

Linköping Studies in Science and Technology. Dissertations.  
No. 1300

# Numerical Solution of Ill-posed Cauchy Problems for Parabolic Equations

Zohreh Ranjbar



**INSTITUTE OF TECHNOLOGY**  
**LINKÖPINGS UNIVERSITET**

Department of Mathematics  
Scientific Computing  
Linköping 2010

Cover page courtesy of Dennis Netzell

Linköping Studies in Science and Technology. Dissertations.  
No. 1300

**Numerical Solution of Ill-posed Cauchy Problems for Parabolic Equations**

Zohreh Ranjbar

*zohreh.ranjbar@liu.se*

*www.mai.liu.se*

*Department of Mathematics*

*Scientific Computing*

*Linköping University*

*SE-581 83 Linköping*

*Sweden*

ISBN 978-91-7393-443-5

ISSN 0345-7524

Copyright © 2010 Zohreh Ranjbar

Printed by LiU-Tryck, Linköping, Sweden 2010

*To Atra, Mohsen and my parents*



# Abstract

Ranjbar, Z. (2010). Numerical Solution of Ill-posed Cauchy Problems for Parabolic Equations. Doctoral dissertation. ISBN 978-91-7393-443-5. ISSN 0345-7524.

Ill-posed mathematical problem occur in many interesting scientific and engineering applications. The solution of such a problem, if it exists, may not depend continuously on the observed data. For computing a stable approximate solution it is necessary to apply a regularization method. The purpose of this thesis is to investigate regularization approaches and develop numerical methods for solving certain ill-posed problems for parabolic partial differential equations. In thermal engineering applications one wants to determine the surface temperature of a body when the surface itself is inaccessible to measurements. This problem can be modelled by a sideways heat equation. The mathematical and numerical properties of the sideways heat equation with constant convection and diffusion coefficients is first studied. The problem is reformulated as a Volterra integral equation of the first kind with smooth kernel. The influence of the coefficients on the degree of ill-posedness are also studied. The rate of decay of the singular values of the Volterra integral operator determines the degree of ill-posedness. It is shown that the sign of the coefficient in the convection term influences the rate of decay of the singular values.

Further a sideways heat equation in cylindrical geometry is studied. The equation is a mathematical model of the temperature changes inside a thermocouple, which is used to approximate the gas temperature in a combustion chamber. The heat transfer coefficient at the surface of thermocouple is also unknown. This coefficient is approximated via a calibration experiment. Then the gas temperature in the combustion chamber is computed using the convection boundary condition. In both steps the surface temperature and heat flux are approximated using Tikhonov regularization and the method of lines.

Many existing methods for solving sideways parabolic equations are inadequate for solving multi-dimensional problems with variable coefficients. A new iterative regularization technique for solving a two-dimensional sideways parabolic equation with variable coefficients is proposed. A preconditioned Generalized Minimum Residuals Method (GMRS) is used to regularize the problem. The preconditioner is based on a semi-analytic solution formula for the corresponding problem with constant coefficients. Regularization is used in the preconditioner as well as truncating the GMRES algorithm. The computed examples indicate that the proposed PGMRES method is well suited for this problem.

In this thesis also a numerical method is presented for the solution of a Cauchy problem for a parabolic equation in multi-dimensional space, where the domain is cylindrical in one spatial direction. The formal solution is written as a hyperbolic cosine function in terms of a parabolic unbounded operator. The ill-posedness is dealt with by truncating the large eigenvalues of the operator. The approximate solution is computed by projecting onto a smaller subspace generated by the Arnoldi algorithm applied on the inverse of the operator. A well-posed parabolic problem is solved in each iteration step. Further the hyperbolic cosine is evaluated explicitly only for a small triangular matrix. Numerical examples are given to illustrate the performance of the method.



# Populärvetenskaplig sammanfattning

Inom många vetenskapliga och tekniska tillämpningar är det nödvändigt att uppskatta vissa parametrar som kännetecknar ett fysiskt system, men som är oåtkomliga för direkta mätningar. Detta problemområde, så kallade inversa problem, har blivit ett mycket aktivt och väletablerat tvärvetenskapligt forskningsområde under de senaste tre decennierna. Det täcker bl a problem från teknik, industri, medicin, liksom livs- och geovetenskaper.

Ett exempel på ett inverst problem inom värmeteknik är att man vill bestämma ytemperaturen hos ett objekt när ytan i sig är oåtkomlig för mätning. Det kan också vara så att lokalisering av en mätenhet på ytan skulle störa mätningarna så att en felaktig temperatur registreras. I sådana fall är man begränsad till interna mätningar. Detta problem kan modelleras med en värmeledningsekvation, som löses i sidled, dvs i rumsled, till skillnad från standardproblemet som löses framåt i tiden. Inversa problem är ofta illa-ställda. Lösningen till ett illa-ställt matematiskt problem, om den existerar, beror inte kontinuerligt på observerade data. Detta innebär t.ex. att små fel i uppmätta temperaturer kan leda till mycket stora fel i den beräknade lösningen. I praktiken uppstår fel i uppmätta data och det är därför nödvändigt att tillämpa en regulariseringsmetod, som gör lösningen mindre känslig för störningar i uppmätta data.

Syftet med denna avhandling är att undersöka regulariseringsstrategier och utveckla numeriska metoder för att lösa vissa illa-ställda problem för paraboliska partiella differentialekvationer. Vi studerar först påverkan av koefficienterna i värmeledningsekvationen i sidled på graden av illa-ställdhet. Vi löser också en värmeledningsekvation i sidled, där ekvationen är en matematisk modell av temperaturförändringar inuti ett termoelement, som används för att approximera gastemperaturen i en förbränningskammare.

Många metoder för att lösa paraboliska ekvationer i sidled är otillräckliga för att lösa multi-dimensionella problem med variabla koefficienter. En ny iterativ regulariserings-teknik för att lösa en två-dimensionell parabolisk ekvation i sidled med variabla koefficienter föreslås. I en iterativ metod startar man med en begynnelseapproximation, som sedan gradvis förbättras. Eftersom iterationerna för denna typ av problem först förbättrar approximationen men senare försämrar den, kan man regularisera genom att stoppa iterationer vid lämplig tidpunkt.

I denna avhandling presenteras också en numerisk metod för lösning av ett parabolisk inverst problem i ett flerdimensionellt rum, där området är cylindriskt i en rumsriktning. Den approximativa lösningen beräknas genom att projicera på ett underrum genererat av en Krylovsrumsmetod.





# Acknowledgments

Through out the long and occasionally rocky process of this thesis I have been supported by many people. It is a pleasure to convey my thanks to all of them who made this work possible.

I wish to express my sincerest gratitude to my supervisor Prof. Lars Eldén for his encouraging and stubborn guidance during this work. I am also very grateful for his most meticulous and thorough revision, professional insights and tireless generosity.

I would like to thank Dr. Fredrik Berntsson whose expertise and interesting discussions helped very much along the work. I am grateful to Prof. Dan Loyd and Elisabeth Blom at the Department of Management and Engineering, Linköping University, for helpful discussions about heat transfer problems. I am also indebted to present and former colleagues at the Department of Mathematics, particularly at the Division of Scientific Computing, for providing a good working environment and sharing experiences with me. I am grateful to Dr. Martin Ohlsson for letting me use the LaTeX layout of his thesis. I really thank the administrative staff for all their support in administering my fellowship.

I would also like to take the chance and thanks my family, my husband Mohsen for his valuable support and continuous encouragement and my parents for their unconditional love and dedication and the many years of support during my undergraduate studies that provided the foundation for this work. I deeply thank my sister Zahra and her family who supported me from the first day I came to Sweden. Thanks also to my other siblings in Iran for their love and for believing in me. I am also very grateful to my friends, my parents-in-law and other relatives who helped me during these challenging years.

*Linköping, February 25, 2010*

*Zohreh Ranjbar*



---

# Contents

<b>1</b>	<b>Introduction and Overview</b>	<b>1</b>
1	Inverse Ill-Posed Problems and Ill-Conditioning . . . . .	1
2	Cauchy Problems for Parabolic Equations . . . . .	2
2.1	Sideways Heat Equations . . . . .	2
2.2	Ill-Posedness and Singular Values . . . . .	4
3	Direct Regularization Methods . . . . .	5
3.1	Truncated Singular Value Decomposition . . . . .	5
3.2	Tikhonov Regularization . . . . .	6
3.3	Method of Lines . . . . .	6
4	Iterative Regularization Methods . . . . .	6
4.1	Classical Stationary Methods . . . . .	7
4.2	Krylov Subspace Methods . . . . .	7
5	Choice of Regularization Parameter . . . . .	8
<b>2</b>	<b>Summary of Papers</b>	<b>9</b>
	<b>Bibliography</b>	<b>11</b>
	<b>Appended Manuscripts</b>	<b>17</b>
<b>I</b>	<b>Numerical Analysis of an Ill-Posed Cauchy Problem for a Convection-Diffusion Equation</b>	<b>19</b>
1	Introduction . . . . .	22
2	Derivation of a Volterra Integral Equation . . . . .	23
2.1	The Kernel Function for Different Values of $a$ and $b$ . . . . .	28
3	Singular Value Analysis of the Volterra Equation . . . . .	28

4	Eigenvalue Analysis of the Cauchy Problem . . . . .	32
5	Numerical Experiments . . . . .	35
6	Concluding Remarks . . . . .	36
A	Appendix . . . . .	38
B	Appendix . . . . .	39
	References . . . . .	40
<b>II A Sideways Heat Equation Applied to the Measurement of the Gas Temperature in a Combustion Chamber</b>		<b>43</b>
1	Introduction . . . . .	46
2	Mathematical Modelling and Computational Procedures . . . . .	48
3	Computation of the Gas Temperature . . . . .	50
3.1	Approximating the Surface Temperature and Heat Flux . . . . .	50
3.2	Solving the Inverse Problem in the Region of Magnesium Oxide . . . . .	51
3.3	Solving the Inverse Problem in the Steel Domain . . . . .	53
3.4	Approximating the Gas Temperature . . . . .	54
4	Calibration . . . . .	54
4.1	Approximating the Surface Temperature and Heat Flux . . . . .	54
4.2	Computing $h$ . . . . .	56
5	Numerical Experiments . . . . .	56
6	Concluding remarks . . . . .	63
7	Acknowledgment . . . . .	66
A	Appendix . . . . .	66
	References . . . . .	68
<b>III A Preconditioned GMRES Method for Solving a Sideways Parabolic Equation in Two Space Dimensions</b>		<b>71</b>
1	Introduction . . . . .	74
2	Preconditioned GMRES . . . . .	76
3	The One-Dimensional Sideways Heat Equation . . . . .	77
3.1	Circulant Preconditioning . . . . .	78
3.2	1D Numerical Experiments . . . . .	81
4	The Two-Dimensional Sideways Parabolic Equation . . . . .	87
4.1	Constant Coefficients: Analysis . . . . .	87
4.2	Preconditioned GMRES for the 2D Problem . . . . .	93
4.3	Preconditioner . . . . .	94
4.4	Numerical Experiments . . . . .	95
5	Conclusions . . . . .	101
A	Appendix . . . . .	103
B	Appendix . . . . .	104
	References . . . . .	105
<b>IV Numerical Solution of a Cauchy Problem for a Parabolic Equation in Two or more Space Dimensions by the Arnoldi Method</b>		<b>109</b>
1	Introduction . . . . .	112
2	Ill-posedness and Regularization . . . . .	113

---

2.1	Regularization Based on Fourier Transform and Eigenvalue Expansion . . . . .	113
3	Arnoldi Recursion and Decomposition . . . . .	115
3.1	Implementation . . . . .	117
4	Arnoldi-Truncated Schur Factorization . . . . .	117
4.1	Accuracy of Truncated Approximation . . . . .	118
5	Arnoldi-TSVD Method . . . . .	120
6	Numerical Examples . . . . .	120
7	Summary and Future Work . . . . .	121
A	Appendix . . . . .	129
A.1	Proof of Lemma 2.1 . . . . .	129
A.2	Proof of Theorem 2.1 . . . . .	130
	References . . . . .	131



# 1

---

## Introduction and Overview

IN many scientific and engineering applications there is a need to estimate some parameters characterizing a physical system, which is inaccessible to direct measurements. This problem area, so called *inverse problems*, has become a very active, interdisciplinary and well-established research area over the past three decades. It covers problems from engineering, industry, medicine, as well as life and earth sciences. Some examples of inverse problems are computerized tomography [50], inverse scattering problems [24], inverse problems in geophysics [25]. One particular area of inverse problems is in *heat conduction* [1], where the goal is to reconstruct the values of the parameters characterizing the system from a noisy measured temperature. A classic problem of inverse heat conduction is the *backward problem*, where the initial conditions (temperature) are to be found from later measurements. Numerical solutions of this problem have been considered in [17, 61, 60, 40, 42]. Another interesting problem is Sideways Heat Equation (SHE) problem, where the unknown temperature at the boundary of the object is to be approximated based on measurements of the accessible temperature of the object. The *heat equation* is a prototype parabolic partial differential equation (PDE), used to model heat conduction in a given region over time. The aim of this thesis is to investigate the numerical solution of certain sideways parabolic PDE problems.

### 1 Inverse Ill-Posed Problems and Ill-Conditioning

Inverse problems are often *ill-posed*, as opposed to the well-posed problems introduced by Hadamard [31]. Consider the linear operator equation

$$Kf = g, \tag{1.1}$$

where  $K : \mathcal{H}_1 \rightarrow \mathcal{H}_2$  is a bounded linear operator between Hilbert spaces  $\mathcal{H}_1$  and  $\mathcal{H}_2$ .

**Definition 1.1.** The problem of solving (1.1) is called *well-posed* if:

1. Existence: a solution exists for any data  $g$  in the data space.
2. Uniqueness: the solution  $f$  is unique in the solution space.
3. Stability: the solution  $f$  depends continuously on the data  $g$ .

Conditions 1 and 2 are equivalent to saying that the operator  $K$  has a well defined inverse  $K^{-1}$  and that the range of  $K$  is all of the data space. The condition 3 is equivalent to  $K^{-1}$  being continuous or bounded. For inverse problems this stability condition is most often violated. To stabilize the solution, one needs to incorporate additional a priori information into the problem, so called *regularization*.

In many linear ill-posed problems that arise in science and engineering, instead of the exact right hand side  $g$ , only a perturbation of it,  $g_\delta = g + \delta$ , is available. When the inverse operator  $K^{-1}$  is unbounded, it means that if the solution  $f$  exists then the solution  $f_\delta = K^{-1}g_\delta$  is usually a poor approximation of  $f$ , even for very small values of  $\delta$ .

While inverse problems are often formulated in infinite dimensional spaces, limitations to a finite number of measurements, and the practical consideration of recovering only a finite number of unknown parameters leads to stating the problem in discrete form. Following [35], a problem is called *discrete ill-posed* when it is highly sensitive to high-frequency perturbations and the solution operator has very large norm.

## 2 Cauchy Problems for Parabolic Equations

A parabolic Cauchy problem (initial-boundary value problem) is a PDE that satisfies certain conditions which are given on the boundary of the domain. As a simple example of a one-dimensional ill-posed Cauchy problem for the heat equation we have,

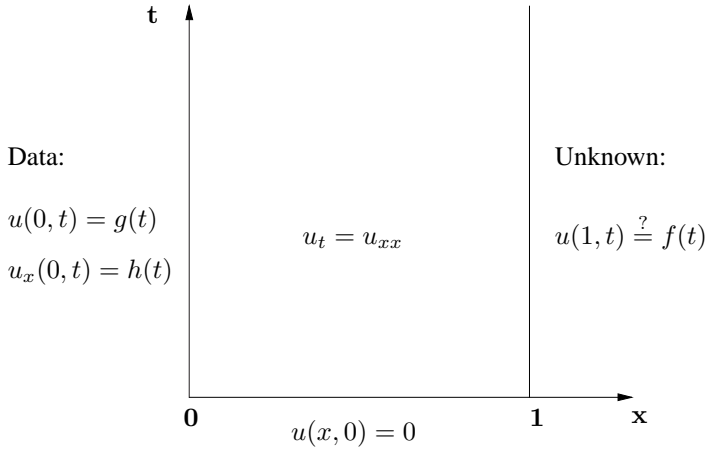
$$\begin{aligned}
 u_t &= u_{xx}, & 0 < x < 1, & \quad 0 \leq t \leq 1, \\
 u(x, 0) &= 0, & 0 \leq x \leq 1, & \\
 u(0, t) &= g(t), & 0 \leq t \leq 1, & \\
 u_x(0, t) &= h(t), & 0 \leq t \leq 1. &
 \end{aligned} \tag{1.2}$$

From the data at the left boundary we want to determine the solution at the right boundary  $u(1, t) = f(t)$ , see Figure 1.1. This is a sideways heat equation in a bounded domain. From now on we consider all the involved functions to be in  $L^2$ .

### 2.1 Sideways Heat Equations

The sideways heat equation (SHE) (1.2) is an ill-posed Cauchy problem for a parabolic equation. It is sometimes referred as the inverse heat conduction problem [1, 49]. We label it the SHE in order to distinguish it from other inverse problems for a parabolic equation [12]. In this definition the initial temperature distribution is considered known. The linearity of the differential equation implies that initial data can easily be taken equal to zero. In Paper II we consider a SHE as a simple model of the heat transfer inside a thermocouple of a suction pyrometer. The suction pyrometer [8], is used for measuring and controlling the gas temperature in a combustion chamber. The numerical experiments in this paper, with synthetic data, indicate that it is possible to organize the measurements





**Figure 1.1:** Determination of function  $f$  from the interior measurements  $g$  and  $h$ .

with the suction pyrometer in such a way that the gas temperature can be computed with sufficient accuracy. For more industrial examples modelled by SHE see [1, 5, 16, 62, 63].

Two types of problems can be formulated:

- *The quarter plane problem* is a problem in a semi-infinite region,  $x \in [0, \infty)$ , where one wants to compute  $f(t)$  at  $x = 0$  from the known data function  $g(t)$  (Dirichlet boundary condition) at  $x = l$  for  $0 < l < \infty$ , with the additional condition that the solution is bounded, as  $x$  tends to infinity.
- *The bounded interval problem:* the requirement of boundedness of the solution in quarter plane is replaced by the measurement of the heat flux at  $x = l$  (Neumann boundary condition). The equation problem (1.2) is a bounded interval problem. All problems studied in this thesis are considered in a bounded region in space.

Both problems can be reformulated as a Volterra integral equation of the first kind [11, 12],

$$g(t) = (Kf)(t) = \int_0^t k(t - \tau) f(\tau) d\tau, \quad 0 \leq t \leq 1, \quad (1.3)$$

with different kernel functions  $k$ . However the kernel functions have similar mathematical properties, e.g. the smoothing property [12, 18].

Recall that the SHE is not well-posed [1] and the solution does not depend continuously on the data. Further the measured data are usually a corrupted version of the exact quantities since we are never able to measure exactly in practice. But in both the quarter and bounded interval problems one can obtain stability of logarithmic convexity type by applying an a priori bound on the solution and bounded measurement error, i.e.,

$$\|f\|_{L^2} \leq M \quad \text{and} \quad \|g - g_\delta\|_{L^2} < \epsilon,$$

see [12, 26, 45, 46, 52]. Stability estimate for more general parabolic equation can be found in [41].

In the Volterra integral equation (1.3) we have a *causality principle* [19] in the sense that what happens at the “solution” boundary at time  $t_0$  can only affect the data  $g(t)$  for  $t \geq t_0$ . Therefore the solution  $f(t)$  can not be reconstructed for  $t$  close to the final time 1. This is another reason of ill-posedness of the SHE beside the smoothness of the Volterra operator. Note that the coefficients of SHE play a role for the smoothness of the Volterra operator (ill-posedness) which is analyzed and illustrated in Paper I.

A common family of methods for solving the SHE transforms the problem into an integral equation of first kind. The weak point of these methods is that often the kernel in the corresponding integral equation is not known explicitly, e.g., when the differential equations has variable coefficients.

## 2.2 Ill-Posedness and Singular Values

Singular values and singular functions of the operator give information about the nature of ill-posedness, for more details see [24, chapter 2]. If in (1.3) the kernel function  $k \in L_2([0, 1] \times [0, 1])$  then the operator  $K$  is compact and the inverse operator  $K^{-1}$  exists and is unbounded [12]. For any compact operator we have the following definition of a singular system.

**Definition 2.1.** The set  $(\sigma_n, u_n, v_n)_{n=1}^{\infty}$  is the *singular system* of the compact operator  $K : \mathcal{H}_1 \rightarrow \mathcal{H}_2$ , if

$$Kv_n = \sigma_n u_n, \quad K^*u_n = \sigma_n v_n,$$

where the singular values are ordered,  $\sigma_1 \geq \sigma_2 \geq \dots > 0$ , and the sets of singular functions  $\{u_n\}_{n=1}^{\infty}$  and  $\{v_n\}_{n=1}^{\infty}$  constitute complete orthonormal systems.

The operator  $K^* : \mathcal{H}_2 \rightarrow \mathcal{H}_1$  is the adjoint of  $K$ . For compact operators the singular values have only one accumulation point 0, which means  $\lim_{n \rightarrow \infty} \sigma_n = 0$ . The discrete analogue of the above singular system is a singular value decomposition (SVD) of a rectangular matrix [28, p.70], and is considered later in this chapter. The singular value expansion (SVE) of the operator is

$$Kf = \sum_{n=1}^{\infty} \sigma_n (f, v_n) u_n, \quad K^*g = \sum_{n=1}^{\infty} \sigma_n (g, u_n) v_n.$$

Formally the solution of  $Kf = g$  can be written

$$f = K^\dagger g = \sum_{n=1}^{\infty} \frac{(g, u_n)}{\sigma_n} v_n, \quad (1.4)$$

The operator  $K^\dagger$  is called the *Moore-Penrose pseudo-inverse* [24]. The following condition for the existence of a solution is called the *Picard criterion*,

$$\|f\|_{L^2}^2 = \sum_{n=1}^{\infty} \frac{|(g, u_n)|^2}{\sigma_n^2} < \infty. \quad (1.5)$$

This implies that  $(g, u_n)$  must decay more rapidly as  $n \rightarrow \infty$  than  $\sigma_n$ , which means that the data function  $g$  that satisfies the Picard condition must be very smooth. In practice, due

to the measurement error we have inexact data  $g_\delta = g + \delta$ . Since the measurement errors are usually stochastic we can not assume that the function  $\delta$  satisfies the Picard condition. Therefore in the case of measurement errors (even very small) any naive solution via the infinite sum (1.4) usually diverges or has a very large norm. The analogue of the condition (1.5), which should be satisfied by the solution of a finite dimensional linear system is called the *discrete Picard condition*, introduced in [34].

The Volterra operator (1.3) in discrete form is a triangular Toeplitz matrix which is extremely ill-conditioned. Even for noise free measured data  $g$ , applying the least squares solution of solving this ill-conditioned system always exhibits very large oscillations due to round-off error in the computer arithmetic.

Therefore there is a need to regularize the problem. There are various approaches to regularizing and stabilizing the ill-posedness of parabolic Cauchy problems, see e.g., [24, 40, 3] and the references therein. In the following we will give a short presentation of some regularization methods for discrete ill-posed problems.

### 3 Direct Regularization Methods

Direct regularization method can be based on some decomposition in numerical linear algebra like, e.g. Singular Value Decomposition (SVD) or orthogonal transformation. These methods require a direct access to all elements of matrix  $K$  when solving the linear system  $Kf = g$ . Some methods based on *Fourier transform* where the ill-posedness is dealt with by cutting off the high frequencies are proposed in [2, 22, 53, 59]. In this thesis the following direct methods are employed: Tikhonov regularization in discrete form (Papers I-III), truncated SVD (Papers III, IV), a method of lines combined with the approximation of the time derivative by a bounded operator (Paper I-III). These methods will be discussed shortly in following subsections.

Other examples of regularization methods for solving ill-posed Cauchy parabolic problems are the method of *Beck* [1], *mollification* [48] and *variational methods* [44, 38].

#### 3.1 Truncated Singular Value Decomposition

The association of small singular values with ill-posedness has been discussed in the previous section. Therefore an obvious idea to regularize the problem is to truncate the small singular values of the operator i.e. truncate the series (1.4). Suppose that the operator  $K$  in (1.1) is discretized to a  $n \times n$  matrix with the following singular value decomposition

$$K = \sum_{i=1}^n \sigma_i u_i v_i^T,$$

where  $\sigma_1 > \sigma_2 > \dots > \sigma_n \geq 0$  are the singular values and  $u_k$  and  $v_k$  are the left and right singular vectors, respectively. The solution to  $Kf = g_\delta$  can be written

$$f = \sum_{i=1}^n \frac{u_i^T g_\delta}{\sigma_i} v_i.$$

Recall that small perturbations in the coefficients  $u_i^T g_\delta$  are magnified extremely by a factor  $\sigma_i^{-1}$  for  $i$  large enough, because the most of singular values  $\{\sigma_i\}$  are very small.

The truncated singular value decomposition (TSVD) method only utilizes the  $N \leq n$  largest singular values for the solution and damps the effects caused by division by the small singular values, i.e. the TSVD solution is

$$f_N = \sum_{i=1}^N \frac{u_i^T g \delta}{\sigma_i} v_i.$$

The number of terms  $N$  is the regularization parameter which should be properly selected to get a good accuracy of the approximated solution.

### 3.2 Tikhonov Regularization

Tikhonov regularization is one of the most commonly used methods for regularization of ill-posed problems. The goal is to minimize  $\|g - Kf\|^2$  subject to a constraint on the size or smoothness of the  $f$ . The regularized solution solves the problem,

$$\min_f \|g - Kf\|^2 + \lambda \|Lf\|^2,$$

where  $\lambda > 0$  is the regularization parameter and the matrix  $L$  is either the identity matrix or a discrete differentiation operator. The parameter  $\lambda$  controls the smoothness of the solution. In other words it is a trade-off between fitting the data and reducing a norm of the solution. Both Tikhonov and TSVD are expensive to implement for large-scale applications. For more details about these two methods we refer to [24, 35].

### 3.3 Method of Lines

The idea of the method of lines is to rewrite the original PDE (1.2) as a system of Ordinary Differential Equation (ODE). The source of ill-posedness is that the time derivative  $\partial u / \partial t$  is unbounded, see [19, 21, 55]. Therefore by replacing the time derivative by a bounded approximation one can regularize the problem. Afterwards the resulting initial-value problem can be solved numerically essentially as an ODE in the space variable. This is a reason to treat the space and time discretization separately. There are some methods to approximate the time derivative, like difference quotient [20], wavelet-Galerkin [55, 56], mollification approximation [39, 48], spectral in terms of Fast Fourier Transform (FFT) [2], spline approximation [4]. We have used the last two methods in Papers I and II.

## 4 Iterative Regularization Methods

Iterative regularization methods are based on iteration schemes that access the matrix  $K$  only via matrix-vector multiplications. This property is suitable for sparse matrices and also when solving problems, where the matrix is not explicitly available. Many iterative methods have a self regularizing property in that early termination of the iterative process has a regularizing effect. The approximate solution initially tends to the true solution and then it diverges to some other undesired vector in later stages of iteration. This is called the *semi-convergence* phenomenon of iterative methods applied to ill-posed problems [24,

chapter 6]. In other words, the iteration number can be considered as a regularization parameter. This is due to the fact that in its first few steps the iterative method approximates mainly solution components associated with the largest singular values. Then gradually the smaller singular values start to influence the solution and finally after many steps, those singular values that are close to zero are approximated, which makes the solution explode. Therefore iterative methods may give useful results if terminated early.

## 4.1 Classical Stationary Methods

One of the first iterative regularization methods is the Landweber iteration, which is a variant of the steepest-descent method for least square problems, see [24, chapter 6]. Such methods are known as stationary methods. The Landweber iteration method has very slow convergence compared to Krylov subspace methods. The Landweber method is most used in signal and image processing, see e.g., [6, 54] and references therein. The iterative method proposed in [15] also can be viewed as a Landweber type method.

## 4.2 Krylov Subspace Methods

Some of the best known Krylov subspace methods are the conjugate gradient (CG), Arnoldi and generalized minimum residual (GMRES) methods, see [58]. The CG algorithm is used for solving sparse symmetric positive definite (SPD) linear systems [30]. In [42, 57] a CG type method based on minimizing a certain functional is proposed to solve a backward heat conduction problem. For a description about the regularization property of CG we refer to [24, chapter 7].

The Arnoldi method is used to solve both large and sparse linear systems and eigenvalue problems by projecting the problem onto a Krylov subspace of smaller dimension  $m < n$ . Given  $K \in \mathbb{R}^{n \times n}$  and  $g \in \mathbb{R}^n$  the *Krylov subspace* of dimension  $m$  is defined by

$$\mathcal{K}_m(K, g) = \text{span}\{g, Kg, K^2g, \dots, K^{m-1}g\}.$$

Let  $v_1 = g/\|g\|$  then the orthonormal basis  $V_m = [v_1, \dots, v_m]$  of Krylov subspace  $\mathcal{K}_m(K, g)$  can be obtained one vector at a time by computing  $Kv_j$  and orthonormalizing this vector against all previous  $v_i$ 's by modified Gram-Schmidt procedure. This gives a relation of the form

$$KV_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^T, \quad (1.6)$$

where  $H_m$  is a  $m \times m$  Hessenberg matrix containing the orthonormalization coefficients. Further by regularizing the Hessenberg matrix we can find a good approximation of the original problem recovered from the solution of projected problem [7, 23, 27, 51].

The GMRES method is based on the Arnoldi recursion and can be used for solving linear systems of equations (1.1) with a arbitrary (non-symmetric) square matrix  $K$ . At step  $n$  we approximate the exact solution  $f = K^{-1}g$  by a vector  $f_m \in \mathcal{K}_m(K, r_0)$  such that residual

$$\|r_m\|_2 = \|g - Kf_m\|_2,$$

is minimized, see Paper III and the references therein. The regularizing properties of the GMRES method have recently been studied in several papers [10, 14, 13, 37, 43, 9].

Usually preconditioning (for well-posed problems) is implemented to speed up the convergence process by clustering the singular values of the iteration matrix. In our work in Paper III preconditioning (for an ill-posed problem) is meant to reduce the number of iterations required to reconstruct the information from the large singular values, may improve the quality of the computed solution. But the small singular values still remain and should be suppressed. This means that the preconditioner should only precondition the well-posed part of operator (cluster the larger singular values of the operator) and it must not precondition the ill-posed part of the operator. In some papers the preconditioner of ill-posed problems acts upon the ill-posed part of the problem with the identity operator [33, 32]; in Paper III we simply truncate the ill-posed part. The problem in Paper III is a two-dimensional sideways parabolic equation with variable coefficients. As a preconditioner we take the solution of an ill-posed Cauchy problem for an equation corresponding to original ill-posed problem with constant coefficients. Thus we regularize the problem by regularizing the preconditioner as well as truncating the GMRES iteration.

## 5 Choice of Regularization Parameter

The regularization parameter in any regularization scheme is a quantity that is used to control the degree of regularization of the solution. Techniques for choosing the regularization parameter can be considered in two categories: those which are based on knowledge of error norms in the data e.g., the Morozov discrepancy principle [47], and those that use just the information in the data, e.g., the L-curve criterion [36] and the method of generalized cross validation [29]. The discrepancy principle is most widely used method for selecting the level of regularization. Basically the discrepancy principle states that the optimal solution is that in which the discrepancy between the true and predicted data is compatible with the estimated data error. However when the estimate of the noise level is not available, then the discrepancy principle cannot be used. For such cases heuristic methods are needed. These parameter choice approaches depend on both the regularization method and the inverse problem in a complex way, i.e., there is not one best approach, see [24] for more details. In this thesis we have used the discrepancy principle and the L-curve method to choose the parameters.

---

## Summary of Papers

### **Paper I: Analysis of an Ill-Posed Cauchy Problem for a Convection-Diffusion Equation**

In this paper we investigate mathematical and numerical properties of an ill-posed problem for a convection-diffusion equation. We study the influence of the coefficients on the degree of ill-posedness. The problem is reformulated as a Volterra integral equation of the first kind with a smooth kernel. Then we compute numerically the singular values of the Volterra operator. The rate of decay of the singular values of the integral operator determines the degree of ill-posedness. In this paper it is shown that the sign of the coefficient in the convection term influences the rate of decay of the singular values. The problem is also analyzed by taking the Fourier transform, giving a linear ordinary differential equation. The eigenvalues of the matrix of the differential equation is then computed. Numerical experiments confirm our results.

### **Paper II: A Sideways Heat Equation Applied to the Measurement of the Gas Temperature in a Combustion Chamber**

We propose an approach to approximate the gas temperature in a combustion chamber, when a shielded aspirated thermocouple has been used to calibrate the temperature sensor. The gas temperature and the heat transfer coefficient at the surface of thermocouple are unknown. The mathematical model of the temperature changes inside the thermocouple is described as a sideways heat equation problem. Since this is an inverse problem which is severely ill-posed, regularization methods are accomplished to determine the solution. The gas temperature and the heat transfer coefficient at the surface of thermocouple are unknown. First the coefficient is approximated via a calibration experiment. Since the thermocouple is made of two different materials, magnesium oxide and steel, the coefficients in the inverse problem are functions of radial distance. Therefore the problem in the space domain is divided into two parts. In the first part, where the material is mag-

nesium oxide, the problem is more ill-posed and the inverse problem is reformulated as a Volterra integral equation. In order to rule out unphysical solutions, we impose a monotonicity constraint on the regularized solution when applying Tikhonov regularization in the calibration experiment. Using the approximate heat transfer coefficient and finding the temperature and heat flux at the surface of thermocouple we compute an approximation of the gas temperature with a relatively high accuracy.

### **Paper III: A Preconditioned GMRES Method for Solving a Sideways Parabolic Equation in Two Space Dimensions**

We present a new iterative regularization technique for solving a two-dimensional sideways parabolic equation with variable coefficients using a preconditioned Generalized Minimum Residuals Method (GMRES). Large-scale ill-posed problems are often solved using iterative methods, in particular Krylov methods, e.g. GMRES, where the number of iterations serves as a regularization parameter. But for this type of problem we can not make such an iteration converge to a reasonable solution at all. Therefore we use preconditioned GMRES, with a preconditioner based on a semi-analytic solution formula for the corresponding problem with constant coefficients. Since the preconditioning operator is singular and a pseudo-inverse is used. Regularization is used in the preconditioner as well as truncating the GMRES algorithm. An important feature of the preconditioner is that it is based on a truncated expansion in terms of trigonometric functions. Therefore it can be implemented using fast discrete trigonometric transforms, in combination with the solution of a relatively small number of simple 1D sideways parabolic problems. The Discrepancy principle is used for determining when to terminate the iteration process [10]. Regularizing the preconditioner stabilizes the convergence behavior of the PGMRES iteration makes which in its turn the quality of the solution less sensitive to choice of regularization parameter (number of PGMRES steps). The computed examples indicate that the proposed PGMRES method is well suited for the solution of 2D sideways parabolic problems with variable coefficients.

### **Paper IV: Numerical Solution of a Cauchy Problem for a Parabolic Equation in Two or more Space Dimensions by the Arnoldi Method**

In this paper we consider the numerical solution of a Cauchy problem for a parabolic equation in multi-dimensional space, where the domain is cylindrical in one spatial direction. It is desired to find the lower boundary values from the Cauchy data on the upper boundary. This problem is severely ill-posed. The formal solution is written as a hyperbolic cosine function in terms of a multi-dimensional parabolic (unbounded) operator. The approximate solution is computed by projecting onto a smaller subspace generated by the Arnoldi algorithm applied on the inverse of the operator. A well-posed parabolic problem is solved in each iteration step. Further the hyperbolic cosine is evaluated explicitly only for a small triangular matrix. Numerical examples are given to illustrate the performance of the method.



---

## Bibliography

- [1] J. V. Beck, B. Blackwell, and S. R. Clair. *Inverse Heat Conduction. Ill-Posed Problems*. Wiley, New York, 1985.
- [2] F. Berntsson. A spectral method for solving the sideways heat equation. *Inverse Problems*, 15:891–906, 1999.
- [3] F. Berntsson. *Numerical Methods for Inverse Heat Conduction Problems*. PhD thesis, Linköping Studies in Science and Technology, Dissertations No. 723, Linköping University, Department of Mathematics, 2001.
- [4] F. Berntsson. Boundary identification for an elliptic equation. *Inverse Problems*, 18(6):1579–1592, 2002.
- [5] F. Berntsson and Lars Eldén. An inverse heat conduction problem and an application to heat treatment of aluminium. In M. Tanaka and G.S. Dulikravich, editors, *Inverse Problems in Engineering Mechanics II. International Symposium on Inverse Problems in Engineering Mechanics 2000 (ISIP 2000)*, Nagano, Japan, pages 99–106. Elsevier, 2000.
- [6] M. Bertero and P. Boccacci. *Introduction to Inverse Problems in Imaging*. Institute of Physics Publishing, Bristol, 1998.
- [7] Å. Björck, E. Grimme, and P. Van Dooren. An implicit shift bidiagonalization algorithm for ill-posed systems. *BIT*, 34:510–534, 1994.
- [8] E. Blom, P. Nyqvist, and D. Loyd. Suction pyrometer analysis of the instrument and guide for users,. *Varmeforsk*, 2004. in Swedish with a summary in English.
- [9] P. Brianzi, P. Favati, O. Menchi, and F. Romani. A framework for studying the regularizing properties of Krylov subspace methods. *Inverse Problems*, 22:1007–1021, 2006.

- 
- [10] D. Calvetti, B. Lewis, and L. Reichel. On the regularizing properties of the GMRES method. *Numer. Math.*, 91:605–625, 2002.
- [11] J. R. Cannon. *The One-Dimensional Heat Equation*. Addison-Wesley, Reading, MA, 1984.
- [12] A. S. Carasso. Determining surface temperatures from interior observations. *SIAM J. Appl. Math.*, 42:558–574, 1982.
- [13] B. Lewis D. Calvetti and L. Reichel. GMRES-type methods for inconsistent systems. *Linear Alg. Appl.*, 316:157–169, 2000.
- [14] B. Lewis D. Calvetti and L. Reichel. GMRES, L-curves, and discrete ill-posed problems. *BIT*, 42:44–65, 2002.
- [15] Youjun Deng and Zhenhai Liu. Iteration methods on sideways parabolic equations. *Inverse Problems*, 25(9):095004 (14pp), 2009.
- [16] Herbert Egger, Yi Heng, Wolfgang Marquardt, and Adel Mhamdi. Efficient solution of a three-dimensional inverse heat conduction problem in pool boiling. *Inverse Problems*, 25(9):095006 (19pp), 2009.
- [17] L. Eldén. Regularization of the backward solution of parabolic problems. In G. Anger, editor, *Inverse and improperly posed problems in differential equations*, Berlin, 1979. Akademie-Verlag.
- [18] L. Eldén. The numerical solution of a non-characteristic Cauchy problem for a parabolic equation. In P. Deuffhard and E. Hairer, editors, *Numerical Treatment of Inverse Problems in Differential and Integral Equations, Proceedings of an International Workshop, Heidelberg, 1982*, pages 246–268. Birkhäuser, Boston, 1983.
- [19] L. Eldén. Numerical solution of the sideways heat equation. In H. Engl and W. Rundell, editors, *Inverse Problems in Diffusion Processes*, pages 130–150. SIAM, Philadelphia, 1995.
- [20] L. Eldén. Numerical solution of the sideways heat equation by difference approximation in time. *Inverse Problems*, 11:913–923, 1995.
- [21] L. Eldén. Solving the sideways heat equation by a 'method of lines'. *J. Heat Transfer, Trans. ASME*, 119:406–412, 1997.
- [22] L. Eldén, F. Berntsson, and T. Regińska. Wavelet and Fourier methods for solving the sideways heat equation. *SIAM J. Sci. Comput.*, 21(6):2187–2205, 2000.
- [23] L. Eldén and V. Simoncini. A numerical solution of a Cauchy problem for an elliptic equation by krylov subspaces. *Inverse Problems*, 25(6), 2009.
- [24] H. Engl, M. Hanke, and A. Neubauer. *Regularization of Inverse Problems*. Kluwer Academic Publishers, Dordrecht, the Netherlands, 1996.
- [25] H. W. Engl, A. K. Louis, and W. Rundell, eds. *Inverse Problems in Geophysics*. SIAM, Philadelphia, 1996.

- [26] H. W. Engl and P. Manselli. Stability estimates and regularization for an inverse heat conduction problem in semi-infinite and finite time intervals. *Numer. Funct. Anal. Optimiz.*, 10:517–540, 1989.
- [27] E. Gallopoulos and Y. Saad. Efficient solution of parabolic equations by Krylov approximation methods. *SIAM J. Scient. Stat. Comput.*, 13(5):1236–1264, 1992.
- [28] G. H. Golub and C. F. Van Loan. *Matrix Computations*. 3rd ed. Johns Hopkins Press, Baltimore, MD., 1996.
- [29] Gene H. Golub, Michael Heath, and Grace Wahba. Generalized cross-validation as a method for choosing a good ridge parameter. *Technometrics*, 21(2):215–223, 1979.
- [30] Gene H. Golub and Charles F. Van Loan. *Matrix Computations (Johns Hopkins Studies in Mathematical Sciences)(3rd Edition)*. The Johns Hopkins University Press, 3rd edition, October 1996.
- [31] J. Hadamard. *Lectures on Cauchy’s problem in linear partial differential equations*. Yale University Press, New Haven, 1923.
- [32] M. Hanke. Iterative regularization techniques in image reconstruction. In *Proceedings of the Conference Mathematical Methods in Inverse Problems for Partial Differential Equations*. Mt.Holyoke, pages 35–52. Springer-Verlag, 1998.
- [33] M. Hanke, J. Nagy, and R. Plemmons. *Preconditioned Iterative Regularization for Ill-Posed Problems*, pages 141–163. Numerical Linear Algebra, ed. L. Reichel and A. Ruttan and R. S. Varga. de Gruyter, Berlin, New York, 1993.
- [34] P. C. Hansen. The discrete Picard condition for discrete ill-posed problems. *BIT*, 30:658–672, 1990.
- [35] P. C. Hansen. *Rank-Deficient and Discrete Ill-Posed Problems. Numerical Aspects of Linear Inversion*. Society for Industrial and Applied Mathematics, Philadelphia, 1997.
- [36] P. C. Hansen. *Rank-deficient and discrete ill-posed problems: numerical aspects of linear inversion*. Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 1998.
- [37] P. C. Hansen and T. K. Jensen. Smoothing-norm preconditioning for regularizing minimum-residual methods. *SIAM Journal on Matrix Analysis and Applications*, 29(1):1–14, 2006.
- [38] D. N. Hao. A noncharacteristic cauchy problem for linear parabolic equations i: Solvability, ii: A variational method, iii: A variational method and its approximation schemes. Technical Report Preprint Nr. A-91-36 - 37 - 38, Fachbereich Mathematik, Freie Universitat Berlin, 1991.
- [39] D. N. Hao. A mollification method for ill-posed problems. *Numer. Math.*, 68:469–506, 1994.

- 
- [40] Dinh Nho Hào. *Methods for Inverse Heat Conduction Problems*. Peter Lang, Frankfurt am Main, 1998.
- [41] Dinh Nho Hao and H-J Reinhard. On a sideways parabolic equation. *Inverse Problems*, 13:297–309, 1997.
- [42] D. N. Hào, N. T. Thành, and H. Sahli. Splitting-based conjugate gradient method for a multi-dimensional linear inverse heat conduction problem. *Journal of Computational and Applied Mathematics*, 232(2):361 – 377, 2009.
- [43] T.K. Jensen and P.C. Hansen. Iterative regularization with minimum-residual methods. *BIT Numerical Mathematics*, 47(1):103–120, 2007.
- [44] B. Tomas Johansson and Daniel Lesnic. A variational method for identifying a spacewise-dependent heat source. *IMA J Appl Math*, 72(6):748–760, 2007.
- [45] P. Knabner and S. Vessella. The optimal stability estimate for some ill-posed Cauchy problems for a parabolic equation. *Math. Methods Appl. Sciences*, 10:575–583, 1988.
- [46] H.A. Levine. Continuous data dependence, regularization, and a three lines theorem for the heat equation with data in a space like direction. *Ann. Mat. Pura Appl.*, 134(1):267–286, 1983.
- [47] V. A. Morozov. On the solution of functional equations by the method of regularization. *Soviet Math. Dokl.*, 7:414–417, 1966.
- [48] D. A. Murio. *The Mollification Method and the Numerical Solution of Ill-Posed Problems*. J. Wiley & Sons, New York, 1993.
- [49] D. A. Murio, Y. Liu, and H. Zheng. Numerical experiments in multidimensional IHCP on bounded domains. In H. Engl and W. Rundell, editors, *Inverse Problems in Diffusion Processes*, pages 151–180. SIAM, Philadelphia, 1995.
- [50] F. Natterer. *The mathematics of computerized tomography*. Society for Industrial and Applied Mathematics, Philadelphia, 2001.
- [51] Dianne P. O’Leary and John A. Simmons. A bidiagonalization-regularization procedure for large scale discretizations of ill-posed problems. *SIAM Journal on Scientific and Statistical Computing*, 2(4):474–489, 1981. Multiplication Toeplitz-vector using FFT.
- [52] L.E. Payne. Improved stability estimates for classes of illposed Cauchy problems. *Applicable Anal.*, 19:63–74, 1985.
- [53] Zhi Qian and Chu-Li Fu. Regularization strategies for a two-dimensional inverse heat conduction problem. *Inverse Problems*, 23:1053–1068, 2007.
- [54] R Ramlau, G Teschke, and M Zhariy. A compressive landweber iteration for solving ill-posed inverse problems. *Inverse Problems*, 24(6):065013 (26pp), 2008.

- [55] T. Regińska and L. Eldén. Solving the sideways heat equation by a wavelet-Galerkin method. *Inverse Problems*, 13:1093–1106, 1997.
- [56] T. Regińska and L. Eldén. Stability and convergence of a Wavelet-Galerkin method for the sideways heat equation. *J. Inverse Ill-Posed Problems*, 8:31–49, 2000.
- [57] H. J. Reinhardt and Dinh Nho Hào. A sequential conjugate gradient method for the stable numerical solution to inverse heat conduction problems. *Inverse Problems in Engineering*, 2:1068–2767, 1996.
- [58] Y. Saad. *Iterative Methods for Sparse Linear Systems, 2nd ed.* SIAM, Philadelphia, 2003.
- [59] T. Seidman and L. Eldén. An optimal filtering method for the sideways heat equation. *Inverse Probl.*, 6:681–696, 1990.
- [60] T. I. Seidman. Optimal filtering for the backward heat equation. *SIAM J. Numer. Anal.*, 33:162–170, 1996.
- [61] U. Tautenhahn and T. Schröter. On optimal regularization methods for the backward heat equation. *J. Anal. Appl.*, 15:475–493, 1996.
- [62] J. Wang. The multi-resolution method applied to the sideways heat equation. *Journal of Mathematical Analysis and Applications*, 309(2):661 – 673, 2005.
- [63] P. L. Woodfield, M. Monde, and Y. Mitsutake. Implementation of an analytical two-dimensional inverse heat conduction technique to practical problems. *Int. J. Heat Mass Transfer*, 49:187–197, 2006.

