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# CMMSE-2019 Mean-based iterative methods for solving nonlinear Chemistry problems

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**Abstract** The third-order iterative method designed by Weerakoon and Fernando includes the arithmetic mean of two functional evaluations in its expression. Replacing this arithmetic mean with different means, other iterative methods have been proposed in the literature. The evolution of these methods in terms of order of convergence implies the inclusion of a weight function for each case, showing an optimal fourth-order convergence, in the sense of Kung-Traub's conjecture. The analysis of these new schemes is performed by means of complex dynamics. These methods are applied on the solution of the nonlinear Colebrook-White equation and the nonlinear system of the equilibrium conversion, both frequently used in Chemistry.

**Keywords** Nonlinear equations · Iterative method · Weight functions · Complex dynamics · Basin of attraction · Chemical applications

**Mathematics Subject Classification (2010)** MSC 65H05

## 1 Introduction

In this manuscript, we are interested in the determination of simple roots of the nonlinear equation $f(x) = 0$, where $f : I \subseteq \mathbb{R} \to \mathbb{R}$ is a nonlinear function defined in the open interval $I$. In general, it is not possible to solve analytically this kind of problems and it is necessary to use iterative methods in order to estimate their solutions. The best known iterative scheme is Newton's procedure, given by

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}, k = 0, 1, 2, \dots$$

which has quadratic convergence for simple roots under particular conditions on $f$. One of the first multipoint variants of Newton's method was designed by Weerakoon and Fernando in [18] as

$$\begin{aligned} y_k &= x_k - \frac{f(x_k)}{f'(x_k)}, \\ x_{k+1} &= x_k - \frac{2f(x_k)}{f'(x_k) + f'(y_k)},\ k = 0, 1, 2, \dots \end{aligned}$$

whose order of convergence is three. The main idea in this method is the use of the arithmetic mean of the derivatives $f'(x_k)$ and $f'(y_k)$ in the denominator of the second step. This allowed the authors to increase the order of convergence of Newton's scheme by adding one functional evaluation. This idea has been extended by

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other authors by replacing the arithmetic mean by other ones: Özban in [13] used the harmonic mean, Ababneh in [1] employed the contraharmonic mean and the centroidal, Heronian, generalized and Lehmer means were used in [17], [16], [19] and [9], respectively. All these methods reach, at most, order of convergence three.

On the other hand, Kung and Traub introduced the concept of optimality in [11] to classify the existing iterative schemes without memory (i.e., by using only $x_k$ in order to calculate $x_{k+1}$). They conjectured that the order of convergence of an iterative methods without memory, which uses $d$ functional evaluations per iteration is bounded by $2^{d-1}$. When this bound is reached, the scheme is called optimal. All the methods previously mentioned use three functional evaluations per iteration and have third-order of convergence; so, they are not optimal schemes.

In order to reach the optimality, we introduce in this paper weight functions in the iterative expressions. They allow us to increase the order of convergence in one unit without adding more functional evaluations. The technique of weight functions have been successfully employed by other authors to construct optimal methods of different orders (a good overview can be found in [2,14]). In this paper, we get fourth-order optimal methods that hold the structure of the different means of the derivatives involved in the iterative expression.

The paper is organized as follows. In Section 2, a set of known iterative methods for solving nonlinear equations based on different expressions of means are introduced. These methods are modified including weight functions to increase the order of convergence of the original ones, reaching the optimality. Furthermore, some extension of the methods are introduced to make them suitable for solving nonlinear systems. Section 3 covers the representation of the basins of attraction of the involved iterative schemes. In Section 4, the methods are applied for solving two common problems in Chemistry, such as the nonlinear Colebrook-White equation and the equilibrium conversion nonlinear system, both with numerical tables and dynamical representations. Finally, Section 5 collects the main conclusions of the study.

## 2 Iterative methods based on different means

The third-order method of Weerakoon and Fernando [18] has the iterative expression

$$x_{k+1} = x_k - \frac{f(x_k)}{M_A\left[f'(x_k), f'(y_k)\right]}, \quad k = 0, 1, 2, \ldots \tag{1}$$

where $y_k$ is the Newton step, and

$$M_A\left[x, y\right] = \frac{x+y}{2}$$

is the arithmetic mean. From now on, instead of using the arithmetic mean, other expressions of means are applied to generate the iterative methods.

### 2.1 Methods with different expressions of the mean

There are different papers in the literature that replace the arithmetic mean of (1) by other expressions, collected in [9]. For instance,

– Özban [13] uses the harmonic mean $M_{Ha}$,

$$M_{Ha}[x, y] = 2\left(\frac{1}{x} + \frac{1}{y}\right)^{-1},$$

– Singh et al. [16] use the Heronian mean $M_{He}$,

$$M_{He}[x, y] = \frac{2}{3}\frac{x+y}{2} + \frac{1}{3}\sqrt{xy}.$$

– Lukić and Ralević in [12] employ the geometric mean $M_G$,

$$M_G[x, y] = \sqrt{xy},$$

– Xiaojian in [19] utilizes the quadratic mean $M_Q$,

$$M_Q[x, y] = \sqrt{\frac{1}{2}\left(x^2 + y^2\right)}.$$

Replacing $M_A$ the expressions of the means $M_{Ha}$, $M_{He}$, $M_G$ and $M_Q$ in equation (1), the obtained iterative schemes satisfy the following result.

**Theorem 1** *Let us suppose that $f : I \subset \mathbb{R} \to \mathbb{R}$ is a sufficiently differentiable function in an open interval $I$ and $\bar{x} \in I$ is a simple root of $f(x) = 0$. If the initial guess $x_0$ is close enough to $\bar{x}$, then the methods based on (1), replacing the arithmetic mean by the harmonic mean, the geometric mean, the Heronian mean and the quadratic mean are third-order convergent, being its error equation*

$$e_{k+1} = Me_k^3 + \mathcal{O}\left(e_k^4\right),$$

*where $e_k = x_k - \bar{x}$ and $M \neq 0$.*

The iterative method of Weerakoon and Fernando [18] can be rewritten using a weight function. In this way, the iterative expression results as

$$x_{k+1} = x_k - G(t_k, u_k), \quad k = 0, 1, 2, \ldots, \tag{2}$$

where $t = \dfrac{f'(y_k)}{f'(x_k)}$, $u = \dfrac{f(x_k)}{f'(x_k)}$ and $G(t, u) = \dfrac{2u}{1+t}$.

In a similar way, the iterative methods based of different means can be also expressed by means of this weight function $G(t, u)$. Their corresponding functions are

– Harmonic mean,

$$G_{Ha}(t, u) = \frac{u}{2}\left(1 + \frac{1}{t}\right), \tag{3}$$

– Geometric mean,

$$G_G(t, u) = \frac{u}{\sqrt{t}}, \tag{4}$$

– Heronian mean,

$$G_{He}(t, u) = \frac{3u}{1 + t + \sqrt{t}}, \tag{5}$$

– Quadratic mean,

$$G_Q(t, u) = \frac{u}{\sqrt{\frac{1}{2} + \frac{1}{2}t^2}}. \tag{6}$$

## 2.2 Increase of the order of convergence

The inclusion of a dumping parameter $\lambda$ in the Newton step generates the J family of iterative methods, whose general expression is

$$\begin{aligned} y_k &= x_k - \lambda\frac{f(x_k)}{f'(x_k)}, \\ x_{k+1} &= x_k - J(t_k, u_k), \quad k = 0, 1, 2, \ldots \end{aligned} \tag{7}$$

where $\lambda \in \mathbb{R} \sim \{0\}$.

**Theorem 2** *Let us suppose that $f : I \subset \mathbb{R} \longrightarrow \mathbb{R}$ is a sufficiently differentiable function in an open interval $I$ and $\bar{x} \in I$ is a simple root of $f(x) = 0$. If the initial guess $x_0$ is close enough of $\bar{x}$, and $J : \mathbb{R}^2 \to \mathbb{R}$ is a function of class $\mathcal{C}^4$ in $\mathbb{R}^2$ such that $J(1,0) = J_{10}(1,0) = J_{02}(1,0) = J_{20}(1,0) = J_{03}(1,0) = J_{30}(1,0) = J_{12}(1,0) = 0$, $J_{01}(1,0) = 1$ and $J_{11}(1,0) = -\frac{1}{2\lambda}$, $J_{21}(1,0) = \frac{1}{2\lambda^2}$, where*

$$J_{ij}(t, j) = \frac{\partial^{i+j}}{\partial t^i \partial u^j} J(t, u),$$

*then J family (7) is third-order convergent, being its error equation*

$$e_{k+1} = \frac{1}{2}(3\lambda - 2)c_3 e_k^3 + \mathcal{O}(e_k^4),$$

*where $c_j = \frac{1}{j!}\frac{f^{(j)}(\bar{x})}{f'(\bar{x})}$, for $j \geq 2$. Let us observe that, for $\lambda = 2/3$, J family is fourth-order convergent, that is, an optimal iterative method, whose error equation is*

$$e_{k+1} = \left(5c_2^3 - c_3c_2 + \frac{c_4}{9}\right)e_k^4 + \mathcal{O}\left(e_k^5\right).$$

*Proof* Using the Taylor expansion for $f(x)$ and $f'(x)$ around $\bar{x}$,

$$f(x_k) = f'(\bar{x})\left(e_k + c_2 e_k^2 + c_3 e_k^3 + c_4 e_k^4 + c_5 e_k^5\right) + \mathcal{O}\left(e_k^6\right),$$

$$f'(x_k) = f'(\bar{x})\left(1 + 2c_2 e_k + 3c_3 e_k^2 + 4c_4 e_k^3 + 5c_5 e_k^4\right) + \mathcal{O}\left(e_k^5\right),$$

the quotient $u = \frac{f(x)}{f'(x)}$ is

$$\begin{aligned} u_k &= \tfrac{f(x_k)}{f'(x_k)} \\ &= e_k - c_2 e_k^2 + \left(2c_2^2 - 2c_3\right) e_k^3 + \left(-4c_2^3 + 7c_3c_2 - 3c_4\right) e_k^4 + \left(8c_2^4 - 20c_3c_2^2 + 10c_4c_2 + 6c_3^2 - 4c_5\right) e_k^5 \\ &\quad + \mathcal{O}\left(e_k^6\right), \end{aligned}$$

and the first step results in

$$\begin{aligned} y_k &= x_k - \lambda \frac{f(x_k)}{f'(x_k)} \\ &= (1-\lambda)e_k + c_2\lambda e_k^2 - 2\lambda\left(c_2^2 - c_3\right) e_k^3 + \left(4c_2^3 - 7c_3c_2 + 3c_4\right)\lambda e_k^4 \\ &\quad -2\lambda\left(4c_2^4 - 10c_3c_2^2 + 5c_4c_2 + 3c_3^2 - 2c_5\right) e_k^5 + \mathcal{O}\left(e_k^6\right). \end{aligned}$$

Expanding $f'(y)$ around $\bar{x}$,

$$\begin{aligned} f'(y_k) &= f'(\bar{x})\left[1 - 2\left(c_2(\lambda-1)\right) e_k + \left(3c_3(\lambda-1)^2 + 2c_2^2\lambda\right) e_k^2\right. \\ &\quad +2\left(-2c_4(\lambda-1)^3 - 2c_2^3\lambda + c_2c_3\lambda(5-3\lambda)\right) e_k^3 \\ &\quad \left.+\left(5c_5(\lambda-1)^4 - 12c_3^2\lambda(\lambda-1) + 8c_2^4\lambda + c_2^2c_3\lambda(15\lambda-26) + 6c_2c_4\lambda(2(\lambda-2)\lambda+3)\right) e_k^4\right] + \mathcal{O}\left(e_k^5\right). \end{aligned}$$

The weight variable $t$ has the expression

$$\begin{aligned} t_k &= \frac{f'(y_k)}{f'(x_k)} \\ &= 1 - 2\left(c_2\lambda\right) e_k + 3\lambda\left(c_3(\lambda-2) + 2c_2^2\right) e_k^2 - 4\left(\lambda\left(c_4\left(\lambda^2 - 3\lambda + 3\right) + c_3c_2(3\lambda-7) + 4c_2^3\right)\right) e_k^3 \\ &\quad +\lambda\left(2c_4c_2\left(10\lambda^2 - 24\lambda + 25\right) + 5c_5\left(\lambda^3 - 4\lambda^2 + 6\lambda - 4\right) + c_3c_2^2(39\lambda - 100) + c_3^2(30 - 21\lambda) + 40c_2^4\right) e_k^4 \\ &\quad +\mathcal{O}\left(e_k^5\right). \end{aligned}$$

Since $u_k \to 0$ and $t_k \to 1$ when $k \to \infty$, the expansion of $J(t,u)$ around $(1,0)$ is

$$\begin{aligned} J(t_k,u_k) &= J(1,0) + J_{10}(1,0)(t_k-1) + J_{0,1}(1,0)u_k \\ &\quad +\tfrac{1}{2}\left(J_{20}(1,0)(t_k-1)^2 + 2J_{11}(1,0)(t_k-1)u_k + J_{02}(1,0)u_k^2\right) \\ &\quad +\tfrac{1}{6}\left(J_{30}(1,0)(t_k-1)^3 + J_{21}(1,0)(t_k-1)^2u_k + J_{12}(1,0)(t_k-1)u_k^2 + J_{03}(1,0)u_k^3\right) \\ &= J(1,0) + e_k\left(J_{01}(1,0) - 2c_2J_{10}(1,0)\lambda\right) + e_k^2\left(-c_2(J_{01}(1,0) + 2J_{11}(1,0)\lambda) + 2c_2^2\lambda(3J_{10}(1,0)\right. \\ &\quad +2J_{20}(1,0)\lambda) + 3c_3J_{10}(1,0)(\lambda-2)\lambda + J_{02}(1,0)) + e_k^3\left(2c_2^2(J_{01}(1,0) + 2\lambda(2J_{11}(1,0)\right. \\ &\quad +J_{21}(1,0)\lambda)) + c_3(3J_{11}(1,0)(\lambda-2)\lambda - 2J_{01}(1,0)) - 2c_2(J_{02}(1,0) + J_{12}(1,0)\lambda) \\ &\quad -8c_2^3\lambda(2J_{10}(1,0) + \lambda(3J_{20}(1,0) + J_{30}(1,0)\lambda)) - 4c_3c_2\lambda(J_{10}(1,0)(3\lambda-7) + 3J_{20}(1,0)(\lambda-2)\lambda) \\ &\quad -4c_4J_{10}(1,0)\lambda((\lambda-3)\lambda+3) + J_{03}(1,0)) + e_k^4\left(c_2\left(c_3(7J_{01}(1,0) + \lambda(J_{11}(1,0)(38-15\lambda)\right.\right. \\ &\quad -12J_{21}(1,0)(\lambda-2)\lambda)) + 2c_4\lambda(J_{10}(1,0)(2\lambda(5\lambda-12)+25) + 8J_{20}(1,0)\lambda((\lambda-3)\lambda+3)) \\ &\quad -3J_{03}(1,0)) - 2c_2^3(2J_{01}(1,0) + \lambda(13J_{11}(1,0) + 14J_{21}(1,0)\lambda)) - c_4(3J_{01}(1,0) \\ &\quad +4J_{11}(1,0)\lambda((\lambda-3)\lambda+3)) + c_2^2\left(c_3\lambda(J_{10}(1,0)(39\lambda-100) + 4\lambda(J_{20}(1,0)(21\lambda-46)\right. \\ &\quad +9J_{30}(1,0)(\lambda-2)\lambda)) + 5(J_{02}(1,0) + 2J_{12}(1,0)\lambda)) + c_3(3J_{12}(1,0)(\lambda-2)\lambda - 4J_{02}(1,0)) \\ &\quad +4c_2^4\lambda(10J_{10}(1,0) + \lambda(25J_{20}(1,0) + 18J_{30}(1,0)\lambda)) + 3c_3^2\lambda\left(J_{10}(1,0)(10-7\lambda)\right. \\ &\quad \left.+3J_{20}(1,0)\lambda(\lambda-2)^2\right) + 5c_5J_{10}(1,0)(\lambda-2)\lambda((\lambda-2)\lambda+2)) + \mathcal{O}\left(e_k^5\right). \end{aligned}$$

Therefore,

$$\begin{aligned} e_{k+1} &= e_k - J(t_k,u_k) \\ &= -J(1,0) + e_k\left(2c_2J_{10}(1,0)\lambda - J_{01}(1,0) + 1\right) + e_k^2\left(c_2\left(-2c_2\lambda(3J_{10}(1,0) + 2J_{20}(1,0)\lambda) + J_{01}(1,0)\right.\right. \\ &\quad +2J_{11}(1,0)\lambda) - 3c_3J_{10}(1,0)(\lambda-2)\lambda - J_{02}(1,0)) + e_k^3\left(-2c_2^2(J_{01}(1,0) + 2\lambda(2J_{11}(1,0)\right. \\ &\quad +J_{21}(1,0)\lambda)) + c_3(2J_{01}(1,0) - 3J_{11}(1,0)(\lambda-2)\lambda) + 2c_2\left(2c_3\lambda(J_{10}(1,0)(3\lambda-7)\right. \\ &\quad +3J_{20}(1,0)(\lambda-2)\lambda) + J_{02}(1,0) + J_{12}(1,0)\lambda) + 8c_2^3\lambda(2J_{10}(1,0) + \lambda(3J_{20}(1,0) + J_{30}(1,0)\lambda)) \\ &\quad +4c_4J_{10}(1,0)\lambda((\lambda-3)\lambda+3) - J_{03}(1,0)) + e_k^4\left(c_2\left(c_3(\lambda(J_{11}(1,0)(15\lambda-38) + 12J_{21}(1,0)(\lambda-2)\lambda)\right.\right. \\ &\quad -7J_{01}(1,0)) - 2c_4\lambda(J_{10}(1,0)(2\lambda(5\lambda-12)+25) + 8J_{20}(1,0)\lambda((\lambda-3)\lambda+3)) + 3J_{03}(1,0)) \\ &\quad +c_2^3\left(4J_{01}(1,0) + 26J_{11}(1,0)\lambda + 28J_{21}(1,0)\lambda^2\right) + c_4(3J_{01}(1,0) + 4J_{11}(1,0)\lambda((\lambda-3)\lambda+3)) \\ &\quad +c_2^2\left(c_3\lambda(J_{10}(1,0)(100-39\lambda) + 4\lambda(J_{20}(1,0)(46-21\lambda) - 9J_{30}(1,0)(\lambda-2)\lambda)) - 5(J_{02}(1,0)\right. \\ &\quad +2J_{12}(1,0)\lambda)) + c_3(4J_{02}(1,0) - 3J_{12}(1,0)(\lambda-2)\lambda) - 4c_2^4\lambda(10J_{10}(1,0) + \lambda(25J_{20}(1,0) \\ &\quad +18J_{30}(1,0)\lambda)) - 3c_3^2\lambda\left(J_{10}(1,0)(10-7\lambda) + 3J_{20}(1,0)\lambda(\lambda-2)^2\right) \\ &\quad -5c_5J_{10}(1,0)(\lambda-2)\lambda((\lambda-2)\lambda+2)) + \mathcal{O}\left(e_k^5\right). \end{aligned}$$

Setting $J(1,0) = J_{10}(1,0) = J_{02}(1,0) = J_{20}(1,0) = J_{03}(1,0) = J_{30}(1,0) = J_{12}(1,0) = 0,\ J_{01}(1,0) = 1$ and $J_{11}(1,0) = -\frac{1}{2\lambda}$, $J_{21}(1,0) = \frac{1}{2\lambda^2}$, the first and second order term vanish and the error equation is

$$e_{k+1} = \frac{1}{2}c_3(3\lambda-2)e_k^3 + \left(c_4\left(-2\lambda^2+6\lambda-3\right) - \frac{3}{2}c_3c_2\lambda + 5c_2^3\right)e_k^4 + \mathcal{O}\left(e_k^5\right).$$

For $\lambda = 2/3$, the family is fourth-order convergent and its error equation is

$$e_{k+1} = \left(5c_2^3 - c_3c_2 + \frac{c_4}{9}\right)e_k^4 + \mathcal{O}\left(e_k^5\right).$$

□

To hold the optimal fourth-order of convergence and to include the mean-based weight function $G(t,u)$, function $J(t,u)$ is constructed as the product of $G(t,u)$ and another weight function $H(t)$. So, expression is re-written as (7),

$$\begin{aligned} y_k &= x_k - \lambda\frac{f(x_k)}{f'(x_k)}, \\ x_{k+1} &= x_k - G(t_k,u_k)H(t_k), \quad k = 0,1,2,\ldots \end{aligned} \tag{8}$$

From now on, the weight function $H(t)$ for each iterative method based on means is presented. Family (8) is fourth-order convergent if $\lambda = 2/3$ and,

- for the arithmetic mean of Weerakoon and Fernando,

$$G(t,u) = G_{WF}(t,u) = \frac{2u}{1+t}, \text{ and } H(t) = H_{WF}(t) = \frac{3}{4}t^2 - \frac{7}{4}t + 2, \tag{9}$$

  being its error equation

$$e_{k+1} = \frac{1}{9}\left(c_2^3 - 9c_2c_3 + c_4\right)e_k^4 + \mathcal{O}\left(e_k^5\right).$$

- for the harmonic mean,

$$G(t,u) = G_{Ha}(t,u), \text{ and } H(t) = H_{Ha}(t) = \frac{1}{2}t^2 - \frac{5}{4}t + \frac{7}{4}, \tag{10}$$

  and its error equation is

$$e_{k+1} = \left(\frac{79}{27}c_2^3 - c_2c_3 + \frac{1}{9}c_4\right)e_k^4 + \mathcal{O}\left(e_k^5\right).$$

- for the geometric mean,

$$G(t,u) = G_G(t,u), \text{ and } H(t) = H_G(t) = \frac{5}{8}t^2 - \frac{3}{2}t + \frac{15}{8}, \tag{11}$$

  being

$$e_{k+1} = \left(\frac{89}{27}c_2^3 - c_2c_3 + \frac{1}{9}c_4\right)e_k^4 + \mathcal{O}\left(e_k^5\right).$$

- for the Heronian mean,

$$G(t,u) = G_{He}(t,u), \text{ and } H(t) = H_{He}(t) = \frac{7}{8}t^2 - 2t + \frac{17}{8}, \tag{12}$$

  and the corresponding error equation is

$$e_{k+1} = \left(\frac{109}{27}c_2^3 - c_2c_3 + \frac{1}{9}c_4\right)e_k^4 + \mathcal{O}\left(e_k^5\right).$$

- for the quadratic mean,

$$G(t,u) = G_Q(t,u), \text{ and } H(t) = H_Q(t) = \frac{17}{24}t^2 - \frac{5}{3}t + \frac{47}{24}, \tag{13}$$

  being its error equation

$$e_{k+1} = \left(\frac{287}{81}c_2^3 - c_2c_3 + \frac{1}{9}c_4\right)e_k^4 + \mathcal{O}\left(e_k^5\right).$$

### 2.3 Extension to solve nonlinear systems

It is not always possible to directly extend an scalar iterative method to the multidimensional case $F(x) = 0$, where $F : D \subseteq \mathbb{R}^n \to \mathbb{R}^n$ is a vectorial function defined in a convex set $D$. Even when it is possible, it is not guaranteed that the order is preserved. Some of the proposed schemes can not be directly extended as square roots of matrices are necessary; however, two of them can be used for solving nonlinear systems, preserving their order of convergence. It is the case of the arithmetic mean scheme

$$\begin{aligned} y^{(k)} &= x^{(k)} - \tfrac{2}{3}\left[F'(x^{(k)})\right]^{-1} F(x^{(k)}), \\ x^{(k+1)} &= x^{(k)} - G_{WF}\left(t^{(k)}, u^{(k)}\right) H_{WF}(t^{(k)}), \quad k = 0, 1, 2, \ldots, \end{aligned} \tag{14}$$

where $F'(x)$ is the Jacobian matrix associated to $F$,

$$[G_{WF}(t,u) = 2\,[I+t]^{-1}\,u, \text{ and } H_{WF}(t) = \frac{3}{4}t^2 - \frac{7}{4}t + 2I, \tag{15}$$

being $t = \left[F'(y^{(k)})\right]^{-1} F'(x^{(k)})$, $u = \left[F'(x^{(k)})\right]^{-1} F(x^{(k)})$ and $I$ the identity matrix.

On the other hand, the fourth-order multidimensional scheme based on harmonic mean is obtained by replacing in expression (14) weight functions $G_{WF}(t,u)$ and $H_{WF}(t)$ by

$$G_{Ha} = \frac{1}{2}\left(u + \left[F'\left(y^{(k)}\right)\right]^{-1} F\left(x^{(k)}\right)\right), \text{ and } H_{Ha}(t) = \frac{1}{2}t^2 - \frac{5}{4}t + \frac{7}{4}I, \tag{16}$$

respectively.

In Section 4, it will be numerically checked that these extensions can solve vectorial nonlinear chemical problems holding the fourth-order of convergence.

## 3 Stability analysis

A wide stability analysis of an iterative method covers an in-depth study on the rational function that results from the application of the method to a nonlinear function, such as [3,4,6]. However, the most of the proposed methods include square roots in their iterative expressions and therefore, their associate fixed point functions are not rational. Another kind of study consists of the representation of the basins of attraction of a method on standard nonlinear equations, and an idea of their stability properties can be deduced from them.

Let $R : \hat{\mathbb{C}} \to \hat{\mathbb{C}}$ be a fixed point function, where $\hat{\mathbb{C}}$ is the Riemann sphere. Each iterative method has its own fixed point operator when it is applied on a nonlinear function, but it is not always rational. Table 1 collects the expressions of the fixed point operators obtained when the methods are applied on the quadratic polynomials $f(z) = z^2 + c, c \in \{-1, 0, 1\}$.

**Table 1** Fixed point operators resulting from the application of the proposed methods to quadratic polynomials

| Method | $z^2 \mp 1$ | $z^2$ |
|---|---|---|
| (9) | $\dfrac{1 \mp 4z^2 + 21z^4 \pm 6z^6}{4z^3 \pm 20z^5}$ | $\dfrac{3z}{10}$ |
| (10) | $\dfrac{83z^8 \pm 343z^6 + 3z^4 \pm z^2 + 2}{144z^5(\pm 1 + 2z^2)}$ | $\dfrac{83z}{288}$ |
| (11) | $\dfrac{\pm 5\sqrt{3} - 21\sqrt{3}z^2 \pm 99\sqrt{3}z^4 + \left(-83\sqrt{3} + 144\sqrt{2 \pm \frac{1}{z^2}}\right) z^6}{144z^5\sqrt{2 \pm \frac{1}{z^2}}}$ | $\dfrac{(288 - 83\sqrt{6})z}{288}$ |
| (12) | $\dfrac{\pm 121z^4 - 27z^2 + \left(16\sqrt{3}\sqrt{2 \pm \frac{1}{z^2}} - 5\right) z^6 \pm 7}{16z^3\left(\pm 1 + \left(\sqrt{3}\sqrt{2 \pm \frac{1}{z^2}} + 5\right) z^2\right)}$ | $\dfrac{\left(16\sqrt{6} - 5\right) z}{16\left(\sqrt{6} + 5\right)}$ |
| (13) | $\dfrac{\pm 303\sqrt{2}z^4 - 69\sqrt{2}z^2 + \left(144\sqrt{\frac{1}{z^4} \pm \frac{4}{z^2} + 13} - 251\sqrt{2}\right) z^6 \pm 17\sqrt{2}}{144\sqrt{\frac{1}{z^4} \pm \frac{4}{z^2} + 13}z^5}$ | $\dfrac{\left(-251\sqrt{26} + 1872\right) z}{1872}$ |

Let us define the orbit of a point $z_0$ as the set of successive applications of the operator $R$. It can be expressed as

$$\text{orbit}(z_0) = \{z_0, R(z_0), R^2(z_0), \ldots, R^n(z_0), \ldots\}.$$

Moreover, the basin of attraction of an attracting fixed point $\mathcal{A}(z^*)$ is the set of initial points $z_0$ whose orbit tends to the attracting fixed point $z^*$ (that is, a point satisfying $|R'(z^*)| < 1$). It can be defined by

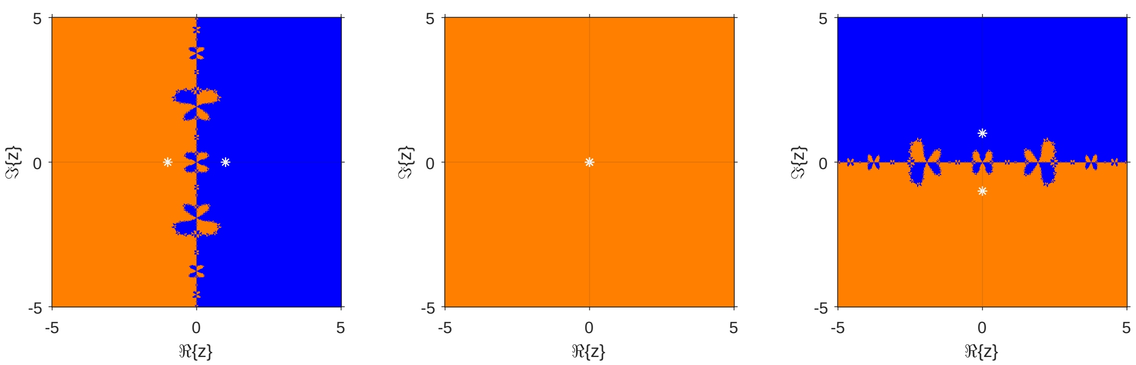
$$\mathcal{A}(z^*) = \{z_0 \in \hat{\mathbb{C}} : R^n(z_0) = z^*, n \to \infty\}.$$

It can be checked that the attracting fixed points $z^*$ of the operators appearing in Table 1 match with the roots of the polynomials. In this sense, $z^* \in \{-1, 1\}$ for $f(z) = z^2 - 1$, $z^* = 0$ for $f(z) = z^2$ and $z^* \in \{-i, i\}$ for $f(z) = z^2 + 1$. So, our methods can only converge to the roots of our nonlinear equations. The dynamical planes represent the basins of attraction of an iterative method, based on its fixed point operator. The orbit of a set of initial points in a mesh of points having real part $\Re\{z\} \in [-5, 5]$ and imaginary part $\Im\{z\} \in [-5, 5]$ has been obtained for each one of the fourth-order proposed methods, following the guidelines of [5]. The attracting fixed points have been represented as white stars, while the color of the basins of attraction follow the mapping of Table 2.

**Table 2** Color mapping of the basins of attraction.

| Function | Attracting fixed point $z^*$ | Color (RGB) |
|---|---|---|
| $f(z) = z^2 - 1$ | $-1$ | Orange $(255, 128, 0)$ |
| | $1$ | Blue $(0, 0, 255)$ |
| $f(z) = z^2$ | $0$ | Orange $(255, 128, 0)$ |
| $f(z) = z^2 + 1$ | $-i$ | Orange $(255, 128, 0)$ |
| | $i$ | Blue $(0, 0, 255)$ |

Figures 1–5 represent the basins of attraction of the methods (9)–(13) when they are applied on quadratic polynomials $f(z) = z^2 + c, c \in \{-1, 0, 1\}$.



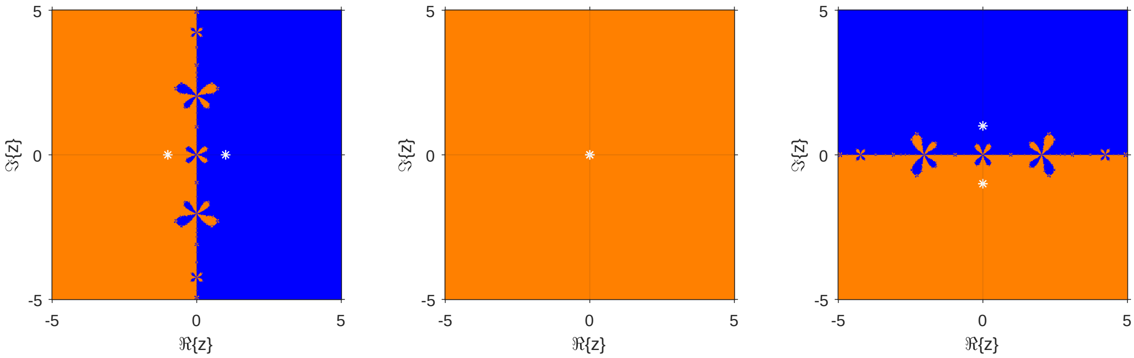

(a) $f(z) = z^2 - 1$ (b) $f(z) = z^2$ (c) $f(z) = z^2 + 1$

**Fig. 1** Dynamical planes for iterative method based on arithmetic mean (9)

For the five methods under study, each iterative expression for every quadratic polynomial converge to the expected roots, as Figures 1–5 confirm. Moreover, the dynamical planes corresponding to $f(z) = z^2 - 1$ and $f(z) = z^2 + 1$ are a rotation of $\pi/2$ radians clockwise. So, these fourth-order schemes perform in a very stable way on quadratic polynomials. In the following section, we test their performance on other nonlinear problems.

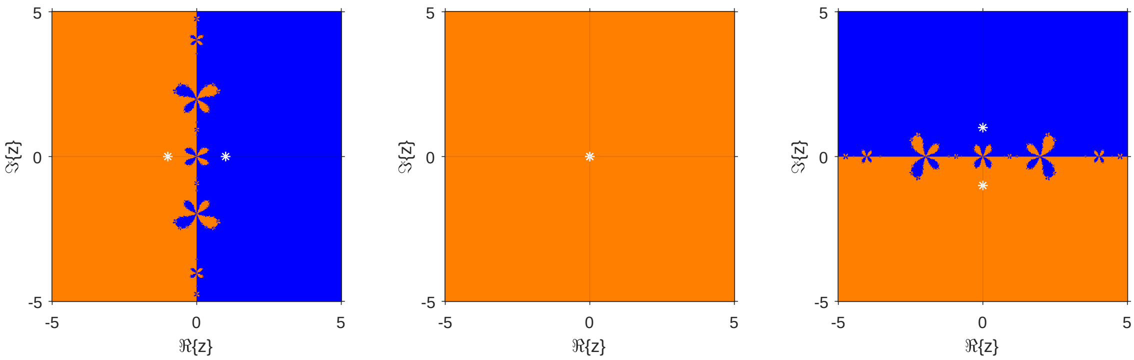
## 4 Numerical performance

In order to check the applicability of the iterative methods in terms of robustness and accuracy, some nonlinear problems appearing in Chemistry are solved. The numerical tests have been performed with Matlab version R2017b, with variable precision arithmetics of 2000 digits of mantissa.



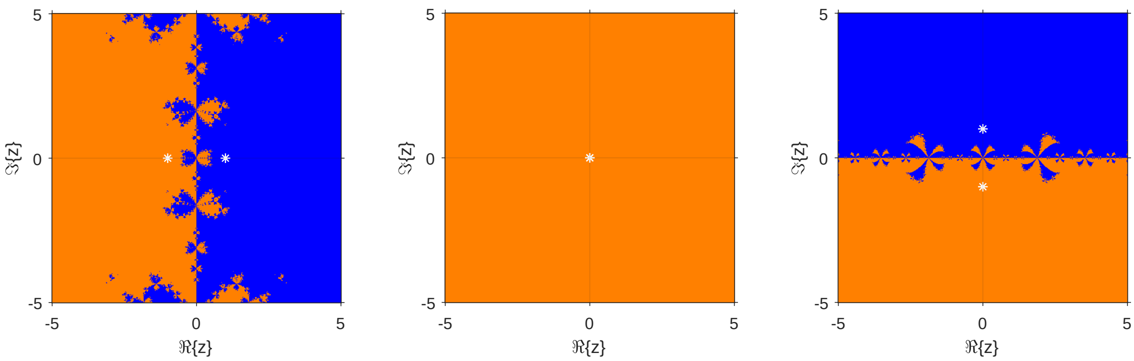

(a) $f(z) = z^2 - 1$ (b) $f(z) = z^2$ (c) $f(z) = z^2 + 1$

**Fig. 2** Dynamical planes for iterative method based on harmonic mean (10)




(a) $f(z) = z^2 - 1$ (b) $f(z) = z^2$ (c) $f(z) = z^2 + 1$

**Fig. 3** Dynamical planes for iterative method based on geometric mean (11)

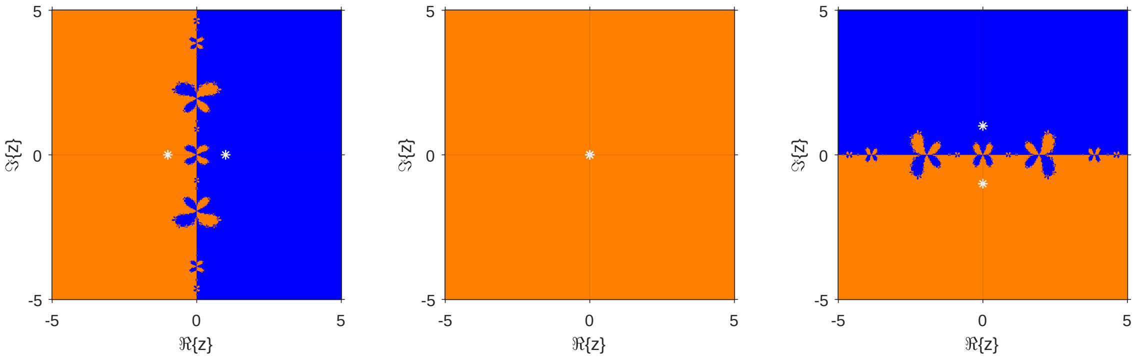



(a) $f(z) = z^2 - 1$ (b) $f(z) = z^2$ (c) $f(z) = z^2 + 1$

**Fig. 4** Dynamical planes for iterative method based on Heronian mean (12)

On the one hand, we estimate the solution of the nonlinear equation involved in the obtention of the friction factor of a pipe. For solving numerically this nonlinear equation, the stopping criteria is set at either $|f(x_{k+1})| < 10^{-500}$ or $|x_{k+1} - x_k| < 10^{-500}$; both residuals will be included in the table of results, joint with the number of iterations needed and the initial guess used.

On the other hand, the equilibrium conversion of some chemical reactions. In this case, a nonlinear system of equations is solved. The stopping criteria in this case is either $\left\| F\left(x^{(k+1)}\right)\right\| < 10^{-500}$ or $\left\|x^{(k+1)} - x^{(k)}\right\| < 10^{-500}$, appearing also these residuals in Table 4, as well as the initial estimations used and the number of iterations needed to reach the solution with the required precision.




(a) $f(z) = z^2 - 1$ (b) $f(z) = z^2$ (c) $f(z) = z^2 + 1$

**Fig. 5** Dynamical planes for iterative method based on quadratic mean (13)

### 4.1 Friction factor

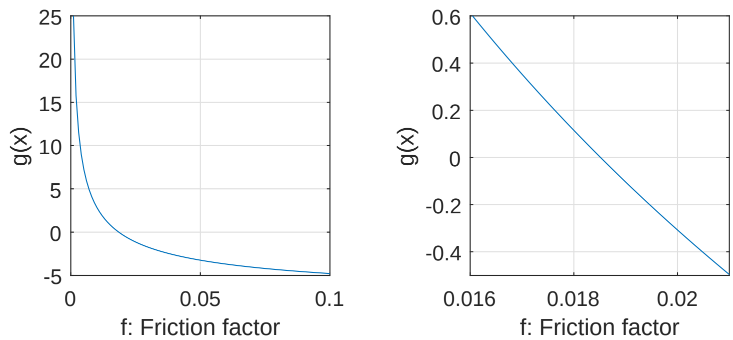
A key value for obtaining the pressure drop in a pipeline at a given flow rate is the friction factor $f$ [15]. The Colebrook-White equation [7] is a relationship between the friction factor, the Reynolds number $R$, the pipe roughness $\epsilon$ and the inner diameter of the pipe $D$. Its expression, for $R > 4000$, is

$$\sqrt{\frac{1}{f}} = -2\log_{10}\left(\frac{\epsilon/D}{3.7} + \frac{2.51}{R\sqrt{f}}\right). \tag{17}$$

The application of the iterative methods requires the solution of $g(x) = 0$. Therefore, equation (17) gets into

$$g(x) = \sqrt{\frac{1}{f}} + 2\log_{10}\left(\frac{\epsilon/D}{3.7} + \frac{2.51}{R\sqrt{f}}\right). \tag{18}$$

For the test cases, $\epsilon/D = 10^{-4}$ and $R = 10^5$. Figure 6 represents function $g(x)$ described in (18).




(a) $0 \leq x \leq 0.1$ (b) $0.016 \leq x \leq 0.021$

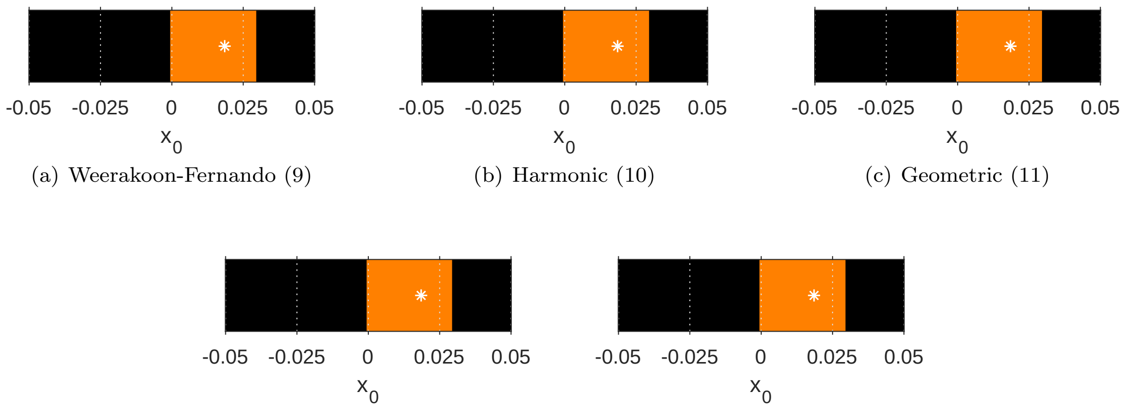
**Fig. 6** Friction factor

Table 3 collects the data from the application of the different iterative methods to the problem defined by (18), for three different initial estimations $x_0 \in \{0.01, 0.0185, 0.02\}$. The solution of (18) is $\bar{f} \approx 0.01851387$. It is deduced from Table 3 that every method finds the solution of the nonlinear problem, with similar accuracy, with a high number of iterations. This is a proof of the difficult nature of the equation to be solved.

In order to observe the dependence of the methods on initial estimations, we use the dynamical lines in Figure 7. Each dynamical line represents the performance of the methods for solving the friction factor problem (17) when different iterative methods are applied, showing in orange color the set of initial guesses that converge to the solution $\bar{f}$. This solution is represented with a white star. The set of initial guesses, for every method, covers the values in the interval $x_0 \in (0, 0.035)$, as can be seen in Figure 7 and it can be observed that the range of converging starting estimations is approximately the same for all the proposed methods.

**Table 3** Numerical results for proposed iterative methods solving the Colebrook-White equation (17)

| $x_0$ | Method | Iterations | $\lvert x_{k+1} - x_k \rvert$ | $\lvert g(x_{k+1}) \rvert$ |
|---|---|---|---|---|
| 0.01 | (9) | 33 | $4.30 \cdot 10^{-502}$ | $8.51 \cdot 10^{-517}$ |
| 0.01 | (10) | 33 | $7.10 \cdot 10^{-503}$ | $1.41 \cdot 10^{-517}$ |
| 0.01 | (11) | 33 | $1.02 \cdot 10^{-502}$ | $2.02 \cdot 10^{-517}$ |
| 0.01 | (12) | 33 | $6.00 \cdot 10^{-501}$ | $1.19 \cdot 10^{-515}$ |
| 0.01 | (13) | 33 | $7.42 \cdot 10^{-503}$ | $1.47 \cdot 10^{-517}$ |
| 0.0185 | (9) | 31 | $3.69 \cdot 10^{-492}$ | $7.30 \cdot 10^{-507}$ |
| 0.0185 | (10) | 31 | $2.67 \cdot 10^{-492}$ | $5.29 \cdot 10^{-507}$ |
| 0.0185 | (11) | 31 | $3.18 \cdot 10^{-492}$ | $6.30 \cdot 10^{-507}$ |
| 0.0185 | (12) | 31 | $4.20 \cdot 10^{-492}$ | $8.31 \cdot 10^{-507}$ |
| 0.0185 | (13) | 31 | $3.52 \cdot 10^{-492}$ | $6.97 \cdot 10^{-507}$ |
| 0.02 | (9) | 32 | $4.76 \cdot 10^{-497}$ | $9.42 \cdot 10^{-512}$ |
| 0.02 | (10) | 32 | $9.43 \cdot 10^{-498}$ | $1.87 \cdot 10^{-512}$ |
| 0.02 | (11) | 32 | $2.27 \cdot 10^{-497}$ | $4.49 \cdot 10^{-512}$ |
| 0.02 | (12) | 32 | $9.09 \cdot 10^{-497}$ | $1.80 \cdot 10^{-511}$ |
| 0.02 | (13) | 32 | $3.76 \cdot 10^{-497}$ | $7.45 \cdot 10^{-512}$ |




(a) Weerakoon-Fernando (9) (b) Harmonic (10) (c) Geometric (11)

(d) Heronian (12) (e) Quadratic (13)

**Fig. 7** Dynamical lines for iterative methods on the Colebrook-White equation (17)

## 4.2 Equilibrium conversion

Consider the reversible chemical reactions [8]

$$\begin{aligned} 2A + B \leftrightarrow C, \;\; K_1 = \frac{C_C}{C_A^2 C_B}, \\ A + D \leftrightarrow C, \;\; K_2 = \frac{C_C}{C_A C_D}. \end{aligned} \tag{19}$$

In order to find the equilibrium conversion of the reactions, the concentrations of the components can be calculated from the equilibrium concentration of the components $x_1$ and $x_2$ of the above reactions and the initial concentrations with the expressions

$$\begin{aligned} C_A &= C_{A0} - 2x_1 C_{B0} - x_2 C_{D0}, \\ C_B &= (1 - x_1) C_{B0}, \\ C_C &= C_{C0} + x_1 C_{B0} + x_2 C_{D0}, \\ C_D &= (1 - x_2) C_{D0}. \end{aligned} \tag{20}$$

Therefore, the nonlinear system of equations $G(x_1, x_2) = (g_1(x_1, x_2), g_2(x_1, x_2)) = (0, 0)$ describing the problem is defined by its coordinate functions

$$\begin{cases} g_1(x_1, x_2) = \dfrac{C_C}{C_A^2 C_B} - K_1 = \dfrac{C_{C0} + x_1 C_{B0} + x_2 C_{D0}}{(C_{A0} - 2x_1 C_{B0} - x_2 C_{D0})^2 (1 - x_1) C_{B0}} - K_1, \\ g_2(x_1, x_2) = \dfrac{C_C}{C_A C_D} - K_2 = \dfrac{C_{C0} + x_1 C_{B0} + x_2 C_{D0}}{(C_{A0} - 2x_1 C_{B0} - x_2 C_{D0})(1 - x_2) C_{D0}} - K_2. \end{cases} \tag{21}$$

In the numerical calculations, the values of the initial concentrations are $C_{A0} = 40$, $C_{B0} = 15$, $C_{C0} = 0$ and $C_{D0} = 10$, while the equilibrium constants are $K_1 = 5 \cdot 10^{-4}$ and $K_2 = 4 \cdot 10^{-2}$. Applying these values to system (21), the numerical problem to be solved is defined by

$$\begin{cases} g_1(x_1, x_2) = \dfrac{1}{6000}\left(-3 - 20\dfrac{3x_1 + 2x_2}{(x_1 - 1)(-4 + 3x_1 + x_2)^2}\right), \\ g_2(x_1, x_2) = \dfrac{1}{50}\left(-2 + \dfrac{5}{2}\dfrac{3x_1 + 2x_2}{(x_2 - 1)(-4 + 3x_1 + x_2)}\right). \end{cases} \tag{22}$$

Table 4 collects the results of the application of the proposed iterative methods for solving nonlinear systems to the equilibrium concentration problem. The solution of the nonlinear system (22) is

$$(\bar{x}_1, \bar{x}_2) \approx (0.12026665, 0.47867067).$$

For different initial estimations of the concentrations of $x_1$ and $x_2$, the table shows the number of iterations, the distance between the two last iterations and the norm of the value of the system in the last iteration. In addition, the approximated computational order of convergence ACOC [10] is also displayed.

**Table 4** Numerical results for extended proposed methods solving the equilibrium concentration nonlinear system (22)

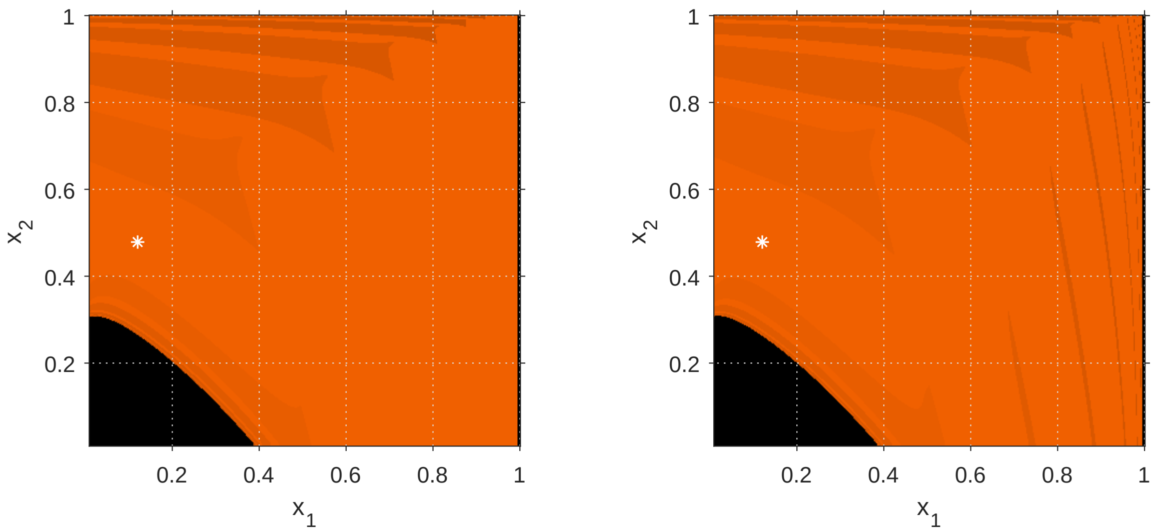
| $x^{(0)}$ | Method | Iterations | $\|x^{(k+1)} - x^{(k)}\|$ | $\|G(x^{(k+1)})\|$ | ACOC |
|---|---|---|---|---|---|
| $[0.2, 0.6]$ | (15) | 7 | $1.77 \cdot 10^{-388}$ | $1.34 \cdot 10^{-1551}$ | 3.9965 |
| $[0.2, 0.6]$ | (16) | 7 | $1.88 \cdot 10^{-424}$ | $1.23 \cdot 10^{-1695}$ | 3.9968 |
| $[0.5, 0.5]$ | (15) | 8 | $6.99 \cdot 10^{-363}$ | $4.59 \cdot 10^{-1450}$ | 4.0013 |
| $[0.5, 0.5]$ | (16) | 8 | $2.41 \cdot 10^{-432}$ | $5.39 \cdot 10^{-1728}$ | 4.0010 |
| $[0.05, 0.95]$ | (15) | 9 | $3.72 \cdot 10^{-298}$ | $2.57 \cdot 10^{-1190}$ | 4.0000 |
| $[0.05, 0.95]$ | (16) | 9 | $1.54 \cdot 10^{-420}$ | $5.59 \cdot 10^{-1680}$ | 4.0000 |

For every case in Table 4, the extension of the methods for solving nonlinear systems finds the solution of the problem. Let us remark that the solution using method (16) is slightly better than that obtained by (15) method, since the residuals are smaller with the same number of iterations. Moreover, the numerical estimation of the order of convergence (ACOC) confirms that these schemes hold the theoretical order of convergence of their scalar partners.

In order to check the dependence of these extended vectorial methods on the initial estimations, we show in Figure 8 the dynamical planes associated to the equilibrium conversion problem (22) when the methods based on the arithmetic and the harmonic means are applied. Each plane represents in orange color the set of initial guesses that converges to the solution $(\bar{x}_1, \bar{x}_2)$, while the black color is devoted to the divergence.' Let us remark that a wide region of initial values $x^{(0)}$ reach the solution using these methods for solving nonlinear systems in a low number of iterations.

## 5 Conclusions

Based on the third-order method of Weerakoon and Fernando, that includes an arithmetic mean of $f'(x_k)$ and $f'(y_k)$, some known third-order iterative methods have been generated by using other definitions of means. To increase the order of convergence without including memory, two weight functions $G(t, u)$ and $H(t)$ have been designed that allows us to define a set of optimal fourth-order schemes, that still preserve the shape of each original mean. Some of them have been extended to the vectorial case. The dynamics of the iterative methods guarantee the convergence of the procedures for quadratic polynomials. The solution of two well-known problems




(a) Weerakoon-Fernando (15) (b) Harmonic (16)

**Fig. 8** Dynamical planes for iterative methods on the equilibrium conversion nonlinear system (22)

in Chemistry, such as Colebrook-White nonlinear equation or the equilibrium conversion nonlinear system, has been obtained by means of the introduced iterative schemes, both in numerical and dynamical tests, for a wide set of initial estimations.

## References

1. Ababneh, O.: New Newton's method with third order convergence for solving nonlinear equations. World Acad. Sci. Eng. Technol. **61**, 1071–1073 (2012)
2. Amat, S., Busquier, S.: Advances in Iterative Methods for Nonlinear Equations, chap. 5, pp. 79–111. SEMA SIMAI Springer Series Vol. 10. Springer, Berlin (2016)
3. Behl, R., Sarría, Í., González, R., Magreñán, Á.A.: Highly efficient family of iterative methods for solving nonlinear models. Journal of Computational and Applied Mathematics **346**, 110–132 (2019)
4. Campos, B., Canela, J., Vindel, P.: Convergence regions for the Chebyshev-Halley family. Communications in Nonlinear Science and Numerical Simulation **56**, 508–525 (2018)
5. Chicharro, F.I., Cordero, A., Torregrosa, J.R.: Drawing dynamical and parameters planes of iterative families and methods. The Scientific World Journal **780513**, 1–11 (2013)
6. Chicharro, F.I., Cordero, A., Torregrosa, J.R.: Dynamics of iterative families with memory based on weight functions procedure. Journal of Computational and Applied Mathematics **354**, 286–298 (2019)
7. Colebrook, C.F., White, C.M.: Experiments with fluid friction in roughened pipes. Proc. Royal Soc. London **161**, 367–381 (1937)
8. Constantinides, A., Mostoufi, N.: Numerical methods for chemical engineers with MATLAB applications. Prentice-Hall (1999)
9. Cordero, A., Franceschi, J., Torregrosa, J.R., Zagati, A.C.: A convex combination approach for mean-based variants of Newton's method. Symmetry **11**, 1062 (2019)
10. Cordero, A., Torregrosa, J.R.: Variants of Newton's method using fifth order quadrature formulas. Appl. Math. Comput. **190**, 686–698 (2007)
11. Kung, H.T., Traub, J.F.: Optimal order of one-point and multipoint iteration. J. Assoc. Comput. Math. **21**, 643–651 (1974)
12. Lukić, T., Ralević, N.: Geometric mean Newton's method for simple and multiple roots. Applied Mathematics Letters **21**, 30–36 (2008)
13. Özban, A.: Some new variants of Newton's method. Applied Mathematical Letters **17**, 677–682 (2004)
14. Petković, M., Neta, B., Petković, L., Džunić, J.: Multipoint Methods for Solving Nonlinear Equations. Academic Press, Cambridge (2013)
15. Shashi, E.: Transmission Pipeline Calculations and Simulations Manual, chap. Fluid Flow in Pipes, pp. 149–234. Elsevier (2015)
16. Singh, M.K., Singh, A.K.: A new-mean type variant of Newton's method for simple and multiple roots. International Journal of Mathematics Trends and Technology **49**, 174–177 (2017)
17. Verma, K.: On the centroidal mean Newton's method for simple and multiple roots of nonlinear equations. Int. J. Comput. Sci. Math. **7**, 126–143 (2016)
18. Weerakoon, S., Fernando, T.G.I.: A variant of Newton's method with third-order convergence. Applied Mathematical Letters **13**, 87–93 (2000)
19. Xiaojian, Z.: A class of Newton's methods with third-order convergence. Applied Mathematics Letters **20**, 1026–1030 (2007)