



# Family of fourth-order optimal classes for solving multiple-root nonlinear equations

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## Abstract

We present a new iterative procedure for solving nonlinear equations with multiple roots with high efficiency. Starting from the arithmetic mean of Newton's and Chebyshev's methods, we generate a two-step scheme using weight functions, resulting in a family of iterative methods that satisfies the Kung and Traub conjecture, yielding an optimal family for different choices of weight function. We have performed an in-depth analysis of the stability of the family members, in order to select those members with the highest stability for application in solving mathematical chemistry problems. We show the good characteristics of the selected methods by applying them on four relevant chemical problems.

**Keywords** Nonlinear · Dynamics · Multiple-root · Chemical application

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## 1 Introduction

Throughout history, physical phenomena have been modeled through mathematical expressions. On many occasions, it is necessary to obtain the solution of the nonlinear equation  $f(x) = 0$ ,  $f : D \subseteq \mathbb{R} \rightarrow \mathbb{R}$ . However, it is not always possible to obtain an analytical solution to such a problem and we have to resort to approximate solutions. Iterative methods obtain approximations to the solution as accurate as we need. The best known and most widely used scheme is Newton's method

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

Under the convergence conditions – initial estimate close to the root and sufficiently differentiable function – Newton's method converges quadratically as long as we look for a simple root. But there are many physical phenomena in which we have to look for a multiple root, and there the convergence is impaired.

Nonlinear equations  $f(x) = 0$  with multiple roots of multiplicity  $m > 1$  satisfy  $f(r_m) = f'(r_m) = \dots = f^{(m-1)}(r_m) = 0$  and  $f^{(m)}(r_m) \neq 0$ . Many authors have designed iterative methods for this purpose [1–6]. Kansal et al. [7] designed two-step optimal methods of fourth order, starting from the arithmetic mean between second order methods for multiple roots, and including weight functions and accelerating parameters in the final scheme. Behl et al. [8, 9] followed a similar strategy to reach order of convergence four.

In this paper we propose the design and analysis of an iterative class taking the arithmetic mean of the accelerated Newton's method [10]

$$x_{n+1} = x_n - m \frac{f(x_n)}{f'(x_n)}, \quad n = 0, 1, 2, \dots$$

and Chebyshev's iterative scheme [11]

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} - \frac{f(x_n)^2 f''(x_n)}{2 f'(x_n)^3}, \quad n = 0, 1, 2, \dots,$$

obtaining the following iterative method:

$$x_{n+1} = x_n - \left[ \frac{m+1}{2} + \frac{1}{4} t_n \right] \frac{f(x_n)}{f'(x_n)}, \quad n = 0, 1, 2, \dots, \quad (1)$$

where  $t_n = \frac{f(x_n) f''(x_n)}{f'(x_n)^2}$ .

Our aim is to design an optimal method in the sense of the Kung-Traub conjecture [11] which states that the order of convergence  $p$  of an iterative scheme without memory is at most  $2^{d-1}$ , where  $d$  is the number of different functional evaluations performed by the iterative algorithm, reaching the optimality when  $p = 2^{d-1}$ . Moreover, Traub showed in [11] that in order to design a one-step method with order of

convergence  $p$ , its iterative expression must contain derivatives at least up to order  $p - 1$ .

Let us notice that (1) is a one-step iterative method that uses three different functional evaluations on each iterative step, being one of them a second-order derivative of the function. With these features, its order of convergence is at most three, so this method cannot reach the optimality. For this reason, we add an extra step in (1) to obtain a two-step iterative scheme that does not require derivatives of order two and uses only three functional evaluations so that according to the Kung-Traub conjecture it could be possible to reach the optimal order of convergence 4.

The paper is structured as follows. Section 2 analyzes the convergence of the introduced family. Section 3 studies the stability of the family, in order to find its best members in terms of initial guesses. In Sect. 4 a numerical analysis is performed, showing the validity of the method in chemistry and academic problems. Finally, Sect. 5 collects the main conclusions of the manuscript.

## 2 Design of the fourth-order optimal family

Consider the Newton-type iterative method for multiple roots

$$x_{n+1} = x_n - \frac{2m}{m+2} \frac{f(x_n)}{f'(x_n)}, \quad n = 0, 1, 2, \dots$$

Using Taylor series developments around  $x = x_n$ , we have:

$$f' \left( x_n - \frac{2m}{m+2} \frac{f(x_n)}{f'(x_n)} \right) \approx f'(x_n) - \frac{2m}{m+2} \frac{f(x_n)f''(x_n)}{f'(x_n)}. \quad (2)$$

From (2), the second derivative of the function can be approximated as

$$f''(x_n) \approx \frac{(m+2)f'(x_n)(f'(x_n) - f'(y_n))}{2mf(x_n)},$$

being  $y_n = x_n - \frac{2m}{m+2} \frac{f(x_n)}{f'(x_n)}$ . In addition, we can write

$$t_n = \frac{f(x_n)f''(x_n)}{f'(x_n)^2} \approx \frac{(m+2)(f'(x_n) - f'(y_n))}{2mf'(x_n)}. \quad (3)$$

Replacing (3) in (1), we obtain

$$\begin{cases} y_n = x_n - \frac{2m}{m+2} \frac{f(x_n)}{f'(x_n)}, \\ x_{n+1} = x_n - \left[ \frac{m+1}{2} + \frac{1}{4}t_n \right] \frac{f(x_n)}{f'(x_n)}, \end{cases} \quad n = 0, 1, 2, \dots \quad (4)$$

with  $t_n = \frac{(m+2)(f'(x_n) - f'(y_n))}{2mf'(x_n)}$ .

It can be proved the linear convergence of (4). Also, although the derivative of order two is not used, it is not an optimal method because three functional evaluations are still carried out. Based on its iterative structure we design another method with higher order of convergence. In this sense, we add two free parameters  $a$  and  $b$  in (4). Then the biparametric family is

$$\begin{cases} y_n = x_n - \frac{2m}{m+2} \frac{f(x_n)}{f'(x_n)}, \\ x_{n+1} = x_n - [a(m+1) + bt_n] \frac{f(x_n)}{f'(x_n)}, \end{cases} \quad n = 0, 1, 2, \dots \quad (5)$$

The convergence of family (5) is analyzed below.

**Theorem 1** Let  $r_m$  be a multiple zero with a multiplicity  $m \geq 1$  of a sufficiently differentiable function  $f : I \subseteq \mathbb{R} \rightarrow \mathbb{R}$  defined in an open interval  $I$  such that  $r_m \in I$ . If the initial estimation  $x_0$  is close enough to  $r_m$ , then the iterative scheme defined by (5) has order of convergence three when parameters  $a$  and  $b$  are defined as following:

$$a = \frac{m(4 + 2m + m^2 - m^{2-m}(2+m)^m)}{4(m+1)}, \quad b = \frac{1}{2}m^{4-m}(2+m)^{m-1}.$$

In this case, the error equation of the resulting method is given by

$$e_{n+1} = \frac{2c_1^2}{m^3}e_n^3 + \mathcal{O}(e_n^4),$$

being  $c_i = \frac{m!}{(m+i)!} \frac{f^{(m+i)}(r_m)}{f^{(m)}(r_m)}$ ,  $i \geq 1$ , and  $e_n = x_n - r_m$ ,  $\forall n \in \mathbb{N}$ .

**Proof** Using Taylor series developments around  $x = r_m$  and taking into account  $f^{(j)}(r_m) = 0$  when  $0 \leq j \leq m-1$  and  $f^{(m)}(r_m) \neq 0$ , we can write

$$f(x_n) = \frac{f^{(m)}(r_m)}{m!}e_n^m(1 + c_1e_n + c_2e_n^2 + c_3e_n^3 + c_4e_n^4) + \mathcal{O}(e_n^5), \quad (6)$$

and its derivative

$$\begin{aligned} f'(x_n) &= \frac{f^{(m)}(r_m)}{m!}e_n^{m-1}(m + (m+1)c_1e_n + (m+2)c_2e_n^2 + (m+3)c_3e_n^3 \\ &\quad + (m+4)c_4e_n^4) + \mathcal{O}(e_n^5), \end{aligned} \quad (7)$$

From (6) and (7), we obtain

$$\frac{f(x_n)}{f'(x_n)} = \frac{1}{m}e_n - \frac{c_1}{m^2}e_n^2 + \left( \frac{(m+1)c_1^2 - 2mc_2}{m^3} \right) e_n^3 + \mathcal{O}(e_n^4). \quad (8)$$

Then we have

$$\begin{aligned}
 y_n - r_m &= e_n - \frac{2m}{m+2} \frac{f(x_n)}{f'(x_n)} \\
 &= \frac{m}{2+m} e_n + \frac{2c_1}{m(2+m)} e_n^2 + \left( \frac{-2(m+1)c_1^2 + 4mc_2}{m^2(2+m)} \right) e_n^3 + \mathcal{O}(e_n^4)
 \end{aligned}$$

and then

$$\begin{aligned}
 f'(y_n) &= \frac{f^{(m)}(r_m)}{m!} (y_n - r_m)^{m-1} (m + (m+1)c_1(y_n - r_m) + (m+2)c_2(y_n - r_m)^2 \\
 &\quad (m+3)c_3(y_n - r_m)^3) + \mathcal{O}(e_n^4)
 \end{aligned}$$

can be written as

$$\begin{aligned}
 f'(y_n) &= \frac{f^{(m)}(r_m)}{m!} e_n^m \left( \frac{m}{2+m} \right)^m \left[ \frac{2+m}{e_n} + \frac{(-4+2m+3m^2+m^3)c_1}{m^2} \right. \\
 &\quad + \frac{-4(m-2)c_1^2 + m^2(-8+4m+4m^2+m^3)c_2}{m^4} e_n \\
 &\quad + \frac{1}{3m^6(2+m)^2} \left( 4(2+m)^2(-12+4m-4m^2+5m^3+m^4)c_1^3 \right. \\
 &\quad \left. \left. - 12m^2(2+m)^2(-8+4m+m^2)c_1c_2 + \beta \right) e_n^2 \right] + \mathcal{O}(e_n^3),
 \end{aligned} \tag{9}$$

where  $\beta = 3m^4(-48 - 24m + 36m^2 + 30m^3 + 9m^4 + m^5)c_3$ .

Now, from (7) and (9) we have

$$\begin{aligned}
 t_n &= \frac{(m+2)(f'(x_n) - f'(y_n))}{2mf'(x_n)} \\
 &= \frac{(m+2)(m - m^m(m+2)^{m-1})}{2m^2} + 2m^{m-4}(m+2)^{m-1}c_1e_n \\
 &\quad - 2 \left( m^{m-6}(m+2)^{m-1}((2+m^2)c_1^2 - 2m^2c_2) \right) e_n^2 + \mathcal{O}(e_n^3).
 \end{aligned} \tag{10}$$

Using (8) and (10) on the second step of the iterative scheme we obtain the error equation

$$\begin{aligned}
 e_{n+1} &= e_n - [a(m+1) + bt_n] \frac{f(x_n)}{f'(x_n)} \\
 &= \left[ 1 - \frac{a(m+1)}{m} - \frac{b(m+2)(m - m^m(m+2)^{1-m})}{2m^3} \right] e_n \\
 &\quad + \frac{am^3(1+m) - 2bm^m(2+m)^{1-m} + \frac{1}{2}bm(m+2)(m - m^m(m+2)^{1-m})}{m^5} c_1e_n^2 \\
 &\quad + \mathcal{O}(e_n^3).
 \end{aligned}$$

From the error equation, the iterative class (5) can achieve cubic order when it holds

$$\begin{cases} 1 - \frac{a(m+1)}{m} - \frac{b(m+2)(m-m^m(m+2)^{1-m})}{2m^3} = 0 \\ am^3(1+m) - 2bm^m(2+m)^{1-m} + \frac{1}{2}bm(m+2)(m-m^m(m+2)^{1-m}) = 0 \end{cases}$$

Equivalently, the order is cubic when parameters  $a$  and  $b$  take the value

$$a = \frac{m(4+2m+m^2-m^{2-m}(2+m)^m)}{4(m+1)}, \quad b = \frac{1}{2}m^{4-m}(2+m)^{m-1}.$$

and then the error equation of the method results into

$$e_{n+1} = \frac{2c_1^2}{m^3}e_n^3 + \mathcal{O}(e_n^4).$$

□

In order to construct a fourth-order optimal method with less than three different functional evaluations, we propose the introduction of a weight function on (5) obtaining

$$\begin{cases} y_n = x_n - \frac{2m}{m+2} \frac{f(x_n)}{f'(x_n)}, \\ x_{n+1} = x_n - [a(m+1) + bt_n] Q \left( \frac{f'(y_n)}{f'(x_n)} \right) \frac{f(x_n)}{f'(x_n)}, \end{cases} \quad n = 0, 1, 2, \dots, \quad (11)$$

where  $t_n = \frac{(m+2)(f'(x_n) - f'(y_n))}{2mf'(x_n)}$  and

$$a = \frac{m(4+2m+m^2-m^{2-m}(2+m)^m)}{4(m+1)}, \quad b = \frac{1}{2}m^{4-m}(2+m)^{m-1},$$

and  $Q \in \mathcal{C}^2(\mathbb{R})$  is a real variable weight function. The following result shows the conditions that the weight function  $Q$  must satisfy in (11) to reach the optimal order of convergence four.

**Theorem 2** *Let  $r_m$  be a multiple zero with a multiplicity  $m \geq 1$  of a sufficiently differentiable function  $f : I \subseteq \mathbb{R} \rightarrow \mathbb{R}$  defined in an open interval  $I$  such that  $r_m \in I$ . If the initial estimation  $x_0$  is close enough to  $r_m$ , then the iterative scheme defined by (11) has order of convergence four when the weight function  $Q$  satisfies:*

- $Q(\mu) = 1$ ,
- $Q'(\mu) = 0$ ,
- $Q''(\mu) = \frac{1}{4}m^{3-2m}(2+m)^{2m}$ ,
- $|Q'''(\mu)| < \infty$ ,

where  $\mu = \left(\frac{m}{2+m}\right)^{m-1}$ . Under these conditions, the following error equation is hold:

$$e_{n+1} = \left[ \frac{m^4[12 + m(-8 + m(2 + m(2 + m)))] + 32 \left(\frac{m}{2+m}\right)^{3m} Q'''(\mu)c_1^3}{3m^9} - \frac{c_1c_2}{m} + \frac{mc_3}{(2+m)^2} \right] e_n^4 + \mathcal{O}(e_n^5),$$

being  $c_i = \frac{m!}{(m+i)!} \frac{f^{(m+i)}(r_m)}{f^{(m)}(r_m)}$ ,  $i \geq 1$ , and  $e_n = x_n - r_m, \forall n \in \mathbb{N}$ .

**Proof** From (6) and (7), we can write

$$\begin{aligned} \frac{f'(y_n)}{f'(x_n)} &= \left(\frac{m}{2+m}\right)^{m-1} - 4m^{m-3}(2+m)^{-m}c_1e_n \\ &+ m^{m-5}(2+m)^{-m}(4(2+m^2)c_1^2 - 8m^2c_2)e_n^2 \\ &- \frac{8}{3} \left(m^{m-7}(2+m)^{m-2} \left((2+m)^2(6+m+m^2(5+(m-1)m))c_1^3 \right. \right. \\ &\left. \left. - 3m^2(2+m)^2(4+m^2)c_1c_2 + 3m^4(6+m(6+m))c_3\right)\right) e_n^3 + \mathcal{O}(e_n^4). \end{aligned} \tag{12}$$

Now we can write  $\frac{f'(y_n)}{f'(x_n)} = \mu + v$ , being  $\mu = \left(\frac{m}{2+m}\right)^{m-1}$ . From (12), the difference holds  $v = \frac{f'(y_n)}{f'(x_n)} - \mu \sim \mathcal{O}(e_n)$ , so we consider the Taylor series expansion of the weight function  $Q\left(\frac{f'(y_n)}{f'(x_n)}\right) = Q(\mu + v)$  around  $\mu$

$$Q\left(\frac{f'(y_n)}{f'(x_n)}\right) = Q(\mu) + Q'(\mu)v + \frac{Q''(\mu)}{2!}v^2 + \frac{Q'''(\mu)}{3!}v^3 + \mathcal{O}(e_n^4). \tag{13}$$

Using (8), (10) and (13) in the iterative expression (11), the error equation holds

$$\begin{aligned} e_{n+1} &= e_n - [a(m+1) + bt_n] Q\left(\frac{f'(y_n)}{f'(x_n)}\right) \frac{f(x_n)}{f'(x_n)} \\ &= K_1e_n + K_2e_n^2 + K_3e_n^3 + \mathcal{O}(e_n^4), \end{aligned} \tag{14}$$

where

$$\begin{aligned} K_1 &= 1 - Q(\mu), \\ K_2 &= 4m^{m-3}(2+m)^{-m}Q'(\mu)c_1, \\ K_3 &= m^{-6}(2+m)^{-2m} \left(2m^3(2+m)^{2m}Q(\mu) - 4m^{m+1}(2+m)^m(2+m^2)Q'(\mu) \right. \\ &\left. - 8m^{2m}Q''(\mu)\right) c_1^2 + 16m^{3+m}(2+m)^mQ'(\mu)c_2. \end{aligned}$$

To obtain an optimal family of iterative methods of order 4, the coefficients of  $e_n$ ,  $e_n^2$  and  $e_n^3$  in the error Eq. (14) must be zero simultaneously. Solving for  $K_1 = 0$ ,  $K_2 = 0$  and  $K_3 = 0$  we obtain the following conditions to cancel the terms up to order three of Eq. (14)

$$\begin{cases} Q(\mu) = 1, \\ Q'(\mu) = 0, \\ Q''(\mu) = \frac{1}{4}m^{3-2m}(2+m)^{2m}, \\ |Q'''(\mu)| < \infty. \end{cases} \quad (15)$$

Using the previous conditions, the error equation of family (11) shows that the order of convergence is four:

$$e_{n+1} = \left[ \frac{m^4(12 + m(-8 + m(2 + m(2 + m)))) + 32 \left(\frac{m}{2+m}\right)^{3m} Q'''(\mu)}{3m^9} c_1^3 - \frac{c_1 c_2}{m} + \frac{m c_3}{(2+m)^2} \right] e_n^4 + \mathcal{O}(e_n^5).$$

□

According to Theorem 2, we have designed a two-step family of iterative methods that only performs three functional evaluations on each iteration and reaches the optimal order of convergence  $p = 4$ .

In the following, we will try to simplify the iterative expression of (11). First, using the notation  $u_n = \frac{f'(y_n)}{f'(x_n)}$  we can write

$$t_n = \frac{(m+2)(f'(x_n) - f'(y_n))}{2mf'(x_n)} = \frac{m+2}{2m}(1 - u_n)$$

and then

$$\begin{aligned} a(m+1) + bt_n &= \frac{m(4+2m+m^2-m^{2-m}(2+m)^m)}{4} + \frac{1}{4}m^{3-m}(2+m)^m(1+u_n) \\ &= a_1 + b_1(1 - u_n), \end{aligned}$$

being  $a_1 = \frac{m(4+2m+m^2-m^{2-m}(2+m)^m)}{4}$  and  $b_1 = \frac{1}{4}m^{3-m}(2+m)^m$ .

On the other hand, from Theorem 2, the weight function can be written as

$$Q\left(\frac{f'(y_n)}{f'(x_n)}\right) = 1 + \frac{1}{8}m^{3-2m}(2+m)^{2m} \left(\frac{f'(y_n)}{f'(x_n)} - \mu\right)^2 + \frac{\alpha}{6} \left(\frac{f'(y_n)}{f'(x_n)} - \mu\right)^3,$$



where  $\alpha = Q'''(\mu)$ ,  $|Q'''(\mu)| < \infty$  and  $\mu = \left(\frac{m}{2+m}\right)^{m-1}$ . Finally, defining  $H$  with the previous expressions

$$H(u_n) = [a_1 + b_1(1 - u_n)] Q(u_n),$$

family (11) can be simplified as

$$\begin{cases} y_n = x_n - \frac{2m}{m+2} \frac{f(x_n)}{f'(x_n)}, \\ x_{n+1} = x_n - H(u_n) \frac{f(x_n)}{f'(x_n)}, \end{cases} \quad n = 0, 1, 2, \dots, \quad (16)$$

being  $\alpha \in \mathbb{C}$  a free parameter. A new family of optimal iterative methods belonging to (11) is designed. Let us denote the iterative class (16) by NC4 family. Next section is devoted to perform a dynamical analysis of NC4 family in order to choose the best members in terms of stability.

### 3 Stability of the family of methods

The stability analysis of a family of iterative methods studies the behaviour of the schemes for a wide set of initial guesses. In this sense, this analysis discriminates whether the methods are useful to solve the nonlinear problems or not.

In section 3.1 the scaling theorem is introduced, and the Möbius transformation is applied to reduce the amount of parameters involved. Section 3.2 analyzes fixed and critical points. Finally, section 3.3 is devoted to select the members of the family with better stability behaviour.

Complex dynamics is used to study the dynamical behaviour of the rational operator associated to family NC4 applied on polynomials. The concepts can be reviewed in more detail at [12–15].

#### 3.1 Operator simplification through Möbius transformation

The iterative family is applied for solving the general nonlinear multiple-root polynomial  $p(z) = (z - \delta_1)^2(z - \delta_2)$ . Theorem 3 points that family NC4 satisfies the scaling theorem, in order to simplify the stability analysis.

**Theorem 3** (Scaling theorem for family NC4) *Let  $f$  be an analytic function in  $\hat{\mathbb{C}}$ , and let  $T(z) = \beta z + \gamma$ ,  $\beta \neq 0$ , an affine map. Let  $g(z) = \lambda (f \circ T)(z) = \lambda f(T(z))$ ,  $\lambda \neq 0$ . Let  $O_f(z)$  the fixed point operator of family (16). Then,  $(T \circ O_g \circ T^{-1})(z) = O_f(z)$ , that is,  $O_g$  and  $O_f$  are affine conjugated by  $T$ .*

Since family (16) satisfies the scaling theorem, the fixed point operators associated to family NC4 applied to analytic functions are affine conjugated by an affine map.

The rational operator of family NC4 applied on  $p(z) = (z - \delta_1)^2(z - \delta_2)$  is

$$O_p(z) = z - \frac{(\delta_1 - z)(z - \delta_2)}{\delta_1 + 2\delta_2 - 3z} A_p B_p, \quad (17)$$

where

$$A_p = 6 - \frac{8(\delta_1 + \delta_2 - 2z)(\delta_1^2 + \delta_1(\delta_2 - 3z) + 4\delta_2^2 - 9\delta_2z + 6z^2)}{(\delta_1 + 2\delta_2 - 3z)^3},$$

$$B_p = \frac{\alpha(\delta_1 - z)^3(\delta_1^2 - 2\delta_1\delta_2 - 2\delta_2^2 + 6\delta_2z - 3z^2)^3}{48(\delta_1 + 2\delta_2 - 3z)^9} + \frac{4(\delta_1 - z)^2(\delta_1^2 - 2\alpha\delta_2 - 2\delta_2^2 + 6\delta_2z - 3z^2)^2}{(\delta_1 + 2\delta_2 - 3z)^6} + 1.$$

Note that (17) depends on the variable  $z$ , the parameter  $\alpha$  and the roots  $\delta_1$  and  $\delta_2$ . In order to overcome the dependence on the roots, we consider the Möbius transformation [12]

$$M(z) = \frac{z - \delta_1}{z - \delta_2},$$

obtaining its affined conjugated operator

$$O(z) = \left( M \circ O_p \circ M^{-1} \right) (z) = z^4 \frac{N_{10}(z)}{D_{13}(z)}, \quad (18)$$

where

$$N_{10}(z) = 24z^{10} + (\alpha + 864)z^9 - 16(\alpha - 396)z^8 + 50(\alpha + 864)z^7 + 4(11\alpha + 58176)z^6 + (744192 - 220\alpha)z^5 - 16(13\alpha - 86976)z^4 + 8(37\alpha + 195840)z^3 + 16(35\alpha + 66816)z^2 + 64(5\alpha + 6528)z + 64(\alpha + 1152),$$

$$D_{13}(z) = (\alpha + 264)z^{13} - 16(\alpha + 33)z^{12} + (50\alpha - 4224)z^{11} + 4(11\alpha + 3264)z^{10} - 4(55\alpha - 7584)z^9 - 16(13\alpha + 15984)z^8 + 8(37\alpha - 133632)z^7 + 80(7\alpha - 19584)z^6 + 320(\alpha - 1440)z^5 + 64(\alpha + 28608)z^4 + 3194880z^3 + 2555904z^2 + 1081344z + 196608.$$

Since  $M(\delta_1) = 0$ ,  $M(\delta_2) = \infty$  and  $M(\infty) = 1$ , Möbius transformation maps roots  $\delta_1$  and  $\delta_2$  with 0 and  $\infty$ , respectively, while the divergent behaviour will be at 1.

### 3.2 Analysis of fixed and critical points

Recalling [12, 13], the fixed points of family (18) are those that satisfy  $O(z) = z$ :

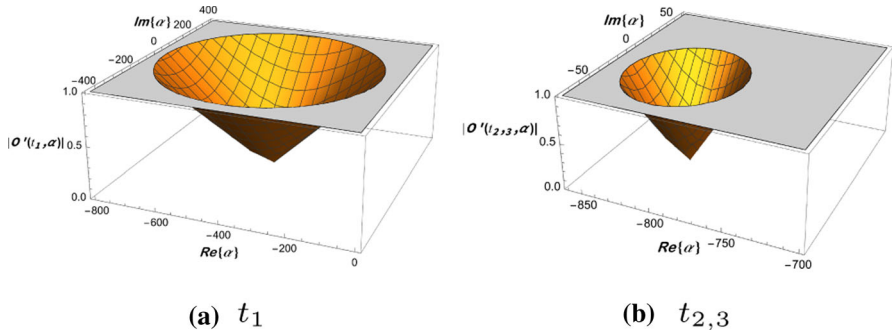


Fig. 1 Stability diagrams of the  $\alpha$ -independent strange fixed points  $t_{1,2,3}$

- $z = 0$ , that corresponds to the root of multiplicity two, whose asymptotical behaviour is superattracting,
- $z = \infty$ , that corresponds to the single root, whose asymptotical behaviour is attracting,
  - attracting, if  $|264 + \alpha| < 24$ ,
  - neutral, if  $|264 + \alpha| = 24$ , and
  - repelling, if  $|264 + \alpha| > 24$ ,
- $z = 1$ , that is a strange fixed point that maps the original divergence and it is
  - attracting, if  $|68472 + 11\alpha| > 472392$ ,
  - neutral, if  $|68472 + 11\alpha| = 472392$ , and
  - repelling, if  $|68472 + 11\alpha| < 472392$ ,
- the  $\alpha$ -independent strange fixed points  $t_i, i \in \{1, 2, 3\}$ , that match with the roots of the polynomial  $q(z) = z^3 - 10z^2 - 16z - 8$ , and the  $\alpha$ -dependent strange fixed points  $s_j, j \in \{1, 2, \dots, 9\}$ , that match with the roots of the polynomial  $r(z, \alpha) = z^9(\alpha + 240) + z^8(1248 - 6\alpha) + z^7(6\alpha + 4608) + z^6(16\alpha + 26112) + z^5(100608 - 12\alpha) + z^4(216576 - 24\alpha) + z^3(279552 - 8\alpha) + 227328z^2 + 110592z + 24576$ , whose asymptotical behaviour is analyzed numerically using the stability diagrams of Figures 2 and 4.

Figure 1 represents the stability diagram of the strange fixed points  $t_1, t_2$  and  $t_3$ . Values of  $\alpha$  in the interval  $[0, 1]$  show the region where the strange fixed points are attracting.

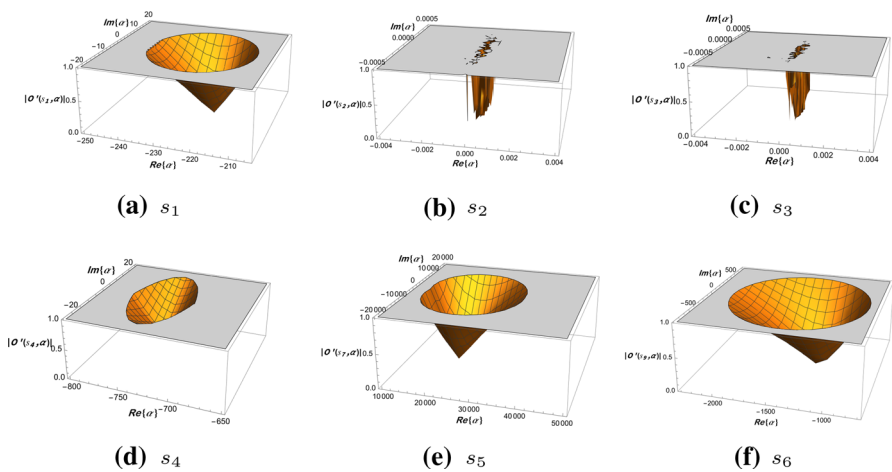
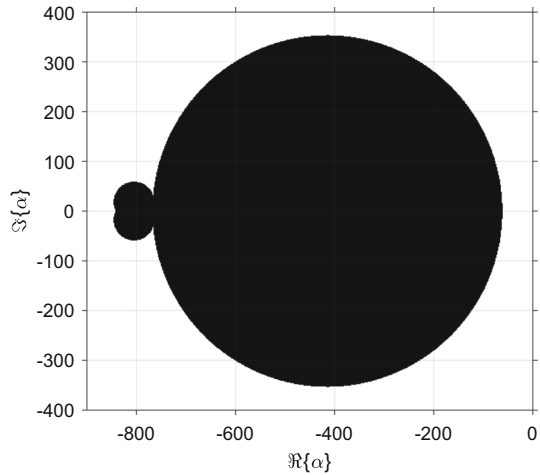
The unified stability diagram [16] represents in black the values of  $\alpha$  such that one strange fixed point is attracting. Figure 2 represents the unified stability diagram of fixed points  $t_1, t_2$  and  $t_3$ .

Figure 3 represents the stability diagram of the strange fixed points  $s_j, j \in \{1, \dots, 6\}$ . Values of  $\alpha$  in the interval  $[0, 1]$  show the region where the strange fixed points are attracting.

It can be shown that  $s_7, s_8$  and  $s_9$  are repelling for every value of  $\alpha$ .

Figure 4 represents the unified stability diagram of fixed points  $s_j, j \in \{1, \dots, 6\}$ . The critical points of family (18) are those that satisfy  $O'(z) = 0$ :

**Fig. 2** Unified stability diagram of the  $\alpha$ -independent strange fixed points  $t_{1,2,3}$

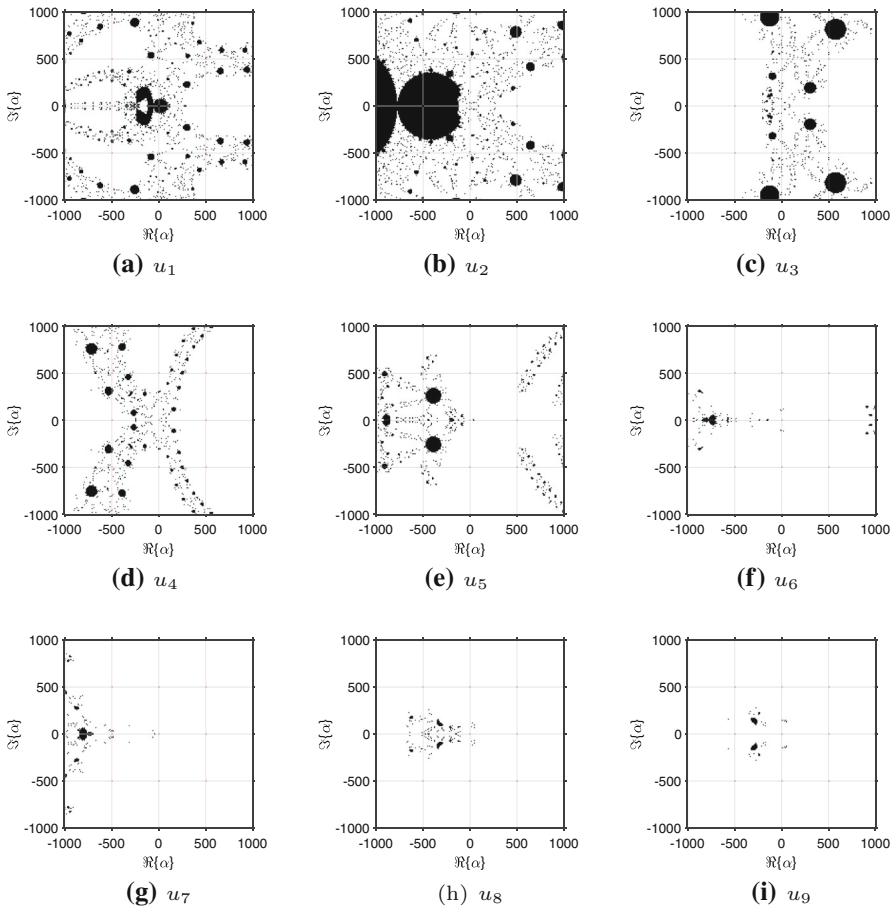
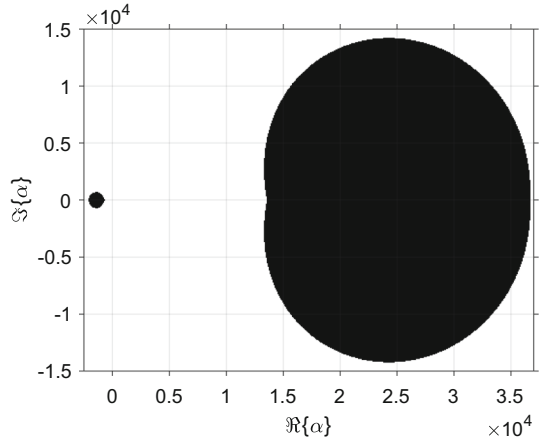


**Fig. 3** Stability diagrams of the  $\alpha$ -dependent strange fixed points  $s_j, j \in \{1, \dots, 6\}$

- $z = 0$ ,
- $z = -2$ , that is a pre-image of  $z = 1$ , and
- the free critical points  $u_k, k \in \{1, \dots, 11\}$  that match with the roots of the polynomial  $v(z, \alpha) = z^{11}(\alpha + 264) + z^{10}(-56\alpha - 7392) + z^9(544\alpha + 6336) + z^8(132480 - 1308\alpha) + z^7(-924\alpha - 215424) + z^6(4032\alpha - 1880064) + z^5(2064\alpha - 2078208) + z^4(2617344 - 4176\alpha) + z^3(7520256 - 2496\alpha) + z^2(2240\alpha + 6881280) + z(2240\alpha + 3072000) + 512\alpha + 589824$ .

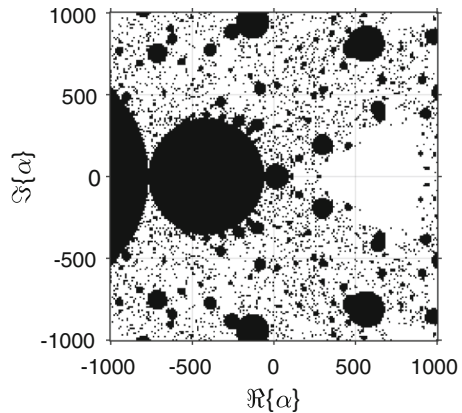
Figure 5 represents the parameter planes of the free critical points, using a similar routine than [14]. In this case, a mesh of  $200 \times 200$  points in the rectangle  $[\Re\{\alpha\}, \Im\{\alpha\}] = [-1000, 1000] \times [-1000, 1000]$  has been selected. White points represent convergence to one of the roots of polynomial, while black points show divergence and, therefore, unstable behaviour. The parameter planes of critical points

**Fig. 4** Unified stability diagram of the  $\alpha$ -dependent strange fixed points  $s_j, j \in \{1, \dots, 6\}$



**Fig. 5** Parameter planes of free critical points

Fig. 6 Unified parameter plane



$u_{10}$  and  $u_{11}$  have not been represented, since both converge only to the roots of the polynomial.

The information of the parameter planes of Figure 5 is summarized via the unified parameter plane of Figure 6. It represents in black the values of  $\alpha$  such that at least one free critical point do not converge to one root of the polynomial.

### 3.3 Selection of the best members of the family

The analysis performed in section 3.2 allows the selection of the parameter  $\alpha$  in terms of stability.

Below we are representing some dynamical planes associated to specific values of  $\alpha$  to show the different behaviours. The dynamical planes represent the basins of attraction of every initial guess in the rectangle  $[\Re\{z\}, \Im\{z\}] = [-30, 30] \times [-30, 30]$ , taking a mesh of  $200 \times 200$  points, in a similar manner than [14]. Orange and blue points represent the convergence to 0 or  $\infty$ , respectively. Black points represent convergence to a point different from the roots.

Selecting a value of  $\alpha$  in the black region of Figure 2 or 4 results in a set of initial guesses that converge to a strange attracting fixed point. Figure 7 shows two samples.

Figure 7(a) represents the dynamical plane of the method  $\alpha = -400 + 200i$ . A wide set of initial estimations converge to the root 0. However, some initial guesses converge to the strange attracting fixed point  $t_1 \approx 11.4574$  represented in white star. A similar behaviour is represented in Figure 7(b), for the method corresponding to  $\alpha = -1500$ , where some initial estimations converge to the strange attracting fixed point  $s_1 \approx 7.9661$ , represented in white star.

Free critical points can have their own basin of attraction, different from the roots of the polynomial. Selecting a value of  $\alpha$  in the black region of Figure 6 results in iterative methods whose free critical points converge to their own root. Figure 8 illustrates this behaviour.

Figure 8(a) represents the dynamical plane of the method  $\alpha = 0$ . In this case,  $u_1 \approx 26.8431$ —represented in white square— is inside a basin of attraction of a two-periodic orbit. Figure 8(b) is the corresponding dynamical plane to  $\alpha = -119 + 157i$ .

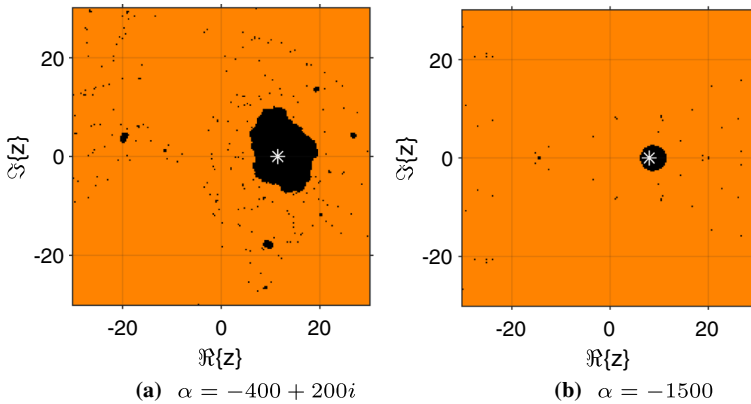


Fig. 7 Dynamical planes for values of  $\alpha$  such that at least one strange fixed point is attracting

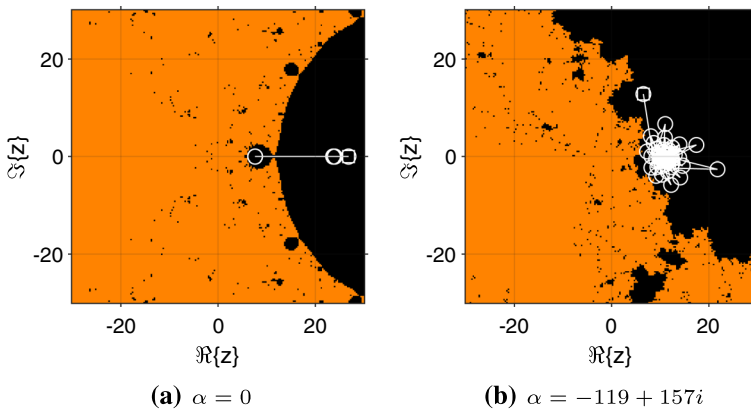


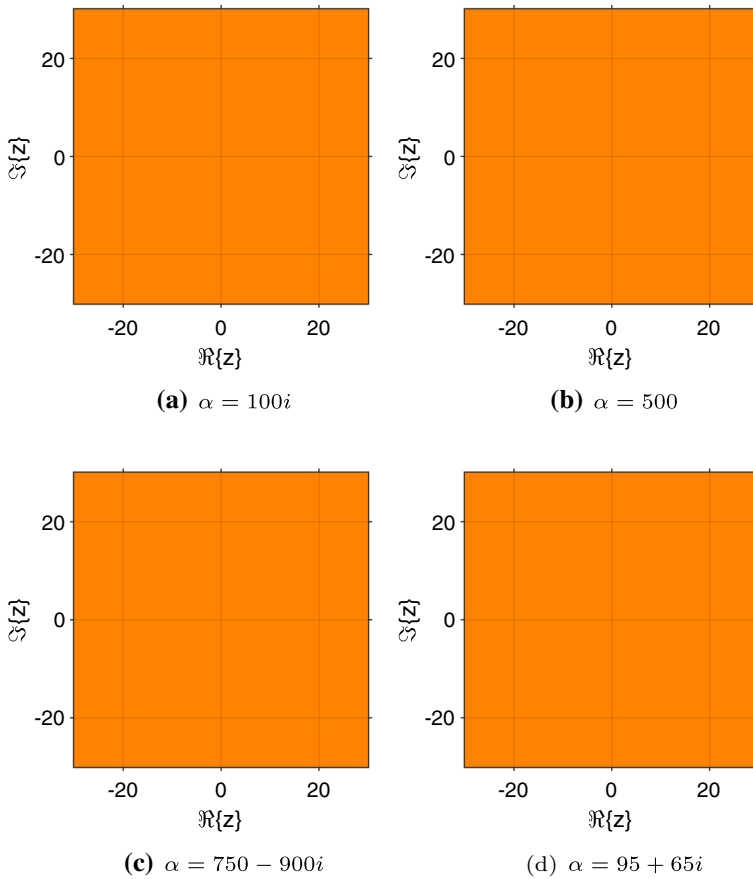
Fig. 8 Dynamical planes for values of  $\alpha$  such that at least one free critical point do not converge to the roots of the polynomial

The free critical point  $u_2 \approx 6.5275 + 12.8139i$  is inside de basin of attraction of  $t_1 \approx 11.4574$ .

In order to show the good stability of the family for a wide set of values of  $\alpha$ , we select specific members in the white regions of Figures 2, 4 and 6. Figure 9 shows four dynamical planes for specific values of  $\alpha$ .

### 4 Numerical tests

In this section we compare the introduced method NC4 with relevant methods of the literature. The selected methods can be found in Sharma and Sharma [17] denoted as SS, Behl et al [9] denoted as B4, and Sharifi et al. [18] denoted as SH. The comparison is performed on different chemical nonlinear equations that involve multiple roots. For



**Fig. 9** Dynamical planes with full convergence

the NC4 family, several parameters – extracted from Figures 7, 8 and 9 – have been selected.

The numerical results of each problem are displayed in a table. In particular, each method is applied until  $|f(x_{k+1})| < tol$  or  $|x_{k+1} - x_k| < tol$ . If it is not stated differently,  $tol = 10^{-300}$  is used along the following examples. Both values are shown in the result tables for the last iterate computed. If the targeted solution is available, we introduce the value of  $|x_{k+1} - \alpha|$ . Furthermore, we include the number of iterates (it) required to reach those tolerances and the approximated computational order of convergence ACOC [19].

#### 4.1 Non-ideal gas model

The Van der Waals gas equation describes the evolution of a non-ideal gas from its idealised version. It uses two parameters  $a_1$  and  $a_2$  to study the nonideality of the gas.



The equations are described as follows:

$$\left(P + \frac{a_1 n^2}{V^2}\right) (V - na_2) = nRT,$$

where  $P$  is the pressure of the gas,  $V$  is its volume,  $n$  are the moles of gas,  $R$  is the universal constant of ideal gases and  $T$  is the absolute temperature of the gas.

Taking proper values for  $n$ ,  $P$  y  $T$  and the constants  $a_1$  and  $a_2$  we end up with equation

$$f_1(x) = x^3 - 5.22x^2 + 9.0825x - 5.2675.$$

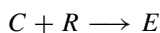
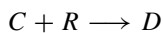
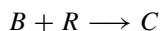
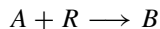
This is a polynomial with a double root at 1.75 and a simple root at 1.72. Table 1 shows the results for the Non-ideal gas model.

We observe that for the parameter  $-1500$  the NC4 method does not converge, this can be expected since the parameter is in the region where at least one of the strange fixed points is attracting.

#### 4.2 Stirred-tank reactor

Let us consider a stirred tank reactor in which an isothermal fluid is stirred continuously, given in Constantinides and Mostoufi [20].

Two components  $A$  and  $R$  are injected in the reactor at ratios  $Q$  and  $q - Q$  respectively. The following reactions occurs in the reactor



Douglas [21] proposes a *feedback control* system in order to control the velocity of the reaction. After his analysis the equation of the transfer function of the reaction is

$$K_c \frac{2.98(x + 2.25)}{(x + 1.45)(x + 2.85)^2(x + 4.35)} = -1,$$

where  $K_c$  is the proportional gain of the controller in the control system. The control is stable for those values of  $K_c$  with negative real part of the transfer function. In control theory, the locatoin the poles of the transfer function improves the knowledge of the behaviour of the controller. Therefore, we are interested finding the roots of equation

$$f_2(x) = x^4 + 11.5x^3 + 47.49x^2 + 83.06325x + 51.23266875 = 0.$$

Here,  $x = -2.85$  is a root of multiplicity 2. There are two other roots located at  $x = -1.45$  and  $x = -4.35$ . The results are displayed in Table 2.

**Table 1** Numerical results for the Non-ideal gas model

Method	$x_0$	$\log( f(x_n) )$	$\log( x_n - \alpha )$	$\log( x_n - x_{n-1} )$	It.	ACOC
NC4(-400+200i)	1.80	-2775.6	-1387.0	-347.8	7	4.00
NC4(-1500)	1.80	-3560.9	-1779.7	-445.8	7	4.00
NC4(0)	1.80	-2542.0	-1270.2	-318.6	7	4.00
NC4(-119+157i)	1.80	-2603.4	-1300.9	-326.3	7	4.00
NC4(100i)	1.80	-2540.4	-1269.4	-318.4	7	4.00
NC4(500)	1.80	-9216.3	-4607.4	-1152.9	8	4.00
NC4(750-900i)	1.80	-8599.1	-4298.8	-1075.8	8	4.00
NC4(95+65i)	1.80	-2491.9	-1245.2	-312.3	7	4.00
SS	1.80	-2508.5	-1253.5	-314.4	7	4.00
SH	1.80	-2505.4	-1252.0	-314.0	7	4.00
B4	1.80	-9342.4	-4670.4	-1168.7	8	4.00
NC4(-400+200i)	-3.00	-2623.8	-1311.1	-328.8	14	4.00
NC4(-1500)*	-3.00	-	-	-	-	-
NC4(0)	-3.00	-6880.6	-3439.5	-860.9	12	4.00
NC4(-119+157i)	-3.00	-7761.6	-3880.0	-971.0	13	4.00
NC4(100i)	-3.00	-4913.9	-2456.2	-615.1	12	4.00
NC4(500)	-3.00	-8838.7	-4418.6	-1105.7	14	4.00
NC4(750-900i)	-3.00	-2486.4	-1242.5	-311.7	12	4.00
NC4(95+65i)	-3.00	-7773.0	-3885.7	-972.5	12	4.00
SS	-3.00	-891.8	-1.5	-445.3	14	2.00
SH	-3.00	-8269.4	-4133.9	-1034.5	15	4.00
B4	-3.00	-5902.4	-2950.4	-738.7	14	4.00

\* Does not converge

**Table 2** Numerical results for the Stirred-tank reactor model

Method	$x_0$	$\log( f(x_n) )$	$\log( x_n - \alpha )$	$\log( x_n - x_{n-1} )$	It.	ACOC
NC4(-400+200i)	-3.00	-5085.4	-0.1	-635.5	8	4.00
NC4(-1500)	-3.00	-5741.6	-0.1	-717.5	8	4.00
NC4(0)	-3.00	-4922.0	-0.1	-615.1	8	4.00
NC4(-119+157i)	-3.00	-4967.3	-0.1	-620.8	8	4.00
NC4(100i)	-3.00	-4921.3	-0.1	-615.0	8	4.00
NC4(500)	-3.00	-4742.9	-0.1	-592.7	8	4.00
NC4(750-900i)	-3.00	-4629.9	-0.1	-578.6	8	4.00
NC4(95+65i)	-3.00	-4885.4	-0.1	-610.5	8	4.00
SS	-3.00	-4870.9	-0.1	-608.7	8	4.00
SH	-3.00	-5510.2	-0.1	-688.6	8	4.00
B4	-3.00	-4726.0	-0.1	-590.6	8	4.00
NC4(-400+200i)	10.50	-8264.3	-0.1	-1032.9	11	4.00
NC4(-1500)*	10.50	-	-	-	-	-
NC4(0)*	10.50	-	-	-	-	-
NC4(-119+157i)**	10.50	-	-	-	-	-
NC4(100i)**	10.50	-	-	-	-	-
NC4(500)	10.50	-9308.6	-0.1	-1163.4	11	4.00
NC4(750-900i)*	10.50	-	-	-	-	-
NC4(95+65i)	10.50	-7120.6	-0.1	-889.9	25	4.00
SS**	10.50	-1030.1	0.3	-515.5	13	2.00
SH*	10.50	-	-	-	-	-
B4*	10.50	-	-	-	-	-

\* There is no convergence of the method.

\*\* Converges to a simple root

Two different initial conditions have been considered. The second one is far from the root, and therefore, several of the methods do not converge. Three of the parameters tested are able to converge to the desired solution. We observe that the SS method converges to a simple root, yielding an undesired result.

### 4.3 Oceanic acidity

The  $CO_2$  concentration of the ocean is modelled according to McHugh et al. [22] and developed by Babajee [23] and Kansal et al [24].

The model computes the acidity levels of the ocean by computing the roots of a fourth order polynomial. The hypothesis considered by Babajee [23] in order to simplify the problem are

- The  $CO_2$  concentration only depends on the upper layer of the ocean. The model does not consider deeper layers of ocean.
- The carbon is distributed as a perfect mixing in the ocean upper layer. That implies that the spatial variables can be neglected.

The dilution of  $CO_2$  involves several chemical reactions, resulting in an increase of the hydrogen ion concentration  $[H^+]$  and, therefore, the acidification of the ocean. The problem of the concentration of hydrogen can be solved by finding the root of the nonlinear function

$$p([H^+]) = \sum_{n=0}^4 r_n [H^+]^n$$

where the coefficients of the polynomials are

$$\begin{cases} r_0 = 2K_0K_1K_2P_tK_B, \\ r_1 = K_0K_1P_tK_B + 2K_0K_1K_2P_t + K_WK_B, \\ r_2 = K_0K_1P_t + BK_B + K_W - AK_B, \\ r_3 = -K_B - A, \\ r_4 = -1. \end{cases}$$

The values  $K_0$ ,  $K_1$ ,  $K_2$ ,  $K_W$  and  $K_B$  are the equilibrium constants of the reactions that involve the acidification process. The parameter  $A$  represents the alkalinity of the ocean water,  $P_t$  is the partial pressure of  $CO_2$ .

In [24] the values  $A = 2.050$  and  $B = 0.409$  are taken from [25, 26] and obtained from [23]:  $P_t = 200$ ,  $K_0 = 3.347(-5)$ ,  $K_1 = 9.747(-4)$ ,  $K_2 = 8.501(-7)$ ,  $K_W = 6.46(-9)$ ,  $K_B = 1.881(-6)$ ,

The values of the constants  $K_i$  can be extracted from [23]. The value of  $P_t$  is a variable that we set in  $P_t = 148.508$ . Under these conditions, we obtain the polynomial

$$f_3(x) = -x^4 + \frac{2309x^3}{250} + r_2 \frac{484274251612376668581111x^2}{5000000000000000000} - \frac{631234663625036799161187633x}{5000000000000000000} + \frac{162684846663854470538576580159111}{12500000000000000000000000} = 0,$$

that has a double root at  $x = 178.977$  and two simple roots at  $x = -360.003$   $y$   $x = 11.2859$ .

Table 3 shows the numerical results to find the zero of multiplicity 2 for taht equation. In that case the tolerance required is  $10^{-200}$ .

#### 4.4 Fixed points in a bi-electron model

A classical problem in chemistry is study of the movement of an electron in the hydrogen atom with a circularly polarised microwave field [27].

The dynamics of this model are given by the Hamiltonian

$$H = \frac{1}{2} (p_x^2 + p_y^2) - x \cdot p_y + y \cdot p_x - \frac{1}{\sqrt{x^2 + y^2}} + K \cdot x,$$

where  $K$  is the intensity of the microwave field. If a a negative charged nucleus is considered instead of positive one, the resulting model is the bi-electron model

$$H = \frac{1}{2} (p_x^2 + p_y^2) - x \cdot p_y + y \cdot p_x + \frac{1}{\sqrt{x^2 + y^2}} + K \cdot x.$$

One is interested in searching in the fixed points of that model. Once computed the dynamical equations it is clear that  $y = 0$  and  $x$  must verify:

$$f_4(x) = x^3 - Kx^2 + \text{sign}(x) = 0.$$

Considering  $K = 2$  this equation has one double root for  $x = 1$  and one single root at  $x = 0$ . Table 4 shows the results for the bi-electron model.

### 5 Conclusion

In the present paper we have introduced a parametric family of order 4 to find roots of multiplicity greater than 2 of nonlinear equations. In order to select the most stable members of the class, a complete study on the stability and the parameters of the

**Table 3** Numerical results for the ocean acidity model

Method	$x_0$	$\log( f(x_n) )$	$\log( x_n - \alpha )$	$\log( x_n - x_{n-1} )$	It.	ACOC
NC4(-400+200i)	200.00	-998.4	-95.8	-275.6	6	4.00
NC4(-1500)	200.00	-998.4	-95.8	-277.0	6	4.00
NC4(0)	200.00	-998.4	-95.8	-257.5	6	4.00
NC4(-119+157i)	200.00	-998.4	-95.8	-261.9	6	4.00
NC4(100i)	200.00	-998.4	-95.8	-257.3	6	4.00
NC4(500)	200.00	-998.4	-95.8	-241.8	6	4.00
NC4(750-900i)	200.00	-998.4	-95.8	-231.3	6	4.00
NC4(95+65i)	200.00	-998.4	-95.8	-253.9	6	4.00
SS	200.00	-998.4	-95.8	-254.4	6	4.00
SH*	200.00	-	-	-	-	-
B4	200.00	-998.4	-95.8	-242.9	6	4.00

\* There is no convergence of the method

**Table 4** Numerical results for the ocean acidity model

Method	$x_0$	$\log( f(x_n) )$	$\log( x_n - \alpha )$	$\log( x_n - x_{n-1} )$	It.	ACOC
NC4(-400+200i)	4.00	-7735.3	-3867.6	-966.8	8	4.00
NC4(-1500)	4.00	-2641.6	-1320.8	-330.0	7	4.00
NC4(0)	4.00	-6993.5	-3496.8	-874.1	8	4.00
NC4(-119+157i)	4.00	-7188.9	-3594.4	-898.5	8	4.00
NC4(100i)	4.00	-6988.5	-3494.2	-873.5	8	4.00
NC4(500)	4.00	-6247.1	-3123.6	-780.8	8	4.00
NC4(750-900i)	4.00	-5756.1	-2878.0	-719.5	8	4.00
NC4(95+65i)	4.00	-6834.4	-3417.2	-854.2	8	4.00
SS	4.00	-6892.5	-3446.3	-861.5	8	4.00
SH	4.00	-5067.4	-2533.7	-633.3	8	4.00
B4	4.00	-6354.6	-3177.3	-794.3	8	4.00
NC4(-400+200i)	200.00	-7188.3	-3594.2	-898.4	10	4.00
NC4(-1500)	200.00	-3138.7	-1569.3	-392.1	9	4.00
NC4(0)	200.00	-5916.9	-2958.4	-739.5	10	4.00
NC4(-119+157i)	200.00	-6247.8	-3123.9	-780.9	10	4.00
NC4(100i)	200.00	-5907.4	-2953.7	-738.3	10	4.00
NC4(500)	200.00	-4676.0	-2338.0	-584.4	10	4.00
NC4(750-900i)	200.00	-3799.4	-1899.7	-474.9	10	4.00
NC4(95+65i)	200.00	-5647.3	-2823.6	-705.8	10	4.00
SS	200.00	-5777.9	-2888.9	-722.1	10	4.00
SH*	200.00	-	-	-	-	-
B4	200.00	-4888.9	-2444.4	-611.0	10	4.00

\* There is no convergence of the method

family has been performed. The application of these schemes is supported with several numerical experiments in the field of mathematical chemistry, showing the good properties of the introduced methods.

**Author Contributions** Conceptualization: Francisco I. Chicharro; Methodology: Neus Garrido; Formal analysis and investigation: Julissa Jerezano, Daniel Pérez-Palau; Writing - original draft preparation: Julissa Jerezano, Daniel Pérez-Palau; Writing - review and editing: Francisco I. Chicharro, Neus Garrido; Funding acquisition: Francisco I. Chicharro, Daniel Pérez-Palau; Resources: Julissa Jerezano; Supervision: Neus Garrido.

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## Declarations

**Conflict of interest** The authors declare they have no competing interests

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