

Solving nonlinear problems by Ostrowski–Chun type parametric families

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Abstract In this paper, by using a generalization of Ostrowski' and Chun's methods two bi-parametric families of predictor–corrector iterative schemes, with order of convergence four for solving system of nonlinear equations, are presented. The predictor of the first family is Newton's method, and the predictor of the second one is Steffensen's scheme. One of them is extended to the multidimensional case. Some numerical tests are performed to compare proposed methods with existing ones and to confirm the theoretical results. We check the obtained results by solving the molecular interaction problem.

Keywords Iterative schemes · Nonlinear equation · System of nonlinear equations · Divided differences · Optimal · Efficiency index

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1 Introduction

Solving nonlinear equations and systems is an important task in theory and practice, not only for Applied Mathematics, but also for many branches of Science and Engineering. A glance at the survey [1] and the references therein show a high level of contemporary interest. In case of problems coming from Chemistry, nonlinear equations regularly appear: in the reaction–diffusion equations that arise in autocatalytic chemical reactions (see [2]), iterative methods can be applied; also in the analysis of electronic structure of the hydrogen atom inside strong magnetic fields (see [3]). Moreover, numerical performance of some chemical problems allows us to check the models of observable phenomena [4]. Even more, many problems from Chemistry consist in finding chemical potentials that are basic for studying other thermodynamic properties: the modeling of such potential leads to nonlinear integral equations that can be reduced to a set of nonlinear algebraic equations (see [5] and [6] for example).

Let us consider the problem of finding a simple zero of the nonlinear function $f : I \subset \mathbb{R} \rightarrow \mathbb{R}$, that is, a solution $\xi \in I$ of the nonlinear equation $f(x) = 0$. The most used iterative techniques to determine these roots can be classified as: (a) methods that require only functional evaluations of f , and (b) schemes whose formula require evaluations of the function and its derivatives. There are two simple and effective known methods that represent these classes: Steffensen's scheme [7]

$$x_{k+1} = x_k - \frac{f(x_k)}{f[\omega_k, x_k]}, \quad (1)$$

where $\omega_k = x_k + f(x_k)$ and $f[\omega_k, x_k] = \frac{f(\omega_k) - f(x_k)}{\omega_k - x_k}$, and Newton's procedure (see [8])

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

where $f'(x)$ is the first derivative of function $f(x)$. The order of convergence of both methods is two.

Multipoint methods have been developed as a result of the search for iterative methods to solve nonlinear equations with fast convergence and small number of operations or functional assessments per iteration. The most important class of multistep schemes are the optimal methods in the sense of Kung–Traub conjecture [9].

The problem of solving a system of nonlinear equations is avoided as far as possible. Generally, the nonlinear system is approximated by a system of linear equations. When this is not satisfactory, the problem must be confronted directly. The direct way is to adapt the methods designed for the scalar case to several variables. A scalar variable is replaced by a vector incorporating all the variables. Hence arises the greatest difficulty to get new iterative methods for nonlinear systems, since not always the methods of nonlinear equations are extensible to systems directly.

Recently, the weight-function procedure has been used, with some restrictions, in the development of high order iterative methods for systems: see, for example the papers of Sharma et al. [10,11] and Abad et al. [12], where the authors apply the designed method to the software improvement of the Global Positioning System.

On the other hand, a common way to generate new schemes is the direct composition of known methods with a later treatment to reduce the number of functional evaluations (see [13–16], for example). A variant of this technique is the so called Pseudocomposition, introduced in [17, 18].

The aim of this work is to design new parametric families of iterative methods for nonlinear equations by using some of the known methods and subsequently extend one of them to systems of nonlinear equations. For this purpose we have used Ostrowski' [19] and Chun's [20] methods with iterative schemes

$$x_{k+1} = y_k - \frac{f(x_k)}{f(x_k) - 2f(y_k)} \frac{f(y_k)}{f'(x_k)}, \quad (3)$$

$$x_{k+1} = y_k - \frac{f(x_k) + 2f(y_k)}{f(x_k)} \frac{f(y_k)}{f'(x_k)}, \quad (4)$$

respectively, where y_k is the step of Newton's method. These methods will be denoted by OM1 and CM1, respectively.

The paper is organized as follows: we start in Sect. 2 with the design of the families of iterative methods for nonlinear equations, with and without derivatives. Section 3 is devoted to the extension of the obtained family with derivatives to systems of nonlinear equations by using the divided difference operator. By means of standard test functions and the problem of molecular interaction, in Sect. 4, we confirm the theoretical results. We finalize the paper with some concluding remarks in Sect. 5.

2 Design of the families for nonlinear equations

We propose a new family as a generalization of Ostrowski' and Chun's methods in the form:

$$y_k = x_k - \alpha \frac{f(x_k)}{f'(x_k)},$$

$$x_{k+1} = y_k - \left[\frac{f(x_k)}{a_1 f(x_k) + a_2 f(y_k)} + \frac{b_1 f(x_k) + b_2 f(y_k)}{f(x_k)} \right] \frac{f(y_k)}{f'(x_k)}, \quad (5)$$

where α , a_1 , a_2 , b_1 and b_2 are real parameters. In the following result we show which values of the parameters are necessary to guarantee the order of convergence is at least 4.

Theorem 1 *Let $f : I \subseteq \mathbb{R} \rightarrow \mathbb{R}$ be a sufficiently differentiable function in an open interval I , such that $\xi \in I$ is a simple solution of the nonlinear equation $f(x) = 0$. Then, the sequence $\{x_k\}_{k \geq 0}$ obtained by using expression (5) converges to ξ with local order of convergence at least four if $\alpha = 1$, $a_2 = a_1^2(b_2 - 2)$, $b_1 = 1 - \frac{1}{a_1}$ and for all a_1 and $b_2 \in \mathbb{R}$ with $a_1 \neq 0$. Then, the error equation is*

$$e_{k+1} = \left((5 - a_1(b_2 - 2))^2 c_2^3 - c_2 c_3 \right) e_k^4 + \mathcal{O}[e_k^5],$$

where $e_k = x_k - \xi$ and $c_q = \left(\frac{1}{q!}\right) \frac{f^{(q)}(\xi)}{f'(\xi)}$, $q \geq 2$.

Proof To prove the local convergence of our iterative process to the solution of $f(x) = 0$ we use the Taylor series expansion of the functions involved around the solution

$$f(x_k) = f'(\xi)[e_k + c_2e_k^2 + c_3e_k^3 + c_4e_k^4] + \mathcal{O}[e_k^5] \tag{6}$$

$$f'(x_k) = f'(\xi)[1 + 2c_2e_k + 3c_3e_k^2 + 4c_4e_k^3 + 5c_5e_k^4] + \mathcal{O}[e_k^5]. \tag{7}$$

By direct division of (6) and (7) and substituting the obtained result in the first step of the proposed iterative method (5) we obtain:

$$y_k = \xi - (1 - \alpha)e_k + \alpha c_2 e_k^2 - 2\alpha(c_2^2 - c_3)e_k^3 - \alpha(-4c_2^3 + 7c_2c_3 - 3c_4)e_k^4 + \mathcal{O}[e_k^5].$$

By using again the Taylor series expansion we obtain:

$$f(y_k) = A_1e_k + A_2e_k^2 + A_3e_k^3 + A_4e_k^4 + \mathcal{O}[e_k^5],$$

where $A_1 = 1 - \alpha$, $A_2 = (1 - \alpha + \alpha^2)c_2$, $A_3 = -2\alpha^2c_2^2 + (1 - \alpha + 3\alpha^2 - \alpha^3)c_3$ and $A_4 = (1 - \alpha + 6\alpha^2 - 4\alpha^3 + \alpha^4)c_4 + 5\alpha^2c_2^3 - \alpha^2(10 - 3\alpha)c_2c_3$. Hence, substituting $f(x_k)$, $f'(x_k)$ and $f(y_k)$ in (5) we obtain the following error equation for the new family:

$$e_{k+1} = B_1e_k + B_2e_k^2 + B_3e_k^3 + B_4e_k^4 + \mathcal{O}[e_k^5],$$

where $B_1 = (1 - \alpha)\left(1 - b_1 - b_2 + b_2\alpha - \frac{1}{a_1 + a_2 - a_2\alpha}\right)$. If $\alpha = 1$ then $B_1 = 0$ and the error equation for the iterative method (5) takes the form:

$$e_{k+1} = B'_2e_k^2 + B'_3e_k^3 + B'_4e_k^4 + \mathcal{O}[e_k^5],$$

where $B'_2 = \left(1 - \frac{1}{a_1} - b_1\right)c_2$. In this case, if $b_1 = \frac{a_1 - 1}{a_1}$, then $B'_2 = 0$ and we obtain for the error equation the following expression:

$$e_{k+1} = B''_3e_k^3 + B''_4e_k^4 + \mathcal{O}[e_k^5],$$

where $B''_3 = \frac{(a_2 - a_1^2(-2 + b_2))c_2^2}{a_1^2}$. We see that if $a_2 = a_1^2(b_2 - 2)$, then $B''_3 = 0$ and

$$e_{k+1} = \left(5 - a_1(b_2 - 2)^2\right)c_2^3 - c_2c_3 e_k^4 + \mathcal{O}[e_k^5], \tag{8}$$

so the order of convergence is at least four. □

Therefore, we obtain the following iterative formula for the bi-parametric family

$$\begin{aligned}
 y_k &= x_k - \frac{f(x_k)}{f'(x_k)}, \\
 x_{k+1} &= y_k - \frac{1}{a_1} \left[\frac{f(x_k)}{f(x_k) + a_1(b_2 - 2)f(y_k)} + \frac{(a_1 - 1)f(x_k) + a_1b_2f(y_k)}{f(x_k)} \right] \frac{f(y_k)}{f'(x_k)}, \tag{9}
 \end{aligned}$$

We present some particular cases of (9):

1. If $b_2 = 2$, the parameter a_1 disappears and the resulting scheme is Chun’s method.
2. When $a_1 = 1$, the iterative formula takes the form:

$$x_{k+1} = y_k - \left[\frac{f(x_k)}{f(x_k) + (b_2 - 2)f(y_k)} + \frac{b_2f(y_k)}{f(x_k)} \right] \frac{f(y_k)}{f'(x_k)}$$

and we have a one parametric family including the original methods as particular cases: (a) if $b_2 = 2$, as we have said, we have Chun’s method (4) and (b) if $b_2 = 0$, we get Ostrowski’s scheme (3).

3. For any $a_1 \neq 0$ and $b_2 = 0$, the iterative formula is:

$$x_{k+1} = y_k - \frac{f(x_k) - 2(a_1 - 1)f(y_k)}{f(x_k) - 2a_1f(y_k)} \frac{f(y_k)}{f'(x_k)}.$$

If we denote $-2(a_1 - 1) = \beta$, then $-2a_1 = \beta - 2$ and we get King’s family [21]

$$x_{k+1} = y_k - \frac{f(x_k) + \beta f(y_k)}{f(x_k) + (\beta - 2)f(y_k)} \frac{f(y_k)}{f'(x_k)}.$$

4. For any $a_1 \neq 0$ and $b_2 = 1$, the iterative formula takes the form:

$$x_{k+1} = y_k - \frac{1}{a_1} \left[\frac{f(x_k)}{f(x_k) - a_1f(y_k)} + \frac{(a_1 - 1)f(x_k) + a_1f(y_k)}{f(x_k)} \right] \frac{f(y_k)}{f'(x_k)}.$$

At this point, can we get a similar family by approximating the derivatives by divided differences and preserving the order of convergence? The answer is given in the following result, where a technique describe in [22].

Theorem 2 *Let $f : I \subseteq \mathbb{R} \rightarrow \mathbb{R}$ be a sufficiently differentiable function in an open interval I , such that $\xi \in I$ is a simple solution of the nonlinear equation $f(x) = 0$. Then, the sequence $\{x_k\}_{k \geq 0}$ obtained by using the expression*

$$\begin{aligned}
 y_k &= x_k - \alpha \frac{f(x_k)}{f[z_k, x_k]}, \\
 x_{k+1} &= y_k - \left[\frac{f(x_k)}{a_1f(x_k) + a_2f(y_k)} + \frac{b_1f(x_k) + b_2f(y_k)}{f(x_k)} \right] \frac{f(y_k)}{f[z_k, x_k]}, \tag{10}
 \end{aligned}$$

where $z_k = x_k + f(x_k)^2$ and $f[z_k, x_k] = \frac{f(z_k) - f(x_k)}{z_k - x_k}$, converges to ξ with order of convergence at least four if $\alpha = 1$, $a_2 = a_1^2(b_2 - 2)$, $b_1 = 1 - \frac{1}{a_1}$ and for all a_1 and $b_2 \in \mathbb{R}$, with $a_1 \neq 0$. The error equation is

$$e_{k+1} = \left((5 - a_1(-2 + b_2))^2 c_2^3 - c_2 c_3 + \gamma c_2^2 \right) e_k^4 + \mathcal{O}[e_k^5],$$

where $e_k = x_k - \xi$, $\gamma = f'(\xi)^2$ and $c_q = \left(\frac{1}{q!} \right) \frac{f^{(q)}(\xi)}{f'(\xi)}$, $q \geq 2$.

Proof By using the Taylor series expansion of the function $f(x_k)$ around ξ (6), we obtain the following expressions:

$$\begin{aligned} z_k &= e_k + \gamma [e_k^2 + 2c_2 e_k^3 + (c_2^2 + 2c_3) e_k^4 + 2(c_2 c_3 + c_4) e_k^5 \\ &\quad + (c_3^2 + 2c_2 c_4 + 2c_5) e_k^6] + \mathcal{O}[e_k^7], \\ f(z_k) &= f'(\xi) [e_k + (c_2 + \gamma) e_k^2 + (c_3 + 4\gamma c_2) e_k^3 + c_4 + \gamma(5c_2^2 + 5c_3 + \gamma c_2) e_k^4 \\ &\quad + (c_5 + \gamma(2c_2^3 + 12c_2 c_3 + 6c_4 + \gamma(4c_2^2 + 3c_3))) e_k^5] + \mathcal{O}[e_k^6], \\ f[z_k, x_k] &= f'(\xi) [1 + 2c_2 e_k + (c_3 + 4\gamma c_2) e_k^3 + (4c_4 + \gamma(2c_2^2 + 3c_3)) e_k^5] + \mathcal{O}[e_k^4]. \end{aligned}$$

Hence, substituting these expressions in (10), we obtain the following result for y_k :

$$y_k = (1 - \alpha) e_k + \alpha (2c_3 - 2c_2^2 + \gamma c_2) e_k^2 + \alpha (4c_2^3 - 7c_2 c_3 - \gamma c_2^2 + 3c_4 + 3\gamma c_3) e_k^4 + \mathcal{O}[e_k^5].$$

By using the Taylor series expansion again, we obtain the following expression:

$$f(y_k) = A_1 e_k + A_2 e_k^2 + A_3 e_k^3 + A_4 e_k^4 + \mathcal{O}[e_k^5],$$

where $A_1 = 1 - \alpha$, $A_2 = (1 - \alpha + \alpha^2) c_2$, $A_3 = \alpha(\gamma - 2\alpha c_2) c_2 + (1 - \alpha + 3\alpha^2 - \alpha^3) c_3$ and $A_4 = (1 - \alpha + 6\alpha^2 - 4\alpha^3 + \alpha^4) c_4 + \alpha(3\gamma c_3 + \gamma(1 - 2\alpha) c_2^2 + 5\alpha c_2^3 + \alpha(3\alpha - 10) c_2 c_3)$. Through these results we get the following error equation for the iterative scheme (10):

$$e_{k+1} = B_1 e_k + B_2 e_k^2 + B_3 e_k^3 + B_4 e_k^4 + \mathcal{O}[e_k^5],$$

where $B_1 = (1 - \alpha) \left(1 - b_1 - b_2 + b_2 \alpha - \frac{1}{a_1 + a_2 - a_2 \alpha} \right)$.

If $\alpha = 1$, then $B_1 = 0$ and the error equation takes the form:

$$e_{k+1} = B'_2 e_k^2 + B'_3 e_k^3 + B'_4 e_k^4 + \mathcal{O}[e_k^5],$$

where $B'_2 = \left(1 - \frac{1}{a_1} - b_1 \right) c_2$. In this case, if $b_1 = \frac{a_1 - 1}{a_1}$, $B'_2 = 0$ and we obtain for the error equation the following expression:

$$e_{k+1} = B''_3 e_k^3 + B''_4 e_k^4 + \mathcal{O}[e_k^5],$$

where $B_3'' = \frac{(a_2 - a_1^2(-2 + b_2))c_2^2}{a_1^2}$. We see that if $a_2 = a_1^2(b_2 - 2)$, then $B_3'' = 0$ and

$$e_{k+1} = ((5 - a_1(-2 + b_2))^2)c_2^3 - c_2c_3 + \gamma c_2^2 e_k^4 + \mathcal{O}[e_k^5], \tag{11}$$

so the order of convergence is at least four. □

Then, we obtain the following iterative formula for the bi-parametric family

$$y_k = x_k - \frac{f(x_k)}{f[z_k, x_k]},$$

$$x_{k+1} = y_k - \frac{1}{a_1} \left[\frac{f(x_k)}{f(x_k) + a_1(b_2 - 2)f(y_k)} + \frac{(a_1 - 1)f(x_k) + a_1b_2f(y_k)}{f(x_k)} \right] \frac{f(y_k)}{f[z_k, x_k]}, \tag{12}$$

and we define the following particular cases of the (12):

1. If $b_2 = 2$, then parameter a_1 is canceled in the iterative expression, that corresponds to the derivative-free Chun’s scheme (CM2).
2. When $a_1 = 1$, the iterative formula takes the form:

$$x_{k+1} = y_k - \left[\frac{f(x_k)}{f(x_k) + (b_2 - 2)f(y_k)} + \frac{b_2f(y_k)}{f(x_k)} \right] \frac{f(y_k)}{f[z_k, x_k]}$$

and we have a one parametric family that includes the derivative-free versions of original schemes: (a) if $b_2 = 2$, we have derivative-free Chun’s method, whose iterative expression is

$$x_{k+1} = y_k - \frac{f(x_k) + 2f(x_k)}{f(x_k)} \frac{f(y_k)}{f[z_k, x_k]},$$

and (b) if $b_2 = 0$, we obtain derivative-free Ostrowski’s method (OM2), with the iterative expression

$$x_{k+1} = y_k - \frac{f(x_k)}{f(x_k) - 2f(x_k)} \frac{f(y_k)}{f[z_k, x_k]}.$$

3. When $a_1 \neq 0$ and $b_2 = 0$, the iterative formula takes the form:

$$x_{k+1} = y_k - \frac{f(x_k) - 2(a_1 - 1)f(y_k)}{f(x_k) - 2a_1f(y_k)} \frac{f(y_k)}{f[z_k, x_k]}.$$

If we denote $-2(a_1 - 1) = \beta$, then $-2a_1 = \beta - 2$ and we get the derivative-free King’s family

$$x_{k+1} = y_k - \frac{f(x_k) + \beta f(y_k)}{f(x_k) + (\beta - 2)f(y_k)} \frac{f(y_k)}{f[z_k, x_k]}.$$

4. When $a_1 \neq 0$ and $b_2 = 1$, the resulting iterative formula is:

$$x_{k+1} = y_k - \frac{1}{a_1} \left[\frac{f(x_k)}{f(x_k) - a_1 f(y_k)} + \frac{(a_1 - 1)f(x_k) + a_1 f(y_k)}{f(x_k)} \right] \frac{f(y_k)}{f[z_k, x_k]}.$$

3 Extension to systems of nonlinear equations

The objective of this section is to give a generalization to several variables of one of the families obtained in Sect. 2, preserving the local order of convergence. In order to get this aim, we are going to use the divided difference operator.

Let us consider a sufficiently differentiable function $F : \Omega \subseteq \mathbb{R}^n \rightarrow \mathbb{R}^n$ in a convex set $\Omega \subset \mathbb{R}^n$ and let $\xi \in \Omega$ be a solution of the nonlinear system $F(x) = 0$. The divided difference operator of F on \mathbb{R}^n is a mapping $[\cdot, \cdot; F] : \Omega \times \Omega \subset \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathcal{L}(\mathbb{R}^n)$ (see [8]) such that

$$[x, y; F](x - y) = F(x) - F(y), \quad \text{for any } x, y \in \Omega.$$

In the proof of the following result, we will use the Genochi-Hermite formula (see [8])

$$[x, y; F] = \int_0^1 F'(x + t(x - y))dt,$$

for all $(x, y) \in \mathbb{R}^n \times \mathbb{R}^n$.

The extension to multivariate case of family (5) requires to rewrite the iterative expression in such a way that no functional evaluation of the nonlinear function remain at the denominator, as they will become vectors in the multivariate case. To get this aim, let us consider that, being the first step of the iterative process $y_k = x_k - \alpha \frac{f(x_k)}{f'(x_k)}$, $f(x_k)$ can be expressed as $f(x_k) = \frac{1}{\alpha}(x_k - y_k)f'(x_k)$. By using this, we can rewrite the quotient $\frac{f(y_k)}{f(x_k)}$ as

$$\frac{f(y_k)}{f(x_k)} = 1 - \alpha \frac{f[x_k, y_k]}{f'(x_k)}.$$

By using this transformation, the proposed family (5) is fully extensible to several variables,

$$\begin{aligned} y^{(k+1)} &= x^{(k)} - \alpha [F'(x^{(k)})]^{-1} F(x^{(k)}) \\ x^{(k+1)} &= y^{(k)} - \left(G_1(x^{(k)}, y^{(k)}) + G_2(x^{(k)}, y^{(k)}) \right) [F'(x^{(k)})]^{-1} F(y^{(k)}), \\ G_1(x^{(k)}, y^{(k)}) &= \left[(a_1 + a_2)I - \alpha a_2 [F'(x^{(k)})]^{-1} [x^{(k)}, y^{(k)}; F] \right]^{-1}, \\ G_2(x^{(k)}, y^{(k)}) &= (b_1 + b_2)I - \alpha b_2 [F'(x^{(k)})]^{-1} [x^{(k)}, y^{(k)}; F], \end{aligned} \tag{13}$$

where

$$G_1(x^{(k)}, y^{(k)}) = \left[(a_1 + a_2)I - \alpha a_2 [F'(x^{(k)})]^{-1} [x^{(k)}, y^{(k)}; F] \right]^{-1},$$

$$G_2(x^{(k)}, y^{(k)}) = (b_1 + b_2)I - \alpha b_2 [F'(x^{(k)})]^{-1} [x^{(k)}, y^{(k)}; F],$$

and $[x^{(k)}, y^{(k)}; F]$ denotes the divided difference operator of F on $x^{(k)}$ and $y^{(k)}$, identity matrix is denoted by I and $F'(x^{(k)})$ is the Jacobian matrix of the system. In the proof of the following result we are going to use the notation introduced in [23].

Theorem 3 *Let $F: \Omega \subseteq \mathbb{R}^n \rightarrow \mathbb{R}^n$ be a sufficiently differentiable function in a convex set Ω and $\xi \in \Omega$ be a solution of $F(x) = 0$. Let us suppose that $F'(x)$ is continuous and nonsingular at ξ . Then, the sequence $\{x^{(k)}\}_{k \geq 0}$ obtained by using the iterative scheme (13), converges to ξ with order of convergence at least four if $\alpha = 1$, $a_2 = a_1^2(b_2 - 2)$, $b_1 = 1 - \frac{1}{a_1}$ and for all a_1 and $b_2 \in \mathbb{R}$ with $a_1 \neq 0$. The error equation is*

$$e_{k+1} = -[(a_1(b_2 - 2)^2 - 5)C_2^3 + C_2C_3]e_k^4 + \mathcal{O}[e_k^5],$$

where $e_k = x^{(k)} - \xi$ and $C_q = \left(\frac{1}{q!}\right) [f'(\xi)]^{-1} F^{(q)}(\xi)$, $q \geq 2$.

Proof By using Taylor expansion around ξ , we obtain:

$$F(x^{(k)}) = F'(\xi)(e_k + C_2e_k^2 + C_3e_k^3 + C_4e_k^4) + \mathcal{O}[e_k^5],$$

$$F'(x^{(k)}) = F'(\xi)(I + 2C_2e_k + 3C_3e_k^2 + 4C_4e_k^3) + \mathcal{O}[e_k^4].$$

Let us consider

$$[F'(x^{(k)})]^{-1} = (I + X_2e_k + X_3e_k^2 + X_4e_k^3)[F'(\xi)]^{-1} + \mathcal{O}(e_k^4).$$

Forcing $[F'(x^{(k)})]^{-1} F'(x^{(k)}) = I$, we get $X_2 = -2C_2$, $X_3 = 2C_2^2 - 3C_3$ and $X_4 = -4C_4 + 6C_3C_2 - 4C_2^3 + 6C_2C_3$. These expressions allow us to obtain

$$y^{(k)} = x^{(k)} - \alpha [F'(x^{(k)})]^{-1} F(x^{(k)})$$

$$= \xi + (1 - \alpha)e^{(k)} - \alpha(A_2e_k^2 + A_3e_k^3 + A_4e_k^4) + \mathcal{O}[e_k^5], \tag{14}$$

where $A_2 = -C_2 - X_2$, $A_3 = -C_3 - C_2X_2 - X_3$ and $A_4 = -C_4 - C_3X_2 - C_2X_3 + X_4$. By using (14) and the Taylor series expansion around ξ we obtain

$$F(y^{(k)}) = F'(\xi)(B_1e_k + B_2e_k^2 + B_3e_k^3 + B_4e_k^4) + \mathcal{O}[e_k^5],$$

where $B_1 = \beta$, $B_2 = (\alpha + \beta^2)C_2$, $B_3 = -\alpha A_3 + 2\alpha\beta C_2A_3 + 3\alpha\beta^2 C_3C_2 + \beta^4 C_4$, $B_4 = -\alpha A_4 + \alpha^2 C_2^3 - 2\alpha\beta C_2A_3 + 3\alpha\beta^2 C_3C_2 - 2 + \beta^4 C_4$ and $\beta = 1 - \alpha$. We

calculate the Taylor expansion of $[x^{(k)}, y^{(k)}; F]$ by using (14),

$$[x^{(k)}, y^{(k)}; F] = F'(\xi) \left[I + D_2 e_k + D_3 e_k^2 + D_4 e_k^3 \right] + \mathcal{O}[e_k^4],$$

where $D_2 = (2 - \alpha)C_2$, $D_3 = \alpha C_2^2 + (3 - 3\alpha + \alpha^2)C_3$ and $D_4 = 2\alpha C_2 C_3 + \alpha(3 - 2\alpha)C_3 C_2 - (4 - 6\alpha + 4\alpha^2 - \alpha^3)C_4$. Then,

$$\begin{aligned} M &= (a_1 + a_2)I - \alpha a_2 [F'(x^{(k)})]^{-1} [x^{(k)}, y^{(k)}; F] \\ &= a_1 + E_2 e_k + E_3 e_k^2 + E_4 e_k^3 + \mathcal{O}[e_k^4], \end{aligned}$$

where $E_2 = \alpha a_2 C_2$, $E_3 = \alpha C_2^3 + \alpha(\alpha - 3)C_3$ and $E_4 = 6\alpha C_2 C_3 - 2\alpha C_2^3 - 4C_4 + 5\alpha(2 - \alpha)C_3 C_2 + (4 - 6\alpha + 4\alpha^2 - \alpha^3)C_3 C_4$. So, we obtain $G_1(x^{(k)}, y^{(k)})$ as the inverse of matrix M :

$$G_1(x^{(k)}, y^{(k)}) = I + Y_2 e_k + Y_3 e_k^2 + Y_4 e_k^3 + \mathcal{O}[e_k^4],$$

where $Y_2 = \frac{\alpha a_2}{a_1} C_2$, $Y_3 = \frac{\alpha a_2}{a_1^2} [(\alpha a_2 - 3)C_2^2 + (\alpha - 3)C_3]$, $Y_4 = \frac{\alpha a_2}{a_1^3} [(8a_1 + 3\alpha a_1 a_2 + 3\alpha a_2 - \alpha^2 a_2^2)C_2^3]$ and

$$G_2(x^{(k)}, y^{(k)}) = b_1 + F_2 e_k + F_3 e_k^2 + F_4 e_k^3 + F_5 e_k^4 + \mathcal{O}[e_k^5],$$

where $F_2 = \alpha b_2 C_2$, $F_3 = -\alpha b_2 [3C_2^2 - (\alpha - 3)C_3]$ and $F_4 = b_2 [\alpha(6 - 4\alpha + \alpha^2)C_4 - 6\alpha(2 - \alpha)C_3 C_2 + 4(\alpha + 1)C_2^3 - 6(\alpha + 1)C_2 C_3]$.

Thus, we obtain the error equation of the proposed method

$$e_{k+1} = H_1 e_k + H_2 e_k^2 + H_3 e_k^3 + H_4 e_k^4 + \mathcal{O}[e_k^5],$$

where $H_1 = \frac{1}{a_1} (1 + a_1(b_1 - 1))(\alpha - 1)$. If $\alpha = 1$, then $H_1 = 0$ and the error equation takes the form:

$$e_{k+1} = H_2' e_k^2 + H_3' e_k^3 + H_4' e_k^4 + \mathcal{O}[e_k^5],$$

where $H_1' = -\frac{1}{a_1} (1 + a_1(b_1 - 1))C_2$. We note that if $b_1 = \frac{a_1 - 1}{a_1}$, then $H_2' = 0$. We introduce this value of b_1 and obtain the new form of the error equation

$$e_{k+1} = H_3''' e_k^3 + H_4''' e_k^4 + \mathcal{O}[e_k^5],$$

where $H_3''' = \frac{a_2 - a_1^2(b_2 - 2)}{a_1^2} C_2^2$. Finally, if $a_2 = a_1^2(b_2 - 2)$, the error equation is:

$$e_{k+1} = -[(a_1(b_2 - 2)^2 - 5)C_2^3 + C_2 C_3] e_k^4 + \mathcal{O}[e_k^5] \tag{15}$$

and this shows that the proposed method has order of convergence at least four. \square

Under the assumptions made in the previous result, the iterative scheme of the bi-parametric family (13) takes the form:

$$\begin{aligned}y^{(k)} &= x^{(k)} - [F'(x^{(k)})]^{-1} F(x^{(k)}), \\x^{(k+1)} &= y^{(k)} - G(x^{(k)}, y^{(k)}) [F'(x^{(k)})]^{-1} F(y^{(k)}), \\G(x^{(k)}, y^{(k)}) &= \frac{1}{a_1} \left[(1 + a_1 b_2 - 2a_1) I - a_1 (b_2 - 2) [F'(x^{(k)})]^{-1} [x^{(k)}, y^{(k)}; F] \right]^{-1} \\&\quad + \frac{1}{a_1} \left((a_1 + a_1 b_2 - 1) I - b_2 [F'(x^{(k)})]^{-1} [x^{(k)}, y^{(k)}; F] \right). \quad (16)\end{aligned}$$

In the following we propose some particular cases:

1. As in the scalar case, if $b_2 = 2$,

$$G(x^{(k)}, y^{(k)}) = 3I - 2[F'(x^{(k)})]^{-1} [x^{(k)}, y^{(k)}; F]$$

and the resulting scheme is the extended Chun's method for nonlinear systems (CM3).

2. When $a_1 = 1$,

$$\begin{aligned}G(x^{(k)}, y^{(k)}) &= [(b_2 - 1)I - (b_2 - 2)[F'(x^{(k)})]^{-1} [x^{(k)}, y^{(k)}; F]]^{-1} \\&\quad + b_2 I - b_2 [F'(x^{(k)})]^{-1} [x^{(k)}, y^{(k)}; F]\end{aligned}$$

and we have a parametric family. Some particular cases of this class are the following:

- (a) If $b_2 = 2$, we have Chun's method transferred to systems

$$x^{(k+1)} = y^{(k)} - \left(I - 2[F'(x^{(k)})]^{-1} [x^{(k)}, y^{(k)}; F] \right) [F'(x^{(k)})]^{-1} F(y^{(k)}).$$

- (b) If $b_2 = 0$, we get Ostrowski's method transferred to systems (OM3)

$$x^{(k+1)} = y^{(k)} - \left(-I + 2[F'(x^{(k)})]^{-1} [x^{(k)}, y^{(k)}; F] \right)^{-1} [F'(x^{(k)})]^{-1} F(y^{(k)}).$$

3. For any $a_1 \neq 0$ and $b_2 = 0$,

$$G(x^{(k)}, y^{(k)}) = \frac{a_1 - 1}{a_1} I + \left[a_1 (1 - 2a_1) I + 2a_1^2 [F'(x^{(k)})]^{-1} [x^{(k)}, y^{(k)}; F] \right]^{-1}.$$

4. For any $a_1 \neq 0$ and $b_2 = 1$,

$$\begin{aligned}x^{(k+1)} &= y^{(k)} - \frac{1}{a_1} \left[(1 - a_1) I + a_1 [F'(x^{(k)})]^{-1} [x^{(k)}, y^{(k)}; F] \right]^{-1} [F'(x^{(k)})]^{-1} \\&\quad F(y^{(k)}) + \frac{1}{a_1} \left[(2a_1 - 1) I - [F'(x^{(k)})]^{-1} [x^{(k)}, y^{(k)}; F] \right] [F'(x^{(k)})]^{-1} F(y^{(k)}).\end{aligned}$$

4 Numerical results

In this section we show the numerical behavior of the proposed methods on some standard equations and systems and also on an applied problem. In the tests made, variable precision arithmetics has been used, with 4,000 digits of mantissa (in the numerical tests for nonlinear equations) and 1,000 digits of mantissa (in the numerical tests for systems of nonlinear equations) in MATLAB R2013a. These tests have been made by using the stopping criterium $\|F(x^{(k+1)})\| < 10^{-700}$ or $\|x^{(k+1)} - x^{(k)}\| < 10^{-700}$. We will also use the approximated computational order of convergence ρ (usually called ACOC), defined by Cordero and Torregrosa in [25]

$$\rho = \frac{\ln(\|x^{(k+1)} - x^{(k)}\|/\|x^{(k)} - x^{(k-1)}\|)}{\ln(\|x^{(k)} - x^{(k-1)}\|/\|x^{(k-1)} - x^{(k-2)}\|)}.$$

4.1 Academic test functions

Firstly, to check the behavior of the proposed methods with derivatives for solving nonlinear equations, we use the following elements of the family of obtained methods:

1. **MA1**: $a_1 = \frac{5}{4}$ and $b_2 = 0$

$$x_{k+1} = y_k - \frac{f(x_k) - \frac{1}{2}f(y_k)}{f(x_k) - \frac{5}{2}f(y_k)} \frac{f(y_k)}{f'(x_k)},$$

2. **MB1**: $a_1 = 1$ and $b_2 = 1$

$$x_{k+1} = y_k - \left(\frac{f(x_k)}{f(x_k) - f(y_k)} + \frac{f(y_k)}{f(x_k)} \right) \frac{f(y_k)}{f'(x_k)},$$

3. **MC1**: $a_1 = 1$ and $b_2 = 3$

$$x_{k+1} = y_k - \left(\frac{f(x_k)}{f(x_k) + f(y_k)} + \frac{3f(y_k)}{f(x_k)} \right) \frac{f(y_k)}{f'(x_k)},$$

where y_k is Newton’s step. In these numerical experiments, we compare MA1, MB1 and MC1 with Newton’s method (NM), Ostrowski’s method (OM) (3), Chun’s method (CM) (4) and Jarratt’s method (JM) [24]

$$y_k = x_k - \frac{2}{3} \frac{f(x_k)}{f'(x_k)}$$

$$x_{k+1} = x_k - \frac{1}{2} \frac{3f'(x_k) + f'(y_k)}{3f'(x_k) - f'(y_k)} \frac{f(x_k)}{f'(x_k)}.$$

Tables 1, 2, 3 and 4 show, for each initial estimation x_0 and every method, the approximated computational order of convergence ρ , the number of iterations, and two measures of the error, specifically, $\|x^{(k+1)} - x^{(k)}\|$ and $\|F(x^{(k+1)})\|$.

Table 1 Test functions and numerical results for methods with derivatives

Method	ρ	Iter	$ x_{k+1} - x_k $	$ f(x_{k+1}) $
$f_1(x) = \sin x - x^2 + 1, x_0 = 1$ and $\xi \approx 1.409624004002596$				
NM	2.0000	10	1.867e-273	5.205e-546
JM	4.0000	5	7.315e-139	1.307e-553
OM	4.0000	6	3.774e-196	4.751e-782
CM	4.0000	5	4.093e-139	1.268e-554
MA1	4.0000	5	1.389e-178	5.588e-716
MB1	4.0000	7	2.005e-959	2.697e-2,008
MC1	4.0000	5	3.938e-090	4.497e-358
$f_2(x) = x^2 - \exp(x) - 3x + 2, x_0 = 0.8$ and $\xi \approx 0.257530285439861$				
NM	2.0000	8	4.472e-190	7.062e-380
JM	4.0000	5	1.756e-258	1.622e-1,033
OM	4.0000	5	7.970e-271	1.909e-1,083
CM	4.0000	5	3.475e-286	3.363e-1,114
MA1	4.0000	5	8.287e-257	9.502e-1,027
MB1	4.0000	6	8.005e-1065	0.0
MC1	4.0000	5	4.385e-266	2.889e-1,064
$f_3(x) = \cos x - x, x_0 = 1$ and $\xi \approx 0.739085133215161$				
NM	2.0000	8	7.118e-167	1.872e-333
JM	4.0000	5	4.214e-296	1.350e-1,183
OM	4.0000	5	1.102e-268	1.693e-1,073
CM	4.0000	5	1.632e-299	2.793e-1,197
MA1	4.0000	5	1.594e-309	1.599e-1,237
MB1	4.0000	6	1.026e-1093	1.349e-2,008
MC1	4.0000	5	2.233e-273	2.409e-1,092
$f_4(x) = \cos x - x \exp x + x^2, x_0 = 0.5$ and $\xi \approx 0.639154096332008$				
NM	2.0000	9	1.068e-243	2.168e-486
JM	4.0000	5	4.140e-293	1.019e-1,170
OM	4.0000	5	3.505e-182	7.589e-726
CM	4.0000	5	5.909e-289	4.679e-1,154
MA1	4.0000	5	3.485e-254	1.219e-1,014
MB1	4.0000	5	1.929e-770	1.349e-2,008
MC1	4.0000	5	2.034e-196	6.597e-783

At the sight of the results in Table 1, we conclude that the new methods have an excellent behavior, giving the best error estimations in all cases.

Now, the elements of the family of derivative-free methods that we are going to use are:

Table 2 Test functions and numerical results for methods without derivatives

Method	ρ	Iter	$ x_{k+1} - x_k $	$ f'(x_{k+1}) $
$f_1(x) = \sin x - x^2 + 1, x_0 = 1$ and $\xi \approx 1.409624004002596$				
ST	2.0000	10	3.249e-274	2.615e-547
LZM	4.0000	5	5.953e-239	5.950e-954
CT4	4.0000	5	6.200e-151	1.855e-601
OM2	4.0000	6	5.935e-277	6.793e-1,105
CM2	4.0000	5	1.012e-91	3.771e-364
MA2	4.0000	6	8.754e-246	3.492e-980
MB2	4.0000	6	2.311e-240	5.332e-959
MC2	4.0000	5	3.938e-90	4.497e-358
$f_2(x) = x^2 - \exp(x) - 3x + 2, x_0 = 0.8$ and $\xi \approx 0.257530285439861$				
ST	2.0000	9	3.979e-175	1.554e-349
LZM	4.0000	5	4.687e-163	6.775e-651
CT4	4.0000	5	1.336e-166	4.202e-665
OM2	-	n.c.	-	-
CM2	4.0000	10	4.367e-111	1.697e-442
MA2	-	n.c.	-	-
MB2	4.0000	5	4.436e-266	3.025e-1,064
MC2	4.0000	5	4.385e-266	2.889e-1,064
$f_3(x) = \cos x - x, x_0 = 1$ and $\xi \approx 0.739085133215161$				
ST	2.0000	8	4.380e-178	4.776e-356
LZM	4.0000	4	1.190e-84	1.460e-338
CT4	4.0000	5	6.809e-309	4.167e-1,235
OM2	4.0000	5	2.492e-238	7.160e-952
CM2	4.0000	5	1.281e-286	3.064e-1,145
MA2	4.0000	5	1.433e-231	8.582e-925
MB2	4.0000	5	1.154e-237	1.717e-1,093
MC2	4.0000	5	2.233e-273	2.409e-1,092
$f_4(x) = \cos x - x \exp x + x^2, x_0 = 0.5$ and $\xi \approx 0.639154096332008$				
ST	2.0000	9	1.412e-219	5.402e-438
LZM	4.0000	5	1.071e-256	1.266e-1,024
CT4	4.0000	5	1.242e-276	1.671e-1,104
OM2	4.0000	5	2.656e-209	4.187e-834
CM2	4.0000	5	3.987e-220	9.449e-878
MA2	4.0000	5	2.132e-207	1.980e-826
MB2	4.0000	5	3.318e-193	4.676e-770
MC2	4.0000	5	2.034e-196	6.597e-783

Table 3 Test functions and results for nonlinear systems, F_1 and F_2

Method	ρ	Iter	$\ x^{(k+1)} - x^{(k)}\ $	$\ F(x^{(k+1)})\ $
$F_1(x_1, x_2) = (\exp x_1 \exp x_2 + x_1 \cos x_2, x_1 + x_2 - 1)$ $x^{(0)} = (3, -2)$ and $\xi_1 \approx 3.4675009642402$, $\xi_2 \approx -2.4675009642402$				
NM	2.0000	9	1.141e-397	4.802e-795
TM	3.0000	6	2.905e-336	5.671e-1,008
JM	4.0000	5	5.597e-254	5.671e-1,008
OM3	4.0000	5	3.978e-266	5.671e-1,008
CM3	4.0000	5	9.701e-261	5.671e-1,008
MA3	4.0000	5	3.749e-268	9.301e-1,072
MB3	4.0000	5	7.966e-262	3.762e-1,046
MC3	4.0000	5	7.972e-262	3.773e-1,046
$F_2(x_1, x_2, x_3, x_4) = (x_1x_3 + x_4(x_2 + x_3), x_1x_3 + x_4(x_1 + x_3), x_1x_2 + x_4(x_1 + x_2), x_1x_2 + x_1x_3 + x_2x_3 - 1)$, $x_0 = (1, 1, 1, -0.5)$ and $\xi_1 = \xi_2 = \xi_3 = 0.5773502691896257$, $\xi_4 = -0.2886751345948129$				
NM	2.0000	11	4.407e-586	3.007e-1,008
TM	3.0000	7	3.003e-341	2.835e-1,008
JM	4.0000	6	4.407e-586	2.835e-1,008
OM3	4.0000	6	4.407e-586	2.835e-1,008
CM3	4.0000	6	9.920e-425	0.0
MA3	4.9996	5	7.717e-340	4.202e-1,697
MB3	4.0000	6	6.486e-447	1.508e-1,785
MC3	4.0000	6	1.555e-442	4.982e-1,768

1. *MA2*: $a_1 = \frac{5}{4}$ and $b_2 = 0$

$$x_{k+1} = y_k - \frac{f(x_k) - \frac{1}{2}f(y_k)}{f(x_k) - \frac{5}{2}f(y_k)} \frac{f(y_k)}{f[z_k, x_k]}$$

2. *MB2*: $a_1 = 1$ and $b_2 = 1$

$$x_{k+1} = y_k - \left(\frac{f(x_k)}{f(x_k) - f(y_k)} + \frac{f(y_k)}{f(x_k)} \right) \frac{f(y_k)}{f[z_k, x_k]}$$

3. *MC2*: $a_1 = 1$ and $b_2 = 3$

$$x_{k+1} = y_k - \left(\frac{f(x_k)}{f(x_k) + f(y_k)} + \frac{3f(y_k)}{f(x_k)} \right) \frac{f(y_k)}{f[z_k, x_k]}$$

where $y_k = x_k - \frac{f(x_k)}{f[z_k, x_k]}$, $f[z_k, x_k] = \frac{f(z_k) - f(x_k)}{z_k - x_k}$ and $z_k = x_k + f(x_k)^2$. In this case, we compare our schemes with Steffensen’s method (SM) [7], LZM [26]

Table 4 Test functions and results for nonlinear systems F_3 and F_4

Method	ρ	Iter	$\ x^{(k+1)} - x^{(k)}\ $	$\ F(x^{(k+1)})\ $
$F_3(x_1, x_2) = (x_1^2 - x_1 - x_2^2 - 1, \sin x_1 + x_2), x_0 = (-0.15, -0.15)$ and $\xi_1 \approx -0.8452567390376772, \xi_2 \approx -0.7481414932526368$				
NM	1.9995	11	3.892e-594	0.0
TM	2.9972	7	4.061e-266	6.803e-798
JM	3.9754	6	2.257e-476	5.845e-1,008
OM3	3.9874	6	8.591e-480	5.845e-1,008
CM3	3.9770	6	2.545e-240	3.598e-960
MA3	3.9831	5	6.832e-184	1.298e-734
MB3	4.0078	6	1.531e-274	2.237e-1,096
MC3	4.0097	6	3.831e-244	6.833e-974
$F_4(x_1, x_2, x_3) = (x_1^2 + x_2^2 + x_3^2 - 9, x_1 x_2 x_3 - 1, x_1 + x_2 - x_3^2), x_0 = (2, -1.5 - 0.5)$ and $\xi_1 \approx 2.140258122005175, \xi_2 \approx -2.090294642255235, \xi_3 \approx -0.2235251210713019$				
NM	2.0002	11	4.822e-478	3.078e-955
TM	3.0000	8	1.534e-311	3.709e-933
JM	4.0009	6	3.163e-477	4.454e-1,007
OM3	4.0010	6	8.695e-479	2.286e-1,007
CM3	3.9996	7	2.695e-475	2.273e-1,007
MA3	3.9964	6	7.193e-566	2.696e-2,008
MB3	3.9998	7	2.890e-628	2.224e-2,007
MC3	4.0000	10	3.285e-288	1.729e-1,150

$$y_k = x_k - \frac{f(x_k)^2}{f(z_k) - f(x_k)}, \quad z_k = x_k + f(x_k),$$

$$x_{k+1} = y_k - \frac{f[x_k, y_k] - f[y_k, z_k] + f[x_k, z_k]}{f[x_k, y_k]^2} f(y_k),$$

and CT4 [27] (with $\gamma = 1, a = 1, b = 1, c = 1$ and $d = 0$)

$$y_k = x_k - \frac{\gamma f(x_k)^2}{f(z_k) - f(x_k)}, \quad z_k = x_k + \gamma f(x_k),$$

$$x_{k+1} = y_k - \frac{f(y_k)}{\frac{af(y_k)-bf(z_k)}{y_k-z_k} + \frac{cf(y_k)-df(x_k)}{y_k-x_k}}.$$

From the results shown in Table 2, it can be stated that the proposed schemes are quite competitive respect to the known ones, being best ones in some cases.

In Tables 3 and 4, we show the results obtained by using the following elements of the family (16), for the following values of a_1 and b_2 :

1. MA3: $a_1 = \frac{5}{4}$ and $b_2 = 0$
2. MB3: $a_1 = 1$ and $b_2 = 1$
3. MC3: $a_1 = 1$ and $b_2 = 3$

In these numerical experiments, we compare the extension for systems of Ostrowski's method (OM3) and Chun's method (CM3), MA3, MB3 and MC3 with Newton's method (NM), Jarratt's method (JM) and Traub's method (TM):

$$\begin{aligned}y^{(k)} &= x^{(k)} - \left[F'(x^{(k)}) \right]^{-1} F(x^{(k)}) \\x^{(k+1)} &= y^{(k)} - \left[F'(x^{(k)}) \right]^{-1} F(y^{(k)}).\end{aligned}$$

In order to preserve the local order of convergence we use in our computations a symmetric divided difference operator.

In general, numerical results confirm theoretical ones. The proposed methods for systems behave better or equal to Jarratt's scheme, that is widely used as fourth-order method for systems. Moreover, the transferred Ostrowski' and Chun's methods for solving nonlinear systems have also a good performance.

4.2 Molecular interaction problem

To solve the equation of molecular interaction, (see [28])

$$\begin{aligned}u_{xx} + u_{yy} &= u^2, \quad (x, y) \in [0, 1] \times [0, 1] \\u(x, 0) &= 2x^2 - x + 1, \quad u(x, 1) = 2 \\u(0, y) &= 2y^2 - y + 1, \quad u(1, y) = 2.\end{aligned}\tag{17}$$

we need to deal with a boundary value problem with a nonlinear partial differential equation of second order. To estimate its solution numerically, we have used central divided differences in order to transform the problem in a nonlinear system of equations, which is solved by using the proposed methods of order four and five.

The discretization process yields to the nonlinear system of equations,

$$u_{i+1,j} - 4u_{i,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - h^2 u_{i,j}^2 = 0, \quad i = 1, \dots, nx, \quad j = 1, \dots, ny,\tag{18}$$

where $u_{i,j}$ denotes the estimation of the unknown $u(x_i, y_j)$, $x_i = ih$ with $i = 0, 1, \dots, nx$, $y_j = jh$ with $j = 0, 1, \dots, ny$, are the nodes in both variables, being $h = \frac{1}{nx}$, $k = \frac{1}{ny}$ and $nx = ny$.

In this case, we fix $nx = ny = 4$, so a mesh of 5×5 is generated. As the boundary conditions give us the value of the unknown function at the nodes (x_0, y_j) , (x_4, y_j) for all j and also at (x_i, y_0) , (x_i, y_4) for all i , we have only nine unknowns, that are renamed as:

$$\begin{aligned}x_1 &= u_{1,1}, \quad x_2 = u_{2,1}, \quad x_3 = u_{3,1}, \quad x_4 = u_{1,2}, \\x_5 &= u_{2,2}, \quad x_6 = u_{3,2}, \quad x_7 = u_{1,3}, \quad x_8 = u_{2,3}, \quad x_9 = u_{3,3}.\end{aligned}$$

So, the system can be expressed as

$$F(x) = Ax + \phi(x) - b = 0,$$

Table 5 Numerical results for molecular interaction problem

$x^{(0)} = (1, \dots, 1)^T$				
Method	ρ	Iter	$\ x^{(k+1)} - x^{(k)}\ $	$\ F(x^{(k+1)})\ $
NM	1.9999	9	1.482e-413	6.448e-828
TM	2.9988	6	1.153e-355	2.545e-1,007
JM	3.9954	5	1.482e-413	1.976e-1,007
OM3	3.9964	5	1.482e-413	1.618e-1,007
CM3	3.9959	5	1.998e-353	1.618e-1,007
MA3	4.0519	5	5.362e-510	1.707e-2,007
MB3	3.9960	5	7.123e-362	1.049e-1,449
MC3	3.9960	5	3.110e-362	3.811e-1,451

where

$$A = \begin{pmatrix} M & -I & 0 \\ -I & M & -I \\ 0 & -I & M \end{pmatrix},$$

being $M = \begin{pmatrix} 4 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 4 \end{pmatrix}, \phi(x) = h^2(x_1^2, x_2^2, \dots, x_9^2)^T,$

I is the 3×3 identity matrix and $b = (\frac{7}{4}, 1, \frac{27}{8}, 1, 0, 2, \frac{27}{8}, 2, 4)^T$. In this case, $F'(x) = A + 2h^2 \text{diag}(x_1, x_2, \dots, x_9)$.

Now, we will check the performance of the methods by means of some numerical tests, by using variable precision arithmetics of 1,000 digits of mantissa. These tests have been made by using the stopping criterium $\|F(x^{(k+1)})\| < 10^{-700}$ or $\|x^{(k+1)} - x^{(k)}\| < 10^{-700}$. In Table 5, we show the numerical results obtained for the problem of molecular interaction (18). We show, the approximated computational order of convergence, the number of iterations, the difference between the two last iterations and the residual of the function at the last iteration.

In Table 5 we can observe that all the new methods converge to the solution of the problem, that appears in Table 6. It can be noticed that the lowest error of the test corresponds to method MA3, duplicating the number of exact digits respect the other ones.

5 Concluding remarks

We have presented two family of iterative methods for solving nonlinear equations with and without derivatives, respectively. In addition, by using the first family we obtain a class of iterative methods for finding the solution of nonlinear systems.

The numerical results obtained in Sect. 4 confirm the theoretical results. Summarizing, we can conclude that the novel iterative methods have a good performance for

Table 6 Approximated solution

	ξ
$u_{1,1}$	1.0259117...
$u_{2,1}$	1.2097139...
$u_{3,1}$	1.5167030...
$u_{1,2}$	1.2097139...
$u_{2,2}$	1.3877038...
$u_{3,2}$	1.6258725...
$u_{1,3}$	1.5167030...
$u_{2,3}$	1.6258725...
$u_{3,3}$	1.7642995...

solving nonlinear equations and systems. In the applied example, the new methods show good stability and precision in the results.

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