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Research Article

Computational Analysis of Nonlinear Models Arising from Van der Waals Fluids and Planck's Radiation Law

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Abstract: Nonlinear equations and systems of nonlinear equations arise in many physical and engineering models, such as equations of state for real gases and thermal radiation laws. Newton-type methods for these problems require derivatives or Jacobian matrices, which may be unavailable or expensive to evaluate. This study presents a derivative-free three-step iterative scheme, denoted PS6 (proposed sixth-order scheme), in which the first two steps use first-order divided differences and the derivative in the third step is approximated by a cubic Hermite interpolating polynomial. For scalar equations, PS6 converges with order six and uses four function evaluations per iteration, giving an efficiency index of $6^{1/4} \approx 1.565$. The scheme is extended to systems of nonlinear equations without evaluating Jacobian matrices, and its sixth-order convergence is proved for both cases by Taylor expansion. The computational efficiency index of PS6 exceeds those of four existing fourth-, fifth- and sixth-order schemes for every system size. In numerical experiments on models arising from the Van der Waals equation of state, Planck's radiation law and particle interaction, and on two coupled nonlinear systems, PS6 required the same number of iterations as or fewer iterations than the compared methods, attained the smallest errors and residuals, and had the shortest central processing unit (CPU) time on both systems; the computational order of convergence agreed with the theoretical order. Basins of attraction for three test polynomials show that 71–92% of the initial points in the square $[-1, 1] \times [-1, 1]$ converge, mostly within three iterations. PS6 is therefore an accurate and efficient alternative for nonlinear problems in which derivatives are unavailable or costly.

Keywords: Derivative-free iterative methods, Hermite interpolation, Systems of nonlinear equations, Van der Waals equation, Planck's radiation law, Computational efficiency, Basins of attraction.

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1. INTRODUCTION

Many problems in physics, chemistry and engineering reduce to the solution of a nonlinear equation $f(\mu) = 0$, where $f: D \subseteq \mathbb{R} \to \mathbb{R}$, or of a system of nonlinear equations $F(\mu) = 0$, where $F: D \subseteq \mathbb{R}^n \to \mathbb{R}^n$ [1, 2]. Typical examples are equations of state for real gases, laws of thermal radiation, chemical equilibrium conditions and force balances between interacting particles [3-5]. Because such equations rarely admit closed-form solutions, they are solved by iterative methods, which should combine a high order of convergence, a low cost per iteration and a wide region of convergence.

Newton's method is the classical iterative method for both scalar equations and systems and converges quadratically to simple roots [1, 2, 6]. Its main limitation is that every iteration requires the derivative $f'(\mu)$ or, for systems, the Jacobian matrix $F'(\mu)$, which may be unavailable, expensive to compute or ill-conditioned. Steffensen [7] removed this requirement by replacing the derivative with a first-order divided difference while preserving quadratic convergence. Since then, many derivative-free multipoint methods of higher order have been constructed by combining divided differences with weight functions or interpolation [8-18].

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Jarratt [19] proposed a fourth-order two-step method that uses one function evaluation and two derivative evaluations per iteration, and Ostrowski [6] introduced the efficiency index that is widely used to compare iterative methods. Weerakoon and Fernando [20] proposed a variant of Newton's method with accelerated third-order convergence, and the local convergence of fourth-order methods based on the Adomian decomposition method and a 3-node quadrature rule was analyzed by Babajee *et al.* [21]. In the present study, the fourth-order Jarratt-type scheme of Soleymani [22], denoted S4, is used for comparison. Sharma *et al.* [23] proposed a fourth-order Weighted-Newton method, and Xiao and Yin [24] extended this idea to obtain a three-step fifth-order scheme (XY5) and a three-step sixth-order scheme (XH6). The sixth-order scheme C6, which originates from the work of Traub [2], was modified for systems by Cordero *et al.* [25]; the same group also proposed sixth-order schemes based on Newton–Jarratt compositions [26]. To reduce the cost per iteration, Amiri *et al.* [27] designed low-complexity Jacobian-free schemes in which the divided-difference operator uses an m-th power of the function so that the order of convergence is preserved, and Cordero *et al.* [28] constructed a stable class of Jacobian-free iterative processes for nonlinear vectorial problems.

Despite this progress, extending high-order scalar methods to systems remains difficult. A method that is accurate and stable for scalar equations need not retain these properties for systems, because each scalar division is replaced by the solution of a linear system whose coefficient matrix is a divided-difference operator; this step dominates the computational cost and can amplify rounding errors [29-31]. In addition, replacing derivatives by divided differences may reduce the order of convergence unless the divided differences are chosen carefully, and many high-order schemes require several different divided-difference operators, and hence several lower–upper (LU) factorizations, per iteration [27, 31]. Recent methods of order four to six include a derivative-free optimal fourth-order scheme [32], a parameter-dependent fourth-order family with a dynamical analysis [33], and a two-step fifth-order Jacobian-free method for systems [34].

To address these issues, this paper constructs a three-step derivative-free scheme, denoted PS6, which combines a Steffensen-type first step, a Traub-type second step [2] and a third step in which the derivative is approximated by the derivative of a cubic Hermite interpolating polynomial. The main contributions are as follows: (i) for scalar equations, PS6 converges with order six using four function evaluations per iteration, so that its efficiency index is $6^{1/4} \approx 1.565$; (ii) PS6 is extended to systems of nonlinear equations without evaluating Jacobian matrices, and its sixth-order convergence is proved; (iii) its computational efficiency index is derived and compared with those of four existing schemes; and (iv) its accuracy, cost and dynamical behaviour are assessed on nonlinear models arising from the Van der Waals equation of state, Planck's radiation law and particle interaction, and by means of basins of attraction.

The remainder of the paper is organized as follows. Section 2 describes the construction of PS6, proves its order of convergence for scalar equations, extends it to systems of nonlinear equations with the corresponding convergence analysis, and evaluates its computational efficiency. Section 3 presents the numerical experiments on scalar and vector models and the basins-of-attraction analysis. Section 4 summarizes the conclusions and outlines future work.

2. MATERIALS AND METHODS

2.1. Construction of the Proposed Scheme

The construction starts from a three-step scheme whose first step is Newton's method,

$$\upsilon^k = \mu^k - \frac{f(\mu^k)}{f'(\mu^k)} \tag{1}$$

whose second step is the Traub-type correction [2],

$$z^k = \upsilon^k - \frac{1}{f'(\mu^k)}\left\{2 - \frac{f'(\upsilon^k)}{f'(\mu^k)}\right\} f(\upsilon^k) \tag{2}$$

and whose third step is the Newton-type correction used by Amiri *et al.* [27],

$$\mu^{k+1} = z^k - \frac{f(z^k)}{f'(\upsilon^k)} \tag{3}$$

The aim is to obtain a derivative-free scheme of order six that uses as few function evaluations per

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iteration as possible. The derivatives in the first two steps are therefore approximated by first-order divided differences:

$$f'(\mu^k) \approx f[\omega^k, \mu^k] \approx \frac{f(\omega^k)-f(\mu^k)}{\omega^k-\mu^k} \quad (4)$$

where $\omega^k = \mu^k + f(\mu^k)^3$, and

$$f'(v^k) \approx f[v^k, \mu^k] \approx \frac{f(v^k)-f(\mu^k)}{v^k-\mu^k} \quad (5)$$

If the derivative in the third step is evaluated at a point r^k to be specified, the scheme becomes:

$$\begin{cases} v^k = \mu^k - \frac{f(\mu^k)}{f'(\mu^k)} \\ z^k = v^k - \frac{1}{f'(\mu^k)}\left\{2 - \frac{f'(v^k)}{f'(\mu^k)}\right\} f(v^k) \\ \mu^{k+1} = z^k - \frac{f(z^k)}{f'(r^k)} \end{cases} \quad (6)$$

Scheme (6) still requires five function evaluations per iteration. To avoid the additional evaluation, $f'(r^k)$ is approximated by $h_3'(z^k)$, where h_3 is the cubic Hermite polynomial that interpolates the available data $f(\mu)$, $f'(\mu)$, $f(v)$ and $f(z)$:

$$h_3(t) = a_0 + a_1(t-\mu) + a_2(t-\mu)^2 + a_3(t-\mu)^3 \quad (7)$$

Its derivative with respect to t is:

$$h_3'(t) = a_1 + 2a_2(t-\mu) + 3a_3(t-\mu)^2 \quad (8)$$

The coefficients are determined by the interpolation conditions:

$$h_3(\mu) = f(\mu), h_3(v) = f(v), h_3(z) = f(z), \\ h_3'(\mu) = f'(\mu) \quad (9)$$

Setting $t = \mu$ in (7) and (8) gives $a_0 = f(\mu)$ and $a_1 = f'(\mu)$. The conditions at $t = v$ and $t = z$ then yield:

$$a_2 = \frac{(z-\mu)f[v,z]}{(z-v)(v-\mu)} - \frac{(v-\mu)f[v,z]}{(z-v)(z-\mu)} - f'(\mu)\left(\frac{1}{z-\mu} - \frac{1}{v-\mu}\right) \quad (10)$$

$$a_3 = \frac{f[\mu,z]}{(z-v)(z-\mu)} - \frac{f[v,\mu]}{(z-v)(v-\mu)} + \frac{f'(\mu)}{(z-\mu)(v-\mu)} \quad (11)$$

Substituting a_1, a_2 and a_3 into (8), setting $t = z$ and replacing $f'(\mu)$ by $f[\omega, \mu]$ from (4) gives:

$$h_3'(z) = 2\big[f[\mu,z] - f[v,\mu]\big] + f[v,z] + \frac{v-z}{v-\mu}\big[f[v,\mu] - f[\omega,\mu]\big] \quad (12)$$

Finally, replacing the derivatives in Equation (6) by the approximations, Equations (4), (5) and (12) yields the proposed derivative-free scheme PS6:

$$\begin{cases} v^k = \mu^k - \frac{f(\mu^k)}{f[\omega^k,\mu^k]} \\ z^k = v^k - \left\{2 - \frac{f[v^k,\mu^k]}{f[\omega^k,\mu^k]}\right\}\frac{f(v^k)}{f[\omega^k,\mu^k]} \\ \mu^{k+1} = z^k - \frac{f(z^k)}{h_3'(r)} \end{cases} \quad (13)$$

where $h_3'(r)$ denotes the value (12) computed at the current iterates. Each iteration of Equation (13) uses only the four function values $f(\mu^k)$, $f(\omega^k)$, $f(v^k)$ and $f(z^k)$, and no derivatives.

2.2. Convergence Analysis for Scalar Equations

Theorem 1. *Let $f: D \subseteq \mathbb{R} \to \mathbb{R}$ be sufficiently differentiable in an open interval D containing a simple root α of f, and let the initial estimate μ^0 be sufficiently close to α. Then the sequence $\{\mu^k\}$ generated by* (13) *converges to α with order six, and its error satisfies:*

$$\mu^{k+1} - \alpha = A_2^5 e^6 + O(e^7) \quad (14)$$

where,

$$e = \mu^k - \alpha$$

and

$$A_i = \frac{1}{i!}[f'(\alpha)]^{-1} f(\alpha), i \geq 2$$

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Proof. Expanding $f(\mu^k)$ and its derivatives in Taylor series about α and using $f(\alpha) = 0$ gives:

$$f(\mu^k) = f'(\alpha)\left(e + A_2\, e^2 + A_3\, e^3 + A_4\, e^4 + A_5\, e^5 + A_6\, e^6 + O(e^7)\right) \tag{15}$$

$$f'(\mu^k) = f'(\alpha)\left(I + 2A_2\, e + 3\, A_3\, e^2 + 4\, A_4\, e^3 + 5A_5\, e^4 + 6A_6\, e^5 + O(e^6)\right) \tag{16}$$

$$f''(\mu^k) = f'(\alpha)\left(2A_2 + 6\, A_3\, e + 12\, A_4\, e^2 + 20A_5\, e^3 + 30A_6\, e^4 + O(e^5)\right) \tag{17}$$

$$f'''(\mu^k) = f'(\alpha)\left(6\, A_3 + 24\, A_4 e + 60A_5\, e^2 + 120A_6 e^3 + O(e^4)\right) \tag{18}$$

$$f^4(\mu^k) = f'(\alpha)\left(24\, A_4 + 120A_5\, e + 360A_6 e^2 + O(e^3)\right) \tag{19}$$

$$f^5(\mu^k) = f'(\alpha)\left(120A_5 + 720A_6 e + O(e^2)\right) \tag{20}$$

$$f^6(\mu^k) = f'(\alpha)720A_6 + O(e), \tag{21}$$

$$f[\omega^k, \mu^k] = \frac{f(\omega^k) - f(\mu^k)}{\omega^k - \mu^k} = f'(\mu^k) + \frac{1}{2!}f''(\mu^k)(\omega^k - \mu^k) + \frac{1}{3!}f'''(\mu^k)(\omega^k - \mu^k)^2 + \frac{1}{4!}f^4(\mu^k)(\omega^k - \mu^k)^3 + O(e^4) = f'(\alpha) + 2A_2 f'(\alpha)e + 3A_3 f'(\alpha)e^2 + \left(A_2 f'(\alpha)^4 + 4A_4 f'(\alpha)\right)e^3 + O(e^4) \tag{22}$$

Hence, the error of the first step is

$$v^k - \alpha = e - \frac{f(\mu^k)}{f[\omega^k, \mu^k]} = Q_0 e^2 + Q_1 e^3 + Q_2 e^4 + O(e^5) \tag{23}$$

where,

$$Q_0 = A_2,\ Q_1 = -2A_2^2 + 2A_3,\ Q_2 = A_2 f(\mu^k)^3 + 4A_2^3 - 7A_2 A_3 + 3A_4 \tag{24}$$

Expanding $f(v^k)$ and its derivatives about α in the same way gives:

$$f(v^k) = f'(\alpha)\left((v^k - \alpha) + A_2\,(v^k - \alpha)^2 + A_3\,(v^k - \alpha)^3 + A_4\,(v^k - \alpha)^4 + O(e^5)\right), \tag{25}$$

$$f'(v^k) = f'(\alpha)(1 + 2\, A_2(v^k - \alpha) + 3A_3(v^k - \alpha)^2 + O(e^4)) \tag{26}$$

$$f''(v^k) = f'(\alpha)(2\, A_2 + 6A_3(v^k - \alpha) + O(e^3)) \tag{27}$$

$$f'''(v^k) = f'(\alpha)(6A_3 + O(e^2)), \tag{28}$$

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$$f[v^k,\mu^k]=\frac{f(v^k)-f(\mu^k)}{v^k-\mu^k}=f'(v^k)+\frac{1}{2!}f''(v^k)(v^k-\mu^k)+\frac{1}{3!}f'''(v^k)(v^k-\mu^k)^2+\frac{1}{4!}f^4(v^k)(v^k-\mu^k)^3+O(e^5)=f'(\alpha)+A_2f'(\alpha)e+\left(A_2^2f'(\alpha)+A_3f'(\alpha)\right)e^2+\left(-2A_2^3f'(\alpha)+3A_2A_3f'(\alpha)+A_4f'(\alpha)\right)e^3+\left(A_2^2f'(\alpha)^4+4A_2^4f'(\alpha)-8A_2^2A_3f'(\alpha)+4A_2A_4f'(\alpha)+2A_3^2f'(\alpha)+A_5f'(\alpha)\right)e^4+O(e^5) \quad (29)$$

so that the error of the second step is:

$$z^k-\alpha=v^k-\alpha-\left\{2-\frac{f[v^k,\mu^k]}{f[\omega^k,\mu^k]}\right\}\frac{f(v^k)}{f[\omega^k,\mu^k]}=A_2^2e^3+(-2A_2^3+3A_2A_3)e^4+O(e^5) \quad (30)$$

$$f[\mu^k,z^k]=\frac{f(\mu^k)-f(z^k)}{\mu^k-z^k}==f'(\mu^k)+\frac{1}{2!}f''(\mu^k)(\mu^k-z^k)+\frac{1}{3!}f'''(\mu^k)(\mu^k-z^k)^2+\frac{1}{4!}f^4(\mu^k)(\mu^k-z^k)^3+O(e^5)=f'(\alpha)(1+A_2e+A_3e^2+(A_2^3+A_4)e^3+(-2A_2^4+4A_2^2A_3+A_5)e^4+(A_2^3f'(\alpha)^3-3A_2^5-8A_2^3+5A_2^2A_4+5A_2A_2^3+A_6)e^5+(2A_2^4f'(\alpha)^3+41A_2^6+5A_2^2A_3f'(\alpha)^3-39A_2^4A_3-9A_2^3A_4-8A_2^2A_3^2+6A_2^2A_5+12A_2A_3A_4+2A_3^3)e^6)+O(e^7) \quad (31)$$

$$f[v^k,z^k]=\frac{f(v^k)-f(z^k)}{v^k-z^k}=f'(v^k)+\frac{1}{2!}f''(v^k)(v^k-z^k)+\frac{1}{3!}f'''(v^k)(v^k-z^k)^2+\frac{1}{4!}f^4(v^k)(v^k-z^k)^3+O(e^5)=f'(\alpha)(1+A_2^2e^2+(-A_2^3+2A_2A_3)e^3+(A_2^2f'(\alpha)^3+2A_2^4-3A_2^2A_3+3A_2A_4)e^4+(-A_2^3f'(\alpha)^3-11A_2^5+3A_2A_3f'(\alpha)^3+11A_2^3A_3-6A_2^2A_4+4A_2A_5)e^5+(4A_2^4f'(\alpha)^3+57A_2^6+4A_2^2A_3f'(\alpha)^3-80A_2^4A_3+6A_2A_4f'(\alpha)^3+22A_2^3A_4+14A_2^2A_3^2-8A_2^2A_5-6A_2A_3A_4+4A_3^3+5A_2A_6)e^6)+O(e^7) \quad (32)$$

Substituting Equations (22), (29), (31) and (32) into the third step of Equation (13) gives the error equation:

$$e^{k+1}=\mu^{k+1}-\alpha=z^k-\alpha-\frac{f(z^k)}{h_3'(r)}=A_2^5e^6+O(e^7) \quad (33)$$

which shows that PS6 converges with order six. Because each iteration uses four function evaluations, the efficiency index of PS6 is $6^{1/4}\approx 1.565$.

2.3. Extension to Systems of Nonlinear Equations

Let $F: D\subseteq\mathbb{R}^n\to\mathbb{R}^n$ be sufficiently differentiable, let $\overline{\mu}$ be a solution of $F(\mu)=0$, and let $[x,y;F]$ denote the first-order divided-difference operator of F [1]. Scheme (13) extends to systems as:

$$\begin{cases} v^k=\mu^k-[\omega^k,\mu^k;F]^{-1}F(\mu^k) \\ z^k=v^k-[\omega^k,\mu^k;F]^{-1}\,\psi\,F(v^k) \\ \mu^{k+1}=z^k-H_3'^{-1}F(z^k) \end{cases} \quad (34)$$

where $\omega^k=\mu^k+F(\mu^k)^3$ (the cube is taken componentwise), $\psi=\{2\,I-[v^k,\mu^k;F]\,[\omega^k,\mu^k;F]^{-1}\}$, and $H_3'=2\left[[\mu^k,z^k;F]-[v^k,\mu^k;F]\right]+[v^k,z^k,F]+\frac{v^k-z^k}{v^k-\mu^k}\left[[v^k,\mu^k;F]-\left[\mu^k+F(\mu^k)^3,\ \mu^k;F\right]\right]$. Each

iteration of (34) evaluates F at the four points $\mu^{(k)}$, $\omega^{(k)}$, $\upsilon^{(k)}$ and $z^{(k)}$ and requires no Jacobian matrix. The linear systems in the first two steps share the coefficient matrix $[\omega^{(k)}, \mu^{(k)}; F]$, so a single LU factorization serves both steps, and one further factorization is needed for $H_3{}'$ in the third step.

2.4. Convergence Analysis for Systems

Theorem 2. *Let $F: D \subseteq \mathbb{R}^n \to \mathbb{R}^n$ be sufficiently differentiable in an open convex neighbourhood D of a solution $\overline{\mu}$ of $F(\mu) = 0$, and let $F'(\overline{\mu})$ be nonsingular and continuous at $\overline{\mu}$. Then, for an initial estimate $\mu^{(0)}$ sufficiently close to $\overline{\mu}$, the sequence $\{\mu^{(k)}\}$ generated by* (34) *converges to $\overline{\mu}$ with order six, and its error satisfies:*

$$e^{(k+1)} = Q_2^5 e^{(k)^6} + O\left(e^{(k)^7}\right) \tag{35}$$

where $e^{(k)} = \mu^k - \overline{\mu}$ and $Q_i = \frac{1}{i!}\,[F'(\overline{\mu})]^{-1} F(\overline{\mu}), i \geq 2$.

Proof. Expanding $F(\mu^{(k)})$ and its derivatives in Taylor series about $\overline{\mu}$ gives:

$$F\left(\mu^k\right) = F'(\overline{\mu})\left(e^{(k)} + Q_2\, e^{(k)^2} + Q_3\, e^{(k)^3} + Q_4\, e^{(k)^4} + Q_5\, e^{(k)^5} + Q_6\, e^{(k)^6}\right) + O\left(e^{(k)^7}\right), \tag{36}$$

$$F'\left(\mu^k\right) = F'(\overline{\mu})\left(I + 2Q_2\, e^{(k)} + 3\,Q_3\, e^{(k)^2} + 4\,Q_4\, e^{(k)^3} + 5Q_5\, e^{(k)^4} + 6Q_6\, e^{(k)^5}\right) + O\left(e^{(k)^6}\right), \tag{37}$$

$$F''\left(\mu^k\right) = F'(\overline{\mu})\left(2Q_2 + 6\,Q_3\, e^{(k)} + 12\,Q_4\, e^{(k)^2} + 20Q_5\, e^{(k)^3} + 30Q_6\, e^{(k)^4}\right) + O\left(e^{(k)^5}\right), \tag{38}$$

$$F'''\left(\mu^k\right) = F'(\overline{\mu})\left(6\,Q_3 + 24\,Q_4 e^{(k)} + 60Q_5\, e^{(k)^2} + 120Q_6 e^{(k)^3}\right) + O\left(e^{(k)^4}\right), \tag{39}$$

$$F^4\left(\mu^k\right) = F'(\overline{\mu})\left(24\,Q_4 + 120Q_5\, e^{(k)} + 360Q_6 e^{(k)^2}\right) + O\left(e^{(k)^3}\right) \tag{40}$$

$$F^5\left(\mu^k\right) = F'(\overline{\mu})\left(120Q_5 + 720Q_6 e^{(k)}\right) + O\left(e^{(k)^2}\right), \tag{41}$$

$$F^6\left(\mu^k\right) = F'(\overline{\mu})720Q_6 + O\left(e^{(k)}\right), \tag{42}$$

The Genocchi–Hermite formula [1] gives the Taylor expansion of the divided-difference operator:

$$[\mu + h, \mu; F] = \int_0^1 F'(\mu + th)dt = F'(\mu) + \frac{1}{2!}F''(\mu)h + \frac{1}{3!}F'''(\mu)h^2 + Oh^3 \tag{43}$$

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from which, together with Equations (37) - (42), we obtain:

$$[\omega^k, \mu^k; F] = F'(\overline{\mu})\left(I + 2Q_2\, e^{(k)} + 3\, Q_3\, e^{(k)^2}\right) + O\left(e^{(k)^3}\right), \tag{44}$$

and hence,

$$[\omega^k, \mu^k; F]^{-1} = \left(I - 2Q_2 e^{(k)} + (4Q_2^2 - 3Q_3)e^{(k)^2}\right)F'(\overline{\mu})^{-1} + O\left(e^{(k)^3}\right), \tag{45}$$

From Equations (34), (36) and (45), the error of the first step is:

$$e_v^{(k)} = v^k - \overline{\mu} = e^{(k)} - [\omega^k, \mu^k; F]^{-1} F\left(\mu^k\right) = Q_2 e^{(k)^2} + O\left(e^{(k)^3}\right), \tag{46}$$

Using Equations (34), (43), (37) - (42), and (46) we have:

$$[v^k, \mu^k; F] = F'(\overline{\mu})(I + Q_2\, e^{(k)} + (Q_2^2 + Q_3)e^{(k)^2} + (-2Q_2^3 + 3Q_2\, Q_3 + Q_4)e^{(k)^3}) + O(e^{(k)^4}) \tag{47}$$

and therefore:

$$[v^k, \mu^k; F][\omega^k, \mu^k; F]^{-1} = I + (-Q_2)e^{(k)} + (3Q_2^2 - 2Q_3)e^{(k)^2} + (-Q_2F'(\overline{\mu})^3 - 8Q_2^3 + 10Q_2\, Q_3 - 3Q_4)e^{(k)^3} + O(e^4), \tag{48}$$

By a similar argument,

$$[\omega^k, \mu^k; F]^{-1}\, \psi = F'(\overline{\mu})^{-1}\left(I - Q_2 e^{(k)} + (-Q_2^2 + Q_3)e^{(k)^2} + (10Q_2^3 - 5Q_2Q_3 - Q_4)e^{(k)^3}\right) + O(e^4) \tag{49}$$

Moreover,

$$F\left(v^k\right) = F'(\overline{\mu})\left(Q_2 e^{(k)^2} + (-2Q_2^2 + 2Q_3)e^{(k)^3}\right) + O\left(e^{(k)^4}\right) \tag{50}$$

From Equations (34), (46), (49) and (50), the error of the second step is:

$$e_z^{(k)} = z^k - \overline{\mu} = e_v^{(k)} - [\omega^k, \mu^k; F]^{-1}\psi F\left(v^k\right) = Q_2^2 e^{(k)^3} + O(e^4) \tag{51}$$

The remaining divided-difference operators and the inverse of $H_3{}'$ have the expansions:

$$[\mu^k, z^k; F] = F'(\overline{\mu})\left(I + Q_2 e^{(k)} + Q_3 e^{(k)^2} + (Q_2^3 + Q_4)e^{(k)^3} + (-2Q_2^4 + 4Q_2^2Q_3 + Q_5)e^{(k)^4} + \left(Q_2^3F'(\overline{\mu})^3 - 3Q_2^5 - 8Q_2^3 + 5Q_2^2Q_4 + 5Q_2Q_2^3 + Q_6\right)e^{(k)^5} + (2Q_2^4F'(\overline{\mu})^3 + 41Q_2^6 + 5Q_2^2Q_3F'(\overline{\mu})^3 - 39Q_2^4Q_3 - 9Q_2^3Q_4 - 8Q_2^2Q_3^2 + 6Q_2^2Q_5 + 12Q_2Q_3Q_4 + 2Q_3^3)e^{(k)^6}\right) + O\left(e^{(k)^7}\right) \tag{52}$$

$$[v^k, z^k, F] = F'(\overline{\mu})\left(I + Q_2^2 e^{(k)^2} + (-Q_2^3 + 2Q_2Q_3)e^{(k)^3} + (Q_2^2F'(\overline{\mu})^3 + 2Q_2^4 - 3Q_2^2Q_3 + 3Q_2Q_4)e^{(k)^4} + \left(-Q_2^3F'(\overline{\mu})^3 - 11Q_2^5 + 3Q_2Q_3F'(\overline{\mu})^3 + 11Q_2^3Q_3 - 6Q_2^2Q_4 + 4Q_2Q_5\right)e^{(k)^5} + (4Q_2^4F'(\overline{\mu})^3 + 57Q_2^6 + 4Q_2^2Q_3F'(\overline{\mu})^3 - 80Q_2^4Q_3 + 6Q_2Q_4F'(\overline{\mu})^3 + 22Q_2^3Q_4 + 14Q_2^2Q_3^2 - 8Q_2^2Q_5 - 6Q_2Q_3Q_4 + 4Q_3^3 + 5Q_2Q_6)e^{(k)^6}\right) + O\left(e^{(k)^7}\right) \tag{53}$$

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$$H_3' = F'(\bar{\mu})\big(I + 2Q_2^3 e^{(k)^3} + (Q_2^2 F'(\bar{\mu})^3 - 4Q_2^4 + 6Q_2^2 Q_3 + Q_2 Q_4)e^{(k)^4} + \big(3Q_2^3 F'(\bar{\mu})^3 - 6Q_2^5 + 5Q_2 Q_3 F'(\bar{\mu})^3 - 12Q_2^3 Q_3 + 5Q_2^2 Q_4 + 4Q_2 Q_3^2 + 2Q_2 Q_5 + 2Q_3 Q_4\big)e^{(k)^5} + (Q_2^2 F'(\bar{\mu})^6 + 3Q_2^4 F'(\bar{\mu})^3 + 82Q_2^6 + 14Q_2^2 Q_3 F'(\bar{\mu})^3 - 71Q_2^4 Q_3 + 10Q_2 Q_4 F'(\bar{\mu})^3 + 6Q_2^3 F'(\bar{\mu})^3 - 10Q_2^3 Q_4 - 4Q_2^2 Q_3^2 + 5Q_2^2 Q_5 + 3Q_2 Q_6 + 4Q_3 Q_5 + 3Q_4^2)e^{(k)^6}\big) + O\big(e^{(k)^7}\big) \quad (54)$$

$$H_3'^{-1} = F'(\bar{\mu})^{-1}\big(I - 2Q_2^3 e^{(k)^3} + (-Q_2^2 F'(\bar{\mu}) + 4Q_2^4 - 6Q_2^2 Q_3 - Q_2 Q_4)e^{(k)^4} + \big(-3Q_2^3 F'(\bar{\mu}) + 6Q_2^5 - 5Q_2 Q_3 F'(\bar{\mu}) + 12Q_2^3 Q_3 - 5Q_2^2 Q_4 - 4Q_2 Q_3^2 - 2Q_2 Q_5 - 2Q_3 Q_4\big)e^{(k)^5} + (-Q_2^2 F'(\bar{\mu})^4 - 3Q_2^4 F'(\bar{\mu}) - 78Q_2^6 - 14Q_2^2 Q_3 F'(\bar{\mu}) + 71Q_2^4 Q_3 - 10Q_2 Q_4 F'(\bar{\mu}) - 6Q_2^3 F'(\bar{\mu}) + 10Q_2^3 Q_4 + 4Q_2^2 Q_3^2 - 5Q_2^2 Q_5 - 3Q_2 Q_6 - 4Q_3 Q_5 - 3Q_4^2)e^{(k)^6}\big) + O(e^{(k)^7}) \quad (55)$$

and

$$F(z^k) = F'(\bar{\mu})\big(Q_2^2 e^{(k)^3} + (-2Q_2^3 + 3Q_2 Q_3)e^{(k)^4} + (Q_2^2 F'(\bar{\mu})^3 - 3Q_2^4 - 6Q_2^2 Q_3 + 4Q_2 Q_4 + 2Q_3^2)e^{(k)^5} + \big(2Q_2^3 F'(\bar{\mu})^3 + 42Q_2^5 + 4Q_2 Q_3 F'(\bar{\mu})^3 - 37Q_2^3 Q_3 - 7Q_2^2 Q_4 - 2Q_2 Q_3^2 + 5Q_2 Q_5 + 5Q_3 Q_4\big)e^{(k)^6}\big) + O\big(e^{(k)^7}\big) \quad (56)$$

Substituting Equations (51), (55) and (56) into the third step of Equation (34) gives the error equation:

$$e^{(k+1)} = \mu^{k+1} - \bar{\mu} = e_z^{(k)} - H_3'^{-1} F(z^k) = Q_2^5 e^{(k)^6} + O\big(e^{(k)^7}\big) \quad (57)$$

which proves that the scheme (34) converges with order six.

2.5. Computational Efficiency

The efficiency of an iterative method depends on its order of convergence and on its cost per iteration. Ostrowski's efficiency index (IE) [6] is $IE = p^{\frac{1}{d}}$, where p is the order of convergence and d is the number of function evaluations per iteration. For systems, the cost of the linear algebra must also be considered; therefore, the computational efficiency index (CEI), $CEI = p^{\frac{1}{d+op}}$, of Cordero *et al.* [26] is used, where op is the number of products and quotients per iteration.

Solving m linear systems of size n with the same coefficient matrix by LU factorization requires $(\frac{1}{3}n^3 + mn^2 - \frac{1}{3}n)$ products and quotients. The remaining operations are counted as follows: n products for a vector–vector product, n^2 for a matrix–vector product, n^3 for a matrix–matrix product, n^2 quotients for a divided-difference operator, $\frac{1}{3}(n^3 - n)$ for an LU decomposition and n^2 for the solution of the resulting triangular systems. Table 1 lists the resulting values of p, d and $d + op$ for PS6 and for the comparison methods S4, XY5, XH6 and C6.

Among the three sixth-order methods, PS6 has the smallest total cost $d + op$ for every $n \geq 1$, and its cost is also smaller than that of XY5 and S4. Consequently, PS6 has the largest CEI for every system size.

Figure 1 plots the CEI of the five methods against the system size n. For $n = 2$, the CEI of PS6 is 1.066, compared with 1.048 for XY5 and C6, 1.042 for XH6 and 1.039 for S4 (Figure 1(a)). The CEI of all methods decreases towards 1 as n increases because the cubic cost of the LU factorizations dominates. The logarithmic scale of Figure 1(b) shows that PS6 retains the largest CEI up to $n = 50$, although the differences among the sixth-order methods become small for large systems.

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Table 1. Order of convergence (p), number of scalar function evaluations (d) and total cost per iteration ($d + op$) of the compared methods for a system of size n; CEI = $p^{1/(d+op)}$.

Method	p	d	$d + op$
PS6	6	$4n^2$	$(2/3)n^3 + 6n^2 - (2/3)n$
S4	4	$2n^2 + n$	$(7/3)n^3 + 4n^2 + n$
XY5	5	$2n^2 + 3n$	$(2/3)n^3 + 6n^2 + (7/3)n$
XH6	6	$2n^2 + 2n$	$(2/3)n^3 + 9n^2 + (4/3)n$
C6	6	$2n^2 + 3n$	$(2/3)n^3 + 7n^2 + (7/3)n$

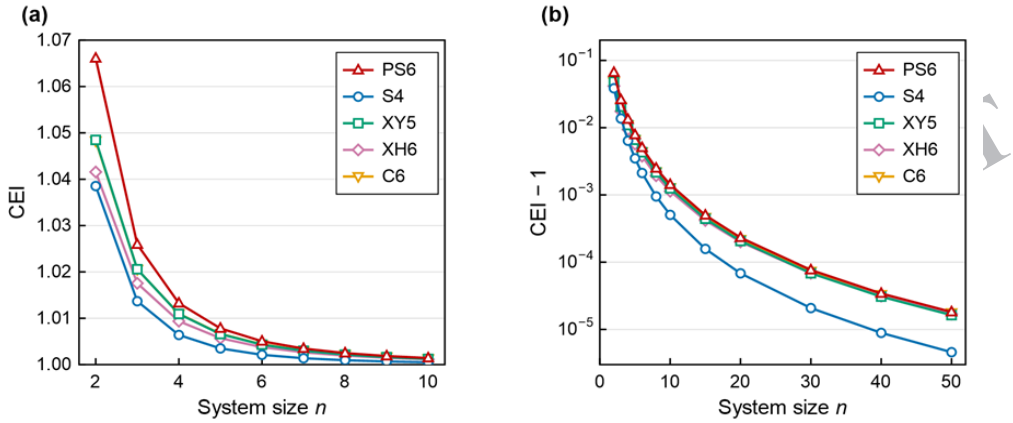

Fig. 1. Computational efficiency index (CEI) of PS6 and of the comparison methods as a function of the system size n: (a) CEI for $n = 2, \ldots, 10$; (b) CEI − 1 on a logarithmic scale for $n = 2, \ldots, 50$.

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3. RESULTS AND DISCUSSION

This section compares PS6 with S4, XY5, XH6 and C6 on three scalar models and two systems of nonlinear equations. All methods were run from the same initial estimate, and computations were carried out in multiple-precision arithmetic so that errors far below double precision could be resolved. For each problem, the tables report the number of iterations (N), the approximate solution (AS) or the central processing unit (CPU) time in seconds, the error between the last two iterates, the residual, and the approximated computational order of convergence [20].

$$\rho \approx \frac{\ln(|\mu^{k+1} - \mu^k| / |\mu^k - \mu^{k-1}|)}{\ln(|\mu^k - \mu^{k-1}| / |\mu^{k-1} - \mu^{k-2}|)} \tag{58}$$

Where the absolute values are replaced by norms for systems. Errors and residuals are reported to three significant digits. In each figure, the bars show $-\log_{10}$ of the error or residual, which approximates the number of correct decimal digits; longer bars therefore indicate higher accuracy.

3.1. Scalar Nonlinear Models

Problem 1 (Van der Waals equation of state). The Van der Waals equation $\left(P + \frac{an^2}{V^2}\right)(V - nb) = nRT$ corrects the ideal gas law for intermolecular attraction (a) and for the finite volume of the molecules (b). For a given gas at prescribed pressure and temperature, it reduces to a cubic equation in the volume; the following instance has been used as a benchmark in [3, 4, 18]:

$$f(\mu) = 0.986\mu^3 - 5.181\mu^2 + 9.067\mu - 5.289 \tag{59}$$

Table 2 compares the methods for the initial estimate $\mu^0 = 2.03$.

PS6 converges in five iterations, as do XH6 and C6, whereas S4 and XY5 require six. With the same number of iterations, PS6 attains the smallest step error, $|\mu^k - \mu^{k-1}| = 3.25 \times 10^{-477}$, and the smallest residual, $|f(\mu^k)| = 8.56 \times 10^{-2857}$; these are more than 100 and 640 orders of magnitude

Table 2. Numerical results for Problem 1 (Van der Waals equation) with the initial estimate $\mu^0 = 2.03$.

Method	N	AS	$\lvert\mu^k - \mu^{k-1}\rvert$	$\lvert f(\mu^k)\rvert$	ρ
PS6	5	1.92985	3.25×10^{-477}	8.56×10^{-2857}	6.00
S4	6	1.92985	2.33×10^{-95}	6.59×10^{-378}	4.00
XY5	6	1.92985	3.62×10^{-150}	8.49×10^{-745}	5.00
XH6	5	1.92985	1.87×10^{-370}	1.95×10^{-2215}	6.00
C6	5	1.92985	4.40×10^{-345}	5.30×10^{-2063}	6.00

N: number of iterations; AS: approximate solution; ρ: approximated computational order of convergence (58).

smaller, respectively, than those of XH6, the most accurate competing method. The computed order $\rho = 6.00$ agrees with Theorem 1.

Figure 2 shows these differences graphically. In Figure 2(a), PS6 attains about 476 correct digits in the step error, compared with 370 for XH6, 344 for C6, 149 for XY5 and 95 for S4. Figure 2(b) shows the same ranking for the residual, with about 2856 digits for PS6. The large gap between the sixth-order methods and S4 and XY5 reflects their lower orders of convergence, whereas the gap between PS6 and the other sixth-order methods reflects the smaller asymptotic error constant of PS6 for this problem.

Problem 2 (Planck's radiation law). Planck's law gives the energy density of blackbody radiation at wavelength λ and absolute temperature T as $\psi(\lambda) = \frac{8\pi hc\lambda^{-5}}{e^{hc/(\lambda k_B T)}-1}$, where h is Planck's constant, c is the speed of light and k_B is Boltzmann's constant. Setting $\psi'(\lambda) = 0$ to locate the wavelength of maximum energy density and substituting $\mu = hc/(\lambda k_B T)$ leads to Equation (60) [35, 36].

$$\square(\mu) = e^{-\mu} - 1 + \frac{\mu}{5} \tag{60}$$

whose nonzero root $\mu \approx 4.96511$ yields Wien's displacement law $\lambda_{\max} T = hc/(4.96511 k_B)$. Table 3 reports the results for the initial estimate $\mu^0 = 4$.

PS6, XH6 and C6 converge in four iterations and S4 and XY5 in five. PS6 again attains the smallest step error (4.11×10^{-322}) and residual (1.80×10^{-1938}), about 26 and 159 orders of magnitude below those of C6, which is the most accurate competing method for this problem. The computed order of every method agrees with its theoretical order.

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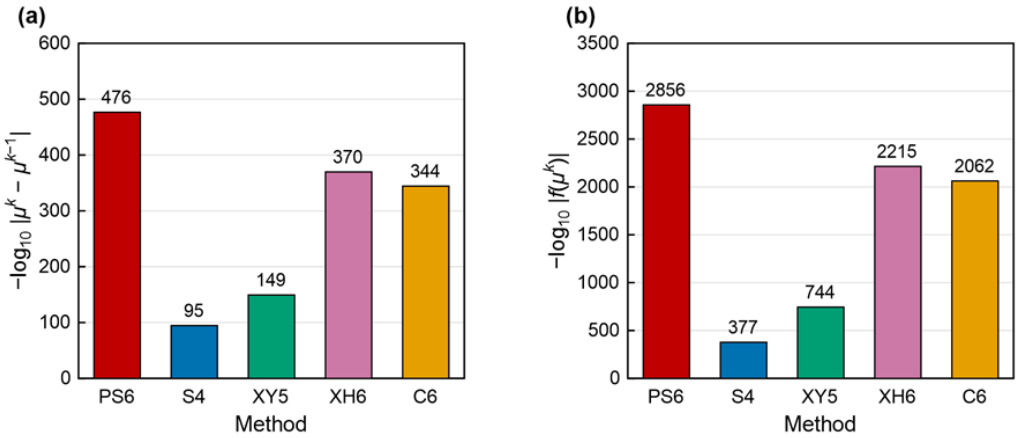

Fig. 2. Accuracy of the compared methods for Problem 1 (Van der Waals equation) with $\mu^0 = 2.03$: (a) $-\log_{10}$ of the error between the last two iterates; (b) $-\log_{10}$ of the residual. The number above each bar is the corresponding value.

Table 3. Numerical results for Problem 2 (Planck's radiation law) with the initial estimate $\mu^0 = 4$.

Method	N	AS	$\lvert\mu^k - \mu^{k-1}\rvert$	$\lvert f(\mu^k)\rvert$	ρ
PS6	4	4.96511	4.11×10^{-322}	1.80×10^{-1938}	6.00
S4	5	4.96511	1.36×10^{-69}	1.86×10^{-280}	4.00
XY5	5	4.96511	5.48×10^{-76}	4.79×10^{-382}	5.00
XH6	4	4.96511	1.18×10^{-223}	1.06×10^{-1344}	6.00
C6	4	4.96511	8.64×10^{-296}	1.54×10^{-1779}	6.00

N: number of iterations; AS: approximate solution; ρ: approximated computational order of convergence (58).

Figure 3 compares the accuracy of the methods for Problem 2. Figure 3(a) shows that the advantage of PS6 over C6 in the step error (321 versus 295 correct digits) is smaller than in Problem 1, whereas XH6 attains only 223 digits. Figure 3(b) shows that the residual of PS6 has about 1938 correct digits, compared with 1779 for C6 and fewer than 400 for S4 and XY5.

Problem 3 (Force between charged particles). The force between charged particles separated by a distance μ is described by the nonlinear model [5],

$$f(\mu) = \frac{q_1 q_2 \mu}{2\epsilon}\left(1 - \frac{\mu}{\sqrt{\mu^2 + r^2}}\right) - F \tag{61}$$

Where q_1 and q_2 are the charges, $\varepsilon = 0.885 \times 10^{-12}\ \mathrm{C}^2/(\mathrm{N}\cdot\mathrm{m}^2)$ is the permittivity of free space and r is a characteristic radius. The distance μ is to be determined for $F = 0.3\ \mathrm{N}$, $q_1 = 2.4 \times 10^{-5}\ \mathrm{C}$, $q_2 = 9.4 \times 10^{-6}\ \mathrm{C}$ and $r = 0.1\ \mathrm{m}$. Table 4 reports the results for the initial estimate $\mu^0 = 1.2$.

All sixth-order methods converge in four iterations, and S4 and XY5 require five. PS6 attains a step error of 1.28×10^{-237} and a residual of 1.39×10^{-1424}, which are about 29 and 173 orders of magnitude smaller than those of XH6.

Figure 4 presents the accuracy for Problem 3. In Figure 4(a), the fifth-order method XY5 (194 correct digits) outperforms C6 (186 digits) in the step error, which shows that the asymptotic error constant can outweigh a one-unit difference in the order of convergence when few iterations are performed. Figure 4(b) shows that PS6 has the most accurate residual, with about 1424 correct digits, followed by XH6 (1251) and C6 (1117).

3.2. Systems of Nonlinear Equations

Problem 4 (Van der Waals fluid in a chemical reactor). A chemical reactor operates at high pressure, where the working fluid deviates

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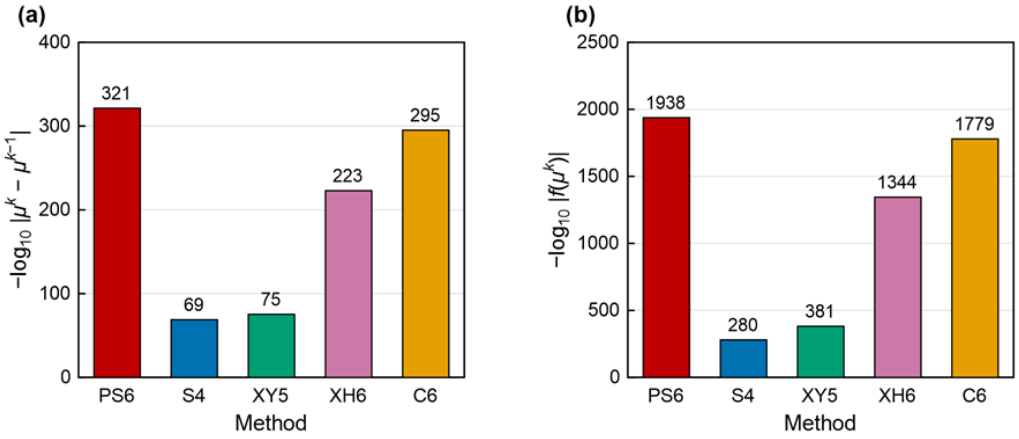

Fig. 3. Accuracy of the compared methods for Problem 2 (Planck's radiation law) with $\mu^0 = 4$: (a) $-\log_{10}$ of the error between the last two iterates; (b) $-\log_{10}$ of the residual.

Table 4. Numerical results for Problem 3 (force between charged particles) with the initial estimate $\mu^0 = 1.2$.

Method	N	AS	$\lvert\mu^k - \mu^{k-1}\rvert$	$\lvert f(\mu^k)\rvert$	ρ
PS6	4	2.12076	1.28×10^{-237}	1.39×10^{-1424}	6.00
S4	5	2.12076	6.05×10^{-75}	1.08×10^{-299}	4.00
XY5	5	2.12076	6.52×10^{-195}	1.09×10^{-975}	5.00
XH6	4	2.12076	7.25×10^{-209}	1.57×10^{-1251}	6.00
C6	4	2.12076	1.02×10^{-186}	3.53×10^{-1118}	6.00

N: number of iterations; AS: approximate solution; ρ: approximated computational order of convergence (58).

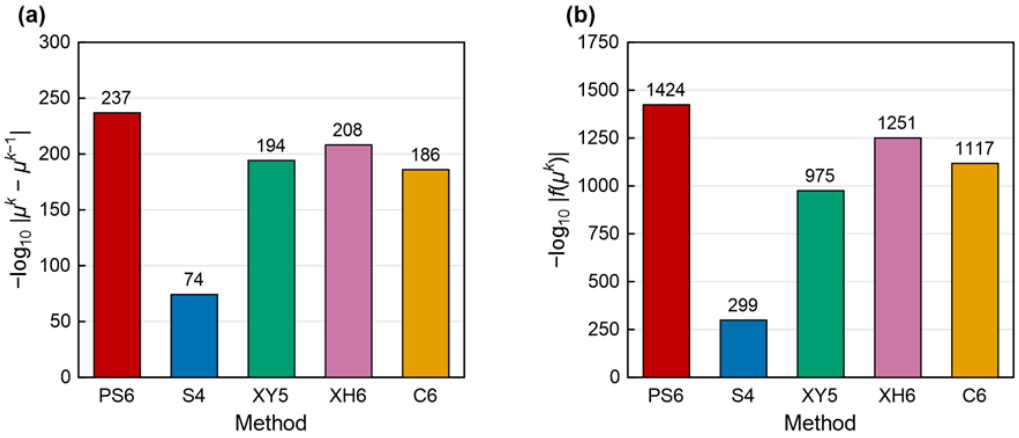

Fig. 4. Accuracy of the compared methods for Problem 3 (force between charged particles) with $\mu^0 = 1.2$: (a) $-\log_{10}$ of the error between the last two iterates; (b) $-\log_{10}$ of the residual.

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from ideal behaviour because of intermolecular attraction and the finite size of the molecules. The thermodynamic equilibrium of the fluid is described by a simplified nondimensional form of the Van der Waals model. Let μ denote the dimensionless reduced molar volume and υ the dimensionless pressure-correction parameter. Because molecular interactions strengthen as the fluid is compressed, the pressure correction is assumed to vary quadratically with the reduced molar volume,

$$\upsilon = \mu^2 - 1. \tag{62}$$

and the balance between compressibility and intermolecular forces gives:

$$\mu = \upsilon^2 - 1. \tag{63}$$

Rearranging Equations (62) and (63) gives the nonlinear system:

$$\begin{cases} \mu^2 - \upsilon = 1 \\ \mu - \upsilon^2 = -1 \end{cases} \tag{64}$$

Table 5 reports the results for the initial estimate $\mu^{(0)} = (-1.1, 0.5)^T$.

PS6 converges in four iterations, as do XH6 and C6, whereas S4 and XY5 require five and six, respectively. PS6 also has the shortest CPU time (0.797 s), which is 28% shorter than that of C6 (1.11 s) and 50% shorter than that of XH6 (1.58 s), in agreement with its lower cost per iteration (Table 1). Its step error (1.80×10^{-462}) and residual (2.31×10^{-2770}) are about 164 and 987 orders of magnitude smaller, respectively, than those of XH6. Figure 5 illustrates the accuracy for Problem 4. Figure 5(a) shows that PS6 attains about 462 correct digits in the step error, whereas the other sixth-order methods attain fewer than 300 and S4 and XY5 fewer than 150. Figure 5(b) shows a similar pattern for the residual norm.

Problem 5 (Steady-state thermal radiation). In thermal radiation, the intensity emitted by a blackbody depends exponentially on temperature,

Table 5. Numerical results for Problem 4 (Van der Waals fluid system) with the initial estimate $\mu^{(0)} = (-1.1, 0.5)^T$.

Method	N	CPU (s)	$\|\mu^{(k)} - \mu^{(k-1)}\|$	$\|F(\mu^{(k)})\|$	ρ
PS6	4	0.797	1.80×10^{-462}	2.31×10^{-2770}	6.00
S4	5	1.20	2.77×10^{-145}	3.35×10^{-722}	4.00
XY5	6	1.20	1.01×10^{-109}	9.02×10^{-544}	5.00
XH6	4	1.58	3.48×10^{-298}	9.52×10^{-1784}	6.00
C6	4	1.11	6.81×10^{-290}	6.85×10^{-1734}	6.00

N: number of iterations; CPU: central processing unit time; ρ: approximated computational order of convergence (58).

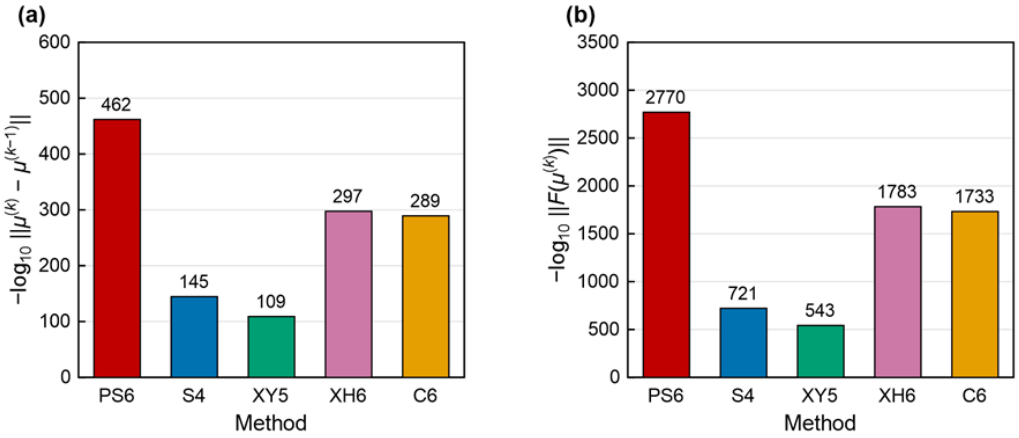

Fig. 5. Accuracy of the compared methods for Problem 4 (Van der Waals fluid system) with $\mu^{(0)} = (-1.1, 0.5)^T$: (a) $-\log_{10}$ of the norm of the error between the last two iterates; (b) $-\log_{10}$ of the residual norm.

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as described by Planck's radiation law. Consider a simplified steady-state radiation model in which μ is the dimensionless inverse temperature and υ is the normalized radiation intensity. The normalized intensity follows the exponential relation:

$$\upsilon = e^{-\mu}, \tag{65}$$

which is a nondimensional form of Planck's radiation law, and the energy balance between absorbed and emitted radiation is approximated by:

$$\mu = \upsilon^2 - 1. \tag{66}$$

Combining (65) and (66) gives the nonlinear system:

$$\begin{cases} \upsilon = e^{-\mu} \\ \mu - \upsilon^2 = -1 \end{cases} \tag{67}$$

Table 6 reports the results for the initial estimate $\mu^{(0)} = (-0.3, 0.5)^T$.

PS6, XH6 and C6 converge in four iterations, S4 in five and XY5 in six. PS6 has the smallest step error (2.41×10^{-622}) and residual (1.87×10^{-3732}) and the shortest CPU time (1.05 s). Its advantage in CPU time over XY5 (1.08 s) is, however, only about 3%, even though XY5 requires two more iterations; compared with XH6 (1.61 s), PS6 is 35% faster.

Figure 6 shows the accuracy for Problem 5. In Figure 6(a), XH6 comes closest to PS6 (583 versus 622 correct digits), whereas XY5 attains only 57 digits after six iterations. Figure 6(b) shows that the residual norm of PS6 has about 3732 correct digits, about 230 more than that of XH6.

3.3. Basins of Attraction

The dependence of PS6 on the initial estimate was examined by means of basins of attraction [16, 28, 33]. The scalar scheme (13) was applied to the polynomials $p_1(z) = z^2 - 1/4$, $p_2(z) = z^4 + 1/64$

Table 6. Numerical results for Problem 5 (thermal radiation system) with the initial estimate $\mu^{(0)} = (-0.3, 0.5)^T$.

Method	N	CPU (s)	$\|\mu^{(k)} - \mu^{(k-1)}\|$	$\|F(\mu^{(k)})\|$	ρ
PS6	4	1.05	2.41×10^{-622}	1.87×10^{-3732}	6.00
S4	5	1.34	9.59×10^{-297}	4.65×10^{-1482}	4.00
XY5	6	1.08	2.19×10^{-57}	4.35×10^{-284}	5.00
XH6	4	1.61	3.96×10^{-584}	1.43×10^{-3502}	6.00
C6	4	1.14	4.10×10^{-517}	4.40×10^{-3100}	6.00

N: number of iterations; CPU: central processing unit time; ρ: approximated computational order of convergence (58).

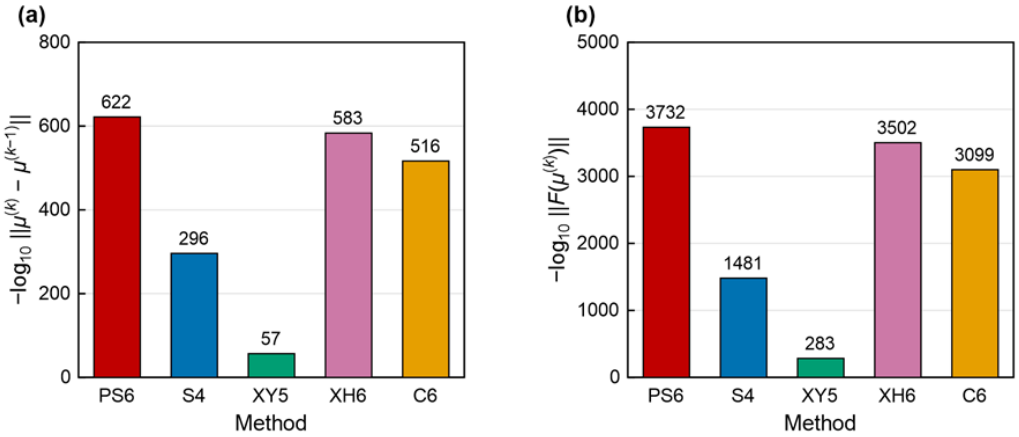

Fig. 6. Accuracy of the compared methods for Problem 5 (thermal radiation system) with $\mu^{(0)} = (-0.3, 0.5)^T$: (a) $-\log_{10}$ of the norm of the error between the last two iterates; (b) $-\log_{10}$ of the residual norm.

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and $p_3(z) = z^2 - 2/3$ from a uniform grid of 700 × 700 initial points (490,000 points) in the square $[-1,1] \times [-1,1]$ of the complex plane. The iteration was stopped when $|p(z^k)| < 10^{-6}$ or $|z^k - z^{k-1}| < 10^{-6}$, with a maximum of 20 iterations. Each initial point was coloured according to the root to which the iteration converged, with darker shades indicating more iterations, and points that did not converge within 20 iterations were coloured black. Table 7 summarizes the results.

Figure 7 shows the dynamical planes of PS6 for p_1. In Figure 7(a), the two basins are wide and connected and contain both roots, and 92.1% of the initial points converge, most of them within two or three iterations (Figure 7(b)). The non-convergent points form a flower-shaped region around the origin, which is the critical point of p_1, and a chain of small regions along the boundary between the basins. Unlike those of Newton's method, the basins are not symmetric with respect to the imaginary axis; this asymmetry arises from the auxiliary point $\omega = \mu + f(\mu)^3$, which is not symmetric under $\mu \to -\mu$.

Figure 8 shows the dynamical planes for p_2, which has four roots. The four basins in Figure 8(a) are of similar size, each attracting about 17–18% of the grid, but the proportion of convergent points decreases to 70.8%. The non-convergent points are concentrated near the origin, where the derivative of p_2 vanishes, along the coordinate axes that separate the basins, and in the corners of the square, far from the roots. Figure 8(b) shows that points inside the basins converge in about three iterations, whereas the boundaries display the fractal structure that is typical of high-order methods applied to polynomials of higher degree.

Figure 9 shows the dynamical planes for p_3, whose roots $\pm\sqrt{2/3} \approx \pm 0.816$ lie farther from the origin than those of p_1. In Figure 9(a), 81.6% of the initial points converge, with a mean of 2.51 iterations, but the basin of the negative root (47.9%)

Table 7. Basin statistics of PS6 for the three test polynomials on a 700 × 700 grid in [−1, 1] × [−1, 1].

Polynomial	Roots	Share of points converging to each root (%)	Convergent points (%)	Mean iterations
$p_1(z) = z^2 - 1/4$	$1/2, -1/2$	43.2, 48.9	92.1	2.50
$p_2(z) = z^4 + 1/64$	$(\pm 1 \pm i)/4$	18.1, 17.3, 17.3, 18.1	70.8	3.32
$p_3(z) = z^2 - 2/3$	$\sqrt{2/3}, -\sqrt{2/3}$	33.7, 47.9	81.6	2.51

Mean iterations are computed over the convergent points. For p_2, the roots are listed counter-clockwise starting from $(1 + i)/4$.

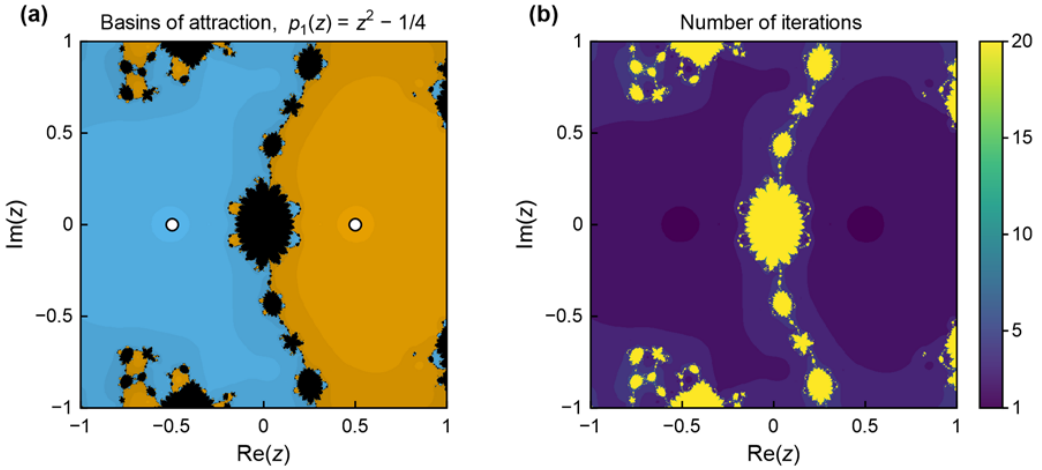

Fig. 7. Dynamical planes of PS6 for $p_1(z) = z^2 - 1/4$: (a) basins of attraction of the roots −1/2 (blue) and 1/2 (orange), with darker shades indicating more iterations, black points not converging within 20 iterations and white circles marking the roots; (b) number of iterations required for convergence.

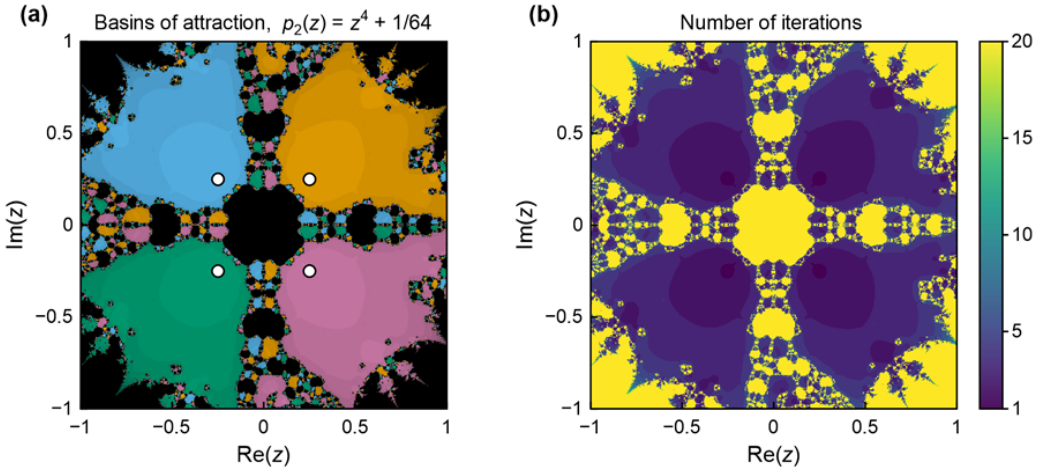

Fig. 8. Dynamical planes of PS6 for $p_2(z) = z^4 + 1/64$: (a) basins of attraction of the roots $(1 + i)/4$ (orange), $(-1 + i)/4$ (blue), $(-1 - i)/4$ (green) and $(1 - i)/4$ (pink), with black points not converging within 20 iterations; (b) number of iterations required for convergence.

is larger than that of the positive root (33.7%), again because of the asymmetric auxiliary point. Figure 9(b) shows that the non-convergent region around the origin is larger than for p_1 and that additional non-convergent regions appear near the upper and lower edges of the square. These results show that PS6 has wide regions of fast convergence, but also that initial estimates close to critical points of the function should be avoided.

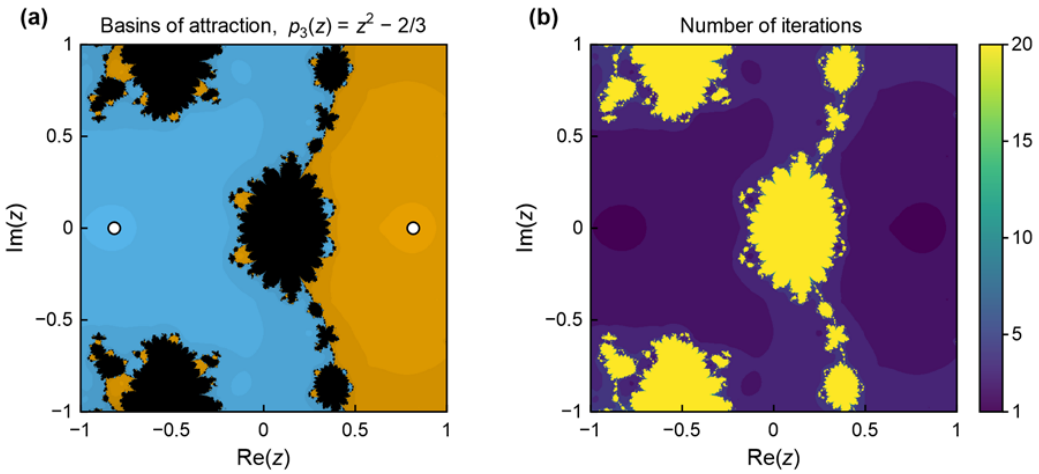

Fig. 9. Dynamical planes of PS6 for $p_3(z) = z^2 - 2/3$: (a) basins of attraction of the roots $-(2/3)^{1/2}$ (blue) and $(2/3)^{1/2}$ (orange), with black points not converging within 20 iterations and white circles marking the roots; (b) number of iterations required for convergence.

4. CONCLUSIONS

A derivative-free three-step iterative scheme, PS6, was developed for scalar nonlinear equations and extended to systems. The first two derivatives are approximated by divided differences and the third by a cubic Hermite interpolating polynomial, so no derivative or Jacobian is evaluated. A Taylor-expansion analysis proves sixth-order convergence in both the scalar and vector cases. In the scalar case the scheme uses four function evaluations per iteration, giving an efficiency index of $6^{1/4} \approx 1.565$.

PS6 has a higher computational efficiency index than S4, XY5, XH6 and C6 for every system size. On five test problems from the Van der Waals equation of state, Planck's radiation law and particle interaction, it needed the same or fewer iterations than the compared methods, gave the smallest errors and residuals, and had the shortest CPU time on both systems. The computed order of convergence matched the theoretical order. Basins of attraction showed that 71–92% of initial points in the test region converge, mostly within three iterations.

PS6 is not optimal in the Kung–Traub sense [37], since an optimal four-evaluation method would have order eight. Its main advantage is the low cost of its extension to systems, and its CPU-time gain over XY5 was small for the two-dimensional system. The auxiliary point makes the basins asymmetric, and initial guesses near critical points may fail to converge. Future work will cover large sparse and constrained systems, semilocal convergence, and parallel implementations.

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6. ETHICAL STATEMENT

This study did not involve human or animal subjects; therefore, ethical approval was not required.

7. CONFLICT OF INTEREST

The authors declare no conflict of interest.

8. FUNDING

No funding was received to conduct this research.

9. AUTHORSHIP CONTRIBUTION STATEMENT

Fatima Siddiqui: Conceptualization, Methodology, Investigation, Writing – Original Draft Preparation. Zubair Ahmed Kalhoro: Supervision, Writing – Review & Editing. Sanaullah Jamali: Visualization & Data Curation. Imran Qasim Memon: Proofreading, Final Manuscript Revision.

10. DECLARATION

The authors declare that (i) the results are original; (ii) the same material is neither published nor under consideration for publication elsewhere; (iii) approval of all authors has been obtained; and (iv) in case the article is accepted for publication, its copyright will be assigned to the Pakistan Academy of Sciences. An AI-based language-editing tool was used to improve the English of the manuscript; the authors reviewed the edited text and take full responsibility for its content.

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