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Research paper



Matrix method for balancing chemical equations of few significant inorganic reactions

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Abstract

Balancing chemical equations provides a unified framework on understanding and quantifying chemical reactions, making it a fundamental tool in chemistry. The prime objectives to balanced chemical equations are to make both sides of the reaction, the reactants as well as the products, possess the same number of atoms per element. It is worth mentioning that understanding how and in what amounts certain molecules are created is made easier with the use of chemical reactions. It also indicates the quantity of reactants required to complete the reaction. These two identities of a chemical reaction are specified by balancing the reaction, which also helps in understanding how to speed up or stop the process. However, balancing long chemical reactions is a difficult and time-consuming task. Employing the principles of mathematical computation to the balancing of chemical equations may come as a remedy to this problem. Thus, in the current paper, we use a matrix-based method, Gauss Elimination mathematical model to balance the chemical equations of a few specific inorganic reactions. Computation work was performed and validated with the help of Python software.

Keywords: *Augmented Matrix; Chemical Equations; Gauss Elimination Method; Linear Equations; Matrix Method.*

1. Introduction

A chemical equation is a figurative illustration of a chemical reaction. In other words, it represents a rearrangement of atoms, molecules, ions etc [1]. To conserve the mass and charge in a reaction, balancing of the chemical equation is vital in Chemistry. In chemical equations, the number of atoms of the reactants and products are altered to make them equal on either side of the reaction. The law of conservation of mass is strictly followed in such cases, according to which, matter can never be created or destroyed [2]. The balancing of chemical equations made its way back in the 18th century, when scientist viz Antoine Lavoisier quantified chemical reactions, for the first time. The development on balancing equations was cemented by Lavoisier's endeavour on the Law of Conservation of Mass. It is noted that balancing chemical equations by inspection is commonly perceived as a trial-and-error method, thereby limiting its use to straightforward chemical reactions and is best suited for miniature reactions. As it possesses certain limitations [3], balancing by inspection fails to provide a systematic assessment of all coefficient sets that could potentially equilibrate an equation [4]. According to Charnock, the algebraic approach to harmonizing both simple and advanced chemical reactions, which are frequently encountered in the secondary chemistry classroom, is superior to the inspection method [5]. Inspection method heavily relies on trial and correction, and therefore, it is effective for simple reactions. However, the algebraic approach is suitable for both simple and advanced reactions that can be transformed into a system of linear equations, which can then be resolved logically and systematically. Further, Risteski in 2010 reported that reconciling chemical reactions is more akin to linear algebra than chemistry. If a chemical process can only produce a vector space, then it can be considered balanced from a scientific perspective. In order to maintain chemical equilibrium, this is a prerequisite which must be satisfied [6]. Shaikh and Yousaf [7] performed a comparative study of few mathematical approaches viz. linear algebra, linear programming, and integer linear programming, which helped in selecting the appropriate techniques for balancing chemical equations based on the complexity of the reactions. Literature survey in [7] additionally reveals that implementing the mathematical concept of linear algebra in balancing chemical equations has also assisted researchers to portray a system's stoichiometry. It provides a captivating platform to researchers in Mathematics and Chemistry to examine linear algebra as a scientific tool. Computational programs and generalized inverses also provide the dais for achieving this equilibrium [8]. When all the elements on either side of a chemical equation are equal, we say that the equation is balanced. Another popular method is the algebraic approach, which treats the coefficients as unknowns and solves for them via a set of equations. This method outperforms the inspection method in terms of balancing both simple and complex reactions, which are common in secondary chemistry instruction [9-10]. The notion of balancing chemical reactions is a topic of applied linear algebra rather than pure chemistry. Scientifically, a chemical reaction can only be balanced if and only if it forms a vector space, which is both necessary and sufficient condition for balancing. A viable reaction is a natural process; consequently, the equation is consistent, leading to a non-trivial solution.

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This assumption is correct and produces no errors. However, if the reaction is not viable, there is only one trivial solution with all coefficients zero. A higher level of mathematical expertise is required to implement numerous strategies for harmonizing chemical processes in both mathematics and chemistry, which rely on generalized matrix inverses [11]. Further, recent progresses in computational chemistry have presented innovative means for balancing chemical equations, moving beyond traditional techniques. Zhang et al. proposed a novel method that views the balancing of chemical equations via the lens of Hilbert bases [12].This approach enables a systematic identification of all possible balanced reactions using a unique set of self-governing elementary reactions, termed Hilbert-basis reactions [12].Again, Phan and his coworkers demonstrated high success rates in rebalancing chemical reactions using SynRBL framework that combines rule-based methods with Maximum Common Substructure (MCS) algorithms [13]. Further, Mohialden et al. in 2023, balanced chemical equations by an automated method employing the Apriori algorithm, which streamlined the balancing process and reduced manual effort [14]. Thus, this paper reports the balancing of a few specific inorganic chemical reactions employing a matrix method, the Gauss Elimination mathematical approach. Python software was used for the computation and validation of the employed mathematical approach. The novelty of this article is that the Gauss Elimination mathematical approach, which is a significant matrix mathematical technique, has not been previously employed by other researchers around the globe to balance the reported chemical equations. This is the first application of Gauss Elimination method to these specific reactions [1-14]. Moreover, this technique provides accurate results which may be lacking in the other trivial methods.

Outlines of the article: The rest of the article is organized as follows: Section 2 contains a general rule for balancing chemical equations and section 3 contains an overview of Gauss Elimination method. Three examples are presented in section 4 and in section 5 a final conclusion is provided on the work.

2. Methods and materials

The general steps to balance a chemical equation are outlined below.

a) Composing the equation that is not balanced.
b) Commencing by formulating the chemical equation by ensuring the accurate representation of chemical formulas for all reactants and products.
c) Quantifying the number of atoms for each element found in both the reactants and products.
d) Altering the coefficients (the numerical values preceding the chemical formulas) in order to achieve equilibrium of atoms for each element on two sides of the equation. Commencing with the most intricate molecule and prioritizing balancing the elements that are present in only one reactant and one product initially.
e) We verify the work by confirming that the quantity of atoms for each element is equal on two sides of the equation. Additionally, the coefficients are to be expressed in the most reduced ratio.
f) Adjustments for charge balance to be made if needed. For redox reactions or ionic equations, the charge should be evenly distributed on both sides of the equation.

2.1. Gauss elimination method

Gauss Elimination method is an iterative scheme generally used to solve systems of linear equations [15-16]. The method is named after Carl Friedrich Gauss.In this method the system of linear equations in matrix form consisting of augmented matrix, is transformed into reduced row echelon form (RREF) [17]. A matrix is said to be in RREF if any zero rows are at the bottom and the first nonzero entry in any row is to the right of the first nonzero entry in any higher row. In RREF all its non-zero rows process a pivot, i.e., a nonzero entry such that all the entries to its left and below it is vanished [18-19]. Elementary row operations are used to transform the system in to its reduced row echelon. Let R_i denotes the i^{th}row and c be any nonzero scalar, then three elementary row operations are common, namely, multiplication a row by a $c(R_i \rightarrow cR_i)$,interchanging rows $(R_i \leftrightarrow R_j)$ and adding one row to another row with a multiple of $c(R_i \rightarrow R_i + cR_j)$. Once the matrix is in RREF, then it is very easy to compute the solution of the system by back substitution. Themethod can be summarized as:

The system of linear equation is expressed in matrix equation given by $Ax = b$.

Then the corresponding augmented matrix will be $[A \mid b]$.

The original matrix can be transformed into the form of $[A' \mid b']$ by performing elementary row operations, where A' is an upper triangular matrix i.e. $a_{ij} = 0$, for $i > j$. The matrix A' is in echelon form.

The solutions of the matrix system $[A' \mid b']$can be obtained by the back-substitution into the higher rows. It is to be noted thatusual elementary row operationsdoesnot alter the solutions of the original system. Therefore, the solution satisfying the $A'x = b'$ are same as that of the original system $Ax = b$.The flow chart of the method is depicted in Figure 1.

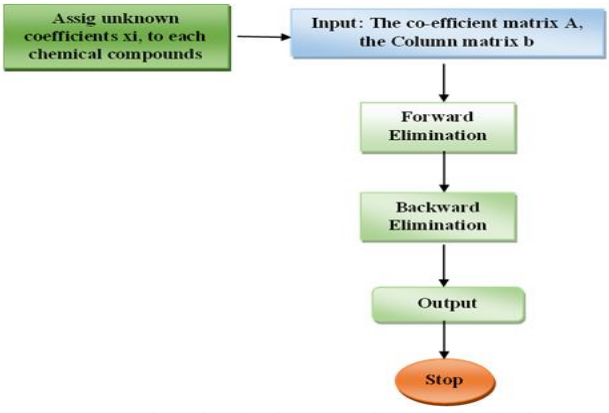


Fig. 1: Flow Chart for the Gauss Elimination Method.

3. Result and discussions

In this section, we consider a few significant inorganic reactions to implement Gauss Elimination method. Computations are performed in the environment of Python with windows 11 operating system.
Example 1: Consider the following chemical reaction:

$$K_4[Fe(SCN)_6] + K_2Cr_2O_7 + H_2SO_4 \rightarrow Fe_2(SO_4)_3 + Cr_2(SO_4)_3 + CO_2 + H_2O + K_2SO_4 + KNO_3$$

This reaction is a complex chemical equation involving the interaction of potassium hexathiocyanoferrate(III) [$K_4[Fe(SCN)_6]$], potassium dichromate ($K_2Cr_2O_7$), and sulfuric acid (H_2SO_4). This equation represents a redox reaction in which several elements experience alterations in their oxidation states. This intricate redox process may be employed in chemical analysis, particularly in oxidation-reduction titrations. It may be utilized in the quantitative analysis of iron, chromium, or other species in solution, considering the precise balance of substantial quantities of each reactant and product in the equation. Chromium, especially in its hexavalent state (Cr6+), is both poisonous and carcinogenic. Reactions that convert Cr(VI) to Cr(III) are environmentally relevant due to the considerably lower toxicity of Cr(III). This reaction may serve as a model or inspiration for chromium detoxification techniques in wastewater treatment. Moreover, the substantial coefficients (such as 97, 355, 36) suggest that this is a well-balanced, large-scale reaction in which minor stoichiometric mistakes may result in incomplete reactions. This renders the equation a compelling task for individuals examining the exact equilibrium of substantial reactions. Once more, sulfuric acid utilized in the reaction acts as a dehydrating agent and a source of sulfate ions that facilitate the formation of sulfate salts. Consequently, it propels the reaction to completion by promoting the dissolution of ionic species in the solution. This equation exemplifies complex multi-step redox chemistry, demonstrating principles of chemical equilibrium, oxidation states, and species transition in industrial and environmental contexts. It is crucial in the examination of redox chemistry, waste management, and industrial chemical operations. The elements make up reaction: Potassium (K); Sulphur (S);Iron (Fe); Carbon (C); Nitrogen (N); Chromium (Cr); Oxygen (O) and Hydrogen (H). The unknown coefficients $x_i, i := 1, 2, \dots \dots \dots, 9$ are assigned to each chemical compounds. The balanced equation can be expressed as follows:

$$x_1K_4[Fe(SCN)_6] + x_2K_2Cr_2O_7 + x_3\ H_2SO_4 \rightarrow x_4Fe_2(SO_4)_3 + x_5Cr_2(SO_4)_3 + x_6\ CO_2 + x_7H_2O + x_8K_2SO_4 + x_9KNO_3$$

Potassium (K): $4x_1+2x_2=2x_8+x_9 \rightarrow 4x_1+2x_2-2x_8-x_9=0$

Iron (Fe): $x_1=2x_4 \rightarrow x_1-2x_4=0$

Sulphur (S): $6x_1+x_3=3x_4+3x_5+x_8 \rightarrow 6x_1+x_3-3x_4-3x_5-x_8=0$

Carbon (C): $6x_1=x_6 \rightarrow 6x_1-x_6=0$

Nitrogen (N): $6x_1=x_9 \rightarrow 6x_1-x_9=0$

Chromium (Cr): $2x_2=2x_5 \rightarrow 2x_2-2x_5=0$

Oxygen (O): $7x_2+4x_3=12x_4+12x_5+2x_6+x_7+4x_8+3x_9 \rightarrow 7x_2+4x_3-12x_4-12x_5-2x_6-x_7-4x_8-3x_9=0$

Hydrogen (H): $2x_3=2x_7 \rightarrow 2x_3-2x_7=0$

It is to be noted that there are eight equations involving nine unknowns. The system of equations is then solved by Gauss Elimination method in python programming as given below:

$$\left[\begin{array}{ccccccccc|c} 4 & 2 & 0 & 0 & 0 & 0 & 0 & -2 & -1 & 0 \\ 1 & 1 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 6 & 0 & 1 & -3 & -3 & 0 & 0 & -1 & 0 & 0 \\ 6 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 2 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 7 & 4 & -12 & -12 & -2 & -1 & -4 & -3 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & -2 & 0 & 0 & 0 \end{array}\right]$$

$$\rightarrow \left[\begin{array}{ccccccccc|c} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1/6 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -97/36 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -355/36 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -1/12 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -97/36 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -355/36 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -91/36 & 0 \end{array}\right]$$

The right-hand side matrix is of RREF; therefore, the required solution of the system can be obtained as

$$\frac{1}{6}x_9 = 0 \Rightarrow x_1 = \frac{1}{6}x_9$$

$$x_2 - \frac{97}{36}x_9 = 0 \Rightarrow x_2 = \frac{97}{36}x_9$$

$x_3 - \frac{355}{36}x_9 = 0 \Rightarrow x_3 = \frac{355}{36}x_9$

$x_4 - \frac{1}{12}x_9 = 0 \Rightarrow x_4 = \frac{1}{12}x_9$

$x_5 - \frac{97}{36}x_9 = 0 \Rightarrow x_5 = \frac{97}{36}x_9$

$x_6 - x_9 = 0 \Rightarrow x_6 = x_9$

$x_7 - \frac{355}{36}x_9 = 0 \Rightarrow x_7 = \frac{355}{36}x_9$

$x_8 - \frac{91}{36}x_9 = 0 \Rightarrow x_8 = \frac{91}{36}x_9$

where, x_9 is a free variable. The particular solution of the above system can be obtained by assigning suitable values to x_9, say $x_9 = 36$. The induced solution set is

$x_1 = 6, x_2 = 97, x_3 = 355, x_4 = 3, x_5 = 97, x_6 = 36, x_7 = 355, x_8 = 91$

Thus, the derived chemical reaction in balanced form is,

$6K_4[Fe(SCN)_6] + 97K_2Cr_2O_7 + 355\ H_2SO_4 \rightarrow 3Fe_2(SO_4)_3 + 97Cr_2(SO_4)_3 + 36\ CO_2 + 355H_2O + 91K_2SO_4 + 36KNO_3$

Example 2: Consider the following chemical reaction

$Mg_3Si_2O_5(OH)_4 + CO_2 \rightarrow MgCO_3 + SiO_2 + H_2O$

This equation depicts a chemical reaction in which serpentine ($Mg_3Si_2O_5(OH)_4$), a prevalent magnesium silicate mineral, reacts with carbon dioxide (CO_2) to yield magnesite ($MgCO_3$), silica (SiO_2), and water (H_2O). This reaction is crucial in both scientific and environmental scenarios. Stable carbonate minerals viz magnesite is formed when serpentine reacts with CO_2saturated air, which is a method for mineral carbonation. This technique is crucial when climate change is taken into consideration. It was observed that $CO_2$is exhausted once sequestered, thus long-term CO_2sequestration has become the need of the hour. Thus, this reaction helps in regulating the atmospheric CO_2levels, thereby contributing to the detention of CO_2 from the atmosphere. This reaction may also help in the capturing of CO_2 emitted during mining activities, thereby counteracting the climate change by eradicating the negative impact of CO_2 emission in nature by mainly the carbon capture and storage activity.The elements make up reaction: Magnesium (Mg); Silicon (Si), Oxygen (O); Carbon (C); Hydrogen (H). The unknown coefficients x_i, $i = 1,2, \ldots\ldots,5$ are assigned to each chemical compound. The balanced equation can be expressed as follows:

$x_1Mg_3Si_2O_5(OH)_4 + x_2CO_2 \rightarrow x_3MgCO_3 + x_4SiO_2 + x_5H_2O$

Magnesium (Mg): $3x_1 = x_3 \Rightarrow 3x_1 - x_3 = 0$

Silicon (Si): $2x_1 = x_4 \Rightarrow 2x_1 - x_4 = 0$

Oxygen (O): $9x_1 + 2x_2 = 3x_3 + 2x_4 + x_5 \Rightarrow 9x_1 + 2x_2 - 3x_3 - 2x_4 - x_5 = 0$

Carbon (C): $x_2 = x_3 \Rightarrow x_2 - x_3 = 0$

Hydrogen (H): $4x_1 = 2x_5 \Rightarrow 4x_1 - 2x_5 = 0$

It is to be noted that there are five equations involving five unknowns. The system of equations is solved by using Gauss Elimination method in python programming as follows:

$$\left[\begin{array}{ccccc|c} 3 & 0 & -1 & 0 & 0 & 0 \\ 2 & 0 & 0 & -1 & 0 & 0 \\ 9 & 2 & -3 & -2 & -1 & 0 \\ 0 & 1 & -1 & 0 & 0 & 0 \\ 4 & 0 & 0 & 0 & -2 & 0 \end{array}\right] \rightarrow \left[\begin{array}{ccccc|c} 1 & 0 & 0 & 0 & -1/2 & 0 \\ 0 & 1 & 0 & 0 & -3/2 & 0 \\ 0 & 0 & 1 & 0 & -3/2 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right]$$

A row of all zeros in RREF of a matrix indicates that one of the original equations was redundant or a linear combination of the other equations. Thus, the solution of the system of equations can be obtained as

$x_1 = \frac{1}{2}x_5$

$x_2 = \frac{3}{2}x_5$

$x_3 = \frac{3}{2}x_5$

$x_4 = x_5$

Where x_5 is a free variable. The particular solution of the system can be obtained by assigning suitable values to x_5, say $x_5 = 2$. The induced solution set is

$x_1 = 1, x_2 = 3, x_3 = 3, x_4 = 2$

Thus, the derived chemical equation in balanced form is,

$Mg_3Si_2O_5(OH)_4 + 3CO_2 \rightarrow 3MgCO_3 + 2SiO_2 + 2H_2O$

Example 3: Consider the following chemical reaction

$Ca_3(PO_4)_2 + SiO_2 \rightarrow P_4O_{10} + CaSiO_3$

This reaction is between calcium phosphate (derived from phosphate rock) and silica to yield phosphorus pentoxide (P_4O_{10}) and calcium silicate ($CaSiO_3$). This equation is essential in the industrial synthesis of phosphorus and its derivatives. Phosphorus pentoxide is an essential stage in the synthesis of elemental phosphorus, which is utilized in fertilizers, phosphoric acid, and several compounds. Calcium silicate is essential in the cement and building sectors. This reaction is essential for phosphorus extraction, facilitating agricultural and many industrial activities, while generating valuable by-products such as calcium silicate used for construction materials. The elements make up reaction: Calcium (Ca); Phosphorus (P); Oxygen (O); Silicon (Si). The unknown coefficients x_1, x_2, x_3, and x_4 are assigned to each chemical compound. The balanced equation can be expressed as follows:

$x_1Ca_3(PO_4)_2 + x_2SiO_2 \rightarrow x_3P_4O_{10} + x_4CaSiO_3$

Calcium (Ca): $3x_1 = x_4 \Rightarrow 3x_1 - x_4 = 0$

Phosphorus (P): $2x_1 = 4x_3$

$\Rightarrow 2x_1 - 4x_3 = 0$

Oxygen (O): $8x_1 + 2x_2 = 10x_3 + 3x_4$

$\Rightarrow 8x_1 + 2x_2 - 10x_3 - 3x_4 = 0$

Silicon (Si): $x_2 = x_4 \Rightarrow x_2 - x_4 = 0$

It is to be noted that there are four equations involving four unknowns. The system of equations is solved by using Gauss Elimination method in python programming as follows:

$$\begin{bmatrix} 3 & 0 & 0 & -1 & 0 \\ 2 & 0 & 4 & 0 & 0 \\ 8 & 2 & 10 & 3 & 0 \\ 0 & 1 & 0 & -1 & 0 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 0 & 0 & -1/3 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & -1/6 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Thus, the solution of the system of equations can be obtained as

$x_1 = \frac{1}{3}x_4$

$x_2 = x_4$

$x_3 = \frac{1}{6}x_4$

Where, x_4 is a free variable. The particular solution of the above system can be obtained by assigning suitable values to x_4, say $x_4 = 6$. The induced solution set is

$x_1 = 2, x_2 = 6, x_3 = 1$

Thus, the derived chemical equation in balanced form is,

$2Ca_3(PO_4)_2 + 6SiO_2 \rightarrow P_4O_{10} + 6\,CaSiO_3$

3.1. Comparative analysis

We compare the Gauss Elimination with Gauss Jordan method adopted in [1], [11], [20] in terms of computational cost. The Gaussian Elimination approach presented in this paper, the linear system induced from the chemical equation is transformed into row echelon form by eliminating entries below the pivot of each column only generating zeros in lower triangular section of the matrix, which also creates a degenerated equation that cannot be solved. This is accomplished by the use of elementary row operations of matrices. The second stage involves using back substitution to solve the system of linear equations. However, in Gauss-Jordan method, it continues to remove entries both above and below the pivots, ultimately resulting in reduced row echelon form and directly solving for the variables. Thus, it requires more computational steps as compared to that of Gauss Jordan method. Therefore, Gauss Elimination method is preferred over Gauss Jordan method in terms of computational cost.

4. Conclusion

Balancing chemical equations is a fundamental tool in chemistry, as it provides a unified framework for comprehending and quantifying chemical reactions. Notably, balancing chemical equations by inspection is often regarded as a trial-and-error approach, which restricts its application to simple chemical reactions and is most effective for small-scale reactions. However, employing mathematical tools in balancing chemical reactions may outperform the inspection method in terms of both simple and complex reactions. Gauss Elimination techniques are known for their scalable properties in solving a spectrum of related problems. In this paper, we reported the balancing of three significant inorganic chemical reactions employing the Gauss elimination mathematical approach. Python code was developed for the computation purpose and it is found that the code works well for balancing chemical reactions. Sometimes, the method yields fractional coefficients that must be multiplied to get whole-number stoichiometric coefficients, adding an extra step that might increase the computational cost. The incorporation of mathematical tools in solving chemical problems has contributed to the interdisciplinary approach of this research, which indeed will help researchers to deal with balancing of chemical equations with large stoichiometry. The potential for Gauss Elimination in evolving computational chemistry is massive, and as future scope further investigation could reveal Gauss novel approaches to addressing organic reactions and other complex chemical systems. Thus, integrating Gauss Elimination into chemistry software like density functional theory, molecular dynamics simulation etc. arise the potential to transform how chemists analyze and model reactions. By mechanizing complex calculations and providing innate tools, such incorporation could improve efficacy in research and development, making advanced computational techniques more reachable to a broader research world.

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Conflict of interest

The authors declare that there is no conflict of interest.

Author contributions

All authors equally contributed to this work.

Ethics approval

Not applicable

Data availability

The data will be available on request

Abbreviation

RREF: Reduced row echelon form

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