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The adjoint method of optimal control for the acoustic monitoring of a shallow water environment

Matthias Meyer

Promoteur:
Prof. Jean-Pierre Hermand

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The adjoint method of optimal control

for the acoustic monitoring of a shallow water environment

This dissertation was discussed in a public defense held at the Université Libre de Bruxelles, Brussels, Belgium, on December 19, 2007. On this occasion, Matthias Meyer was awarded a European Doctorate in engineering sciences.

Composition of the jury:

Frans G. J. Absil
Professor, Royal Netherlands Naval College, Den Helder, The Netherlands
Member of the jury

Mark Asch
Professor, Université de Picardie Jules Verne, Amiens, France
Member of the jury

Christine De Mol
Professor, Université Libre de Bruxelles, Brussels, Belgium
Member of the jury

Frank Dubois
Professor, Université Libre de Bruxelles, Brussels, Belgium
Secretary of the jury

Jean-Pierre Hermand
Professor, Université Libre de Bruxelles, Brussels, Belgium
Thesis supervisor

Michel Verbanck
Professor, Université Libre de Bruxelles, Brussels, Belgium
President of the jury

External referees:

Volker Mellert
Professor, Carl v. Ossietzky Universität Oldenburg, Oldenburg, Germany

Dick G. Simons
Professor, Delft University of Technology, Delft, The Netherlands

Summary

Originally developed in the 1970s for the optimal control of systems governed by partial differential equations, the adjoint method has found several successful applications, e.g., in meteorology with large-scale 3D or 4D atmospheric data assimilation schemes, for carbon cycle data assimilation in biogeochemistry and climate research, or in oceanographic modelling with efficient adjoint codes of ocean general circulation models.

Despite the variety of applications in these research fields, adjoint methods have only very recently drawn attention from the ocean acoustics community. In ocean acoustic tomography and geoacoustic inversion, where the inverse problem is to recover unknown acoustic properties of the water column and the seabed from acoustic transmission data, the solution approaches are typically based on travel time inversion or standard matched-field processing in combination with metaheuristics for global optimization.

In order to complement the adjoint schemes already in use in meteorology and oceanography with an ocean acoustic component, this thesis is concerned with the development of the adjoint of a full-field acoustic propagation model for shallow water environments. In view of the increasing importance of global ocean observing systems such as the European Seas Observatory Network, the Arctic Ocean Observing System and Maritime Rapid Environmental Assessment (MREA) systems for defence and security applications, the adjoint of an ocean acoustic propagation model can become an integral part of a coupled oceanographic and acoustic data assimilation scheme in the future.

Given the acoustic pressure field measured on a vertical hydrophone array and a modelled replica field that is calculated for a specific parametrization of the environment, the developed adjoint model backpropagates the mismatch (residual) between the measured and predicted field from the receiver array towards the source. The backpropagated error field is then converted into an estimate of the exact gradient of the objective function with respect to any of the relevant physical parameters of the environment including the sound speed structure in the water column and densities, compressional/shear sound speeds, and attenuations of the sediment layers and the sub-bottom halfspace. The resulting environmental gradients can be used in combination with gradient descent methods such as conjugate gradient, or Newton-type optimization methods to locate the error surface minimum via a series of iterations. This is particularly attractive for monitoring slowly varying environments, where the gradient information can be used to track the environmental parameters continuously over

time and space.

In shallow water environments, where an accurate treatment of the acoustic interaction with the bottom is of outmost importance for a correct prediction of the sound field, and field data are often recorded on non-fully populated arrays, there is an inherent need for observation over a broad range of frequencies. For this purpose, the adjoint-based approach is generalized for a joint optimization across multiple frequencies and special attention is devoted to regularization methods that incorporate additional information about the desired solution in order to stabilize the optimization process.

Starting with an analytical formulation of the multiple-frequency adjoint approach for parabolic-type approximations, the adjoint method is progressively tailored in the course of the thesis towards a realistic wide-angle parabolic equation propagation model and the treatment of fully nonlocal impedance boundary conditions. A semi-automatic adjoint generation via modular graph approach enables the direct inversion of both the geoacoustic parameters embedded in the discrete nonlocal boundary condition and the acoustic properties of the water column. Several case studies based on environmental data obtained in Mediterranean shallow waters are used in the thesis to assess the capabilities of adjoint-based acoustic inversion for different experimental configurations, particularly taking into account sparse array geometries and partial depth coverage of the water column. The numerical implementation of the approach is found to be robust, provided that the initial guesses are not too far from the desired solution, and accurate, and converges in a small number of iterations. During the multi-frequency optimization process, the evolution of the control parameters displays a parameter hierarchy which clearly relates to the relative sensitivity of the acoustic pressure field to the physical parameters.

The actual validation of the adjoint-generated environmental gradients for acoustic monitoring of a shallow water environment is based on acoustic and oceanographic data from the Yellow Shark '94 and the MREA '07 sea trials, conducted in the Tyrrhenian Sea, south of the island of Elba.

Starting from an initial guess of the environmental control parameters, either obtained through acoustic inversion with global search or supported by archival in-situ data, the adjoint method provides an efficient means to adjust local changes with a couple of iterations and monitor the environmental properties over a series of inversions. In this thesis the adjoint-based approach is used, e.g., to fine-tune up to eight bottom geoacoustic parameters of a shallow water environment and to track the time-varying sound speed profile in the water column. In the same way the approach can be extended to track the spatial water column and bottom structure using a mobile network of sparse arrays.

Work is currently being focused on the inclusion of the adjoint approach into hybrid optimization schemes or ensemble predictions, as an essential building block in a combined ocean acoustic data assimilation framework and the subsequent validation of the acoustic monitoring capabilities with long-term experimental data in shallow water environments.

Statement

This thesis describes original research carried out by the author. This work has not been previously submitted to the Université Libre de Bruxelles or to any other university for the award of any degree. Nevertheless, some chapters of this thesis are partially based on articles that, during his doctoral studies, the author, together with a number of co–workers, has published or submitted for publication in the scientific literature.

The description of the state of the art and the bibliographic review in Chapter 2 is partly based on

M. Meyer and J.-P. Hermand. Backpropagation techniques in ocean acoustic inversion: Time reversal, retrogation and adjoint modelling - A review. In A. Caiti, R. Chapman, J.-P. Hermand, and S. Jesus, editors, *Acoustic Sensing Techniques for the Shallow Water Environment: Inversion Methods and Experiments*, pages 29–47, Dordrecht, 2006. Springer.

The theoretical background for the application of the multiple frequency adjoint-based inversion algorithm in ocean acoustics as described in Chapter 3 is based on

M. Meyer, J.-P. Hermand, M. Asch and J.-C. Le Gac. An iterative multiple frequency adjoint-based inversion algorithm for parabolic-type approximations in ocean acoustics. *Inverse Problems in Science and Engineering*, 14(3):245–65, 2006.

The analytical equivalent applying a closed-form spectral integral approach (Neumann-to-Dirichlet map) as a nonlocal boundary was first presented in

J. S. Papadakis, E. T. Flouri, M. Meyer, and J.-P. Hermand. Analytic derivation of adjoint nonlocal boundary conditions for stratified oceanic environments in parabolic approximation. *Journal of the Acoustical Society of America*, 119(5):3216: 1aSPb5, 2006. Providence, Rhode Island, 5–9 June 2006.

The extension to the wide-angle parabolic equation and the introduction of regularization schemes for the adjoint-based inversion in Chapter 4 are contained in

M. Meyer and J.-P. Hermand. Optimal nonlocal boundary control of the wide-angle parabolic equation for inversion of a waveguide acoustic field. *Journal of the Acoustical Society of America*, 117(5):2937–48, 2005.

The semi-automatic adjoint generation via modular graph approach to enable direct inversion of the geoacooustic parameters embedded in the discrete NLBC as described in Chapter 5 is based on

J.-P. Hermand, M. Meyer, M. Asch, and M. Berrada. Adjoint-based acoustic inversion for the physical characterization of a shallow water environment. *Journal of the Acoustical Society of America*, 119(6):3860–71, 2006.

J.-P. Hermand, M. Meyer, M. Asch, M. Berrada, C. Sorror, S. Thiria, F. Badran, and Y. Stéphan. Semi-automatic adjoint PE modelling for ocean acoustic inversion. In D. Lee, A. Tolstoy, E.C. Shang, and Y.C. Teng, editors, *Theoretical and Computational Acoustics*, pages 53–64. World Scientific Publishing, 2006.

Application of the adjoint approach to acoustic particle velocity modelling was first presented in

M. Meyer, J.-P. Hermand, and K. B. Smith. On the use of acoustic particle velocity fields in adjoint-based inversion. *Journal of the Acoustical Society of America*, 120(5):3356: 5aUW8, 2006. Honolulu, Hawaii, 28 November–2 December 2006.

A unified description of the concept of variational inversion in satellite ocean colour imagery and geoacoustic characterization of the seafloor is further contained in

F. Badran, M. Berrada, J. Brajard, M. Crépon, C. Sorror, S. Thiria, J.-P. Hermand, M. Meyer, L. Perichon, and M. Asch. Inversion of satellite ocean colour imagery and geoacoustic characterization of seabed properties: Variational data inversion using a semi-automatic adjoint approach. *Journal of Marine Systems*, 69(1–2): 126–136, 2007, (in print).

Implementation of the adjoint approach with a stochastic local search strategy, validation with experimental acoustic data and the dynamic sound speed estimation in a time-varying environment as described in Chapter 6 is partly based on

M. Meyer, J.-P. Hermand, M. Berrada and M. Asch. Remote sensing of Tyrrhenian shallow waters using the adjoint of a full-field acoustic propagation model. *Journal of Marine Systems*, 2007, (manuscript submitted).

A list of conference talks held in the course of the thesis and papers published in conference proceedings or as technical reports can be found in the bibliography section on the website of the Environmental Hydroacoustics Laboratory[1]. This thesis, all articles and reports that have been produced in the course of the PhD were typeset by the author using LaTeX 2_ε, in combination with REVTeX[2] and $\mathcal{AMS}$-TeX[3] respectively. Illustrations were generated with the Matlab™ package and other free programs under the GNU General Public License, such as XFig, Gimp and Inkscape.

[1] `http://www.ulb.ac.be/polytech/ehl/web/publications.html`

[2] REVTeX is provided by the the American Physical Society for preparation of manuscript submissions to APS journals

[3] $\mathcal{AMS}$-TeX is the the American Mathematical Society's TeX macro system

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Contents

1 Introduction

The opening chapter of this thesis is intended to position the work in the wider context of current Maritime Rapid Environmental Assessment (MREA), Global Monitoring for Environment and Security (GMES) and more general ocean observation based services (Sec. 1.1–1.2). It is used to briefly introduce inverse problems in ocean acoustics and to familiarize with classical Matched Field Processing (MFP) and the respective global search algorithms, without going into detail (Sec. 1.3). The different subjects will be picked up again and addressed in more detail in the remainder of the thesis. Following a first general description of the adjoint method of optimal control, Sec. 1.4 presents a short historical overview of the adjoint approach in different research fields and gives an outlook on ongoing work and possible applications in ocean acoustics. Section 1.5 concludes the introductory chapter with a detailed outline of the thesis structure.

1.1 Remote sensing of the ocean

Acoustic remote sensing of the ocean interior together with satellite altimetry and scatterometry and as a third observational component freely drifting profilers or tracer sampling systems are today providing complementary basin scale observations of the ocean. While satellite remote sensing can provide high quality information of sea surface and coastal topography, wind stress, ocean colour and chlorophyll concentrations, etc., acoustic techniques provide the most effective means for remote sensing of the ocean interior, for monitoring sea floor processes, and for probing the structure beneath the sea floor. In some cases complementary data from different sensor platforms can be directly merged, as is done e.g., with single- or multi-beam acoustic bathymetry and satellite altimetry data. Similarly, high resolution profilers, such as acoustic Doppler current profilers (ADCPs), and tracer injection and sampling systems can both provide independent estimates of turbulent and diffusive mixing processes in the ocean.

Ocean observation based services nowadays constitute an essential part in many different applications of high socio-economic value, e.g., coastal zone monitoring, electronic charting and sea floor mapping, fisheries, aquaculture and sea bed habitat assessment, monitoring of marine mammals and marine surveillance for ship detection, tracking and oil-spill detection. Other examples include climate change research, oceanographic and meteorological services, search and rescue, off-shore oil and gas exploration, sea ice mapping and monitoring, estimation of geotechnical properties of sea bed materials and investigation of natural geohazards in marine sediments. The world-wide network of hydroacoustic stations as part of the International Monitoring System (IMS) of the United Nations Comprehensive Test Ban Treaty (CTBT) of nuclear weapons, the Global Ocean Observing System (GOOS) under the aegis of the UNESCO, the European Seas Observatory Network (ESONET) or the large-scale acoustic monitoring of the ocean climate in the ATOC project are just a few examples of international ocean observatory networks.

1.2 Environmental assessment

In the general context of Global Monitoring for Environment and Security (GMES) an integrated multi-disciplinary ocean observation system forms the basis for the Maritime Rapid Environmental Assessment (MREA) concept. With the shift of the naval oceanographic focus from deep waters to littoral (i.e., coastal) waters in the mid-1980s also the focus of Meteorology and Oceanography (MetOcean) changed and initiated an increased interest in coastal monitoring and surveillance technologies. Near-coast and inshore environments worldwide house nearly 60% of the world's population and generate approximately 25% of global primary productivity. In this context, pressure from industrial activity in the coastal cities, development of off shore resources as well as international and local shipping traffic continue to threaten the coastal shallow water environment.

Satellite remote sensing, acoustic monitoring and meteorological and oceanographic modelling represent the three essential components in the MREA scheme displayed in Fig. 1.1. Different colours are used to distinguish between high resolution satellite and acoustic data acquisition (blue), respective data processing (red) and meteorology and oceanography modelling (yellow). Freely drifting profilers, tracer sampling systems, CTD casts from previous hydrographic surveys or thermistor chain drifters, though not included as a separate observational component in Fig. 1.1, can be used as an additional input to the MetOcean models. The MetOcean models usually include atmospheric (AGCM) and ocean general circulation models (OGCM) that are coupled together possibly with other additional components such as a sea ice model. Of particular interest for MREA are the specific wind models, nested wave models or near-shore wave simulation and surf models shown in Fig. 1.1.

Acoustic data is typically recorded on sparse arrays of acoustic-oceanographic sensors that are moored to the sea floor or mounted on mobile platforms such as buoys, gliders, autonomous underwater vehicles (AUVs), or other generic robotic sensor agents (RSAs). The acoustic source can either be a controlled, active source that is deployed likewise from a mobile platform or a source of opportunity, e.g., the noise of a passing ship or ambient noise.

For the environmental assessment (light grey colouring, Fig. 1.1) all available

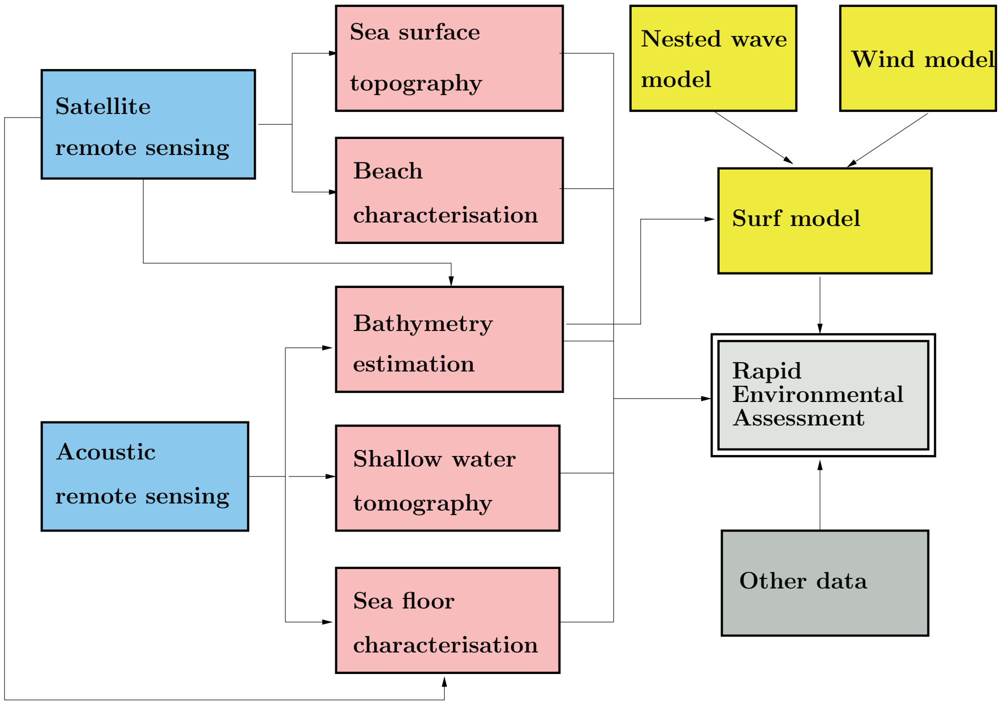

Figure 1.1: REA scheme. Different colours are used to distinguish between high resolution environmental data acquisition (blue), respective data processing (red) and MetOcean modelling (yellow).

information from satellite remote sensing, acoustic monitoring and the output of the MetOcean models is fused in a (central) database to obtain a complete picture of the environment that can then be further processed, stored and distributed via web-based and standardized product searching, retrieval and viewing tools. It can thus serve as an optimal support for the respective application under consideration.

1.3 Inverse problem in ocean acoustics

All the different forms of ocean observation services mentioned in Sec. 1.1 involve detection and measurement of environmental parameters and features in one or more spatial dimensions, observing their dynamics and forecasting their behaviour. In physical terms, the required processing (red colouring, Fig. 1.1) of the initial high resolution data in order to estimate the respective environmental properties typically poses an *inverse problem*.

By definition, most classical problems where the internal structure of a physical system is assumed to be completely prescribed are considered direct problems in the sense that the system's behaviour can be clearly predicted. Inverse problems arise quite naturally if the task consists in determining the unknown internal structure of a physical system (e.g., part of the underlying partial differential equation, its domain or its initial and/or boundary condition) from the systems

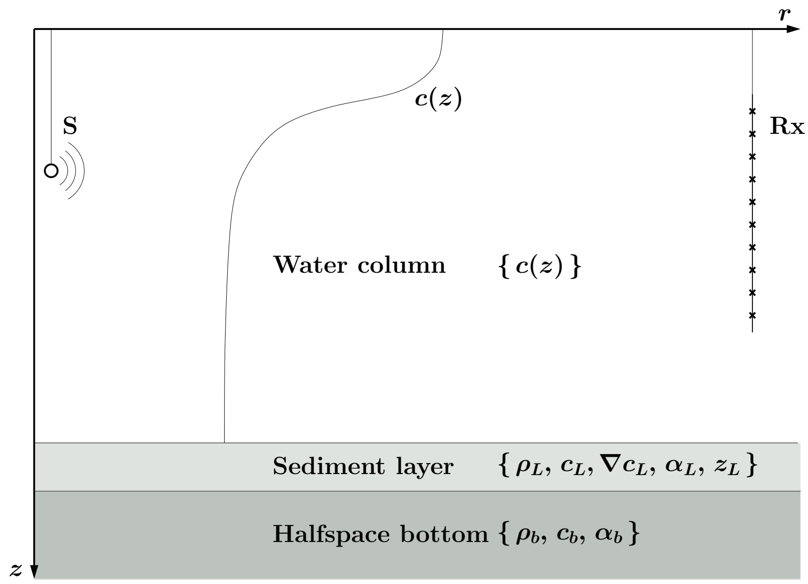

Figure 1.2: The problem in shallow water acoustic tomography and geoacoustic inversion is to recover unknown acoustic properties of the water column and the sea bed from measurable ocean and acoustic field data. 'S' and 'Rx' indicate the acoustic source and the receiver array and the indices 'L' and 'b' refer to the sediment layer and bottom halfspace, respectively.

behaviour, i.e., from available measurements. An important aspect certainly lies in the identification of a set of measurement data that are sufficient for a unique determination of one or several of the physical properties in question. Even if the direct problem is linear, the associated inverse problem is highly non-linear and most often ill-posed.

In the context of ocean acoustic tomography and geoacoustic inversion [1; 2; 3; 4; 5; 6; 7] the problem is to recover unknown acoustic properties of the water column and the seabed from measurable, mid-range ocean and acoustic field data (Fig. 1.2).

The main parameter to be estimated within the water column is the vertical sound speed profile (SSP) $c(z)$, which is in turn determined by static pressure (water depth), salinity and temperature. Relevant geoacoustic properties of the sediment layer(s) and the bottom halfspace typically include compressional and shear sound speeds c, sound speed gradient ∇c, density ρ, attenuation α and layer thickness z_L (see Fig. 1.2). Direct, *in situ* measurement of these properties tends to be highly time-consuming and cost-intensive as it requires an extensive hydrographic campaign in the area and a full seismic survey with subbottom profiler, grab sampling and coring.

By contrast, acoustic sensing techniques provide a powerful methodology for the remote estimation of these parameters typically based on matched-field inversion in combination with meta-heuristic global search algorithms. Classical matched field processing (MFP) [8] is the process of cross-correlation of a measured field with a predicted replica field in order to determine a set of input parameters that yield the highest correlation. The goal is to minimize an objective function that compares the measured acoustic pressure field with a modeled field (replica) that is calculated for a specific parametrization of the water column and the seabed. Then, the parameter set in the model space which gives the highest correlation between the replica of the field and the measured data is taken as the solution.

In MFP the parameter search itself has been principally solved by means of meta-heuristic optimization techniques [9; 10; 11; 12; 13; 14; 15]. Most of these techniques are directed Monte Carlo searches, that are based on analogies with natural optimization processes. As global optimization methods they are designed to widely search the parameter space by using a random process to iteratively update the model and repeatedly solve the forward problem. Since model updates are primarily based on random processes, global methods generally include the ability to escape from local suboptimal solutions but as a consequence they are less efficient at moving downhill, particularly near convergence and for problems involving correlated parameters. Attempts have been made to combine global optimizers such as genetic algorithms and simulated annealing with a local component in so-called hybrid inversions. The Downhill Simplex (DHS) method [16; 17] is a classical, straightforward geometric scheme that has been applied for determining a local downhill step in the objective function in order to improve or replace some of the random steps of the global optimizer [18; 19; 20].

While the DHS method provides a simple, geometric improving-neighbourhood update based on a simplex of possible solutions, numerical finite-difference calculations of the full gradient of the objective function are most often impractical, particularly for higher-dimensional problems. The computational resources required for both DHS and numerical differentiation clearly increase with the number of model parameters as both of them require repeated runs of the forward model for each point on the simplex or each possible variation in the model parameters, respectively. Gradient approximations via numerical differentiation further involve small variations in the model parameters, which may lead to stability and convergence problems.

Effective algorithms that can provide an exact gradient of the objective function are particularly attractive for monitoring slowly time-varying environments, where they can be used in combination with a gradient-based optimizer to track the environmental parameters continuously over time (or range). The concept of data assimilation (DA) in general, aims at an accurate analysis, estimation and prediction of unknown environmental properties or state variables by merging new observations into the physical model once they become available. Typically DA methods are categorized into variational methods based on optimal control theory (Sec. 1.4) and filtering-type methods based on statistical estimation theory. For the latter category, the Kalman filter (KF) [21] – or one of its more recent variants – forms the principal component. In underwater acoustics the state-space model-based processor has been introduced by Candy and Sullivan [22; 23] based on the extended KF. This approach is currently followed up at the Environmental Hydroacoustics Lab by extending it to the unscented and ensemble KF [24].

1.4 The adjoint method of optimal control

The adjoint method at the heart of variational DA provides an elegant mathematical means to calculate exact gradient information of the objective function to be optimized. Therefore, the adjoint system and its boundary conditions are derived from the system of partial differential equations (PDEs) governing the direct problem. A single adjoint model run is used to backpropagate the mismatch (residual) between the measured and modeled acoustic field from the receiver array towards the source. The backpropagated error field is then converted into an estimate of the exact gradient of the objective function with respect to any of the the environmental model parameters, regardless of the dimensionality of the problem. The environmental gradients can be used in combination with gradient descent methods such as conjugate gradient, or Newton-type large-scale optimization methods to locate the error surface minimum via a series of iterations. In contrast to meta-heuristic optimization techniques the inversion procedure itself is directly controlled by the waveguide physics.

Originally, the exact mathematical formulation for the optimal control of systems governed by partial differential equations was introduced by J. L. Lions in 1971 [25] and in a later sequel 1988 [26]. His publication coincided with Jazwinski's, Sage and Melsa's work on filtering and estimation theory [27; 28] and it can be seen in the succession of other seminal works on optimal control theory by Gelfand, Feldbaum, Luenberger and Kirk [29; 30; 31; 32].

There are many industrial and scientific applications that apply non-invasive investigations of physical properties by means of wave phenomena, such as non-destructive testing of materials, imaging and source identification in biomedical engineering, crack localization, remote sensing of earth resources and environmental quality or as an optimal design method. The wave phenomena used in probing the inhomogeneous media are typically of electromagnetic, elastodynamic or acoustic nature.

In this context, the potential of adjoint-based methods has been recently demonstrated for data assimilation, model tuning, and sensitivity analysis in several fields, e.g., in fluid dynamics [33; 34; 35; 36], inverse scattering and elasticity imaging [37; 38; 39; 40; 41], geophysical inversion and seismology [42; 43; 44; 45; 46; 47], meteorology [48; 49; 50], electromagnetic tomography [51; 52] and oceanography [53; 54; 55; 56]. Related problems of adjoint-based exact and approximate boundary controllability are addressed in [57; 58; 59] for the heat equation and systems associated to a Laplace operator on a regular bounded domain in general. In computational fluid dynamics the adjoint approach is successfully being applied as an optimal design method, particularly for aeronautical applications, e.g., [60; 61; 62; 63]. Other applications are inverse problems in the field of electromagnetic induction and resistivity, particle transport and thermal diffusion. Good comparative studies of the different adjoint approaches can be found in [64; 65; 66; 67] dealing respectively with 1D and 2D resistivity problems, inverse scattering problems and shape reconstruction. Recently also second order adjoint techniques have been introduced for the analysis of ill-posed problems in computational fluid dynamics [68; 69] or in meteorology [70].

Despite the variety of applications in other research fields, adjoint methods have only very recently drawn attention from the ocean acoustic community. This might be partly due to the fact that the theoretical derivation of the adjoint of an ocean acoustic propagation model is a challenging task that becomes more and more difficult with the level of complexity in the propagation model. In the optimization with meta-heuristic search methods the propagation model can be any one of the major propagation codes available and little to no insight in the model itself is required for the optimization. By contrast, the derivation of the adjoint PDE and its boundary conditions necessitates complete understanding of the underlying direct model regarding both the theoretical formulation and the numerical implementation. Since many of the available standard propagation codes have grown steadily over the last decades with extensions and fixes to handle many different special cases, the derivation of the corresponding adjoint can be a very cumbersome task. Starting from scratch with a self-written propagation code is in many aspects more straightforward for the adjoint derivation, but it requires much more effort to achieve a level of complexity in the modelling that is sufficient to match realistic ocean-acoustic conditions.

It is in this context that the present thesis aims at investigating the use of the adjoint method of optimal control for the acoustic sensing of shallow water environments. Possible applications of the adjoint method in ocean acoustics are manifold, for the acoustic monitoring of slowly time-varying environments (tracking of environmental parameters), for the inclusion in hybrid optimization schemes or ensemble predictions or as an essential building block in an acoustic data assimilation framework.

Returning to the MREA concept and MetOcean modelling in particular (see Fig. 1.1), the effective implementation of the adjoint method for atmospheric data assimilation has been pioneered by Talagrand, Courtier and Le Dimet [71; 72]. Adjoint models are today being applied in operational weather forecast in large-scale 3D or 4D variational data assimilation schemes, e.g., at Météo-France or the European Centre for Medium-Range Weather Forecasts (ECMWF).

In oceanography the introduction of variational data assimilation is even more recent, see, e.g., the seminal works by Thacker and Long or Sheinbaum and Anderson [73; 74]. Adjoint versions of OGCMs have been constructed, such as the Adjoint MIT Ocean General Circulation Model [75] and most recently the variational assimilaton of Lagrangian data into an OGCM at basin scale has been proposed in [56].

In this context, the combination of an adjoint acoustic propagation model with an adjoint ocean circulation model would provide an excellent platform to unify the two approaches in the future in order to assimilate acoustic data into MetOcean models and vice versa.

1.5 Organizational structure of the thesis

The remainder of the thesis proceeds as follows. Chapter 2 presents a selective bibliographic overview of backpropagation techniques in ocean acoustics which is completed by a general introduction to the main principles of adjoint modelling and a detailed description of the resulting adjoint-based iterative inversion for ocean acoustic purposes. The backpropagation methods covered in the review range from Parvulescu's time reversal to Tappert's original acoustic retrogation but include also the classical MFP approach and a short overview of the most common optimization algorithms via global, local and hybrid search. In the introduction to the adjoint method, special attention is devoted to the classification of adjoint approaches into discrete, continuous and (semi-)automatic adjoint generation. This classification is particularly useful to distinguish the three different adjoint approaches reported in the chapters 3, 4 and 5.

Chapter 3 formally introduces the theoretical background for the application of a multiple frequency adjoint-based inversion algorithm for a shallow water waveguide. The approach presented in this chapter is based on a Standard Parabolic Equation (SPE) model with local boundary conditions (LBCs) at the water-sediment interface and illustrates the inherent need for a joint inversion across multiple frequencies especially for the case of non-fully populated hydrophone arrays. The local impedance boundary condition is used as a range-dependent control parameter of the complex pressure field in the waveguide but the formalism is also extended for tomography purposes where the sound speed profile in the water column plays the role of the control parameter. The chapter is intended as an analytic reference solution for the extension of the approach to higher order PE approximations and more sophisticated boundary conditions in the following chapters. It further proposes an analytical second order adjoint formulation and concludes with a discussion of local *vs.* nonlocal boundary conditions.

Chapter 4 addresses the extension of the approach to the wide angle parabolic equation (WAPE) model with a discrete non local boundary condition NLBC and introduces regularization schemes for the adjoint-based inversion. Following a brief overview of absorbing boundary conditions in general and a first analytical ansatz applying a closed-form spectral integral approach (Neumann-to-Dirichlet map) as a Non Local Boundary Condition (NLBC), the remainder of the chapter deals with the discrete NLBC introduced by Yevick and Thomson. A continuous adjoint approach is derived in order to retrieve generalized coefficients of the nonlocal impedance boundary. These can be used for model tuning to correctly predict the acoustic propagation without knowing the physical parameters of the environment. Such a “through-the-sensor” approach allows, e.g., to generate an effective bottom model for use in sonar signal processing algorithms.

Chapter 5 describes a semi-automatic adjoint generation via modular graph approach that enables direct inversion of the geoacoustic parameters embedded in the discrete NLBC. In this case the control variables represent physical parameters that can be used to characterize an unknown ocean environment and to construct a geoacoustic model of the material properties of the bottom. Starting from a modular graph representation of the Wide Angle Parabolic Equation (WAPE), a programming tool facilitates the generation and coding of both the tangent linear and the adjoint models. The potential of this approach is illustrated with several applications for geoacoustic inversion and ocean acoustic tomography. Additional examples combine the two applications and demonstrate the feasibility of geoacoustic inversion in the presence of an uncertain sound speed profile.

Chapter 6 discusses the application of the semi-automatic adjoint approach to the experimental acoustic data collected during the YS94 sea trial and the oceanographic data obtained in the framework of the MREA07 experiment. It covers some validation tests in order to evaluate the fidelity of the WAPE forward model for simulation of YS94 real data and discusses the choice of an adequate real data cost function. To enhance the performance of the adjoint approach, its implementation in a stochastic local search (SLS) scheme is discussed. Utilization of stochastic choice as an integral part in the so-called Iterated Local Search (ILS) process can lead to significant increases in performance and robustness. First validations of the adjoint-generated environmental gradients are shown using the adjoint ILS scheme with the YS94 experimental acoustic data. For comparison, inversion results are shown with standard metaheuristics, such as genetic algorithms and ant colony optimization. In a concluding example for ocean acoustic tomography, the temporal variability of the MREA07 SSP data set is analyzed in terms of empirical orthogonal functions and the adjoint-based approach is used to track the time-varying sound speed profile of the experimental transect.

Chapter 7 concludes the thesis with some comments and an outlook on future work and the Appendices A – C provide additional details on the finite difference PE solver for discrete NLBCs (A), the use of acoustic particle velocity fields in adjoint-based inversion (B), and uncertainty estimation via Hessian calculation (C).

7 Conclusion

In analogy to meteorological and oceanographic modelling, where adjoint schemes are used in efficient 3D or 4D variational assimilation schemes, this thesis proposes a multiple frequency adjoint approach for a full-field acoustic propagation model that is physically realistic for solving a class of inverse problems in shallow water acoustics.

The developed approach combines the advantages of exact nonlocal boundary conditions for the wide-angle parabolic equation (WAPE) model with the concept of adjoint-based control, and allows for the inversion of both the geoacoustic parameters of the seabed and the acoustic properties of the water column.

In contrast to metaheuristic search algorithms that are mainly based on directed Monte Carlo searches, the adjoint-based optimization is directly controlled by the underlying waveguide physics. The adjoint method provides an exact representation of the gradient of the matched field cost function that depends implicitly on the control parameters to be optimized. The use of these adjoint-generated environmental gradients is particularly attractive for monitoring slowly varying environments, where the gradient information can be used in combination with a Newton-type optimizer to track the environmental parameters continuously over time.

Since regularization schemes are particularly important to enhance the performance of full-field acoustic inversion, special attention has been devoted to the application of penalization methods to the adjoint optimization formalism. Regularization incorporates additional information about the desired solution in order to stabilize the optimization process and identify useful solutions, a feature that is of particular importance for inversion of field data sampled on a sparsely populated vertical receiver array.

Numerical simulations with acoustic observations that are synthesized with environmental data collected in Mediterranean shallow waters, and validations using ocean acoustic data from the Yellow Shark '94 and the Maritime Rapid Environmental Assessment '07 sea trials have been presented that demonstrate the feasibility of the adjoint approach for ocean acoustic tomography and geoacoustic inversion purposes for different source receiver configurations.

Especially when moving from synthesized acoustic observations to experimental data, the accuracy of the acoustic propagation model in matching realistic ocean acoustic conditions becomes an important issue. Particularly at high SNR the main error contribution in the optimization process is due to inadequate forward modeling, i.e., model deficiencies such as neglected physics, etc. For this purpose the WAPE forward modeling capabilities for the YS real-data simulation, have been carefully verified with a coupled normal mode reference model. The fidelity of the forward model is in fact an important issue, since variational approaches such as the adjoint method use the exact model dynamics as a constraint for the optimization (strong constraint assumption).

For application to real data, a multi-frequency maximum likelihood cost function has been implemented that is based on the spatial correlation matrix of the acoustic observations on the vertical receiver array. This formulation has been used earlier in standard matched field processing where it was shown to provide a good maximum likelihood estimate for the case of unknown, frequency-dependent noise.

To further enhance the performance of the adjoint approach in the case of real acoustic data, and to optimize the exploitation of the search space in the vicinity around the local minimum, the implementation of an iterated local search (ILS) scheme has been discussed. The general concept of ILS or so-called large-step Markov chains provide a comprehensive framework for the combination of the adjoint method as a local search, with a stochastic strategy, e.g., using the Metropolis criterion as in simulated annealing. For comparison, the optimization results of the adjoint ILS scheme have been validated with standard metaheuristics, such as genetic algorithms and ant colony optimization.

As a concluding demonstration of dynamic estimation in a time-varying environment, the temporal variability of the MREA07 sound speed profiles has been analyzed in terms of empirical orthogonal functions, and the adjoint-generated gradients are used to track the time-varying sound speed profile of the experimental transect.

In this context, work is currently ongoing in order to extend the acoustic propagation model to take into account range-dependent features of the waveguide, such as the spatial variability of the sound speed profile over the transect of acoustic transmission. As shown for the boundary control of the parabolic equation, the adjoint method can be used to retrieve range-dependent control parameters. In fact, the analytical adjoint formulation for the acoustic tomography problem, allows for an adjustment of the continuous two-dimensional sound speed field $c(r, z)$.

Another interesting aspect related to the dynamic estimation in the framework of the MREA07 experiment arises in the comparison of the variational approach that uses the adjoint method for the updating of the profiles, with sequential methods on the basis of a filtering-type approach. The latter is of stochastic nature and can be regarded complementary to the variational approach. The original state-space model-based processor that had been introduced in underwater acoustics in the 1990s based on the extended Kalman filter, is currently being extended for the unscented and ensemble Kalman filter, respectively. Both the variational and the filtering approaches will be implemented as key components of the coupled ocean acoustic data assimilation scheme for shallow water environments currently under development.

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Acronyms

ABC Absorbing Boundary Condition

ACO Ant Colony Optimization

AD Automatic (or Algorithmic) Differentiation

ADCP Acoustic Doppler Current Profiler

ADIFOR Automatic Differentiation of FORTRAN

ADOL-C Automatic Differentiation of Algorithms Written in C/C++

AGCM Atmospheric General Circulation Model

APC Active Phase Conjugation

ASSA Adaptive Simplex Simulated Annealing

ATOC Acoustic Thermometry of the Ocean Climate

AUV Autonomous Underwater Vehicle

BC Boundary Condition

BFGS Broyden-Fletcher-Goldfarb-Shanno method

BW-CT Backward-Centered Euler scheme

CDE Convection Diffusion Equation

CN Crank Nicolson scheme

CTBT Comprehensive Test Ban Treaty

CTD Conductivity, Temperature and Depth

CW Continuous-Wave

DA Data Assimilation

DE Differential Evolution

DHS Downhill Simplex Method

DPSS Discrete Prolate Spheroidal Sequences

DTBC Discrete Transparent Boundary Condition

ECMWF European Centre for Medium-Range Weather Forecasts

EOF Empirical Orthogonal Function

ESONET European Seas Observatory Network

FAF Focused Acoustic Field experiments

FD Finite Differences

FSA Fast Simulated Annealing

GA Genetic Algorithms

GI Geoacoustic Inversion

GIBC Generalized Impedance Boundary Condition

GMES Global Monitoring for Environment and Security

GOOS Global Ocean Observing System

ILS Iterated Local Search

IMS International Monitoring System

KF Kalman Filter

LBC Local Boundary Conditon

LSMC Large-Step Markov Chains

MBMF Model Based Matched Filter

MESS Matched Equivalent-Space Signal

MetOcean Meteorology and Oceanography

MFP Matched Field Processing

MIMO Multiple Input Multiple Output

MREA Maritime Rapid Environmental Assessment

MREA07 Maritime Rapid Environmental Assessment '07 sea trial

MVDR Minimum Variance Distortionless Response Processor

NCOM Navy Coastal Ocean Model

NLBC Non Local Boundary Condition

NtD Neumann-to-Dirichlet map

OAT Ocean Acoustic Tomography

ODE Ordinary Differential Equation

OGCM Ocean General Circulation Model

OUFP Optimum Uncertainty Field Processor

PCA Principal Component Analysis

PDE Partial Differential Equation

PE Parabolic Equation

PML Perfectly Matched Layer

PPC Passive Phase Conjugation

PSD Power Spectral Density

REA Rapid Environmental Assessment

RII Randomized Iterative Improvement

RSA Robotic Sensor Agent

RW Random Walk

SA Simulated Annealing

SLS Stochastic Local Search

SNR Signal-to-Noise Ratio

SPE Standard Parabolic Equation

SSF Split-Step Fourier Algorithm

SSP Sound Speed Profile

SVD Singular Value Decomposition

SWAT Shallow Water Acoustic Tomography

TAF Transformation of Algorithms in FORTRAN

TAMC Tangent Linear and Adjoint Model Compiler

TBC Transparent Boundary Condition

TL Transmission Loss

TLM Tangent Linear Model

TR Time Reversal

TS TABU Search

VRA Vertical Receiver Array

UNESCO United Nations Educational, Scientific and Cultural Organization

VNS Variable Neighbourhood Search

WAPE Wide Angle Parabolic Equation

XBT Expendable Bathythermograph

YS94 Yellow Shark '94 sea trial