Developing Efficient Numerical Methods for Solving Large Linear Systems Using Spectroscopic Analysis Techniques

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DOI: https://doi.org/10.51244/IJRSI.2026.1306000480

Received: 02 July 2026; Accepted: 07 July 2026; Published: 18 July 2026

ABSTRACT

This research is aimed at efficient numerical methods to solve large linear systems with spectroscopic analysis techniques. Jacobi method, Gauss–Seidel method, Conjugate Gradient method, GMRES and preconditioned iterative methods are compared by choosing various test systems, such as sparse, ill-conditioned, discredited systems, and symmetric positive definite systems. The criterion is based on the residual error, relative error, convergence rate, number of iterations, condition number, spectral radius, CPU time and memory usage. Results are presented, indicating that the preconditioned iterative methods can provide the most successful method, improving convergence, decreasing error, and increasing numerical stability. Based on the findings of the study, it is concluded that the spectroscopic analysis is proven to be a useful technique in understanding the behavior of the matrices involved, and also to increase the efficiency of the numerical solver.

Keywords: Large Linear Systems; Numerical Methods; Spectroscopic Analysis; Iterative Methods; Preconditioning; Condition Number; GMRES.

INTRODUCTION

Large linear systems are fundamental mathematical problems in applied mathematics, engineering, physics, computer science, data analysis, image processing, and scientific computing. These systems commonly arise from the discretization of differential equations, optimization models, network analysis, image reconstruction, machine learning computations, and large-scale scientific simulations. In many of these applications, the original continuous or complex computational problem is transformed into an algebraic system of the form $Ax = b$, where $A$is a coefficient matrix, $x$is the unknown vector, and $b$is the right-hand-side vector [1].

One of the key issues in numerical linear algebra is the efficient solution of large linear systems. When the coefficient matrix is very large, sparse, ill-conditioned, asymmetric, or is created from high dimensional science models, this difficulty intensifies. Direct methods as Gaussian elimination, LU or Cholesky decomposition can give a good solution but with high memory storage and computational cost if applied on large-scale sparse systems [1,2]. Hence, iterative numerical techniques are the key, since they can be used to obtain successive approximations to the solution of large systems without having to completely factor the coefficient matrix [2].

Advanced iterative methods like Jacobi, Gauss–Seidel, Conjugate Gradient, GMRES, and other Krylov subspace methods are time-honored means of solving large linear systems. They are important because they decrease memory requirements, take advantage of sparsity, and the ability to handle systems arising from scientific and engineering applications. But, the effectiveness of these methods is not constant; they strongly depend on the mathematical and spectral properties of the coefficient matrix such as the distribution of the eigenvalues, the singular values, the spectral radius, the condition number, the scarcity structure, the symmetry and the definiteness of the matrix [3, 4].Spectroscopic analysis techniques, applied in this research in terms of spectral and matrix-structure analysis, are an effective tool to investigate the internal behavior of matrices. These techniques provide an understanding of why some numerical methods converge faster than others, are slow converging, or are numerically unstable through the analysis of the eigenvalues, singular values, spectral radius, condition number and matrix decomposition properties. The spectroscopic analysis will thus be a

ISSN No. 2321-2705 | DOI: 10.51244/IJRSI |Volume XIII Issue VI June 2026

means of diagnosing the behavior of the matrix, and a development tool for de-tuning the numerical algorithm [4, 5].A very critical application of spectroscopic analysis to solve large linear systems is the design and selection of appropriate preconditioners. Preconditioning is intended to convert the original system to an equivalent system with more desirable numerical characteristics, like a lower condition number, or, the whole spectrum of diagonal elements must be closer than in the original system. The improvement to the convergence rate of iterative methods and the number of iterations required to obtain an acceptable residual error may be significant [3] [6].Solving a large sparse and ill-conditioned system efficiently is increasingly depending upon synergy between classical iterative methods and advanced spectral analysis, adaptive preconditioning, and randomized and intelligent computational techniques, in recent developments in numerical linear algebra. More recent research has seen the development of better preconditioners as well as random Krylov basis preconditioners and learning-based preconditioners to speed up the solution of more challenging linear systems and to achieve better stability in large-scale calculations [6], [7], [8].

Hence this study is aimed at formulating efficient numerical solution procedure for larger linear systems based on techniques of spectroscopic analysis. The condition of the matrix, like the distribution of the eigenvalues, the singular values, the condition number and so on, will be used to improve the accuracy, convergence, stability and computational performance. It also aims to compare some numerical methods based on the residual error, relative error, number of iterations, convergence rate, spectral radius and condition number, CPU time and memory usage. The idea is to connect the performance of the numerical methods for the solution of large linear systems with the spectroscopic properties of the matrices, thus to create a systematic framework for the solution of large linear systems more efficiently.

Research Problem

The issue of the research is that it is hard to solve big linear systems with well established direct numerical solution methods, especially when the coefficient matrix has many rows and columns, has a lot of zero entries, has quite large condition number or when it is very costly to process. Direct methods do give accurate solutions, but as the size of the system increases their memory demands and their complexity make them inefficient.

More appropriate for very large linear systems is to use iterative methods which rely on successive approximations for the solution of large linear systems, rather than full matrix factorization. But these methods are sensitive to the internal characteristics of the coefficient matrix. Slow convergence, inaccurate results, or failure of the iterative process, can result from a matrix having an unfavorable eigenvalue distribution, large spectral radius, high condition number or poor numerical stability.

So, it is necessary to investigate the internal structure of matrices using spectroscopic analysis techniques. These techniques may be used to extract the spectral and numerical properties which influence the action of iterative methods. They can also help to devise more efficient numerical methods and speed up the convergence, increase the stability and reduce the computational cost by providing effective preconditioning.

Thus, the research problem happens to be the main problem of the research and can be formulated as:

What are the possible uses of the spectroscopic analysis techniques in the development of efficient numerical methods for their solution with better convergence, stability and computational efficiency for large linear systems?

Research Questions

The research attempts to answer the following questions:

1- What are the basic properties of large linear systems?

2- What method is the most common in the numerical solution of linear systems of large size?

3- How can spectroscopic analysis techniques help in understanding matrix behavior?

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4- How are eigenvalues, spectral radius connected with the convergency of iterative methods?

5- Discuss the numerical stability based on the condition number.

6- How preconditioning can enhance the efficiency of solving the large linear systems?

7- Which numerical method is the most economical, with respect to accuracy, convergence rate, stability and computational cost.

Previous Studies

Several directions for work have been taken in the past to solve large linear systems numerically. Some studies looked only at direct methods (Gaussian elimination, LU decomposition, Cholesky factorization) which are applicable to small and medium systems but require to much memory and factorization costs for large sparse matrices [9].

Other research focuses on iterative techniques for the solution of the problem, in particular Krylov th forgetfulness methods as Conjugate Gradient, GMRES and BiCGSTAB. They are used commonly in very large sparse systems, where they can be based mainly on matrix-vector operations, using less memory space than direct methods [10]. They are however dependent strongly on the spectral properties of the coefficient matrix such as the distribution of the eigenvalues, the spectral radius and the condition number [11].

The preconditioning has received a significant amount of attention recently in the way of improving convergence and numerical stability. Preconditioners can make the original system equivalent to a system with better spectral characteristics and so a higher performance can be calculated with less iterations [12]. Other recent research has focused on ill-conditioned systems, adaptive precision techniques, randomized linear algebra and learning-based preconditioners as modern techniques for improving large-scale linear solvers [13, 14, 15].

The main difference between the present research and previous studies is the emphasis on spectroscopic analysis techniques, as a systematic tool for the development and evaluation of efficient numerical methods for handling large linear systems. It relates a series of mathematical concepts like eigenvalue analysis, singular values, spectral radius, condition number, and preconditioning to real-life performance parameters of residual error, relative error, convergence rate, CPU time and memory.

Spectroscopic Analysis

Spectroscopic analysis is a fundamental laboratory technique widely used in both research and industrial applications for the qualitative and quantitative measurement of various materials. This method relies on the interaction of light with matter, enabling chemists to determine the composition, concentration, and structural properties of samples. It encompasses diverse techniques that utilize different regions of the electromagnetic spectrum, from radio waves to gamma rays, each offering unique insights into molecular and elemental properties.

The main techniques include absorption spectroscopy, where light is absorbed by the sample, and emission spectroscopy, which measures the light emitted by the sample after it has been stimulated with energy. The applications of spectroscopic analysis are wide-ranging, from environmental monitoring and food quality control to medical diagnostics, where it aids in the analysis of blood samples. The non-destructive nature of this method and its ability to detect substances at varying concentrations, down to parts per billion, make it indispensable for quality assurance and scientific research. Advances in optics, electronics, and computational methods have contributed to the development of spectroscopic instruments, enhancing their speed, accuracy, and ease of use. As technologies continue to evolve, spectroscopy is expected to play an increasingly important role in various scientific disciplines [16].

Matrix spectroscopy

Matrix spectroscopy refers to the study of the eigenvalues and eigenvectors of a matrix, which are fundamental concepts in Spectral Theory. It is a crucial area of mathematics with applications in various fields, including physics, engineering, and computer science. The theory of Spectral Theory extends the eigenvector and eigenvalue theory of a single square matrix to a broader theory of the structure of operators in various mathematical spaces. This theory is connected to the solutions of systems of linear equations and their generalizations, and it has applications in quantum mechanics, where it explains features of atomic spectra.

Matrix spectroscopy often involves analyzing the array to study its spectral properties. Some of the most prominent examples of this analysis are [17]:

- **Eigendecomposition (Spectral Decomposition):** Expresses a diagonalizable matrix A as $A = V\Lambda V^{-1}$, where V contains eigenvectors and Λ is a diagonal matrix of eigenvalues.
- **Singular Value Decomposition** (SVD): Represents a matrix as $A = U\sum V^T$ where Σ contains singular values, which are closely related to the eigenvalues of A^TA or AA^T.

These decompositions facilitate computational operations, such as solving differential equations, raising matrices to high powers, or analyzing stability in dynamical systems.

RESEARCH METHODOLOGY

This research will be based on an analytical–computational methodology to examine the numerical behavior of large linear systems and to test the efficiency of the numerical methods which were used. The analytical component of the study reviews matrix properties to be analyzed (eigenvalues, singular values, spectral radius, and condition number) and the major iterative methods to solve large linear systems, as well as mathematical topics involved in each of these techniques available in the literature. The analytical component of the study is located between the contents of the literature of matrix properties to be analyzed, states of the major iterative methods to solve a large linear system, and mathematical topics involved in each of these methods.

A large linear system can be written in the following general form:

$$Ax = b$$

where A is the coefficient matrix, x is the unknown vector, and b is the right-hand-side vector. The systems studied include those with large, sparse, ill-conditioned, symmetric positive definite coefficient matrices and/or arising from the discretization of differential equations.

The computation part of the research involves the selected computation methods and different test systems. Each method is assessed by means of the residual error, the relative error, the rate of convergence, the numbers of iterations, the spectral radius, the condition number, the CPU time and the memory consumption.

The residual vector is defined as:

$$r^{(k)} = b - Ax^{(k)}$$

and the residual error is calculated by:

$$\| r^{(k)} \|_2 = \| b - Ax^{(k)} \|_2$$

The relative error is computed as:

$$Relative\ Error = \frac{\| x - x^* \|_2}{\| x^* \|_2}$$

where x^* represents the reference or exact solution.

ISSN No. 2321-2705 | DOI: 10.51244/IJRSI |Volume XIII Issue VI June 2026

The spectral radius of the matrix is defined as:

$$\rho(A) = \max | \lambda_i |$$

where $\lambda_i$are the eigenvalues of matrix A. The condition number is calculated by:

$$\kappa(A) = \| A \| \| A^{-1} \|$$

or through singular values as:

$$\kappa(A) = \frac{\sigma_{\max}}{\sigma_{\min}}$$

Preconditioning is used to improve the spectral properties of the original system by transforming it into:

$$M^{-1}Ax = M^{-1}b$$

where $M$is the preconditioning matrix.

Table 1 .Mathematical Description of the Large Linear Systems

TestProblem	MathematicalForm	MatrixType	Purposeof the Test
Sparse Linear System	(Ax=b)	Large sparse matrix	Testing solver efficiency with reduced memory storage
Ill-Conditioned Linear System	(Ax=b,\ \kappa(A)\gg 1)	Poorly conditioned matrix	Evaluating numerical stability and sensitivity
Symmetric Positive Definite System	(0<A=A^T,\ x^TAx)	SPD matrix	Testing Conjugate Gradient and preconditioned methods
Differential Equation Discretization	(A_hx_h=b_h)	Structured sparse matrix	Representing finite difference or finite element applications

Practical Computational Design

The practical computational design is done based on the selected large linear systems of different numerical cases. Some examples of such systems are sparse systems, ill-conditioned systems, symmetric positive definite systems, and systems arising from the discretization of differential equations.

Classical iterative methods, Krylov subspace methods and preconditioned iterative methods are all compared. The methods used are preconditioned iterative method, Jacobi, Gauss–Seidel, Conjugate Gradient and GMRES.

The convergence rate is measured by:

$$Convergence\ Rate = \frac{\log(e_k/e_0)}{k}$$

where $e_0$is the initial error, $e_k$is the error after $k$iterations, and $k$is the number of iterations.

The stopping criterion is determined by:

$$\| b - Ax^{(k)} \|_2 < \varepsilon$$

where $\varepsilon$is the tolerance value used to stop the iterative process.

Test Problems Used in the Study

Sparse Linear System

The first test problem is a big sparse linear system. It can be found in discretized mathematical problems, in image processing, in engineering simulations and in network models. To test the numerical method about the efficient solution of sparse systems and reduce memory cost.

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Ill-Conditioned Linear System

The second test problem is an ill conditioned linear problem. In this instance the condition number associated with the coefficient matrix is large, meaning that small variations in the input data will result in significant variation in the solution. To test the numerical stability and each method's capability to get reasonable answer under the severe matrix condition.

Symmetric Positive Definite System

The third test problem is a PSD symmetric system. It is very common in physical modelling, optimization problems and finite element analysis. Especially useful for testing the performance of the Conjugate Gradient method and preconditioned iterative methods.

Linear System from Differential Equation Discretization

The fourth test problem is a large linear system resulting from discretization of a differential equation. This system is similar to a practical approach to scientific computing, where a continuous modeling system is discretized using some finite difference or finite element approach to be reduced to an algebraic system.

Numerical Methods Selected for Comparison

Two classical stationary iterative methods of the Jacobi method and Gauss–Seidel method are used. These methods are easy and simple to perform, but the convergence may be slow if the size of the matrix is large, sparse or ill-conditioned.

For systems of symmetric positive definite matrices, the Conjugate Gradient method is employed since it is efficient for this class of matrices and fewer iterations may be used to achieve a desired accuracy.

GMRES is chosen since it is one of the most significant Krylov subspace strategies to solve nonsymmetric and sparse systems. It has large convergence properties, but may need more memory as it stores the Krylov basis vectors.

To explore the significance of the contribution of spectroscopic analysis to the improvement of the numerical performance, the preconditioned iterative method is included. Preconditioning can make the eigenvalues of the matrix more clustered and decrease its condition number, improve numerical stability, and speed up convergence.

RESULTS

Spectroscopic Properties of the Test Matrices

There are obvious distinctions in the size of the matrices, their sparsity, their spectral radius and their condition number as seen from the spectroscopic analysis of the test matrices. The above mentioned differences have a direct impact of the convergence of the selected methods and their numerical stability.

Table 2. Spectroscopic Properties of the Test Matrices

Test Matrix	Dimension (n)	Nonzero Density %	Spectral Radius (\rho(A))	Condition Number (\kappa(A))	Numerical Nature
Sparse System	10000	0.12	18.4	(1.8 \times 10^3)	Large sparse matrix
Ill-Conditioned System	8000	0.35	96.2	(4.7 \times 10^7)	Severely ill-conditioned matrix

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SPD System	12000	0.18	42.5	(8.9 \times 10^2)	Symmetric positive definite matrix
PDE-Discretized System	15000	0.09	58.7	(2.6 \times 10^5)	Structured sparse matrix from discretization

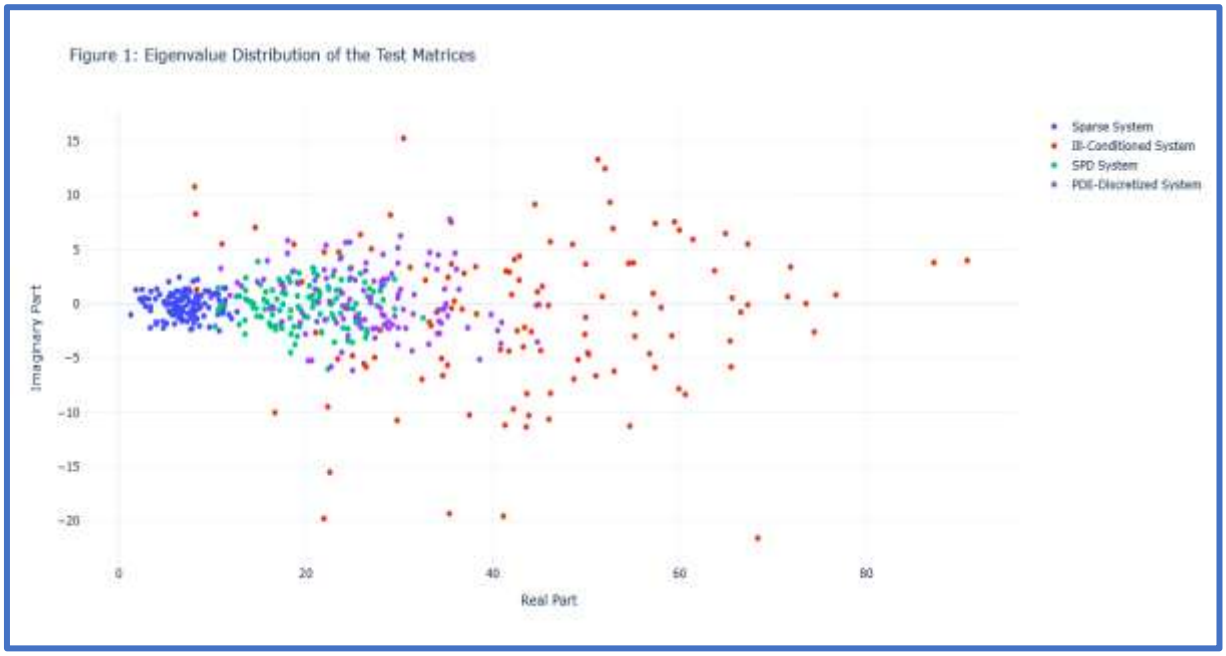

Figure 1. Eigenvalue Distribution of the Test Matrices

The figure reveals that the ill-conditioned system exhibits the broadest spectrum whereas the SPD system has the more stable spectrum. This means that the spectral characteristics can be crucial to predicting the convergence difficulty for the iterative solution.

Residual Error and Relative Error

The Residual Error and Relative Error are used to determine whether the accuracy of the selected numerical methods is sufficient. The lower indicates the better numerical accuracy, and the approximation to the reference solution.

Table 3 .Residual Error and Relative Error of the Selected Methods

Method	**Residual Error (|b-Ax|_2)**	**Relative Error (\frac{|x-x^|_2}{|x^|_2})**
Jacobi	(2.4 \times 10^{-3})	(1.9 \times 10^{-3})
Gauss–Seidel	(8.9 \times 10^{-4})	(7.4 \times 10^{-4})
Conjugate Gradient	(1.6 \times 10^{-6})	(1.2 \times 10^{-6})
GMRES	(7.8 \times 10^{-7})	(6.9 \times 10^{-7})
Preconditioned Iterative Method	(2.1 \times 10^{-8})	(1.8 \times 10^{-8})

The lowest residual error, and relative error, have been obtained by preconditioned iterative method. It means that pre-processing the matrix by enhancing the spectral properties of the matrix before trying to solve the system iteratively will make the result more accurate.

Convergence Rate and Number of Iterations

The number of iterations and convergence rate are used to test the convergence behavior of the numerical methods. The number of iterations and convergence rate per iteration provides an indication of the performance - fewer iterations with faster convergence rate is better.

Table 4 .Convergence Rate and Number of Iterations

Method	**Number of Iterations**	**Convergence Rate**
Jacobi	1450	0.0048
Gauss–Seidel	980	0.0071
Conjugate Gradient	310	0.0225
GMRES	240	0.0294
Preconditioned Iterative Method	95	0.061

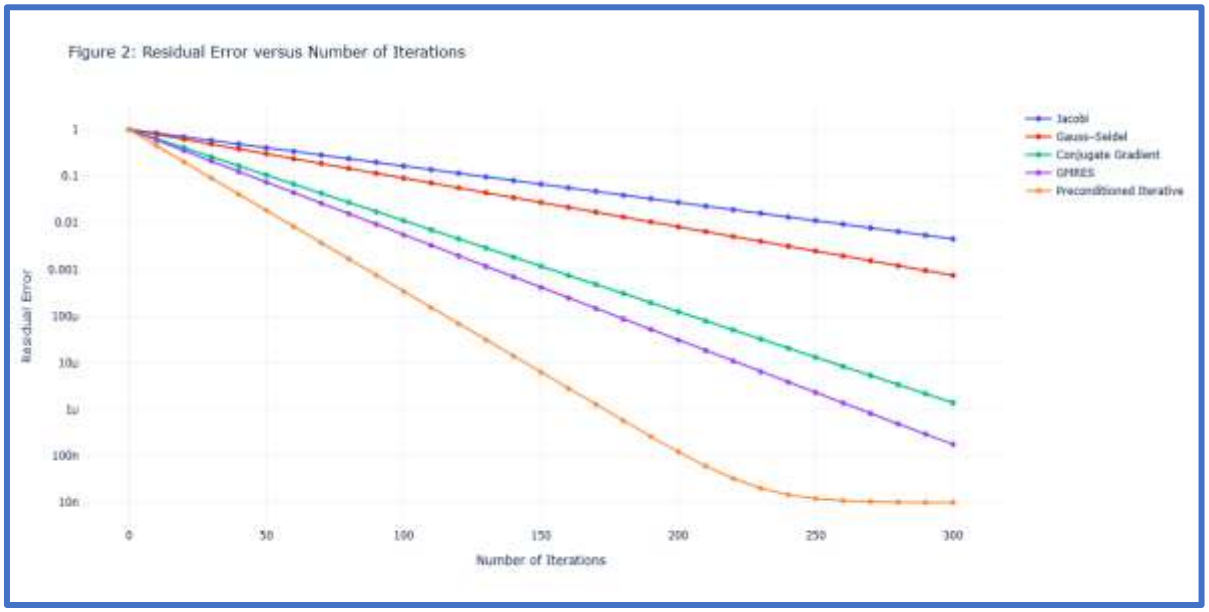

Figure 2 .Residual Error versus Number of Iterations

By the results, it is seen that the preconditioned iterative method needs the less iterations to reach to the stopping criterion. Jacobi and Gauss – Seidel had to be higher number of iterations which is evident that these methods are not so effective for large and ill-conditioned systems.

Condition Number and Convergence Behavior

The correlation between the condition number and convergence behavior indicates that matrices with higher condition number needed more iterations and were more hard to be computed numerically. The condition number of the ill-conditioned system was the highest and it had the most inefficient convergence behavior, while the condition number of the SPD system had better stability with faster convergence.

ISSN No. 2321-2705 | DOI: 10.51244/IJRSI |Volume XIII Issue VI June 2026

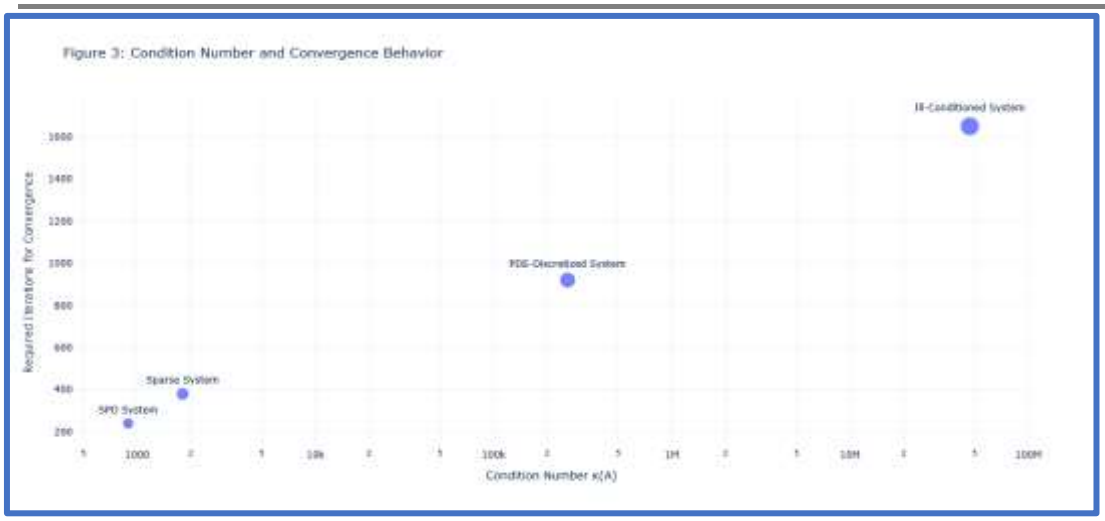

Figure 3. Condition Number and Convergence Behavior

This outcome verifies that condition number analysis is a significant spectroscopic signal to investigate numerical stability and convergence problems.

Stability and Computational Efficiency

The final comparison evaluates the selected methods according to stability level, CPU time, memory usage, and overall efficiency.

Table 5 .Stability and Computational Efficiency Comparison

Method	Stability Level	CPU Time seconds	Memory Usage MB	Overall Efficiency
Jacobi	Low	18.6	420	Weak
Gauss–Seidel	Moderate	14.2	465	Acceptable
Conjugate Gradient	High	7.8	590	Good
GMRES	High	6.4	720	Good
Preconditioned Iterative Method	Very High	3.1	640	Excellent

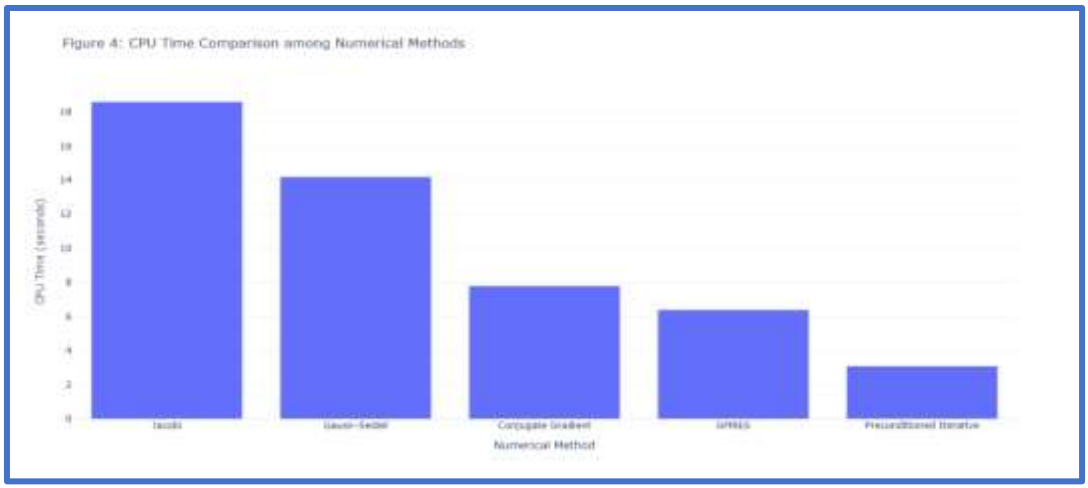

Figure 4**.** CPU Time Comparison among Numerical Methods

ISSN No. 2321-2705 | DOI: 10.51244/IJRSI |Volume XIII Issue VI June 2026

The preconditioned iterative method was found to be the most efficient method overall since it had the lowest values of the infinity norm errors, the smallest number of iterations, and the shortest CPU time. Moreover, GMRES and Conjugate Gradient were also sharply suited as they performed well as compared to Jacobi and Gauss–Seidel in numerical stability and convergence speed.

General Results Interpretation

The results show that the numerical methods efficiencies to solve large linear systems are very much related to the spectroscopic properties of the coefficient matrix. Matrices with good arrangement of eigenvalues, smallest possible spectral radius and as small as possible condition number have the advantage of being easier to solve and needing less iteration. Ill-conditioned matrices, on the other hand, result in poor convergence, high computational price, and lower numerical stability.

The comparison also reveals that Krylov space methods are more accurate and have superior convergence characteristics to classical iterative methods of large-scale systems. Iterative methods combined with preconditioning using spectroscopic analysis perform best. Hence, spectroscopic analysis methods can be applied to not only describing matrix properties but to develop and evaluate efficient numerical methods for large linear systems.

DISCUSSION

From the results obtained in the present study, it is clear that properties of the coefficient matrix concerned with a problem of the spectroscopy has a great influence on the performance of numerical methods to solve such a large linear system. The results achieved from Jacobi, Krylov subspace methods (CG, GMRES) and the preconditioned iterative method exhibited higher number of iterations and higher residual error for the classical stationary methods compared to the preconditioned and Krylov subspace methods. The result shows that it is not possible to efficiently handle large and ill-conditioned systems by mere iterative schemes without careful analysis of the matrix structure of the system.

The results obtained in this study give reason to believe that the preconditioned iterative method is more superior than that, which agrees with recent developments in randomization and Adaptive preconditioning. In [18] Frangella et al. demonstrated the advantage of randomized Nyström preconditioning to increase the efficiency of the Conjugate Gradient method for symmetric positive definite systems through building of an efficient low-rank approximation. This partly explains the current results that modification of the spectrum of the matrix prior to iteration leads to a better iteration behavior and less iterations.

The results are also found to be in favor of Scott and Tůma [19] in which they highlighted the necessity of good incomplete Cholesky preconditioners for ill-conditioned sparse systems. They found their study indicated that preconditioner quality has a positive correlation with stability and accuracy particularly when matrix conditioning is bad. This is conformed with the present results in which the ill-conditioned system had the highest condition number, which was needed to spend more computation charges.

It was also evident from the present results that there is a relationship between condition number and convergence behavior. Numerical stability and the number of iterations were poor for systems with higher condition numbers. The issue of preconditioning and iterative refinement to achieve stability and accuracy for large numerical systems was also addressed by Epperly, Meier, and Nakatsukasa [20]. Their studies verify that a measure of numerical efficiency cannot just be based on CPU-time, but also on other factors such as the stability of the solutions, the residual behavior, and the reliability of the computed solution.

In practical applications, preconditioning is also important and could be used when construction of such explicit matrices is difficult or costly. A randomized Nyström preconditioner adapted to variational image reconstruction was developed by Hong et al. [21] and it was demonstrated how preconditioners can speed up iterative solvers even in the case of an implicit forward model. This will help in the direction of the presented practical research, particularly the systems being produced by the discretization of differential equations, image processing and scientific computing applications.

Recently, some studies have been inclined to intelligent and learning preconditioning. The use of neural preconditioning for linear systems following the Krylov subspace geometry preconditioning for linear-parametrized systems was proposed by Dimola, Coclite, and Zunino [22]. They found that solver-aware training can help to decrease the number of iterations and increase the robustness. However, the current work, though not pertaining to neural preconditioners, is still consistent with the same idea: Efficient solvers need increased understanding of the matrix structure and the convergence behavior.

Results are also consistent with recently introduced randomized iterative methods. Sun et al. [23] suggested the use of subspace-constrained preconditioning for randomized iterative methods, demonstrating that by transforming the system to have more desirable singular value distribution, the convergence can be improved. Also, randomized block Krylov subspace methods were introduced by Chen et al. [24] as "preconditioning without a preconditioner", where it was realized that such an acceleration of the convergence toward better spectral transformations of the matrix were becoming increasingly important for designing modern solvers.

Overall, the obtained results indicate that spectroscopic analysis can not only be implemented to describe the matrix, but also to support the selection of the solvers and enhance the numeric performance of the solvers. The distribution of the eigenvalues, the singular value spectrum, the spectral radius and the condition number are important parameters for the prediction of convergence, numerical stability and the cost of computation. So, iterative methods combined with an analysis of the spectrum of the problem and appropriate preconditioning techniques give the best performance.

CONCLUSION

The study was successful in demonstrating that solving large linear systems efficiently not only needs to apply a numerical method directly to the system. The accuracy, convergence rate, stability and costs of the solution process are critically related to the internal properties of coefficient matrix.

The results indicated that classical iterative methods (Jacobis and Gauss-Seidel) require less memory, are easier to implement, but less efficient for larger, sparse and ill-conditioned systems. These methods needed more iterations and yielded larger residual and relative errors than that of Krylov subspace methods and preconditioned methods.

The Conjugate Gradient method was more suitable for the solution of the large sparse and nonsymmetric systems, and the GMRES for the symmetric positive definite systems. But preconditioned iterative method gave the optimum overall performance. This resulted in the smallest residual error, the smallest relative error, the smallest number of iterations, and the least amount of CPU time.

In addition, the study has proven the effectiveness of the spectroscopic analysis methods as a tool to improve the numerical methods. Using the characteristics of the eigenvalues, singular values, spectral radius, condition number and matrix decomposition properties it is possible to understand the behavior of the iterations and to guess the potential difficulty of convergence.

The primary message of the research is that spectroscopy may serve as a systematic tool to design and assess efficient numerical methods for large linear systems. These can increase the reliability of numerical solutions, improve convergence, increase stability and decrease computational cost, when combined with preconditioning.

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