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DOI
10.1145/3679240.3734600

Publication date
2025

Document Version
Final published version

Published in
E-ENERGY 2025 - Proceedings of the 2025 16th ACM International Conference on Future and Sustainable Energy Systems

Performance of Krylov solvers for gas networks

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Abstract

To integrate renewable energies with our current energy systems, we require interaction between gas and electrical networks. The coupling of networks results in a larger system of equations to be solved. Henceforth, scalable solvers are more suitable for large coupled networks. In this paper, a preliminary research is done, by investigating Krylov solvers on gas networks from the GasLib library. The networks are simulated with steady-state models. The models yield a nonlinear system, which is solved with the Newton-Raphson method. The corresponding Jacobian is non-symmetric, indefinite and sparse. We have considered the following Krylov solvers: GMRES, Bi-CGSTAB and IDR(s). We compare the performance with a direct solver, which is the LU factorisation. Our results show that basic Krylov solvers are ineffective in solving the networks, because most networks have a large condition number and an unfavourable distribution of the eigenvalues. Hence, we have explored several preconditioners, such as Jacobi, Gauss-Seidel and ILU methods. Only the ILU preconditioner with the use of the COLAMD reordering scheme leads to convergence of all networks. For this preconditioner, the fill ratio has to be taken large enough, otherwise the ILU factorisation breaks down due to a zero pivot. The minimum required fill ratio leads to a similar amount of work as the direct solver. Thus the combination of ILU and Krylov solver does not perform better than direct solvers for these medium sized problems.

CCS Concepts

• **Mathematics of computing → Computations on matrices**.

Keywords

Energy Hubs, Gas Networks, Integrated Energy Networks, Multi-carrier Energy Networks, Steady-State Load Flow

ACM Reference Format:
Buu-Van Nguyen, Johan Romate, and Cornelis Vuik. 2025. Performance of Krylov solvers for gas networks. In *The 16th ACM International Conference on Future and Sustainable Energy Systems (E-ENERGY '25), June 17–20, 2025, Rotterdam, Netherlands.* ACM, New York, NY, USA, 6 pages. https://doi.org/10.1145/3679240.3734600

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ACM ISBN 979-8-4007-1125-1/25/06
https://doi.org/10.1145/3679240.3734600

1 Introduction

Large projects related to windfarms are ongoing in the North Sea. Connecting farms with on-shore networks is challenging. One of these challenges is to assure stability to the power grid. Instability arises when supply and demand of electricity does not match. We can stabilise this by incorporating electrolysers. This leads to an integrated energy network with interaction between electricity and gas. If one is interested in modelling the effect of electrolysers, one can look at steady-state load flow analysis. This analysis requires a vast amount of scenarios to be computed for an energy network. The analysis involves many solves of linear systems. Moreover, the linear systems become larger, because future energy systems will become larger through coupling networks. For the steady-state load flow analysis to be practical, it has to be done in a fast way. Numerical solvers suited for this job are Krylov solvers [14]. To use Krylov solvers efficiently, we require knowledge of each single-carrier involved in an integrated energy network.

Performance of Krylov solvers for steady-state electrical networks have been extensively studied in [3]. The coupling between distribution and transmission networks has been investigated in [16] and [7].

For steady-state gas networks, there is still a lot to uncover for Krylov solvers. The closest research covers Krylov solvers for the time-dependent gas flow problem, which is discussed in [13]. Furthermore, an effective preconditioner for the time-dependent gas flow problem is proposed. However, there are some main differences compared to our study. We assume a steady-state flow, the compressibility factor is constant and the friction factor is constant. This results in a different system of equations to be solved, where the Jacobian does not satisfy the condition of a generalised saddle-point matrix.

Other strategies for solving gas networks involves changing the outer solve. In [4], a model order reduction method based on the network topology is proposed. In [19], a semi implicit method to solve the gas networks is applied resulting in a robuster method.

The complexity of modelling gas transport is increased by allowing mixing, which is described in [18]. For more recent advances and applications, see [5]. In our study, we do not take into account mixing of gas and assume that the gas is homogeneous throughout the network.

Furthermore, research of solving integrated energy network usually involves, solving each single-carrier network sequentially, see [19][12][11][2]. However, this cuts the network in smaller parts, where Krylov solvers are less interesting. Since we are interested in Krylov solvers, we want to solve the integrated energy network all at once, this still remains an open challenge.

From the the current body of literature, there is a lack of knowledge of Krylov solvers applied on steady-state gas flow. Henceforth, we focus on investigating the performance of Krylov solvers on gas networks. The key contributions in this paper are the following:

- The performance of Krylov solvers is analysed by investigating the singular values and eigenvalues of the Jacobian from several gas networks obtained from the GasLib library [15].
- A similar analysis is applied with preconditioners: Jacobi, Gauss-Seidel and ILU.

The paper is structured as follows. In Section 2, we briefly explain the model and describe the numerical methods to solve the nonlinear systems resulting from the models. In Section 3, the performance of Krylov solvers with and without preconditioners are discussed. Section 4 concludes the paper and presents recommendations.

2 Model and Solver

We model a gas network as a graph. Each node and link is governed by an equation. At each node we have conservation of mass. Each link consists of a steady-state equation of the corresponding network element. Furthermore, we assume that pipes are homogeneous in diameter and the pipe is not on a slope. As pipe model we take the Weymouth equation [6], $p_{inlet}^2 - p_{outlet}^2 = C^{-2} f|q|q$ with $C = \frac{\pi}{8}\sqrt{\frac{SD^5}{TR_{air}LZ}}$, where q is the gas flow, p denotes the pressure, S is the specific gravity, D is the diameter of the pipe, T is the gas temperature, R_{air} is the specific air constant, L is the pipe length and Z is the compressibility factor. The Weymouth friction factor is $f = (20.64^2 D^{\frac{1}{3}} E^2)^{-1}$, where E is the pipe efficiency. For more details on pipe and compressor models see [9]. The following model is used for resistors $p_{inlet}^2 - p_{outlet}^2 = C_r^{-2}|q|q$, where C_r is a constant.

2.1 System of Equations

Using the models leads to a nonlinear system of equations. Let there be n nodes and l links. This leads to n+l equations and $2n$+l variables from n nodal pressures, n injected flows and l link flows. For steady-state load flow analysis, we need to specify n known variables such that the system has an equal amount of unknown variables and equations. In practice, the in-takes, off-take and reference pressures are given. Resulting in a square system. We define the following notations:

- q_L is a vector containing the flow on the links,
- q_N is a vector with the injected flows,
- q is defined as a vector of all the flows $(q_L, q_N)^T$,
- p is a vector of the the nodal pressures,
- F^N is a vector function corresponding to the nodal equations, which corresponds to the mass conservation equations,
- F^L is a vector function corresponding to the link equations.

This leads to the nonlinear system of equations shown below:

$$F(q,p) = \begin{pmatrix} F^N(q,p) \\ F^L(q,p) \end{pmatrix} = 0$$

This system is solved with the Newton-Raphson (NR) method. The next iterate is updated with $x^{k+1} = x^k + \Delta x^k$. The update is obtained by solving:

$$J(x^k)\Delta x^k = -F(x^k) \quad (1)$$

The NR method terminates when it satisfies the stopping criterion.

2.2 Krylov Solver

The Jacobian J described in Equation (1) is sparse, non-symmetric and indefinite. To solve Equation (1), we use the following Krylov solvers suitable with our matrix properties: GMRES [14], Bi-CGSTAB [14] and IDR(s) [17]. To improve the performance of Krylov solvers a preconditioner can be applied. We opt for left preconditioning:

$$M^{-1}J\Delta x = M^{-1}F$$

where the preconditioner M is a non-singular matrix. We investigate the following preconditioners:

(1) Jacobi: M is a diagonal matrix with the same diagonal entries as J. If the entry is 0, then it is replaced by 1. This guarantees that the preconditioner stays nonsingular and no scaling is applied to the corresponding row.

(2) Gauss-Seidel: M is a lower triangular matrix with the same lower triangular entries as J. The same procedure is followed for the diagonal entries to ensure a nonsingular matrix.

(3) ILUTP: an approximation of the LU factorisation. For the sake of brevity, we refer to this algorithm as ILU(γ), where $\gamma \in [1, \infty)$ is the fill ratio. The algorithm makes use of partial pivoting and a dual threshold criterion, see [8] for more details. For the dual threshold, we have chosen to drop values lower than a tolerance τ and keep the m largest values per row.
In this paper, we choose a fill ratio of $\gamma = 5$. This is the minimum integer value where ILU does not breakdown for the presented gas networks. Moreover, we apply a COLAMD reordering to improve the robustness of the ILU factorisation.

3 Numerical Experiments

We apply a steady-state load flow computation for several networks found in the GasLib dataset [15]. We have applied simplifications to the data, which are described in Section 3.1. To see whether the networks are solvable, we solve the steady-state load flow of each gas network with a direct solver, see Section 3.3. In Section 3.4, we compare 3 Krylov solvers, which are GMRES, Bi-CGSTAB and IDR(s). After the initial investigation on the Krylov solvers, we focus on investigating several preconditioners, which are Jacobi, Gauss-Seidel and ILU, which are discussed in Section 3.5.

3.1 Data

GasLib is an open-source database containing gas transmission networks based on the German gas network [15]. Networks are named with the number of nodes as a postfix. We consider the following networks for the numerical experiments: GasLib-11, GasLib-24, GasLib-40, GasLib-135, GasLib-582 and GasLib-4197. GasLib networks contain the following node elements: source, sinks and junctions. Furthermore, the following link elements are present: pipe, compressor, resistor, short pipe, valve, and control valve.
For our numerical experiments we have made assumptions that simplify the networks. There is only 1 type of gas flowing in the networks, which is natural gas (methane). The temperature and compressibility of the gas is constant in the whole network. Furthermore, each pipe has the same pipe efficiency. The default values

corresponding to these assumptions are shown in Appendix A, Table 5. All compressors are turned off, which means the pressure coming out of the compressor remains unchanged. Furthermore, we assume that all valves are open. Valves and short pipes are link elements that create a relatively small pressure drop, where we model it as a resistor with a coefficient of $C_r = 10^3$.
GasLib does not provide a slack node and reference node, which are essential for our steady-state load flow computations to obtain a unique solution. The first source node present in the GasLib data is changed to a slack node. Thus the injected gas flow variable is set to unknown. In addition, the first source node is also set to a reference node, which means the pressure is known at this node. The reference pressure is set to the largest gas pressure found in the data, see Appendix, A Table 6. Smaller reference pressure values can lead to an unsolveable system.

3.2 Set-up

We apply a per unit scaling as described in [10]. Without this scaling the gas networks do not converge with the NR method. For the NR method, we have chosen the residual as a stopping criterion $\|F\|_2 < 10^{-6}$. The maximum number of iterations is set to 20.
For all Krylov solver we use the relative residual as a stopping criterion $\frac{\|F-J\Delta x\|_2}{\|F\|_2} < 10^{-8}$. We use the following settings for each Krylov solver:

- **GMRES:** At most 100 restart cycles where each restart cycle consists of a maximum of 20 iterations.
- **Bi-CGSTAB:** At most 100 iterations.
- **IDR(s):** At most 100 iterations and we choose $s = 4$.

3.2.1 Initial guess. A flat start is taken for the mass flow. We assume that the gas flows in the defined direction. Thus all mass flows start with positive values. In addition, the mass flow is set to 10% of the largest absolute mass flow value from the in-take or off-take. The initial nodal pressures are chosen from a linear profile based on the ordering of the pressure values. The values start from 95% of the reference pressure and decreases to 90% of the reference pressure.

3.2.2 Negative pressure values. The NR method can converge to negative pressure values, which is physically not possible. This is caused by the pressure drop, $\Delta p = p_{inlet}^2 - p_{outlet}^2$, containing quadratic values of the pressure. In other words, the pressure drop is an even symmetric function. Hence, the pressure drop value remains the same if we change the negative pressure value to positive. Therefore, if the solution of the NR method contains negative pressure values, we take the absolute value after each NR iteration.

3.3 Direct solver

We use an LU factorisation with a forward and backward substitution to solve the system in Equation (1). A COLAMD reordering has been applied to reduce the bandwidth of the matrix. We make use of the superLU package [1]. The direct solver manages to converge for all networks. The number of NR iterations until convergence is shown in Table 1.

Table 1: Number of iterations until convergence for each GasLib network of the Newton-Raphson (NR) method with a direct solver. The NR method requires more iteration when the network grows in size.

Network	System size	Iterations
GasLib-11	21	4
GasLib-24	48	4
GasLib-40	84	5
GasLib-135	304	8
GasLib-582	1190	17
GasLib-4197	8662	11

3.4 Without Preconditioner

Using a Krylov solver instead of a direct solver yields poor results. GMRES and Bi-CGSTAB only converge for the smallest available network, GasLib-11. IDR(s) converges up to GasLib-24. To explain this performance, it is informative to look at the condition number of the Jacobian defined by, $\kappa(J) = \frac{\sigma_1}{\sigma_n}$, where σ_1 is the largest singular value and σ_n is the smallest singular value. Generally, if the condition number is large, then it is quite likely that the iterative method will converge slowly. Table 2 only shows the conditions number at the start of NR, because the condition number changes at most with one order of magnitude throughout all NR iterations.

Table 2: The condition number and extreme singular values of each network.

Network	Condition Number	Smallest σ	Largest σ
GasLib-11	$2.32 \cdot 10^2$	$1.73 \cdot 10^{-2}$	$4.03 \cdot 10^0$
GasLib-24	$3.79 \cdot 10^3$	$1.10 \cdot 10^{-3}$	$4.18 \cdot 10^0$
GasLib-40	$4.08 \cdot 10^2$	$1.11 \cdot 10^{-2}$	$4.52 \cdot 10^0$
GasLib-135	$5.47 \cdot 10^3$	$1.11 \cdot 10^{-3}$	$6.07 \cdot 10^0$
GasLib-582	$7.97 \cdot 10^{10}$	$2.90 \cdot 10^{-9}$	$2.31 \cdot 10^2$
GasLib-4197	$4.58 \cdot 10^{10}$	$6.98 \cdot 10^{-10}$	$3.20 \cdot 10^1$

The condition number for GasLib-582 and GasLib-4197 are significantly larger compared to the other networks by at least a factor of 10^6. Note that the condition number for GasLib-40 is in the same order of magnitude as GasLib-11, but the Krylov methods do not converge. The condition number does not explain this behaviour. Therefore, we extend our analysis by investigating the distribution of the eigenvalues. We have observed complex eigenvalues for all networks. The eigenvalues are scattered, which leads to bad performance of Krylov solvers. Furthermore, with increasing size of the network, we see that the eigenvalues are contained in a disc, see Appendix B, Figure 5. Moreover, a cluster of eigenvalues is forming around the origin.

3.5 With Preconditioner

To deal with the problematic singular values and eigenvalues, we use preconditioning methods that can change these values. Also, in this section, we focus on the results from the preconditioned GMRES method, because the results from Bi-CGSTAB and IDR(s) are similar. The ILU preconditioning is used, which leads to convergence for all networks. The other preconditioners do not improve the performance. For GMRES+ILU(5), the number of iterations required for convergence at the first and last NR iterations are shown in Table 3. The number of iterations remained nearly constant for all networks, except for GasLib-582 and GasLib-4197. For GasLib-582, throughout the 17 NR iterations, the Krylov solver remained between 7 and 13 iterations. For GasLib-4197, the last two NR iterations required twice as much iterations from the Krylov solver compared to the other NR iterations. The performance is not surprising when we investigate the condition number and eigenvalues of the preconditioned system. In Table 4, we show the condition number of each network.

Table 3: Overview of iterations until convergence with GMRES+ILU(5).

Network	First NR	Last NR
GasLib-11	4	4
GasLib-24	1	1
GasLib-40	1	1
GasLib-135	1	1
GasLib-582	7	13
GasLib-4197	15	56

Table 4: The condition number and extreme singular values with ILU(5) as a preconditioner.

Network	Condition Number	Smallest σ	Largest σ
GasLib-11	$9.78 \cdot 10^3$	$1.09 \cdot 10^{-2}$	$1.07 \cdot 10^2$
GasLib-24	$1.00 \cdot 10^0$	$1.00 \cdot 10^0$	$1.00 \cdot 10^0$
GasLib-40	$1.00 \cdot 10^0$	$1.00 \cdot 10^0$	$1.00 \cdot 10^0$
GasLib-135	$1.00 \cdot 10^0$	$1.00 \cdot 10^0$	$1.00 \cdot 10^0$
GasLib-582	$5.93 \cdot 10^1$	$2.67 \cdot 10^{-1}$	$1.58 \cdot 10^1$
GasLib-4197	$2.96 \cdot 10^{10}$	$1.08 \cdot 10^{-5}$	$3.21 \cdot 10^5$

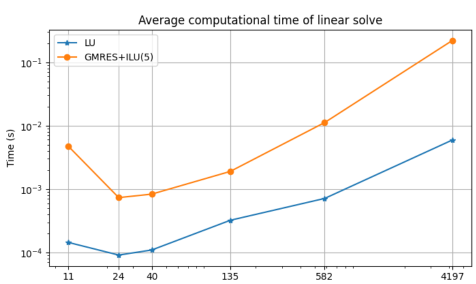

Figure 1: A comparison between the computational time of the LU factorisaton and GMRES+ILU(5) applied on the inner solve in the NR method. The LU factorisation is faster than GMRES+ILU(5).

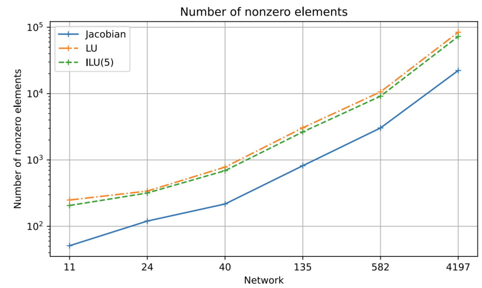

Figure 2: The number of nonzero elements of the lower triangular part of the LU and ILU(5) factorisation are compared with the number of nonzero elements of the Jacobian J.

The condition number has significantly decreased for most networks, except for GasLib-11 and GasLib-4197. GMRES+ILU(5) still manages to solve the aforementioned networks, because the eigenvalues are mostly clustered around 1. See Appendix C for figures. Figure 1 shows the computational time of the inner solve compared with LU and GMRES+ILU(5). The computational time of the direct solver is at least an order lower than the iterative solver. This is not surprising, because the number of nonzero elements in the ILU factorisation is close to the number of nonzero elements in the LU factorisation, see Figure 2. Note that the preconditioned Krylov solver requires a solve with the preconditioner on top of its regular algorithm, which results in a larger computational time.
Motivated by our observations, it is not worth the effort to solve the linear systems resulting from the presented GasLib network formulations with a preconditioned Krylov solver where ILU is the preconditioner. However, the systems of equations are small, where direct solvers remain the better choice. Moreover, future energy systems deal with decentralised energy sources, which requires modelling both transmission and distribution networks. This leads to larger systems of equations of an order of at least 10^6. At this size we might see better performance from Krylov solvers. Hence, it is premature to end on a definite conclusion with our results.

4 Conclusion and Recommendations

We have investigated several Krylov solvers, because these solvers scale well with the problem size. Our numerical results show that Krylov solvers without preconditioning are ineffective in solving the presented gas transmission networks from the GasLib dataset. The condition number is large and the eigenvalues are unfavourably distributed. Hence, we applied several preconditioning techniques, where only the ILU factorisation leads to convergence for all networks. However, the ILU preconditioner requires nearly the same amount of work as an LU factorisation. Thus the ILU factorisation is not a suitable preconditioner if one has to recompute the factorisation at every NR iteration.
For further research, we suggest to keep the same ILU factorisation until the nonlinear system has changed sufficiently based on a quantifier (Inexact-Newton method). Furthermore, this work serves as a precursor for solving multi-carrier energy networks. In the future, insight of preconditioning methods shown in this paper will be compared with GasLib networks coupled with a different energy carrier such as electricity.

Acknowledgments

This work is funded by NWO (Dutch Research Council) with grant number NEAT: ESI-BiDa 647.003.002.

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A Data

Table 5: Pipe parameter values used for the simplified GasLib networks.

	E	R_{air}	S	T	Z
Value	1	287.002	0.589	273.15 K	1

Table 6: Reference pressure for each gas network.

Network	Pressure (Bara)
GasLib-11	70
GasLib-24	70
GasLib-40	81
GasLib-135	81
GasLib-582	121
GasLib-4197	101

B Eigenvalues without Preconditioner

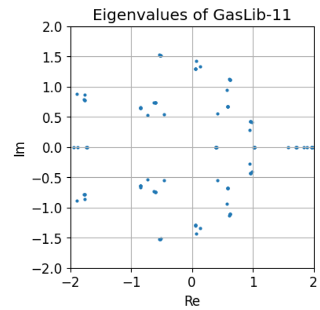

Figure 3: Eigenvalues of GasLib-11 The eigenvalues are scattered.

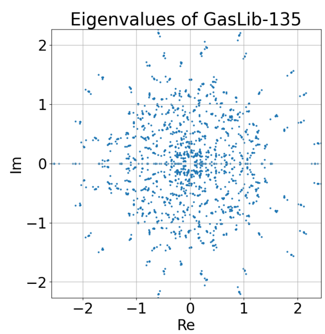

Figure 4: Eigenvalues of GasLib-135. The eigenvalues are scattered.

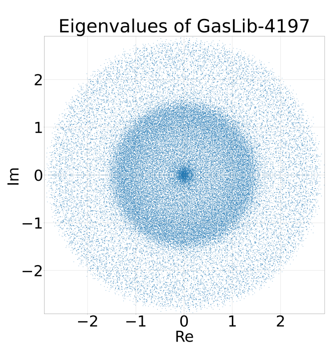

Figure 5: Eigenvalues of GasLib-4197. It becomes more distinct that the eigenvalue are contained in a disc.

C Eigenvalues with Preconditioner

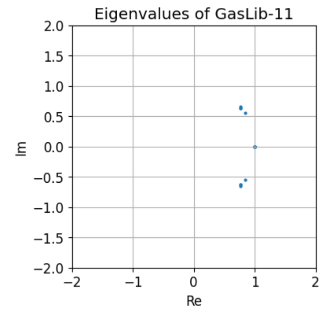

Figure 6: Eigenvalues of the preconditioned system with ILU(5) of GasLib-11. Most eigenvalues equal 1.

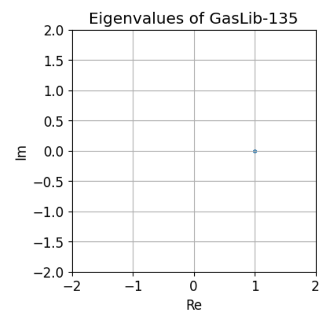

Figure 7: Eigenvalues of the preconditioned system with ILU(5) of GasLib-135. All eigenvalues equal 1.

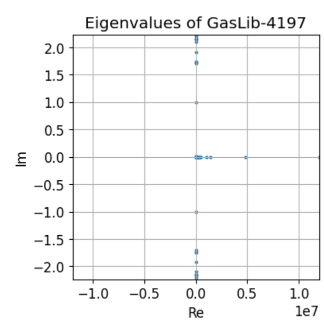

Figure 8: Eigenvalues of the preconditioned system with ILU(5) of GasLib-4197. Most eigenvalues equal 1.