CHEMNITZ SYMPOSIUM ON INVERSE PROBLEMS 2023

on tour in Würzburg

November 08-10, 2023

Annual meeting of the German-Speaking Inverse Problems Society (GIP)

Book of Abstracts

Scientific Committee:
Alfio Borzì (Würzburg)
Claudia Schillings (Berlin)
Thomas Schuster (Saarbrücken)
Frank Werner (Würzburg)

Local Organization Team:
Petra Markert-Autsch
Frank Werner

https://www.mathematik.uni-wuerzburg.de/csip/

The Chemnitz Symposium on Inverse Problems in its present form was initiated by Bernd Hofmann in 2002 and has taken place annually since then, both in Chemnitz and various 'on tour' locations around the world. The Symposium is also traditionally an occasion for young researchers to present their work to the community. Since 2019 it also serves as the annual meeting of the German-Speaking Inverse Problems Society (GIP).

CONTENTS

1 ORGANIZATION

INVITED SPEAKERS

Christina Brandt, University of Hamburg
Andreas Hauptmann, University of Oulu, Finland
Tim Jahn, University of Bonn
Aretha Teckentrup, University of Edinburgh, UK

VENUE

The symposium takes place in the heart of Würzburg, more precisely in the Juliusspital Tagungszentrum Zehntscheune. You can access the grounds via Klinikstraße and Juliuspromenade, but access by car is only possible via the parking garage in Koellikerstraße. All talks will take place in the 1st floor.

WIFI ACCESS

WiFi is available at the conference site via the guest WLAN of Juliusspital:

SSID:	gaeste
password:	Gae$teWLAN!3056

FOOD AND BEVERAGES

Coffee breaks as well as soft drinks are included in the conference fee. Lunch is not included but there are certain cafes and restaurants in Würzburg close to the symposium site, including the Mensa Röntgenring.

SOCIAL PROGRAM

There is an ice breaker session on the evening of Wednesday, November 8th, where sandwiches and soft drinks are available. Afterwards, there will be a guided winery tour through the cellar of the Juliusspital, including a wine tasting.

2 SCHEDULE

Day 1 (Wednesday, November 8th)

8.00	-	8.50	Registration
8.50	-	9.00	Opening
9.00	-	9.50	Andreas Hauptmann
9.50	-	10.20	William Rundell
10.20	-	10.50	Coffee break
10.50	-	11.20	Jannik Rönsch
11.20	-	11.50	Tram Nguyen
11.50	-	12.20	Annalena Albicker
12.20	-	14.00	Lunch break
14.00	-	14.30	Sarah Eberle-Blick
14.30	-	15.00	Alfio Borzì
15.00	-	15.30	Luis Ammann
15.30	-	16.00	Coffee break
16.00	-	16.30	Michael Quellmalz
16.30	-	17.00	Kristina Meth
17.00	-	17.30	Simon Hackl
17.30	-	19.00	Ice breaker session
19.00	-	21.00	Guided winery tour (with tasting)

Day 2 (Thursday, November 9th)

9.00	-	9.50	Aretha Teckentrup
9.50	-	10.20	Vesa Kaarnioja
10.20	-	10.50	Coffee break
10.50	-	11.40	Tim Jahn
11.40	-	12.10	Marcello Carioni
12.10	-	12.40	Dehan Chen
12.40	-	14.00	Lunch break
14.00	-	14.30	Alfred K. Louis
14.30	-	15.00	Otmar Scherzer
15.00	-	15.30	Barbara Kaltenbacher
15.30	-	16.00	Peter Mathé
16.00	-	16.30	Coffee break
16.30	-	17.00	Sergei Pereverzyev
17.00	-	17.30	Yu Deng
19.00	-	21.00	General Assembly of the GIP (Oswald-Külpe-Hörsaal)

Day 3 (Friday, November 10th)

9.00	-	9.50	Christina Brandt
9.50	-	10.20	Oleh Melnyk
10.20	-	10.50	Coffee break
10.50	-	11.20	Lukas Weissinger
11.20	-	11.50	Christian Aarset
11.50	-	12.20	Kathrin Hellmuth
12.20	-	14.00	Lunch break
14.00	-	14.30	Fabio Frommer
14.30	-	15.00	Phuoc Truong Huynh
15.00	-	15.15	Closing

3 ABSTRACTS

DAY 1 (WEDNESDAY, NOVEMBER 8TH)

Learned reconstruction methods and convergent regularization: linear plug-and-play denoiser

Andreas Hauptmann (University of Oulu)

The question if a reconstruction algorithm provides a convergent regularization has been long studied in inverse problems, as it provides more than just the knowledge that a solution can be computed at a certain noise level. It tells us that stable solutions exist for all noise realizations and even more importantly that in the limit case, when noise vanishes, we obtain a solution of the underlying operator equation. In other words, we can guarantee mathematically that obtained solutions are indeed solutions to the inverse problem. This is in contrast to the majority of novel data-driven approaches where we may only guarantee that obtained solutions are minimizers of the empirical loss, given suitable training data. Consequently, the concept of convergent data-driven reconstructions has gained considerable interest very recently. In this talk we shortly give an overview of learned reconstruction methods with and without convergence guarantees and then continue to discuss the popular framework of plug-and-play (PnP) denoising, which uses of the shelf denoisers in an iterative framework. We will specifically consider linear denoisers and propose a novel spectral filtering technique to control the strength of regularization arising from the denoiser. This allows us to show that PnP with linear denoisers does provide indeed a convergent regularization scheme.

Recovering coefficients in nonlinear wave equations

William Rundell (Texas A&M University)

The main equation considered is the Westervelt model for ultrasound. There are several important coefficients in the model that have physical and, in particular, imaging significance. We will show that it is possible to recover these from measurement data and explore the level of ill-conditioning inherent in the process.

Geometric regularization in three-dimensional inverse obstacle scattering

Jannik Rönsch (Georg-August-Universität Göttingen)

We study the classical inverse problem to determine the shape of a three-dimensional scattering obstacle from measurements of scattered waves or their far-field patterns. Previous research on this subject has mostly assumed the object to be star-shaped and imposed a Sobolev penalty on the radial function or has defined the penalty term in some other ad-hoc manner which is not invariant under coordinate transformations. For the case of curves in $\mathbb{R}^2$, Julian Eckardt suggests in his PhD thesis to use the bending energy as regularization functional and proposes Tikhonov regularization and regularized Newton methods on a shape manifold. The case of surfaces in $\mathbb{R}^2$ is considerably more demanding. First, a suitable space (manifold) of shapes is not obvious. The second problem is to find a stabilizing functional for generalized Tikhonov regularization which on the one hand should be bending-sensitive and on the other hand prevent the surface from self-intersections during the reconstruction. The tangent-point energy is a parametrization-invariant and repulsive surface energy that is constructed as the double integral over a power of the tangent point radius with respect to two points on the surface, i.e. the smallest radius of a sphere being tangent to the first point and intersecting the other. The finiteness of this energy also provides $C^{1,\alpha}$ Hölder regularity of the surfaces. Using this energy as the stabilizing functional, we choose general surfaces of Sobolev-Slobodeckij regularity, which are naturally connected to this energy. The proposed approach works for surfaces of arbitrary (known) topology. In numerical examples we demonstrate that the flexibility of our approach in handling rather general shapes.

Bi-level iterative regularization for inverse problems in nonlinear PDEs

Tram Nguyen (Max Planck Institute for Solar System Research, Göttingen)

We investigate the ill-posed inverse problem of recovering unknown spatially dependent parameters in nonlinear evolution PDEs from linear measurements. We propose a bi-level Landweber scheme, where the upper-level parameter reconstruction embeds a lower-level state approximation. This can be seen as combining the classical reduced setting and the newer all-at-once setting, allowing us to, respectively, utilize well-posedness of the parameter-to-state map, and to bypass having to solve nonlinear PDEs. Using this, we derive stopping rules for lower- and upper-level iterations and convergence of the bi-level method. We discuss application to parameter identification for the Landau-Lifshitz-Gilbert equation in magnetic particle imaging.

Monotonicity in inverse scattering for Maxwell's equations

Annalena Albicker (Karlsruhe Institute of Technology)

We consider an inverse scattering problem for time-harmonic Maxwell's equations in unbounded free space. The goal is to recover the position and shape of scattering objects by means of far field observations of the scattered electromagnetic waves. The media are supposed to be penetrable, non-magnetic and non-absorbing but the electric permittivity may be inhomogeneous inside the scattering objects. First, we establish monotonicity relations for the eigenvalues of the far field operator which maps superpositions of plane wave incident fields to the far field patterns of the corresponding scattered waves. In addition, we discuss the existence of localized vector wave functions that have arbitrarily large energy in some prescribed region whereas at the same time having arbitrarily small energy in some other prescribed region. Combining the monotonicity principle and the localized vector wave functions leads to rigorous characterizations of the support of the scattering objects. Finally, we present shape reconstruction algorithms and give numerical examples to illustrate the reconstruction procedure.

The monotonicity method for the time-harmonic elastic wave equation

Sarah Eberle-Blick (Goethe University Frankfurt)

We consider the problem of reconstructing inhomogeneities in an isotropic elastic body using time-harmonic waves and solve the corresponding inverse problem of linear elasticity. Here, we extend the monotonicity method for inclusion detection and show how to detect and reconstruct inhomogeneities. More specifically, we give an insight into this method, which is based on the monotonicity properites of the Neumann-to-Dirichlet operator with respect to the Lamé parameters and the density as well as the techniques of localized potentials. Finally, we present some first numerical results for the time-harmonic case.

A new approach to high contrast and resolution reconstruction in quantitative photoacoustic tomography

Alfio Borzì (Julius-Maximilians-Universität Würzburg)

A new approach for the reconstruction of optical diffusion and absorption coefficients in quantitative photoacoustic tomography (QPAT) is presented. This approach is based on a Tikhonov-type functional with a regularization term promoting sparsity of the absorption coefficient and a prior involving a Kubelka-Munk absorption-diffusion relation that allows to obtain superior reconstructions. The reconstruction problem is formulated as the minimization of this functional subject to the differential constraint given by a photon-propagation model. This problem is solved in the framework of the Pontryagin maximum principle. Results of numerical experiments are presented that demonstrate the ability of the proposed framework to obtain reconstructions of the optical coefficients with high contrast and resolution for different objects. This is joint work with Anwesa Dey and Souvik Roy. This work was partially supported by the BMBF Project iDeLIVER.

Full Waveform Inversion via Optimal Control

Luis Ammann (Universität Duisburg-Essen)

Full-waveform inversion (FWI) is a recent technique in seismic tomography to reconstruct physical parameters sampled by waves. Compared with other methods relying only on partial waveform information such as travel times or phase velocities, FWI exploits the entire wave- form content. In this talk, we discuss an optimal control method for acoustic FWI. The aim is to reconstruct the speed wave parameter entering the hyperbolic PDE model in the coefficient of the second-order time derivative of the acoustic pressure. For the given optimization problem, we present necessary first-order optimality conditions based on adjoint techniques where the adjoint state has only low regularity properties. This is particularly favorable since then no Sobolev smoothing effect occurs in the optimal solution. Further, under specific regularity and compatibility assumptions, we present second-order sufficient optimality conditions and discuss the essential ideas of the non-standard proof.

Sliced optimal transport on the sphere

Michael Quellmalz (Technische Universität Berlin)

Sliced optimal transport reduces optimal transport on multi-dimensional domains to transport on the line. More precisely, sliced optimal transport is the concatenation of the well-known Radon transform and the cumulative density transform, which analytically yields the solutions of the reduced transport problems. Inspired by this concept, we propose two adaptions for optimal transport on the 2-sphere. Firstly, as counterpart to the Radon transform, we introduce the vertical slice transform, which integrates along all circles orthogonal to a given direction. Secondly, we introduce a semicircle transform, which integrates along all half great circles with an appropriate weight function. Both transforms are generalized to arbitrary measures on the sphere. While the vertical slice transform can be combined with optimal transport on the interval and leads to a sliced Wasserstein distance restricted to even probability measures, the semicircle transform is related to optimal transport on the circle and results in a different sliced Wasserstein distance for arbitrary probability measures. The applicability of both novel sliced optimal transport concepts on the sphere is demonstrated by proof-of-concept examples dealing with the interpolation and classification of spherical probability measures. The numerical implementation relies on the singular value decompositions of both transforms and fast Fourier techniques. For the inversion with respect to probability measures, we propose the minimization of an entropy-regularized Kullback–Leibler divergence, which can be numerically realized using a primal-dual proximal splitting algorithm.

L^1-data fitting for Inverse Problems with subexponentially-tailed data

Kristina Meth (Julius-Maximilians-Universität Würzburg)

Outgoing from the papers by Hohage & Werner (SINUM 2014) and König, Hohage & Werner (SINUM 2016), we analyze variational regularization with L^1 data fidelity. We investigate discrete models with regular data in the sense that the tails decay subexponentially. Therefore, error bounds are provided and numerical simulations of convergence rates are presented.

Ultrasound Aberration Correction for Layered Media

Simon Hackl (Johann Radon Institute for Computational and Applied Mathematics, Linz)

Ultrasound diagnostics is an important, non-invasive examination method in modern medicine and the reconstruction of an observed object is an inverse problem of current scientific interest. With focused ultrasound waves, one can look deep inside the human body without causing harm. However, a crucial assumption in the theory of focused ultrasound imaging is that the sound speed in the observed medium is constant, which is not the case in most clinical applications. It is possible to incorporate a space dependent sound speed into the model, but at the cost of significantly higher complexity, which makes this approach not applicable in clinical practice. In this talk, we present a mathematical framework for modeling the aberrations caused by a layered medium. First, we propose a new focusing algorithm that takes into account the layered structure of observed media, which has to be known. By calculating travel time differences from the individual transducer elements to the focus point and shifting the output accordingly, focusing is achieved. In the second part of the talk, a parameter reconstruction algorithm that calculates the a-priori unknown sound speeds and layer thicknesses of the medium necessary for focusing, is introduced. Reconstruction is achieved by measuring the travel times that the soundwaves take along different paths. Sound speeds as well as thickness of the layers are then obtained from the variations of these measured travel times. The effectiveness of both proposed methods is demonstrated through numerical simulation using the k-Wave toolbox for Matlab. This work is a collaboration with S. Hubmer (RICAM) and R. Ramlau (JKU).

DAY 2 (WEDNESDAY, NOVEMBER 9TH)

Deep Gaussian processes: theory and applications

Aretha Teckentrup (University of Edinburgh)

Deep Gaussian processes have proved remarkably successful as a tool for various statistical inference tasks. This success relates in part to the flexibility of these processes and their ability to capture complex, non-stationary behaviors. In this talk, we will introduce the general framework of deep Gaussian processes, in which many examples can be constructed, and demonstrate their superiority in inverse problems including computational imaging and regression. We will discuss recent algorithmic developments for efficient sampling, as well as recent theoretical results which give crucial insight into the behavior of the methodology.

Quasi-Monte Carlo for Bayesian Optimal Experimental Design Problems Governed by PDEs

Vesa Kaarnioja (Freie Universität Berlin)

The goal in Bayesian optimal experimental design (OED) is to maximize the expected information gain for the reconstruction of unknown quantities given a limited budget for collecting measurement data. This leads to optimization problems, where the objective functional involves nested high-dimensional integrals. To this end, we derive efficient rank-1 lattice quasi-Monte Carlo (QMC) cubature rules to reduce the computational burden in Bayesian OED problems governed by PDEs. Numerical experiments are presented to assess the theoretical results.

Discretization-adaptive regularization of inverse problems

Tim Jahn (Universität Bonn)

We consider linear inverse problems under white (non-Gaussian) noise. For the solution we have to discretize the problem, and we consider a sequence of discretization schemes with increasing complexity. Starting from the coarsest discretization, we sequentially solve the discretized problems with standard methods (e.g., spectral cut-off and Landweber method together with the (heuristic) discrepancy principle). We additionally take into account the dynamics of the regularization parameters to decide when to stop the procedure adaptively. We discuss the accuracy and the computational costs of the final approximation.

Sparse optimization of inverse problems regularized with infimal-convolution-type functionals

Marcello Carioni (University of Twente)

The infimal convolution of functionals is a convex-preserving operation that have been used to construct regularizers for inverse problems by optimally combining features of two or more functionals. In this talk, we first introduce a variational framework capable to construct regularizers through the repeated application of infimal convolution operations and linear operators. Then, we propose a variant of the previous approach that is based on the infimal convolution of a continuously parametrized family of functionals. Finally, we illustrate how to design optimization methods able to take advantage of the sparsity in the parameter space.

Tikhonov regularization: convergence rates with applications to inverse PDEs problems

Dehan Chen (University of Duisburg-Essen)

This talk presents some developments of Tikhonov regularizations in Hilbert and Banach settings. We first propose and analyze variational source conditions (VSC) for the Tikhonov regularization methods with Lp-penalties applied to an ill-posed operator equation in a Banach space. Our analysis is built on the celebrated Littlewood-Paley theory and the concept of (Rademacher) R-boundedness. With these two analytical principles, we validate the proposed VSC under a conditional stability estimate in terms of a dual Triebel-Lizorkin-type norm. On the other hand, we will presents the applications of VSCs in some inverse PDEs problems.

Bernd Hofmann - A German Pioneer of Ill-Posed Problems

Alfred K. Louis (Universität des Saarlandes)

Laudatio on the occasion of Bernd Hofmann’s 70th birthday.

Gauss-Newton method for solving linear inverse problems with neural network coders

Otmar Scherzer (Universität Wien)

Neural networks functions are supposed to be able to encode the desired solution of an inverse problem very efficiently. We therefore consider the problem of solving linear inverse problems with neural network coders. A Gauss-Newton method is suitable for solving encoded linear inverse problems, which is supported by a local convergence result. Some numerical experiments are presented to support the theoretical findings.

Convergence guarantees for variational and Newton type methods via range invariance

Barbara Kaltenbacher (University of Klagenfurt)

A proof of convergence of iterative methods for parameter identification problems in partial differential equations PDEs from boundary measurements, as relevant, e.g., in tomographic applications, has been a long-standing open problem due to the fact that the convergence analysis of these methods can only be carried out under restrictions on the nonlinearity of the forward operator that could not be verified for such PDE coefficient identification problems so far. Likewise, although at a first glance not burdened with such restrictive assumptions on the forward operator, Tikhonov regularization requires the computation of a global minimizer of a functional whose (local) convexity can only be verified under similar restrictions on the nonlinearity. The goal of this talk is to revisit one of these conditions – range invariance of the linearized forward operator – and show that an extension of variability of the searched for parameter often allows for its verification. Since this counteracts unique identifiability of the parameter, we restore the original restricted dependency of the parameter by a proper penalization within the reconstruction method. We concretize the abstract convergence analysis in a framework typical of parameter identification in PDEs in a reduced and an all-at-once setting. This is further illustrated by three examples of coefficient identification from boundary observations in elliptic and parabolic PDEs. If time permits, we will also dwell on convergence rates under variational source conditions, a topic that has been coined by Bernd Hofmann over the last decade.

Tikhonov regularization with oversmoothing penalty: Error bounds in terms of distance functions

Peter Mathé (Weierstrass Institut für Angewandte Analysis und Stochastik, Berlin)

On the occasion of Bernd's 70th birthday I will review some of our joint contributions at the example of a most recent project.

A Strategy for identifying informative variables for the prediction from imbalanced dataset

Sergei Pereverzyev (Johann Radon Institute for Computational and Applied Mathematics, Linz)

We discuss the problem of detecting the most informative coordinates of input vectors that allow an accurate reconstruction of the corresponding outputs from previously unseen inputs. This problem appears in a wide variety of applications. In our study we are motivated by predicting neurodevelopmental outcomes of preterm neonates from the ratios of the amplitudes of the peaks of metabolite spectra provided by magnetic proton spectroscopy (MRS).

The degree of ill-posedness for some composition governed by the Cesaro operator

Yu Deng (Chemnitz University of Technology)

In this talk, we consider the singular value asymptotics of compositions of compact linear operators mapping in the Hilbert space $L^2(0,1)$. Specifically, the composition is given by the compact simple integration operator followed by the non-compact Cesaro operator possessing a non-closed range. We show that the degree of ill-posedness of that composition is two, which means that the Cesaro operator increases the degree of ill-posedness by the amount of one compared to the simple integration operator.

DAY 3 (WEDNESDAY, NOVEMBER 10TH)

Improving time dependent image reconstruction in magnetic particle imaging

Christina Brandt (Universität Hamburg)

Magnetic particle imaging (MPI) is a tracer-based medical imaging technique invented by Gleich and Weizenecker in 2005. It allows for the reconstruction of the spatial distribution of magnetic nanoparticles injected into the blood flow via exploiting their non-linear magnetization response to changing magnetic fields. MPI has the potential to be a fast imaging technique which make it interesting for applications such as blood flow imaging and instrument tracking. Therefore, one might not only be interested in the reconstruction of the particle distribution but also of the motion or flow itself. Current systems are using a field-free line (FFL) or field-free point (FFP) for spatial encoding and model based reconstruction is performed under ideal assumptions such as static particle distributions, ideal magnetic fields and lack of motion. In the case of a sequential line rotation of the FFL, the MPI data can be linked to Radon transformed particle distributions. Nevertheless, most scanners are based on the FFP excitation and measurements of the forward operator to avoid limitations of the model based approaches. However, in both cases field imperfections and motion may occur which results in artifacts in the reconstructed images. We will give on overview about different strategies in magnetic particle imaging to reduce these artifacts and show numerical reconstruction results from simulated as well as real dynamic data.

Blind Ptychography via gradient methods

Oleh Melnyk (Technische Universität Berlin)

Ptychography is an imaging technique that aims to reconstruct the object of interest from a set of diffraction patterns obtained by illuminating its small regions. When the distribution of light within the region is known, the recovery of the object from ptychographic measurements becomes a special case of the phase retrieval problem. In the other case, also known as blind ptychography, the recovery of both the object and the distribution is necessary. One of the well-known reconstruction methods for blind ptychography is extended Ptychographic Iterative Engine. Despite its popularity, there was no known analysis of its performance. Based on the fact that it is a stochastic gradient descent method, we derive its convergence guarantees if the step sizes are chosen sufficiently small. The second considered method is a generalization of the Amplitude Flow algorithm for phase retrieval, a gradient descent scheme for the minimization of the amplitude-based squared loss. By applying an alternating minimization procedure, the blind ptychography is reduced to phase retrieval subproblems, which can be solved by performing a few steps of Amplitude Flow. The resulting procedure converges to a critical point at a sublinear rate.

An inverse problems approach to pulse wave analysis in the human brain

Lukas Weissinger (Johann Radon Institute for Computational and Applied Mathematics, Linz)

Cardiac pulsations in the human brain have recently garnered interest due to their potential involvement in the pathogenesis of neurodegenerative diseases. The (pulse) wave, which describes the velocity of blood flow along an intracranial artery, consists of a forward (anterograde) and back- ward (retrograde, reflected) part, but the measurement usually consists of a superposition of these components. In this talk, we provide a mathematical framework for the inverse problem of estimating the pulse wave velocity as well as the forward and backward component of the pulse wave separately, using MRI measurements on the middle cerebral artery. Additionally, we provide an analysis of the problem, which is necessary for the application of a solution method based on an alternate direction approach. The proposed method's applicability is demonstrated through numerical experiments using simulation data. This is a joint work with S. Hubmer, R. Ramlau (RICAM) and H. Voss (Cornell University)

Optimal design for aeroacoustics with correlation data

Christian Aarset (Georg-August-Universität Göttingen)

A key problem in aeroacoustics is the inverse problem of estimating an unknown random source from correlation data sampled from surrounding sensors. We study optimal design for this and related problems, that is, we identify the sensor placement minimizing covariance of the solution to the inverse random source problem. To achieve this, we discuss the assumption of gaussianity and how to adapt this to our setting of correlation data, and demonstrate how this model can lead to sparse designs for aeroacoustic experiments.

Parameter identification for a model of mathematical biology

Kathrin Hellmuth (Julius-Maximilians-Universität Würzburg)

In mathematical biology, the motion of individuals, e.g. bacteria, in response to an external stimulus can be described by a partial differential equation for the propagation of the bacteria density. Chemotaxis is one such example, where, in the mesoscopic regime, the motion is driven by a parameter accounting for the individual velocity change. We consider the inverse parameter identification problem of determining this mesoscopic parameter from macroscopic, i.e. directionally averaged data. This introduces additional difficulty, which will be bridged by the use of time dependent interior domain data. In particular, we present results on the existence and uniqueness of the reconstruction, its macroscopic limiting behavior and the numerical inversion. This is joint work with Christian Klingenberg (Würzburg, DE), Qin Li (Madison, Wisc., USA) and Min Tang (Shanghai, China).

The Henderson Problem and the relative Entropy functional in the thermodynamic limit

Fabio Frommer (University of Mainz)

The inverse Henderson problem of statistical mechanics is the theoretical foundation for many bottom-up coarse-graining techniques for the numerical simulation of complex soft matter physics. This inverse problem concerns classical particles in continuous space which interact according to a pair potential depending on the distance of the particles. Roughly stated, it asks for the interaction potential given the equilibrium pair correlation function of the system. In 1974 Henderson proved that this potential is uniquely determined in a canonical ensemble and recently it has been argued by Rosenberger et al. that this potential minimizes a relative entropy. Here we provide a rigorous extension of these results for the thermodynamical limit and define a corresponding relative entropy density for this. We investigate further properties of this functional for suitable classes of pair potentials.

Towards optimal sensor placement for sparse inverse problems

Phuoc Truong Huynh (University of Klagenfurt)

In this talk, we study parameter identification problems from a finite number of measurements under a sparsity assumption. Since the data is contaminated by Gaussian noise, a statistical framework for its recovery is considered. It relies on two main ingredients, first, a convex but nonsmooth Tikhonov point estimator over the space of Radon measures and, second, a suitable mean-squared error based on its Hellinger-Kantorovich (H-K) distance to the ground truth. Assuming standard non-degenerate source conditions as well as applying careful linearization arguments, we derive a sharp upper bound for the H-K distance between the aforementioned ground truth and an estimator. On the one hand, this allows to derive asymptotic convergence results for the mean-squared error, which is later used as a crucial tool for sensor placement problem. Finally, we present some numerical results to illustrate our theory. This is a joint work with Konstantin Pieper and Daniel Walter.