\boldsymbol{y} \in \mathbb{R}^M$,find $\nu \in \mathcal{V}_u^*$ such that: $\|\boldsymbol{y} - (\boldsymbol{H}(\boldsymbol{\theta})\nu)\|_* \stackrel{!}{=} \min$ with: $\phi_m(\boldsymbol{r}) = -(W\nu)(\boldsymbol{r})$ $\boldsymbol{r} \in \Omega$

3.3.4 Discretization

The space \mathcal{V}_u^* is infinite dimensional. For the numerical solution of boundary integral equations one needs to describe the boundary condition ν by functions that depend on a finite number of parameters [52]. One therefore proceeds in the same way as for the finite-element methods, and approximates ν by locally supported basis functions on a boundary mesh.

The boundary mesh is defined via the *boundary elements* τ_l , forming the decomposition

$$\partial\Omega = \bigcup_{l=0}^{N} \tau_l. \tag{3.34}$$



Figure 3.2: Higher order surface parameterization based on the unit square.

Throughout this thesis the boundary elements are defined via the surface parameterizations, based on the unit square

$$\gamma_l : \Box := [0, 1]^2 \mapsto \tau_l \subset \partial\Omega. \tag{3.35}$$

Such a parameterization is illustrated in Fig. 3.2.

The stream function ν is approximated in the finite dimensional approximation space S_u . If $S_u \subset V_u$, the approximation space is said to be conforming, which is a requirement for uniqueness and convergence of the approximated boundary value problem (see [43] theorem 8.1 (Cea's Lemma)). The function space S_u may be constructed by globally continuous basis functions $\varphi_k^{\rm D}$. The approximation of ν in S_u is denoted by ν_h and is constructed by using the locally supported basis functions $\varphi_k^{\rm D}$, according to

$$\nu(\mathbf{r}) \approx \nu_h(\mathbf{r}) = \sum_{k=1}^{K} \nu_k \varphi_k^{\mathrm{D}}(\mathbf{r}), \quad \in \mathcal{S}_u \qquad \mathbf{r} \in \partial \Omega$$
(3.36)

3.3.5 The discrete observation operator

Following the discretization scheme presented in section 3.3.4, one can derive a discrete version of the observation operator $H : (\nu, \theta) \mapsto \tilde{y}$. This operator will be written as a function of the vectors ν and θ , according to $\tilde{y} = H(\nu, \theta)$.

This section focuses on the indirect double-layer formulation according to definition 6. The derivations for the approximations of other representation formulas follow the same principle.

The density function ν is approximated with

$$\nu(\mathbf{r}') \approx \nu_h(\mathbf{r}') = \sum_{k=1}^{K} \nu_k \varphi_k^{\mathrm{D}}(\mathbf{r}') \quad \in \mathcal{S}_u \qquad \mathbf{r}' \in \partial\Omega,$$
(3.37)

where the state vector of the magnetic field (short state vector) is $\boldsymbol{\nu} = (\nu_1, ..., \nu_K)^T$.

Central to the construction of the discrete observation operator $H(\nu, \theta)$ is the evaluation operation $f(r_m)$: $S_u \ni \nu \mapsto B(r_m) \in \mathbb{R}^3$, where $r_m \in \Omega$ is a measurement position. $f(r_m)$ may be derived from Eq. (3.26) and the approximated surface current density $s_h = \operatorname{curl}_{\partial\Omega} \nu_h(\boldsymbol{r})$

$$\begin{split} \boldsymbol{B}(\boldsymbol{r}_{m}) &= -\mu_{0} \int_{\partial\Omega} \operatorname{curl}_{\boldsymbol{r}} \left(u^{*}(\boldsymbol{r}_{m},\boldsymbol{r}')\boldsymbol{s}_{h}(\boldsymbol{r}') \right) d\boldsymbol{r}' \\ &= -\mu_{0} \int_{\partial\Omega} \operatorname{grad}_{\boldsymbol{r}} u^{*}(\boldsymbol{r}_{m},\boldsymbol{r}') \times \boldsymbol{s}_{h}(\boldsymbol{r}') d\boldsymbol{r}' \\ &= -\mu_{0} \sum_{k=1}^{K} \nu_{k} \sum_{\tau_{l} \in \operatorname{supp}(\varphi_{k}^{\mathrm{D}}) \frac{1}{\tau_{l}}} \operatorname{grad}_{\boldsymbol{r}} u^{*}(\boldsymbol{r},\boldsymbol{r}') \big|_{\boldsymbol{r}=\boldsymbol{r}_{m}} \times \operatorname{curl}_{\partial\Omega} \varphi_{k}^{\mathrm{D}}(\boldsymbol{r}') d\boldsymbol{r}'. \end{split}$$
(3.38)

In the first step, the product rule for the curl was used, along with the fact that s_h does not depend on r. supp $(\varphi_k^{\rm D})$ denotes the support of the basis function $\varphi_k^{\rm D}$ on $\partial\Omega$.

It is advantageous to evaluate the integrals over the reference element \Box rather than $\tau_l \in \mathbb{R}^3$. To this end, the local basis function $\hat{\varphi}_{k,l}^{\mathrm{D}}$ on \Box is defined by

$$\hat{\varphi}_{k,l}^{\mathsf{D}} := \left. \varphi_{k}^{\mathsf{D}} \right|_{\tau_{l}} \circ \boldsymbol{\gamma}_{l} : \quad \Box \to \mathbb{R}.$$
(3.39)

For $t = (t_1, t_2) \in \Box$, it holds that (see [53] chapter 4.1.8)

$$\kappa_{l}(\boldsymbol{t})\operatorname{curl}_{\partial\Omega} \left. \varphi_{k}^{\mathrm{D}} \right|_{\tau_{l}}(\boldsymbol{r}) \circ \boldsymbol{\gamma}_{l}(\boldsymbol{t}) = \boldsymbol{J}_{l}(\boldsymbol{t}) \left(\partial_{v}, -\partial_{u} \right)^{T} \hat{\varphi}_{k,l}^{\mathrm{D}}(\boldsymbol{t}),$$
(3.40)

where $\kappa_l(t)$ is the surface measure

$$\kappa_l(t) := \|\partial_u \gamma_l(t) \times \partial_v \gamma_l(t)\|_2, \tag{3.41}$$

and $J_l(t)$ the Jacobian

$$\boldsymbol{J}_{l}(\boldsymbol{t}) := (\partial_{u}\boldsymbol{\gamma}_{l}(\boldsymbol{t}), \partial_{v}\boldsymbol{\gamma}_{l}(\boldsymbol{t})) = \begin{pmatrix} \partial_{u}\boldsymbol{\gamma}_{l,x}(\boldsymbol{t}) & \partial_{v}\boldsymbol{\gamma}_{l,x}(\boldsymbol{t}) \\ \partial_{u}\boldsymbol{\gamma}_{l,y}(\boldsymbol{t}) & \partial_{v}\boldsymbol{\gamma}_{l,y}(\boldsymbol{t}) \\ \partial_{u}\boldsymbol{\gamma}_{l,z}(\boldsymbol{t}) & \partial_{v}\boldsymbol{\gamma}_{l,z}(\boldsymbol{t}) \end{pmatrix}.$$
(3.42)

In this way, the integral in Eq. (3.38) can be re-parameterized:

$$\boldsymbol{B}(\boldsymbol{r}_{m}) = -\mu_{0} \sum_{k=1}^{K} \nu_{k} \sum_{\tau_{l} \in \operatorname{supp}(\varphi_{k}^{\mathrm{D}})} \int_{\Box} \operatorname{grad}_{\boldsymbol{r}} u^{*}(\boldsymbol{r}, \boldsymbol{\gamma}_{l}(\boldsymbol{t}))|_{\boldsymbol{r}=\boldsymbol{r}_{m}} \times \boldsymbol{J}_{l}(\boldsymbol{t}) \left(\partial_{v}, -\partial_{u}\right)^{T} \hat{\varphi}_{k,l}^{\mathrm{D}}(\boldsymbol{t}) \, \mathrm{d}\boldsymbol{t},$$
(3.43)

where the integrals are formulated on the reference elements.

To give an example for the explicit formulation of an observation operator, a linear combination of \boldsymbol{B} according to $y_m = \boldsymbol{n}_x \cdot \boldsymbol{B}(\boldsymbol{r}_m)$ at M positions $\boldsymbol{r}_m \in \Omega$ for m = 1, ..., M is now considered as the measurement operation. In the following, the vector $\boldsymbol{n}_x \in \mathbb{R}^3$ is a constant sensor orientation vector, but it could also depend on the sensor parameters $\boldsymbol{\theta}$. The predicted measurements at the positions \boldsymbol{r}_m can be assembled into the vector $\tilde{\boldsymbol{y}} = (y_1, ..., y_M)^T$, which is related to the state vector $\boldsymbol{\nu}$ via the equation system

$$\tilde{y} = H\nu. \tag{3.44}$$

In this case, sensor parameters have been neglected and the observation operator $H : \nu \mapsto \tilde{y}$ establishes a linear relationship between boundary data and the predicted measurements. The elements of the matrix H are given by

$$[\boldsymbol{H}]_{m,k} = -\mu_0 \sum_{\boldsymbol{\tau}_l \in \text{supp}(\varphi_k^{\text{D}})} \boldsymbol{n}_x \cdot \int_{\Box} \operatorname{grad}_{\boldsymbol{r}} u^*(\boldsymbol{r}, \boldsymbol{\gamma}_l(\boldsymbol{t}))|_{\boldsymbol{r}=\boldsymbol{r}_m} \times \boldsymbol{J}_l(\boldsymbol{t}) \left(\partial_v, -\partial_u\right)^T \hat{\varphi}_{k,l}^{\text{D}}(\boldsymbol{t}) \, \mathrm{d}\boldsymbol{t}.$$
(3.45)

3.3.6 Iso-geometric analysis in boundary element methods

So far no explicit definitions for the basis functions $\varphi_k^{\rm D}$ and surface parameterizations γ_l have been given. The algorithms presented in this thesis have been developed in C++, using the Boundary Element Method Based Engineering Library (BEMBEL) [54]. In BEMBEL, higher-order basis splines, short *B-splines*, are used to span the approximation spaces. B-splines enjoy great popularity for interpolation problems in general, as they enable arbitrarily-smooth interpolations, while using locally supported basis functions. Univariate B-splines may be computed according to definition 8 and are illustrated in Fig. 3.3 for different spline degrees. Two dimensional B-splines for $\varphi_k^{\rm D}$ are constructed from the tensor product of univariate splines on a regular grid (see Fig. 3.4).

Moreover, BEMBEL makes use of non-uniform rational basis spline (NURBS) mappings for the surface parameterization. NURBS mappings are commonly used in computer aided design (CAD) as they can represent arbitrary geometries without approximation and enable flexible modification. Using NURBS mappings in electromagnetic computations, one can bypass the intermediate step of meshing and directly perform the computations on the CAD geometry representation. This avoids an additional level of approximation and is in the spirit of *iso-gemometric analysis* (IGA) [55]. Details about NURBS mappings and B-splines in the context of BEM are found in [56], [57] and [58].

Using higher-order surface parameterizations such as NURBS mappings, complex geometries can be modelled exactly. This has been proven useful for the computation of resonance frequencies in radio frequency cavities [59]. In this work, the exact geometry of a, possibly curved, vacuum chamber may be used as boundary for the computational domain. However the use of basis splines in combination with higher-order surface parameterizations has some peculiarities, because the surface evaluations are computationally costly.

Definition 8 *B-splines* [60] Let $0 \le p \le k$ and consider the *p*-open knot vector $\Xi = (\underbrace{\xi_0 = \ldots = \xi_p}_{=0} \le \ldots \le \underbrace{\xi_k = \ldots = \xi_{k+p}}_{=1}) \in [0,1]^{k+p+1}.$ (3.46)

The lowest degree (p = 0) B-spline basis functions b_i^0 are given by

$$b_{j}^{0}(x) = \begin{cases} 1, & \text{if } \xi_{j} \le x \le \xi_{j+1} \\ 0, & \text{else} \end{cases}$$
(3.47)

Higher degree (p > 0) B-spline basis functions are constructed according to

$$b_j^p(x) = \frac{x - \xi_j}{\xi_{j+p} - \xi_j} b_j^{p-1}(x) + \frac{\xi_{j+p+1} - x}{\xi_{j+p+1} - \xi_{j+1}} b_{j+1}^{p-1}(x).$$
(3.48)

In Fig. 3.3 B-splines of different degrees are shown. Such B-splines are locally supported on finite intervals and a spline of degree p is C^{p-1} continuous. A basis spline can be expressed as a superposition of *Bernstein polynomials*, which are element-wise defined on the underlying grid [61].

Fig. 3.4 shows a two dimensional, cubic B-spline, on a grid over the xy-plane. The grid is generated by separating the x and y axes into four intervals, yielding 16 grid elements. This spline is C^2 -continuous,



Figure 3.3: Univariate B-splines of degrees zero to three. Each interval is occupied by p + 1 B-splines. When all knots are distinct, a spline of degree p is C^{p-1} -continuous.

and on each element the spline can be expressed by means of a superposition of locally defined Bernstein polynomials.

Global approximation spaces for $\varphi_k^{\rm D}$ and $\varphi_k^{\rm N}$ are built on a set of two-dimensional B-splines, overlapping on multiple elements of the computational grid, in a way that the values of the B-splines sum up to 1 at each position. They are therefore said to form a *partition of unity*. Evaluating the boundary integral equation, involves integrating over these basis functions. One might be temped iterating over the basis functions and evaluating the integrals basis function by basis function. As basis functions are overlapping, this would require "visiting" each element of the grid multiple times and evaluating the surface for spatial integration. However, evaluating the higher-order surface parameterizations is computationally costly.

The efficiency can be improved by exploiting the Bernstein basis. To this end, one iterates over the grid elements and integrates over the Bernstein polynomials. When integrating over all Bernstein polynomials at once, the approach is most efficient, as the surface is evaluated only once for all polynomials. This is the standard approach of matrix assembly when using IGA in boundary-element methods.

As an example, the construction of the matrix H according to (3.45) based on the approximated stream function $\nu_h \in S_u$ is now considered. Denoting by ψ_n the *n*-th of all locally defined two-dimensional Bernstein polynomials, according to Fig. 3.4, the function space $W_{\text{disc}} := \text{span}(\psi_1, ..., \psi_N)$ spanned by ψ_n can be defined. W_{disc} is said to be *discontinuous*, to emphasize its difference to S_u in continuity. The dimension of the discontinuous space W_{disc} is higher than the dimension of S_u , i.e., $\dim(W_{\text{disc}}) > \dim(S_u)$. A vector $\boldsymbol{\nu} \in S_u$ may be expressed as a linear combination of a vector $\boldsymbol{\psi} \in W_{\text{disc}}$ by means of the sparse projection matrix $\boldsymbol{P} \in \mathbb{R}^{N \times K}$

$$\boldsymbol{\nu} = \boldsymbol{\psi} \boldsymbol{P}. \tag{3.49}$$



Figure 3.4: A cubic basis spline is expressed as a composition of Bernstein polynomials.

It is possible to assemble the integral operator H in W_{disc} , and then transfer it to the continuous space S_u , by using the projection operator

$$H = H_{\rm disc} P. \tag{3.50}$$

 H_{disc} is constructed by integrating over the two-dimensional Bernstein polynomials ψ_n in (3.45). A drawback of this approach is the large memory consumption accompanied with storing the matrix in the high-dimensional, discontinuous space W_{disc} . It is thus advantageous to directly project into the low dimensional matrix H when assembling the equation system. This can be accomplished by temporally storing the matrix elements into sparse matrices. The principle is illustrated in Fig. 3.5. Considering limited computational resources, this approach is indispensable to attain high dimensions for S_u when using higher order basis splines and dense matrices. As an example, take the result presented in Fig. 6.11. 13 402 degrees of freedom using cubic basis splines require a discontinuous space of dim $(W_{\text{disc}}) = 137$ 216. Moreover, M = 110 076 measurements are considered. This requires an H_{disc} matrix of 120 GB, which would be impossible to handle on a desktop computer.



Figure 3.5: Using sparse matrices for the memory efficient matrix assembly in boundary element methods using IGA. The evaluation operator H is considered. A small block of the matrix H_{disc} has been assembled in \mathcal{W}_{disc} . This block has been stored in \widetilde{H}_{disc} in a sparse matrix format. The H matrix can be incremented by applying the projector P to \widetilde{H}_{disc} on the fly.

3.3.7 Incorporating a gauge condition

For a unique formulation of the inverse problem, the space \mathcal{V}_u^* was restricted to stream functions with vanishing mean (see remark 1),

$$\int_{\partial\Omega} \nu(\mathbf{r}') \,\mathrm{d}\mathbf{r}' = 0. \tag{3.51}$$

This condition can be incorporated into the equation system by matrix manipulation.

Consider the state vector $\boldsymbol{\nu} = (\nu_1, ..., \nu_K)^T \in \mathbb{R}^K$ and the gauge condition $\boldsymbol{a} \cdot \boldsymbol{\nu} = 0$, which has been derived from (3.51). The coefficients a_k of the vector $\boldsymbol{a} \in \mathbb{R}^K$ are given by

$$a_k = \int_{\partial\Omega} \varphi_k^{\rm D}(\mathbf{r}') \,\mathrm{d}\mathbf{r}'. \tag{3.52}$$

Since

$$\nu_1 = -\frac{1}{a_1} \sum_{k=2}^{K} \nu_k a_k, \tag{3.53}$$

it holds

$$\tilde{\boldsymbol{y}} = \boldsymbol{H}\boldsymbol{\nu} = \begin{pmatrix} \sum_{n=1}^{K} H_{1,k}\nu_{k} \\ \vdots \\ \sum_{n=1}^{K} H_{M,k}\nu_{k} \end{pmatrix} = \begin{pmatrix} \sum_{n=2}^{K} \left(H_{1,k} - \frac{H_{1,1}a_{k}}{a_{1}}\right)\nu_{k} \\ \vdots \\ \sum_{n=2}^{K} \left(H_{M,k} - \frac{H_{M,1}a_{k}}{a_{1}}\right)\nu_{k} \end{pmatrix}, \quad (3.54)$$

for the product of ν with the matrix H that contains the elements $[H]_{m,k} = H_{m,k}$. One may therefore define the reduced matrix $H_r \in \mathbb{R}^{M \times K-1}$ and the gauge matrix G according to

$$\boldsymbol{H}_{\mathrm{r}} = \begin{pmatrix} H_{1,2} & \dots & H_{1,K} \\ \vdots & \ddots & \vdots \\ H_{M,2} & \dots & H_{M,K} \end{pmatrix}, \qquad \boldsymbol{G} = -\frac{1}{a_1} \begin{pmatrix} H_{1,1} \\ \vdots \\ H_{M,1} \end{pmatrix} \otimes (a_2, \dots, a_K), \tag{3.55}$$

where $C = A \otimes B$ denotes the Kronecker product of the matrices $A \in \mathbb{R}^{K \times L}$ and $B^{M \times N}$ according to $[C]_{km,ln} = [A]_{k,l}[B]_{m,n}$ with $C \in \mathbb{R}^{KM \times LN}$.

In this way the product $H\nu$ can be computed on the reduced state vector $\nu_{\rm r} = (\nu_2, ..., \nu_K) \in \mathbb{R}^{K-1}$

$$\tilde{\boldsymbol{y}} = (\boldsymbol{H}_{\mathrm{r}} + \boldsymbol{G})\boldsymbol{\nu}_{\mathrm{r}}.\tag{3.56}$$

3.3.8 The Aubin-Nitsche formalism and the design of the measurement procedure

The Aubin-Nitsche formalism allows to derive point-wise error estimates for the evaluation of the approximated boundary integral equations (see [43, Theorem 12.8], [53, Example 4.2.15]). For the solution of the Neumann problem, using the indirect double layer potential and, assuming a sufficiently smooth boundary, this yields the estimate [62, Theorem 7.1]

$$|(W\nu)(\mathbf{r}) - (W\nu_h)(\mathbf{r})| \lesssim c(\mathbf{r})h^{2p+1}, \qquad \mathbf{r} \in \Omega.$$
(3.57)

 ν_h is the approximated stream function using B-splines of polynomial degree p, and h is a mesh parameter, which is often identified with the maximum edge length of all boundary elements.

In Fig. 3.6, the convergence for the implementation in BEMBEL is shown and compared to the theoretical limits. Two domains are considered: (left) the ball $\Omega = \{x, y, z : \sqrt{x^2 + y^2 + z^2} < 1\}$, and (right) the cube $\Omega = [-1/2, 1/2]^3$. In both cases, the Neumann problem based on the indirect double layer potential, given the manufactured solution

$$\phi_{\rm m}(\mathbf{r}) = 4x^2 - 3y^2 - z^2, \tag{3.58}$$

is solved.

The matrices involved in the solution of the indirect Neumann problem are found in appendix 8.3. The error is evaluated in the l^{∞} -norm, computing the maximum value of the absolute difference between $\phi_{\rm m}$ and $(W\nu_h)$ on a grid inscribed into the domains. In both figures, the errors are normalized with respect to the maximum potential value in the evaluation grid.

Whereas the boundary of the ball is continuously differentiable, the cube contains corners and is therefore only Lipschitz continuous. However, similar convergence rates are reported also for the cube. Moreover, in this specific case, the B-splines of degree p = 2 are performing better than expected.

The term c in (3.57) depends on the evaluation position $r \in \Omega$. Even when considering an exact numerical integration, this term tends to infinity for r approaching the domain boundary.

A numerical experiment is designed to investigate the impact. The stream function ν is approximated on the surface of the cube, by solving the Neumann problem based the indirect double-layer potential [62], given the manufactured solution (3.58). The flux density is then evaluated on the lines defined by the vectors $p_1 = (1/2, 0, 0)^T$ and $p_2 = (1/2, 1/2, 1/2)^T$, starting from the origin. The cube, as well as the vectors p_1 and p_2 are illustrated in Fig. 3.7. For the following analysis, the cube is refined four times, yielding boundary elements with edge length h = 1/16.

The approximation errors are investigated in the flux density B, by means of the relative error

relative error
$$= \frac{\|B(r) - B_h(r)\|_2}{\max \|B(r)\|_2},$$
 (3.59)



Figure 3.6: Convergence of the BEM approximation in case of the indirect Neumann problem. In both cases, the manufactured solution according to (3.58), provides a Neumann condition for the magnetic scalar potential. The problem is solved in the ball (left) and cube (right). The errors are measured in the l^{∞} -norm in the interior of the domain and normalized with respect to the maximum potential.



Figure 3.7: Numerical experiment for the investigation of approximation errors for field evaluations close to the domain boundary.



Figure 3.8: Performance of the indirect formulation for field evaluation close to the domain boundary. Left: Evaluations approaching the smooth part of the boundary along p_1 . Right: Evaluations approaching the corner of the cube along p_2 . The boundary mesh and the lines p_1 and p_2 are illustrated in Fig. 3.7.

where B(r) is the flux density computed from the manufactured solution according to (3.58), and B_h is the approximation by the BEM.

In Fig. 3.8 the relative errors are shown for the evaluations along p_1 and p_2 for different polynomial degrees p. On the left, the evaluation along p_1 is shown. For p > 1, the relative errors are below 10^{-4} , with a distance larger than h. As found in Fig. 3.6 (right) already, the B-splines with polynomial degrees p = 2 and 3 are performing equally well.

Larger relative errors in the range of 10^{-3} and 10^{-2} are found for the evaluation approaching the corner (see Fig. 3.8 right). This is a known drawback of indirect boundary element methods, in the cases where the domain boundary contains sharp corners (see [63] remark 3). The reason for this behavior is that indirect methods make use of the jumping boundary data between interior and exterior domain. Approximating the trace operators by boundary elements is harder at places where the boundary admits sharp, re-entrant corners, and the corners of the cube are re-entrant for the exterior domain. This problem can be accommodated either by smoothing out edges in the definition of $\partial\Omega$, or by extending the domain boundary to shift the corners outside of the domain of interest.

Fig. 3.8 illustrates how the approximation errors at the boundary are smoothed out for the evaluation in Ω . Concerning the solution of the inverse problem according to definition 7, this smoothing property is both a blessing and a curse. With an approximation ν_h at hand, the smoothing effect is exploited to obtain a field reconstruction of high precision. However, for the inverse computations the smoothing effect is a curse, as it inevitably leads to ill-conditioned problems.

This aspect must be investigated for the design of the measurement process. Due to the trade-off between smoothing and approximation error, the measurements should be placed within a distance of h to the boundary.

This gives an inscribed boundary surface, which can be covered with measurements. The mesh parameter h is usually given in accordance with the size of the domain and the desired approximation accuracy. The remaining question is how many measurements are needed to identify the approximated stream function ν_h ?

To this end, the conditioning of the inverse problem formulated in definition 7 needs to be investigated. Measuring the error by means of the sum of squared residuals

$$\|\boldsymbol{y}_{\text{det}} + \boldsymbol{\epsilon} - (\boldsymbol{H}(\boldsymbol{\theta})\nu_h)\|_2^2, \tag{3.60}$$

and assuming a linear observation operator H independent of θ , the minimizer ν_{LS} is found by solving the linear equation system

$$\boldsymbol{H}^{T}\boldsymbol{H}\boldsymbol{\nu}_{\text{LS}} = \boldsymbol{H}^{T}\left(\boldsymbol{y}_{\text{det}} + \boldsymbol{\epsilon}\right). \tag{3.61}$$

The quality of the least-squares solution depends on the mesh parameter h, the error term ϵ , and the *measurement resolution* h_M , assuming that the measurements are placed equidistantly. Numerical experiments, such as the one presented in Fig. 3.9, have been performed to study the accuracy of the least squares solution. Considering that the three components of the magnetic flux density B are measured, and that the elements of the error term have a standard deviation of $\sigma(\epsilon) = 10^{-3} \max |\mathbf{y}_{det}|$, an accuracy of 10^{-4} for the field evaluation is obtained for a measurement resolution of $h_M < h/3$. However, the domain of validity for this statement, based on the parameters h, $\sigma(\epsilon)$, and h_M has not been found yet, and should be investigated more deeply in future research.

3.3.9 The benefits of the indirect formulation

This subsection summarizes the advantages of the indirect double layer potential formulation for the field reconstruction form measurement data.

In the representation formula according to (3.15), two integrals are to evaluate. These integrals are involving the Dirichlet and Neumann data u and g. As it is discussed in appendix 8.1, the Dirichlet and Neumann data are dependent by a linear operator. The inverse problem therefore needs to be formulated in terms of u or g, and the missing boundary data needs to be computed by means of the solution of a linear equation system. These equation systems are derived in appendix 8.2 and 8.3.

To give an example, the discrete observation operator $H_{\text{direct BEM}}$ formulated in terms of the approximated Dirichlet data u, based on (3.15) takes on the form

$$\tilde{y} = \tilde{V}g - Wu = \underbrace{\left(\tilde{V}V^{-1}K - W\right)}_{:=H_{\text{direct BEM}}}u.$$
(3.62)

 \tilde{V} and W are the discretized single layer and double layer potentials according to (3.15). The matrices V and K are found in appendix 8.2. In this case, the inverse of the matrix V is needed to construct $H_{\text{direct BEM}}$. This inverse matrix can only be computed explicitly in low dimensional problems.

As an alternative to BEM, a field representation by finite element methods (FEM) would be plausible. In FEM, the whole domain Ω , is discretized and equipped with local basis functions. Usually a magnetic potential is expressed by means of a linear combination of the local basis functions, in order to represent the field. Denoting by x the coefficients of this linear combination, the finite element method for the Dirichlet problem results in an equation system of the kind

$$Ax = Fu, \tag{3.63}$$



Figure 3.9: Design of the measurement resolution. The cube with h = 1/16, illustrated in Fig. 3.7 is considered. The polynomial degree is p = 2. The measurements are placed equidistantly on the surface of an inscribed cube Ω_{eval} , with a distance of one mesh parameter h to the boundary. The solution of the Neumann problem ν_h is used to generate flux density evaluations on Ω_{eval} , with a measurement resolution of h_M . The three flux density components on each evaluation position are filling the vector y_{det} . An error term with $\sigma(\epsilon) = 10^{-3} \max |y_{\text{det}}|$ is added to perturb the right hand side of (3.61). The least-squares solution is then computed to obtain ν_{LS} . In both, the blue and the orange lines, the least-squares solution ν_{LS} is compared to the approximation ν_h , and not to the manufactured solution. In this way, approximation errors do not contribute to the differences. The L2-norm of the difference $\nu_{\text{LS}} - \nu_h$ is given in blue, normalized with respect to $(\int_{\partial\Omega} \nu_h^2(\mathbf{r}') \, d\mathbf{r}')^{1/2}$. Moreover, the errors in the potential evaluation are measured in the l^{∞} -norm and are given in orange, normalized with respect to the maximum value of ϕ_{m} . The potentials are computed on a 3D grid in $[-1/3, 1/3]^3$. All errors are averaged over 50 trials. For comparison, the mesh parameter h is marked in red. where A is the so-called Galerkin matrix and F is a projector operator for the Dirichlet data u [64]. As the observation operator acts on the field inside the domain, it needs to be constructed on x. This means that in the case of finite element methods

$$\tilde{\boldsymbol{y}} = \underbrace{\boldsymbol{S}\boldsymbol{A}^{-1}\boldsymbol{F}}_{:=\boldsymbol{H}_{\text{FEM}}}\boldsymbol{u},\tag{3.64}$$

where S is a matrix which is mapping the coefficients x to the predicted measurements \tilde{y} [65]. Also here the construction of the observation operator requires a matrix inverse.

Whenever the right hand sides in (3.62) and (3.64) are changed and the field is to be evaluated, a linear equation system needs to be solved. This linear equation system is of the same dimension as the BEM or FEM approximation spaces, even if the field is to be evaluated at a single measurement position only. In contrast, the discrete observation operator when using the indirect formulation according to section 3.3.5, takes on the form

$$\tilde{\boldsymbol{y}} = \boldsymbol{H}\boldsymbol{\nu},\tag{3.65}$$

where a direct relationship between \tilde{y} and ν is established, without the need for the solution of an equation system. This is particularly beneficial for data assimilation, as a small amount of measurements can be treated efficiently.

The benefits of the indirect formulation by means of the double layer potential are now summarized.

- 1. The discrete observation operator does not require a matrix inverse.
- 2. A magnetic vector potential is accessible by means of an integral evaluation according to definition 6.
- 3. High convergence rates are obtained for the evaluation of B, A and ϕ_m , and also their spatial derivatives.

3.3.10 The multilevel fast-multipole method

Matrices arising in boundary element methods are fully populated, as the Green's kernel is globally supported. Therefore the algorithms presented so far scale badly with increasing number of measurements and basis functions. To make boundary element methods scalable, an efficient compression technique for matrix-vector products is indispensable. To this end, a multilevel fast multipole method (MLFMM), according to [66] can be applied to the evaluation operators in an iso-geometric framework.

Fundamental to the approach is the harmonic expansion of the Green's kernel and the hierarchical clustering of observations and sources. First, the inverse distance $||\mathbf{r} - \mathbf{r}'||$ with $\mathbf{r} = (r, \theta, \varphi)$ and $\mathbf{r}' = (\rho, \alpha, \beta)$ in spherical coordinates is expanded according to

$$\frac{1}{\|\boldsymbol{r} - \boldsymbol{r}'\|} = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \rho^n \tilde{Y}_n^{-m}(\alpha, \beta) \frac{\tilde{Y}_n^m(\theta, \varphi)}{r^{n+1}}.$$
(3.66)

The definition of the spherical harmonics in (3.66) is slighly different, to the one presented in 3.10.

$$\tilde{\boldsymbol{Y}}_{n}^{m}(\boldsymbol{\theta},\boldsymbol{\varphi}) = \sqrt{\frac{(n-|m|)!}{(n+|m|)!}} P_{n}^{|m|}(\cos(\boldsymbol{\theta})) \exp(jm\boldsymbol{\varphi}).$$
(3.67)

This is done to express the transformations between multipoles, which are central to the MLFMM, in a more elegant way.



Figure 3.10: Bisecting the computational domain into cells. Blue: Lowest level, covering all sources and observations. Level 1 (orange) and level 2 (green) are obtained by bisecting the cells of the parent cells into eight. Not all cells need to be occupied with entities. Plane computational domains can be treated in the same way.

Secondly, the computational domain is divided into boxes according to the refinement scheme presented in Fig. 3.10. Starting with an outer cell at level 0, enclosing all sources and observations, one bisects each cell in each level by eight to obtain an a hierarchical decomposition into parent and child cells in an octree structure. Cells that are not enclosing any sources or measurements and cells that are hosting at most a certain minimal amount of entities are not refined.

The MLFMM relies on local multipole expansions of type (3.66) within the cells and on transformations between them. These transformations are found in [66], Theorem 5.1 to 5.3.

Fig. 3.11 is inspired by [67]. The green dots on the left side are representing the sources, i.e., fictitious magnetic monopoles, double layers or surface currents. The blue dots in the red cell on the right side represent the measurement data, such as Hall voltages or magnetic fluxes.

Given a distribution of sources (green), one computes the values for the measurements in the target cell (red). Instead of computing all interactions between sources and measurements, the domain is split into near and far field cells and only the near field interactions are computed directly by evaluating the underlying integral equation.

For the far field cells the sources within each cell on the lowest level are expanded into multipoles. One then translates these multipoles to the higher tree levels by means of *multipole-to-multipole* (M2M) transformations. Each cell on each level then carries a local multipole expansion, representing the far field due to the enclosed sources.

The measurements within the target cell are expressed as a superposition of near field and far field interactions. The far field interactions are computed by passing through the tree from top to bottom.

On the highest level, the multipole expansions of cells, which are sufficiently far away are transferred to the cell enclosing the target cell by means of *moment-to-local* transformations (M2L). Sufficiently far away means that there is at least one cell between source and target cell on the corresponding level.

The cell *A* on level *l* is called the father of a cell *B* on level l + 1, if it contains cell *B*. Conversely, *B* is the son of cell *A*. On the lower tree levels, the local expansions of the father cells are transferred to their sons by means of *local-to-local* transformations (L2L). The collection of cells between the near and far fields is called



Figure 3.11: The multilevel fast multipole method in two dimensions. In each step, information is transferred from green to blue dots. The target cell is highlighted in red.

interaction region. On each level, all multipole moments from the interaction region are considered by means of M2L transformations. This is illustrated in Fig. 3.11 (middle right), where multipoles in the interaction region are transferred directly to the target cell.

On the lowest level, the direct field evaluation of the near field cells is superimposed with the evaluation of the local multipole expansion, which accounts for all cells in the interaction region as well as the far field.

The performance of the implementation is reported in Fig. 3.12. $N = 6\,938$ (blue) and $N = 26\,138$ (orange) cubic polynomials are used to approximate a stream function ν on the boundary of a unit cube. This boundary data is then used to compute the magnetic scalar potential at M measurement positions inside the domain. The measurements are placed on an inscribed cube, which is one mesh parameter separated from the domain boundary. p = 20 multipoles are used and the tree refinement is stopped after 5 levels. The result of the dense matrix-vector product $\phi_{m,dense}$ is computed and compared to the result of the MLFMM $\phi_{m,mlfmm}$. The relative error is computed as max $|\phi_{m,mlfmm} - \phi_{m,dense}|/\max|\phi_{m,dense}|$. It is at about 10^{-6} in all cases.

The advantage of the MLFMM is most pronounced in terms of assembly time and memory allocation, where one order of magnitude is gained. The solution time is dominated by the assembly time, which is usually the case for higher order methods. However, in most cases the matrix assembly is required only once and matrices can be stored in memory. They are then employed for matrix-vector products whenever needed. This is why



Figure 3.12: Performance of the MLFMM. In all figures: dashed: dense operation, solid: MLFMM, blue: $N = 6\,938$, orange: $N = 26\,138$. As the number of basis functions N is fixed, the dense operations as well as the storage requirements scale linearly when increasing the number of measurements M. The incline is smaller for the MLFMM in all cases. The computations were distributed on 16 CPUs of type Intel(R) Core(TM) Processor (Broadwell, IBRS) @ 2.194 GHz.

the memory requirements and computation times for matrix-vector products are more critical criteria than assembly times.

Computing the matrix-vector product faster than a linear algebra package like Eigen is challenging, as routines are optimized for high performance in terms of memory assignment and parallelization. The implementation of the MLFMM was parallelized using OpenMPI [68]. At this point there is room for improvement, as the distribution of the computations is based on splitting the moment-to-local transformations, level by level. The total load is not necessarily split equally within the tasks, which is why the curves for the computation times for the matrix-vector product show discontinuities.

However, also the MLFMM implementation of the matrix-vector product is faster than the dense operation for very large problems. It should also be emphasized, that the requirements for the relative maximum errors reported in Fig. 3.12 are stronger than what is usually necessary in computational electromagnetics. This is because the implementation shall later be used for inverse calculation and uncertainty quantification, and sensor systems for magnetic measurements are reaching precisions in the 10^{-4} range. If the requirements are lower, the advantage of the MLFMM would emphasize even more drastically.



Figure 3.13: Performance of the interpolation based FMM [62] for the indirect Neumann problem using the double layer potential. The time to solution includes the assembly of the equation system, as well as its solution. The solution was computed by the GMRES method, with a restart after 2000 iterations. The relative maximum error was computed with respect to a manufactured solution. Here *p* is the degree of the B-splines (*p*-refinement). Each dot represents a mesh refinement level (*h*-refinement). These computations were performed on a Intel(R) Core(TM) i7-8550U CPU @ 1.80GHz, on 8 CPUs.

In principle, the same procedure can be applied to obtain a compression of the dense matrices arising from the mappings between Dirichlet and Neumann data (see appendix 8.2 and 8.3). The measurements, which were to be evaluated previously, would be replaced by the integrals over the boundary values. It is possible to compress the operations even further by exploiting the tree structure also in the construction of the mesh and basis functions.

For the Neumann problem using the double layer potential, the interpolation-based, fast-multiple method presented in [62] has therefore been implemented. This compression technique reaches even a linear complexity for the computation of matrix-vector products. Results are presented in Fig. 3.13. The performance reported in [62, Fig. 17], is recovered. However, as it is shown in Fig. 3.13 right, the memory requirements are large, as the hierarchical matrix requires four times the resources as a similar compression of the single layer operator V (see [62] for details).

4 Magnetic Measurement Techniques

The most common magnetic measurement techniques exploit Faraday's law of induction to generate a measurable voltage U_{ind} proportional to the rate of change of the magnetic flux Φ_A linked with the sensor surface A,

$$U_{\rm ind} = -\frac{\mathrm{d}\Phi_{\mathcal{A}}}{\mathrm{d}t}.\tag{4.1}$$

In the case of induction coils, conducting wires are wound around a coil former to span the sensor surface A. A voltage signal is generated by ramping the magnetic field or moving (rotating or translating) the coil through a static magnetic field. In the latter case, expressing the velocity vector by v, one may exploit the convective derivative [69, (4.100)] to obtain an expression for the induced voltage,

$$U_{\text{ind}} = \int_{\partial \mathcal{A}} (\boldsymbol{v} \times \boldsymbol{B}) \cdot d\boldsymbol{r}.$$
(4.2)

Equation (4.2) is exploited extensively in static magnetic field measurements. Rotating coil systems employ induction coils mounted on shafts that are rotated in the static magnetic field. Stretched-wire systems can be regarded as coils with a single turn. The stretched part of the wire covers the whole spatial extension of the magnetic field. The flux linked with a surface traced out by the wire is proportional to the integrated voltage induced during the displacement of the wire. More recent developments use translating coils, which are mounted on sleds moved longitudinally through the magnetic field [15].

The fact that the induced voltage is proportional to the rate of change in Φ_A makes it necessary to move the sensor in the case of static magnetic field measurements, and therefore leads to multi-physics problems. In fact, most of the measurement uncertainty in modern day rotating and translating coil systems is traced back to mechanical vibrations and positioning errors [70].

A second class of measurement systems exploits the so-called Hall effect to generate a voltage, which is proportional to a component the magnetic field B. The physical principle of the Hall effect is best understood considering the configuration illustrated in Fig. 4.1. The semiconductor (gray) is located in the *xy*-plane. A current density J is impressed across the semiconductor along x. Under the influence of an external magnetic field B, the Lorenz force acts on the charge carriers, which gives rise to a force proportional to $J \times B$, and hence perpendicular to J. The equilibrium of forces within the material is maintained by the appearance of a measurable electric field E across the *y*-axis.

The Hall voltage is proportional to $J \times B$ and hence dependent on the Hall current I_H used to provide the current density J in the semiconductor. The sensitivity function $s : (B, I_H) \mapsto \mathbb{R}$ of a Hall sensor can be expressed in terms of the sensor parameter I_H and at first approximation given by the linear, axial model

$$s(\boldsymbol{B}, I_{\rm H}) = s_{\rm H} I_{\rm H} \, \boldsymbol{n}_{\rm H} \cdot \boldsymbol{B} + U_0(I_{\rm H}), \tag{4.3}$$

where $n_{\rm H}$ is the unit vector of the probe orientation, $s_{\rm H}$ is the probe's linear sensitivity given in VA⁻¹T⁻¹, and $U_0(I_{\rm H})$ is a zero field offset voltage.



Figure 4.1: An illustration of the Hall effect in a semiconductor. The Lorentz force generated by the product $v \times B$ gives rise to a field E, in a way that the equilibrium of forces is maintained.

Modern Hall-effect devices are reaching typical sensitivities between 50 and $500 \text{VA}^{-1} \text{T}^{-1}$, [71] by using semiconductors such as gallium arsenide or layers of graphene as active elements [72]. Although this technology enables nearly point-wise sampling of the magnetic field, with active areas below 1 mm², as well as the capability to measure static magnetic fields, Hall sensors are usually not the first choice for magnetic measurements in particle accelerator magnets. This is due to the following reasons:

- 1. Point-wise sampling for the components of the magnetic field is often not required, as small induction coils are providing adequate spatial resolutions.
- 2. In order to perform spatial sampling, the sensors need to be moved through the magnetic field, yielding the same susceptibility towards mechanical vibrations and positioning errors.
- 3. The Hall effect has a non-negligible temperature dependency, yielding tough requirements for temperature control and calibration.
- 4. The sensor transfer function suffers from nonlinearities and the influence of planar field components, which require a careful calibration procedure.
- 5. In contrast to the induced voltage in an induction coil, the Hall voltage depends on the excitation current, which is provided by an external power supply. The signal quality is highly dependent on the stability of the Hall current.

The most accurate measurement technology for homogeneous fields above mT is nuclear magnetic resonance (NMR), generating an electromagnetic signal with a frequency proportional to the magnitude of the magnetic field |B| [73]. Such NMR measurements are reaching relative accuracies in the 10^{-6} range and are therefore used extensively for the calibration of magnets, induction coils, and Hall probes. Moreover they find great popularity as field markers in case of online field monitoring, this means type (4) measurements according to Fig. 1.1.

The following section focuses on Hall probe measurements and the metrological characterization of a new *three-axes Hall-probe mapper*. Its commissioning, characterization, as well as the design and implementation of measurement routines has been the practical part of this thesis. The next section starts with a summary of all all relevant components related to the three-axes Hall probe mapper. Then the most dominant error sources are investigated.

4.1 The three-axes Hall probe mapper

Field mapping relies on local field measurements by means of Hall probes. Fig. 4.2 shows a picture of the three-axes Hall probe mapper (short *3D mapper*). A three-axes Hall probe (A) is mounted on the tip of the mapper arm (B). The arm is segmented and consists of an aluminum as well as a carbon-fiber-reinforced plastic part, in a way that its length can be adjusted from 1 to 2 m.



Figure 4.2: The three-axes Hall probe mapper.



Figure 4.3: The Leica absolute laser tracker AT960.

The mapper arm is mounted to the stages of a coordinate measuring machine (CMM) (C). The CMM is equipped with three linear encoders, with a sensor precision of 5 μ m (D). The *x* and *y* axes of the CMM use air bearings for contact-free linear motion. The overall measurable volume of the system using *x*, *y* and *z* axes is 1 m × 1 m × 3 m.

The CMM is specified for a dynamic positioning accuracy of 0.1 mm and a nominal velocity of $v_N = 20 \text{ mm s}^{-1}$. This means that the maximum positioning errors, for moves inside the $1 \text{ m} \times 1 \text{ m} \times 3 \text{ m}$ domain with v_N fall below this threshold. The specifications have been validated by optical measurements on several occasions.

The linear encoders can be set up to generate trigger pulses when the stage passes a certain distance. In this way a read out of the Hall voltages can be launched on the fly, i.e., during the movement of the stages. This is a critical aspect, as it considerably reduces the measurement duration with respect to measurements in start-stop mode.

For the acquisition of the Hall voltages, three 8.5 digit, digital multimeters of type 3458A from Keysight technologies are used. The integration period of the multimeters can be set up between 100 ns and 1 s, and is adjusted with respect to the trigger frequency for optimal signal-to-noise ratios. The trigger generation and on-the-fly acquisition of three multimeters has been tested for trigger frequencies of up to 100 Hz. Higher frequencies are not required.

A critical aspect for the signal-to-noise ratio is the proper shielding of the signal cables of the Hall probe. The signal cables of 18 m length for the Hall voltages need to be routed closely to the power cables of the linear stages. In the commissioning phase of the machine, large electromagnetic compatibility issues were found. The shielding of the signal cables, all the way from the multimeters to the Hall sensor, and the removal of ground loops could fix these issues.

The position measurements of the linear encoders do not per se relate to a useful coordinate system. Field maps need to be referred to the magnet geometry. Therefore, a relation between the encoder position and the magnet coordinates needs to be found. This procedure is called *fiducialization*.

Optical measurements are indispensable for the fiducialization. The absolute Laser tracker AT960 from Leica is used for this purpose. A picture of the device is shown in Fig. 4.3. The laser tracker provides absolute position measurements of reflector targets, in three dimensional space, with an accuracy in the range of $20 \,\mu\text{m}$. Usually, some targets are mounted on fixed reference positions on the magnet geometry. From these reference positions a magnet coordinate system is constructed.

The position measurements of the linear encoders must be linked to the magnet coordinate system. This can be achieved by moving the Hall sensor to a known position in magnet coordinates. For this reason, a cone quadrupole magnet was built in permanent magnet technology, providing a distinct zero field in the magnet center. The magnet is shown in Fig. 4.4 (right). The tolerances in magnet production were kept tight in order to guarantee a certain relation between zero field and three reflector target holders on the top of the magnet. The Hall sensor is moved into the center of the magnet, by searching the zero-field position in the Hall voltages. Having measured the reflector targets of the cone quadrupole, this position can then be related to the magnet coordinates.

In section 4.2 the laser tracker will be used extensively to characterize the mechanical system. These optical measurements are only used in the phase of metrological characterization and not during the field mapping. The optical measurements are merely used to derive noise models for the arm vibration. None of the approaches presented in chapter 6 uses other position measurements than the ones provided by the linear encoders.





Figure 4.4: Cone dipole and quadrupole magnets. As it will be useful in the following discussion, a spherical coordinate system is inscribed in the center of the cone quadrupole. The r and φ coordinates are illustrated. The gap height of the cone quadrupole is denoted by H.

4.1.1 Sensor noise

In electronics, noise is an unwanted disturbance in an electrical signal [74]. In the following it is shown how the noise of a sensor can be characterized based on experimental measurements. The noise characterization is fundamental for the derivation of realistic noise models used in the quantification of measurement uncertainties.

It is beneficial to characterize the sensor noise in the frequency domain, because different physical effects may affect different frequency regimes. For instance, thermal noise and other *white noise* sources, usually govern the noise characteristics for high frequencies, whereas 50 Hz noise is often related to the power-line frequency.

Fundamental to the following discussion is the *power spectral density* of a signal. Denoting by $y : \mathbb{R} \to \mathbb{R}$ a signal in time and by $w_T(t)$ a windowing function

$$w_T(t) = \begin{cases} 1, & |t| < T, \\ 0, & \text{else,} \end{cases}$$

the power spectral density of y(t) is defined as

$$S_{yy}(f) := \lim_{T \to \infty} \frac{1}{T} |Y_T(f)|^2,$$
(4.4)

where $Y_T(f)$ is the Fourier transform of the windowed signal $y_T(t) = y(t)w_T(t)$. It describes how the power of the signal y is distributed over the frequencies f.



Figure 4.5: Amplitude power spectral density of a graphene Hall sensor compared to 1/f noise.

Noise of $1/f^{\alpha}$ -type is characterized by a power spectral density of type $S_{yy}(f) \propto 1/f^{\alpha}$, and it dominates the low-frequency regime in almost all electronic devices. Dependent on the parameter α , different *noise colors* may be classified, such as white noise $\alpha = 0$, pink noise $\alpha = 1$ and Brownian noise $\alpha = 2$.

As an example, measurement data taken with a graphene Hall sensor is considered [72]. The sensor is placed into a "zero Gauss" chamber, isolating it from external electromagnetic fields. A National Instruments PXI-6289 acquisition card [75] is used to sample the Hall voltage with a frequency of f = 625 kHz. From the discrete time series $\mathbf{y} = (y(t=0), ..., y(t=(M-1)\Delta t))^T$, where M = 100000 and $\Delta t = 1/f$, the power spectral density according to (4.4), is estimated by [76]

$$S_{yy}(f) \approx \frac{\Delta t}{M} \left| \sum_{m=0}^{M-1} y(m\Delta t) \exp\left(-j2\pi f m\Delta t\right) \right|^2.$$
(4.5)

It is common practice to average $S_{yy}(f)$ over several trials. In this case 1000 trials are taken. For the noise characterization, the mean value of y is usually subtracted from the signal before computing $S_{yy}(f)$.

As a figure of merit, the amplitude power spectral density, rather than the power spectral density, is commonly used to quantify electronic noise. This is because variations in the amplitude power-spectral density relate more directly to signal variations in cases of flat noise spectra. The amplitude power-spectral density is simply the square root of the power spectral density and is illustrated in Fig. 4.5.

The observed amplitude power-spectral density is typical for semiconductor devices such as Hall probes. A regime of 1/f noise, is followed by a plateau of generation recombination (GR) noise (see [71] Fig. 2.15), at about 1 kHz. As the signal was amplified with an analogue amplifier, hosting a 10 kHz low-pass filter [77], a

second cut off is visible around this frequency. The peaks between 1 kHz and 10 kHz could origin from noise in the power supply, which is providing the Hall current.

Given the power-spectral density, it is possible to derive a Gaussian model for the sensor noise. To this end it is assumed that the statistical properties of the process do not change over time, which is a reasonable assumption as long as the operation conditions are constant. For instance, characterizing the sensor noise in some controlled environment, the statistical properties are expected to be the same over longer time spans.

The stochastic process is expected to be wide-sense stationary according to definition 9, that is, the signal mean and auto-covariance depend only on the lag $\tau := t_2 - t_1$ between two instances.

Definition 9 Wide-sense stationary process A stochastic process generating the signal $y : \mathbb{R} \to \mathbb{R}$ is said to be wide-sense stationary, if its mean and auto-covariance functions are time invariant.

$$\mathbf{E}[y(t)] =: \mu = \text{const.}, \quad \forall t \in \mathbb{R},$$
(4.6)

$$\mathbf{E}\left[\left(y(t_1)-\mu\right)\left(y(t_2)-\mu\right)\right] =: R_{yy}(\tau), \quad \forall t_1, t_2 \in \{x, y \in \mathbb{R} \mid \tau = y - x\}.$$
(4.7)

In case of a wide sense stationary process, the power spectral density is the inverse Fourier transformation of the auto-correlation function $r_{yy}(\tau)$

$$S_{yy}(f) = \int_{-\infty}^{\infty} r_{yy}(\tau) \exp\left(j2\pi f\tau\right) \,\mathrm{d}\tau,\tag{4.8}$$

which is known as the Wiener-Khinchin theorem [78]. The auto-correlation function is defined as

$$r_{yy}(\tau) := \mathbb{E}\left[y(t_1)y(t_2)\right] = R_{yy}(\tau) - \mu^2, \tag{4.9}$$

where $R_{yy}(\tau)$ is the auto-covariance according to definition 9. If the considered signal is mean free, $\mu = 0$, the auto-covariance is equal to the auto-correlation function.

Having characterized the sensor noise by means of the power spectral density, one can estimate a signal covariance matrix by sampling with a given frequency. Considering that the measurement vector $\boldsymbol{y} = (y(t=0), ..., y(t=(M-1)\Delta t))^T$ is acquired by sampling the sensor voltage M times, with a frequency of $f = 1/\Delta t$, the signal may be considered as a realization of the Gaussian process $\boldsymbol{y} \sim \mathcal{N}(\mathbf{E}(\boldsymbol{y}), \boldsymbol{R}_y)$, where $\mathbf{E}(\boldsymbol{y})$ is the mean vector and the elements of the sensor noise covariance matrix \boldsymbol{R}_y are given by

$$[\mathbf{R}_{y}]_{i,j} = R_{yy}(\tau), \quad \text{with:} \quad \tau = (j-i)\Delta t. \tag{4.10}$$

This means that an estimate for the measurement covariance can be computed by evaluating $R_{yy}(\tau)$ for the lag τ between two instances.

For the measurement data given in Fig. 4.5, the auto-covariance $R_{yy}(\tau)$ is computed and evaluated for 1000 steps between $\tau = 0$ and 40 ms. In Fig. 4.6 left, the square root of the auto-covariance function is illustrated units of μ V. For comparison, the result of 1/f noise is shown. For lags above 10 ms, the correlations between measurements are below 1μ V, which is equivalent to 5μ T for this sensor. Such small effects are negligible for measurements in the 1 T range.



Figure 4.6: Estimation of a noise covariance matrix from the auto-covariance function. Left: Square root of the measured auto-covariance function compared to 1/f noise. Right: Resulting covariance matrix constructed from R_{yy} .

The matrix \mathbf{R}_y is illustrated in Fig. 4.6 right, for lags below 1.4 ms. In this case, the power spectral density is flat enough, that for moderate sampling rates $f > (10 \text{ ms})^{-1}$, the measurement covariance can be expressed by a diagonal matrix in good approximation. This, however, is not necessarily the case and has to be investigated for each individual sensor system and sampling frequency. If signal filtering, such as integration in time, is applied to the raw signal, an appropriate digital filter can be applied to the time series before computing the power spectral density according to 4.5.

4.1.2 Temperature effects

The electrical characteristics of semiconductor devices are strongly dependent on the temperature range of operation. For Hall sensors, this results in a temperature dependency of the sensitivity function s. The temperature coefficient TC_I is often defined as [71]

$$TC_I = \frac{1}{s_{\rm H}} \frac{\partial s_{\rm H}}{\partial T},\tag{4.11}$$

using the linear sensitivity $s_{\rm H}$ according to (4.3) for a reference operation condition. In [71, section 5.1.4], temperature coefficients are listed for different types of semiconductors. For gallium arsenid (GaAs), a typical temperature coefficient of $0.3 \times 10^{-3} \,\mathrm{K}^{-1}$ is observed [79]. To avoid relative errors in the 10^{-4} range, it is therefore necessary to either stabilize the temperature of the device within 1 K, or to calibrate TC_I and monitor the Hall temperature within the same range. Fig. 4.7 illustrates a temperature versus Hall voltage measurement, for one of the three axes used in the AS-3DC Hall probe from Projekt Elektronik [80]. A linear fit to the data yields $-4.11 \times 10^{-3} \,\mathrm{mV K}^{-1}$, which results in a temperature coefficient of $-0.082 \times 10^{-3} \,\mathrm{K}^{-1}$, as the probe's linear sensitivity for the given excitation current is $5 \,\mathrm{V T}^{-1}$.



Figure 4.7: Temperature calibration of the AS-3DC.

4.1.3 Hall effects in three dimensions

Another limitation of Hall probes for high accuracy magnetic field measurements, is their sensitivity towards planar field components, yielding Hall effects in three-dimensions.

The so-called *planar Hall effect* origins from a spread in the charge carrier drift velocity, in a combination with the thickness of the device [71][81]. An illustrative description of planar Hall effects is given in the caption of Fig. 4.8. In this figure and in the following, a local coordinate system (u, v, w) is fixed to the Hall sensor, in a way that w is oriented along the probe's orientation vector.

A more general description of the electric field in a semiconductor, due to the current density J and incident field B, is given by [71]

$$\boldsymbol{E} = \rho_B \boldsymbol{J} - R_H (\boldsymbol{J} \times \boldsymbol{B}) + P_H (\boldsymbol{J} \cdot \boldsymbol{B}) \boldsymbol{B}.$$
(4.12)

The resistance ρ_B is dependent on B due to magnetoresistive effects. The second term in the above equation corresponds to the classical Hall effect, which generates an electric field perpendicular to J and B. The third term generates an electric field oriented along B and is the source for what is called the planar Hall voltage U_{PHE} .

The measurable Hall voltage is determined by integrating the electric field E across the device. For the contribution of the planar Hall voltage this means

$$U_{ ext{PHE}} \propto (oldsymbol{J} \cdot oldsymbol{B})(oldsymbol{e} \cdot oldsymbol{B})_{ ext{PHE}}$$

where *e* is a vector indicating the direction along which the Hall voltage is measured (see Fig. 4.9).

The planar Hall voltage is zero if B is perpendicular to J, but also for B perpendicular to e. It is thus expected to have a double angular dependence in the uv-plane, which is often denoted as

$$U_{\text{PHE}} = c_{\text{PHE}} I |\boldsymbol{B}|^2 \sin(\theta) \sin(2\varphi).$$
(4.13)

Here c_{PHE} is a constant that depends on the geometry and material properties of the device, and θ , φ are the polar and azimuthal angles of the incident flux density, as shown in Fig. 4.9.



Figure 4.8: An illustrative description of the planar Hall effect. Consider the active area of the device to be located in the uv-plane and a planar magnetic flux density vector $B_{||}$. A spread in the charge carrier drift velocity δv will cause some charge carriers to drift with higher, or lower velocity than average. These carriers will be deflected from the equilibrium, due to the magnetic force generated by $\delta v \times B_v$, which is a force directed along w. As soon as the drift velocity contains a vertical component, the carriers are affected by a force $\propto |B_u|$ along v. The new equilibrium will result in a measurable voltage across the v axis, which is known as planar Hall voltage. The overall effect vanishes for both, $|B_u| = 0$ or $|B_v| = 0$. [82]



Figure 4.9: The local coordinate system (u, v, w) and the Hall element. The vector \boldsymbol{B} in (u, v, w) coordinates is described by $|\boldsymbol{B}|$, the polar angle θ and the azimuth angle φ .



Figure 4.10: Rotary stages for the three dimensional Hall probe calibration. The rotors are marked with the labels (A), and (B). The (u, v, w)-coordinates are fixed to the rotary tares in a way that the uv-plane is parallel to the rotor (B).

An approach for the three dimensional Hall probe calibration including the planar Hall effects was first presented in [83]. The Hall voltage is expanded by means of the solid harmonics $|\mathbf{B}|^l Y_l^m$, where $|\mathbf{B}|$ takes on the role of the radial coordinate

$$U(|\boldsymbol{B}|, \theta, \varphi) = \sum_{l=0}^{L} \sum_{m=-l}^{l} c_{l,m} |\boldsymbol{B}|^{l} Y_{l}^{m}(\theta, \varphi).$$
(4.14)

The term l = 0 is independent of |B| and corresponds to the sensor's zero field offset voltage U_0 . By (4.14), three dimensional phenomena can be characterized by means of the coefficients $c_{l,m} \in \mathbb{C}$, where $m \neq 0$. As an example, the planar Hall voltage corresponds to the coefficient $c_{2,\pm 2}$, assuming that the probe is oriented according to Fig. 4.9.

The calibration of the coefficients $c_{l,m}$ requires the possibility to manipulate the incident angles θ and φ of the excitation field B with a high accuracy. For this reason, calibration stages have been built using non-magnetic piezo-electric rotary stages. The rotors are equipped with rotary encoders with a measurement accuracy of 25 µrad. The whole assembly was designed to fit into a reference dipole magnet of 80 mm gap-height. It is shown in Fig. 4.10.

The azimuthal and polar angles θ and φ according to Fig. 4.9 may be related to the piezo rotors according to Fig. 4.10, assuming that the field is oriented along w for $\theta = \varphi = 0$. If this is not the case, the resulting harmonic expansion can be rotated in the post-processing. In this way, a possible stage misalignment with respect to the field direction can be accommodated.

The following results were used to characterize the planar Hall effect for new Hall effect devices using graphene technology [72]. As the planar Hall effect is related to the device thickness, it is expected that Hall probes based on mono-layers of graphene show reduced sensitivity towards planar fields.



Figure 4.11: Measurement positions for the three dimensional Hall probe calibration in the (u, v, w)-frame.

The rotary stages are equipped with the Hall probe and are mounted inside a calibration magnet, which is powered with a current I_{cal} in order to provide the desired absolute field |B|. The absolute field |B| is measured with an NMR probe. As NMR probe and Hall sensor cannot be placed at the same point, either a sufficient field homogeneity, or a prior magnet calibration is necessary.

The angular positions of the rotary stages are set in a way that the Hall probe's orientation vector is performing a full three dimensional rotation around the field vector. This means that the whole range $(0 < \theta < \pi, -\pi < \varphi < \pi)$ for θ and φ according to Fig. 4.9 is covered with measurements. In total 382 measurement positions are set. These positions are shown in Fig. 4.11 as points in the (u, v, w) frame.

In Fig. 4.12 (right) the Hall voltage is plotted as a response surface over the 382 measurement positions. This response surface can be interpreted in the following way: The distance of the response surface to the origin of the coordinates is proportional to the measured Hall voltage at this angular position. Also the color of the response surface encodes the Hall voltage in order to obtain the information about its sign.

The solid harmonics according to (4.14) are fitted to the signal by least squares. In total L = 15 harmonics are needed, yielding $(L + 1)^2 = 256$ coefficients to obtain a residual of $3.8 \cdot 10^{-8}$ V between measurements and fit. In Fig. 4.12 (right), the sensor imperfection is shown as a response surface. This imperfection is computed by suppressing all solid harmonic coefficients with l < 2.

In Fig. 4.13, the coefficients $c_{l,m}$ are scaled with $|\mathbf{B}|^l$ and plotted as bars for l < 10. Even- and odd multipoles are separated to limit the number of bars in each plot. The results are scaled with respect to the main coefficient $c_{1,0}$ and given in units of per mille. Coefficients with m = 0 correspond to the axial sensor response, without dependency on φ . These coefficients encode the probe's non-linear transfer function towards axial fields and can be determined without rotations by axial calibration.



Figure 4.12: Hall voltage response and sensor imperfection. Left: Hall probe voltage response for a full three dimensional rotation in a reference magnet. Right: Sensor imperfection. This means: Voltage response suppressing solid harmonic coefficients with l < 2. The imperfection is normalized with respect to the l = 1 coefficient and given in parts per mille.

Planar effects relate to coefficients with $m \neq 0$. For the device under test, planar effects are well below 10^{-4} with respect to the main sensitivity $c_{1,0}$. This proves the expected benefits for using graphene technology for Hall effect devices.

4.1.4 Orthogonality errors

Three-axes Hall probes are designed to measure the three components of the magnetic flux density in an orthogonal coordinate system. In Fig. 4.14 two examples are shown. The picture on the left shows a Hall cube of type HE444 from HE Hoeben electronics [84], integrated in an electronic circuit board for signal conditioning. The three Hall elements are embedded into the Hall cube of 3.3 mm width. In such small dimensions it is particularly challenging to mount the three axes orthogonally. The orthogonality errors can be assessed by mounting the sensor onto rotary stages and detecting the orientation of the sensor response surfaces in three dimensions. To this end, one extracts the coefficients $c_{l,m}$ as it was explained in section 4.1.3. From the coefficients with l = 1 one can compute the angular orientation by means of the spherical coordinates.

$$\varphi_{\max} = -\arg(c_{1,1}),\tag{4.15}$$

$$\theta_{\max} = \arg\left(c_{1,0} + j\sqrt{2}\sqrt{\operatorname{Re}\{c_{1,1}\}^2 + \operatorname{Im}\{c_{1,1}\}^2}\right),\tag{4.16}$$

where $\arg(z)$ is the argument of $z \in \mathbb{C}$. This follows from the definition of the spherical harmonics and trigonometric relations (see appendix 8.4). Given the angles φ_{\max} and θ_{\max} , the probe orientation may be



Figure 4.13: Expansion coefficients recovered from the measurements illustrated in Fig. 4.12. Only axial effects with coefficients m = 0 yield voltages above 10^{-4} , with respect to the maximum voltage. The measurement was performed at $|\mathbf{B}| = 0.9993$ T.

	relative angle [deg.]	orthogonality error [deg.]
x - y	89.7725	-0.2274
x-z	90.0493	0.04931
y-z	90.0755	0.07551

Table 4.1: Measured orthogonality errors for the HE444 Hall cube.

expressed by means of the orientation vector

$$\boldsymbol{n}_{\rm H}(\theta_{\rm max},\varphi_{\rm max}) = \begin{pmatrix} \sin(\theta_{\rm max})\cos(\varphi_{\rm max})\\ \sin(\theta_{\rm max})\sin(\varphi_{\rm max})\\ \cos(\theta_{\rm max}) \end{pmatrix}.$$
(4.17)

Computing the orientation vectors of all the three Hall probes, the angles between the probes can be determined. The orthogonality errors are then found in the differences to 90 degree. For the HE444 Hall cube, errors smaller than 0.5 degree are obtained. This is an impressing result considering the small dimensions, but still yields cross sensitivity errors above 10^{-4} and therefore requires calibration.

Integrated three-dimensional Hall cubes are expensive. Moreover, as angular orientation errors are unavoidable and need to be calibrated, custom-made solutions such as the assembly shown in Fig. 4.14 (right) are becoming attractive. Here three axial Hall probes of type HE244 from HE Hoeben electronics [85] are glued onto a ceramic cube. Including the cube, the price of the assembly is roughly a tenth of the integrated Hall cube. However, sensor packaging forbids placing the sensors closer than 1.2 mm to one another which makes it necessary to calibrate the relative sensor positions as well.



Figure 4.14: Examples for three-axes Hall probes. Left: HE444 embedded in an electronic circuit board for signal conditioning. Right: Three HE244 Hall probes glued on a ceramic cube. Details about the sensors can be found in [85].



Figure 4.15: Hall voltages for a full rotation of the HE444 as response surfaces in three dimensions.

4.1.5 Absolute position and sensor orientation

Mounting the sensor onto the tip of the mapper arm, it is not guaranteed that the probe orientation vectors are aligned with the stage coordinates. Moreover, the position of the Hall cube, relative to the stage and magnet coordinates, is only roughly estimated from the arm length and the sensor position within the measuring head. A fiducialisation is needed in order to relate the sensor position and orientation to the magnet coordinates.

Cone dipole and quadrupole magnets have been built especially for this purpose. These magnets are shown in Fig. 4.4 and are using permanent magnets to generate the magnetic fields. The assemblies are symmetric around the vertical axis¹. Poles of electrical steel are employed to shape dipole and quadrupole type fields around the magnets' geometric centers. The dipole magnet provides a vertical B-field, which can be used to align one of the sensor axes. The quadrupole magnet is used to identify the sensor position in three dimensional space, as its field exhibits a distinct zero in the geometric magnet center.

The support structure of the mapper arm is equipped with precision alignment screws, allowing to rotate and tilt the arm in order to align one of the senors to the field. This procedure was found to be difficult, however, as the arm deformation due to sag yields large tilt angles that need to be corrected. Moreover, the alignment needs to be based on detecting a signal maximum within a small range of variation. This is a challenging task, as the maximum of a signal $\propto \cos(\delta)$ needs to be found in an interval of δ in the range of only a few degrees.

The measured and simulated cone quadrupole fields in the xz and xy-planes are illustrated in Figures 4.16 and 4.17. Due to the orthogonality errors, the Hall voltages are zero along three non-orthogonal planes and the magnetic center may be found in the intersection of the planes in which $n_i \cdot B = 0$ holds $\forall i \in \{x, y, z\}$. The vectors n_i , for $i \in \{x, y, z\}$ are denoting the orientations of the three Hall probes.

First approaches to implement root finding algorithms were based on the detection of zero crossings in the Hall voltages and on gradient based iterations, minimizing the absolute value of |B| until convergence. In both cases, poor reproduction of results was experienced, as one relies on the stage positioning accuracy within a small volume around the magnet center and on the sensor accuracy for measuring small field amplitudes. Moreover, while the algorithms detect the |B| = 0 position, they cannot locate the positions of the individual Hall elements within the three zero planes. The position errors in a setup like Fig. 4.14 (right) might be in the range of millimeters.

For these reasons, a macroscopic approach is adopted, distributing measurements within a sphere around the magnet center. Sampling the field inside a larger volume is superior to local measurements around the magnet center, because the sensors are driven in their desired range of operation. As the approach is using the theory of chapter 5, details and results will be given in chapter 6.

4.2 A magneto-mechanical model for the three-axes Hall probe mapper

The use case of the three-axes Hall probe mapper is the measurement of local effects in inhomogeneous magnetic fields. With the elaborate probe calibration presented in the previous sections, most of the remaining measurement uncertainty is attributed to positioning errors of the stages and arm vibrations.

¹Except for the return yoke of the cone dipole.



Figure 4.16: Measured and simulated field of the cone quadrupole. The field simulation was performed in FEMM [86]. Differences between measurements and simulations are explained by the tolerances for the magnetization of the permanent magnets. The coordinates x, z as well as the spherical coordinates r and φ are illustrated in Fig. 4.4



Figure 4.17: Hall voltages measured in the *xy*-plane of the cone quadrupole. The dashed lines indicate the "zero planes", where $n_{\rm H} \cdot B = 0$. The normal vectors of these planes give evidence for the probe orientations with respect to the *xyz*-frame. In this plot, the dashed lines have been drawn with contour function of matplotlib [87].


Figure 4.18: Example for a three-axes Hall probe measurement suffering from mapper arm vibrations. Even in the homogeneous region of the magnet, the U_z voltage is affected, as the vibration deforms the arm in the yz-plane.

The arm of the 3D mapper can be considered as a cantilever beam, supported by the stages of the CMM on one side, carrying the Hall probe on the other. Due to leverage effects, small positioning perturbations of the stage motion introduce arm vibrations with amplitudes orders of magnitudes larger at the sensor position. In this way, arm vibrations influence the measurement result not only in the fringe fields, but also in the homogeneous region, where a changing field incident angle influences the measured voltages. This effect is seen in the signals plotted in Figure 4.18, where Hall probe measurements in a dipole field are given. To emphasize the effects, this measurement was performed with a velocity of 50 mm s^{-1} , larger than the nominal speed.

In the following sections, a mathematical model for the arm deformation is derived. This model will lay the foundation for the uncertainty quantification employed in chapters 5 and 6.

The mapper arm as a cantilever beam

The mapper arm under consideration is shown in Fig. 4.19 (left). It is a composition of an aluminum and carbonfiber-reinforced plastic (CFRP) tube, connected by means of a Polyoxymethylene (POM) joint. The measuring head hosting the sensor is mounted at the tip of the mapper arm. Without loss of generality, it is assumed that the arm's axis is aligned to the z-axis, as shown in Fig 4.19 (right).

In structural mechanics, deformations are commonly expressed by means of a deformation field $w : r' \rightarrow r \in \mathbb{R}^3$, mapping a coordinate r' in some reference configuration to a position r inside the deformed body. Considering that deformations are small and the arm cross section is axisymmetric, it is assumed that vertical and horizontal movements are decoupled and no axial effects are present. The arm's shape may be described



Figure 4.19: The mapper arm and the numerical model. Left: Composite mapper arm consisting of tubes of aluminum and carbon-fiber-reinforced plastic. Right: Numerical model by means of a cantilever beam in xz and yz-planes. Axial rotations are neglected.

by means of the deformation field

$$\boldsymbol{w}(x,y,z,t) = \begin{pmatrix} w_x(z,t) \\ w_y(z,t) \\ -x\varphi_x(z) - y\varphi_y(z) \end{pmatrix},$$
(4.18)

with the displacements w_x , w_y and the rotations φ_x and φ_y , which are drawn in Fig. 4.19 (right).

Because the mapper arm is long compared to its cross section, the derivatives $\partial w_x/\partial z$ and $\partial w_y/\partial z$ are approximately

$$\frac{\partial w_x}{\partial z} \approx \varphi_x, \qquad \frac{\partial w_y}{\partial z} \approx \varphi_y.$$
 (4.19)

This approximation distinguishes the so-called *Euler-Bernoulli* beam theory, from more sophisticated theories of linear elasticity.

Dropping the subscripts for w_x and w_y and considering either the xz or yz plane, the Euler-Bernoulli beam is governed by the partial differential equation [88]

$$(Lw)(z,t) + (C\frac{d}{dt}w)(z,t) + M(z)\frac{d^2}{dt^2}w(z,t) = p(z),$$
(4.20)

where L is the linear self-adjoint differential operator

$$L := \frac{\partial^2}{\partial z^2} \left(EI \frac{\partial^2}{\partial z^2} \right), \tag{4.21}$$

specifying the beam's *stiffness*, by means of the *elastic modulus* E and the *second moment of area* I, which is given by

$$I = \iint_{\mathcal{A}} y^2 \, \mathrm{d}x \, \mathrm{d}y, \tag{4.22}$$

for a beam with cross section A in the xy-plane, deformed in the yz-plane. A similar equation for I holds for the deformation in the xz-plane. M is the beam's mass per unit length and C is a model for the beams *internal* structural damping. C is parameterized by the constant parameters μ and λ , according to the Rayleigh model

$$C = 2\mu M + \lambda L. \tag{4.23}$$

Finally, p(z) is the distributed load. Since all beam parameters E, I, C and M are dependent on z, and the support condition at the clamped side is not trivial, solutions to Eq. (4.20) are computed by means of a finite element method (FEM). Details about the implementation are given in Appendix 8.5.

Using an approximation by finite elements, the displacement field w is expressed by means of the vector \hat{w} , encoding the values of w(z) and $\partial w(z)/\partial z$ at the nodes $z_1, ..., z_K$

$$\hat{\boldsymbol{w}} := \left(w(z_1), \left. \frac{\partial w}{\partial z} \right|_{z=z_1}, ..., w(z_K), \left. \frac{\partial w}{\partial z} \right|_{z=z_K} \right)^T.$$
(4.24)

With \hat{w} , (4.20), yields the linear ordinary differential equation system

$$\boldsymbol{M}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\hat{\boldsymbol{w}}(t) + \boldsymbol{C}\frac{\mathrm{d}}{\mathrm{d}t}\hat{\boldsymbol{w}}(t) + \boldsymbol{K}\hat{\boldsymbol{w}}(t) = \boldsymbol{f}(t), \qquad (4.25)$$

where M, K and C are the mass, stiffness and damping matrices, respectively. The right hand side f accounts for support conditions and applied loads.



Figure 4.20: Mapper arm and support, mounted onto the stages of the CMM.

Support motion

Fig. 4.20 shows the support structure of the mapper arm, which consists of an aluminum holder with brass clamps. This support is modeled by means of a combination of spring-mass dampers at the bearing points, see Fig. 4.21. Imperfections of the stage motion are causing the mapper arm to vibrate. These imperfections can be expressed by means of the support condition a(t) according to Fig. 4.21. Accounting for both stiffness and damping in the support model, the right hand side f may be decomposed into

$$\boldsymbol{f} = \boldsymbol{p} + \boldsymbol{k} \, \boldsymbol{a}(t) + \boldsymbol{d} \, \dot{\boldsymbol{a}}(t), \tag{4.26}$$

where p is a time independent load vector. See Appendix 8.5 for the definitions of k and d.



Figure 4.21: Support condition of the mapper arm in one dimension. This model is an approximation of the real support shown in Fig. 4.20. The support condition a(t) is allowed to vary in time, introducing vibrations to the structure.

The mapper arm transfer function

Considering an harmonic excitation by means of the spectral coefficients $a_n \in \mathbb{C}$, at frequencies $\omega_n \in \mathbb{R}$, where $a_n = a_{-n}^*$, and n = -N, ..., N according to

$$a(t) = \sum_{n=-N}^{N} a_n \exp\left(j\omega_n t\right),\tag{4.27}$$

it is beneficial to decompose also the arm deformation in the frequency domain:

$$\hat{\boldsymbol{w}}(t) = \sum_{n=-N}^{N} \boldsymbol{w}_n \exp\left(j\omega_n t\right), \qquad (4.28)$$

with $w_n \in \mathbb{C}$ and $w_n = w_{-n}^*$. Exploiting orthogonality yields for the *n*-th excitation frequency

$$\underbrace{\left(-\omega_n^2 M + j\omega_n C + K\right)}_{:=T(\omega_n)} \boldsymbol{w}_n = a_n (\boldsymbol{k} + j\omega_n \boldsymbol{d}).$$
(4.29)

Solving this equation system in the frequency range of interest allows one to derive an arm transfer function, mapping any harmonic support motion a_n to the tip displacement $w_n(z_s)$ and rotation $\varphi_n(z_s)$ at the sensor position z_s . To this end, the matrices: $\mathbf{F} : \hat{\mathbf{w}} \mapsto w(z_s)$ and $\partial \mathbf{F} : \hat{\mathbf{w}} \mapsto \varphi(z_s)$ are defined, in order to evaluate the displacement and rotation at the sensor position z_s , based on the FEM vector $\hat{\mathbf{w}}$. The transfer functions are given by

$$a_n T_w(z_{\mathbf{s}},\omega_n) := a_n \boldsymbol{F}(z_{\mathbf{s}}) \boldsymbol{T}(\omega_n)^{-1} (\boldsymbol{k} + j\omega_n \boldsymbol{d}) = w_n(z_{\mathbf{s}},a_n),$$

$$a_n T_{\varphi}(z_{\mathbf{s}},\omega_n) := a_n \partial \boldsymbol{F}(z_{\mathbf{s}}) \boldsymbol{T}(\omega_n)^{-1} (\boldsymbol{k} + j\omega_n \boldsymbol{d}) = \varphi_n(z_{\mathbf{s}},a_n).$$
(4.30)

Fig. 4.22 shows the transfer functions $T_w(z_s, \omega)$ and $T_{\varphi}(z_s, \omega)$ resulting from the FEM analysis in the vertical plane.

Measuring the tip deformation

Without knowledge about the spectrum of a(t), little is gained by the transfer functions shown in Fig. 4.22. To quantify the impact of arm deformations on the measured voltages, one desires to measure the support motion a(t) and apply the transfer function to recover amplitudes and frequencies of the tip deformation. Measuring a(t) directly, however, requires the measurement of displacement errors in the µm range, which is a non-trivial task, as particular instrumentation is required and environmental noise needs to be insulated carefully. It is beneficial to estimate the tip deformation from displacement measurements close to the sensor position where displacements in the 100 µm range can be observed. In the following, it is explained how the tip deformation can be estimated from optical measurements and the transfer functions derived from the FEM model.

Fig. 4.23 shows the signal path and an illustration of the mapper arm equipped with a retro reflector target, mounted at position z_t . The position of this target in three dimensional space is measured with a Leica laser tracker. Sampling with a frequency of $1\,000\,\text{Hz}$, this gives the signal $w_y(z_t, t)$ by means of a time series.



Figure 4.22: Transfer functions $T_w(z_s, \omega = 2\pi f)$ and $T_{\varphi}(z_s, \omega = 2\pi f)$ for the arm shown in Fig. 4.19, left. These functions can be computed from the FEM model and will be used to propagate the support motion to the tip displacement.

 $w_y(z_t, t)$ is Fourier transformed to obtain the spectrum of $w_y(\omega_n)$. Then, the transfer functions $T_{w,y}(z_s, \omega_n)/T_{w,y}(z_t, \omega_n)$ and $T_{\varphi,y}(z_s, \omega_n)/T_{w,y}(z_t, \omega_n)$ are applied to transfer the vertical displacement at z_t to the displacement $w_y(z_s, \omega_n)$ and rotation $\varphi_y(z_s, \omega_n)$ at the sensor position z_s . In the last step, the inverse Fourier transformation provides the signals $w_y(z_s, t)$ and $\varphi_z(z_s, t)$ as time series. The same approach is applied to the xz-plane.

4.2.1 The covariance matrix of mechanical perturbations

It will be beneficial for some of the approaches presented in chapter 6 to derive a statistical model for the arm deformation at the sensor position. The *mechanical state vector* d is introduced, in order to describe the mechanical vibrations and positioning errors at the sensor position. The result of this section is a statistical model for d given by means of a Gaussian distribution $p(d) \sim \mathcal{N}(0, D)$, with the *covariance matrix of mechanical perturbations* D. Chapter 5 contains an explanation of probability density functions, Gaussian distributions, and covariance matrices.

Considering a series of magnetic measurements taken at times t_m for m = 1, ..., M, one can assemble the five state vectors $d_{w,i}$ with $i \in \{x, y, z\}$ and $d_{\varphi,i}$ for $i \in \{x, y\}$ according to the scheme

$$\boldsymbol{d}_{w,i} = (w_i(z_{\mathsf{s}}, t_1), ..., w_i(z_{\mathsf{s}}, t_M))^T, \qquad \boldsymbol{d}_{\varphi,i} = (\varphi_i(z_{\mathsf{s}}, t_1), ..., \varphi_i(z_{\mathsf{s}}, t_M))^T.$$
(4.31)

The mechanical state vector is then assembled according to

$$\boldsymbol{d} = (\boldsymbol{d}_{w,x}^T, \boldsymbol{d}_{w,y}^T, \boldsymbol{d}_{w,z}^T, \boldsymbol{d}_{\varphi,y}^T, \boldsymbol{d}_{\varphi,y}^T)^T.$$
(4.32)

It is considered as zero mean, colored Gaussian noise $d \sim \mathcal{N}(0, D)$ (see section 4.1.1). The estimation of the covariance matrix D is the objective of this section.



Figure 4.23: Signal path for the measurement of displacement and rotation at the sensor position. The arm transfer function is applied to the measured signal in the Fourier domain. The deformation at the sensor position in the time domain is then recovered from the inverse transformation.

It is assumed that the motion is decoupled between the axes such that

$$\operatorname{cov}(\boldsymbol{d}_{w,i}, \boldsymbol{d}_{w,j}) = 0, \qquad \operatorname{cov}(\boldsymbol{d}_{\varphi,i}, \boldsymbol{d}_{\varphi,j}) = 0, \quad \text{for } i \neq j.$$
(4.33)

All other matrix blocks, $cov(d_{w,i}, d_{w,i})$, $cov(d_{w,i}, d_{\varphi,j})$ and $cov(d_{\varphi,j}, d_{\varphi,j})$ for $i \in \{x, y, z\}$ and $j \in \{x, y\}$, will be estimated from optical measurements according to section 4.2.

Remark 2 Also the positioning along the mapper arm axis is imperfect. Without loss of generality this axis is denoted by z. Although these positioning errors do not contribute to arm vibrations, they are still taken into account in the following analysis. The transfer function for w_z is therefore set to identity and the $d_{w,z}$ vector is filled with the differences between the measurements obtained from the encoder and the laser tracker. To this end, the laser tracker has been synchronized with the distance trigger of the positioning stages of the CMM.

With the assumption that the stochastic process for d is wide-sense stationary according to definition 9, the statistical properties between two observations are dependent only on the time difference between two measurements. The covariance can then be expressed by the auto-covariance, meaning that it can be estimated from a single time series, comparing the signal with shifted versions of itself. To this end, a total amount of 2K measurements are taken. Denoting by $d_{w,x}^{(k)}$ the sampled time series of $d_{w,x}$ shifted by k samples and assuming that $E[d_{w,x}] = 0$, the covariance matrix $cov(d_{w,x}, d_{w,x})$ is computed by

$$\operatorname{cov}(\boldsymbol{d}_{w,x}, \boldsymbol{d}_{w,x}) = \frac{1}{K-1} \left(\boldsymbol{d}_{w,x}^{(1)}, ..., \boldsymbol{d}_{w,x}^{(K)} \right) \cdot \left(\boldsymbol{d}_{w,x}^{(1)}, ..., \boldsymbol{d}_{w,x}^{(K)} \right)^{T},$$
(4.34)

here K is half of the number of samples available, in order to be able to shift the signals accordingly. Similar equations are used for all other matrix blocks.

This approach overestimates the positioning precision for very low frequencies, because the displacement measurements are based on the best fit of a line to the measured positions and computing the position errors



Figure 4.24: Blocks of the covariance matrix D, corresponding to horizontal and vertical displacements $d_{w,x}$ and $d_{w,y}$. The covariance is estimated for 1 000 measurements with $\Delta t = 10$ ms. Different frequencies are excited for $d_{w,x}$ and $d_{w,y}$.

with respect to this line. The resulting displacements are indeed zero mean. However, the machine coordinates are imperfect; the position of the best fit line may be displaced with respect to the desired position. To get a more realistic estimator for low frequencies, the positioning precision for moves in the full volume of 3 m^3 was observed. The maximum positioning error is 0.1 mm. This value is therefore set as three standard deviations and added to the matrix blocks $cov(d_{w,i}, d_{w,i})$ for $i \in \{x, y, z\}$.

The resulting covariance structures only depend on the time difference between two observations, and therefore naturally lead to Toeplitz matrices. This has two significant advantages: 1) Only a single row of the matrix needs to be stored. 2) If the Toeplitz matrix is diagonally dominant, $|[D]_{1,1}| > \sum_{k \neq 1} |[D]_{1,k}|$ and $[D]_{1,1} > 0$, the matrix will be positive semi-definite and therefore a proper covariance matrix. Fig. 4.24 illustrates the covariance matrix blocks for the vertical perturbation recovered from a horizontal move.

4.2.2 The perturbed observation operator

Arm deformation and positioning errors are perturbing the measurement positions and therefore the measured voltages. Some of the applications presented in chapter 6 aim for the precise quantification of measurement uncertainties due to mechanical perturbations. Therefore, a perturbed observation operator is now derived.

Consider the 3D mapper equipped with a three-axis Hall sensor. The measurements of the three probes are assembled into the vector $\tilde{\boldsymbol{y}}$ according to the scheme $\tilde{\boldsymbol{y}} = (\tilde{\boldsymbol{y}}_x^T, \tilde{\boldsymbol{y}}_y^T, \tilde{\boldsymbol{y}}_z^T)^T$. Therefore, in case of the 3D mapper, the vector $\tilde{\boldsymbol{y}}$ is of size \mathbb{R}^{3M} , where *M* is the number of measurement *positions*.

Assuming, without loss of generality, that the mapper arm is oriented along z and the probe is centered transversely within the arm, it holds that x = y = 0 in (4.18). The position of the probe is then given by

$$\boldsymbol{r}(t) = \boldsymbol{r}_s(t) + \boldsymbol{w}(z_s, t) = \boldsymbol{r}_s(t) + \begin{pmatrix} w_x(z_s, t) \\ w_y(z_s, t) \\ w_z(z_s, t) \end{pmatrix}.$$
(4.35)

 $r_s(t)$ is the position of the Hall probe, assuming infinite stiffness of the mapper arm², and $w(z_s, t)$ is the arm deformation evaluated at the sensor position z_s . Comparing (4.18) to (4.35), the *z* coefficient $w_z(z_s, t)$ is introduced. In this way, a possible axial displacement can be described. The axial transfer function for $w_z(z_s, t)$ may be set to identity, to account for longitudinal positioning errors of the stages, which do not contribute to the arm deformation (see remark 2).

In addition to deformations, the rotations φ_x and φ_y at the sensor position must be taken into account. As only transverse motions are of concern, axial rotations (see Fig. 4.19) can be neglected. As is was discussed in section 4.2.1, w_x , w_y , w_z as well as φ_x and φ_y are the elements of the mechanical states vectors d. The same sorting scheme for d, which was used in (4.32) is now adopted.

Denoting by ν the state vector of the magnetic field, for instance the degrees of freedom of the BEM approximation space, the discrete observation operator H can be formulated in terms of both the magnetic and mechanical state vectors,

$$\boldsymbol{H}: (\boldsymbol{\nu}, \boldsymbol{d}) \to \mathbb{R}^M,$$
 (4.36)

where the mechanical state vector d is treated as a sensor parameter. In almost all cases, the dependency of H on d is complicated. Since the displacements are small perturbations around r_s , the observation operator may be linearized according to

$$\begin{aligned} \boldsymbol{H}(\boldsymbol{\nu},\boldsymbol{d}) &\approx \boldsymbol{H}(\boldsymbol{\nu},\boldsymbol{d}) = \boldsymbol{H}(\boldsymbol{\nu},\boldsymbol{0}) + \partial_{x}\boldsymbol{H}(\boldsymbol{\nu},\boldsymbol{d})|_{\boldsymbol{d}=\boldsymbol{0}} d_{\boldsymbol{w},\boldsymbol{x}} \\ &+ \partial_{y}\boldsymbol{H}(\boldsymbol{\nu},\boldsymbol{d})|_{\boldsymbol{d}=\boldsymbol{0}} d_{\boldsymbol{w},\boldsymbol{y}} \\ &+ \partial_{z}\boldsymbol{H}(\boldsymbol{\nu},\boldsymbol{d})|_{\boldsymbol{d}=\boldsymbol{0}} d_{\boldsymbol{w},\boldsymbol{z}} \\ &+ \partial_{\varphi_{x}}\boldsymbol{H}(\boldsymbol{\nu},\boldsymbol{d})|_{\boldsymbol{d}=\boldsymbol{0}} d_{\varphi,\boldsymbol{x}} \\ &+ \partial_{\varphi_{y}}\boldsymbol{H}(\boldsymbol{\nu},\boldsymbol{d})|_{\boldsymbol{d}=\boldsymbol{0}} d_{\varphi,\boldsymbol{y}}. \end{aligned}$$
(4.37)

The terms $\partial_j \boldsymbol{H}(\boldsymbol{\nu}, \boldsymbol{d})|_{\boldsymbol{d}=\boldsymbol{0}}$ are matrices in $\mathbb{R}^{3M \times M}$, as three Hall voltages are measured at M positions. The matrices have the meanings of the derivatives of the discrete observation operator with respect to $j \in \{x, y, z, \varphi_x, \varphi_y\}$, evaluated for $\boldsymbol{d} = \boldsymbol{0}$ and some particular $\boldsymbol{\nu}$.

To understand the structure of the matrices $\partial_j H(\nu, d)|_{d=0}$, the rows of the discrete observation operator $H(\nu, d)$ are denoted according to

$$H(\nu, d) = \begin{pmatrix} H_{x,1}(\nu, d) \\ \vdots \\ H_{x,M}(\nu, d) \\ H_{y,1}(\nu, d) \\ \vdots \\ H_{y,M}(\nu, d) \\ H_{z,1}(\nu, d) \\ \vdots \\ H_{z,M}(\nu, d) \end{pmatrix},$$
(4.38)

which is in-line with the sorting scheme $\tilde{y} = (\tilde{y}_x^T, \tilde{y}_y^T, \tilde{y}_z^T)^T$ for the predicted measurements. The element $H_{j,m}$ denotes the observation operator for the *j*-th sensor at the *m*-th measurement position. Adopting this

 $^{{}^{2}\}boldsymbol{r}_{s}(t)$ will be identified with the position measurements of the linear encoders.

notation, the matrices $\left.\partial_{j}\boldsymbol{H}(\boldsymbol{\nu},\boldsymbol{d})\right|_{\boldsymbol{d}=\boldsymbol{0}}$ are given explicitly by

$$\partial_{j} \boldsymbol{H}(\boldsymbol{\nu}, \boldsymbol{d})|_{\boldsymbol{d}=\boldsymbol{0}} = \begin{pmatrix} \partial_{j} H_{x,1}(\boldsymbol{\nu}, \boldsymbol{d})|_{\boldsymbol{d}=\boldsymbol{0}} & 0 & \cdots & 0 \\ 0 & \partial_{j} H_{x,2}(\boldsymbol{\nu}, \boldsymbol{d})|_{\boldsymbol{d}=\boldsymbol{0}} & \cdots & 0 \\ \vdots & \cdots & \ddots & \vdots \\ 0 & 0 & \cdots & \partial_{j} H_{x,M}(\boldsymbol{\nu}, \boldsymbol{d})|_{\boldsymbol{d}=\boldsymbol{0}} \\ \partial_{j} H_{y,1}(\boldsymbol{\nu}, \boldsymbol{d})|_{\boldsymbol{d}=\boldsymbol{0}} & 0 & \cdots & 0 \\ 0 & \partial_{j} H_{y,2}(\boldsymbol{\nu}, \boldsymbol{d})|_{\boldsymbol{d}=\boldsymbol{0}} & \cdots & 0 \\ \vdots & \cdots & \ddots & \vdots \\ 0 & 0 & \cdots & \partial_{j} H_{y,M}(\boldsymbol{\nu}, \boldsymbol{d})|_{\boldsymbol{d}=\boldsymbol{0}} \\ \partial_{j} H_{z,1}(\boldsymbol{\nu}, \boldsymbol{d})|_{\boldsymbol{d}=\boldsymbol{0}} & 0 & \cdots & 0 \\ \vdots & \cdots & \ddots & \vdots \\ 0 & 0 & \cdots & \partial_{j} H_{z,M}(\boldsymbol{\nu}, \boldsymbol{d})|_{\boldsymbol{d}=\boldsymbol{0}} \end{pmatrix}.$$
(4.39)

One may introduce the short-handed notation

$$\left. \partial_{j} \boldsymbol{H}(\boldsymbol{\nu}, \boldsymbol{d}) \right|_{\boldsymbol{d}=\boldsymbol{0}} = \begin{pmatrix} \operatorname{diag} \left(\partial_{j} \boldsymbol{H}_{x}(\boldsymbol{\nu}, \boldsymbol{d}) \right|_{\boldsymbol{d}=\boldsymbol{0}} \\ \operatorname{diag} \left(\partial_{j} \boldsymbol{H}_{y}(\boldsymbol{\nu}, \boldsymbol{d}) \right|_{\boldsymbol{d}=\boldsymbol{0}} \\ \operatorname{diag} \left(\partial_{j} \boldsymbol{H}_{z}(\boldsymbol{\nu}, \boldsymbol{d}) \right|_{\boldsymbol{d}=\boldsymbol{0}} \end{pmatrix} \right),$$
(4.40)

where H_i is the observation operator of probe *i* for i = x, y, z, and diag(x) is a diagonal matrix with diagonal elements x.

In (4.37), a linear relationship between the predicted measurements \tilde{y} and the mechanical state vector d is established. The operator \tilde{H} will be denoted as the *perturbed observation operator*. One may combine the $\partial_i H$ matrices and write

$$\overline{H}(\nu, d) = H(\nu, 0) + \partial H(\nu) d, \qquad (4.41)$$

where

$$\partial \boldsymbol{H}(\boldsymbol{\nu}) := \left(\left. \partial_x \boldsymbol{H}(\boldsymbol{\nu}, \boldsymbol{d}) \right|_{\boldsymbol{d}=\boldsymbol{0}}, \left. \partial_y \boldsymbol{H}(\boldsymbol{\nu}, \boldsymbol{d}) \right|_{\boldsymbol{d}=\boldsymbol{0}}, \left. \partial_z \boldsymbol{H}(\boldsymbol{\nu}, \boldsymbol{d}) \right|_{\boldsymbol{d}=\boldsymbol{0}}, \left. \partial_{\varphi_x} \boldsymbol{H}(\boldsymbol{\nu}, \boldsymbol{d}) \right|_{\boldsymbol{d}=\boldsymbol{0}}, \left. \partial_{\varphi_y} \boldsymbol{H}(\boldsymbol{\nu}, \boldsymbol{d}) \right|_{\boldsymbol{d}=\boldsymbol{0}} \right).$$
(4.42)

The matrix $\partial \boldsymbol{H}(\boldsymbol{\nu}) \in \mathbb{R}^{3M \times 5M}$ gives the linearized relationship between the measurements and the mechanical state vector \boldsymbol{d} , it is therefore denoted as *mechanical perturbation matrix*. In case of a BEM field representation, the spatial derivatives in $\partial \boldsymbol{H}(\boldsymbol{\nu})$ can be computed by deriving the Green's function analytically. The angular derivatives are obtained by expressing the Hall voltage as a function of the probe's orientation vector $\boldsymbol{n}(\varphi_x, \varphi_y)$, and differentiating the resulting expression with respect to φ_x and φ_y . It is beneficial to perform the integration for all $\partial_j \boldsymbol{H}$ matrices at once, to avoid multiple evaluations of the surface elements on the domain boundary.

5 Statistical inference

Statistical inference is the process of using data analysis to infer properties of an underlying distribution of probability [89]. Assessing estimators and credible intervals for the boundary data ν and sensor parameters θ based on erroneous measurement data, is a classical example for statistical inference. This chapter gives an introduction into the concept of Bayesian inference, which will be of particular importance for the applications presented in chapter 6. The focus lies on the derivation of algorithms for the solution of inference problems for linear and nonlinear problems, as they will be applied to several applications in chapter 6. This shall provide the link between the physical modeling presented in the previous chapters and the application part in chapter 6.

Referring to the blueprint, this chapter shall provide the framework to blend measurement data with the physical model and prior knowledge. The blueprint notation for the state vector $\boldsymbol{\nu}$, sensor parameters $\boldsymbol{\theta}$ and measurements \boldsymbol{y} is adopted. In cases where a distinction between $\boldsymbol{\nu}$ and $\boldsymbol{\theta}$ is irrelevant, both variables will be joint in the vector $\boldsymbol{x} = \{\boldsymbol{\nu}, \boldsymbol{\theta}\} \in \mathbb{R}^N$ and denoted as *state variables*, defined over the *sampling space* \mathbb{R}^N . The observation operator will then be denoted $\boldsymbol{H} : \boldsymbol{x} \in \mathbb{R}^N \to \mathbb{R}^M$. In the following, \boldsymbol{H} might be linear or nonlinear in \boldsymbol{x} , and it relates to the measurement data \boldsymbol{y} via the additive noise model

$$\boldsymbol{y} = \boldsymbol{H}(\boldsymbol{x}) + \boldsymbol{\epsilon}. \tag{5.1}$$

In light of the discussion in chapter 1, the deterministic part y_{det} is identified with H(x) in (5.1). ϵ is the error term, able to encode microscopic or macroscopic physical effects which can be expressed by means of a noise model. In this work, this means a probability density function. A typical example is the colored Gaussian noise model, which has been derived in section 4.1.1 for the electronic noise in Hall-probe measurements. Expressing ϵ as a random variable following a certain probability density function, the measurement vector y may be interpreted as a realization of a stochastic process with probability density function p(y). For the aspects covered in this thesis, the rather informal discussion about probability density functions over continuous random variables given in definition 10 is sufficient. This definition is inspired by [17, p. 1.2.1].

In statistical inference, variables which are not directly observed, but inferred by means of a mathematical model, are called *latent variables*. As in magnetic measurements all measurement data is provided by voltages and their integrals over small time windows, the state variables are never observed directly and always need to be inferred through a mathematical model (for the sensor and the field). Therefore x, ν and θ are latent variables. It is common practice to denote variables which are influencing the measurement process, but not the process of drawing predictions from the numerical model, as *nuisance* parameters. As θ is related to the sensor model and not the field model, θ is also a nuisance parameter.

The definitions of some important statistical properties are found in table 5.1. The two most important probability density functions for this thesis are found in definition 11 and 12.

parameter	notation	definition	estimator
mean	$E(\boldsymbol{x})$	$\int_{\mathbb{R}^N} oldsymbol{x} p(oldsymbol{x}) \mathrm{d}oldsymbol{x}$	$rac{1}{K}\sum_k oldsymbol{x}_k$
covariance	$\operatorname{cov}({m x},{m y})$	$E\left(\left(\boldsymbol{x}-E\left(\boldsymbol{y}\right)\left(\boldsymbol{y}-E\left(\boldsymbol{x}\right)\right) ight) ight)$	$\left \begin{array}{c} rac{1}{K-1} \sum_k (oldsymbol{x}_k - { t E}[oldsymbol{x}]) (oldsymbol{y}_k - { t E}(oldsymbol{y})^T \end{array} ight.$
variance	$var(\boldsymbol{x})$	$\mathrm{E}\left(oldsymbol{x}-\mathrm{E}\left(oldsymbol{x} ight)^{2} ight)$	$rac{1}{K-1}\sum_k \left(\left(oldsymbol{x}_k - \operatorname{E}\left(oldsymbol{x} ight) ight)^2$

Table 5.1: Definition of some important statistical properties. p(x) is the probability density function for x defined over \mathbb{R}^N . It is defined in definition 10

Definition 10 (Probability density functions over continuous random variables) The probability density function p(x) is defined as a function $x \in \mathbb{R}^N \to \mathbb{R}$, such that the probability for x falling in an infinitesimal volume δx , containing the point x is given by $p(x)\delta x$. This probability density function must satisfy [17, Section 1.2.1]

$$p(\boldsymbol{x}) \ge 0, \qquad \forall \boldsymbol{x} \in \mathbb{R}^N$$
 (5.2)

$$\int_{\mathbb{R}^N} p(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = 1. \tag{5.3}$$

Definition 11 (Gaussian distributions) The multivariate Gaussian distribution (short Gaussian distribution), is defined over $x \in \mathbb{R}^N$ and given by the probability density function

$$p(\boldsymbol{x}) = \frac{1}{\sqrt{2\pi}^{N} \det(\boldsymbol{\Sigma})} \exp\left(-\frac{1}{2} \left(\boldsymbol{x} - \boldsymbol{m}\right)^{T} \boldsymbol{\Sigma}^{-1} \left(\boldsymbol{x} - \boldsymbol{m}\right)\right).$$
(5.4)

Herein, m is the mean value and Σ is the covariance matrix according to the definitions in table 5.1. One writes

$$p(\boldsymbol{x}) \sim \mathcal{N}(\boldsymbol{m}, \boldsymbol{\Sigma}).$$
 (5.5)

Definition 12 (Gamma distributions) The gamma distribution is defined over $x \in \mathbb{R}$ and given by the probability density function

$$p(x) = \begin{cases} \frac{b^p}{\Gamma(p)} x^{p-1} \exp(-bx), & x > 0\\ 0, & x \le 0. \end{cases}$$
(5.6)

It is parameterized by the scale and rate parameters b and $p \in \mathbb{R}$. Mean and variance are related to b and p by:

$$E(x) = \frac{p}{b}, \quad var(x) = \frac{p}{b^2}.$$
 (5.7)

One writes

$$p(x) \sim \Gamma(p, b). \tag{5.8}$$

5.1 Bayesian inference

In Bayesian inference, the uncertainty in the state variables x is expressed in terms of a probability density function p(x). The aim is to infer the probability density function p(x), based on a collection of observed, dependent variables y. In the context of magnetic measurements y has the meaning of measurement data, and the relation between x and y is given by the observation operator H according to Eq. (5.1).

The explicit form of the observation operator H is derived by linking the sensor sensitivity function $s(\theta, B)$ with the numerical model for the field B dependent on ν

$$\boldsymbol{H}(\boldsymbol{x}) = s(\boldsymbol{\theta}, \boldsymbol{B}) \circ \boldsymbol{B}(\boldsymbol{\nu}).$$

Due to the random character of the error term, it is natural to ask how likely a measurement y is, given a vector of parameters x. The probability of a measurement y may be described by means of the conditional probability density function p(y|x), expressing the probability density function for y given a value for x. The resulting function, when considering p(y|x) for a fixed measurement outcome y over the parameters x, is called the *likelihood function*. Identifying p(y|x) is a question of metrological characterization of the measurement system, as discussed in chapter 4.

As an example, consider the Gaussian noise model with mean value E(y) and covariance matrix \mathbf{R} ; $p(\mathbf{y}) \sim \mathcal{N}(E(\mathbf{y}), \mathbf{R})$. The measurement outcome \mathbf{y} depends on the magnetic field at the measurement position, and therefore on the state variables \mathbf{x} . The conditional probability density function $p(\mathbf{y}|\mathbf{x})$ is obtained by substituting the observation operator for $E(\mathbf{y})$ in $p(\mathbf{y})$, yielding the distribution $p(\mathbf{y}|\mathbf{x}) \sim \mathcal{N}(\mathbf{H}(\mathbf{x}), \mathbf{R})$. The likelihood function is then determined by fixing the \mathbf{y} variable in $\mathcal{N}(\mathbf{H}(\mathbf{x}), \mathbf{R})$ and considering the result as a function over \mathbf{x} .

Fundamental to Bayesian inference is Bayes' rule of probability. In this thesis, the focus lies on probability density functions over continuous random variables, according to definition 10. Considering x and y as dependent realizations of random variables, the Bayes rule is a direct consequence of the definition of the conditional probability density function

$$p(\boldsymbol{y}|\boldsymbol{x}) = \frac{p(\boldsymbol{x}, \boldsymbol{y})}{p(\boldsymbol{x})}.$$
(5.9)

p(y|x) is the conditional probability density function for y given a value for x, p(x, y) is the joint probability density function over x and y, and p(x) is the marginal probability density function for variable x. Exchanging the order of x and y in (5.9) the Bayes rule of probability yields

$$p(\boldsymbol{x}|\boldsymbol{y}) = \frac{p(\boldsymbol{y}|\boldsymbol{x})p(\boldsymbol{x})}{p(\boldsymbol{y})}.$$
(5.10)

The role of the denominator p(y) in the Bayes rule is for normalization and can therefore be omitted from now on. Then follows the proportionality relation

$$\underbrace{p(\boldsymbol{x}|\boldsymbol{y})}_{\text{Posterior}} \propto \underbrace{p(\boldsymbol{y}|\boldsymbol{x})}_{\text{Likelihood}} \underbrace{p(\boldsymbol{x})}_{\text{Prior}}.$$
(5.11)

The posterior $p(\boldsymbol{x}|\boldsymbol{y})$ is the probability density function for the state variables, which describes their "belief" based on the observations \boldsymbol{y} . $p(\boldsymbol{y}|\boldsymbol{x})$ is the likelihood function discussed before and the prior $p(\boldsymbol{x})$ encodes knowledge about the state variables \boldsymbol{x} .

The Bayesian paradigm differs from the so-called frequentist paradigms. As stated in [17]: In both the Bayesian and frequentist paradigms, the likelihood function p(y|x) plays a central role. However, the manner in which it is used is fundamentally different in the two approaches. In a frequentist setting, x is considered to be a fixed parameter, whose value is determined by some form of 'estimator', and errors bars on this estimate are obtained by considering the distribution of possible data sets y. By contrast, from the Bayesian viewpoint there is only a single data set y (namely the one that is actually observed), and the uncertainty in the parameters is expressed through a probability distribution over x.

In view of the Bayesian and frequentist paradigms, the approaches presented in this thesis differ from classical uncertainty quantification used in the post-processing of magnetic measurement data. Error bars are usually derived by investigating the spread of the measurement result after repeated observations. In rotating coil measurements, for instance, multipole errors are computed for several turns of the rotating coil and mean and standard deviations are estimated from the sampled statistical moments of the resulting population. Data acquisition for the whole population takes only seconds and the post-processing is computed on the fly. In some cases however, repeating a measurement several times may be a time consuming process. A full three dimensional field map, taken with the Hall-probe mapper, may easily require a full day of measurements. Following the Bayesian paradigm allows one to derive error bars from the posterior distribution based on a single data set only.

There is a great flexibility in choosing the prior p(x). Although strictly speaking, uniform distributions over the whole sampling space in \mathbb{R}^N do not exist (as it would contradict the requirements formulated in definition 10), it is always possible to assume a sufficiently flat prior that is approximately constant over the relevant sampling space $p(x) \approx \text{const.}$ This yields proportionality relations between posterior and likelihood relying on measurements only. Throughout this thesis, these priors will be denoted as *flat priors*, and they will be used to initialize the active learning algorithm.

It is also plausible to use results from numerical field simulations as prior knowledge in order to regularize ill-posed inverse problems. In these cases however, it is often difficult to assign reasonable values to the prior covariance matrix.

In the following sections, some explicit algorithms for the computation of p(x|y) based on Bayes rule of probability are presented, as they will be applied extensively in chapter 6.

5.2 Maximum likelihood solutions

In the following, a linear observation operator is investigated, such that $\tilde{y} = Hx$. Considering a Gaussian noise model for $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{R})$, with covariance matrix \mathbf{R} in (5.1), the likelihood function is given by $p(y|x) \sim \mathcal{N}(H(x), \mathbf{R})$. Choosing a sufficiently flat prior p(x), such that $p(x) \approx \text{const over the relevant sampling space}$, the posterior probability density function is given by

$$p(\boldsymbol{x}|\boldsymbol{y}) \propto \exp\left(-\frac{1}{2}\left(\boldsymbol{y} - \boldsymbol{H}\boldsymbol{x}\right)^{T}\boldsymbol{R}^{-1}\left(\boldsymbol{y} - \boldsymbol{H}\boldsymbol{x}\right)\right).$$
 (5.12)

It can be shown that this is a Gaussian distribution over x. To see this, one may perform the multiplications in the exponent to obtain

$$p(\boldsymbol{x}|\boldsymbol{y}) \propto \exp\left(-\frac{1}{2}\left(\boldsymbol{y}^{T}\boldsymbol{R}^{-1}\boldsymbol{y} - 2\boldsymbol{x}^{T}\boldsymbol{H}^{T}\boldsymbol{R}^{-1}\boldsymbol{y} + \boldsymbol{x}^{T}\boldsymbol{H}^{T}\boldsymbol{R}^{-1}\boldsymbol{H}\boldsymbol{x}\right)\right).$$
(5.13)

The same can be done for a standard Gaussian distribution $p(x) \sim \mathcal{N}(m, \Sigma)$

$$p(\boldsymbol{x}) \propto \exp\left(-\frac{1}{2}\left(\boldsymbol{m}^{T}\boldsymbol{\Sigma}^{-1}\boldsymbol{m} - 2\boldsymbol{x}^{T}\boldsymbol{\Sigma}^{-1}\boldsymbol{m} + \boldsymbol{x}^{T}\boldsymbol{\Sigma}^{-1}\boldsymbol{x}\right)\right).$$
 (5.14)

One then finds the mean m and covariance matrix Σ of the posterior by comparing the coefficients in the exponents,

$$\boldsymbol{\Sigma} = \left(\boldsymbol{H}^T \boldsymbol{R}^{-1} \boldsymbol{H}\right)^{-1}, \qquad (5.15)$$

$$\boldsymbol{\Sigma}^{-1}\boldsymbol{m} = \boldsymbol{H}^T \boldsymbol{R}^{-1} \boldsymbol{y}. \tag{5.16}$$

This procedure to identify the mean and covariance matrix in the posterior is known as *completing the squares* and the solution $m = \Sigma H^T R^{-1} y$ is known as *maximum likelihood solution*. The posterior probability density function is defined by the mean m and covariance matrix Σ .

It is possible to generate samples x_k from the posterior p(x|y) by solving the randomized linear equations system

$$(\boldsymbol{H}^{T}\boldsymbol{R}^{-1}\boldsymbol{H})\boldsymbol{x}_{k} = \boldsymbol{H}^{T}\boldsymbol{R}^{-1}\boldsymbol{y} + \boldsymbol{H}^{T}\boldsymbol{R}^{-1/2}\boldsymbol{\epsilon}_{k}, \quad \boldsymbol{\epsilon}_{k} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I}_{M}).$$
(5.17)

 I_M is an identity matrix of dimension $M \times M$ and $\mathbf{R}^{1/2}$ denotes the square root matrix of \mathbf{R} such that $\mathbf{R} = \mathbf{R}^{1/2}\mathbf{R}^{1/2}$. A square root of a symmetric, positive definite matrix can be computed by the Cholesky factorization. This functionality is available in the Cholesky module of the Eigen C++ library [90]. Although the covariance matrix might be of a large dimension $\mathbf{R} \in \mathbb{R}^{M \times M}$, it is sparse in all the considerations to follow. In cases of measurements with the 3D mapper, typically only 1% of the matrix is populated.

To prove that x_k follows the desired posterior distribution, consider a multivariate Gaussian random variable $x \sim \mathcal{N}(m, \Sigma)$ and the affine transformation w = c + Bx. From the linearity of Gaussian distributions it follows that $w \sim \mathcal{N}(c + Bm, B\Sigma B^T)$ (see [91, chapter 1.2]). Substituting the right-hand-side of (5.17) according to

$$egin{aligned} m{m} &\mapsto m{0}, \ m{\Sigma} &\mapsto m{I}_M, \ m{c} &\mapsto m{H}^T m{R}^{-1} m{y}, \ m{B} &\mapsto m{H}^T m{R}^{-1/2}. \end{aligned}$$

one finds that

$$\boldsymbol{w} \sim \mathcal{N} \left(\boldsymbol{H}^T \boldsymbol{R}^{-1} \boldsymbol{y}, \boldsymbol{H}^T \boldsymbol{R}^{-1} \boldsymbol{H} \right).$$
(5.18)

Now consider another linear transformation

$$\boldsymbol{x} = \left(\boldsymbol{H}^T \boldsymbol{R}^{-1} \boldsymbol{H}\right)^{-1} \boldsymbol{w}.$$
 (5.19)

Following the same arguments as before,

$$\boldsymbol{x} \sim \mathcal{N}\left(\left(\boldsymbol{H}^{T}\boldsymbol{R}^{-1}\boldsymbol{H}\right)^{-1}\left(\boldsymbol{H}^{T}\boldsymbol{R}^{-1}\boldsymbol{y}\right), \left(\boldsymbol{H}^{T}\boldsymbol{R}^{-1}\boldsymbol{H}\right)^{-1}\right),$$
(5.20)

which has the desired mean and covariance given in (5.16) and (5.15).

Generating samples according to (5.17) is of advantage in the high-dimensional case, because $(\mathbf{H}^T \mathbf{R}^{-1} \mathbf{H})$ does not need to be inverted to assess the statistical properties of the posterior. Instead, the mean and covariance matrix can be estimated from the samples \mathbf{x}_k according to table 5.1.

The observation operator H may be available in compressed form by means of a multilevel fast multipole matrix. In such cases, samples are drawn matrix-free by using conjugate gradient solvers (CG), only requiring the execution of matrix-vector and matrix-transpose-vector products. The Eigen C++ library provides templates for CG solvers, enabling matrix free iterations in a straight-forward fashion (see [92]). It is shown in appendix 8.7 how to enforce a common gauge condition to all samples generated when using compressed matrices.

5.3 The Kálmán filter

The Kálmán filter equations are derived from the Bayes rule, assuming a linear observation operator H and Gaussian distribution for the likelihood function, as well as the prior. Denoting the prior distribution by $p(x) \sim \mathcal{N}(x_0, \delta^{-1}Q)$, with prior mean x_0 and covariance matrix $\delta^{-1}Q$, the posterior is given by

$$p(\boldsymbol{x}|\boldsymbol{y}) \propto \exp\left(-\frac{1}{2}\left((\boldsymbol{y} - \boldsymbol{H}\boldsymbol{x})^T \, \boldsymbol{R}^{-1} \left(\boldsymbol{y} - \boldsymbol{H}\boldsymbol{x}\right) + (\boldsymbol{x} - \boldsymbol{x}_0)^T \,\delta \boldsymbol{Q}^{-1} \left(\boldsymbol{x} - \boldsymbol{x}_0\right)\right)\right). \tag{5.21}$$

Here a regularization parameter $\delta \in \mathbb{R}$ is introduced, which can be used to tune the impact of the prior.

Completing the squares, as it was done in section 5.2 yields

$$p(\boldsymbol{x}|\boldsymbol{y}) \sim \mathcal{N}(\boldsymbol{m}, \boldsymbol{\Sigma})$$
 (5.22)

where

$$\boldsymbol{\Sigma} = \left(\boldsymbol{H}^T \boldsymbol{R}^{-1} \boldsymbol{H} + \delta \boldsymbol{Q}^{-1}\right)^{-1}, \qquad (5.23)$$

and

$$\boldsymbol{\Sigma}^{-1}\boldsymbol{m} = \boldsymbol{H}^T \boldsymbol{R}^{-1} \boldsymbol{y} + \delta \boldsymbol{Q}^{-1} \boldsymbol{x}_0. \tag{5.24}$$

This is the update step of a linear Kálmán filter [18]. A well established alternative representation for the equations (5.23) and (5.24) is given by

$$\boldsymbol{\Sigma} = \delta^{-1} \left(\boldsymbol{I}_N - \boldsymbol{K} \boldsymbol{H} \right) \boldsymbol{Q}, \tag{5.25}$$

and

$$\boldsymbol{m} = \boldsymbol{x}_0 + \boldsymbol{K} \left(\boldsymbol{y} - \boldsymbol{H} \boldsymbol{x}_0 \right), \tag{5.26}$$

where K is the Kálmán gain

$$\boldsymbol{K} = \delta^{-1} \boldsymbol{Q} \boldsymbol{H}^{T} \left(\delta^{-1} \boldsymbol{H} \boldsymbol{Q} \boldsymbol{H}^{T} + \boldsymbol{R} \right)^{-1}.$$
(5.27)

The equivalence of the above equations can be shown by using the Sherman-Morrison-Woodbury formula [93] [94] (see appendix 8.6).

The posterior probability density function $p(\boldsymbol{x}|\boldsymbol{y}) \sim \mathcal{N}(\boldsymbol{m}, \boldsymbol{\Sigma})$ is defined by the updated mean \boldsymbol{m} and covariance matrix $\boldsymbol{\Sigma}$.

In order to compute the posterior covariance matrix, the inversion of a matrix is required. This computational effort to perform this matrix inversion scales badly with respect to the number of degrees of freedom of the state variables N. In the high dimensional case it is more efficient to estimate the statistical properties from an ensemble of K random vectors $\mathbf{X} = {\mathbf{x}_1, ..., \mathbf{x}_K}$, where $\mathbf{x}_k \sim p(\mathbf{x}|\mathbf{y})$. It is often sufficient to use K < N, which yields a large benefit in computational complexity [26]. Formulas to estimate mean and covariance from the ensembles are found in the right column of table 5.1. A sample \mathbf{x}_k can be computed by solving the randomized linear equation system

$$(\boldsymbol{H}^{T}\boldsymbol{R}^{-1}\boldsymbol{H} + \delta\boldsymbol{Q}^{-1})\boldsymbol{x}_{k} = \boldsymbol{H}^{T}\boldsymbol{R}^{-1}\boldsymbol{y} + \delta\boldsymbol{Q}^{-1}\boldsymbol{x}_{0} + \left(\boldsymbol{H}^{T}\boldsymbol{R}^{-1/2}, \delta^{1/2}\boldsymbol{Q}^{-1/2}\right)\boldsymbol{\epsilon}_{k}, \qquad (5.28)$$
$$\boldsymbol{\epsilon}_{k} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I}_{M+N}).$$

 I_{M+N} is an identity matrix of dimension $(M+N) \times (M+N)$. The prove that x_k follows the desired posterior distribution is completely analogous to section 5.2 and is therefore not performed explicitly at this stage. In the above relations, $Q^{1/2}$ denotes the square root matrix of Q such that $Q = Q^{1/2}Q^{1/2}$.

The sampling approach is of advantage in the high-dimensional case and when H is not available in closed form. Problematic, however, is the appearance of the inverse of the prior covariance matrix Q in all the equations. This limits the applicability of (5.28) to simple prior covariance structures or low dimensional problems. If the prior is available by means of an ensemble x, which could have been obtained from (5.17), Q must be approximated, which may be inaccurate in cases with K < N. An approach to perform the Kálmán update directly on the prior ensemble is desired. The *ensemble Kálmán filter* has been developed especially for this purpose [20].

5.4 The ensemble Kálmán filter

The ensemble Kálmán filter solves the issues related the prior covariance matrix Q. A good introduction into the concept of ensemble Kálmán filtering and its efficient implementation is found in [22].

It is now considered that a prior ensemble of K state variables $\{x_k\}$ is available, which is providing prior information for distribution of the parameters x. This prior ensemble might have been computed by solving the randomized linear equation system according to (5.17) or (5.28).

The notation x_k^{prior} and x_k^{post} is now used to distinguish between the prior and posterior state vectors. The prior ensemble matrix $X^{\text{prior}} \in \mathbb{R}^{N \times K}$ is defined as

$$\boldsymbol{X}^{\text{prior}} := \left(\boldsymbol{x}_1^{\text{prior}}, ..., \boldsymbol{x}_K^{\text{prior}}\right).$$
(5.29)

The mean and the covariance matrix of the prior ensemble can be computed by

$$\mathbf{E}\left(\boldsymbol{X}^{\text{prior}}\right) = \frac{1}{K} \sum_{k=1}^{K} \boldsymbol{x}_{k}^{\text{prior}}, \qquad \boldsymbol{Q}^{\text{prior}} = \frac{\boldsymbol{U}\boldsymbol{U}^{T}}{K-1},$$
(5.30)

with

$$\boldsymbol{U} = \boldsymbol{X}^{\text{prior}} - \mathbb{E}\left(\boldsymbol{X}^{\text{prior}}\right) \boldsymbol{I}_{1 \times K}, \qquad (5.31)$$

where $I_{1 \times K}$ is a row vector $(1, ..., 1) \in \mathbb{R}^{1 \times K}$.

The measurement data is randomized as it was done in equations (5.17) and (5.28), according to the measurement covariance matrix \mathbf{R} for the measurement vector \mathbf{y} . To this end, the data matrix $\mathbf{Y} \in \mathbb{R}^{M \times K}$ is defined as

$$\boldsymbol{Y} := (\boldsymbol{y}_1, ..., \boldsymbol{y}_K), \quad \text{with:} \quad \boldsymbol{y}_i = \boldsymbol{y} + \boldsymbol{\epsilon}_i, \quad \boldsymbol{\epsilon}_i \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{R}).$$
 (5.32)

The Kálmán update yields the posterior ensemble

$$\boldsymbol{X}^{\text{post}} = \boldsymbol{X}^{\text{prior}} + \frac{1}{K-1} \boldsymbol{U} \left(\boldsymbol{H} \boldsymbol{U} \right)^T \boldsymbol{P}^{-1} \left(\boldsymbol{Y} - \boldsymbol{H} \boldsymbol{X}^{\text{prior}} \right), \qquad (5.33)$$

where $\boldsymbol{H} \in \mathbb{R}^{M \times N}$ is the matrix related to the linear observation operator and

$$\boldsymbol{P} = \frac{1}{K-1} \boldsymbol{H} \boldsymbol{U} \left(\boldsymbol{H} \boldsymbol{U} \right)^{T} + \boldsymbol{R} \qquad \in \mathbb{R}^{M \times M}.$$
(5.34)

Equation (5.33) follows directly from (5.26) by substituting the sampled covariance matrix Q^{prior} according to (5.30) for $\delta^{-1}Q$ in the definition of the Kálmán gain in (5.27). The variables used in (5.33) and (5.34) are summarized in table 5.2

In the case of a non-linear observation operator H, or when the observation operator is available in compressed form only, an observation matrix-free implementation is possible. One therefore defines the matrices HX^{prior} and HU according to

$$HX^{\text{prior}} := (H(x_1), ..., H(x_K)),$$
 (5.35)

$$\boldsymbol{H}\boldsymbol{U} := \left(\boldsymbol{H}(\boldsymbol{x}_1) - \mathbb{E}\left(\boldsymbol{H}(\boldsymbol{x})\right), ..., \boldsymbol{H}(\boldsymbol{x}_K) - \mathbb{E}\left(\boldsymbol{H}(\boldsymbol{x})\right)\right),$$
(5.36)

where

$$\mathsf{E}(\boldsymbol{H}(\boldsymbol{x})) := \frac{1}{N} \sum_{k=1}^{K} \boldsymbol{H}(\boldsymbol{x}_{k}),$$
(5.37)

and substitutes the resulting matrices for HU and HX^{prior} in (5.33) and (5.34).

By working with a nonlinear observation operator in ensemble Kálmán filtering one suffers from approximation errors, as the true nonlinear update is fitted with a Gaussian model. In complex high dimensional systems the ensemble Kálmán filter still enjoys great popularity, as it is often the only way to do approximate inference. Alternative techniques can only be applied to highly simplified versions of the original problem [26].

In this work the ensemble Kálmán filter will be used to update the prior ensemble X^{prior} in regions of the magnet where the remaining measurement uncertainty is large. Comparing to the initialization, less measurements will be used for such local updates. The P matrix will therefore be of a reasonable size $M \ll N$. For high dimensional updates $M \gg N$, it is shown in [22] how to reformulate P to obtain linear complexity in M.

5.5 Nonlinear observation operators

In case of a nonlinear observation operator H, the posterior is not a Gaussian distribution and the statistical moments of the posterior cannot be identified by completing the squares in the exponent as it was done before. If nonlinearities are small, it is common practice to linearize H in order to recover a Gaussian

variable	meaning	definition
N	dimension of the parameter vector $oldsymbol{x}$	
M	dimension of the measurement vector \boldsymbol{y}	
K	size of the ensemble	
\boldsymbol{y}	measurement vector	\mathbb{R}^{M}
$X^{ m prior}$	prior ensemble	$\mathbb{R}^{N \times K}$
X^{post}	posterior ensemble	$\mathbb{R}^{N \times K}$
Y	data matrix	$\mathbb{R}^{M \times K}$
U	centered prior ensemble	$\mathbb{R}^{N \times K}$
$oldsymbol{Q}^{ ext{prior}}$	prior ensemble covariance matrix	$\mathbb{R}^{N \times N}$
H	linear observation operator	$\mathbb{R}^{M \times N}$

Table 5.2: Summary of all variables used in the ensemble Kálmán filter.

posterior. This is the basic principle of *extended Kálmán filtering*. Linearizations will be used in some applications in chapter 6, and the details about these approaches will depend strongly on the specific use case.

The focus of this section lies in the estimation of statistical moments for nonlinear problems without linearization. A good overview about the different approaches can be found in [95]. The basic principle of Markov-Chain-Monte-Carlo (MCMC) methods is similar to using 5.28, where random numbers are generated from the posterior and statistical moments are estimated by means of the sampled statistical moments. This allows to derive matrix-free algorithms, which are efficient for high dimensional problems. All implementations and derivations given below are based on [91, Chapter 6]. In the following, the concept of maximum a-posteriori solutions for nonlinear problems is discussed, before a result-oriented summary on MCMC methods is given.

In the spirit of section 5.3, the algorithms are based on a Gaussian prior $p(\mathbf{x}) \sim \mathcal{N}(\mathbf{x}_0, \mathbf{Q})$, which is available from the mean vector \mathbf{x}_0 and the prior covariance matrix \mathbf{Q} , rather than an ensemble of state variables.

5.5.1 Maximum a-posteriori solutions

For normal-distributions of noise and prior, the posterior probability density function takes on the least-squares form

$$p(\boldsymbol{x}|\boldsymbol{y}) \propto \exp\left(-\frac{1}{2}\|\boldsymbol{A}(\boldsymbol{x}) - \boldsymbol{b}\|_{2}^{2}\right)$$
 (5.38)

where

$$\boldsymbol{A}(\boldsymbol{x}) := \begin{pmatrix} \boldsymbol{R}^{-1/2} \boldsymbol{H}(\boldsymbol{x}) \\ \delta^{1/2} \boldsymbol{Q}^{-1/2} \boldsymbol{x} \end{pmatrix}, \text{ and } \boldsymbol{b} := \begin{pmatrix} \boldsymbol{R}^{-1/2} \boldsymbol{y} \\ \delta^{1/2} \boldsymbol{Q}^{-1/2} \boldsymbol{x}_0 \end{pmatrix}.$$
(5.39)

The maximum a-posteriori solution x_{MAP} is maximizing the posterior p(x|y) that is equivalent to

$$\boldsymbol{x}_{\text{MAP}} = \arg\min_{\boldsymbol{x}} \left(\frac{1}{2} \|\boldsymbol{A}(\boldsymbol{x}) - \boldsymbol{b}\|^2 \right).$$
(5.40)



Figure 5.1: Random walk in Markov-Chain-Monte-Carlo methods. The probability for drawing a new sample does only depend on the current state and not on the whole history of the chain.

It is important to mention that x_{MAP} is not the expected value of x for nonlinear inference problems. Moreover, a maximum a-posteriori solution alone does not give information about the statistical properties of the posterior, which are needed to quantify uncertainties.

5.5.2 Metropolis Hastings in Markov-Chain-Monte-Carlo methods

In MCMC methods, the successive computation of random vectors x_k describes a random walk through the probability space. This random walk is designed to draw samples from the desired posterior distribution. The random walk in MCMC methods is a Markov-Chain, where the probability for drawing a new sample depends only on the current state, and not the whole history of the sequence. The probability for drawing a sample x_{k+1} given the current state x_k is expressed by means of a transition kernel $K(x_{k+1}|x_k)$. This principle is illustrated in Fig. 5.1.

Different version of MCMC methods exist, all varying in the choice of the transition kernel $K(x_{k+1}|x_k)$. In Metropolis Hastings (MH), the goal is to construct $K(x_{k+1}|x_k)$ such that

$$p(\boldsymbol{x}_{k+1}) = \int K(\boldsymbol{x}_{k+1}|\boldsymbol{x}_k) p(\boldsymbol{x}_k) \, \mathrm{d}\boldsymbol{x}_k.$$
(5.41)

 $p(x_k)$ is said to be an invariant density for the transition kernel $K(x_{k+1}|x_k)$. In this way it is guaranteed that the Markov chain converges in distribution to p(x) [91].

Choosing

$$p(\mathbf{x}_k)K(\mathbf{x}_{k+1}|\mathbf{x}_k) = p(\mathbf{x}_{k+1})K(\mathbf{x}_k|\mathbf{x}_{k+1})$$
 (5.42)

it is shown in [96] that p is an invariant density for $K(x_{k+1}|x_k)$. Eq. (5.42) is practical to derive transition kernels in MH. To this end one may choose a proposal q according to

$$K(\boldsymbol{x}_{k+1}|\boldsymbol{x}_k) = \alpha(\boldsymbol{x}_{k+1}, \boldsymbol{x}_k)q(\boldsymbol{x}_{k+1}|\boldsymbol{x}_k),$$
(5.43)

and modify α such that Eq. (5.42) is satisfied. Explicitly, this yields for α [91]

$$\alpha(\boldsymbol{x}_{k+1}, \boldsymbol{x}_k) = \min\left(1, \frac{p(\boldsymbol{x}_{k+1})q(\boldsymbol{x}_k|\boldsymbol{x}_{k+1})}{p(\boldsymbol{x}_k)q(\boldsymbol{x}_{k+1}|\boldsymbol{x}_k)}\right).$$
(5.44)

The advantage of MH is that samples can be generated using a known proposal density, allowing for efficient evaluation. The function α is then used as to derive acceptance or rejection rules for the proposed samples, as it is known from rejection sampling. Without explicitly specifying the proposal q and function α , the MH algorithm to sample from a given posterior probability density function $p(\boldsymbol{x}|\boldsymbol{y})$ can now be summarized in algorithm 1.

Algorithm 1 Sampling from the posterior $p(\boldsymbol{x}|\boldsymbol{y})$

```
Initialize x_0

for k = 1, ..., number of samples K do

Generate a proposal \tilde{x} \sim q(x_k | x_{k-1})

Compute \alpha = \alpha(\tilde{x}, x_{k-1})

Draw sample from a uniform distribution u \sim \mathcal{U}(0, 1)

if u < \alpha then

accept proposal x_k = \tilde{x}

else

reject proposal x_k = x_{k-1}

end if

end for
```

The function α follows from the definition of the proposal q and the probability density function $p(\boldsymbol{x}|\boldsymbol{y})$ and is computed by (5.44). An example for how to choose the proposal q is given in the next subsection.

5.5.3 The randomize-then-optimize proposal for Metropolis Hastings

So far, the proposal used in MH has not been given explicitly. The choice of the proposal is critical for the efficiency of the sampling algorithm. In the optimal case, the proposal is tailored tightly to the posterior distribution, such that most of the proposed samples are accepted. This however might be impossible when using simple proposal distributions, such as uniform or Gaussian distributions. In this thesis, all nonlinear MCMC implementations make use of the so called *randomize-then-optimize* (RTO) proposal in Metropolis Hastings, as it fits tightly to nonlinear problems with Gaussian priors and noise models. In these cases, the posterior probability density function can be formulated in the least-squares form according to 5.38. Details about the RTO proposal are found in [91]. The key ideas and equations needed for implementation are given in the following.

The randomize-then-optimize proposal is chosen as

$$q_{\text{RTO}}(\boldsymbol{x}|\boldsymbol{y}) = \underbrace{|\boldsymbol{Q}_{\text{qr}}^T \boldsymbol{J}(\boldsymbol{x})|}_{:= c(\boldsymbol{x})} \underbrace{\exp\left(-\frac{1}{2} \|\boldsymbol{Q}_{\text{qr}}^T (\boldsymbol{A}(\boldsymbol{x}) - \boldsymbol{b})\|\right)}_{:= q(\boldsymbol{x}|\boldsymbol{y})}$$
(5.45)

where Q_{qr} is the matrix Q_1 of the thin QR-factorization of the Jacobian $J(x_{MAP})$ of A(x), according to definition 13, evaluated for the maximum a-posteriori solution x_{MAP} .

The proofs for the following statements are found in [91, 6.3.1 and 6.3.2]. The advantage of the RTO proposal is that it appears to fit tightly to the posterior given in (5.38) and it allows to compute samples efficiently by solving the nonlinear stochastic optimization problem

$$\tilde{\boldsymbol{x}} = \arg\min_{\boldsymbol{x}} \|\boldsymbol{Q}_{qr}^T \boldsymbol{A}(\boldsymbol{x}) - (\boldsymbol{b} + \boldsymbol{\epsilon})\|^2, \qquad \boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I}_{M+N}).$$
(5.46)

 I_{M+N} is an identity matrix of dimensions $(M + N) \times (M + N)$. The algorithm to draw a sample from the RTO proposal can now be summarized in algorithm 2. This algorithm can be used to generate the proposal \tilde{x}

Algorithm 2 Sampling from the RTO proposal for MHCompute x_{MAP} from (5.40)Compute Q_{qr} from QR-factorization of $J(x_{MAP})$ Compute \tilde{x} from (5.46)

in algorithm 1, whereas the maximum a-posteriori solution and the QR factorization can be performed once before iterating over k.

It remains to derive the acceptance rule based on the function α in algorithm 1. To this end, one substitutes $q(\tilde{x}|y)$ and $q(x_{k-1}|y)$, defined in (5.45), in the definition of α according to (5.44) to obtain [91, p. 6.3.3]

$$\alpha(\tilde{\boldsymbol{x}}, \boldsymbol{x}_{k-1}) = \min\left(1, \frac{c(\boldsymbol{x}^{k-1})}{c(\tilde{\boldsymbol{x}})}\right).$$
(5.47)

Definition 13 (The QR-factorization) The QR-factorization of a matrix $A \in \mathbb{R}^{M \times N}$ with $M \geq N$ is defined as

$$\boldsymbol{A} = (\boldsymbol{Q}_1, \boldsymbol{Q}_2) \begin{pmatrix} \boldsymbol{R}_1 \\ \boldsymbol{0} \end{pmatrix} = \boldsymbol{Q}_1 \boldsymbol{R}_1, \tag{5.48}$$

where $\mathbf{R} \in \mathbb{R}^{N \times N}$ is an upper triangular matrix and $\mathbf{Q}_1 \in \mathbb{R}^{M \times N}$ and $\mathbf{Q}_2 \in \mathbb{R}^{M \times (M-N)}$ have orthogonal columns. $\mathbf{A} = \mathbf{Q}_1 \mathbf{R}_1$ is called the thin QR-factorization.

The algorithmic implementation of the QR-factorization is available in the "qr" function of the linear algebra package of scipy [97]. The thin QR-factorization is available by using the mode parameter "economic".

5.6 Regularization parameter selection

The regularization parameter δ in the posteriors according to (5.21) and (5.38), has the same role as the regularization parameters known from the Tikhonov regularization methods [91, Chapter 2.2]. In said approaches, δ is considered as a known value, and is estimated prior to the computation of x. In this thesis, the approach presented in [91, Chapter 5.2] is chosen. The regularization parameter is treated as an additional random variable, a so-called *hyper parameter*.

Following [91], a prior in form of a gamma distribution $\Gamma(p, b)$, according to definition 12 is used for the regularization parameter δ . This is a standard choice in the Gaussian framework, as the full posterior $p(x, \delta | y)$, for x and δ is of the form

$$p(\boldsymbol{x},\delta|\boldsymbol{y}) \propto \delta^{N/2+p-1} \exp\left(-\|\boldsymbol{A}(\boldsymbol{x},\delta) - \boldsymbol{b}(\delta)\|^2 - b\delta\right).$$
(5.49)

Considering either x or δ as given, the conditionals $p(x|\delta, y)$ and $p(\delta|x, y)$ are given by

$$p(\boldsymbol{x}|\delta, \boldsymbol{y}) \propto \exp\left(-\|\boldsymbol{A}(\boldsymbol{x}, \delta) - \boldsymbol{b}(\delta)\|^2\right),$$
(5.50)

and

$$p(\delta|\boldsymbol{x}, \boldsymbol{y}) \propto \delta^{N/2+p-1} \exp\left(\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{x}_0)^T \boldsymbol{Q}(\boldsymbol{x}-\boldsymbol{x}_0) - b\right)\delta\right).$$
(5.51)

The conditional $p(\boldsymbol{x}|\boldsymbol{\delta},\boldsymbol{y})$ is of a least squares form (Gaussian, if \boldsymbol{H} is linear), whereas the conditional $p(\boldsymbol{\delta}|\boldsymbol{x},\boldsymbol{y})$ is gamma distributed with new scale and rate parameters

$$p(\delta | \boldsymbol{x}, \boldsymbol{y}) \sim \Gamma(N/2 + p, -\frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}_0)^T \boldsymbol{Q}(\boldsymbol{x} - \boldsymbol{x}_0) - b).$$
 (5.52)

Therefore the same forms of the prior distributions are recovered in the conditionals of the posterior. This relationship between prior distributions and posteriors is known as conjugacy, and it allows to derive sampling algorithms based on known probability density functions in standard forms. In the above, the dependency of A and **b** on δ was denoted explicitly, to highlight that **A** and **b** are functions of δ .

5.7 The two stage Gibbs sampling

Gibbs sampling can be seen as a special case of Metropolis Hastings, in which the proposals q are identified from conditional posterior density functions. Even though more general multi-stage Gibbs samplers are plausible, this work focuses on two stage Gibbs sampling, as it is introduced in [98, Chapter 9].

Considering two random variables a and b with joint probability density function p(a, b) the two stage Gibbs sampler generates a Markov chain by sampling from the conditionals p(a|b), p(b|a) according to algorithm 3 [98]. The samples a_k, b_k of the Markov chain converge in distribution to the joint distribution p(a, b) under

```
Algorithm 3 The two stage Gibbs sampler
```

```
Initialize a_0
for k = 1, ..., number of samples K do
      Compute \boldsymbol{b}_k \sim p(\boldsymbol{b}|\boldsymbol{a}_k)
      Compute \boldsymbol{a}_k \sim p(\boldsymbol{a}|\boldsymbol{b}_k)
end for
```

mild conditions (see [98], Theorem 9.6).

Returning to the posterior in section 5.6, samples from the posterior $p(x, \delta | y)$ may be computed by using algorithm 4.

Algorithm 4 Sampling from the posterior $p(\boldsymbol{x}, \delta \boldsymbol{y})$
Initialize $\boldsymbol{x}_0, \delta_0$
for $k = 1,,$ number of samples K do
Compute $\delta_k \sim p(\delta \boldsymbol{x}_{k-1}, \boldsymbol{y})$
Compute $oldsymbol{x}_k \sim p(oldsymbol{x} \delta_k, oldsymbol{y})$
and for

The initial stage of any MCMC chain is called burn-in, when the elements of the chain move from their starting values to the region of relatively high probability of the target density [91]. The burn-in samples are usually omitted, in order to avoid a possible bias in the sampled statistics. After the burn-in, a MCMC chain is said to be in equilibrium, and it can be assumed that the samples are collected from the target distribution [91]. The so called *Geweke* test [99] will be applied to the samples δ_k generated from algorithm 4, in order to assess the equilibrium of the Markov-Chain. The Geweke test is based on hypothesis testing, and the central limit theorem, details and derivations are found in [99] and [91, page 85].

variable	meaning
<i>K</i> ₁₀	largest integer less than $(K - K_{bi})/10$
K_{50}	largest integer less than $(K - K_{bi})/2$
$\overline{\delta}_{10}$	mean value of the first 10 percent of all samples δ_k with
	$k > K_{\rm bi}$
$\overline{\delta}_{50}$	mean value of the last 50 percent of all samples δ_k with
	$k > K_{\rm bi}$
$\hat{S}_{10}(0)$	variance estimated from the 0 coefficient of the spectral den-
	sity of the first 10 percent of all samples δ_k with $k > K_{bi}$
$\hat{S}_{50}(0)$	variance estimated from the 0 coefficient of the spectral den-
	sity of the last 50 percent of all samples δ_k with $k > K_{\rm bi}$

Table 5.3: Variables needed for the computation of R_{Geweke} .

For the Geweke test, all samples δ_k with $k > K_{bi}$ are considered, where K_{bi} is the number of burn in samples. If the Geweke test fails for K_{bi} , one usually increases K_{bi} and tests the new chain for equilibrium. The Geweke test is based on the statistic R_{Geweke} defined as

$$R_{\text{Geweke}} = \frac{\overline{\delta}_{10} - \overline{\delta}_{50}}{\sqrt{\hat{S}_{10}(0)/K_{10} + \hat{S}_{50}(0)/K_{50}}}.$$
(5.53)

The variables needed for the computation of R_{Geweke} in (5.53) are given in table 5.3. From R_{Geweke} , the Geweke *p*-value is computed as the probability that $|z| > |R_{\text{Geweke}}|$ for $z \sim \mathcal{N}(0, 1)$, meaning that $\mathcal{N}(0, 1)$ is integrated for $|z| > |R_{\text{Geweke}}|$ to obtain *p*. This value can be interpreted as the probability of observing a value at least as extreme as R_{Geweke} , given that chain is in equilibrium. *p*-values larger than 0.95 provide strong evidence, that the chain is in equilibrium.

6 Applications

In this chapter, four inference problems related to the post-processing of magnetic measurement data are presented. The physical meanings of the latent variables ν and θ will change depending on the application. The tools for the statistical inference and numerical modeling, which have been discussed in the previous chapters, will now be applied to real measurement data.

Section 4.1.5. The first problem deals with the three-axes, Hall probe mapper. The main objective is the identification of sensor parameters θ by statistical inference. More precisely, it aims to infer sensor positions and orientations based on a field map in a cone-quadrupole field. This application is challenging, because the cone-quadrupole field is provided by permanent magnets, which are affected by manufacturing tolerances and temperature dependence. The temperature effects are characterized by long time constants. The field can therefore be considered stable within the measurement campaign of less than one hour, not, however, within hours and days. Under these conditions, the inference can not be performed with respect to a fixed reference field, which is why a model for the magnetic field by means of ν is necessary. The resulting algorithm has developed into a powerful fiducialization tool. This tool admits the localization of the sensor positions in three dimensional space, with respect to magnet coordinates. This fiducialization procedure is now well established in the setup phase of the 3D mapper.

Section 6.2. The second application uses the sensor parameters identified previously as fixed variables, to reconstruct the three-dimensional magnetic field based on boundary measurements in an accelerator magnet, by means of a mathematical model based on the boundary-element method. The state variables for the magnetic field ν correspond to equivalent surface currents at the domain boundary and are to be identified from dependent measurements y for given sensor parameters θ .

The challenge in this application lies in the construction of the approximation space and the large dimensionality of the problem. A residual-based mesh refinement is presented, which uses a stopping criterion derived from the expected residual due to mechanical vibration and positioning uncertainties, which are estimated from the experiments explained in chapter 4 and a least squares solution for ν .

The least squares solution does not provide the feedback necessary for uncertainty quantification, as it neglects the measurement covariance matrix, which is mostly affected by mechanical vibrations and positioning errors. As the impact of these error sources depends on the magnetic field, the covariance matrix is dependent on ν , yielding a complicated likelihood function. In the over-sampled case, according to the discussions in section 3.3.8, the least squares solution provides a good estimate for the parameters ν and is therefore used to estimate the measurement covariance matrix. This covariance structure is then used for the inference of ν by drawing samples from the posterior probability density function.

It will be shown, how positioning uncertainties propagate to field evaluations in the fringe field region and how local update measurements can be incorporated to improve the estimates by ensemble Kálmán filtering. An algorithm is presented, which is exploring the physical space dependent on the uncertainty.

Finally, the advantages of the BEM based post processing are showcased by comparing to the "naive" approach of mapping the field directly on a 3D grid.

Section 6.3. In the third example, the dependency on a least squares solution for the estimation of the error covariance matrix is relaxed. The perturbation of the sensor position and orientation is considered by means of the nuisance parameters θ and is estimated together with ν by means of Gibbs sampling. As this approach requires the successive computation of field gradients and measurement derivatives, it requires large computational resources to store all derivative evaluations in the format of dense matrices. The fast multipole method, presented in chapter 3 would provide a tool to solve this issue, however, the derivative operations for the fast multipole method have so far not been implemented in the code. Therefore, a small scaled field map in the fringe field of a magnet is taken as a proof of principle. Results are verified by recovering the sensor displacement from θ and comparing it to an optical position measurement.

6.1 The absolute position and orientation problem

This section ties in with the discussion in section 4.1.5. Based on a field map around the center of the cone quadrupole magnet, the primary goal is to infer the absolute positions o_i and orientation vectors n_i for the three axes of a Hall cube, $i \in \{x, y, z\}$. The mapper is equipped with a 3D Hall probe of type AS-3DC [80] from Projekt Elektronik including an electronic board for signal conditioning, which provides linearized output voltages for the three axes. In case of the AS-3DC, planar Hall effects are neglectable and the Hall voltages can be described by the linear axial model

$$U_i(\boldsymbol{r} + \boldsymbol{o}_i) = s_i \, \boldsymbol{n}_i \cdot \boldsymbol{B}(\boldsymbol{r} + \boldsymbol{o}_i) + U_{i,0}, \tag{6.1}$$

for the three axes of the Hall sensor $i \in \{x, y, z\}$, the sensitivities s_i and offset voltages $U_{i,0}$ have been determined in a prior probe calibration.

In the linear axial model, there are 15 degrees of freedom, three for each o_i , and two for each n_i . In some cases, one might have calibrated the relative orientation between the three axes of the Hall cube already, for instance, by using rotations in a calibration dipole (see section 4.1.5). This information could then be used to reduce three degrees of freedom, as the angular orientation problem reduces to the determination of three rigid body rotations¹. Alternatively, this information can be encoded by means of a prior, allowing to correct for miscalibration.

The 15 degrees of freedom related to the Hall cube are filling the vector θ and are shown in Fig. 6.1. For the definition of the sensor orientations, two angles are used for each orientation vector. The naming convention and the axes of rotation for each angle are found in table 6.1. As the following analysis extensively uses spherical harmonics and coordinates, it is beneficial to denote by *z* the vertical axis, i.e., the cone-quadrupole's symmetry axis. The three orientation vectors are given explicitly in (6.2).

$$\boldsymbol{n}_{x} = \begin{pmatrix} \cos(\gamma_{x})\cos(\beta_{x})\\ \sin(\gamma_{x})\cos(\beta_{x})\\ -\sin(\beta_{x}) \end{pmatrix}, \quad \boldsymbol{n}_{y} = \begin{pmatrix} -\sin(\gamma_{y})\cos(\alpha_{y})\\ \cos(\gamma_{y})\cos(\alpha_{y})\\ \sin(\alpha_{y}) \end{pmatrix}, \quad \boldsymbol{n}_{z} = \begin{pmatrix} \sin(\beta_{z})\cos(\alpha_{z})\\ -\sin(\alpha_{z})\\ \cos(\beta_{z})\cos(\alpha_{z}) \end{pmatrix}. \quad (6.2)$$

sensor	name	rotation axis
x	β_x	y
x	γ_x	z
y	α_y	x
y	γ_y	z
z	α_z	x
z	β_z	y

Table 6.1: Naming convention for the six angular degrees of freedom.

The only knowledge about the magnetic field in the cone quadrupole is coming from a numerical field simulation (see Fig. 4.16). Tolerances in permanent magnet magnetization as well as temperature effects with long time constants influence the magnetic field. For this reason, one cannot fiducialize versus a known field gradient. The field is therefore considered as unknown and parameterized by means of the state vector

¹This would also be the approach followed if planar Hall effects were not negligible.



Figure 6.1: Three-axes Hall sensor and sensor parameters.

 ν . To this end, a spherical coordinate system $\mathbf{r} = (r, \theta, \varphi)^T$, is placed in the center of the cone quadrupole. The field inside a sphere of radius r < R, where R = H/2, and H is the gap height (see Fig. 4.4 (right)), can be expressed by means of the solid harmonic expansion

$$\phi_{\mathrm{m}}(r,\theta,\varphi) = \sum_{l=2}^{L} \nu_{l,0} r^{l} Y_{l}^{0}(\theta,\varphi).$$
(6.3)

By setting $\nu_{l,n} = 0$, for $n \neq 0$ the axisymmetry of the cone quadruple is implied in this ansatz. Moreover, constant potentials and dipole fields have been excluded by l > 1. In the following, the series expansion is truncated by setting L = 8. These assumptions are found valid as long as the magnet is aligned well with respect to gravity and the evaluation radius does not exceed H/2.

The problem of determining the latent variables θ and ν from dependent measurements y is a classical inference problem, according to the blueprint presented in chapter 1. Following the naming convention of table 6.2, the observation operator can be expressed by

$$\boldsymbol{H}(\boldsymbol{\nu},\boldsymbol{\theta}) + \boldsymbol{U}_{0} := \begin{pmatrix} s_{x} \boldsymbol{n}_{\boldsymbol{x}}(\beta_{x},\gamma_{x}) \cdot \boldsymbol{B}(\boldsymbol{r}_{1} + \boldsymbol{o}_{x},\boldsymbol{\nu}) \\ \vdots \\ s_{x} \boldsymbol{n}_{\boldsymbol{x}}(\beta_{x},\gamma_{x}) \cdot \boldsymbol{B}(\boldsymbol{r}_{M} + \boldsymbol{o}_{x},\boldsymbol{\nu}) \\ s_{y} \boldsymbol{n}_{\boldsymbol{y}}(\alpha_{y},\gamma_{y}) \cdot \boldsymbol{B}(\boldsymbol{r}_{1} + \boldsymbol{o}_{y},\boldsymbol{\nu}) \\ \vdots \\ s_{y} \boldsymbol{n}_{\boldsymbol{y}}(\alpha_{y},\gamma_{y}) \cdot \boldsymbol{B}(\boldsymbol{r}_{M} + \boldsymbol{o}_{y},\boldsymbol{\nu}) \\ s_{z} \boldsymbol{n}_{\boldsymbol{z}}(\alpha_{z},\beta_{z}) \cdot \boldsymbol{B}(\boldsymbol{r}_{1} + \boldsymbol{o}_{z},\boldsymbol{\nu}) \\ \vdots \\ s_{z} \boldsymbol{n}_{\boldsymbol{z}}(\alpha_{z},\beta_{z}) \cdot \boldsymbol{B}(\boldsymbol{r}_{M} + \boldsymbol{o}_{z},\boldsymbol{\nu}) \end{pmatrix} + \begin{pmatrix} U_{x,0} \\ \vdots \\ U_{x,0} \\ U_{y,0} \\ \vdots \\ U_{y,0} \\ U_{z,0} \\ \vdots \\ U_{z,0} \end{pmatrix}$$
(6.4)

Here s_i for $i \in \{x, y, z\}$ are the Hall probe's sensitivity functions and the orientation vectors n_i for $i \in \{x, y, z\}$ are dependent on the field incident angles and therefore on the angular degrees of freedom. The sensor offsets o_i for $i \in \{x, y, z\}$ are changing the evaluation position of the *B*-vectors at the measurement positions. The field evaluations are therefore dependent on o_i . The vector U_0 accounts for the probe's zero-field offset voltages.

variable	meaning		
ν	vector of solid harmonic coefficients		
	$oldsymbol{ u}=(u_2^0,, u_L^0)\in\mathbb{R}^{L-1}$		
θ_x	x sensor parameters		
	$oldsymbol{ heta}_x = (oldsymbol{o}_x^T,eta_x,\gamma_x) \in \mathbb{R}^5$		
$oldsymbol{ heta}_y$	y sensor parameters		
	$oldsymbol{ heta}_y = (oldsymbol{o}_y^T, lpha_y, \gamma_y) \in \mathbb{R}^5$		
θ_z	z sensor parameters		
	$oldsymbol{ heta}_z = (oldsymbol{o}_z^T, lpha_z, eta_z) \in \mathbb{R}^5$		
θ	all sensor parameters		
	$oldsymbol{ heta} = (oldsymbol{ heta}_x^T, oldsymbol{ heta}_y^T, oldsymbol{ heta}_z^T)^T \in \mathbb{R}^{15}$		
$oldsymbol{y}_x$	voltages of sensor x		
	$oldsymbol{y}_x \in \mathbb{R}^M$		
$oldsymbol{y}_y$	voltages of sensor y		
	$oldsymbol{y}_y \in \mathbb{R}^M$		
$oldsymbol{y}_z$	voltages of sensor z		
	$oldsymbol{y}_z \in \mathbb{R}^M$		
y	voltages of sensors x, y, z		
	$oldsymbol{y} = (oldsymbol{y}_x^T, oldsymbol{y}_y^T, oldsymbol{y}_z^T)^T \in \mathbb{R}^{3M}$		
R	measurement covariance matrix $\in \mathbb{R}^{3M \times 3M}$		
r_m	position of the m -th measurement $\in \mathbb{R}^3$		

Table 6.2: Naming convention for all variables related to the absolute position and orientation problem.



Figure 6.2: Measurement data, initial guess and maximum likelihood solution of the absolute orientation problem. The initial guess uses the numerical field simulation as well as the design values for the sensor parameters. The measurement vector contains the voltages of the three Hall probes. The moves where performed along lines, which are filling a spherical domain in the center of the cone quadrupole.

Assuming a Gaussian noise model according to section 4.1.1, the posterior probability density function takes the form

$$p(\boldsymbol{x}|\boldsymbol{y}) \propto \exp\left(-\frac{1}{2}\left(\boldsymbol{y} - \boldsymbol{U}_0 - \boldsymbol{H}(\boldsymbol{x})\right)^T \boldsymbol{R}^{-1}\left(\boldsymbol{y} - \boldsymbol{U}_0 - \boldsymbol{H}(\boldsymbol{x})\right)\right),$$
 (6.5)

with the state vector $\boldsymbol{x} = (\boldsymbol{\nu}^T, \boldsymbol{\theta}^T)^T$. In the above, a sufficiently flat prior was used, but also Gaussian priors could be considered without reservation. Due to the non-linearity of \boldsymbol{H} , this is not a Gaussian distribution in \boldsymbol{x} .

One can estimate the model parameters x by computing a maximum likelihood solution x_{ML} , which is defined as the state vector x, maximizing the probability density function (6.5). This is equivalent to the minimization problem

$$\boldsymbol{x}_{\mathrm{ML}} = \arg\min_{\boldsymbol{x}} \left((\boldsymbol{y} - \boldsymbol{U}_0 - \boldsymbol{H}(\boldsymbol{x}))^T \, \boldsymbol{R}^{-1} \left(\boldsymbol{y} - \boldsymbol{U}_0 - \boldsymbol{H}(\boldsymbol{x}) \right) \right). \tag{6.6}$$

A maximum likelihood solution can be computed with iterative solvers, such as the Levenberg-Marquardt algorithm, which is available in the linear algebra package of scipy [97].

Fig. 6.2 illustrates the measurement data y, the initial guess $H(x_0)$, as well as the result obtained from the maximum likelihood solution $H(x_{ML})$. Here x_0 is computed from the design values and the field simulation. In the bottom, the residuals between y, $H(x_0)$ and $H(x_{ML})$ are drawn. The RMS error is 0.103 mV, which is equivalent to $\sim 20 \,\mu\text{T}$ as the sensitivity of the sensors is $\sim 5 \,\text{VT}^{-1}$.

The maximum likelihood solution does not provide any information about the uncertainties in the parameters x. In principle, one could apply algorithm 1 to generate samples from the posterior distribution and estimate the statistical moments from samples. However, as the probe nonlinearity is small and the sensor parameters are small deviations from the design values, the linearization

$$\boldsymbol{H}(\boldsymbol{x}) \approx \boldsymbol{H}(\boldsymbol{x}_{\mathrm{ML}}) + \left(\partial_{\boldsymbol{x}} \boldsymbol{H}|_{\boldsymbol{x}_{\mathrm{MI}}}\right) (\boldsymbol{x} - \boldsymbol{x}_{\mathrm{ML}}), \tag{6.7}$$

is justified for the computation of the posterior covariance matrix. Here x_{ML} is the maximum likelihood solution, and $\partial_x H|_{x_{ML}}$ is the Jacobian of H evaluated for $x = x_{ML}$. This matrix encodes the derivatives of the observation function, evaluated at the maximum likelihood solution x_{ML} . The derivatives with respect to ν , as well as the angular derivatives are comprising the first and second order derivatives of the solid harmonics, and have been implemented based on analytic formulas, whereas the partial derivatives with respect to o_i are computed by numerical approximation.

The linearized posterior is a Gaussian distribution with the covariance matrix

$$\boldsymbol{\Sigma}_{\text{lin}} = \left(\partial_{\boldsymbol{x}} \boldsymbol{H} |_{\boldsymbol{x}_{\text{ML}}}^{T} \boldsymbol{R}^{-1} \left. \partial_{\boldsymbol{x}} \boldsymbol{H} \right|_{\boldsymbol{x}_{\text{ML}}} \right)^{-1}.$$
(6.8)

The advantage of using a linearization for the uncertainty quantification, is a considerable gain in computational complexity, compared to the sampling from the nonlinear posterior.

To prove that the linearized estimate is expressing the correct uncertainty, 1 000 samples from the nonlinear posterior are drawn by algorithm 1. In Figs. 6.3 to 6.5 the samples are drawn in histograms. The three standard deviations, estimated from the MCMC samples are indicated in the ticks of the horizontal axes. A Gaussian is fitted to all histo-plots (orange) and compared to the linear estimator (dashed-green). The differences between both estimators might be related to the approximation from 1 000 samples, or the linearization, but they are tolerable for this application. The resulting field solution has been plotted in Fig. 4.16 and differs from the field simulation most certainly due to the tolerances in permanent magnet magnetization and temperature effects.

For a better comparison of the numerical values, the mean values, design values, and the standard deviations are summarized in table 6.3.

The position estimate is cross validated, by moving the y sensor into the zero plane manually and monitoring the vertical position of the linear encoder. The estimated position is recorded in table 6.4 and compared to the encoder position measurement. The difference is 6 μ m, which is in the range of the positioning accuracy of the linear stages.



Figure 6.3: Histo-plots for the field solution. Blue: samples from the posterior generated by MCMC-RTO. Solid-orange: Fitted Gaussian distribution. Dashed-green: Gaussian distribution after linearizing the posterior. As all distributions sum up to one, or $1\,000$ samples, the frequencies on the y axis have been omitted in all cases. The coefficients are scaled to a reference radius $r_{\rm ref} = 5$ mm, and divided by μ_0 to give a value in T.



Figure 6.4: Histo-plots for the probe orientations. Blue: samples from the posterior generated by MCMC-RTO. Solid-orange: Fitted Gaussian distribution. Dashed-green: Gaussian distribution after linearizing the posterior.

variable	mean	design	σ	difference	unit
$c_2^0 r_{ m ref}/\mu_0$	95.9	96.49	0.041	-0.59	mT
$c_{3}^{0}r_{\rm ref}^{2}/\mu_{0}$	0.13	0	0.058	0.13	mT
$c_4^0 r_{\rm ref}^3 / \mu_0$	4.6	12.50	0.055	-7.9	mТ
$c_{5}^{0}r_{\rm ref}^{4}/\mu_{0}$	0.05	0	0.049	0.05	mТ
$c_{6}^{0}r_{ref}^{5}/\mu_{0}$	0.16	0	0.042	0.16	mТ
$c_{7}^{0}r_{\rm ref}^{6}/\mu_{0}$	0.02	0	0.037	0.02	mТ
$c_8^0 r_{\rm ref}^7 / \mu_0$	0.02	0	0.024	0.02	mT
α_y	87.20	90	0.032	-2.80	deg
α_z	-92.25	-90	0.025	-2.25	deg
β_x	0.79	0	0.017	0.79	deg
β_z	75.44	0	0.456	75.44	deg
γ_x	178.70	180	0.030	-1.3	deg
γ_y	-3.17	0	1.015	-3.17	deg
o_x^x	2.08	2	0.002	0.08	mm
o_x^y	0.05	0	0.050	-0.05	mm
o_x^z	0.01	0	0.020	-0.01	mm
o_y^x	0.05	0	0.019	-0.05	mm
o_y^y	0.04	0	0.017	-0.04	mm
o_{y}^{z}	-2.09	-2	0.001	-0.09	mm
o_z^x	0.29	0	0.050	-0.29	mm
$o_z^{\tilde{y}}$	0.28	0.2	0.003	0.08	mm
o_z^z	-0.25	0	0.023	-0.25	mm

Table 6.3: Results of the fiducialisation. The coefficients of the solid harmonic expansion are scaled to a reference radius of 5 mm and divided by μ_0 to give a value in T. The angle β_z rotates the *z*-sensor around the *y* axis of the magnet coordinates. As the *z*-sensor's orientation vector is nearly parallel to the magnets *y*-axis (see Fig. 6.1), a large deviation with respect to the design value is expected for this rotation. The angle γ_y rotates around the symmetry axis of the magnet. This explains the large standard deviations for these two parameters.

$[\boldsymbol{P}_0^y]_y$ estimated	$[\boldsymbol{P}_0^y]_y$ measured	difference [µm]
228.345	228.351	6

Table 6.4: Validation of the position fiducialisation. Moving the stages to the coordinates P_0^y , places the y-sensor in the center of the cone quadrupole. For validation, the vertical coordinate $[P_0^y]_y$ is measured by moving the sensor into the zero plane and reading out the encoder position manually. This position is compared to the estimated vertical position based on the numerical model. The difference between measurement and estimate is at 6 µm, which is in the range of the precision of the linear encoder.


Figure 6.5: Histo-plots for the probe offsets. Blue: samples from the posterior generated by MCMC-RTO. Solid-orange: Fitted Gaussian distribution. Dashed-green: Gaussian distribution after linearizing the posterior.

6.2 Field mapping in three dimensions

This section deals with the main objective of this research: the extraction of boundary data from distributed Hall probe measurements in accelerator magnets. Field maps are commonly demanded for spectrometers, detector magnets and also for strongly curved magnets, as integrated field measurements alone do not provide the feedback necessary for particle beam dynamics and magnet design. Mapping only the boundary and using a numerical model to predict the field in the enclosed domain comes with tremendous savings in terms of measurement duration.

In the following, the curved, C-shaped dipole magnet shown in Fig. 6.6 (left) is considered. The magnet is a bending dipole for the extra low energy antiproton ring (ELENA) [100]. Numerical field simulations have been used to compute the three dimensional field distribution, which was considered for particle tracking applications in [7]. It will be shown how a field representation by boundary data, derived only from magnetic measurements, is capable to provide the same information and can therefore be considered as an alternative to the magnet simulation. This is of importance when beam tracking has to be performed with the magnetic field distribution of the magnet as built. In order to provide a fully independent result from the numerical simulations, no prior knowledge from the simulations will be used.

The goal of this section is not only to derive a three dimensional field representation by boundary data, but also the implementation of an active learning algorithm, which explores the physical space dependence on uncertainties. The mathematical tools, such as the boundary element method, as well as the ensemble Kálmán filter have been discussed in chapters 3 and 5, respectively. An outline of the active learning algorithm has been shown in Fig. 1.5.

The following procedure is best separated into two steps:

- 1. Initialization: A field map is taken along a boundary, enclosing the domain of interest. The domain is over-sampled in a way that no prior for regularization is needed, and the inverse problem is solvable, relying only on measurement data. The result of the initialization step is an ensemble for the state vector for the magnetic field ν , obtained by sampling from the posterior (which in this case, equals the likelihood), according to section 5.2. This ensemble represents the statistical properties of the parameters, given the initialization measurements.
- 2. Active learning: The uncertainties are propagated to the *B*-field along a reference trajectory. New measurements are identified, dependent on the local uncertainty in |B|. The ensemble Kálmán filter is used to update the prior ensemble move-by-move. The algorithm is stopped when the uncertainty in the quantity of interest falls below a certain threshold.

The quantity on interest in this case, is the field integral

$$I_{B_y} := \int_s B_y \,\mathrm{d}s,\tag{6.9}$$

where s is the path length along the reference trajectory.

As a stopping criterion, the relative 3σ standard deviation defined by

$$3\sigma_{\rm rel}(I_{B_y}) := 3\frac{\sigma(I_{B_y})}{{\rm E}(I_{B_y})} = 3\frac{\sqrt{{\rm var}(I_{B_y})}}{{\rm E}(I_{B_y})},\tag{6.10}$$



Figure 6.6: ELENA dipole magnet and mapper moves for magnetic measurements. Left: Spare dipole magnet for the Extra Low Energy Antiproton ring (ELENA). Right: Mapper moves to sample the curved domain of interest. The black arrows indicate the move direction. For better visibility, the moves are separated by 25 mm, whereas the field map was taken with a higher resolution of 4 mm.



Figure 6.7: The steps of the post processing procedure for the ELENA field mapping.

with the mean and variance operations defined in table 5.1 is used. The algorithm shall provide a result for I_{B_y} with $3\sigma_{\rm rel}(I_{B_y}) < 2 \times 10^{-4}$.

As part of the machine setup, the analysis presented in section 6.1 was performed in order to determine the probe positions and orientation vectors in a coordinate system related to the magnet geometry. The results have already been reported in table 6.3. Therefore, the 15 degrees of freedom of the Hall cube are considered as fixed parameters.

In the next subsection the initialization step will be discussed.

6.2.1 Initialization

The initialization step is illustrated in Fig. 6.7. It makes sense to separate the following discussion into four parts: 1) measurements, 2) construction of the ansatz space, 3) Bayesian inference, and 4) prediction.

1) Measurements

First, the domain boundary is sampled along a curved spiral, using horizontal and vertical moves according to the scheme in Fig. 6.6 (right). For better visibility, the moves in this visualization are separated by 25 mm, whereas for the measurements shown in Fig. 6.7 a step size of 4 mm is selected. One acquisition for the three Hall voltages is triggered by the encoder whenever a distance of 3 mm has been travelled. The three multimeters are set up for an integration time of 10 ms. With a nominal velocity of 20 mm s^{-1} , this corresponds to an integration length of 0.2 mm. In total, the three Hall voltages are sampled at 36 692 positions yielding $110\,076$ measurements. The overall measurement duration needed to fully cover the domain is four hours.

2) Construction of the ansatz space

A boundary mesh needs to be generated. This is a critical step, as the quality of the approximation depends on the ansatz space and therefore, on the mesh generation. A trade-off is to be found between the accuracy for the reconstruction of fine details on one side, and the smoothing of local measurement uncertainties on the other. A BEM ansatz space is constructed for different mesh refinement stages and B-spline degrees. For each ansatz space, a least squares solution (LS) is computed and the approximation error is observed in the residual. In this way, the complexity of the approximation space is increased until the global root-mean-squared (RMS) residual

$$\operatorname{res}_{\mathrm{RMS}} = \sqrt{\frac{1}{3M} (\boldsymbol{y} - \boldsymbol{H}(\boldsymbol{\nu}_{\mathrm{LS}}))^T (\boldsymbol{y} - \boldsymbol{H}(\boldsymbol{\nu}_{\mathrm{LS}}))},$$
(6.11)

falls below a threshold, which will be derived in the following. In the above ν_{LS} is the least squares solution

$$\boldsymbol{\nu}_{\text{LS}} := \arg\min_{\boldsymbol{\nu}} \|\boldsymbol{y} - \boldsymbol{H}\boldsymbol{\nu}\|_2^2, \tag{6.12}$$

and M is the number of measurement positions. As there are three Hall probes, $y \in \mathbb{R}^{3M}$. Since in all refinement stages, the boundary data is over-sampled, according the discussion in section 3.3.8, over-fitting is not a matter of concern. Otherwise, the following procedure could be applied to a separated validation set, taken with a higher spatial resolution.



Figure 6.8: Stages of the adaptive mesh refinement for constructing the BEM ansatz space.



Figure 6.9: Residual with respect to a least square solution for each of the mesh refinement stages shown in Fig. 6.8. Here, p = 3.

To assess parts of the mesh in the fringe fields, which require local mesh refinement, also the observation of the local residuals is necessary. Fig. 6.8 shows the boundary mesh for three *h*-refinement stages. The corresponding residual error is shown in Fig. 6.9 for cubic B-splines (p = 3). The remaining residual for h = 3 is located mainly in the fringe field region. This is expected, as positioning errors and vibrations, resulting in measurement errors proportional to the field gradient, are largest in these regions.

A reasonable threshold for the global RMS residual res_{RMS} needs to be estimated. To this end, an ensemble of K = 100 samples for the arm deformation is drawn from the mechanical model of the mapper arm; $d_k \sim \mathcal{N}(\mathbf{0}, \mathbf{D})$ (see section 4.2.1) and added to the measurement positions. The expected measurement errors due to d_k are estimated by

$$\boldsymbol{\epsilon}_{k} = \partial \boldsymbol{H}(\boldsymbol{\nu}_{\text{LS}})\boldsymbol{d}_{k} \tag{6.13}$$

using the mechanical perturbation matrix according to (4.41).

The expected measurement errors ϵ_k are computed for each stage of the adaptive mesh refinement. The

h	p	$\epsilon_{\rm RMS}$ [mT]	residual RMS [mT]
1	1	0.457	34.848
1	2	0.301	12.966
1	3	0.193	6.823
1	4	0.139	3.861
2	1	0.167	5.866
2	2	0.092	1.674
2	3	0.083	0.629
2	4	0.080	0.233
3	1	0.080	0.285
3	2	0.079	0.072
3	3	0.079	0.049

Table 6.5: RMS residuals of the least squares solutions used for adaptive mesh refinement. ϵ_{RMS} is the expected RMS error due to positioning errors. As the residual falls below ϵ_{RMS} for p = h = 3, it is assumed that the remaining residual origins from positioning errors and vibrations.

estimated global RMS error is denoted by ϵ_{RMS} and is defined by

$$\epsilon_{\text{RMS}} := \frac{1}{K} \sum_{k=1}^{K} \sqrt{\frac{\boldsymbol{\epsilon}_k^T \boldsymbol{\epsilon}_k}{3M}}.$$

It is given in table 6.5 and compared to the residuals of the least squares solutions. For convenience, both residuals are transferred to units of mT, by dividing with the probes sensitivity of 5 V T^{-1} .

As it is seen from table 6.5, the estimated residual ϵ_{RMS} saturates at 0.079 mT for h = 3, p = 2. This is reasonable, as with increasing complexity, the field model will properly describe the field distribution in the fringe fields, but miss the flexibility to fit to the mechanical vibrations. The residual of the least squares fit falls below ϵ_{RMS} for h = 3, p = 2. This justifies the assumption that the remaining residual is traced back to positioning errors and not to under-fitting. In the following the approximation space with h = p = 3 is selected. This choice is debatable, as the residual falls below the expected threshold for p = 2already.

The least squares solution used for the construction of the ansatz space does not provide feedback about uncertainties. Moreover, in the least squared sense residuals are equally weighted, without incorporating the measurement uncertainties properly.

The initialization ensemble shall be drawn based on realistic assumptions on the measurement uncertainties. Therefore a sensor noise covariance matrix needs to be estimated, which properly accounts for sensor noise and positioning uncertainties. The derivation of this covariance matrix is the subject of the next subsection.

A decorrelated noise model by linearization

The mechanical perturbation matrix $\partial H(\nu)$, depends on the state vector for the magnetic field. The way how arm vibrations and positioning errors are influencing the measured voltages can therefore not be estimated a-priori. The mechanical noise is correlated with the field, which yields a complicated noise structure.

However, as it was indicated by the investigations in section 3.3.8, the least squares solution ν_{LS} provides a good estimate for the expected value of ν in the over-sampled case where dim $(\nu) \ll \dim(y)$. In this case, it is possible to use the least squares solution to estimate the impact of the mechanical perturbations, a-priori. To this end, one substitutes ν_{LS} for ν in the mechanical perturbation matrix $\partial H(\nu)$ and writes

$$H(\nu, \theta) \approx \partial H(\nu, \theta = 0) + H(\nu_{\rm LS})\theta, \tag{6.14}$$

to drop the dependency of ∂H on ν . In this way, the mechanical noise is decorrelated from $H(\nu, \theta = 0)$, which gives rise to the decorrelated Gaussian noise model

$$p(\boldsymbol{y}|\boldsymbol{x}) \sim \mathcal{N}(\boldsymbol{H}(\boldsymbol{\nu}, \boldsymbol{\theta} = \boldsymbol{0}), \underbrace{\partial \boldsymbol{H}(\boldsymbol{\nu}_{\mathrm{LS}}) \boldsymbol{D} \partial \boldsymbol{H}(\boldsymbol{\nu}_{\mathrm{LS}})^{T}}_{:=\boldsymbol{R}_{d}} + \boldsymbol{R}_{y}),$$
 (6.15)

 R_y is the sensor noise covariance matrix, which takes the form

$$\boldsymbol{R}_{y} = \begin{pmatrix} \boldsymbol{R}_{U_{x}} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{R}_{U_{y}} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{R}_{U_{z}} \end{pmatrix},$$
(6.16)

assuming that the measurement vector is ordered according to the scheme

$$\boldsymbol{y} = (U_x(\boldsymbol{r}_1), ..., U_x(\boldsymbol{r}_M), U_y(\boldsymbol{r}_1), ..., U_y(\boldsymbol{r}_M), U_z(\boldsymbol{r}_1), ..., U_z(\boldsymbol{r}_M))^T.$$
(6.17)

The blocks of R_y in (6.16), are identified by experiments according to (4.10) in section 4.1.1, for each of the three Hall probes (see (4.10)).

D is the covariance matrix of mechanical perturbations, $d \sim \mathcal{N}(0, D)$ (see section 4.2.1). The term $R_d = \partial H(\nu_{\text{LS}}) D \partial H(\nu_{\text{LS}})^T$ is the mechanical noise covariance matrix, and it accounts properly for the measurement errors due to mapper arm vibration and positioning errors, assuming that $E(\nu) = \nu_{\text{LS}}$. Since individual moves can be considered as uncorrelated, it is a block-wise sparse matrix and can be constructed "move-by-move". Fig. 6.2.1 gives an example for R_d which has been constructed from nine mapper moves.

3) Bayesian inference

Denoting by R the total measurement covariance $R := R_d + R_y$, the posterior probability density function is

$$p(\boldsymbol{\nu}|\boldsymbol{y}) \propto \exp\left(-\frac{1}{2}\left(\boldsymbol{y} - \boldsymbol{H}\boldsymbol{\nu}\right)^T \boldsymbol{R}^{-1}\left(\boldsymbol{y} - \boldsymbol{H}\boldsymbol{\nu}\right)\right),$$
 (6.18)

where a sufficiently flat prior has been selected. To avoid the inversion of a large matrix, 10 000 samples from the posterior are drawn by solving the linear equation system according to (5.17). The matrix R is sparse and positive definite by construction, as correlations between moves are neglected. In this application, only 1% of the matrix elements are populated. A square root matrix of R is computed using the sparse Cholesky factorization as it is implemented in Eigen's SimplicialLLT function [90]. To avoid direct matrix inversions, the sample ν_k is computed in four steps:

- 1. solve $\mathbf{RC} = \mathbf{H}$ for \mathbf{C}
- 2. solve $\mathbf{R}\mathbf{u} = \mathbf{y}$ for \mathbf{u}



- Figure 6.10: Example for the covariance structure using the decorrelated noise model. Here the covariance of nine moves is shown. 362 measurements are taken, therefore the matrix is of dimension $1\,086 \times 1\,086$. The entries of the covariance matrix are given in V², and correspond to the covariances between the measurements, due to mechanical perturbations.
 - 3. solve $\mathbf{R}^{1/2} \mathbf{l}_k = \boldsymbol{\epsilon}_{k}$ for \mathbf{l}_k
 - 4. solve $\boldsymbol{H}^T \boldsymbol{C} \boldsymbol{\nu}_k = \boldsymbol{H}^T (\boldsymbol{u} + \boldsymbol{l}_k)$ for $\boldsymbol{\nu}_k$

where steps 1 and 2, as well as the computation of $H^T Q$ can be performed once and be reused for all samples. The matrix $H^T Q$ can be factorized once before the sampling. In this way, step 4 requires solely a backward substitution to draw a new sample.

From the collection of ν_k , the mean and covariance can be estimated. In the bottom plot of Fig 6.11, the boundary is colored according to the mean $E(\nu)$, whereas the logarithm of $|var(\nu)|$ is given in the top plot. Due to the positioning errors and vibrations the variances are largest in the fringe field region.

4) Prediction

More important than the statistics in ν is the uncertainty for field evaluations inside the domain. Denoting by $F\nu$ the linear prediction operator for the evaluation of B, the covariance $\operatorname{cov}[B]$ is a linear transformation of $\operatorname{cov}(\nu)$, according to $\operatorname{cov}(B) = F\operatorname{cov}(\nu)F^T$. The covariance $\operatorname{cov}(\nu)$ is approximated from the sampled covariance matrix of the ensemble ν_k , according to table 5.1.

In Fig. 6.12, the field is evaluated along a reference trajectory inside the domain. The uncertainty in ν is propagated towards the three components of B. The dashed lines illustrate the 3σ error bars for each component. The uncertainty is largest for B_y and B_z in the fringe-field, where the 3σ bars are reaching 7 mT for B_y .

The value of $3\sigma_{rel}(I_{B_y})$ after the initialization is given by

$$3\sigma_{\rm rel}(I_{B_y}) = 22.29 \times 10^{-4}.$$
 (6.19)



Figure 6.11: Mean and variance computed from 10000 samples at the boundary of the domain. Here 13402 cubic basis splines are approximating the boundary data.

6.2.2 Active learning

With the prior ensemble computed before, the active learning algorithm can start. Whereas the uncertainties in the magnet's homogeneity region are below 10^{-4} T (see Fig. 6.12), the remaining uncertainty in the fringe field yields an uncertainty in the field integral, which is exceeding the desired value. For this reason, update measurements are taken in the fringe field region where the uncertainty is largest (see Fig. 6.12).

The resulting positions are shown in Fig. 6.13. The moves are denoted by j = 1, ..., J. In total, J = 400 moves in the left and right fringe field are taken, and the spatial resolution is increased to 2 mm. This gives $25\,000$ new measurement positions. The positions are illustrated in Fig. 6.13. The overall measurement duration for the update measurements is 2 hours.

In the following, the update steps presented in section 5.4 are applied to the J update moves. The superscripts *prior* and *post* are replaced with the superscripts j - 1 and j, respectively. In this way the updates can be expressed by means of a loop over j.

For the first move j = 1, the samples generated from section 6.2.1 are treated as prior ensemble, filling the columns of the matrix $\mathbf{X}^0 := (\mathbf{\nu}_1^0, ..., \mathbf{\nu}_K^0) \in \mathbb{R}^{N \times K}$.

The ensemble Kálmán filter, presented in section 5.4, provides the way to update the prior ensemble based on the new set of observations. The measurement vector of move j is denoted by y^j and the covariance matrix is denoted by \mathbf{R}^j . The latter is computed in the same way as it was done in section 6.2.1, replacing the least squares solution ν_{LS} with the mean of the prior ensemble

$$\mathbf{E}\left(\boldsymbol{X}^{j-1}\right) = \frac{1}{K} \sum_{k=1}^{K} \boldsymbol{\nu}_{k}^{j-1}.$$
(6.20)



Figure 6.12: Mean values (solid) and three standard deviations (dashed) for the field evaluation along a reference trajectory.



Figure 6.13: Measurement data taken in the fringe field to update the the field map.

The ensemble is now updated move-by-move, following the steps presented in section 5.4. In this case, the number of measurements in every update is not greater than M = 303, since the domain width is 202 mm, and the measurements for the three Hall voltages are triggered in steps of 2 mm.

Iterating over the moves j, the update from the ensemble X^{j-1} to X^j is computed according to the following six steps:

- 1. compute $m{Y}^j := \left(m{y}^j + m{\epsilon}_1, ..., m{y}^j + m{\epsilon}_K
 ight), \quad ext{with:} \quad m{\epsilon}_k \sim \mathcal{N}(m{0}, m{R}_j)$
- 2. compute $U^{j-1} = X^{j-1} \mathbb{E}(X^{j-1}) I_{1 \times K}$
- 3. compute $H^{j}U^{j-1}$ and $H^{j}X^{j-1}$
- 4. compute $P^{j} = \frac{1}{K-1} H_{j} U^{j-1} \left(H^{j} U^{j-1} \right)^{T} + R^{j}$
- 5. solve $P^j Z^j = Y^j H^j X^{j-1}$ for Z^j
- 6. update $X^{j} = X^{j-1} + \frac{1}{K-1} U^{j-1} (H^{j} U^{j-1})^{T} Z^{j}$.

Including the assembly of the H^{j} matrix, each update takes about 30 s on a desktop computer.

In Fig. 6.14 the 3σ standard deviation for the evaluation of the absolute field along the reference trajectory is shown. It has been evaluated for the prior X^0 , the posterior ensemble after updating with the first 200 measurements X^{200} as well as the posterior ensemble after updating using the remaining 200 measurements X^{400} . Using the local updates, the 3σ standard deviation in |B| could be reduced by a factor of ten, from values of about 7 mT to 0.7 mT.

The value of $3\sigma_{rel}(I_{B_y})$ after all 400 updates are taken is

$$3\sigma_{\rm rel}(I_{B_y}) = 1.78 \times 10^{-4},\tag{6.21}$$

which falls below the desired threshold.

In Fig. 6.15, the measurement uncertainty is propagated to B_y in the *xy*-plane, in the center of the domain, this means s = 0 comparing to Fig. 6.12.

6.2.3 Discussion

In this section, the advantages of the field representation by boundary data are summarized.

Expressing the field by means of boundary integral equations, one benefits from a smoothing property towards random measurement errors. To show this effect, measurements in the xy-plane, central to the magnet (see Fig. 6.15) are taken and the flux density B at the measurement position is computed via the point-wise (pw) axial sensor model

diag
$$(s_x, s_y, s_z) \cdot (\boldsymbol{n}_x, \boldsymbol{n}_y, \boldsymbol{n}_z)^T \boldsymbol{B}_{pw}(\boldsymbol{r}_m) = \boldsymbol{U}(\boldsymbol{r}_m) - \boldsymbol{U}_0,$$
 (6.22)

with the sensor orientations according to (6.2) resulting from the analysis of section 4.1.5. The definitions of all variables in this equations are found in table 6.6.



Figure 6.14: Three standard deviations for the evaluation of the absolute field |B| along the reference trajectory. The blue curve is computed using the ensemble V_0 , which is the result of the initialization step. The orange curve results from the ensemble V_{200} which was obtained after updating with the measurements in the left fringe field. The green curve shows the result when using the ensemble V_{400} which results after updating V_{200} with the measurements in the right end of the magnet.



variable	meaning
s_x	sensitivity of <i>x</i> -sensor
s_y	sensitivity of <i>y</i> -sensor
s_z	sensitivity of <i>z</i> -sensor
n_x	orientation vector of x-sensor
n_y	orientation vector of <i>y</i> -sensor
n_z	orientation vector of <i>z</i> -sensor
U_0	zero field offset voltage of x, y and z sensor
ig U	measurement vector
r_m	measurement position

Table 6.6: Variables in the point-wise axial sensor model.

In the top plot of Fig. 6.16 the vertical field component $B_y(x, y)$ is reconstructed by BEM and given as a field map. The value of $B_y(0,0) = 0.42819$ T in the center of the domain is taken as a reference and the field quality Q is defined as

$$Q = \log_{10} \left| \frac{B_y(x, y) - B_y(0, 0)}{B_y(0, 0)} \right|.$$
(6.23)

Q is plotted in the central plot of Fig. 6.16, whereas the boundary-element method is used to compute $B_y(x, y)$. In the bottom plot, B_y is computed from Eq. (6.22), based on direct measurements inside the domain. In both cases, Q was referred to the same reference field of $B_y(0,0) = 0.42819$ T, which validates the capability of the field model to predict the correct field distribution. Of course, a smoothing filter applied to the direct measurements would provide similar results. The advantage is, that no measurements inside the domain were needed to predict the field, saving enormously in terms of measurement duration.

The predictions are validated also by comparing the results to an alternative measurement device, namely a nuclear magnetic resonance (NMR) sensor. The results are given in Fig. 6.17. There is a systematic difference of 0.1 mT, between the field reconstruction and the NMR measurement. Such difference is not unusual for Hall probe measurements, as temperature effects, offset drifts and the calibration of the acquisition card might influence the signal in this range. It is common practice for field maps taken by Hall probes to correct the remaining difference by means of an NMR reference measurement.

So far, the advantages of the BEM field model have been pointed out. To finish this chapter, the benefits of the mathematical sensor model shall be investigated. To this end, the flux density B is recovered from the point-wise axial sensor model, according to (6.22), and compared to the prediction of BEM. Every fifth sample of the boundary measurements shown in Fig. 6.9 is considered in the following analysis. In Fig. 6.18, the error measured in the euclidean norm $||B_{\text{BEM}} - B_{\text{pw}}||_2$, between the predicted flux density B_{BEM} and the direct measurements, using a point-wise approximation B_{pw} is shown. The BEM reconstruction not only smooths out the random measurement errors, it also avoids systematic errors, as the sensor model correctly accounts for the three sensor positions. The errors related to a point wise-approximation would reach values of up to 27 mT in the fringe-field region.







Figure 6.17: Prediction of |B| validated by NMR measurements. A systematic difference of $0.1 \,\mathrm{mT}$ was found.



Figure 6.18: Error measured in the euclidean norm for the boundary measurements when using the point-wise approximation according to Eq. (6.22).

6.3 A two stage Gibbs sampler for positioning uncertainty quantification

The uncertainty quantification presented in the previous section made use of a least-squares solution to estimate the measurement derivatives, which were needed to estimate the influence of the mechanical noise. The field and mechanical models with parameters ν and θ were decoupled, and the influence of mechanical perturbations was considered as a colored Gaussian noise contribution, estimated with the help of the least-squares solution. From an engineering perspective, this approach seems plausible in cases where the mechanical noise is filtered out in the least-squares solution. However a domain of validity for this statement, has not been determined yet and should be investigated more deeply in the future research. Especially, since it is expected that the filtering property of the BEM approximation performs worse for low-frequency vibrations, and because the frequencies of vibration decrease with the length of the mapper arm, the decorrelation by means of a least-squares solution is questionable in such circumstances.

For this reason, an alternative approach for uncertainty quantification is now presented, which avoids the use of a least squares solution. To this end, the mechanical state vector d is now considered as unknown nuisance parameter, and the two stage Gibbs sampler presented in section 5.7 is applied to the joint posterior density function $p(\nu, d|y)$.

For y, the Gaussian noise model

$$\boldsymbol{y} \sim \mathcal{N}(\mathrm{E}(\boldsymbol{y}), \boldsymbol{R}_{y})$$
 (6.24)

is now assumed, where R_y is the same block matrix as it was used in Eq. (6.16), given that the y vector is sorted accordingly. It was discussed in section 4.1.1, that this noise model excludes the mechanical noise.

Referring to sections 4.2.1 and 4.2.2, d describes the 5M degrees of freedom of freedom correspond to a rigid body motion of the sensor, five for each measurement position. These mechanical degrees of freedom are can be considered as a nuisance parameter, as they are affecting the predicted measurements, but not the quantities of interest.

The two-stage Gibbs sampler introduced in section 5.7 is applied to draw samples for stage vector of the magnetic field $\boldsymbol{\nu} \in \mathbb{R}^N$ and the mechanical state vector $\boldsymbol{d} \in \mathbb{R}^{5M}$. Substituting the observation operator $\boldsymbol{H}(\boldsymbol{\nu}, \boldsymbol{d})$ for the mean $\mathbb{E}(\boldsymbol{y})$ in Eq. 6.24 yields the likelihood

$$p(\boldsymbol{y}|\boldsymbol{\nu},\boldsymbol{\theta}) \sim \exp\left(-\frac{1}{2}\left(\boldsymbol{y} - \boldsymbol{H}(\boldsymbol{\nu},\boldsymbol{d})\right)^T \boldsymbol{R}_y^{-1}\left(\boldsymbol{y} - \boldsymbol{H}(\boldsymbol{\nu},\boldsymbol{d})\right)\right),$$
 (6.25)

and applying Bayes rule gives the posterior

$$p(\boldsymbol{\nu}, \boldsymbol{\theta} | \boldsymbol{y}) \propto \exp\left(-\frac{1}{2} \left(\boldsymbol{y} - \boldsymbol{H}(\boldsymbol{\nu}, \boldsymbol{d})\right)^T \boldsymbol{R}_{\boldsymbol{y}}^{-1} \left(\boldsymbol{y} - \boldsymbol{H}(\boldsymbol{\nu}, \boldsymbol{d})\right)\right)$$
$$\exp\left(-\frac{1}{2} \left(\boldsymbol{\nu} - \boldsymbol{\nu}_0\right)^T \boldsymbol{Q}^{-1} \left(\boldsymbol{\nu} - \boldsymbol{\nu}_0\right)\right)$$
$$\exp\left(-\frac{1}{2} \boldsymbol{d}^T \boldsymbol{D}^{-1} \boldsymbol{d}\right).$$
(6.26)

In this case Gaussian priors have been implied for ν and d, using the prior covariance matrices Q and D. The zero mean prior for d is used to the distribution for d around 0 and the covariance matrix of mechanical perturbations D is used to enforce the physical correlations between the degrees of freedom based on the mechanical model (see section 4.2.1).

The Gibbs sampler is based on the conditionals $p(\nu|d, y)$ and $p(d|\nu, y)$. According to (5.9) these functions can be computed by dividing the joint probability density function $p(\nu, d|y)$ by either p(d) or $p(\nu)$, and then, interpreting the results as functions of d or ν , with the remaining parameter as a given variable.

In this case, the resulting conditionals are

$$p(\boldsymbol{\nu}|\boldsymbol{d},\boldsymbol{y}) \propto \exp\left(-\frac{1}{2}\left(\boldsymbol{y} - \widetilde{\boldsymbol{H}}(\boldsymbol{\nu},\boldsymbol{d})\right)^{T} \boldsymbol{R}^{-1}\left(\boldsymbol{y} - \widetilde{\boldsymbol{H}}(\boldsymbol{\nu},\boldsymbol{d})\right)\right)$$
$$\exp\left(-\frac{1}{2}\left(\boldsymbol{\nu} - \boldsymbol{\nu}_{0}\right)^{T} \boldsymbol{Q}^{-1}\left(\boldsymbol{\nu} - \boldsymbol{\nu}_{0}\right)\right),$$
(6.27)

$$p(\boldsymbol{d}|\boldsymbol{\nu}, \boldsymbol{y}) \propto \exp\left(-\frac{1}{2}\left(\boldsymbol{y} - \widetilde{\boldsymbol{H}}(\boldsymbol{\nu}, \boldsymbol{d})\right)^T \boldsymbol{R}^{-1}\left(\boldsymbol{y} - \widetilde{\boldsymbol{H}}(\boldsymbol{\nu}, \boldsymbol{d})\right)\right)$$
$$\exp\left(-\frac{1}{2}\boldsymbol{d}^T \boldsymbol{D}^{-1}\boldsymbol{d}\right).$$
(6.28)

Following the discussion in section 4.2.2, and noticing that the arm displacements are small, the above conditionals are formulated in terms of the perturbed observation operator \widetilde{H} , according to (4.41). If \widetilde{H} is linear in ν , both of the above conditionals are Gaussian distributions.

With algorithm 3 and the conditionals, the two-stage Gibbs sampler for the posterior in (6.26) is summarized in algorithm 5.

Algorithm 5 Sampling from the posterior $p(\boldsymbol{\nu}, \boldsymbol{d} \boldsymbol{y})$	
$d_0 = 0$	initialize mechanical state vector
for $k = 1,,$ number of samples K do	
$oldsymbol{ u}_k \sim p(oldsymbol{ u} oldsymbol{d}_{k-1},oldsymbol{y})$	sample state vector for the magnetic field
for $j = 1,,$ number of moves J do	
$oldsymbol{ heta}_{k,j} \sim p(oldsymbol{d}_j oldsymbol{ u}_{k-1}, oldsymbol{y}_j)$	\triangleright sample mechanical state vector for move j
end for	
$m{d}_k = (m{d}_{k,1}^T,,m{d}_{1,J}^T)^T$	collect mechanical state vectors
end for	

As it is usually the case, the measurement data is taken move-by-move and the inference is applied to the collection of all measurements, see for instance Fig. 6.6 (right). In algorithm 5, J denotes the total number of mapper moves and the mechanical state vector is considered to be deccorrelated between them. In this way, the sampling for the high-dimensional mechanical state vector $d \in \mathbb{R}^{5M}$ is split into J parts of smaller dimension.

At this point, the equations are getting intuitive. Having sampled a state vector for the magnetic field ν one computes the derivatives $\partial H(\nu)$, which are then used to determine a sample for the mechanical state vector d. This d is then used to compute a new sample for ν . Measurements in regions where the derivative $\partial H(\nu)$ is small do not yield any information about the positioning error, but the zero mean prior ties the distribution for d to zero. This has the effect of a regularization.

A major drawback of algorithm 5 when using BEM as a field model, is that the derivative of the observation operator $\partial H(\nu)$, is required in every step. This increases the memory requirements of the algorithm by a factor



Figure 6.19: Field map taken with the Hall probe mapper in a cylindrical domain.

of six. At this point, the MLFMM presented in section 3.3.10 becomes indispensable for high-dimensional problems.

As a proof of concept, the measurements and boundary mesh illustrated in Fig. 6.19 is now considered. The measurements have been taken in the fringe field region of a magnet, in a way that evidence for the sensor position is available by means of a field gradient and the overall problem size is manageable for a desktop computer with 16 GB RAM. For validation, a move through the center of the domain of interest is taken, and the sensor position of this move is measured by means of a Leica laser tracker. The validation move is taken through the center of the domain, as the magnet geometry did not allow for mounting a reflector target for the boundary moves.

Fig. 6.20 shows the residual between measurements y and the prediction $\widetilde{H}(\nu_1, d=0)$,

$$\operatorname{res} := \boldsymbol{y} - \widetilde{\boldsymbol{H}}(\boldsymbol{\nu}_1, \boldsymbol{d} = \boldsymbol{0}), \tag{6.29}$$

based on the initializing field solution ν_1 in blue. For comparison, the expected residual, based on the measured sensor displacements is computed by

$$\operatorname{res}_{\exp} := \partial H d_{\operatorname{meas}},\tag{6.30}$$

where d_{meas} is the measured mechanical state vector. This vector needs to be determined according to section 4.2, using the FEM model of the mapper arm, in order to transfer the measured displacements to the arm deformation and rotation at the sensor position. It is plotted in orange. It becomes clear, that the residual provides evidence for the mechanical state vector *d*, as frequencies and amplitudes of the residual are matching with the expectations.

1 000 samples from the posterior are now drawn from algorithm 5. The sampled mean, as well as the maximum and minimum values for the vertical arm displacement w_y are shown in Fig. 6.21, and compared to the optical measurements. The differences are within the range of the measurement accuracy of laser tracker of ~ 20 µm. Fig. 6.22 shows the resulting mean value of the boundary data, as well as the variance, estimated from the diagonal of the sampled posterior covariance matrix. The values for the displacements w_y are directly accessible in the d_k -vectors, according to (4.32).



Figure 6.20: Residual in the measurement operation after the initialization step (blue) and the expected residual based on optical measurements (orange). As the field component affecting the U_z measurement is small, the vibrations are hidden under the nose floor, which is why only U_x and U_y are plotted.



Figure 6.21: Estimated vertical arm displacement compared to optical measurements for validation. Red: Mean value based on 1 000 samples from the posterior. Blue: Optical measurement using a Leica laser tracker and the numerical FEM model. Gray: Maximum and minimum values for w_y based on the ensemble d_k . As d_k stores the mechanical perturbations at the measurement times, the values for w_y are found in the corresponding rows of the d_k vector according to (4.32).



Figure 6.22: Resulting boundary data and standard deviation in logarithmic scale, estimated from $1\,000$ samples of the Gibbs sampler.

The advantage of algorithm 5 is that the sensor-noise model is simplified with respect to the one used in (6.15), since the effect of mechanical noise is encoded by the nuisance parameter d and not by means of a prior field solution. With a suitable compression technique for the dense mathematical operations involving the observation operators H and ∂H , the approach may also be considered for large dimensional problems. This has been the main motivation for the implementation of the MLFMM. Moreover, also iso-geometric finite element methods might be considered for future research, as their advantage for the memory efficient evaluation of field derivatives is undeniable and state-of-the-art approaches are reaching high accuracy [101].

7 Conclusion and Outlook

The main objective of this thesis, was to apply boundary element methods for the field reconstruction in accelerator magnets, mainly with the ambition to make three-dimensional field mapping more efficient. Although it was a long way to obtain coherent results using the combination of boundary-element methods and Hall probe measurements, this goal can be considered as achieved.

In the scope of this doctoral thesis, a new three-axes Hall probe mapper was commissioned and metrologically characterized. It uses the stages of a coordinate measurement machine and provides spatial sampling of the three flux density components of the magnetic field. Moreover, acquisition software and measurement procedures were developed and implemented, and new calibration routines for the three-dimensional probe calibration have been designed. On several occasions, the mapper system has been proven a useful contribution to the portfolio of measurement systems of the TE-MSC-TM section at CERN.

The first coherency problems were mainly due to the cross sensitivity between the axes of the Hall probe, and their spatial offsets. Wrong assumptions about these parameters yield large errors in the field reconstruction in the fringe fields (see Fig. 6.18). The development of the cone quadrupole calibration approach can be considered as a break-through, as it provides the required evidence for the sensor positions and orientations in three-dimensions.

It quickly became clear that the remaining bottleneck for the Hall-probe mapper system is the positioning accuracy. Positioning errors in the 0.1 mm range yield field errors of 1 mT in gradient fields with 10 T m^{-1} . Gradients in this range are quite common in the extremities of accelerator magnets. For this reason, the mechanical system was investigated deeply, resulting in a magneto-mechanical model for the precise quantification of positioning perturbations. This model lays the foundation for the discrimination between approximation and positioning errors and is employed for the systematic construction of the BEM approximation spaces, as it is shown in Fig. 6.9.

A complete boundary measurement, covering a volume of $\Omega = (0.1 \times 0.05 \times 2) \text{ m}^3$, including the fiducialization procedure and update measurements in the fringe fields (see chapter 6) requires roughly half of a working day of measurement time. To put this into perspective, mapping the field in the volume Ω as mentioned before, with a spatial resolution of 5 mm requires 4 000 moves when mapping along the *x*-axis. The boundary map, however, would require only 860 moves. With the nominal speed of 20 mm s⁻¹, this reduces the measurement duration from 11 to roughly 2.5 hours. Moreover, because of the model-based approach, there is no limit in spatial resolution for the field map generation from boundary data and the maps are exact magneto-static solutions.

The accuracy of the system strongly depends on the capability to stabilize the temperature within the Hall probe. Even in the controlled environment of CERN's measurement laboratories, relative sensitivity drifts in the range of 3×10^{-4} have been observed, which are in accordance with the temperature calibration and the measured ambient temperature fluctuations. As the temperature drifts are long-term effects, field maps can be corrected by NMR measurements, however, the monitoring and control of the Hall probes temperature

would provide the feedback necessary to mitigate the accuracy issues. To this end, the developments on a new Hall probe measuring head and a temperature calibration setup have already been started during this PhD thesis.

The Bayesian framework been has proven useful for the quantification of measurement uncertainties and the development of active learning schemes to update field maps with new data in locations where uncertainties remain large. In this way, field maps are obtained even more efficiently by exploring the physical space dependent on uncertainties. All error sources affecting the measurement outcome need to be understood for a useful uncertainty quantification, which is the basis for the active learning scheme. The magneto-mechanical model of the mapper system provides the tool which is necessary to estimate the impact of positioning errors. Not only the efficiency on the data acquisition side was improved by using the Bayesian framework. It allows also to separate large inverse problems into small Bayesian updates. Each of these updates is usually faster than the measurement acquisition itself, and can be performed on-the-fly during the acquisition, at the test bench.

The potential of Bayesian inference in the context of magnetic measurements is far from exhausted. In the view of the author, future research related to the field should focus on the following aspects:

- The domains of validity for the identifiability of the boundary data requires a deeper investigation. This analysis could follow the ideas presented in [102].
- Future research should investigate information theoretical aspects, to measure the information gain by means of the relative entropy (see [103]). In this way, sufficiency criteria can be derived, which can be used to decide when to stop exploring, based on the information the measurement system is capable to provide.
- This research has just started by bringing sensor parameters into the game. Systematic error sources are not only treated as uncertainty, but leveraged in order to draw better conclusions, based on the data and the correlations to the magnetic field. This has proven beneficial to the solution of the absolute position and orientation problem in the cone quadrupole calibration and also for the quantification of positioning perturbations during the field mapping. Future research could make used of a variety of different sensor systems, such as temperature probes or strain gauges, and fuse the measurement data in a way to explore a more extensive multiphysical model comprising the magnetic field, the sensor and also the mechanical system. The concept of sensor fusion is well established in robotics [104] [105].
- The iso-geometric analysis (IGA) based, finite element approaches presented in [11] should be investigated for future research as an alternative to BEM. The mathematical operations for the efficient computation of measurement derivatives in the context of fast multipole methods and BEM are quickly getting exhaustive. The advantages of the local support of the IGA ansatz spaces and the sparsity of the mathematical operations are not to deny. Moreover, as these methods discretize the domain already, they have the potential to establish a more direct link to particle tracking, bypassing the need for local expansions from boundary integral equations.

8 Appendix

8.1 The Calderón projector

The fact that both, the potential $\phi_{\rm m}$ and that normal derivative $\partial_n \phi_{\rm m}$ appear on the right hand side of (3.15) does not mean that one can inscribe both quantities independently. This is because the scalar potential is uniquely defined by means of a Dirichlet boundary condition already. Dirichlet and Neumann data are dependent by a linear operator. One can express this dependency by means of a boundary integral equation, taking the limit of the representation formula for $r \rightarrow \partial \Omega$. To this end, one searches for the correct trace operators for electromagnetic fields. A trace operator is a linear mapping that extracts suitable boundary values from a field [106]. The interior Dirichlet trace γ_0 may be introduced by

$$(\gamma_0 \phi_{\mathbf{m}})(\boldsymbol{r}) = \lim_{\boldsymbol{r} \to \boldsymbol{r}'} \phi_{\mathbf{m}}(\boldsymbol{r}), \quad \text{for } \boldsymbol{r}' \in \partial\Omega, \, \boldsymbol{r} \in \Omega.$$
(8.1)

Moreover, for smooth parts of the boundary and continuously differentiable functions, one can define the the *interior Neumann trace*, γ_1 as:

$$(\gamma_1 \phi_m)(\boldsymbol{r}) = \lim_{\boldsymbol{r} \to \boldsymbol{r}'} \boldsymbol{n}(\boldsymbol{r}') \cdot \operatorname{grad} \phi_m(\boldsymbol{r}), \quad \text{for } \boldsymbol{r}' \in \partial\Omega, \ \boldsymbol{r} \in \Omega.$$
(8.2)

Care must be taken when carrying out the limit $r \to \partial \Omega$ due to the singularity of the fundamental solution for r = r'. For a the derivation of the following equations see [107, Chapter 1].

Without elaborating further on their properties, the function spaces V_u and V_g^* , according to (3.8) and (3.9), are used for the Dirichlet and Neumann traces

$$(\gamma_0 \phi_{\mathbf{m}})(\mathbf{r}) \in \mathcal{V}_u, \quad (\gamma_1 \phi_{\mathbf{m}})(\mathbf{r}) \in \mathcal{V}_q^*.$$
 (8.3)

For details, the reader is referred to [53, Chapter 3].

In the following, it is assumed that the boundary $\partial\Omega$ is sufficiently smooth, such that the Dirichlet and Neumann traces may be identified by the restrictions $(\gamma_0\phi_m)(\mathbf{r}) = \phi_m|_{\partial\Omega} = u$ and $(\gamma_1\phi_m)(\mathbf{r}) = \partial_n\phi_m|_{\partial\Omega} = g$, where the same notation used in section 3.1, is adopted for Dirichlet and Neumann data, u and g. The definitions for the smooth case can be extended to the general case [108].

Taking the Dirichlet trace of the representation formula yields the boundary integral equation

$$u(\mathbf{r}) = (Vg)(\mathbf{r}) + \sigma(\mathbf{r})u(\mathbf{r}) - (Ku)(\mathbf{r}), \quad \text{for } \mathbf{r} \in \partial\Omega,$$
(8.4)

with the single layer operator

$$V := \gamma_0 \circ \widetilde{V} \tag{8.5}$$

and the double layer operator

$$(Ku)(\mathbf{r}) = \lim_{\epsilon \to 0} \int_{\mathbf{r}' \in \partial \Omega: |\mathbf{r} - \mathbf{r}'| \ge \epsilon} \mathbf{n}(\mathbf{r}') \cdot \operatorname{grad}_{\mathbf{r}'} u^*(\mathbf{r}, \mathbf{r}') u(\mathbf{r}') \, \mathrm{d}\mathbf{r}'.$$
(8.6)

 $\sigma(\mathbf{r})$ results from the limit of the double layer potential and is related to the interior angle of Ω in $\mathbf{r} \in \partial \Omega$. On smooth parts of the boundary, $\sigma(\mathbf{r}) = 1/2$. A similar boundary integral equation is derived by taking the Neumann trace of the representation formula

$$g(\mathbf{r}) = \sigma(\mathbf{r})g(\mathbf{r}) + (K'g)(\mathbf{r}) + (Du)(\mathbf{r}), \quad \text{for } \mathbf{r} \in \partial\Omega,$$
(8.7)

with the hypersingular operator

$$D := -\gamma_1 \circ W \tag{8.8}$$

and the adjoint double layer operator

$$(K'g)(\mathbf{r}) := \lim_{\epsilon \to 0} \int_{\mathbf{r}' \in \partial\Omega: |\mathbf{r} - \mathbf{r}'| \ge \epsilon} \mathbf{n}(\mathbf{r}) \cdot \operatorname{grad}_{\mathbf{r}} u^*(\mathbf{r}, \mathbf{r}') g(\mathbf{r}') \, \mathrm{d}\mathbf{r}'.$$
(8.9)

Equations (8.4) and (8.7) provide linear maps between Dirichlet and Neumann data. It is common to summarize both equations in a linear equation system¹.

$$Vg = ((1/2)I + K)u,$$
(8.10)

$$Du = ((1/2)I - K')g, \tag{8.11}$$

where I denotes the identity operator. The single layer² V as well as the hypersingular operator D are bounded, elliptic and semi-elliptic respectively [107]. These properties are the basis for uniqueness and convergence proofs for the discrete linear equation systems when following the Galerkin discretization scheme according to section 3.3.4 (assuming a suitable regularization for D is applied, see [107, Chapter 2.3]). Moreover it yields symmetric positive definite matrices suited for the iterative solution via conjugate gradient solvers. For these reasons, it is common practice working with 8.10 as a basis for *Dirichlet-to-Neumann* maps, whereas 8.11 is used to derive *Neumann-to-Dirichlet* maps. The latter is of particular importance for the post processing of measurement data, because measured voltages are proportional to fluxes or flux densities, and therefore relate to the Neumann data.

8.2 The discrete Dirichlet-to-Neumann map

One can understand the Galerkin scheme, as substituting the approximations for $u(\mathbf{r})$ and $g(\mathbf{r})$ in 8.4, multiplying by $\varphi_l^{\mathrm{N}}(\mathbf{r})$, for l = 1, ..., L and integrating over the domain boundary. In this way one obtains the Galerkin equations

$$\left\langle Vg_{h},\varphi_{l}\right\rangle_{\partial\Omega} = \left\langle \left(\frac{1}{2}I+K\right)u_{h},\varphi_{l}\right\rangle_{\partial\Omega}, \quad \text{for} \quad l=1,...,L.$$
 (8.12)

¹A smooth boundary is assumed; $\sigma = 1/2$.

²At this point the condition $R > \text{diam}(\Omega)$, must hold for the single layer operator V to be elliptic in two dimensions.

Here and in the following

$$\langle u, v \rangle_{\partial\Omega} := \int_{\partial\Omega} u(\mathbf{r}') v(\mathbf{r}') \,\mathrm{d}\mathbf{r}'.$$
 (8.13)

This gives rise to the matrix $V \in \mathbb{R}^{L \times L}$ with

$$[\mathbf{V}]_{i,j} := \left\langle V\varphi_i^{\mathbf{N}}(\mathbf{r}), \varphi_j^{\mathbf{N}}(\mathbf{r}) \right\rangle_{\partial\Omega}, \tag{8.14}$$

and the matrix $\boldsymbol{K} \in \mathbb{R}^{L \times K}$ with

$$[\mathbf{K}]_{i,j} := \left\langle \left(\frac{1}{2}I + K\right) \varphi_i^{\mathsf{D}}(\mathbf{r}), \varphi_j^{\mathsf{N}}(\mathbf{r}) \right\rangle_{\partial\Omega},$$
(8.15)

such that the discrete Dirichlet-to-Neumann map is given by

$$Vg = Ku. \tag{8.16}$$

where $\boldsymbol{g} = (g_1, ..., g_L)^T \in \mathbb{R}^L$ and $\boldsymbol{u} = (u_1, ..., u_K)^T \in \mathbb{R}^K$.

8.3 The discrete Neumann-to-Dirichlet map

There are two reasons for which the hypersingular operator *D* requires special treatment. 1) *The integral operator does not exhibit an explicit representation as a Cauchy singular value* [107], as the required limit does not exist. 2) The operator has a non-trivial kernel.

The cure to 1) is to apply integration by parts in order to bring the linear form $\langle Du, v \rangle_{\partial\Omega}$ into the form

$$\langle Du, v \rangle_{\partial\Omega} = \frac{1}{4\pi} \iint_{\partial\Omega} \frac{\operatorname{curl}_{\partial\Omega} u(\boldsymbol{r}) \cdot \operatorname{curl}_{\partial\Omega} v(\boldsymbol{r})}{\|\boldsymbol{r} - \boldsymbol{r}'\|_2} d\boldsymbol{r} d\boldsymbol{r}'.$$
(8.17)

Here $\operatorname{curl}_{\partial\Omega} u(\boldsymbol{r})$ is the vectorial surface curl

$$\operatorname{curl}_{\partial\Omega} u(\boldsymbol{r}) = -\boldsymbol{n}(\boldsymbol{r}) \times \operatorname{grad}_{\boldsymbol{r}} \widetilde{u}(\boldsymbol{r}), \quad \text{for } \boldsymbol{r} \in \partial\Omega,$$
(8.18)

and \widetilde{u} is the local extension of u.

A commonly applied cure to 2) is to gauge out the averaged Dirichlet data

$$\int_{\partial\Omega} u(\mathbf{r}') \,\mathrm{d}\mathbf{r}' = 0. \tag{8.19}$$

This can be accommodated by considering the extended variational problem [107]

$$\langle Du, v \rangle_{\partial\Omega} + \langle u, 1 \rangle_{\partial\Omega} \langle v, 1 \rangle_{\partial\Omega} = \left\langle \left(\frac{1}{2}I - K'\right)g, v \right\rangle_{\partial\Omega}.$$
 (8.20)

Applying a Galerkin scheme one sets $u \to u_h$, $g \to g_h$ and $v \to \varphi_k^D$ for k = 1, ..., K to obtain the equation system

$$\underbrace{\left(\widetilde{D} + aa^{T}\right)}_{:=\widetilde{D}_{a}} u = K'g.$$
(8.21)

The matrices \tilde{D} and K' follow from approximating (8.17) and the right hand side of (8.20). Details are found in [107] chapter 2.3.2. a is the stabilization vector

$$[\boldsymbol{a}]_{i} = \int_{\partial\Omega} \varphi_{i}^{\mathrm{D}}(\boldsymbol{r}') \mathrm{d}\boldsymbol{r}'.$$
(8.22)



Figure 8.1: Finite beam element and nodal forces.

8.4 Computing the sensor orientation from solid harmonics

Considering only the coefficients with l = 1, the Hall voltage is given explicitly by

$$U(|\boldsymbol{B}|,\theta,\varphi) = |\boldsymbol{B}|\sqrt{\frac{3}{4\pi}} \left(\frac{1}{\sqrt{2}} \left(c_{1,-1} \exp(-j\varphi) - c_{1,1} \exp(j\varphi) \right) \sin(\theta) + c_{1,0} \cos(\theta) \right).$$
(8.23)

The Hall voltage is a real signal, this means that the coefficients must satisfy

$$\operatorname{Re}\{c_{1,1}\} = -\operatorname{Re}\{c_{1,-1}\}, \qquad \operatorname{Im}\{c_{1,1}\} = \operatorname{Im}\{c_{1,-1}\}.$$
(8.24)

In the *xy*-plane, it holds $\theta = \frac{\pi}{2}$ and therefore

$$U(|\boldsymbol{B}|, 0, \varphi) \propto |\boldsymbol{B}| \left(-\operatorname{Re}\{c_{1,1}\}\cos(\varphi) + \operatorname{Im}\{c_{1,1}\}\sin(\varphi) \right).$$
(8.25)

The maximum of this signal is found from trigonometric relations

$$\varphi_{\max} = -\arg\left(c_{1,1}\right). \tag{8.26}$$

The angle θ_{\max} is found in the $\varphi = \varphi_{\max}$ plane. Here

$$U(|\mathbf{B}|, \theta, \varphi_{\max}) \propto |\mathbf{B}| \left(c_{1,0} \cos(\theta) + \sqrt{2} \sqrt{\text{Im}\{c_{1,1}\}^2 + \text{Re}\{c_{1,1}\}^2} \sin(\theta) \right).$$
(8.27)

This follows from (8.23), with (8.24), after substituting $\varphi = \varphi_{max}$. The maximum angle θ_{max} is found from trigonometric relations

$$\varphi_{\max} = \arg\left(c_{1,0} + j\sqrt{2}\sqrt{\operatorname{Im}\{c_{1,1}\}^2 + \operatorname{Re}\{c_{1,1}\}^2}\right).$$
(8.28)

8.5 Finite element approximation of the Euler-Bernoulli beam

The beam is divided into subsections according to Fig. 8.1. Each interval of length h_i is parameterized by a



Figure 8.2: Hermite basis function on the unit interval.

linear transformation $\gamma_i : [0, h_i] \rightarrow [z_i, z_{i+1}]$. The displacement w(z, t) on $z \in [z_i, z_{i+1}]$ is then approximated by:

$$w(z) \approx \begin{pmatrix} N_1(\gamma_i^{-1}(z)) \\ N_2(\gamma_i^{-1}(z)) \\ N_3(\gamma_i^{-1}(z)) \\ N_4(\gamma_i^{-1}(z)) \end{pmatrix}^T \cdot \begin{pmatrix} w_s(z_i) \\ \theta_s(z_i) \\ w_s(z_{i+1}) \\ \theta_s(z_{i+1}) \end{pmatrix} = \boldsymbol{N}_i^T(z) \cdot \boldsymbol{w}_i, \qquad z \in [z_i, z_{i+1}]$$
(8.29)

with the Hermite basis functions on $\hat{z} \in [0,h_i]$ according to:

$$N_{1}(\hat{z}) = \frac{1}{h_{i}^{3}} \left(2\hat{z}^{3} - 3h_{i}\hat{z}^{2} + h_{i}^{3} \right)$$

$$N_{2}(\hat{z}) = \frac{1}{h_{i}^{3}} \left(h_{i}\hat{z}^{3} - 2h_{i}^{2}\hat{z}^{2} + h_{i}^{3}\hat{z} \right)$$

$$N_{3}(\hat{z}) = \frac{1}{h_{i}^{3}} \left(-2\hat{z}^{3} + 3h_{i}\hat{z}^{2} \right)$$

$$N_{4}(\hat{z}) = \frac{1}{h_{i}^{3}} \left(h_{i}\hat{z}^{3} - h_{i}^{2}\hat{z}^{2} \right).$$
(8.30)

 N_1 to N_4 are illustrated in Fig. 8.2. Approximating w(z,t) in (4.20) and testing with the functions $N_j(z)$, in a Galerkin scheme yields on element *i*:

$$[\mathbf{M}]_{i} \ddot{\mathbf{w}}_{i}(t) + [\mathbf{C}]_{i} \dot{\mathbf{w}}_{i}(t) + [\mathbf{K}]_{i} \mathbf{w}_{i}(t) = \mathbf{f}_{i} + \mathbf{p}_{i}.$$
(8.31)

Here, $(\dot{\cdot})$ and $(\ddot{\cdot})$ denote the first and second temporal derivatives. K is the *stiffness matrix*

$$[\mathbf{K}]_{i} = \int_{0}^{h_{i}} EI - \frac{\partial^{2}}{\partial z^{2}} \mathbf{N}_{i}^{T} \frac{\partial^{2}}{\partial z^{2}} \mathbf{N}_{i} \, \mathrm{d}\hat{z} = \frac{E_{i}I_{i}}{h_{i}^{3}} \begin{pmatrix} 12 & 6h_{i} & -12 & 6h_{i} \\ 6h_{i} & 4h_{i}^{2} & -6h_{i} & 2h_{i}^{2} \\ -12 & -6h_{i} & 12 & -6h_{i} \\ 6h_{i} & 2h_{i}^{2} & -6h_{i} & 4h_{i}^{2} \end{pmatrix},$$
(8.32)

 $[\boldsymbol{p}]_i$ the load vector

$$[\mathbf{p}]_i = \int_0^{h_i} p \mathbf{N}_i \,\mathrm{d}\hat{z} \tag{8.33}$$

$$=h_i p_i \begin{pmatrix} 1/2 \\ h_i/12 \\ 1/2 \\ -h_i/12 \end{pmatrix},$$
(8.34)

and f_i the force vector

$$\boldsymbol{f}_{i} = (f_{i}, m_{i}, f_{i+1}, m_{i+1})^{T}, \qquad (8.35)$$

with the nodal forces and moments depicted in Fig. 8.1.

The matrices K, M and the load vector p given above are valid whenever E, I, $p \neq f(z)$ for $z \in [z_i, z_{i+1}]$, and therefore in case of a uniform cross section within the finite element. f_i contains forces and moments acting on the nodes of the finite elements (see Fig. 8.1). If no additional forces are applied to the structure, this vector is in balance with neighboring elements and vanishes.

Global system matrices are assembled by iterating over the finite elements and adding up the local contributions of $[M]_i$, $[K]_i$ and $[p]_i$. Degrees of freedom can interact with multiple segments, which allows to model segmented beams, made out of different materials, such as the one illustrated in Fig. 8.3. Moreover, realistic support boundary conditions can be modeled by introducing force terms acting at the global degrees of freedom of the FEM approximation.

Support Model

The beam is attached to the stages by the means of an aluminum holder with brass clamps, as it is illustrated in Fig. 4.20. To account for the structure's elasticity and structural damping, the support is modeled by two elastic dampers as illustrated in Fig. 4.21. This support model is applied in both, the xz and yz plane, with different damping and stiffness parameters. Whereas the support's stiffness is estimated by attaching known weights to different positions along the beam, the damping coefficients can be chosen to match a measured frequency response after exciting the structure with an impulse hammer. Considering that the support is attached at position z_i , and that z_i is a FEM node such that the displacement $w(z_i)$ is given by the global degree of freedom $[w]_n = w(z_i)$, the deformation is accompanied by a repelling force:

$$F(z_i) = -k(w(z_i, t) - a(t)),$$
(8.36)

where k is the supports elasticity, and a(t) is the support motion. Similarly, an elastic bending moment is modeled, by means of the support condition

$$m(z_i) = -r\theta(z_i, t). \tag{8.37}$$

A support damping is introduced by means of the force term

$$F(z_i) = -d(\dot{w}(z_i, t) - \dot{a}(t)).$$
(8.38)

The support forces and moments are assembled into the vector f. The global equation system is then given by

$$\boldsymbol{M}\ddot{\boldsymbol{w}}(t) + \boldsymbol{C}\dot{\boldsymbol{w}}(t) + \boldsymbol{K}\boldsymbol{w}(t) = \boldsymbol{p} + \boldsymbol{f}.$$
(8.39)



Figure 8.3: Numerical model of mapper arm with three parts. (i) Aluminium tube, (ii) Polyoxymethylene (POM) joint (iii) carbon fiber tube. At the tip, an additional fixation (POM) for the Hall probe measuring head is mounted.

The right hand side can be rewritten according to

$$\boldsymbol{f} = -\boldsymbol{K}_s \boldsymbol{w}(t) - \boldsymbol{C}_s \dot{\boldsymbol{w}}(t) + \boldsymbol{k}(t) + \dot{\boldsymbol{c}}(t). \tag{8.40}$$

The matrices K_s and C_s and the vectors k and c encode the elasticity and damping of the support according to (8.36) to (8.38).

$$[\mathbf{K}_s]_{n,n} = \begin{cases} k_n & \text{if } n & \text{is support displacement,} \\ r_n & \text{if } n & \text{is support rotation,} \\ 0 & \text{else,} \end{cases}$$
$$[\mathbf{C}_s]_{n,n} = \begin{cases} d_n & \text{if } n & \text{is support displacement,} \\ 0 & \text{else,} \end{cases}$$

The vectors $\boldsymbol{k}(t)$ and $\dot{\boldsymbol{c}}(t)$ are given by:

$$[\mathbf{k}(t)]_n = k_n a(t)$$
 if *n* is support displacement, 0 else,
 $[\dot{\mathbf{c}}(t)]_n = d_n \dot{a}(t)$ if *n* is support displacement, 0 else.

(8.41)

Finally the governing system of equations is found to be

$$M\ddot{w}(t) + (C + C_s)\dot{w}(t) + (K + K_s)w(t) = q + k(t) + \dot{c}(t).$$
 (8.42)

8.6 The Kálmán gain

The Sherman-Morrison-Woodbury formula reads [93] [94]

$$(UCV + A)^{-1} = A^{-1} - A^{-1}U (C^{-1} + VA^{-1}U)^{-1} VA,$$
(8.43)

for the matrices $A \in \mathbb{R}^{N \times N}$, $U \in \mathbb{R}^{N \times M}$, $C \in \mathbb{R}^{M \times M}$ and $V \in \mathbb{R}^{M \times N}$.

Applying this formula to the posterior covariance matrix in 5.23 gives

$$(\boldsymbol{H}^{T}\boldsymbol{R}^{-1}\boldsymbol{H} + \boldsymbol{Q}^{-1})^{-1} = \boldsymbol{Q} - \boldsymbol{Q}\boldsymbol{H}^{T} (\boldsymbol{R} + \boldsymbol{H}\boldsymbol{Q}\boldsymbol{H}^{T})^{-1} \boldsymbol{H}\boldsymbol{Q}.$$

$$= (\boldsymbol{I}_{M} - \boldsymbol{K}\boldsymbol{H}) \boldsymbol{Q},$$

$$(8.44)$$

where it was set $\delta = 1$ to simplify the notations. The Kálmán gain K is defined as

$$\boldsymbol{K} := \boldsymbol{Q}\boldsymbol{H}^T \left(\boldsymbol{R} + \boldsymbol{H}\boldsymbol{Q}\boldsymbol{H}^T \right)^{-1}.$$
(8.45)

The posterior mean is therefore given by

$$m = \left(Q - QH^{T} \left(R + HQH^{T}\right)^{-1} HQ\right) \left(H^{T}R^{-1}y + Q^{-1}x_{0}\right)$$

$$= x_{0} + QHR^{-1}y - K \left(HQH^{T}R^{-1}y - Hx_{0}\right),$$

$$= x_{0} + QH \left(R + HQH^{T}\right)^{-1} \left(R + HQH^{T}\right) R^{-1}y - K \left(HQH^{T}R^{-1}y - Hx_{0}\right),$$

$$= x_{0} + K \left(R + HQH^{T}\right) R^{-1}y - K \left(HQH^{T}R^{-1}y - Hx_{0}\right),$$

$$= x_{0} + K \left(y - Hx_{0}\right).$$
(8.46)

8.7 Enforcing gauged formulations using matrix-free CG iterations

It is well known that conjugate gradient solvers converge to a solution even if $H^T R^{-1} H$ is positive semi-definite, provided that the right-hand-side is strictly contained in the range of the matrix. This is intrinsically the case when working with potential sources, as any function $x + cI_{N\times 1}$, for $c \in \mathbb{R}$ and $I_{N\times 1} \in \mathbb{R}^{N\times 1}$, yields the same observation. However, it is possible to enforce a gauge condition for all samples x_k arithmetically, manipulating the products Hx and H^Ty . This procedure is described in the following.

As it was shown in section 3.3.7, it is possible to compute the matrix vector product $H\nu$ on the reduced vector $x_r = (x_2, ..., x_N) \in \mathbb{R}^{N-1}$ according to

$$\boldsymbol{y} = (\boldsymbol{H}_{\mathrm{r}} + \boldsymbol{G})\boldsymbol{x}_{\mathrm{r}},\tag{8.47}$$

with the reduced H matrix as well as the gauge matrix G according to (3.55). The transposed matrix vector product $u = (H_r + G)^T y$ is given by

$$\boldsymbol{u} = (\boldsymbol{H}_{\mathbf{r}}^{T} + \boldsymbol{G}^{T})\boldsymbol{y} = \begin{pmatrix} H_{1,2} & \dots & H_{M,2} \\ \vdots & \ddots & \vdots \\ H_{1,N} & \dots & H_{M,N} \end{pmatrix} \boldsymbol{y} - \frac{1}{a_{1}} \begin{pmatrix} H_{1,1}a_{2} & \dots & H_{M,1}a_{2} \\ \vdots & \ddots & \vdots \\ H_{1,1}a_{N} & \dots & H_{M,1}a_{N} \end{pmatrix} \boldsymbol{y}.$$
 (8.48)

For the second product it holds

$$-\frac{1}{a_{1}}\begin{pmatrix}H_{1,1}a_{2}&\dots&H_{M,1}a_{2}\\\vdots&\ddots&\vdots\\H_{1,1}a_{N}&\dots&H_{M,1}a_{N}\end{pmatrix}\boldsymbol{y} = -\frac{1}{a_{1}}\begin{pmatrix}a_{2}(H_{1,1},\dots,H_{1,M})^{T}\boldsymbol{y}\\\vdots\\a_{N}(H_{1,1},\dots,H_{1,M})^{T}\boldsymbol{y}\end{pmatrix} = -\frac{[\boldsymbol{H}]_{:,1}^{T}\boldsymbol{y}}{a_{1}}\begin{pmatrix}a_{2}\\\vdots\\a_{N}\end{pmatrix},\quad(8.49)$$

where $[\boldsymbol{H}]_{:,1} = (H_{1,1}, ..., H_{1,M})^T$ denotes the first column of \boldsymbol{H} .

Computing the same product using the full H matrix one finds

$$\boldsymbol{u}^{*} = \begin{pmatrix} u_{1}^{*} \\ \vdots \\ u_{N}^{*} \end{pmatrix} = \boldsymbol{H}^{T} \boldsymbol{y} = \begin{pmatrix} H_{1,1} & \dots & H_{M,1} \\ \vdots & \ddots & \vdots \\ H_{1,N} & \dots & H_{M,N} \end{pmatrix} \boldsymbol{y}.$$
(8.50)

Comparing the columns n = 2 to N of this result to u in (8.48), one obtains

$$\boldsymbol{u} = \begin{pmatrix} u_2^* \\ \vdots \\ u_N^* \end{pmatrix} - \frac{[\boldsymbol{H}]_{:,1}^T \boldsymbol{y}}{a_1} \begin{pmatrix} a_2 \\ \vdots \\ a_N \end{pmatrix}.$$
(8.51)

This equation is of advantage, in cases where H is available in compressed form only, for instance when using the MLFMM. Here, it is not possible to impose a gauge condition by manipulating the matrix. Instead, the vector u^* is computed using the full H matrix. The result is then corrected according to (8.51), using only the first column $[H]_{:,1}$, as well as the vectors y and a. In this way, it can be guaranteed that the same gauge condition is enforced for all samples x_k . The column $[H]_{:,1}$ needs to be computed once and can be stored in memory together with the compressed matrix.

List of acronyms

3D	three dimensional
BEM	boundary element method
BEMBEL	boundary element method based engineering library
BFF	Bessel-Fourier-Fourier
CAD	computer aided design
CCT	canted cosine theta
CMM	coordinate measuring machine
ELENA	extra low energy antiproton ring
FCC-ee	future circular electron collider
FEM	finite element method
FEMM	finite element method magnetics
NURBS	non-uniform rational basis spline
GaAs	gallium arsenide
GR	generation recombination
IGA	iso-gemometric analysis
L2L	local to local
LS	least squares
M2L	moment to local
M2M	moment to moment
MAP	maximum a-posteriori
MCMC	Markov chain Monte-Carlo
MLFMM	multilevel fast multipole method
NbTi	niobium titanium
NMR	nuclear magnetic resonance
PCB	printed circuit board
PHE	planar Hall effect
RMS	root mean square
RTO	randomize then optimize

List of symbols

Particle beam dynamics

Symbol	Unit	Description
\boldsymbol{z}	mixed	particle state vector
$oldsymbol{F}$	Ν	force vector
q	m	coordinate vector
$m{p}^{ ext{mech}}$	${ m kg}{ m m}{ m s}^{-1}$	momentum vector
p	$ m kgms^{-1}$	canonical momentum vector
L	J	Lagrangian
H	J	Hamiltonian

Linear theory of elasticity

Symbol	Unit	Description
w	m	deformation field
D	m, rad	covariance matrix of mechanical perturbations
$\varphi_x, \varphi_y, \varphi_z$	rad	beam rotations around x, y and z axes
E	${ m N}{ m m}^{-2}$	elastic modulus
M	${ m kg}{ m m}^{-1}$	distributed mass
Ι	m ⁴	second moment of area
p	${ m N}{ m m}^{-1}$	distributed load
μ		mass proportional Rayleigh damping coefficient
λ		stiffness proportional Rayleigh damping coefficient
a	m	support condition

Maxwell's equations

Symbol	Unit ¹	Description
B	Т	magnetic flux density
H	$\mathrm{A}\mathrm{m}^{-1}$	magnetic field strength
$oldsymbol{E}$	${ m V}{ m m}^{-1}$	electric field strength
J	$\mathrm{A}\mathrm{m}^{-2}$	current density
\boldsymbol{A}	${ m Vsm^{-1}}$	magnetic vector potential
\boldsymbol{n}		outward directed unit vector
s	$\mathrm{A}\mathrm{m}^{-1}$	surface current density
$oldsymbol{s}_h$	$\mathrm{A}\mathrm{m}^{-1}$	approximated surface current density
ν	p.d.	state vector of the magnetic field
ν	p.d.	boundary data, mostly by means of a stream function
$ u_h$	А	approximated stream function
u	А	Dirichlet data
g	$\mathrm{A}\mathrm{m}^{-1}$	Neumann data
$\phi_{\rm m}$	А	magnetic scalar potential
U	V	voltage
$U_{\rm ind}$	V	induced voltage
$U_{\rm PHE}$	V	planar Hall voltage
\tilde{V}	А	single layer potential
\tilde{W}	А	double layer potential
μ_0	$V s A^{-1} m^{-1}$	vacuum permeability

 $^1\mathrm{The}$ abbreviation p.d. is used for units which are problem dependent.

Probability theory

Symbol Unit¹

p.d.	prior covariance matrix
V, V s	measurement covariance matrix
V	data matrix
V	data matrix
p.d.	prior ensemble
p.d.	posterior ensemble
p.d.	centered prior ensemble
p.d.	prior ensemble covariance matrix
p.d.	sampled state vector from the posterior
	regularization parameter
	number of samples i.e. ensemble size
	p.d. V, V s V p.d. p.d. p.d. p.d. p.d.

Description

 $^1\mathrm{The}$ abbreviation p.d. is used for units which are problem dependent.
Magnetic measurements

Symbol	Unit	Description
y	V, V s	measurement data
$oldsymbol{y}_{ ext{det}}$	V, V s	deterministic part of y
$ ilde{oldsymbol{y}}$	V, V s	predicted measurement
H	V, V s	observation operator
\widetilde{H}	V, V s	perturbed observation operator
$\partial oldsymbol{H}$	V, V s	mechanical perturbation matrix
d	m, rad	mechanical state vector
r_s	m	position of the 3D mapper measured by the linear encoders
$m{n}_x, m{n}_y, m{n}_z, m{n}_{ m H}$		sensor orientation vectors
R_y	V^2	sensor noise covariance matrix
$\ddot{R_d}$	V^2	mechanical noise covariance matrix
θ	m, rad	sensor parameters
$oldsymbol{U}_0$	V	vector of offset voltages
\boldsymbol{v}	${ m ms^{-1}}$	velocity vector
M		number of measurements
s	V	sensitivity function
s_{H}	$V A^{-1} T^{-1}$	linear sensitivity
I_{H}	А	Hall current
U_0	V	offset voltage
h_M	m^{-1}	measurement resolution
$v_{ m N}$	${ m ms^{-1}}$	nominal velocity
y	V	measurement signal
μ	V	signal mean
w_T		windowing function
y_T	V	windowed signal
Y_T	Vs	Fourier transformation of a windowed signal
S_{yy}	$V^2 Hz^{-1}$	power spectral density
R_{yy}	V^2	auto-covariance function
r_{yy}	V^2	auto-correlation function
$c_{l,m}$	VT^{-l}	coefficient for the 3D Hall probe calibration
I_{cal}	А	calibration magnet current
I_{B_y}	Τm	field integral along a reference trajectory

Mathematical functions

Symbol Description

P_l^n	associated Legendre polynomials of degree l and order n
Y_l^n	spherical harmonic function of degree l and order n
\tilde{Y}_{l}^{m}	definition of the spherical harmonic function of degree l and order m , according to [66]
$arphi_k^{\mathrm{D}}$	basis function $\in \mathcal{S}_u$

 \mathbb{R}^3

Mathematical notations

Symbol Description

j	imaginary unit
\mathbb{Z}	set of all integers
\mathbb{R}	set of real numbers
\mathbb{R}^n	<i>n</i> -dimensional real space
\mathbb{C}	set of complex numbers
	unit square
\mathbb{C}^n	<i>n</i> -dimensional complex space
C^k	set of k-times continuously differential functions
$\operatorname{Re}\{x\}$	real part of a complex number x
$\operatorname{Im}\{x\}$	imaginary part of a complex number x
Ω	compact (closed and bounded) domain of interest $\subset \mathbb{R}^2$ or \subset
$\partial \Omega$	boundary of Ω
Δ	Laplace operator
\mathcal{V}	function space for the potential function
\mathcal{V}_{u}	function space for the Dirichlet data
\mathcal{V}_g	function space for the Neumann data
\mathcal{S}_{u}	\mathcal{V}_u conforming approximation space
grad	gradient of a vector field
div	divergence of a vector field
curl	curl of a vector field
$\operatorname{curl}_{\partial\Omega}$	vectorial surface curl
$oldsymbol{\gamma}_l$	surface parameterization
h	mesh parameter

List of publications and scientific presentations

Publications in scientific journals

Journal	Title	Year	Reference
International Journal of Modern Physics A	Challenges in extracting pseudo-multipoles from magnetic measurements	2019	[109]
IEEE Transactions on Magnetics	Boundary-Element Methods for Field Reconstruc- tion in Accelerator Magnets	2020	[5]
Nuclear Instruments and Methods in Physics Research Section A	Local field reconstruction from rotating coil mea- surements in particle accelerator magnets	2021	[10]

Conference proceedings reports and poster sessions

Conference	Title	Year	Reference
22nd International Conference on the Computation of Electromagnetic Fields (COMPUMAG 2019)	Boundary-Element Methods for Field Reconstruc- tion in Accelerator Magnets	2019	[110]
12th International Particle Accelera- tor Conference (IPAC2021)	Magnetic Measurements at Warm of the First FCC- ee Final Focus Quadrupole Prototype	2021	[111]

Scientific presentations

Event	Title	Year	Reference
Workshop on Advances in Electro- magnetic Research (KWT 2018)	Boundary Element Methods for Post-Processing of Magnetic Measurement Data	2018	[112]
Workshop on Advances in Electro- magnetic Research (KWT 2019)	Solving the Inverse Problem to Extract Boundary Data from Translating Coil Measurements	2019	[113]
24th IMEKO TC4 International Symposium	Distance Calibration of Large PCB Induction-Coil Arrays in Active Mode	2020	[114]
The 13th International Conference on Scientific Computing in Electrical Engineering (SCEE)	Boundary-Element Methods for Field Reconstruc- tion in Accelerator Magnets	2020	[115]
TE-MSC Seminar	Computation of Electromagnetic Boundary Data from Magnetic Measurements in Accelerator Mag- nets	2020	[116]
Workshop on Advances in Electro- magnetic Research (KWT 2020)	Efficient 3D mapping in accelerator magnets	2020	[117]
Workshop on Advances in Electro- magnetic Research (KWT 2021)	Three dimensional field reconstruction in strongly curved magnets from magnetic measurement data	2021	[118]

Code availability

Some of the codes which have been implemented in the scope of this research are available in three github repositories under the link https://github.com/MelvinLie. In the following the repositories are listed and short descriptions about the implementations are given.

Absolute position and orientation problem

This repository contains python tools for the solution of the absolute position and orientation problem using a linearization and MCMC-RTO. It includes all the functionality to compute the discrete observation operator, as well as its derivatives, based on the solid harmonic expansion.

Scripts	Description
run_fiducialization.py	Implementation of the MCMC-RTO sampler and comparison to the lin- earization used in section 6.1.

Euler-Bernoulli beam

This repository contains python tools for the finite element approximation of the Euler-Bernoulli beam. It was used to compute the transfer functions of the mapper arm in section 4.2.

Scripts	Description
example transfer function.py	Computation of a transfer function as it was used in section 4.2.

BEMM

This repository contains a modification of the BEMBEL C++ library for the post-processing of magnetic measurement data.

Scripts	Description
example_MLFMM.cpp	Implementation of the multilevel fast multipole method used in section 3.3.10.
example_initialization.cpp	Implementation of the initialization step used in section 6.2.1.
example_ensemble_Kalman_filter.cpp	Implementation of the ensemble Kálmán filter used in sec- tion 6.2.2.
example_gibbs_sampling.cpp	Implementation of the Gibbs sampler used in section 6.3.

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