Test of Iterative Solvers on ITBL

Yoshinari Fukui
RIKEN
yoshinari.fukui@ieee.org

Hidehiko Hasegawa
University of Tsukuba
hasegawa@slis.tsukuba.ac.jp

Abstract

As an example to evaluate algorithms and computing environments, and to provide a free Internet service on the ITBL portal, we developed the TIS system, which is an evaluation system of linear iterative solvers and preconditioners for a system of simultaneous linear equations $Ax = b$. The TIS system can be used to determine an appropriate iterative solver and preconditioner for a matrix A with no programming effort. The TIS system can be used to evaluate new iterative solvers, new preconditioners and new computing environments for the given data. The proposed evaluation system is important for high-quality, high-performance computing.

1 Introduction

At present, the Grid system consists mainly of large-scale distributed computers and distributed file systems. The IT Fundamental Strategy Office of Japan Government announced the "e-Japan Strategy Program" in March 2001 in order to further promote IT technology as national infrastructure in Japan. NIMS, NIED, JAXA(NAL), JAERI, RIKEN and JST are participating in the Information Technology Based Laboratory (ITBL) project[1]. The ITBL is being developed as a virtual laboratory to share research resources that were previously distributed over a network. In addition, the ITBL will investigate new research styles based on IT. As an example, we herein construct an evaluation system for the algorithms and computing environments for a system of simultaneous linear equations $Ax = b$.

Fast solution of linear equations $Ax = b$ for large sparse matrices A is essential in science and engineering. The number of iterations until convergence depends on the iterative solver, the preconditioner, and the problem to be solved. The computation time depends on the computing environment and the storage format of the matrices A. Therefore, determining an appropriate iterative solver and preconditioner with no programming effort would be useful. If an appropriate iterative solver and preconditioner are known, then users may obtain the program based on these solver and preconditioner from somewhere. The user may develop his/her own program, which is tuned to realize higher performance for a particular set of data and environment based on this evaluation result. If the characteristics of data has been changed or a new iterative solver and preconditioner have been proposed, then the user may once again search for a suitable iterative solver and preconditioner.

We are developing the Test of Iterative Solvers (TIS) system by using the computing service function of the ITBL portal, which is used as an example to evaluate algorithms and computing environments. By providing his/her own data, the user can receive a set of solutions and a convergence history graph. The data provided by the user are accumulated in the TIS system and are used for future research concerning iterative solvers and preconditioners. For example, if a certain new iterative solver is proposed, a rough evaluation of the new solver can be performed by applying the new solver to all accumulated data. These data are also used for the evaluation of new computing environments.

2. Evaluation System for Algorithms

Two types of free services are provided on the Internet:

- Programs and data, such as Netlib (http://www.netlib.org/) and MatrixMarket (http://math.nist.gov/MatrixMaket/), are provided
- Results are returned for some input, i.e. information retrieval services such as Google (http://www.google.com/)

Until now, free computing services were difficult to provide because of restricted computing resources. However, since these restrictions will be not present in the Grid computing environment, computing services should be available. Thus, anonymous users should be able to input some computation and obtain the computed result via the Internet. This service enables users to obtain solutions with no programming effort. In addition, this service can provide assistance for building custom software.

The TIS system solves a system of simultaneous linear equations $Ax = b$ by a combination of iterative solvers and preconditioners. After the computation, the TIS system produces a comparison graph and a set of solutions corresponding to the combination of iterative solvers and preconditioners. The TIS system accepts a coefficient matrix A, a right-hand side vector b, and an initial solution vector x_0 of $Ax = b$. The TIS system provides a calculator or a recommendation system for a large system of simultaneous linear equations on the Internet. Previously, although programs and data were available on the Internet, no environment existed to test their combination. A great deal of effort was required in order to prepare the computing environment and perform computation. On the TIS system, many evaluations are easily performed with little effort.

The Grid Test for Large Systems of Equations (Grid TLSE)[2] is based on a similar idea. The Grid TLSE is built using the DIET middleware[3] on a Grid computing environment and provides information regarding the optimal ordering and the optimal sparse direct solver for a given matrix A of a system of simultaneous linear equations $Ax = b$. For solving the equation by the sparse direct solver, computation time depends on the pattern of non-zero elements in the matrix A, the ordering, and the algorithm, but does not depend on the right-hand side b. Although the Grid TLSE does not solve the system $Ax = b$, it can provied information regarding the optimal ordering and the optimal direct solver. The Grid TLSE can provide useful information to users by making available the preprocessing stage of a sparse direct solver via the Internet. The Grid TLSE does not have a large computing cost, because no sparse direct solvers are performed.

On the other hand, for solving a system of simultaneous linear equations using a number of iterative solvers, the number of iterations until convergence depends on the mathematical properties of A, b, x_0, the iterative solvers, and the preconditioners. The computation time also depends on the pattern of non-zero elements in matrix A and the computing environment. The TIS system solves the system $Ax = b$ by a combination of iterative solvers and preconditioners and then provides a comparison result of this combination as a graph and a set of solutions corresponding to the combinations. The computing cost is relatively small on a high-performance computing environment such as the ITBL portal.

In order to offer such service, a certain merit is required. Because it is difficult to continue a free volunteer serevice for a long time. The TIS system has three types of members: users, researchers, and the manager. Users send their problems via the Internet and obtain the computed result. Researchers provide an iterative solver or a preconditioner for public use and obtain the right to use accumulated data for further research. The manager provides and manages the computing resources of the ITBL and obtains timing results for combinations of the problem, the iterative solver, and the preconditioner on the ITBL environment.

Figure 1 shows the relationship between these members. The users are able to determine an appropriate iterative solver and preconditioner for their problem with no programming effort. However, the users must provide their data to the TIS system for future research. The researchers are able to use several types of data sets to develop a new iterative solver and preconditioner. However, the researchers must prepare a number of iterative solvers and preconditioners for public use. The ITBL manager automatically accumulates computation results that can be used to compare computing environments. However, the manager must set up a number of computing environments for public use. We believe that the information exchange between the members of the TIS system will help to develop a new research community.

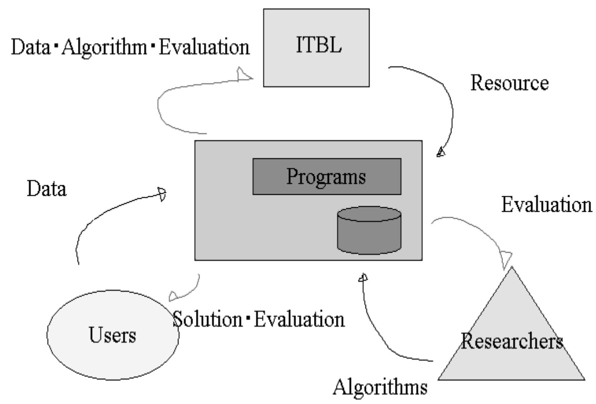

Figure 1. Relationship between the members of the TIS system as a supplier and as a consumer

3. TIS: Test of Iterative Solvers

In order to use the TIS system to determine the appropriate iterative solver and preconditioner for the system $Ax = b$, the user must follow six steps (See Figure 2):

1. Access http://www.itbl.jp/ and obtain an ITBL Portal account.

2. Upload a coefficient matrix A, a right-hand side b, and an initial solution x_0 for the system of simultaneous linear equations $Ax = b$. The initial solution x_0 is optional. The uploaded file must be in ASCII text and must fit the TIS matrix data format. Currently the total size of the matrix and vectors is restricted to 700 MB.

3. Select a combination of iterative solvers and preconditioners. Currently, there are eleven iterative solvers for general real matrices[4]: the BiConjugate Gradient method, the Conjugate Square method, the BiCGSTAB method, the BiCGSTAB(l) method, the General Product type BiCG method[5], the Orthomin method, the GMRES method, the QMR method, the Jacobi method, the Gauss-Seidel method, and the SOR method. In addition, there are six preconditioners: Jacobi, Incomplete LU, SSOR, Hybrid[6], $I+S$ type[7], SAINV[8], and no-precondition. Users can choose either "one iterative solver and many preconditioners" or "many iterative solvers and one preconditioner". The SSI Linear Iterative Solver[9] is used as the computation kernel of the TIS system.

4. Provide information such as the origin of data A, a mathematical property, and a description of the system for future analysis (See Figure 4). This information is optional.

5. Submit the computation. The user obtains the job identification number of the ITBL portal. The TIS server may send this number to the user by mail. This number will be used for inquiry of the job status and retrieval of the computation result.

6. Obtain a graph that shows how many iterations were performed until convergence (See Figure 5). Compare the qualities of all computed solutions to determine the best combination of iterative solver and preconditioner.

The TIS system solves the system $Ax = b$ repeatedly and creates a comparison graph of convergence from the computation results. Data transfer (uploading and downloading) is left up to the user. Neither notification nor sending of results are performed. Management tasks, such as user management, registration of data, accumulation of data, execution of computing, job management, and management of usage statistics are performed using the function of the ITBL portal.

Mathematical properties, such as the number of iterations until convergence, do not depend on the computing environment. However, the computation time strongly depends on the computing environment. If an iterative solver and a preconditioner are used with accumulated data in different computing environment, then the computation time varies depending on some property of its computing environment. The fundamental characteristic data of a new computing environment is also obtained by using the contents of the TIS system. Therefore, the TIS system can be used for the evaluation of computing environments.

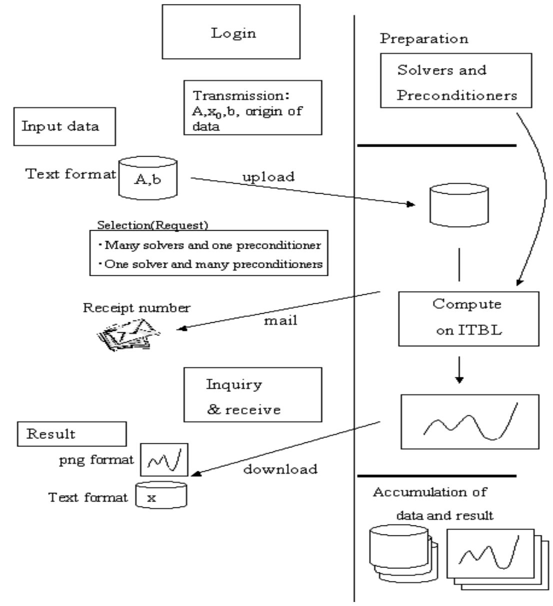

Figure 2. Outline of the TIS service

(1)	(2)	(3)	(4)
%comment	%comment	%comment	%comment
N, NNZ	N, NNZ	N, NNZ	N
$i, j, a_{i,j}$	b	b	$i, j, a_{i,j}$
b	$\{x_0\}$	$i, j, a_{i,j}$	b
$\{x_0\}$	$i, j, a_{i,j}$	$\{x_0\}$	$\{x_0\}$

Figure 3. Matrix and vector data format for the TIS system. N is the dimension of the matrix, and NNZ is the number of non-zero elements of matrix A. An initial solution x_0 is optional. Lines that begin with % are comment lines.

3.1. Matrix Data format

The data format of the TIS system is based on the MatrixMarket Exchange format[10], which has only a coefficient matrix. We prepared an extension of coordinate form of the MatrixMarket Exchange format that includes a right-hand side b, and an initial solution x_0 for iterative solvers. An initial solution x_0 is optional, and so appears just after the right-hand side b in several cases. Lines that begin with % are comment lines. In the TIS system, the information about the received data is added to the header portion of the data as comment lines and is used for future analysis. N is the dimension of the coefficient matrix A, and NNZ is the number of non-zero elements of A. The TIS accepts the four types of matrix data (See Figure 3):

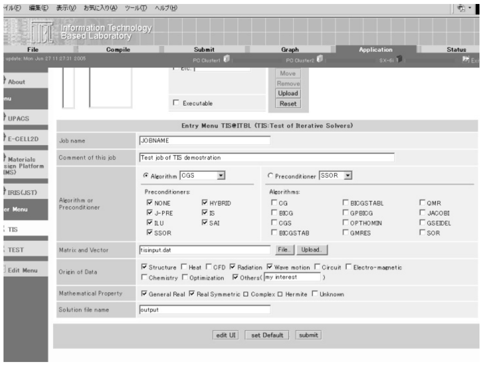

Figure 4. Menu describing $Ax = b$

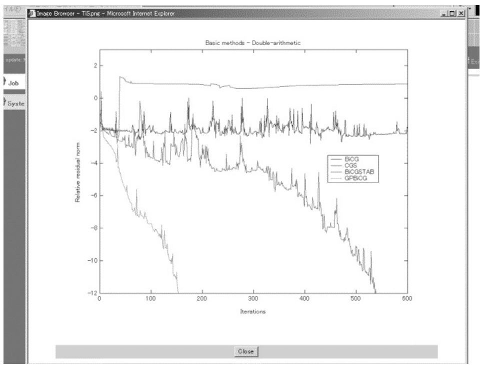

Figure 5. Sample comparison result

4. Conclusion

The TIS system acquires iterative methods, preconditioners, and user data and then solves a system of simultaneous linear equations $Ax = b$ repeatedly on the ITBL portal. This system provides useful information regarding the system $Ax = b$, iterative solvers, preconditioners, and computing environments. If the supplier of the data, the supplier of the algorithms and the supplier of the computing resources cooperate, a new research community may emerge. While this system functions as a virtual laboratory to the general community, the TIS system is also a forerunner of future computing services on the Internet.

From the point of view of researchers and the manager, the TIS system functions as a data gathering system and provides a tool by which to classify the features of data and algorithms. The accumulated real data will be used to classify algorithms and data and to determine their characteristics.

The TIS system provides only the result obtained by applying some iterative methods and preconditioners to the user data. The source program of the algorithms can be kept secret and copy-protected. If the computing accuracy of the system can be improved, then users may be able to realize effectiveness of accurate computing, and then to choose the best computing accuracy for the problem. Constant terms, such as the number of iterations, depend only on mathematics and not on the computing environment. However, variable terms, such as the computation time, strongly depend on the computing environment. In order to perform high-quality, high-performance computing, a balance between constant and variable terms is essential. The TIS system enables to evaluate algorithms and computing environments by real problems easily, and provides a public service. The TIS system is a first step toward these purposes.

Ease of use and the number of algorithms are subjects for future study.

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