INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING
Int. J. Numer. Meth. Engng 2017; **110**:661–674
Published online 11 October 2016 in Wiley Online Library (wileyonlinelibrary.com). DOI: 10.1002/nme.5426

Globalization technique for projected Newton–Krylov methods

Jinhai Chen[1] and Cornelis Vuik[2,*,†]

[1]*Princeton University, Princeton, NJ 08544, USA*
[2]*Delft University of Technology, Mekelweg 4, 2628 CD Delft, The Netherlands*

SUMMARY

Large-scale systems of nonlinear equations appear in many applications. In various applications, the solution of the nonlinear equations should also be in a certain interval. A typical application is a discretized system of reaction diffusion equations. It is well known that chemical species should be positive otherwise the solution is not physical and in general blow up occurs. Recently, a projected Newton method has been developed, which can be used to solve this type of problems. A drawback is that the projected Newton method is not globally convergent. This motivates us to develop a new feasible projected Newton–Krylov algorithm for solving a constrained system of nonlinear equations. Combined with a projected gradient direction, our feasible projected Newton–Krylov algorithm circumvents the non-descent drawback of search directions which appear in the classical projected Newton methods. Global and local superlinear convergence of our approach is established under some standard assumptions. Numerical experiments are used to illustrate that the new projected Newton method is globally convergent and is a significate complementarity for Newton–Krylov algorithms known in the literature. © 2016 The Authors. *International Journal for Numerical Methods in Engineering* Published by John Wiley & Sons Ltd.

Received 29 May 2015; Revised 2 June 2016; Accepted 4 September 2016

KEY WORDS: nonlinear equations with constraints; projected Newton–Krylov method; projected gradient direction; global convergence

1. INTRODUCTION

The mathematical model of chemical vapor deposition typically involves the Navier–Stokes equations associated with the energy equation and a usually large number of advection–diffusion-reaction equations that model the interaction of the reactive species. Because of the different time scales involving the species transport and their conversion as consequence of chemical reactions, the system of species equations is a stiff system of partial differential equations. In order to fulfill stability requirements, the species equations are discretized implicitly in time. This leads to a large-scale system of strongly nonlinear algebraic equations that need to be solved in each time step. In addition to the stability issues, the non-negativity of the species mass fractions is also required to satisfy the physical quantity like the concentrations.

Based on these observations, van Veldhuizen, Vuik, and Kleijn [1] proposed a class of projected Newton–Krylov methods to find the nonnegative solutions of the advection–diffusion-reaction equations arising from laminar reacting flow problems for chemical vapor deposition. More specifically, the authors [1] first used the first-order Euler backward method to discretize the advection–diffusion-reaction equations and then employed projected Newton–Krylov methods to solve the underlying large-scale systems of nonlinear equations in the form of

*Correspondence to: Cornelis Vuik, Delft University of Technology, Mekelweg 4, 2628 CD Delft, The Netherlands.
†E-mail: c.vuik@tudelft.nl

$$\begin{cases} F(\boldsymbol{x}) = 0 \\ \boldsymbol{x} \geqslant 0, \end{cases} \tag{1}$$

where $F : \mathbb{R}^n \to \mathbb{R}^n$ is continuously differentiable. From the class of discretized nonlinear partial differential equations, the size of system (1) is very large; 10^9 or more unknowns are no exception. This type of projected Newton–Krylov methods is very effective, because the authors have used it successfully to solve large advection–diffusion-reaction systems (50 chemical reactions), in which the standard nonlinear solver packages are not easy or impossible to use. In fact, these methods can be considered as a classical projected Newton method that involves preconditioned iterative linear solvers (i.e., Krylov subspace methods, cf. [2]). Although their numerical results are promising, these methods do not overcome the possible non-convergence of the classical projected Newton method. In particular, there is no guarantee for the descent property of search directions (i.e., projected Newton directions) used for minimizing the underlying merit function, see Example 7 in Section 3.

On the other hand, as is well known in optimization, a projected gradient direction on a constraint set is usually a descent direction[‡], see, for example [3–6]. This actually motivates us to modify the projected Newton–Krylov methods in [1] by means of introducing a series of projected gradient directions. Roughly speaking, we will use a projected gradient direction as a descent direction to calculate the next iterate when the current projected Newton direction is not descent. As will be shown in Section 2, this modification will not only ensure the global convergence of the projected Newton–Krylov methods in [1] but also inherit the computational advantages of these methods, such as the capacity of solving extreme large-scale problems mentioned earlier, the matrix-free operation, and preconditioning technique, and so on, see, for example, [7]. In other words, we extend the theory of Newton–Krylov methods in [2, 8] fully to the projected case. In particular, we add new descent feasibility of the projected Newton–Krylov methods in [1], under reservation of the computational advantages of these methods.

In order to accomplish the purposes of this paper in a very general setting, we consider the numerical solution of the following constrained system of nonlinear equations

$$\begin{cases} F(\boldsymbol{x}) = 0 \\ \boldsymbol{x} \in \Omega, \end{cases} \tag{2}$$

where Ω is a convex constraint set of $\mathbb{R}^n$, such as the well known box constraint set $\{\boldsymbol{x} \in \mathbb{R}^n \mid \boldsymbol{l} \leqslant \boldsymbol{x} \leqslant \boldsymbol{u}\}$, $l_i \in \{\mathbb{R} \cup \{-\infty\}\}$ and $u_i \in \{\mathbb{R} \cup \{-\infty\}\}$, $l_i < u_i$, $i = 1, \ldots, n$, $F : \mathbb{R}^n \to \mathbb{R}^n$ is continuously differentiable on Ω. Note that constraints $\boldsymbol{x} \geqslant 0$ in system (1) are special cases of box constraints.

In addition to appearing in systems of discretized partial differential equations, compare with [1], system (2) also arises from optimization and equilibrium problems, compare with [3, 9]. Great efforts have been made to find a solution of nonlinear equations (2) by solving an equivalently constrained minimization problem

$$\min \Theta(\boldsymbol{x}) = \frac{1}{2}\|F(\boldsymbol{x})\|^2, \quad \boldsymbol{x} \in \Omega, \tag{3}$$

see [3, 10–14] and references therein. In particular, Gould, Leyffer, and Toint [10] developed a multidimensional filter algorithm for the solution of systems of nonlinear equations and nonlinear least-squares problems with $\Omega = \mathbb{R}^n$. This algorithm combines the efficiency of filter techniques and the robustness of trust-region methods. Moveover, the algorithm was later extended to find vectors satisfying general sets of nonlinear equations and/or inequalities on $\mathbb{R}^n$ [11]. For a general set Ω, Kanzow, Yamashita, and Fukushima [12] discussed a global projected Levenberg–Marquardt method for the numerical solution of the general nonsquare systems of bound-constrained nonlinear equations. The method proposed by Ulbrich [13] is based on a Newton-like method with projection

[‡]A direction $\boldsymbol{d} \in \mathbb{R}^n$ is a descent direction for a continuous differentiable function $\Theta(\boldsymbol{x})$ at $\boldsymbol{x}$ if

$$\left.\frac{\mathrm{d}\Theta(\boldsymbol{x} + t\boldsymbol{d})}{\mathrm{d}t}\right|_{t=0} = \nabla\Theta(\boldsymbol{x})^\top \boldsymbol{d} < 0.$$

wrapped into a trust-region technique. It requires the minimization of quadratic problems on Ω and achieves quadratic convergence. In [14], Wang, Monteiro, and Pang described a potential reduction type interior point method for the solution of constrained problems.

The remainder of this paper is organized as follows. In Section 2, we give a detailed statement of our new feasible projected Newton–Krylov method and establish its global and local convergence. In Section 3, we provide numerical examples to illustrate the necessity of a projected gradient direction, in the case of a projected Newton direction being not descent. We give some concluding comments in Section 4.

A few words about the notation used throughout the paper. Given a continuously differentiable function $F : \mathbb{R}^n \to \mathbb{R}^n$, its Jacobian matrix at $\boldsymbol{x} \in \mathbb{R}^n$ is denoted by $F'(\boldsymbol{x})$, and its transposed Jacobian matrix by $\nabla F(\boldsymbol{x})$. $\|\cdot\|$ denotes the Euclidean norm, and $\mathscr{P}(\cdot)$ is the orthogonal projection operator onto Ω.

2. FEASIBLE PROJECTED NEWTON–KRYLOV METHOD

In this section, we illuminate a new feasible projected Newton–Krylov method, by introducing projected gradient directions. In our feasible projected Newton–Krylov method, a simple and practical but effective switching strategy between projected Newton directions and projected gradient directions is employed to ensure the descent feasibility of search directions, which overcome the possible non-convergence of classical projected Newton methods. The convergence analysis of our new approach is also presented.

We start by giving our feasible projected Newton–Krylov method as follows. We remark that the forcing term $\{\eta_k\}$ in our feasible projected Newton–Krylov method can be chosen according to the strategy for inexact Newton method without projection in [8, 15–18], because the nonexpansiveness of the projection operator [3, 4] does not affect the local convergence of the projected Newton method. Thus, inequality (5) is always satisfied as iterative point $\boldsymbol{x}^k$ is close enough to the solution of $F(\boldsymbol{x})$ on Ω, see Theorem 5 stated in the succeeding text. Moreover, if the Newton direction $\boldsymbol{d}^k$ in step 2 exists, that is, inequality (4) is solvable, then inequality (5) is also satisfied with $\Omega = \mathbb{R}^n$, see [8, Lemma 3.1].

Our feasible projected Newton–Krylov method (i.e., Algorithm 1) can be traced back to the ones in [1] and thus inherits the computational advantages of these methods, such as the capacity of solving extreme large-scale problems, the matrix-free operation, and preconditioning technique. Moveover, Algorithm 1 in this paper has some peculiar characteristics of its own. For example, we exploit a projected gradient direction $\mathcal{P}(\boldsymbol{x}^k - \lambda\nabla\Theta(\boldsymbol{x}^k)) - \boldsymbol{x}^k$ to generate next iterate $\boldsymbol{x}^{k+1}$, in the case when projected Newton direction is unavailable or fails to be a direction of descent for the projected Newton–Krylov algorithms in [1]; in addition, we make use of a simple indicator variable $\mathrm{FLAG_{NG}}(= 0 \text{ or } 1)$, to determine the switching between a projected Newton direction and a projected gradient direction. As will be shown in this section (i.e., Lemma 3), the projected gradient direction $\mathcal{P}(\boldsymbol{x}^k - \lambda\nabla\Theta(\boldsymbol{x}^k)) - \boldsymbol{x}^k$ is always descent. Consequently, inequality (6) can be always satisfied, in particular, when inequality (5) is not valid. Therefore, our feasible projected Newton–Krylov method is well-defined.

In what follows, we give a theoretical analysis of the feasible projected Newton–Krylov method, that is, Algorithm 1. We first recall some basic properties of a projection operator.

Lemma 1 (see [4, Lemma 2.1]*)*
Let $\mathscr{P}$ be the projection into Ω.

(a) If $z \in \Omega$ then $(\mathscr{P}(\boldsymbol{x}) - \boldsymbol{x}, z - \mathscr{P}(\boldsymbol{x})) \geqslant 0$ for all $\boldsymbol{x} \in \mathbb{R}^n$.
(b) $\mathscr{P}$ is a monotone operator, that is $(\mathscr{P}(\boldsymbol{y}) - \mathscr{P}(\boldsymbol{x}), \boldsymbol{y} - \boldsymbol{x}) \geqslant 0$ for $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n$. If $\mathscr{P}(\boldsymbol{y}) \neq \mathscr{P}(\boldsymbol{x})$ then strict inequality holds.
(c) $\mathscr{P}(\boldsymbol{x})$ is a nonexpansive operator, that is, $\|\mathscr{P}(\boldsymbol{y}) - \mathscr{P}(\boldsymbol{x})\| \leqslant \|\boldsymbol{y} - \boldsymbol{x}\|$ for $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n$.

The next lemma is given by Gafni and Bertsekas in [5, Lemma 3] and [6, Lemma 1.a)], and reconsidered with a simple proof by Calamai and Moré in [4, Lemma 2.2].

DOI: 10.1002/nme

Algorithm 1 Feasible projected Newton–Krylov method

Require: $\boldsymbol{x}^0 \in \Omega$, $t, \sigma \in (0,1)$, $\eta_{\max} \in [0,1)$, $0 < \lambda_{\min} \leqslant \lambda_0 \leqslant \lambda_{\max} < 1$, $m_{\max} \in \mathbb{N}$, and $\text{FLAG}_{NG} = 0$

for $k = 0$ step 1 until convergence **do**
  if $\text{FLAG}_{NG} = 0$ and a preconditioned Krylov subspace method finds some $\eta_k \in [0, \eta_{\max}]$ and a vector $\boldsymbol{d}^k$ satisfying

$$\|F(\boldsymbol{x}^k) + F'(\boldsymbol{x}^k)\boldsymbol{d}^k\| \leqslant \eta_k \|F(\boldsymbol{x}^k)\| \tag{4}$$

  then
    $m = 0, \lambda = \lambda_0$
    while $\lambda \in [\lambda_{\min}, 1]$ and $m < m_{\max}$ **do**
      $\lambda \leftarrow \lambda_0^m$
      if

$$\|F(\mathcal{P}(\boldsymbol{x}^k + \lambda \boldsymbol{d}^k))\| \leqslant (1 - t\lambda(1-\eta_k))\|F(\boldsymbol{x}^k)\| \tag{5}$$

      then
        $\boldsymbol{x}^{k+1} = \mathcal{P}(\boldsymbol{x}^k + \lambda \boldsymbol{d}^k), m = m_{\max}, \text{FLAG}_{NG} = 0$
      else
        $m = m + 1, \text{FLAG}_{NG} = 1$
      end if
    end while
  else
    $\boldsymbol{d}^k = -\nabla\Theta(\boldsymbol{x}^k)$
    $m = 0, \lambda = \lambda_0$
    while $\lambda \in (0, 1]$ and $m < m_{\max}$ **do**
      $\lambda \leftarrow \lambda_0^m$
      if

$$\Theta(\mathcal{P}(\boldsymbol{x}^k + \lambda \boldsymbol{d}^k)) \leqslant \Theta(\boldsymbol{x}^k) + \sigma \nabla\Theta(\boldsymbol{x}^k)^\top (\mathcal{P}(\boldsymbol{x}^k + \lambda \boldsymbol{d}^k) - \boldsymbol{x}^k) \tag{6}$$

      then
        $\boldsymbol{x}^{k+1} = \mathcal{P}(\boldsymbol{x}^k + \lambda \boldsymbol{d}^k)$ and $m = m_{\max}, \text{FLAG}_{NG} = 0$
      else
        $m = m + 1$
      end if
    end while
  end if
end for

Lemma 2
Let $\mathscr{P}$ be the projection into Ω. Given $\boldsymbol{x} \in \mathbb{R}^n$ and $\boldsymbol{d} \in \mathbb{R}^n$, then function ψ defined by

$$\psi(\alpha) = \frac{\|\mathscr{P}(\boldsymbol{x} + \alpha \boldsymbol{d}) - \boldsymbol{x}\|}{\alpha}, \; \alpha > 0, \tag{7}$$

is antitone (nonincreasing).

With these properties for the projection operator $\mathscr{P}$, we can show that the projected Newton–Krylov method is well-defined.

Lemma 3
Suppose that $\boldsymbol{x}^k$ is not a stationary point of (3) and $\lambda \in (0,1]$. Then $\mathcal{P}(\boldsymbol{x}^k - \lambda\nabla\Theta(\boldsymbol{x}^k)) - \boldsymbol{x}^k$ is a descent direction of (6).

Proof
In fact, let $\boldsymbol{x} = \boldsymbol{x}^k - \lambda \nabla\Theta(\boldsymbol{x}^k)$ and $\boldsymbol{z} = \boldsymbol{x}^k$ in the part (a) of Lemma 1. An immediate consequence of the part (a) of Lemma 1 yields that

$$\begin{aligned} 0 &\leqslant \left(\mathscr{P}\left(\boldsymbol{x}^k - \lambda\nabla\Theta(\boldsymbol{x}^k)\right) - \left(\boldsymbol{x}^k - \lambda\nabla\Theta(\boldsymbol{x}^k)\right), \boldsymbol{x}^k - \mathscr{P}\left(\boldsymbol{x}^k - \lambda\nabla\Theta(\boldsymbol{x}^k)\right)\right) \\ &\leqslant \left(\mathscr{P}\left(\boldsymbol{x}^k - \lambda\nabla\Theta(\boldsymbol{x}^k)\right) - \boldsymbol{x}^k, \boldsymbol{x}^k - \mathscr{P}\left(\boldsymbol{x}^k - \lambda\nabla\Theta(\boldsymbol{x}^k)\right)\right) \\ &\quad + \left(\lambda\nabla\Theta(\boldsymbol{x}^k), \boldsymbol{x}^k - \mathscr{P}\left(\boldsymbol{x}^k - \lambda\nabla\Theta(\boldsymbol{x}^k)\right)\right) \\ &\leqslant -\left\|\mathscr{P}\left(\boldsymbol{x}^k - \lambda\nabla\Theta(\boldsymbol{x}^k)\right) - \boldsymbol{x}^k\right\|^2 - \lambda\nabla\Theta(\boldsymbol{x}^k)^\top\left(\mathcal{P}\left(\boldsymbol{x}^k - \lambda\nabla\Theta(\boldsymbol{x}^k)\right) - \boldsymbol{x}^k\right). \end{aligned} \tag{8}$$

By (8), we have

$$\nabla\Theta(\boldsymbol{x}^k)^\top\left(\mathcal{P}\left(\boldsymbol{x}^k - \lambda\nabla\Theta(\boldsymbol{x}^k)\right) - \boldsymbol{x}^k\right) \leqslant -\frac{1}{\lambda}\left\|\mathcal{P}\left(\boldsymbol{x}^k - \lambda\nabla\Theta(\boldsymbol{x}^k)\right) - \boldsymbol{x}^k\right\|^2 < 0, \tag{9}$$

which establishes the assertion. □

Now, we are ready to state and prove the promised convergence result of the feasible projected Newton–Krylov method. To this end, we assume that the feasible projected Newton–Krylov method does not terminate at a stationary point at any finite step.

Theorem 4
Assume that $\{\boldsymbol{x}^k\} \subset \Omega$ is a sequence generated by the feasible projected Newton–Krylov method. Then any accumulation point of $\{\boldsymbol{x}^k\}$ is at least a stationary point of (3). Further, if (5) is satisfied by the projected Newton direction for all but finitely many k, then $\boldsymbol{x}^*$ is a zero of $F(\boldsymbol{x})$ on Ω.

Proof
Let $\boldsymbol{x}^*$ be an accumulation point of a sequence $\{\boldsymbol{x}^k\}$ generated by the feasible projected Newton–Krylov method. We consider two cases. Suppose first that the projected Newton direction is used (i.e., (5) holds) for infinitely many iterations. It follows immediately that $F(\boldsymbol{x}^*) = 0$. So $\boldsymbol{x}^*$ is a stationary point.

On the other hand, suppose that the projected gradient direction is used (i.e., (6) holds) for all but finitely many iterations. It follows from (6) that $\{\Theta(\boldsymbol{x}^k)\}$ is monotonically decreasing (unless the method terminates at a stationary point at any finite step) and is bounded below by zero. Hence, it converges and

$$\lim_{k\to\infty}\left(\Theta(\boldsymbol{x}^{k+1}) - \Theta(\boldsymbol{x}^k)\right) = 0. \tag{10}$$

By (6), this implies that

$$\lim_{k\to\infty}\nabla\Theta(\boldsymbol{x}^k)^\top\left(\mathcal{P}\left(\boldsymbol{x}^k - \lambda_0^{m_k}\nabla\Theta(\boldsymbol{x}^k)\right) - \boldsymbol{x}^k\right) = 0. \tag{11}$$

Let $\{\boldsymbol{x}^k, k \in K\}$ be a subsequence converging to $\boldsymbol{x}^*$. We consider two subcases for (11).
Case 1: Assume

$$\liminf_{k(\in K)\to\infty}\lambda_0^{m_k} > 0.$$

By (11) and (9) in Lemma 3, it follows that for some infinite subset $K' \subseteq K$,

$$\lim_{k(\in K')\to\infty} -\left\|\mathcal{P}\left(\boldsymbol{x}^k - \lambda_0^{m_k}\nabla\Theta(\boldsymbol{x}^k)\right) - \boldsymbol{x}^k\right\|^2 = 0. \tag{12}$$

Hence, $\boldsymbol{x}^*$ is a stationary point of (3).
Case 2: Assume that there is a subsequence $\{\boldsymbol{x}^k\}_{k\in J}$, $J \subseteq K$, with

DOI: 10.1002/nme

$$\lim_{k(\in J)\to\infty} \lambda_0^{m_k} = 0. \tag{13}$$

Then, for sufficiently large $k(\in J)$, $\boldsymbol{x}^k$ is not a stationary point. Otherwise, if $\boldsymbol{x}^k$ is a stationary point, then $\lambda_0^{m_k} = 1$ follows from (6). This is in contradiction to (13). Therefore, for sufficiently large $k(\in J)$, it holds that

$$\left\| \mathcal{P}\left(\boldsymbol{x}^k - \lambda_0^{m_k-1}\nabla\Theta(\boldsymbol{x}^k)\right) - \boldsymbol{x}^k \right\| > 0. \tag{14}$$

In addition, it follows from (6) that

$$\Theta\left(\mathcal{P}\left(\boldsymbol{x}^k - \lambda_0^{m_k-1}\nabla\Theta(\boldsymbol{x}^k)\right)\right) - \Theta(\boldsymbol{x}^k) > \sigma\nabla\Theta(\boldsymbol{x}^k)^\top \left(\mathcal{P}\left(\boldsymbol{x}^k - \lambda_0^{m_k-1}\nabla\Theta(\boldsymbol{x}^k)\right) - \boldsymbol{x}^k\right). \tag{15}$$

Moveover, by the mean value theorem, we know

$$\begin{aligned}
&\Theta\left(\mathcal{P}\left(\boldsymbol{x}^k - \lambda_0^{m_k-1}\nabla\Theta(\boldsymbol{x}^k)\right)\right) - \Theta(\boldsymbol{x}^k)\\
&\quad = \nabla\Theta(\xi^k)^\top \left(\mathcal{P}\left(\boldsymbol{x}^k - \lambda_0^{m_k-1}\nabla\Theta(\boldsymbol{x}^k)\right) - \boldsymbol{x}^k\right)\\
&\quad = \left(\nabla\Theta(\xi^k) - \nabla\Theta(\boldsymbol{x}^k)\right)^\top \left(\mathcal{P}\left(\boldsymbol{x}^k - \lambda_0^{m_k-1}\nabla\Theta(\boldsymbol{x}^k)\right) - \boldsymbol{x}^k\right)\\
&\qquad + \nabla\Theta(\boldsymbol{x}^k)^\top \left(\mathcal{P}\left(\boldsymbol{x}^k - \lambda_0^{m_k-1}\nabla\Theta(\boldsymbol{x}^k)\right) - \boldsymbol{x}^k\right)\\
&\quad > \sigma\nabla\Theta(\boldsymbol{x}^k)^\top \left(\mathcal{P}\left(\boldsymbol{x}^k - \lambda_0^{m_k-1}\nabla\Theta(\boldsymbol{x}^k)\right) - \boldsymbol{x}^k\right),
\end{aligned} \tag{16}$$

where $\boldsymbol{\xi}^k = \tau\boldsymbol{x}^k + (1-\tau)\mathcal{P}(\boldsymbol{x}^k - \lambda_0^{m_k-1}\nabla\Theta(\boldsymbol{x}^k))$ for some $\tau \in (0,1)$, that is, $\boldsymbol{\xi}^k$ is a point in the line segment between $\boldsymbol{x}^k$ and $\mathcal{P}(\boldsymbol{x}^k - \lambda_0^{m_k-1}\nabla\Theta(\boldsymbol{x}^k))$. Consequently,

$$\begin{aligned}
&\left(\nabla\Theta(\boldsymbol{\xi}^k) - \nabla\Theta(\boldsymbol{x}^k)\right)^\top \left(\mathcal{P}\left(\boldsymbol{x}^k - \lambda_0^{m_k-1}\nabla\Theta(\boldsymbol{x}^k)\right) - \boldsymbol{x}^k\right)\\
&\qquad > (1-\sigma)\nabla\Theta(\boldsymbol{x}^k)^\top \left(\boldsymbol{x}^k - \mathcal{P}\left(\boldsymbol{x}^k - \lambda_0^{m_k-1}\nabla\Theta(\boldsymbol{x}^k)\right)\right).
\end{aligned} \tag{17}$$

Further,

$$\begin{aligned}
&\nabla\Theta(\boldsymbol{x}^k)^\top \left(\boldsymbol{x}^k - \mathcal{P}\left(\boldsymbol{x}^k - \lambda_0^{m_k-1}\nabla\Theta(\boldsymbol{x}^k)\right)\right)\\
&\quad < \frac{1}{1-\sigma}\left(\nabla\Theta(\boldsymbol{\xi}^k) - \nabla\Theta(\boldsymbol{x}^k)\right)^\top \left(\mathcal{P}(\boldsymbol{x}^k - \lambda_0^{m_k-1}\nabla\Theta(\boldsymbol{x}^k) - \boldsymbol{x}^k\right)\\
&\quad < \frac{1}{1-\sigma}\left\|\nabla\Theta(\boldsymbol{\xi}^k) - \nabla\Theta(\boldsymbol{x}^k)\right\| \left\|\mathcal{P}\left(\boldsymbol{x}^k - \lambda_0^{m_k-1}\nabla\Theta(\boldsymbol{x}^k)\right) - \boldsymbol{x}^k\right\|.
\end{aligned} \tag{18}$$

On the other hand, by Lemma 2, it follows that $\frac{\|\boldsymbol{x}^k - \mathscr{P}(\boldsymbol{x}^k - \lambda\nabla\Theta(\boldsymbol{x}^k))\|}{\lambda}$ is monotonically nonincreasing with respect to λ. From (9), we then have

$$\begin{aligned}
&\Theta(\boldsymbol{x}^k)^\top \left(\boldsymbol{x}^k - \mathcal{P}\left(\boldsymbol{x}^k - \lambda_0^{m_k-1}\nabla\Theta(\boldsymbol{x}^k)\right)\right)\\
&\quad \geqslant \frac{\left\|\boldsymbol{x}^k - \mathscr{P}(\boldsymbol{x}^k - \lambda_0^{m_k-1}\nabla\Theta(\boldsymbol{x}^k))\right\|^2}{\lambda_0^{m_k-1}}\\
&\quad \geqslant \frac{\left\|\boldsymbol{x}^k - \mathcal{P}(\boldsymbol{x}^k - \lambda_0\nabla\Theta(\boldsymbol{x}^k))\right\|}{\lambda_0}\left\|\boldsymbol{x}^k - \mathcal{P}(\boldsymbol{x}^k - \lambda_0^{m_k-1}\nabla\Theta(\boldsymbol{x}^k))\right\|.
\end{aligned} \tag{19}$$

This, combined with (14) and (18), implies

$$\frac{\left\|\boldsymbol{x}^k - \mathcal{P}(\boldsymbol{x}^k - \lambda_0\nabla\Theta(\boldsymbol{x}^k))\right\|}{\lambda_0} < \frac{1}{1-\sigma}\left\|\nabla\Theta(\boldsymbol{\xi}^k) - \nabla\Theta(\boldsymbol{x}^k)\right\|. \tag{20}$$

Passing to the limit as $k(\in J) \to \infty$, we obtain

$$\frac{\|\mathcal{P}(\boldsymbol{x}^* - \lambda_0 \nabla \Theta(\boldsymbol{x}^*)) - \boldsymbol{x}^*\|}{\lambda_0} = 0, \tag{21}$$

which implies $\boldsymbol{x}^*$ is a stationary point. Therefore, in either case, we establish the assertion. □

We next pass to prove the local convergence of the feasible projected Newton–Krylov method. To this end, we need some basic concepts in convergence analysis of iterative algorithms. Let the sequence $\{\boldsymbol{x}^k\}$ converges a point $\boldsymbol{x}^*$. The convergence rate is said to Q-linear with Q-factor $\sigma \in (0, 1)$ if

$$\|\boldsymbol{x}^{k+1} - \boldsymbol{x}^*\| \leqslant \sigma \|\boldsymbol{x}^k - \boldsymbol{x}^*\|$$

for all large enough k and some norm on $\mathbb{R}^n$. The convergence rate is called to Q-superlinear if

$$\lim_{k \to \infty} \frac{\|\boldsymbol{x}^{k+1} - \boldsymbol{x}^*\|}{\|\boldsymbol{x}^k - \boldsymbol{x}^*\|} = 0$$

for some norm on $\mathbb{R}^n$, see [19, Chapter 9] for details. We call that a function $F(\boldsymbol{x})$ has a strong Fréchet derivative $F'(\boldsymbol{x})$ at $\boldsymbol{x}$ (cf. [19, Defination 3.2.9]) if

$$\lim_{\substack{\boldsymbol{y} \to \boldsymbol{x} \\ \boldsymbol{z} \to \boldsymbol{x}}} \frac{\|F(\boldsymbol{x}) - F(\boldsymbol{y}) - F'(\boldsymbol{x})(\boldsymbol{z} - \boldsymbol{y})\|}{\|\boldsymbol{z} - \boldsymbol{y}\|} = 0. \tag{22}$$

If $F(\boldsymbol{x})$ is continuously differentiable, then $F(\boldsymbol{x})$ is locally Lipschitz continuous at $\boldsymbol{x}$, that is, there exists a constant $L_{\boldsymbol{x}}$ such that for all $\boldsymbol{y}$ sufficiently close to $\boldsymbol{x}$,

$$\|F(\boldsymbol{y}) - F(\boldsymbol{x})\| \leqslant L_{\boldsymbol{x}} \|\boldsymbol{y} - \boldsymbol{x}\|. \tag{23}$$

Further, if $F'(\boldsymbol{x})$ is nonsingular at $\boldsymbol{x}^*$, that is, there exists a constant $C_{\boldsymbol{x}^*}$ such that $\|F'(\boldsymbol{x}^*)^{-1}\| \leqslant C_{\boldsymbol{x}^*}$, then there exists a constant C such that $F'(\boldsymbol{y})^{-1}$ exists, and

$$\|F'(\boldsymbol{y})^{-1}\| \leqslant C \tag{24}$$

for all $\boldsymbol{y}$ sufficiently close to $\boldsymbol{x}^*$, see, for example, [19, Theorem 2.3.3].

Theorem 5
Assume that $\boldsymbol{x}^* \in \Omega$ is a limit point of $\{\boldsymbol{x}^k\}$ generated by the feasible projected Newton–Krylov method. Assume also that $F(\boldsymbol{x}^*) = 0$ and $F'(\boldsymbol{x}^*)$ is nonsingular. Then the whole sequence $\{\boldsymbol{x}^k\}$ converges to $\boldsymbol{x}^*$. Furthermore, for large enough k,

(a) if $\eta_{\max}$ and t are chosen by

$$\begin{cases} \eta_{\max} \in (0, 1), t \in \left[C^2 L, 1\right), & \text{if } C^2 L < 1, \\ \eta_{\max} \in \left(0, \frac{1-t}{C^2 L - t}\right), t \in (0, 1), & \text{if } C^2 L \geqslant 1, \end{cases} \tag{25}$$

where L is the Lipschitz constant of F at $\boldsymbol{x}^*$ (see (28)), and C is an upper bound of inverse of $F(x)$ defined in a neighborhood of $\boldsymbol{x}^*$ (see (30)), then the projected Newton direction is eventually accepted with $\lambda = 1$, that is, no projected gradient direction is carried out;

(b) if

$$\begin{cases} \eta_{\max} \in \left(0, \min\left\{\frac{1}{CL}, 1\right\}\right), t \in \left[C^2 L, 1\right), & \text{if } C^2 L < 1, \\ \eta_{\max} \in \left(0, \min\left\{\frac{1}{CL}, \frac{1-t}{C^2 L - t}\right\}\right), t \in (0, 1), & \text{if } C^2 L \geqslant 1, \end{cases} \tag{26}$$

then the convergence rate is Q-linear;

(c) if $\eta_k \to 0$, the convergence rate is Q-superlinear.

Proof
The nonsingularity of $F'(\boldsymbol{x}^*)$ implies that $\boldsymbol{x}^*$ is an isolated limit point of the sequence $\{\boldsymbol{x}^k\}$. By exploiting the proof of Theorem 4, and the nonexpansiveness of the projection operator $\mathscr{P}$, it follows that

$$\lim_{k\to\infty} \left\| \boldsymbol{x}^{k+1} - \boldsymbol{x}^k \right\| = 0. \tag{27}$$

This indicates that the entire sequence $\{\boldsymbol{x}^k\}$ converges to $\boldsymbol{x}^*$.

Let $\boldsymbol{e}^k = \boldsymbol{x}^k - \boldsymbol{x}^*$. Owing to continuous differentiability of $F(x)$, it follows that $F(x)$ is locally Lipschitz continuous at $x \in \Omega$, and its Fréchet derivative $F'(x)$ at x is strong. Therefore, there exists a constant L such that for all $\boldsymbol{x}^k$ sufficiently close to $\boldsymbol{x}^*$,

$$\left\| F(\boldsymbol{x}^k) - F(\boldsymbol{x}^*) \right\| \leqslant L \left\| \boldsymbol{e}^k \right\|. \tag{28}$$

Also, by the definition of strong Fréchet derivative (i.e., (22)), it follows that

$$\left\| F(\boldsymbol{x}^k) - F(\boldsymbol{x}^*) - F(\boldsymbol{x}^k)\boldsymbol{e}^k \right\| = o\left(\left\| \boldsymbol{e}^k \right\| \right). \tag{29}$$

Furthermore, by making use of the nonsingularity of $F'(\boldsymbol{x}^*)$ again, there exists a constant C such that

$$\left\| F'(\boldsymbol{x}^k)^{-1} \right\| \leqslant C \tag{30}$$

for all $\boldsymbol{x}^k$ sufficiently close to $\boldsymbol{x}^*$.

In addition, for all $\boldsymbol{x}^k$ sufficiently close to $\boldsymbol{x}^*$, it holds that

$$\mathscr{P}(\boldsymbol{x}^k + \boldsymbol{d}^k) - \boldsymbol{x}^* = \mathcal{P}\left(\boldsymbol{x}^k - F'(\boldsymbol{x}^k)^{-1} F(\boldsymbol{x}^k) + F'(\boldsymbol{x}^k)^{-1} \left[F'(\boldsymbol{x}^k)\boldsymbol{d}^k + F(\boldsymbol{x}^k) \right] \right) - \boldsymbol{x}^*.$$

From this and (30), taking into account (28) and (29), we have

$$\begin{aligned}
\|\mathscr{P}(\boldsymbol{x}^k + \boldsymbol{d}^k) - \boldsymbol{x}^*\| &= \|\mathcal{P}\left(\boldsymbol{x}^k - F'(\boldsymbol{x}^k)^{-1} F(\boldsymbol{x}^k) + F'(\boldsymbol{x}^k)^{-1} \left[F'(\boldsymbol{x}^k)\boldsymbol{d}^k + F(\boldsymbol{x}^k) \right] \right) - \boldsymbol{x}^*\| \\
&\leqslant \left\| F'(\boldsymbol{x}^k)^{-1} \left(F'(\boldsymbol{x}^k)\boldsymbol{e}^k - F(\boldsymbol{x}^k) + F'(\boldsymbol{x}^k)\boldsymbol{d}^k + F(\boldsymbol{x}^k) \right) \right\| \\
&\leqslant C \left[\left\| F(\boldsymbol{x}^k) - F(\boldsymbol{x}^*) - F'(\boldsymbol{x}^k)\boldsymbol{e}^k \right\| + \left\| F'(\boldsymbol{x}^k)\boldsymbol{d}^k + F(\boldsymbol{x}^k) \right\| \right] \\
&\leqslant C \left(\left\| F(\boldsymbol{x}^k) - F(\boldsymbol{x}^*) - F'(\boldsymbol{x}^k)\boldsymbol{e}^k \right\| + \eta_k \left\| F(\boldsymbol{x}^k) \right\| \right) \\
&\leqslant C \left(L\eta_k \left\| \boldsymbol{e}^k \right\| + o\left(\left\| \boldsymbol{e}^k \right\| \right) \right) \\
&= C \left(L\eta_k + o(1) \right) \left\| \boldsymbol{e}^k \right\|,
\end{aligned} \tag{31}$$

where the last inequality is due to (28) and (29). In addition,

$$\begin{aligned}
\|\boldsymbol{e}^k\| &= \left\| F'(\boldsymbol{x}^k)^{-1} \left[F'(\boldsymbol{x}^k)\boldsymbol{e}^k - F(\boldsymbol{x}^k) + F(\boldsymbol{x}^*) + F(\boldsymbol{x}^k) \right] \right\| \\
&\leqslant \left\| F'(\boldsymbol{x}^k)^{-1} \right\| \left(\left\| F'(\boldsymbol{x}^k)\boldsymbol{e}^k - F(\boldsymbol{x}^k) + F(\boldsymbol{x}^*) \right\| + \left\| F(\boldsymbol{x}^k) \right\| \right) \\
&\leqslant C \left(o\left(\left\| \boldsymbol{e}^k \right\| \right) + \left\| F(\boldsymbol{x}^k) \right\| \right).
\end{aligned} \tag{32}$$

Consequently,

$$\left\| \boldsymbol{e}^k \right\| \leqslant \frac{C}{1 - Co(1)} \left\| F(\boldsymbol{x}^k) \right\|. \tag{33}$$

DOI: 10.1002/nme

Using (31) and (29), we have

$$\begin{aligned}\left\|F(\mathscr{P}(\boldsymbol{x}^k+\boldsymbol{d}^k))\right\| &\leqslant L\left\|\mathcal{P}(\boldsymbol{x}^k+\boldsymbol{d}^k)-\boldsymbol{x}^*\right\| \\ &\leqslant C\left(L\eta_k\left\|\boldsymbol{e}^k\right\|+o\left(\left\|\boldsymbol{e}^k\right\|\right)\right) \\ &= C\left(L\eta_k+o(1)\right)\left\|\boldsymbol{e}^k\right\| \\ &\leqslant \frac{C^2(L\eta_k+o(1))}{1-Co(1)}\left\|F(\boldsymbol{x}^k)\right\|.\end{aligned} \tag{34}$$

This, together with (5), yields that statement (a) is valid if and only if

$$\frac{C^2(L\eta_k+o(1))}{1-Co(1)} \leqslant 1-t(1-\eta_k) \tag{35}$$

holds. By solving (35) with respect to η_k, and the fact that $t \in (0,1)$, we have

$$\begin{cases}\eta_k \in (0,1), t \in \left[\frac{C^2L}{1-Co(1)}, 1\right), & \text{if } \frac{C^2L}{1-Co(1)} < 1, \\ \eta_k \in \left(0, \frac{(1-t)(1-Co(1))-C^2o(1)}{C^2L-t(1-Co(1))}\right], t \in (0,1), & \text{if } \frac{C^2L}{1-Co(1)} \geqslant 1.\end{cases} \tag{36}$$

An intuitive alternative for (36) is

$$\begin{cases}\eta_k \in (0,1), t \in \left[C^2L, 1\right), & \text{if } C^2L < 1, \\ \eta_k \in \left(0, \frac{1-t}{C^2L-t}\right), t \in (0,1), & \text{if } C^2L \geqslant 1,\end{cases} \tag{37}$$

which is of the form (25). Therefore, if we take $\eta_{\max}$ and t from (37) (e.g., (25)), then statement (a) follows, that is, for large enough k, the method eventually accepts the projected Newton direction with $\lambda = 1$.

To prove assertion (b), we need to show that η_k in (31) satisfies

$$C(L\eta_k+o(1)) < 1. \tag{38}$$

Solving for η_k in (38), we obtain

$$\eta_k < \frac{1-Co(1)}{CL}. \tag{39}$$

This, combined with (36), yields that

$$\begin{cases}\eta_k \in \left(0, \min\left\{\frac{1-Co(1)}{CL}, 1\right\}\right), t \in \left[\frac{C^2L}{1-Co(1)}, 1\right), & \text{if } \frac{C^2L}{1-Co(1)} < 1, \\ \eta_k \in \left(0, \frac{1-Co(1)}{CL}\right) \cap \left(0, \frac{(1-t)(1-Co(1))-C^2o(1)}{C^2L-t(1-Co(1))}\right], t \in (0,1), & \text{if } \frac{C^2L}{1-Co(1)} \geqslant 1.\end{cases} \tag{40}$$

By (40), we obtain the following choices for $\eta_{\max}$ and t,

$$\eta_{\max} \in \begin{cases}\left(0, \min\left\{\frac{1}{CL}, 1\right\}\right), t \in \left[C^2L, 1\right), & \text{if } C^2L < 1, \\ \left(0, \min\left\{\frac{1}{CL}, \frac{1-t}{C^2L-t}\right\}\right), t \in (0,1), & \text{if } C^2L \geqslant 1.\end{cases} \tag{41}$$

This is the expression of (26), so we conclude the assertion (b).

Finally, if $\eta_k \to 0$, then (31) yields

$$\left\|\boldsymbol{e}^{k+1}\right\| = o\left(\left\|\boldsymbol{e}^k\right\|\right). \tag{42}$$

Consequently,

$$\begin{aligned}\left\| F(\mathscr{P}(\boldsymbol{x}^k + \boldsymbol{d}^k))\right\| &= \left\| F(\mathcal{P}(\boldsymbol{x}^k + \boldsymbol{d}^k)) - F(\boldsymbol{x}^*)\right\| \\ &= O\left(\left\|\mathcal{P}(\boldsymbol{x}^k + \boldsymbol{d}^k) - \boldsymbol{x}^*\right\|\right) \\ &= o\left(\left\|\boldsymbol{e}^k\right\|\right) = o\left(\left\|F(\boldsymbol{x}^k)\right\|\right).\end{aligned} \tag{43}$$

This establishes statement (c). □

Remark 6
We note that the choices for $\{\eta_k\}$ in Theorem 5 extend the ones in [8, 15–18, 20], in particular, for the case of Q-linear convergence theory.

3. NUMERICAL TESTS

As illustrated in Section 2, there is no theoretical guarantee of success for calculating the next iterative point via a projected Newton direction in the case in which the current one is far from the solution. To attain an intuitive understanding for this, we consider a two-dimensional example.

Example 7
Solve the following constrained problem for $\boldsymbol{x} = (x_1, x_2)^\top \in \Omega = (-\infty, 1] \times (-\infty, 1]$:

$$\begin{cases} x_1^2 - x_2 - 2 = 0, \\ x_1 - x_2 = 0. \end{cases} \tag{44}$$

The unique solution for this problem on Ω is $\boldsymbol{x}^* = (-1, -1)^\top$. The Jacobian $F'(\boldsymbol{x}) = \begin{pmatrix} 2x_1 & -1 \\ 1 & -1 \end{pmatrix}$. The gradient of its merit function $\Theta(x)$ is

$$\nabla\Theta(\boldsymbol{x}) = \left(2x_1(x_1^2 - x_2 - 2) + x_1 - x_2, -(x_1^2 - x_2 - 2) - (x_1 - x_2)\right)^\top. \tag{45}$$

We take an initial iteration vector $\boldsymbol{x}^0 = \left(1, \frac{1}{2}\right)^\top$. Then it follows from Algorithm 1 that a particular instance of Newton directions at $\boldsymbol{x}^0$ is $\boldsymbol{d}^0 = \left(2, \frac{5}{2}\right)^\top$ as $\eta_0 = 0$ in Algorithm 1. Notice that

$$\nabla\Theta(\boldsymbol{x}^0)^\top \boldsymbol{d}^0 = \left(-\frac{5}{2}, 1\right) \cdot \left(2, \frac{5}{2}\right)^\top = -\frac{5}{2} < 0. \tag{46}$$

Thus, Newton direction $\boldsymbol{d}^0$ is a good candidate for descent directions in the unconstrained case for (44). However, the projected Newton direction $\mathscr{P}(\boldsymbol{x}^0 + \lambda\boldsymbol{d}^0) - \boldsymbol{x}^0$ is not descent for problem (44) on Ω, because

$$\begin{aligned}\mathscr{P}(\boldsymbol{x}^0 + \lambda\boldsymbol{d}^0) - \boldsymbol{x}^0 &= \left(\min\{1 + 2\lambda, 1\}, \min\left\{1, \frac{1}{2} + \frac{5\lambda}{2}\right\}\right)^\top - \left(1, \frac{1}{2}\right)^\top \\ &= \left(0, \min\left\{\frac{1}{2}, \frac{5\lambda}{2}\right\}\right)^\top,\end{aligned} \tag{47}$$

for any $\lambda \in (0, 1]$, and

$$\begin{aligned}\nabla\Theta(\boldsymbol{x}^0)^\top(\mathscr{P}(\boldsymbol{x}^0 + \lambda\boldsymbol{d}^0) - \boldsymbol{x}^0) &= \left(-\frac{5}{2}, 1\right) \cdot \left(0, \min\left\{\frac{1}{2}, \frac{5\lambda}{2}\right\}\right)^\top \\ &= \min\left\{\frac{1}{2}, \frac{5\lambda}{2}\right\} \geqslant 0.\end{aligned} \tag{48}$$

DOI: 10.1002/nme

In contrast, the projected gradient direction $\mathscr{P}(\boldsymbol{x}^0 - \lambda\nabla\Theta(\boldsymbol{x}^0)) - \boldsymbol{x}^0$ is descent. Indeed, for any $\lambda \in (0, 1]$, we have

$$\begin{aligned}\mathscr{P}(\boldsymbol{x}^0 - \lambda\nabla\Theta(\boldsymbol{x}^0)) - \boldsymbol{x}^0 &= \left(\min\left\{1 + \frac{5}{2}\lambda, 1\right\}, \min\left\{1, \frac{1}{2} - \lambda\right\}\right)^\top - \left(1, \frac{1}{2}\right)^\top \\ &= (0, -\lambda)^\top,\end{aligned} \tag{49}$$

and

$$\nabla\Theta(\boldsymbol{x}^0)^\top(\mathscr{P}(\boldsymbol{x}^0 + \lambda\boldsymbol{d}^0) - \boldsymbol{x}^0) = \left(-\frac{5}{2}, 1\right)\cdot(0, -\lambda)^\top = -\lambda < 0. \tag{50}$$

Next, example shows that our feasible projected Newton–Krylov method, ithat is, Algorithm 1, can converge to a solution when a projected Newton direction fails to be a direction of descent. Therefore, Algorithm 1 including projected gradient directions is a significant complement for the projected Newton–Krylov algorithm in [1] from a computational point of view.

Example 8

Consider a system of nonlinear equations for $\boldsymbol{x} = (x_1, \ldots, x_n)^\top$ with $\Omega = \{\boldsymbol{x} \in \mathbb{R}^n \mid x_1 \in [0.8, 2], x_i \in [0.5, 2], 2 \leqslant i \leqslant n\}$.

$$\begin{cases} x_1^2 - 1 = 0, \\ x_1 - x_2^3 = 0, \\ x_2 - x_3^3 = 0, \\ \quad\vdots \\ x_{n-2} - x_{n-1}^3 = 0, \\ x_{n-1} - x_n = 0. \end{cases} \tag{51}$$

The solution for the system of nonlinear equations on Ω is $\boldsymbol{x}^* = (1, \ldots, 1)^\top$.

We test Algorithm 1 with a standard modified Gram-Schmidt GMRES implementation [21]. We use the zero vector to be the initial approximate solution for (4). The termination tolerance rule for

Table I. Output of Algorithm 1 for constrained problem (51) with dimension $n = 100$.

Iterates	λ	$\|F(\boldsymbol{x})\|$	Search direction
1	1	3.4873	PN
2	0.2500	3.4840	PN
3	0.1250	3.4813	PN
4	0.1250	3.4796	PN
5	0.6400	3.4779	PG
6	0.5000	3.8144	PN
7	1	3.6715	PN
8	1	3.6174	PN
9	0.6400	3.6087	PG
10	0.5000	4.1736	PN
11	1	3.7805	PN
12	1	3.7395	PN
13	0.6400	3.7388	PG
14	0.5000	4.9133	PN
15	1	3.8563	PN
16	0.0039	3.5496	PN
17	0.1250	2.3928	PN
18	1	0.5615	PN
19	1	0.1172	PN
20	1	0.0037	PN
21	1	2.6134e-06	PN
22	1	1.1652e-12	PN
23	1	3.8432e-13	PN

the nonlinear iterations is $\|F(\boldsymbol{x}^k)\| \leqslant 10^{-12}$. GMRES iterations terminate when (4) is satisfied with the rule of forcing term η_k proposed in [16] and $\eta_{\max} = 0.9$. For line search technique used in (5) and (6), we take $t = \sigma = 10^{-4}$, $m_{\max} = 20$, $\lambda_0 = 0.5$ in (5), and $\lambda_0 = 0.8$ in (6). In addition, both maximum allowable number of nonlinear iterations and maximum allowable number of GMRES iterations per nonlinear iteration are 100.

We first run our algorithm for constrained problem (51) with $n = 100$, by taking the initial value of nonlinear iterations $\boldsymbol{x}^0$ as $\boldsymbol{x}^0(1:20) = 0.9$ and $\boldsymbol{x}^0(21:100) = 0.5$. Table I shows details of the iterations, that is, step size λ, residual norm $\|F(\boldsymbol{x})\|$, and search direction. In particular, we denote a projected Newton direction and a projected gradient direction by PN and PG, respectively, for the search direction item.

From Table I, we can see that Algorithm 1 enjoys not only a global convergence but also a rapid local superlinear convergence.

We next test Algorithm 1 for the constrained problem (51) with $n = 10^5$. We use the same parameters as mentioned earlier, except for the initial value of nonlinear iterations. In particular, we choose $\boldsymbol{x}^0(1:70000) = 0.9$, and $\boldsymbol{x}^0(70001:100000) = 0.5$. Table II gives details of the partial iterations, including step size λ, residual norm $\|F(\boldsymbol{x})\|$, and search direction. The complete residual norm (i.e., $\|F(\boldsymbol{x})\|$) history is shown in Figure 1.

Table II and Figure 1 illustrate that Algorithm 1 is capable of solving large-scale constrained nonlinear problems with global and local superlinear convergence properties.

Table II. Output of Algorithm 1 for constrained problem (51) with dimension $n = 10^5$.

Iterates	λ	$\|F(\boldsymbol{x})\|$	Search direction
1	1	79.1577	PN
2	1	66.1661	PN
3	1	65.1058	PN
4	0.0625	65.1019	PN
5	0.6400	65.0966	PG
6	0.5000	65.5796	PN
7	0.5120	65.5297	PG
8	0.8000	66.6279	PG
9	0.5000	69.0157	PN
10	1	68.0353	PN
11	1	65.8934	PG
12	0.5000	69.1636	PN
13	0.1250	69.1366	PN
14	1	66.5676	PN
15	1	65.0184	PG
⋮	⋮	⋮	⋮
62	0.5000	66.2263	PN
63	0.6250	66.1883	PN
64	0.5120	66.1252	PG
65	0.5000	69.7062	PN
66	0.2500	69.5956	PN
67	0.5120	69.5064	PG
68	0.5000	79.7120	PN
69	1	68.7289	PN
70	0.2500	26.7161	PN
71	1	6.4583	PN
72	1	0.7691	PN
73	1	0.0661	PN
74	1	0.0014	PN
75	1	8.0587e-07	PN
76	1	2.6112e-13	PN

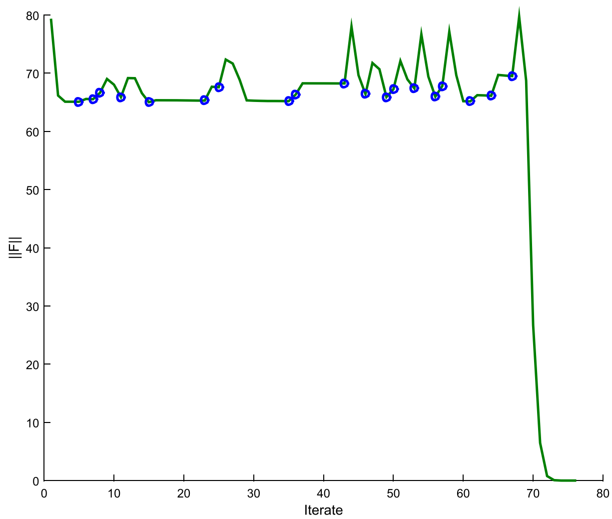

Figure 1. Numerical solution of constrained problem (51) with dimension $n = 10^5$: residual norm ($\| F(\boldsymbol{x}) \|$) at intermediate iterates (solid lines) and used projected gradient direction (circles).

4. SUMMARY AND CONCLUSIONS

This paper developed a new feasible projected Newton–Krylov algorithm for solving constrained system of nonlinear equations. This algorithm can be used to solve very large constrained systems of nonlinear equations. A typical example is a large diffusion reaction system with up to 50 chemical reactions, resulting in a constrained system of nonlinear equations with 10^9 unknowns.

A theoretical analysis is given to analyze the global convergence of the feasible projected Newton-Krylov algorithm. In particular, based on a simple but effective switching strategy between projected Newton directions and projected gradient directions, the feasible projected Newton–Krylov algorithm always ensures its search directions of descent and can converge to a solution when a projected Newton direction is unavailable or fails to be a descent direction. Also the rate of convergence (linear, superlinear) is investigated.

Finally, some examples are given, which show that the new feasible projected Newton–Krylov algorithm converges to a correct solution, whereas the classical projected Newton–Krylov algorithm does not converge. From these experiments, it also follows that the projected Newton–Krylov converges quadratically when the iterates are close to the exact solution.

REFERENCES

1. van Veldhuizen S, Vuik C, Kleijn CR. On projected Newton–Krylov solvers for instationary laminar reacting gas flows. *Journal of Computational Physics* 2010; **229**:1724–1738.
2. Brown PN, Saad Y. Hybrid Krylov methods for nonlinear systems of equations. *SIAM Journal on Scientific and Statistical Computing* 1990; **11**:450–481.
3. Bertsekas DP. *Nonlinear Programming*. Athena Scientific: Belmont MA, 1995.
4. Calamai PH, Moré JJ. Projected gradient methods for linearly constrained problems. *Mathematical Programming* 1987; **39**:93–116.
5. Gafni EH, Bertsekas DP. Convergence of a gradient projection method, Massachusetts Institute of Technology, Laboratory for Information and Decision Systems Report LIDS-P-1201, Cambridge, Massachusetts, 1982.
6. Gafni EH, Bertsekas DP. Two-metric projection methods for constrained optimization. *SIAM Journal on Control and Optimization* 1984; **22**:936–964.
7. Knoll DA, Keyes DE. Jacobian-free Newton–Krylov methods: a survey of approaches and applications. *Journal of Computational Physics* 2004; **193**:357–397.
8. Eisenstat SC, Walker HF. Globally convergent inexact Newton methods. *SIAM Journal of Optimization* 1994; **4**: 393–422.
9. Chen J, Qi L. Pseudotransient continuation for solving systems of nonsmooth equations with inequality constraints. *Journal of Optimization Theory and Applications* 2010; **147**:223–242.

10. Gould NIM, Leyffer S, Toint PL. A multidimensional filter algorithm for nonlinear equations and nonlinear least-squares. *SIAM Journal of Optimization* 2004; **15**:17–38.
11. Gould NIM, Toint PL. FILTRANE, a Fortran 95 filter-trust-region package for solving nonlinear least-squares and nonlinear feasibility problems. *ACM Transactions on Mathematical Software* 2007; **33**(1, Article 3):23.
12. Kanzow C, Yamashita N, Fukushima M. Levenberg–Marquardt methods for constrained non-linear equations with strong local convergence properties. *Journal of Computational and Applied Mathematics* 2004; **172**:375–397.
13. Ulbrich M. Nonmonotone trust-region method for bound-constrained semismooth equations with applications to nonlinear mixed complementarity problem. *SIAM Journal on Optimization* 2001; **11**:889–917.
14. Wang T, Monteiro RDC, Pang JS. An interior point potential reduction method for constrained equations. *Math. Program* 1996; **74**:159–195.
15. Dembo RS, Eisenstat SC, Steihaug T. Inexact Newton methods. *SIAM Journal on Numerical Analysis* 1982; **19**: 400–408.
16. Eisenstat SC, Walker HF. Choosing the forcing terms in an inexact Newton method. *SIAM Journal on Scientific Computing* 1996; **17**:16–32.
17. Idema R, Lahaye DJP, Vuik C. On the convergence of inexact Newton methods, Delft University of Technology, Delft Institute of Applied Mathematics, 2011. Report 11-14.
18. Idema R, Lahaye D. *Computational Methods in Power System Analysis*, Series: Atlantis Studies in Scientific Computing in Electromagnetics, vol. 1. Atlantis Press: Amsterdam, 2014.
19. Ortega JM, Rheinboldt WC. *Iterative Solution of Nonlinear Equations in Several Variables*. Academic Press: New York, 1970.
20. Chen J, Qi L. Globally and superlinearly convergent inexact Newton–Krylov algorithms for solving nonsmooth equations. *Numerical Linear Algebra with Applications* 2010; **17**:155–174.
21. Saad Y, Schultz MH. GMRES: a generalized minimal residual method for solving nonsymmetric linear systems. *SIAM Journal on Scientific and Statistical Computing* 1986; **7**:856–869.

DOI: 10.1002/nme