Transformed Newton's method with a fixed-point iteration for highly nonlinear problems in structural mechanics

*Ngoc M. La¹, †Cuong T. Nguyen², †Minh N. Dinh²

¹Vietnamese German University, Vietnam. ²School of Science and Technology, RMIT University, Vietnam.

*Presenting author: <u>lmngocdhsp@gmail.com</u> †Corresponding authors: <u>cuong.nguyentan@rmit.edu.vn</u>, <u>minh.dinh4@rmit.edu.vn</u>

Abstract

In this paper, a nonlinear solver combining fixed-point iteration and transformed Newton's method is first proposed. The transformed Newton's method was recently introduced to decrease the degree of nonlinearity of problems in solid mechanics. The key contribution behind this work is to modify the starting point of each iteration of the transformed method. Specifically, the transformed method gets started with the previous converged solution while the proposed solver starts at an initial guess theoretically proved to be close to the converged root of the current step. The advantage of the proposed nonlinear solver lies in the simple implementation and the significant reduction in number of iterations compared with the purely transformed Newton's method. Numerical results are presented to show the accuracy and efficiency of the proposed solver in dealing with highly nonlinear problems in structural mechanics.

Keywords: Nonlinear elasticity, Newton's method, fixed-point iteration.

1 Introduction

Nonlinear behavior of solids takes two typical forms: material and geometric nonlinearity. The former occurs when the stress is not linearly proportional to the strain, whereas the latter is important when changes in geometry, however large or small, have a significant effect on the response of structures [1]. Modelling and simulating nonlinear structures require robust solvers for solving the obtained nonlinear system of equations. A well-known and widely used iterative algorithm is Newton's method. The basic idea of Newton's method is to linearize the governing equations for obtaining the solution. Specifically, in each force increment step a successive equation is established to compute iteratively the next estimate closer to the real root. Highly nonlinear problems can lead to slow convergence which results in expensive computational cost.

In biomechanics, the common characteristic of many of the proposed constitutive laws is the exponential relation between stress and strain [2]. The exponential feature drastically increases the level of nonlinearity of problems. Recently, Yue Mei et al. [3] proposed a transform technique toward reducing the nonlinear degree to improve the performance of Newton's method. In particular, Newton's method is modified by applying a transformation before linearization. The transformed problem possesses significantly reduced nonlinearity, and thus convergence properties can be improved.

It is also well-known that the convergence properties of Newton's method depend heavily on the initial guess, poor choices often lead to slow convergence or divergence and it is quite time consuming. The main idea of this study is to develop a technique that leads to a reduction in

nonlinearity and alleviating the limitation of Newton's method in choosing the initial guess. The fixed-point iteration and its corresponding natural Newton's method [4] have been used to improve the initial guess and increase the order of convergence. The mathematical formulation of the proposed approach is introduced in sections 2 and 3. We then illustrate the application of our proposed combination to numerical examples about 1DOF and 2DOF truss systems in section 4. We proceed to assess the performance of the new formulation and show the improved convergence property compared with Newton's method and transformed Newton's method.

2 Fixed point iteration

2.1 Newton's method

Suppose that the nonlinear function f(x) is continuous and there exists its first derivative $f'(x) \neq 0$ for all $x \in (x^* - \delta, x^* + \delta)$, where $f(x^*) = 0$.

Let $x_0 \in (x^* - \delta, x^* + \delta)$ be an initial guess and $|x^* - x_0|$ is sufficiently "small". The function f(x) is evaluated at x^* by expanding in Taylor's series about a point up to second order as follows

$$f(x^{*}) = f(x_{0}) + (x^{*} - x_{0})f'(x_{0}) + \frac{(x^{*} - x_{0})^{2}}{2}f''(\xi(x^{*})), \qquad (1)$$

where $\xi(x^*)$ lies between x^* and x_0 . Since $f(x^*) = 0$, Eq. (1) leads to

$$0 = f(x_0) + (x^* - x_0) f'(x_0) + \frac{(x^* - x_0)^2}{2} f'(\xi(x^*)).$$
⁽²⁾

Newton's method is derived by assuming that $|x^* - x_0|$ is small, thus the term involving $(x^* - x_0)^2$ is much smaller, so

$$0 \approx f(x_0) + (x^* - x_0) f'(x_0).$$

Slightly rearranging this equation leads to $x^* \approx x_0 - \frac{f(x_0)}{f(x_0)} \equiv x_1$. By applying this process

iteratively, we obtain a sequence $\{x_n\}_{n=0}^{\infty}$ which is given by

$$x_{n+1} = x_n - \frac{f(x_n)}{f(x_n)}$$
(3)

in each iteration.

2.2 Iteration function

We would like to find $x = x^*$ such that $f(x^*) = 0$ for a given differentiable function $f: K \to K(K = \mathbb{R} \text{ or } \mathbb{C})$. In order to solve this problem, starting with an initial guess to the solution $x_n = x_0$ the guess is iteratively updated using $x_{n+1} = \Phi(x_n)$, n = 0, 1, 2, ... where the

iteration function $\Phi(x)$ depends on f(x). It is required that $x_n \to x^*$ as $n \to \infty$ for the numerical scheme to be converged to the true solution.

2.3 Choosing the initial guess

Following theorem 2.1 in [4], let $\Phi(x)$ is an iteration function of f(x), $\Phi^{(1)}(x)$ denotes its first derivative and x_0 is an initial guess. If $\|\Phi^{(1)}(x^*)\| < 1$, then there exists a neighborhood of x^* such that for any x_0 in that neighborhood the sequence converges to x^* .

Convergence analysis:

From the proof for theorem 2.1 in [4], by continuity, there is an interval $I_{\rho}(x^*) = (x^* - \rho, x^* + \rho)$

such that
$$\left\| \Phi^{(1)}(x) \right\| \le \frac{1 + \left\| \Phi^{(1)}(x^*) \right\|}{2} = L < 1$$
. Then, if $x_n \in I_{\rho}(x^*)$, we have
 $\left\| x_{n+1} - x^* \right\| \le L \left\| x_n - x^* \right\| \le \left\| x_n - x^* \right\| \le \rho$ (4)

and $x_{n+1} \in I_{\rho}(x^*)$. Moreover,

$$\|x_n - x^*\| \le L^n \|x_0 - x^*\|,$$
(5)

and the sequence $x_{n+1} = \Phi(x_n)$ converges to x^* as $n \to \infty$ because $0 \le L < 1$.

Remark: We assume that $\mathbf{A} \in \mathbb{R}^{n \times n}$ and define the spectral radius of \mathbf{A} by $\rho(\mathbf{A}) \coloneqq \max \{ |\lambda| : \lambda \in \mathbb{C} \text{ is an eigenvalue of } \mathbf{A} \}.$

Then every subordinate matrix norm on $\mathbb{R}^{n \times n}$ satisfies the inequality $\rho(\mathbf{A}) \leq ||\mathbf{A}||$. That leads to $||\mathbf{A}|| < 1$ if and only if $\rho(\mathbf{A}) < 1$. Thus, the main condition of the previous theorem could also be equivalently reformulated as $\rho(\Phi^{(1)}) < 1$. When we extend to *vector* nonlinear equations, $\Phi^{(1)}(\mathbf{x})$ is the Jacobian matrix of $\Phi(x)$ at x,. The norms are defined as

$$\|.\|_{\infty} = \text{row sum norm} \qquad \|\mathbf{M}\|_{\infty} \coloneqq \max_{i=1,\dots,m} \sum_{j=1}^{n} |M_{ij}|$$
(6)

$$\|\mathbf{M}\|_{l} = \text{column sum norm} \qquad \|\mathbf{M}\|_{l} \coloneqq \max_{j=1,\dots,n} \sum_{i=1}^{m} |M_{ij}|$$
(7)

Application:

Newton's method for finding roots of a given function f(x) is Eq. (3)

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}.$$

By choosing $\Phi(x_n) = x_n - \frac{f(x_n)}{f(x_n)}$ is an iteration function, we can rewrite the Newton iteration as the fixed-point iteration: $x_{n+1} = \Phi(x_n)$, then

$$\Phi^{(1)}(x_n) = \frac{f(x_n)f''(x_n)}{f^{'2}(x_n)}.$$
(8)

3 Transformed Newton with fixed-point iteration method

3.1 Degree of nonlinearity

In this section, we summarize the basic idea behind the transformed Newton method presented in [3]. The degree of nonlinearity at the current point x_n is defined as $N(\zeta, x_n) \coloneqq \sup_{\zeta \in (x_n, x^*)} \left| \frac{f''(\zeta)}{2f'(x_n)} \right|$ for $\zeta \in [x_n, x^*]$. We start with a simple exponential function $f(x) \colon Ae^{Bx} = H$. The standard formulation reads:

$$N_{\text{standard}} = \sup_{\zeta \in (x_n, x)} \left| B e^{B(\zeta - x_n)} \right| = B e^{B\Delta x}.$$
(9)

It shows clearly that the error in the Newton's method will rise as when increasing Δx . A more practical model of force–displacement relation is $f(x): A(e^{Bx}-1) = H$, using the transformation $\log[A(e^{Bx}-1)] = \log[H]$, we obtain

$$N_{\text{transform}} = \sup_{\zeta \in (x_n, x)} \left| \frac{-\left(\frac{1}{f(\zeta)} ABe^{B\zeta}\right)^2 + \frac{1}{f(\zeta)} AB^2 e^{B\zeta}}{\frac{1}{f(x_n)} ABe^{Bx_n}} \right| = \frac{B}{e^{Bx_n} - 1}.$$
 (10)

It is worth to note that the nonlinearity in the log formulation is non-zero but does not depend on Δx . It only depends on the initial guess x_n and reduces when increasing x_n . Then, the ideal scenario to apply the transformed method occurs when its degree of nonlinearity is smaller than the one produced by the standard method, i.e.

$$N_{\text{transform}} < N_{\text{standard}} \Longrightarrow \frac{B}{e^{Bx_n} - 1} < \frac{Be^{Bx}}{e^{Bx_n}}.$$
(11)

As can be seen from Eq. (11), when Bx_n is extremely small the standard method is expected to be better than the transform method.

3.2 Transformed Newton's method

In this section, we briefly go through the important steps in the procedure using the transformed technique proposed by Yue Mei et. al. in [3]. Equilibrium equations are established with respect

to the current position by assembling the typical internal forces T_i and the external forces F_i at all nodes (i = 1, 2, ..., N), the residual or out of balance nodal force R_i as the balance between the internal and the external forces as

$$R_i(x) = T_i(x) - F_i(x) = 0 \quad \forall i = 1,..., N.$$
 (12)

We utilize a transformed equation to solve the standard equation Eq. (12)

$$\mathcal{T}(T_i(x)) = \mathcal{T}(F_i(x)) \qquad \forall i = 1, ..., N$$
(13)

for a pre-determined bijective transformation $\mathcal{T} : \mathbb{R} \to \mathbb{R}$.

Our aim is to determine a simple transformation that reduces the nonlinearity. Many of the constitutive models include an exponential function, which is the primary source of nonlinearity. Thus, we suppose a highly-simplified form $\sigma \sim \exp(\lambda)$ which could be reduced the nonlinearity by taking a logarithm, i.e., $\mathcal{T} \equiv \log$. Using finite element discretization, we write the linearized system of equations as

$$\sum_{j} K_{ij} \Delta x_{j} = \overline{R}_{i} \left(x_{n} \right), \tag{14}$$

where the modified residual

$$\overline{R}_{i}(x_{n}) = \begin{cases} T_{i}(x_{n})\log\left(\frac{F_{i}(x_{n})}{T_{i}(x_{n})}\right) & \text{if condition (16) is satisfied} \\ F_{i}(x_{n}) - T_{i}(x_{n}) & \text{otherwise} \end{cases}$$
(15)

and with tolerance TOL, the transformed condition is:

$$|F_i(x_n)| > TOL, |T_i(x_n)| > TOL, \text{ and } \frac{F_i(x_n)}{T_i(x_n)} > 0.$$
 (16)

3.3 Transformed Newton method enhanced by fixed-point iteration

In this section, we present algorithms in detail for applying transformed Newton method approach with fixed-point iteration. For problems of multi degree of freedom (MDOF), the fixed-point iteration requires computing the Jacobian matrix so its algorithm need to be presented separately.

3.3.1 Scalar nonlinear equations for problems of single degree of freedom (SDOF)

Algorithm: Transformed Newton method enhanced by fixed-point iteration for SDOF problems

Input: geometry, material properties, and solution parameters, x: displacement vector, and

f(x): internal force vector.

- Input A: the initial shear modulus

 B: dimensionless parameter
 L: initial length truss
 nincr: number of load increment
 fincr: force increment
 area: initial area
 E: Young modulus
 maxiteration: maximum number of fixed-point iteration
- 3: $TOL \leftarrow$ convergence tolerance
- 4: $x_0 \leftarrow \text{initial guess}$
- 5: Compute the tangent stiffness $K_t(x)$

6: **for** k = 1: nincr **do**

7: $F \leftarrow F + fincr$

8: **for** m = 1:maxiteration **do**

9:
$$r(x) \leftarrow f(x) - F$$
 (residual)
10: $N \leftarrow x - \frac{r(x)}{r(x)}$ (establish the iteration function)

11:
$$dN \leftarrow \frac{r(x)r'(x)}{\left[r'(x)\right]^2}$$
 (typically Eq.(8))

12: if
$$|dN(x = x_0)| < 1$$

- 13: break
- 14: end if

15:
$$x_0 \leftarrow N(x_0)$$

16: end for

17: $x \leftarrow x_0$

18:
$$K \leftarrow K_t(x_0)$$

19:
$$R \leftarrow R - fincr$$

20: while
$$(||R|| / ||F|| > tolerance)$$
 do

21: Solve
$$Ku = R$$

22:
$$x \leftarrow x + u$$

23:
$$T \leftarrow f(x), K \leftarrow K_t(x)$$

24: **if** $|F| > TOL, |T| > TOL$, and $F/T > 0$ **do**

 $R \leftarrow T * \log(F/T)$ 25: 26: else $R \leftarrow F - T$ 27: 28: end if 29: end while 30: $x_0 \leftarrow x$ 31: end for

3.3.2 Vector nonlinear equations for problems of multi degree of freedom (MDOF)

Algorithm 2: Transformed Newton method enhanced by fixed-point iteration for MDOF problems

Input: geometry, material properties, and solution parameters, $u = [u_1; u_2]$: displacement vector, and $f(u_1, u_2)$: internal force vector.

- 1: Input A: the initial shear modulus **B:** dimensionless parameter L: initial length truss nincr: number of load increment fincr: force increment area: initial area E: Young modulus
 - maxiteration: maximum number of fixed-point iteration
- 2: $F \leftarrow [0;0], R \leftarrow [0;0]$
- 3: $TOL \leftarrow$ convergence tolerance
- 4: $u_0 \leftarrow \text{initial guess}$
- 5: Compute the tangent stiffness matrix: $K_t(u_1, u_2)$

6: **for** k = 1: nincr **do**

$$I: \quad F \leftarrow F + funcr$$

8:
$$r(u_1, u_2) \leftarrow f(u_1, u_2) - F$$
 (residual)

 $N(u_1, u_2) \leftarrow [u_1; u_2] - \frac{r(u_1, u_2)}{K_t(u_1, u_2)}$ 10: $DN = jacobian(N, [u_1; u_2])$

 $A \leftarrow DN(\mathbf{u}_0)$ 12:

 $spectral \leftarrow \max(abs(eig(A)))$ 13:

16: end if

17:
$$u_0 \leftarrow N(u_0)$$

19: $u \leftarrow u_0$ $K \leftarrow Kt(u_0)$ 20; $R \leftarrow R - fincr$ 21: while (||R|| / ||F|| > tolerance) do 22: 23: Solve Kx = R24: $u \leftarrow u + x$ $T \leftarrow f(u), K \leftarrow Kt(u)$ 25: for i = 1:2 do 26: if $||F_i|| > TOL$, $||T_i|| > TOL$, and $F_i / T_i > 0$ do 27: $R_i \leftarrow T_i * \log(F_i / T_i)$ 28: 29: else 30: $R_i \leftarrow F_i - T_i$ end if 31: 32: end for 33: end while 34: $u_0 \leftarrow u$ 35: end for

4 Numerical examples

In this section, we consider two truss systems as depicted in Figure 1. The bar elements in these trusses are modelled by human tracheal cartilage with the elastic modulus E = 25 MPa [5], the cross-sectional A = 1 cm². For these bar elements, the difference between the cross-section area in the current configuration, A, and that in the original configuration, A_0 , is negligible. The highly nonlinear component comes from the spring attached at node 2. In particular, the spring represents for a bar made by aortic tissue, which is modelled using an isotropic Veronda-Westmann constitutive law [5][6], with the initial shear modulus A = 0.5 kPa. The aortic tissue bar is in uniaxial stretch and under incompressibility constraint, the first Piola-Kirchhoff stress along stretch direction can be expressed as

$$P(\lambda) = 2A\left(\lambda - \frac{1}{\lambda^2}\right)e^{B\left(\lambda^2 + \frac{2}{\lambda} - 3\right)} - A\left(1 - \frac{1}{\lambda^3}\right),$$

where the stretch $\lambda = l / L$, the initial length is L = 25 cm.



Figure 1. Truss systems: 1DOF (left) and 2DOF (right).

4.1 One degree of freedom problem

In case of 1DOF system as shown in Figure 1, applying the Crisfield truss-element method [1], we first get the reference configuration

$$\mathbf{X}^{e} = \begin{pmatrix} \mathbf{X}^{e1} \\ \mathbf{X}^{e2} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 4 & 3 \end{pmatrix}^{T},$$

and the element displacement vector is expressed as: $\boldsymbol{u}^{e} = \begin{pmatrix} u^{e_{1}} \\ u^{e_{2}} \end{pmatrix} = \boldsymbol{x}^{e} - \boldsymbol{X}^{e} = \begin{pmatrix} 0 & 0 & 0 \end{pmatrix}^{T}$. The

undeformed and deformed lengths are computed as

$$L^{2} = \mathbf{X}^{e} \cdot \mathbf{A} \cdot \mathbf{X}^{e} = 4^{2} + 3^{2} = 25,$$

$$l^{2} = \mathbf{x}^{e} \cdot \mathbf{A} \cdot \mathbf{x}^{e} = (4+0)^{2} + (3+v+0)^{2} = 25 + 6v + v^{2},$$

in which v is the vertical displacement at node 2. We proceed to compute the internal force vector

(a)

$$\boldsymbol{F}_{\text{int}}^{e}\left(\boldsymbol{u}^{e}\right) = \frac{EA}{2L^{3}}\left(l^{2} - L^{2}\right) \begin{pmatrix} a \\ b \\ -a \\ -b \end{pmatrix}, \text{ where } \begin{cases} a = X_{1}^{e1} + u_{1}^{e1} - X_{1}^{e2} - u_{1}^{e2} = -4 \\ b = X_{2}^{e1} + u_{2}^{e1} - X_{2}^{e2} - u_{2}^{e2} = -(3+v) \end{cases}$$

The internal force therefore is reduced to $F_{22}^e = (6v + v^2)(3 + v) = 18v + 9v^2 + v^3$. The stiffness matrix comprises of two parts, geometric and material ones as follows

$$\mathbf{K}^{e} = \mathbf{K}^{e}_{geo} + \mathbf{K}^{e}_{mat} = \frac{EA}{L^{3}} \left(\frac{\left(l^{2} - L^{2}\right)}{2} \begin{pmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{pmatrix} + \begin{pmatrix} a^{2} & ab & -a^{2} & -ab \\ \cdot & b^{2} & -ab & -b^{2} \\ \cdot & \cdot & a^{2} & ab \\ sym. & \cdot & \cdot & b^{2} \end{pmatrix} \right),$$

then $K_{22}^e = K_{geo_{22}}^e + K_{mat_{22}}^e = 18 + 18v + 3v^2$. The current force acting on the aortic tissue bar is calculated as $F_s = P(\lambda)S_0$, where the initial cross-section area $S_0 = 1 \text{ cm}^2$.



Figure 2. 1DOF ($B = 40, \Delta F = 20 N$): Equilibrium path (left) and No. of iterations (right).



Figure 3. 1DOF ($B = 60, \Delta F = 20 N$): Equilibrium path (left) and No. of iterations (right).



Figure 4. 1DOF ($B = 80, \Delta F = 20 N$): Equilibrium path (left) and No. of iterations (right).



Figure 6. 1DOF (B = 80): No. of iterations when $\Delta F = 30 N$ (left) and $\Delta F = 35 N$ (right).

In order to study the performance of transformed Newton's enhanced by fixed-point iteration when applied to highly nonlinear problems, we gradually increase the parameter B, the numerical results are shown in Figure 2-Figure 6. As can be seen from these graphs, all three methods lead to numerical results perfectly matching with the exact solutions. The implementation of Fixed-point Transform method to our scalar nonlinear equation brings us incredible improvements. Notably, the improvement of decreasing the nonlinearity using Fixed-point Transform method is even greater than the Transform method. It can also be noted that when B = 40 the Newton-Raphson method needs a number of iterations that is significantly higher than for Transform and Fixedpoint Transform. If we rise the degree of nonlinearity to B = 60 or B = 80, the numbers of iterations using the Newton's and Transform method increase accordingly, whereas the convergence of Fixed-point Transform remains nearly constant (around 35 or 36 iterations). On the other hand, another significant advantage of using the Fixed-point Transform method is that the number of iterations to converge is deeply smaller than for Newton's and better than Transform method when we increase the force increment ΔF from 20 to 35. In a nutshell, for the scalar nonlinear equation under consideration the enhancement of Transform method by Fixed-point iteration does not increase the computational cost in each force increment step.

4.2 Two degree of freedom problem

Again, following the Crisfield truss-element method, we proceed the same procedure as used in subsection 4.1 to obtain the stiffness matrix

$$\mathbf{K}^{e} = \mathbf{K}^{e}_{geo} + \mathbf{K}^{e}_{mat} = \begin{bmatrix} 5.1u_{1} + 4.89u_{1}^{2} + 9.78u_{2} + 1.63u_{2}^{2} + 63.5 & 9.78u_{1} + 3.26u_{1}u_{2} + 1.7u_{2} + 5.1 \\ 9.78u_{1} + 3.26u_{1}u_{2} + 1.7u_{2} + 5.1 & 1.7u_{1} + 1.63u_{1}^{2} + 29.34u_{2} + 4.89u_{2}^{2} + 29.34 \end{bmatrix}$$

Combining the internal forces inside of two bars and the soft tissue spring leads to the total internal force as follows

$$\boldsymbol{F}_{\text{int}} = \begin{bmatrix} 63.5u_1 + 2.55u_1^2 + 1.63u_1^3 + 9.78u_1u_2 + 1.63u_1u_2^2 + 5.1u_2 + 0.85u_2^2 \\ 5.1u_1 + 4.98u_1^2 + 1.7u_1u_2 + 1.63u_1^2u_2 + 29.34u_2 + 14.67u_2^2 + 1.63u_2^3 + F_s \end{bmatrix}$$



Figure 7. 2DOF ($B = 10, \Delta F = 20 N$): Equilibrium path (left) and No. of iterations (right).



Figure 8. 2DOF ($B = 30, \Delta F = 20 N$): Equilibrium path (left) and No. of iterations (right).



Figure 9. 2DOF ($B = 50, \Delta F = 20 N$): Equilibrium path (left) and No. of iterations (right).











Equilibrium path (left) and No. of iterations (right).

Both Transform and Fixed-point Transform methods work perfectly as shown in Figure 7-Figure 9, the results fit the exact equilibrium paths, the number of iterations to converge of Fixed-point Transform method is lower than those of Transform method. The extension of Fixed-point Transform method to vector nonlinear equations shows that the convergence improved significantly when increasing force increment to a certain high value, e.g. $\Delta F = 300$ N, whereas Transform method diverges (noted that: the horizontal line describes the number of iterations corresponding to external force remain constant which means that it *diverges*). In other words, the Fixed-point Transform method allows us to increase the permissible load step size (Figure 10-Figure 12). One drawback of Fixed-point Transform method is that it slightly increases the computational cost of each iteration since it needs the second derivative. However, the development of newer methods based on symbolic computation and automatic differentiation, this limitation is becoming less important.

5 Conclusion

Nonlinear solvers based on the classical Newton's method to find roots of equations are at the heart of computational science. The combination of fixed-point iteration and the transform Newton's method presented in this work, which results in improving the quality of the initial guess and decreasing the nonlinearity, provides an efficient technique to deal with highly nonlinear problems. This approach is simple in implementation and can be easily integrated into any nonlinear finite element solvers. Hence, it has the potential of attracting the interest of the community of scientific computing to fully explore its capacities in solving highly nonlinear problems with various materials and structures.

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