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Are Magnus Bruaset

# A survey of preconditioned iterative methods

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# A survey of preconditioned iterative methods


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# Contents

# Preface

These notes present a survey of iterative methods for the solution of large linear systems of algebraic equations. In particular, we focus on systems derived as discrete counterparts to partial differential equations. Such systems are usually very *sparse*, i.e., only a small fraction of the coefficient matrix contains nonzero entries. For this type of problems, iterative solvers have proven to be efficient and valuable strategies. This observation is indeed present as technological developments expand our computational power, thus encouraging the numerical solution of larger and larger systems. Moreover, high-performance computing puts us in a position where we are able to study mathematical models at complexity levels far beyond the limits of currently available analytic tools. For these reasons, the development of efficient and reliable procedures for solving linear systems will have continuing impact on computational mathematics.

The main objective of this survey is to present a compact overview of modern iterative solvers. There are already several thousands of papers published in this field, and it may seem as a overwhelming task to search this literature for the information that is relevant to one's own work. Hopefully, this presentation may help non-specialists to find suitable methods for their problems and also serve as a guide to the existing literature. However, due to the vast amount of publications in this area, this survey does not pretend to be exhaustive. Instead it presents a subjective selection of recent developments that presumably is of interest to many groups of users. We apologize therefore to anyone whose work is left out or not given the attention it deserves.

Besides the presentation of several iterative solvers, we also focus on the basic principles behind such methods. Starting with simple stationary iterations like Jacobi and SOR, we end up discussing a framework for a family of Krylov projection solvers such as the conjugate gradient method. We also review further developments that have led to methods like GMRES, BICGSTAB and QMR. In order to achieve a satisfactory convergence behaviour, iterative methods should usually be combined with an appropriate preconditioning strategy. Indeed, when solving general nonsymmetric problems, preconditioning may be required to obtain convergence at all. In the present survey, we pay special attention to algebraic preconditioners such as incomplete factorizations and matrix polynomials. We also outline the construction of some preconditioners that are closely connected to the original continuous problem, e.g. multigrid and domain decomposition.

Realizing that it would be next to impossible to compile this survey without sub-

stantial support, I am grateful to the research council and all individuals that in some way or another have contributed to this project. Financial support has been provided by The Research Council of Norway primarily under grant no. 413.90/002, and partially through the strategic research program STP 28402: *Toolkits in Industrial Mathematics at SINTEF*. Moreover, I want to thank Dr. Aslak Tveito and Professor Ragnar Winther (University of Oslo) for helpful discussions and for encouraging this work. I also highly appreciate the valuable comments on preliminary versions of this survey made by Dr. Torgeir Rusten (SINTEF Applied Mathematics), as well as the constructive suggestions from Professor Åke Björck (University of Linköping) and Professor Magne Espedal (University of Bergen). In addition, I want to thank Dr. Hans Petter Langtangen (University of Oslo) for a stimulating and fruitful teamwork in the development of `Diffpack`, where several of the methods and techniques discussed in this survey have been implemented. Finally, I take this opportunity to thank my family, Helga, Ingeborg and Jørgen, for their neverending support and concern.

Oslo, February 1995
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# 1. Introduction

This survey is devoted to iterative methods for solving large linear systems of algebraic equations

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}, \tag{1.1}$$

where $\boldsymbol{A} \in \mathbb{R}^{n,n}$ is nonsingular and $\boldsymbol{x}, \boldsymbol{b} \in \mathbb{R}^n$. Such systems are natural parts of applications in many different disciplines, e.g. structural analysis, electrical engineering, oil reservoir modeling, computer aided geometric design, atmospheric pollution, chemical engineering and economic modeling. In many cases, some dynamic process is modeled in mathematical terms, e.g. as a partial differential equation, and (1.1) is derived as the discrete counterpart of the continuous model. Even for nonlinear and time-dependent problems, linear systems like (1.1) naturally arise at intermediate steps of the global computation.

Since World War II, and in particular over the last decade, the increased access to computational power has encouraged studies of mathematical models at complexity levels far beyond the limits of currently available analytic tools. There is no doubt that such technological developments, at present ranging from modern workstations to supercomputers with vector and/or parallel processing capabilities, will have continuing impact on mathematical applications. According to Lax [259], the influence of fast computers on mathematics is "comparable to the role of telescopes in astronomy and microscopes in biology". However, due to the gap between theoretical insight and computability, there is urgent need for *robust*, as well as efficient, methods for dealing with intricate mathematical models. In particular, it is observed that the solution of linear algebraic systems is a fundamental, and often the most time-consuming, part of many simulation codes. Thus, we recognize the need for fast and reliable procedures for solving such systems, motivated by practical as well as economical reasons.

## 1.1 A model problem

As indicated above, we are primarily concerned with linear systems obtained by discretization of a corresponding continuous problem. For a typical example, we consider the following elliptic *model problem* in a domain $\Omega \subset \mathbb{R}^d$

$$\mathcal{L}u = -\sum_{i=1}^{d} \frac{\partial}{\partial \xi_i}\left(K^i(\boldsymbol{\xi})\frac{\partial u}{\partial \xi_i}\right) + \sum_{i=1}^{d} V^i(\boldsymbol{\xi})\frac{\partial u}{\partial \xi_i} + H(\boldsymbol{\xi})u = f \tag{1.2}$$

subject to the boundary conditions

$$\mathcal{B}u = \alpha u + \beta \frac{\partial u}{\partial \boldsymbol{n}} = g \tag{1.3}$$

on the piecewise smooth boundary $\partial\Omega$ with outwards directed normal $\boldsymbol{n}$. Denoting the closure of $\Omega$ as $\overline{\Omega} = \Omega \cup \partial\Omega$, we have $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_d) \in \overline{\Omega}$ for some $d \in \{1, 2, 3\}$. The functions $K^i, V^i, H : \overline{\Omega} \mapsto \mathbb{R}$ are assumed to be sufficiently smooth and fulfill the inequalities $K^i \geq K^i_{\min} > 0$ and $H \geq 0$ for $i = 1, \ldots, d$. Choosing $(\alpha, \beta) = (1, 0)$ or $(\alpha, \beta) = (0, 1)$ gives *Dirichlet* or *Neumann* boundary conditions, respectively. When both $\alpha$ and $\beta$ are nonzero, the boundary conditions are said to be of *Robin* type. Allowing the parameters to be functions of the spatial position $\boldsymbol{\xi}$, we are able to assign different types of conditions to specific segments of $\partial\Omega$. Restrictions that ensure the existence of a unique solution $u$ may be found in many textbooks on elliptic boundary value problems, see for instance Gilbarg and Trudinger [192]. To this end, we will assume that these requirements are satisfied and that the corresponding linear system is nonsingular.

Throughout this survey, unless otherwise stated, we consider the linear system (1.1) as a result of discretizing the model problem (1.2), (1.3) by a finite difference method, cf. [113, 275, 313], or a finite element method, cf. [32, 114, 429]. In many situations we will refer to the simplified model problem obtained for $K^i \equiv 1$, $V^i \equiv 0$ and $H \equiv 0$ subject to homogeneous Dirichlet boundary conditions,

$$\begin{aligned} -\Delta u &= f \qquad && \boldsymbol{x} \in \Omega = (0,1)^d, \\ u &= 0 && \boldsymbol{x} \in \partial\Omega. \end{aligned} \tag{1.4}$$

This is the *Poisson equation*, which for $d = 2$ is posed on the unit square. Defining the mesh size $h = 1/(q+1)$ for some positive integer $q$, we introduce the computational grid $\Omega_h$ and its "closure" $\overline{\Omega}_h$:

$$\begin{aligned} \Omega_h &= \{(ih, jh) : (i,j) \in I_h\}, \qquad && I_h = \{(i,j) : 1 \leq i,j \leq q\}, \\ \overline{\Omega}_h &= \{(ih, jh) : (i,j) \in \bar{I}_h\}, && \bar{I}_h = \{(i,j) : 0 \leq i,j \leq q+1\}. \end{aligned} \tag{1.5}$$

A second-order finite difference approximation of problem (1.4) is then given by

$$-u_{i,j-1} - u_{i-1,j} + 4u_{i,j} - u_{i+1,j} - u_{i,j+1} = h^2 f_{i,j}, \quad i,j = 1,2,\ldots,q, \tag{1.6}$$

where $f_{i,j} = f(ih, jh)$ and $u_{i,j}$ is the computed approximation to $u(ih, jh)$ which vanishes on the discretized boundary $\partial\Omega_h = \overline{\Omega}_h \setminus \Omega_h$. This system of equations is of form (1.1) with $n = q^2$ provided $\boldsymbol{A}$ denotes the usual five-point discrete Laplacian, $\boldsymbol{x} = (u_{1,1}, u_{2,1}, \ldots, u_{q,q})^T$ and $\boldsymbol{b} = h^2(f_{1,1}, f_{2,1}, \ldots, f_{q,q})^T$. Similar discretization for $d = 3$ leads to a seven-point difference scheme.

## 1.2 Direct versus iterative methods

Given a linear system $\boldsymbol{Ax} = \boldsymbol{b}$, there are essentially two possible approaches for solution. Traditionally, such problems have been solved by a *direct* method such as Gaussian elimination (or Cholesky decomposition), where the exact factorization of $\boldsymbol{A} = \boldsymbol{LU}$ into lower and upper triangular matrices $\boldsymbol{L}$ and $\boldsymbol{U}$ is computed, see Golub and van Loan [194, Ch. 4]. For the general $n \times n$ problem such procedures need $\mathcal{O}(n^3/3)$ flops, while the solution of the triangular systems $\boldsymbol{Ly} = \boldsymbol{b}$ and $\boldsymbol{Ux} = \boldsymbol{y}$ needs $\mathcal{O}(n^2)$ flops. If $\boldsymbol{A}$ is not needed for other purposes, it may be overwritten by its computed factors $\boldsymbol{L}$ and $\boldsymbol{U}$ in order to save storage.

REMARK 1.1 A *flop* is essentially the cost of the statement `S = S + A(I,K)*B(K,J)`, i.e., a floating point multiplication and addition including some subscripting, cf. [194]. ■

**Direct methods for sparse problems.** Linear systems derived by discretization of elliptic boundary value problems are typically *sparse*. This means that relatively few entries of the coefficient matrix $\boldsymbol{A}$ are nonzero, e.g. five or seven contributions for each row, such that the total number of nonzeros are $\mathcal{O}(n)$. Depending on the geometry of the problem and the chosen discretization procedure, the sparsity pattern of $\boldsymbol{A}$ will be structured or practically random, cf. Figure 1.1. In many cases $\boldsymbol{A}$ has a *banded* structure such that $a_{i,j} = 0$ whenever $i > j + p_1$ or $j > i + p_2$. The constants $p_1$ and $p_2$ are referred to as *lower* and *upper bandwidths*. If $p = p_1 = p_2$, we may also use the term *halfbandwidth*. For the system (1.6) we have $p_1 = p_2 = q = n^{1/2}$. When solving banded systems the operation count for the unpivoted factorization procedure is $\mathcal{O}(np_1p_2)$ flops, since the banded structure is maintained in $\boldsymbol{L}$ and $\boldsymbol{U}$. This estimate is significantly smaller than $n^3/3$ whenever $p_1$ or $p_2$ is much smaller than $n$. In (1.6), the discrete Poisson problem in two dimensions, this estimate is reduced to $\mathcal{O}(n^2)$. Exploiting the symmetry of $\boldsymbol{A}$, the number of arithmetic operations can be further halved. In terms of storage we obtain similar reductions from $n^2$ floating point numbers in the general case to $n(p_1 + p_2 + 1)$ for a banded matrix. Whenever $\boldsymbol{A}$ is symmetric we have $p = p_1 = p_2$, and only $n(p + 1)$ entries need to be stored.

If a direct solver such as Gaussian elimination is applied to a sparse system, we introduce a large number of additional nonzero entries into the coefficient matrix. These *fill-in* values will destroy the sparse structure of the problem and thus increase the storage requirements significantly.

The conditioning of $\boldsymbol{A}$ may have bad influence on the numerical errors that occur during the elimination process, or in any other solution method, see for instance Stewart and Sun [362, Ch. III]. Since problems like (1.2) typically lead to a spectral condition number $\kappa(\boldsymbol{A}) = \mathcal{O}(h^{-2})$, the numerical difficulties increase as we tend to solve larger systems, e.g. as a result of more computational power. To compensate for this behaviour, we may be forced to employ high-precision computations which will further increase the cost of storage and processing. However, there are other remedies

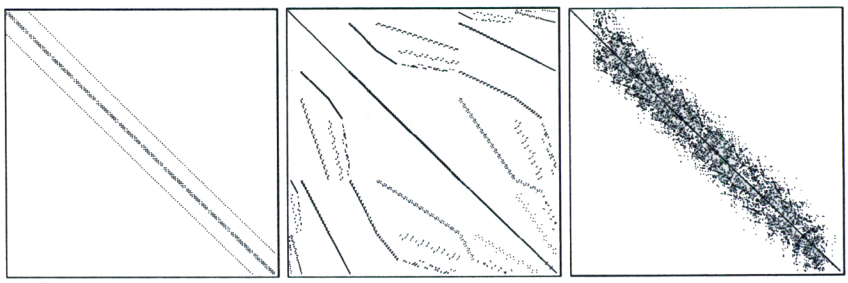

Figure 1.1: *Some examples of sparsity patterns, where the dots indicate nonzero entries. The figure to the left describes a typical five-point finite difference discretization, e.g. the discrete model problem (1.6). From left to right, the system sizes are* $n = 144$, $n = 465$ *and* $n = 991$.

for this problem such as iterative refinement techniques, see Duff et al. [145], Golub and van Loan [194] and Zlatev [430, 431]. There also exist other direct strategies, e.g. nested dissection and frontal methods, that are well suited for solving sparse systems. For a discussion of such methods in the context of finite element discretizations we refer to Axelsson and Barker [32, Ch. 6], while general introductions to this field are provided by George and Liu [191] and Duff et al. [145]. Considerable improvement over simple (banded) Gaussian elimination is achievable by these methods. However, due to their complicated nature, implementation for general problems is a nontrivial task.

**Iterative methods.** As an alternative to direct methods we may apply an iterative solver to the system (1.1), see Golub and van Loan [194, Ch. 10]. Such methods start with an initial guess $\boldsymbol{x}^0$ for the solution $\boldsymbol{x} = \boldsymbol{A}^{-1}\boldsymbol{b}$ and compute a sequence of approximations $\{\boldsymbol{x}^k\}$ which hopefully converges to $\boldsymbol{x}$. When using an iterative method, the coefficient matrix $\boldsymbol{A}$ is involved (directly or indirectly) only in terms of matrix by vector products. Thus there is no need for storing the zero entries of $\boldsymbol{A}$, and it is possible to implement algorithms that are extremely cost-effective with respect to computing time as well as storage, see Example 1.1. In addition to matrix by vector products, many iterative solvers are based on vector operations like $\boldsymbol{y} = a\boldsymbol{x} + \boldsymbol{y}$, $a \in \mathbb{R}$, (commonly called a SAXPY operation) and inner products $(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{x}^T\boldsymbol{y}$. Thus, except for some possible problems related to the global communication needed for the computation of inner products, such iterative methods are well suited for parallel and vectorized implementations, cf. Dongarra et al. [140, Ch. 7] and Saad [339].

EXAMPLE 1.1 Consider the three-dimensional model problem (1.2) posed on the unit cube with

$$K^i(\boldsymbol{\xi}) = 1 + e^{-20[(\xi_1-1/2)^2+(\xi_2-1/2)^2+(\xi_3-1/2)^2]}, \quad i = 1, 2, 3,$$

$V^i \equiv H \equiv 0$ and $f \equiv 1$ subject to $u = 0$ on $\partial\Omega$. We want to solve the associated $n \times n$ system of linear equations obtained by a centered second order difference approximation. In Table 1.1

| $n$ | Direct solver | | Iterative solver | | Ratio | |
|---|---|---|---|---|---|---|
| | CPU (s) | Memory (Mb) | CPU (s) | Memory (Mb) | CPU | Memory |
| 3 375 | 14.4 | 5.9 | 0.2 | 0.29 | 72.3 | 20.3 |
| 8 000 | 109.7 | 24.5 | 0.5 | 0.63 | 219.3 | 38.9 |
| 15 625 | 531.3 | 74.7 | 1.2 | 1.17 | 442.6 | 63.8 |
| 27 000 | 1 922.1 | 185.8 | 2.2 | 1.95 | 924.0 | 95.3 |
| 64 000 | 5.4 hours* | 782.2 | 6.1 | 4.44 | 3 158.1* | 176.2 |
| 125 000 | 1.4 days* | 2 386.1 | 16.3 | 8.46 | 7 503.3* | 282.0 |
| 216 000 | 6.7 days* | 5 935.9 | 32.3 | 14.37 | $1.8 \cdot 10^{4*}$ | 413.1 |
| 512 000 | 83.7 days* | $2.5 \cdot 10^{4}$ | 96.0 | 33.35 | $7.5 \cdot 10^{4*}$ | 749.9 |
| 1 000 000 | 1.7 years* | $7.6 \cdot 10^{4}$ | 221.4 | 64.30 | $2.4 \cdot 10^{5*}$ | 1 186.8 |
| 3 375 000 | 62.8 years* | $5.8 \cdot 10^{5}$ | 929.0 | 213.29 | $2.1 \cdot 10^{6*}$ | 2 716.5 |
| 8 000 000 | 832.0 years* | $2.4 \cdot 10^{6}$ | 2594.8 | 501.21 | $1.0 \cdot 10^{7*}$ | 4 871.2 |

Table 1.1: *Measured CPU times and memory requirements for Example 1.1.*

we show the CPU times and memory requirements for a typical direct method compared to the performance of a well-known iterative solver. The direct method is banded Gaussian elimination adapted to symmetric problems, while the iterative procedure is a conjugate gradient iteration combined with a MILU preconditioner, see Sections 3.3.1 and 4.2.1. Highly optimized versions of both methods have been implemented and executed on a Silicon Graphics Onyx workstation with 1 Gb of memory, running only on a single processor. All computations have been done in double precision arithmetics. The iterative solutions were computed with a relative residual norm less or equal $10^{-6}$, see Section 3.5.

The columns labeled "Ratio" refers to the ratio between values obtained for the direct versus the iterative method. All entries marked $*$ are based on estimated values and not on actual measurements. ■

By its nature, an iterative procedure does not accumulate rounding errors in the same way as a direct method. Nevertheless, the accuracy of the iterative solution is still affected by the conditioning of $\boldsymbol{A}$, see for instance Woźniakowski [413] and Greenbaum [198]. As demonstrated by Brussino and Sonnad [89], iterative methods are very often attractive alternatives to direct solvers. However, a proper strategy should be chosen on basis of the problem we want to solve. On some occasions, direct methods may be preferable to iterative procedures, cf. Howard et al. [229] and Poole et al. [321] for relevant discussions.

In this presentation we regard two widely used classes of iterative methods applicable to the algebraic problem (1.1). First, there are several iterative schemes based on splittings of the coefficient matrix, e.g. $\boldsymbol{A} = \boldsymbol{M} - \boldsymbol{N}$, which include traditional methods like Jacobi, Gauss-Seidel and successive overrelaxation (SOR). Such methods are widely covered in the monographs of Varga [391] and Young [420], see also Hageman and Young [225] and Hadjidimos [223]. Secondly, a large number of methods is based on approximating the exact solution $\boldsymbol{x} = \boldsymbol{A}^{-1}\boldsymbol{b}$ by some $\boldsymbol{x}^m \in \mathcal{K}_m$,