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A robust stress update algorithm for elastoplastic models without analytical

2 derivation of the consistent tangent operator and loading/unloading estimation

3

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4 Abstract

5 A robust and concise implicit stress integration algorithm of elastoplastic models is presented. It does not require the loading/unloading estimation and analytical derivation operation for the stress update. First, the elastoplastic stress 6 7 update problem is recast into an unconstrained minimization problem by utilizing the smooth function to bypass the 8 loading/unloading estimation. Then, the object problem is solved by the line search method instead of the Newton 9 method for better convergence. The consistent tangent operator is evaluated by the complex step derivative 10 approximation without the subtraction cancellation error, which provides the quadratic convergence rate of global iteration. The rationality of the numerical consistent tangent operator is validated by the one obtained by the analytical 11 12 derivation. A recently developed non-orthogonal elastoplastic (NEP) clay model is implemented using the new 13 algorithm. The algorithm is confirmed through comparing the numerical solution and the analytical one for a cavity 14 expansion problem. The algorithm performance is assessed based on a series of geotechnical boundary value problems. 15 It is found that the new algorithm is more robust than the one employed by ABAQUS. The source code of the model 16 implementation can be downloaded from https://github.com/zhouxin615. KEYWORDS: Stress update algorithm; Line search method; Complex step derivative approximation; Smooth 17 18 function; Consistent tangent operator; Constitutive model

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Nomenclature	
ς, σ	deviatoric stress tensor, stress tensor
<i>q</i> , <i>p</i>	generalized shear stress, hydrostatic pressure
$p_{\rm c}$	yield surface size
$\epsilon, \gamma, \varepsilon_v$	total and deviatoric strain tensors, total volume strain
$\boldsymbol{\epsilon}^{\mathrm{p}}, \boldsymbol{\gamma}^{\mathrm{p}}, \boldsymbol{\varepsilon}_{\mathrm{v}}^{\mathrm{p}}$	plastic strain tensor, deviatoric plastic strain tensor, plastic volume strain
V	Poisson's ratio
K, G, E	bulk, shear, and Young's moduli
D	elastic stiffness tensor
f	yield function
λ, κ	compression and swelling indexes in the <i>e</i> -ln <i>p</i> plane
e_{0}, e_{1}	initial void ratio and one at $p = 1$ kPa
C_{κ} , C_{p}	$c_{\kappa} = (1 + e_0)/\kappa$ and $c_{p} = (1 + e_0)/(\lambda - \kappa)$ for convenience in writing.
ΔΠ	vertical distance between the NCL and the CSL in the <i>e</i> -ln <i>p</i> plane
М	slope of the critical state line in triaxial compression conditions
Ν	shape parameter of the elliptical yield curve
μ	fractional order
1, I	second-order and fourth-order unit tensors
$\mathbf{I}^{\mathrm{vol}}$, $\mathbf{I}^{\mathrm{sym}}$	volumetric and symmetric parts of I
h	perturbation value
dø	plastic multiplier
Ψ	merit function
$c_{ m d}$, eta	dimensional parameter, smoothing parameter in the smoothing function
$ ho$, ς	parameters of line search method
α , d	size and direction of search step

23 1. INTRODUCTION

The stress update problem of elastoplastic models is an initial value problem of the ordinary differential equations (ODEs) constrained by inequalities. The ODEs are usually transformed into algebraic equations to solve based on the explicit^{1,2} or implicit³⁻⁶ integral schemes. The implicit algorithm requires the Jacobian matrix in the local stress update iteration, which can be difficult to derive, especially for sophisticated soil models. But it is still preferred because it preserves the quadratic convergence rate of global iteration⁷⁻¹⁰.

29 The most popular implicit stress updating algorithm may be the return-mapping algorithm where the operator splitting technique addresses the inequality constraints and the Newton method¹¹ solves the nonlinear equations¹². This 30 computational paradigm is also followed by the cutting plane algorithm¹³ and the semi-implicit algorithm¹⁴ and has 31 been used widely in the numerical implementation of advanced soil models^{15,16}. But it is found that the iterations may 32 33 not converge for the Newton method when the initial value is far from the final solution or the problem is highly nonlinear due to complex model formulations^{17,18}. The loading/unloading estimation of the operator splitting technique 34 35 also makes the stress update procedure more cumbersome. Therefore, attempts have been made to improve the 36 efficiency of the implicit stress integration method. For instance, one can use the smoothing function to replace the inequality constraints¹⁹⁻²³ or the penalty function²⁴ to bypass loading/unloading judgment. The nonlinear equations can 37 be solved by the homotopy method²⁵, the line search method^{18,19}, or the trust region method ¹⁹ instead of the Newton 38 method. These three methods can achieve better convergence. The line search method, however, is a more cost-39 effective manner from the perspective of conciseness. Compared with the Newton method, it only adds a one-40 dimensional nonlinear problem about the optimal step size in search, since the trust region method requires optimizing 41 42 the multidimensional search direction, and the homotopy method needs to solve homotopy equations to obtain a better 43 initial value. Some contributions worthy of attention in this field can be found in the literature^{18,26,21,27,28}, which initially 44 focused primarily on constitutive models for metal materials. Theoretically, these methods should also have great

45 potential in implementing advanced soil models with complex formulations and deserves further study.

In the implicit model implementation, the derivation operation is required to determine the Jacobian matrix and 46 the consistent tangent operator. The former is used for the solution of local nonlinear stress integral equations and the 47 48 latter is used for global equilibrium iterations. The analytical derivatives of constitutive equations can be obtained 49 easily for some simple cases, e.g., the Mises model, the Mohr-Coulomb model, and others. For elastoplastic soil models with highly nonlinear characteristics²⁹, however, the analytical derivation operation, especially for the 50 51 consistent tangent operator, has become an increasingly cumbersome and even impossible task. Numerical 52 differentiation may be preferred to analytical derivation because it avoids tedious algebraic work and is easy to 53 implement³⁰. There are three practical numerical differentiation methods: the finite difference method³⁰, the complex step derivative approximation (CSDA)³¹, and the Hyper-dual step derivative approximation (HDSDA)³². The essence 54 55 of these methods is to expand the object function on different types of number axes and truncate the higher-order term 56 of the Taylor series to obtain the desired derivative term. The calculation results of HDSDA are almost equivalent to 57 those of analytical derivation, but a lot of function overloading and operator overloading are required to define the 58 operation rules of the Hyper-dual number³³. For the finite difference method, there are two kinds of numerical errors, 59 namely the truncation error and the rounding error dominated by subtraction cancellation error. The former can be reduced effectively with a small perturbation value (i.e., differential step size), but the latter will increase with the 60 decrease of the perturbation value. It is often a prerequisite for the successful application of the finite difference method 61 to determine an optimal perturbation value³⁴. There is no subtraction cancellation error for the CSDA due to the 62 63 absence of subtraction operation. On the other hand, the operation rules of the complex number have been added to

64 mainstream programming languages. Therefore, the CSDA makes it possible for the concise and robust 65 implementation of constitutive models.

This study aims to propose a robust and concise stress update algorithm to reduce the complexity in the implicit 66 numerical implementation of advanced elastoplastic models and to improve its computational efficiency. The root of 67 complexity is that the implicit algorithm needs to calculate the Jacobian matrix of nonlinear equations and consistent 68 tangent stiffness, in which tedious derivative operations are required for complex elastoplastic models. Therefore, the 69 70 proposed algorithm uses the CSDA method with high precision to obtain numerical derivatives instead of analytical 71 derivatives. The loading/unloading estimation for the elastoplastic stress update problem is bypassed by using smooth 72 functions. On the other hand, the main reason for limiting the computational efficiency of implicit algorithms is that 73 the Newton method requires a small load step to ensure the convergence of the solution under strong nonlinear conditions. In the proposed algorithm, the line search strategy will be used to improve the computational efficiency of 74 75 the algorithm, in which a larger load increment step is allowed. This paper is organized as follows: Section 2 gives the 76 implicit integral scheme of the NEP clay model by the Backward Euler method. In Section 3, the complete stress 77 update procedure is given. Section 4 is devoted to the determination of consistent tangent operator from the analytical 78 and numerical perspectives, where different numerical schemes are discussed and compared. In Section 5, the 79 robustness and accuracy of model implementation are assessed and validated by a series of boundary problems.

80

2. NON-ORTHOGONAL ELASTOPLASTIC (NEP) CLAY MODEL

81 The elastoplastic models with the non-orthogonal flow rule have piqued an increasing interest in modelling the mechanical behaviour of geomaterials in recent years, in which some salient material properties (e.g., the dilatancy^{35,36}, 82 strain hardening/softening³⁷, and state-dependence³⁸) can be captured by the fractional derivative. A potential function 83 84 is not required because the direction of plastic flow is given by the fractional gradient of the yield function³⁹. Though these models show excellent predictive capability for different soils^{40,41}, no research has been done on the numerical

86 implementation. A NEP clay model established by Liang et al.³⁵ is employed for the algorithm validation because the

87 consistent tangent operator and Jacobian matrix of this model can be analytically derived due to its relative simplicity.

88 2.1 Brief review of the model concept

The NEP clay model is developed based on the modified Cam-clay (MCC) model⁴². The basic equations of both models are presented in Table 1. They have the same elastic law and hardening law. The elastic stiffness matrix is expressed as

92
$$\mathbf{D} = K\mathbf{1} \otimes \mathbf{1} + 2Kr\left(\mathbf{I} - \frac{1}{3}\mathbf{1} \otimes \mathbf{1}\right)$$
(1)

93 where **I** and **1** denote the fourth-order and second-order unit tensors, respectively. $r = 1.5(1-2\nu)/(1+\nu)$ and ν 94 is Poisson's ratio. The bulk modulus *K* depends on the hydrostatic pressure *p*:

95
$$K = c_{\kappa} p \tag{2}$$

96 where $c_{\kappa} = (1+e_0)/\kappa$, e_0 denotes the initial void ratio. The parameters κ and λ in Table 1 are the swelling and 97 compression indexes of soil in isotropic consolidation conditions, respectively. The calibration method for κ and λ is 98 presented in Section 2.2.

99 In the NEP clay model, the fractional gradient
$$\left(\frac{\partial^{\mu} f}{\partial p^{\mu}}\frac{\partial p}{\partial \mathbf{\sigma}} + \frac{\partial^{\mu} f}{\partial q^{\mu}}\frac{\partial q}{\partial \mathbf{\sigma}}\right)$$
 of the yield function f is used as the

100 plastic flow direction. q and μ represent the generalized shear stress and fractional order, respectively. In general,

101 the Riemann-Liouville fractional derivative operator is employed. $\frac{\partial^{\mu} f}{\partial p^{\mu}}$ and $\frac{\partial^{\mu} f}{\partial q^{\mu}}$ are expressed as follows:

102
$$\frac{\partial^{\mu} f}{\partial p^{\mu}} = \frac{q^2}{p^{\mu} N^2 \Gamma(1-\mu)} + \frac{2p^{2-\mu}}{\Gamma(3-\mu)} - \frac{p_c p^{1-\mu}}{\Gamma(2-\mu)}$$
(3)

103
$$\frac{\partial^{\mu} f}{\partial q^{\mu}} = \frac{2q^{2-\mu}}{N^{2}\Gamma(3-\mu)} + \frac{p(p-p_{c})}{q^{\mu}\Gamma(1-\mu)}$$
(4)

104 where $\Gamma(\cdot)$ is the gamma function, p_c is the yield surface size. More details can refer to the literature^{35,36,43}.

105 The NEP clay model uses a different yield function (See Table 1) in which the ratio of vertical and horizontal 106 axes of the elliptic yield curve at the meridian plane is defined by the parameter *N*. Based on the volume change 107 condition $d\varepsilon_v^p = 0$ at the critical state and Eq. (3), the relationship between parameters μ and *N* is obtained by:

$$N = M\sqrt{2-\mu} \tag{5}$$

109 where the parameter M = (q/p) is the critical state stress ratio in triaxial compression conditions. It should be 110 emphasized that the shape of the yield curve is controlled by the parameter *N*, however, in the NEP clay model, *N* is 111 not an independent material parameter and can be determined by μ and M (Eq. (5)). Therefore, for a given parameter 112 *M*, the change of μ value will cause the change of *N*, leading to the change of the shape of the elliptical yield curves, 113 as shown in Fig. 1 (a). From the perspective of model performance, the stiffness and dilatancy behaviour for different 114 clays can be captured by an appropriate μ value as shown in Fig. 1 (b).

115

Table 1 Basic evaluation equations of two models

Basic equations	MCC model	NEP clay model
Hooke's law	$d\boldsymbol{\sigma} = \mathbf{D}: \left(d\boldsymbol{\epsilon} - d\boldsymbol{\epsilon}^{p}\right)$	$d\boldsymbol{\sigma} = \mathbf{D}: \left(d\boldsymbol{\epsilon} - d\boldsymbol{\epsilon}^{p}\right)$
Hardening law	$\mathrm{d}p_{\mathrm{c}} = \frac{1+e_{0}}{\lambda-\kappa} p_{\mathrm{c}} \mathrm{d}\varepsilon_{\mathrm{v}}^{\mathrm{p}}$	$\mathrm{d}p_{\mathrm{c}} = \frac{1 + e_{\mathrm{0}}}{\lambda - \kappa} p_{\mathrm{c}} \mathrm{d}\mathcal{E}_{\mathrm{v}}^{\mathrm{p}}$
Flow rule	$\mathbf{d}\boldsymbol{\varepsilon}^{\mathrm{p}} = \mathbf{d}\boldsymbol{\phi} \left(\frac{\partial f}{\partial p} \frac{\partial p}{\partial \boldsymbol{\sigma}} + \frac{\partial f}{\partial q} \frac{\partial q}{\partial \boldsymbol{\sigma}} \right)$	$\mathbf{d}\boldsymbol{\varepsilon}^{\mathrm{P}} = \mathbf{d}\boldsymbol{\phi} \left(\frac{\partial^{\mu} f}{\partial p^{\mu}} \frac{\partial p}{\partial \boldsymbol{\sigma}} + \frac{\partial^{\mu} f}{\partial q^{\mu}} \frac{\partial q}{\partial \boldsymbol{\sigma}} \right)$
Yield function	$f = q^2 + M^2 \left(p^2 - p_{\rm c} p \right)$	$f = q^2 + N^2 \left(p^2 - p_{\rm c} p \right)$
Karush-Kuhn-Tucker conditions	$d\phi \ge 0, f \le 0, d\phi f = 0$	$\mathrm{d}\phi \geq 0, f \leq 0, \mathrm{d}\phi f = 0$
Model parameters	Μ, λ, κ, ν	$M, \mu, \lambda, \kappa, \nu$





Fig. 1 NEP clay model: (a) yield curves; (b) stress-strain curves.

118

2.2 Parameter calibration and model validation

119 It can be seen from Table 1 that the NEP clay model has 5 material parameters, i.e., M, μ , λ , κ and v, among which the calibration methods of parameters M, λ , κ and ν can refer to the MCC model. Only one more material 120 parameter μ is added for the NEP clay model. Although the literature³⁵ has provided the detailed parameter calibration 121 122 method of the NEP clay model, a brief review is necessary for the calibration method to facilitate the numerical 123 application of the NEP clay model. First, the parameter $M = 6\sin \varphi/(3 - \sin \varphi)$ can be determined by the internal 124 friction angle φ in triaxial compression conditions. In the isotropic consolidation compression test, the swelling index κ and compression index λ can be determined by the slopes of swelling line (SWL: $e = e_s - \kappa \ln p$) and normally 125 consolidated line (NCL: $e = e_N - \lambda \ln p$) in the *e*-ln*p* plane, as shown in Fig. 2 (a). For the parameter calibration of μ , 126 it is necessary to measure the vertical distance $\Delta\Pi$ between the critical state line (CSL) and the NCL in *e*-ln*p* space. 127 128 It can be seen from Fig. 2 that $\Delta \Pi$ is exactly equal to the plastic void ratio $\Delta e^{\rm p}$ caused by the triaxial compression 129 path A_0A_0' :

130
$$\Delta \Pi = \left(\lambda - \kappa\right) \ln \left(\frac{p_x}{p_0}\right) \tag{6}$$

131 where p_x/p_0 can be obtained by substituting stress point (p_0, Mp_0) into the yield function:

132
$$\frac{p_x}{p_0} = \frac{M^2}{N^2} + 1$$
 (7)

133 Substituting Eqs. (5) and (7) into Eq. (6), the parameter μ can be determined by:

134
$$\mu = 2 - \frac{1}{\exp\left(\frac{\Delta \Pi}{2}\right) - 1}$$
(8)





Fig. 2 Determination of parameter μ : (a) *e*-ln*p* plane; (b) *p*-*q* plane.

In what follows, the drained triaxial compression test of Fujinomori clay (F-clay) reported in literature⁴⁴ and the 136 undrained triaxial compression test of Boston blue clay (BB-clay) reported in literature⁴⁵ are used to demonstrate the 137 138 performance of NEP clay model. The material parameters are determined by the test data provided in the literature and the parameter calibration method mentioned above, as presented in Table 2. The test data of F-clay and the predicted 139 140 curves of NEP clay model ($\mu = 1.23$) are illustrated in Fig. 3 (a), in which the results predicted by the MCC model $(\mu = 1.0)$ are also presented. The prediction results from these two models finally reach the same stress ratio because 141 142 the M-value for the two models is the same. However, the NEP clay model better describes the stress-strain behaviours 143 of clay before the critical state, and reflects the deformation characteristics of soil with different stiffness by 144 introducing fractional order μ . Fig. 3 (b) shows the model predictions and test data under undrained conditions, where ε_a is the axial strain. Comparing with the MCC model, the NEP clay model can more reasonably capture the strength 145 and deformation characteristics of BB-clay under undrained conditions. The reason is that under undrained conditions, 146

the stress path predicted by the model is influenced by the pore pressure which is closely associated with the volume change of soil, as shown in Fig. 3 (c). The NEP clay model can more reasonably describe the dilatancy law of soil by selecting a suitable μ -value.

150

Table 2 Material parameters of the NEP clay model

Material parameters	$\lambda/(1+e_0)$	$\kappa/(1+e_0)$	v	М	μ
F-clay	0.0444	0.0047	0.3	1.36	1.23
BB-clay	0.0883	0.0173	0.1	1.35	1.47

151



Fig. 3 Model validation for: (a) F-clay; (b) stress-strain curve of BB-clay; (c) stress path of BB-clay.

153

154 **2.3 Stress integral equations of the model**

155 Table 1 presents the basic equations of the model defined in the form of the ODEs. In the model implementation,

- 156 the ODEs need to be discretized into the algebraic equations for the time interval $[t_n, t_{n+1}]$. Based on the Backward
- 157 Euler method, the control equations of NEP clay model are given by:

$$\begin{cases} \mathbf{\sigma}_{n+1} = \mathbf{\sigma}_{n} + \overline{\mathbf{D}} \mathbf{c} \Biggl[\Delta \mathbf{\varepsilon}_{n+1} - \Delta \phi_{n+1} \Biggl(\frac{\partial^{\mu} f_{n+1}}{\partial p_{n+1}^{\mu}} \frac{\partial p_{n+1}}{\partial \mathbf{\sigma}_{n+1}} + \frac{\partial^{\mu} f_{n+1}}{\partial q_{n+1}^{\mu}} \frac{\partial q_{n+1}}{\partial \mathbf{\sigma}_{n+1}} \Biggr) \Biggr] \\ p_{c,n+1} = p_{c,n} \exp(c_{p} \Delta \mathcal{E}_{v,n+1}^{p}) \\ \Delta \phi_{n+1} \ge 0, f_{n+1} \le 0, \Delta \phi_{n+1} f_{n+1} = 0 \end{cases}$$
(9)

159 where $c_p = (1 + e_0)/(\lambda - \kappa)$. $\overline{\mathbf{D}} = \mathbf{D}(\overline{K}, \overline{G})$ is the secant elastic stiffness tensor. The secant bulk modulus \overline{K} is:

160
$$\overline{K} = \frac{p_n}{\Delta \varepsilon_{v, n+1}^{\rm e}} \left[\exp\left(c_\kappa \Delta \varepsilon_{v, n+1}^{\rm e}\right) - 1 \right]$$
(10)

161 where $\Delta \varepsilon_{v, n+1}^{e}$ represents elastic volume strain increment and $\Delta \varepsilon_{v, n+1}^{e} = \Delta \varepsilon_{v, n+1} - \Delta \varepsilon_{v, n+1}^{p}$. Eq. (9) contains 8 equality 162 equations and 2 inequality constraints. The number of stress integral equations can be simplified to reduce the difficulty 163 of the solution. The stress tensor $\boldsymbol{\sigma}_{n+1}$ can be decomposed into its isotropic part and deviatoric part:

164
$$\sigma_{n+1} = p_{n+1} \mathbf{1} + \mathbf{s}_{n+1}$$
 (11)

165 where \mathbf{s}_{n+1} is the deviatoric stress tensor. p_{n+1} and \mathbf{s}_{n+1} can be expressed as follows:

166
$$p_{n+1} = \frac{1}{3}\boldsymbol{\sigma}_{n+1} : \mathbf{1} = p_n + \overline{K} \left(\Delta \varepsilon_{\mathbf{v}, n+1} - \Delta \varepsilon_{\mathbf{v}, n+1}^{\mathbf{p}} \right)$$
(12)

$$\mathbf{s}_{n+1} = \mathbf{s}_n + 2\overline{G}(\Delta \mathbf{\gamma}_{n+1} - \Delta \mathbf{\gamma}_{n+1}^{\mathrm{p}})$$
(13)

168 where $\overline{G} = r\overline{K}$ represents the secant shear modulus, $\Delta \gamma_{n+1}$ and $\Delta \gamma_{n+1}^{p}$ denote the total deviatoric strain increment

169 and its plastic part. $\Delta \varepsilon_{v, n+1}^{p}$ and $\Delta \gamma_{n+1}^{p}$ are expressed by:

170
$$\Delta \varepsilon_{\nu,n+1}^{p} = \Delta \varepsilon_{n+1}^{p} : \mathbf{1} = \Delta \phi_{n+1} \left[\frac{q_{n+1}^{2}}{p_{n+1}^{\mu} N^{2} \Gamma(1-\mu)} + \frac{2p_{n+1}^{2-\mu}}{\Gamma(3-\mu)} - \frac{p_{c,n+1}p_{n+1}^{1-\mu}}{\Gamma(2-\mu)} \right]$$
(14)

171
$$\Delta \boldsymbol{\gamma}_{n+1}^{\mathrm{p}} = \mathbf{P} : \Delta \boldsymbol{\varepsilon}_{n+1}^{\mathrm{p}} = 3\Delta \phi_{n+1} \mathbf{s}_{n+1} \left[\frac{q_{n+1}^{1-\mu}}{N^2 \Gamma(3-\mu)} + \frac{p_{n+1} \left(p_{n+1} - p_{c,n+1} \right)}{2q_{n+1}^{1+\mu} \Gamma(1-\mu)} \right]$$
(15)

172 where the fourth-order projection tensor **P** is determined by $\mathbf{P} = \mathbf{I} - \mathbf{1} \otimes \mathbf{1}/3$. Substituting Eq. (15) into Eq. (13),

173 one can get the expression for \mathbf{s}_{n+1} :

$$\mathbf{s}_{n+1} = \frac{\mathbf{s}_n + 2\bar{G}\Delta\gamma_{n+1}}{1+c} \tag{16}$$

175 where

174

176
$$c = 6\bar{G}\Delta\phi_{n+1} \left[\frac{q_{n+1}^{1-\mu}}{N^2 \Gamma(3-\mu)} + \frac{p_{n+1}(p_{n+1}-p_{c,n+1})}{2 q^{1+\mu}\Gamma(1-\mu)} \right]$$
(17)

177 Substituting Eq. (14) into Eq.(12) and considering Eq. (16), the update formulas of p_{n+1} and q_{n+1} can be

178 obtained to replace that of σ_{n+1} in Eq. (9).

179
$$p_{n+1} = p_n \exp\left\{c_\kappa \Delta \varepsilon_{\nu, n+1} - c_\kappa \Delta \phi_{n+1} \left[\frac{q_{n+1}^2}{p_{n+1}^\mu N^2 \Gamma(1-\mu)} + \frac{2p_{n+1}^{2-\mu}}{\Gamma(3-\mu)} - \frac{p_{c, n+1}p_{n+1}^{1-\mu}}{\Gamma(2-\mu)}\right]\right\}$$
(18)

180
$$q_{n+1} = \sqrt{\frac{3}{2}} \frac{\left\| \mathbf{s}_n + 2\bar{G}\Delta\gamma_{n+1} \right\|}{1+c}$$
(19)

181 Finally, the implicit stress integral equations of the NEP clay model can be simplified in the following form:

182
$$\begin{cases} f_{1} \\ f_{2} \\ f_{3} \\ f_{4} \end{cases} = \begin{cases} p_{n+1} - p_{n} \exp(c_{\kappa} \Delta \varepsilon_{v, n+1}^{e}) = 0 \\ q_{n+1} - \sqrt{\frac{3}{2}} \frac{\|\mathbf{s}_{n} + 2\bar{G}\Delta \gamma_{n+1}\|}{1+c} = 0 \\ p_{c, n+1} - p_{c, n} \exp(c_{p}\Delta \varepsilon_{v, n+1}^{p}) = 0 \\ \Delta \phi_{n+1} \ge 0, f_{n+1} \le 0, \Delta \phi_{n+1} f_{n+1} = 0 \end{cases}$$
(20)

where Eq. (20) contains only 4 equalities. Comparing with Eq. (9) containing 8 equalities, the number of nonlinear
equations is significantly reduced.

185 3. UNCONSTRAINED IMPLICIT STRESS UPDATE BASED ON THE LINE SEARCH METHOD

Eq. (20) is non-smooth due to the existence of *KKT* conditions, i.e., Eq. (20)₄, where the inequality constraints mean that the nonlinear equations cannot be solved directly. In the operator splitting technique, the "*elastic prediction*", i.e., $\boldsymbol{\sigma}_{n+1}^{trial} = \boldsymbol{\sigma}_n + \bar{\mathbf{D}}(\bar{K}, \bar{G})$: $\Delta \boldsymbol{\varepsilon}_{n+1}$, is conducted to estimate loading and unloading states of material to address the inequality constraints. If $\boldsymbol{\sigma}_{n+1}^{trial}$ is within the current yield surface, i.e., $f(\boldsymbol{\sigma}_{n+1}^{trial}) < 0$, the stress update follows the elastic Hooke's law and no plastic strain occurs in this step. On the other hand, if $\boldsymbol{\sigma}_{n+1}^{trial}$ exceeds the current yield surface, i.e., $f(\sigma_{n+1}^{trial}) > 0$, Eq. (20) is solved by using $f_{n+1} = 0$ instead of Eq. (20)₄. The stress gradually iterates back from σ_{n+1}^{trial} to the true stress point. The solving process is also known as the "plastic correction". The loading/unloading estimation is required at each increment step, which increases the complexity of the model implementation. To this end, the *KKT conditions* in Eq. (20)₄ are replaced equivalently by the *Fischer-Burmeister* smooth function¹⁹.

196

$$\begin{cases}
f_{1} \\
f_{2} \\
f_{3} \\
f_{4}
\end{cases} = \begin{cases}
p_{n+1} - p_{n} \exp(c_{\kappa} \Delta \varepsilon_{v,n+1}^{e}) = 0 \\
q_{n+1} - \sqrt{\frac{3}{2}} \frac{\|\mathbf{s}_{n} + 2\overline{G}\Delta \gamma_{n+1}\|}{1 + c} = 0 \\
p_{c,n+1} - p_{c,n} \exp(c_{p}\Delta \varepsilon_{v,n+1}^{p}) = 0 \\
\sqrt{(c_{d}\Delta \phi_{n+1})^{2} + f_{n+1}^{2} + 2\beta} - c_{d}\Delta \phi_{n+1} + f_{n+1} = 0
\end{cases}$$
(21)

197 where $c_{d} = \left\| \mathbf{\sigma}_{n} + \mathbf{\overline{D}}(\mathbf{\overline{K}}, \mathbf{\overline{G}}) : \Delta \mathbf{\varepsilon}_{n+1} \right\|^{3}$ and $\beta = 0.5FTOL^{2}$ are the parameters in the smoothing function Eq. (21)₄. 198 *FTOL* is the allowable error for judging the convergence of solutions of nonlinear equations. Fig. 4 shows that the 199 smooth curve will gradually approximate *KKT conditions* as the parameter β decreases. There is no need for the 200 loading/unloading estimation in solving Eq. (21). The calculation results exactly satisfy the *KKT* conditions when the 201 solution of Eq. (21) converges.



Fig. 4 Fischer-Burmeister smooth function.



205
$$\min \quad \psi(\{\mathbf{x}\}_{n+1}) = \frac{1}{2} \{\mathbf{f}(\mathbf{x})\}_{n+1}^{T} \{\mathbf{f}(\mathbf{x})\}_{n+1}$$
(22)

206 The decline of the merit function ψ can be achieved by the iterative search in multi-dimensional space:

207
$$\left\{\mathbf{x}\right\}^{k+1} = \left\{\mathbf{x}\right\}^{k} + \alpha^{k} \left\{\mathbf{d}\right\}^{k}$$
(23)

denotes the search direction, which is usually determined by the Newton direction 208 where **{d**} $\{\mathbf{d}\}^{k} = -\left[\nabla \mathbf{f}(\mathbf{x})\right]_{k}^{-1} \{\mathbf{f}(\mathbf{x})\}^{k}$ to provide the quadratic convergence rate of local stress update iteration, where k denotes 209 the iteration number in the local stress update. $\nabla f(x)$ is the Jacobian matrix of nonlinear equations defined by Eq. 210 211 (20), which can be calculated by the numerical differentiation. Appendix A also provides the analytical expression of $\nabla \mathbf{f}(\mathbf{x})$. α is the step size. The most essential task for the line search technique is to optimize the step size α^k to 212 achieve the maximum benefit of minimizing ψ^k under a given search direction $\{\mathbf{d}\}^k$, which will further produce a 213 one-dimensional sub problem to find α^k . 214

$$\min \quad \psi\left(\left\{\mathbf{x} + \alpha \mathbf{d}\right\}_{n+1}^{k}\right) \tag{24}$$

216 However, the exact minimization of Eq. (24) may be computationally expensive and is usually unnecessary. α^{k} 217 is thus updated by a more practical iterative formula with *Goldstein's condition*:

215

218
$$\begin{cases} Accept \ \alpha_{j}^{k} \ and \ exit \qquad IF \ \psi(\alpha_{j}^{k}) < (1 - 2\rho\alpha_{j}^{k})\psi(0) \\ \alpha_{j+1}^{k} = \frac{\psi(0)}{\psi(0) + 2\psi(\alpha_{j}^{k})} \qquad ELSE \end{cases}$$
(25)

219 where the initial value of α is set to 1. The updated step size α_{j+1}^k needs to be greater than a minimum value to 220 avoid too small a benefit:

221
$$\alpha_{j+1}^{k} = \max\left\{ \varsigma \alpha_{j}^{k}, \frac{\psi(0)}{\psi(0) + 2\psi(\alpha_{j}^{k})} \right\}$$
(26)

where the algorithm parameters ρ and ς are recommended as 10⁻⁴ and 0.1⁴⁶. Eqs. (25) and (26) essentially provide an inexact line search strategy, in which the step size for a given descent direction $\{\mathbf{d}\}^k$ is not a value that minimizes $\psi(\{\mathbf{x} + \alpha \mathbf{d}\}_{n+1}^k)$, but an acceptable range, as shown in Fig. 5. Finally, the complete stress update procedure of the NEP clay model is demonstrated in Fig. 6.



Fig. 5 Inexact line search method.

Input: σ_n , $\Delta \varepsilon_{n+1}$, $p_{c,n}$ Compute σ_{n+1}^{trial} as the initial point of iteration and set *FTOL* Set k = 0, $\{p_{n+1}^0, q_{n+1}^0, p_{c,n+1}^0, \Delta \phi_{n+1}^0\} = \{p_{n+1}^{trial}, q_{n+1}^{trial}, p_{c,n}, 0\}$ and $\beta = FTOL^2/2$, $c_d = \|\mathbf{\sigma}_{n+1}^{trial}\|^2$ Set $\{\mathbf{x}\}_{n+1}^{0} = \{p_{n+1}^{0}, q_{n+1}^{0}, p_{c,n+1}^{0}, \Delta \phi_{n+1}^{0}\}$ and compute $\psi^{0} = \psi(\{\mathbf{x}\}_{n+1}^{0})$ **do while** $\left\| \mathbf{f} \left(\left\{ \mathbf{x} \right\}^k \right) \right\| \le FTOL$ and $k \le k_{\max}$ Compute $\{\mathbf{x}^*\}_{n=1}^{k+1}$ using the line search method $\left\{\mathbf{d}\right\}^{k} = -\left[
abla \mathbf{f}\left(\mathbf{x}\right)\right]_{k}^{-1} \left\{\mathbf{f}\right\}_{n+1}^{k}$, j = 0 , $\alpha_{j}^{k} = 1$ $\psi(0) = \frac{1}{2} \left\| \left\{ \mathbf{f}(\mathbf{x}) \right\}_n \right\|^2$, $\psi(\alpha_j^k) = \frac{1}{2} \left\| \left\{ \mathbf{f}(\mathbf{x} + \alpha_j^k \mathbf{d}) \right\}_{n+1}^k \right\|^2$ **do while** $\psi(\alpha_j^k) \ge (1 - 2\rho \alpha_j^k) \psi(0)$ and $j \le j_{\max}$ $\alpha_{j+1}^{k} = \max\left\{\varsigma\alpha_{j}^{k}, \frac{\psi(0)}{\psi(0) + \psi(\alpha_{j}^{k})}\right\}$ $\psi\left(\alpha_{j+1}^{k}\right) = \frac{1}{2} \left\| \left\{ \mathbf{f}\left(\mathbf{x} + \alpha_{j+1}^{k} \mathbf{d}\right) \right\}_{n+1}^{k} \right\|^{2}$ j = j + 1end do $\{\mathbf{x}\}_{n+1}^{k+1} = \{\mathbf{x}\}_{n+1}^{k} + \alpha_{j}^{k} \{\mathbf{d}\}^{k}$ Set k = k + 1end do State update and compute σ_{n+1} $p_{n+1} = p_{n+1}^k, \ q_{n+1} = q_{n+1}^k, \ p_{c,n+1} = p_{c,n+1}^k, \ \Delta \phi_{n+1} = \Delta \phi_{n+1}^k$ $\mathbf{s}_{n+1} = \frac{\mathbf{s}_n + 2\overline{G}\Delta \mathbf{\gamma}_{n+1}}{1+c}$, $\mathbf{\sigma}_{n+1} = p_{n+1}\mathbf{1} + \mathbf{s}_{n+1}$ Compute the consistent tangent operator $\partial \sigma_{n+1} / \partial \varepsilon_{n+1}$ **Output** : σ_{n+1} , $p_{c, n+1}$, and $\partial \sigma_{n+1} / \partial \varepsilon_{n+1}$

Fig. 6 Algorithm flow of a numerical implementation of the NEP clay model.

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230 4. CONSISTENT TANGENT OPERATOR

The consistent tangent operator of NEP clay model is given by the analytical derivation and the numerical differentiation, respectively. The latter can be easily extended to the implicit calculation of other non-orthogonal models or elastoplastic models.

234 **4.1 Analytical evaluation**

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238

241

235 The consistent tangent operator can be expressed by:

$$\frac{\partial \mathbf{\sigma}_{n+1}}{\partial \boldsymbol{\varepsilon}_{n+1}} = \mathbf{1} \otimes \frac{\partial p_{n+1}}{\partial \boldsymbol{\varepsilon}_{n+1}} + \frac{\partial \mathbf{s}_{n+1}}{\partial \boldsymbol{\varepsilon}_{n+1}}$$
(27)

Taking the derivatives of both Eq. (12) and Eq. (16) over $\mathbf{\epsilon}_{n+1}$, one can obtain:

$$\frac{\partial p_{n+1}}{\partial \boldsymbol{\varepsilon}_{n+1}} = a_1 \boldsymbol{K}_{n+1}^* \mathbf{1} + a_2 \boldsymbol{K}_{n+1}^* \frac{\partial \Delta \phi_{n+1}}{\partial \boldsymbol{\varepsilon}_{n+1}} + a_3 \boldsymbol{K}_{n+1}^* \frac{\partial q_{n+1}}{\partial \boldsymbol{\varepsilon}_{n+1}}$$
(28)

$$\frac{\partial \mathbf{s}_{n+1}}{\partial \boldsymbol{\varepsilon}_{n+1}} = 2a_{8}\mathbf{R}: \left(\bar{G}\mathbf{P} + a_{1}a_{9}\Delta\boldsymbol{\gamma}_{n+1}\otimes\mathbf{1} + a_{2}a_{9}\Delta\boldsymbol{\gamma}_{n+1}\otimes\frac{\partial\Delta\phi_{n+1}}{\partial\boldsymbol{\varepsilon}_{n+1}}\right)$$

$$-2\sqrt{6}a_{8}q_{n+1}\mathbf{R}: \hat{\mathbf{n}}\otimes\left[a_{1}a_{7}a_{9}\Delta\phi_{n+1}\mathbf{1} + a_{7}\left(a_{2}a_{9}\Delta\phi_{n+1} + \bar{G}\right)\frac{\partial\Delta\phi_{n+1}}{\partial\boldsymbol{\varepsilon}_{n+1}} + \frac{\bar{G}\Delta\phi_{n+1}K_{n+1}^{*}}{2q_{n+1}^{1+\mu}\Gamma\left(1-\mu\right)}\left(c_{1}\mathbf{1} + c_{2}\frac{\partial\Delta\phi_{n+1}}{\partial\boldsymbol{\varepsilon}_{n+1}}\right)\right]$$

$$(29)$$

240 where
$$K_{n+1}^* = c_{\kappa} p_n \exp\left(c_{\kappa} \Delta \varepsilon_{\nu,n+1}^{e}\right)$$
.

$$\mathbf{R} = \left\{ \mathbf{I} + 6a_{8}q_{n+1}\Delta\varphi_{n+1} \left[\bar{G} \frac{2q_{n+1}^{-\mu} + N^{2} \left(\mu^{2} - \mu - 2\right) \left(p_{n+1}^{2} - p_{n+1}p_{c,n+1}\right) q_{n+1}^{-2-\mu}}{2N^{2} \left(2 - \mu\right) \Gamma \left(1 - \mu\right)} + \frac{\bar{G}K_{n+1}^{*} \left(2p_{n+1} - p_{c,n+1}\right) a_{3} - \bar{G}K_{n+1}^{*}p_{n+1}a_{6}}{2q_{n+1}^{1+\mu} \Gamma \left(1 - \mu\right)} + a_{3}a_{7}a_{9} \right] \hat{\mathbf{n}} \otimes \tilde{\mathbf{n}} - \sqrt{6}a_{3}a_{8}a_{9}\Delta\gamma_{\mathbf{n+1}} \otimes \tilde{\mathbf{n}} \right\}^{-1}$$
(30)

$$\begin{cases} a = 1 + K_{n+1}^{*} \Delta \phi_{n+1} \left(\frac{2p_{n+1}^{1-\mu}}{\Gamma(2-\mu)} - \frac{\mu q_{n+1}^{2}}{p_{n+1}^{1+\mu} N^{2} \Gamma(1-\mu)} - \frac{p_{c,n+1}}{p_{n+1}^{\mu} \Gamma(1-\mu)} \right) + \frac{p_{c,n+1} c_{p} \Delta \phi_{n+1} p_{n+1}^{1-\mu}}{\Gamma(2-\mu)} \\ a_{1} = \left(1 + \frac{p_{c,n+1} c_{p} \Delta \phi_{n+1} p_{n+1}^{1-\mu}}{\Gamma(2-\mu)} \right) \bigg/ a \\ a_{2} = \left(\frac{p_{c,n+1} p_{n+1}^{1-\mu}}{\Gamma(2-\mu)} - \frac{q_{n+1}^{2}}{p_{n+1}^{\mu} N^{2} \Gamma(1-\mu)} - \frac{2p_{n+1}^{2-\mu}}{\Gamma(3-\mu)} \right) \bigg/ a \\ a_{3} = \frac{-2\Delta \phi_{n+1} q_{n+1}}{n p_{n+1}^{\mu} N^{2} \Gamma(1-\mu)} - \frac{\mu q_{n+1}^{2}}{p_{n+1}^{1+\mu} N^{2} \Gamma(1-\mu)} - \frac{p_{c,n+1}}{p_{n+1}^{\mu} N^{2} \Gamma(1-\mu)} \bigg) \bigg/ a \\ a_{4} = p_{c,n+1} c_{p} \Delta \phi_{n+1} \bigg(\frac{2p_{n+1}^{1-\mu}}{\Gamma(2-\mu)} - \frac{\mu q_{n+1}^{2}}{\Gamma(3-\mu)} - \frac{p_{c,n+1} p_{n+1}^{1-\mu}}{\Gamma(2-\mu)} \bigg) \bigg/ a \\ a_{5} = p_{c,n+1} c_{p} \bigg(\frac{q_{n+1}^{2}}{p_{n+1}^{\mu} N^{2} \Gamma(1-\mu)} + \frac{2p_{n+1}^{2-\mu}}{\Gamma(3-\mu)} - \frac{p_{c,n+1} p_{n+1}^{1-\mu}}{\Gamma(2-\mu)} \bigg) \bigg/ (aK_{n+1}^{*}) \\ a_{6} = \left(2p_{c,n+1} c_{p} \Delta \phi_{n+1} q_{n+1} \right) / \bigg[p_{n+1}^{\mu} N^{2} K_{n+1}^{*} a \Gamma(1-\mu) \bigg] \\ a_{7} = \frac{q_{n+1}^{1-\mu}}{N^{2} \Gamma(3-\mu)} + \frac{p_{n+1}^{2-\mu} - p_{n+1} p_{c,n+1}}{2q_{n+1}^{1-\mu} \Gamma(1-\mu)} \bigg) \\ a_{8} = \left(1 + 6\overline{G} \Delta \phi_{n+1} a_{7} \right)^{-1} \\ a_{9} = r \bigg(K^{*} - \overline{K} \bigg) / \Delta \varepsilon_{v,n+1}^{*}$$
(31)

 $\frac{\partial p_{c,n+1}}{\partial \boldsymbol{\varepsilon}_{n+1}}$ can be derived by taking Eq. (9)₃ with respect to $\boldsymbol{\varepsilon}_{n+1}$: 243

244
$$\frac{\partial p_{c,n+1}}{\partial \boldsymbol{\varepsilon}_{n+1}} = a_4 K_{n+1}^* \mathbf{1} + a_5 K_{n+1}^* \frac{\partial \Delta \phi_{n+1}}{\partial \boldsymbol{\varepsilon}_{n+1}} + a_6 K_{n+1}^* \frac{\partial q_{n+1}}{\partial \boldsymbol{\varepsilon}_{n+1}}$$
(32)

There are four unknowns (i.e., $\partial p_{n+1}/\partial \varepsilon_{n+1}$, $\partial s_{n+1}/\partial \varepsilon_{n+1}$, $\partial p_{c,n+1}/\partial \varepsilon_{n+1}$, and $\partial \Delta \phi_{n+1}/\partial \varepsilon_{n+1}$) in Eqs. (28), (29), 245

and (32). An additional constraint is needed to close the equations involving unknowns. The total differential of Eq. 246 247 $(20)_4$ can yield:

248
$$\frac{\partial f_4}{\partial f} \left[\frac{3\mathbf{s}_{n+1}}{M^2} : \frac{\partial \mathbf{s}_{n+1}}{\partial \mathbf{\epsilon}_{n+1}} + \left(2p_{n+1} - p_{c,n+1} \right) \frac{\partial p_{n+1}}{\partial \mathbf{\epsilon}_{n+1}} - p_{n+1} \frac{\partial p_{c,n+1}}{\partial \mathbf{\epsilon}_{n+1}} \right] + \frac{\partial f_4}{\partial \Delta \phi_{n+1}} \frac{\partial \Delta \phi_{n+1}}{\partial \mathbf{\epsilon}_{n+1}} = 0$$
(33)

From Eqs. (28), (29), (32), and (33), $\frac{\partial p_{n+1}}{\partial \boldsymbol{\varepsilon}_{n+1}}$, $\frac{\partial \mathbf{s}_{n+1}}{\partial \boldsymbol{\varepsilon}_{n+1}}$, $\frac{\partial p_{c,n+1}}{\partial \boldsymbol{\varepsilon}_{n+1}}$, and $\frac{\partial \Delta \phi_{n+1}}{\partial \boldsymbol{\varepsilon}_{n+1}}$ can be derived as follows: 249

250
$$\frac{\partial p_{n+1}}{\partial \varepsilon_{n+1}} = (a_1 + a_2 b_1) K_{n+1}^* \mathbf{1} + (a_2 b_2 + \sqrt{6} a_3 a_8 \overline{G}) K_{n+1}^* \mathbf{\tilde{n}} : \mathbf{R} : \mathbf{P} + \sqrt{6} a_3 a_8 a_9 K_{n+1}^* (a_1 + a_2 b_1) \mathbf{\tilde{n}} : \mathbf{R} : \Delta \gamma_{n+1} \otimes \mathbf{1}$$
(34)

 $+\sqrt{6}a_2a_3a_8a_9b_2K_{n+1}^*\tilde{\mathbf{n}}:\mathbf{R}:\Delta\gamma_{n+1}\otimes\tilde{\mathbf{n}}:\mathbf{R}:\mathbf{P}-6a_3a_8b_4q_{n+1}K_{n+1}^*\tilde{\mathbf{n}}:\mathbf{R}:\hat{\mathbf{n}}\otimes\mathbf{1}-6a_3a_8b_2b_5q_{n+1}K_{n+1}^*\tilde{\mathbf{n}}:\mathbf{R}:\hat{\mathbf{n}}\otimes\tilde{\mathbf{n}}:\mathbf{R}:\mathbf{P}-6a_3a_8b_4q_{n+1}K_{n+1}^*\tilde{\mathbf{n}}:\mathbf{R}:\hat{\mathbf{n}}\otimes\mathbf{1}-6a_3a_8b_2b_5q_{n+1}K_{n+1}^*\tilde{\mathbf{n}}:\mathbf{R}:\hat{\mathbf{n}}\otimes\tilde{\mathbf{n}}:\mathbf{R}:\mathbf{P}-6a_3a_8b_4q_{n+1}K_{n+1}^*\tilde{\mathbf{n}}:\mathbf{R}:\hat{\mathbf{n}}\otimes\mathbf{1}-6a_3a_8b_2b_5q_{n+1}K_{n+1}^*\tilde{\mathbf{n}}:\mathbf{R}:\hat{\mathbf{n}}\otimes\tilde{\mathbf{n}}:\mathbf{R}:\mathbf{R}$

251
$$\frac{\partial \mathbf{s}_{n+1}}{\partial \mathbf{\varepsilon}_{n+1}} = 2a_8 \overline{G} \mathbf{R} : \mathbf{P} + 2a_8 a_9 \left(a_1 + a_2 b_1 \right) \mathbf{R} : \Delta \gamma_{n+1} \otimes \mathbf{1}$$
(35)

$$+2a_2a_8a_9b_2\mathbf{R}:\Delta\gamma_{n+1}\otimes\tilde{\mathbf{n}}:\mathbf{R}:\mathbf{P}-2\sqrt{6}a_8b_4q_{n+1}\mathbf{R}:\hat{\mathbf{n}}\otimes\mathbf{1}-2\sqrt{6}a_8b_2b_5q_{n+1}\mathbf{R}:\hat{\mathbf{n}}\otimes\tilde{\mathbf{n}}:\mathbf{R}:\mathbf{P}$$

252
$$\frac{\partial p_{c,n+1}}{\partial \boldsymbol{\varepsilon}_{n+1}} = a_4 K_{n+1}^* \mathbf{1} + a_5 K_{n+1}^* \frac{\partial \Delta \phi_{n+1}}{\partial \boldsymbol{\varepsilon}_{n+1}} + a_6 K_{n+1}^* \frac{\partial q_{n+1}}{\partial \boldsymbol{\varepsilon}_{n+1}}$$
(36)

$$\frac{\partial \phi_{n+1}}{\partial \boldsymbol{\varepsilon}_{n+1}} = b_1 \mathbf{1} + b_2 \tilde{\mathbf{n}} : \mathbf{R} : \mathbf{P}$$
(37)

where the coefficients

$$\begin{cases} b = 2a_{2}a_{8}a_{9}b_{3}\tilde{\mathbf{n}}: \mathbf{R}: \Delta \gamma_{\mathbf{n}+1} \frac{\partial f_{4}}{\partial f} - 2\sqrt{6}a_{8}b_{3}q_{n+1} \left\{ a_{2}a_{7}a_{9}\Delta \phi_{n+1} + a_{7}\overline{G} + \frac{\overline{G}\Delta \phi_{n+1}K_{n+1}^{*}c_{2}}{2q_{n+1}^{1+\mu}\Gamma(1-\mu)} \right\} \tilde{\mathbf{n}}: \mathbf{R}: \hat{\mathbf{n}} \frac{\partial f_{4}}{\partial f} + K_{n+1}^{*}c_{2} \frac{\partial f_{4}}{\partial f} + \frac{\partial f}{\partial \Delta \phi_{n+1}} \\ b_{1} = -\frac{\partial f_{4}}{\partial f} \left[2a_{1}a_{8}a_{9}b_{3}\tilde{\mathbf{n}}: \mathbf{R}: \Delta \gamma_{\mathbf{n}+1} - 2\sqrt{6}a_{8}b_{3}q_{n+1}\tilde{\mathbf{n}}: \mathbf{R}: \hat{\mathbf{n}} \left(a_{1}a_{7}a_{9}\Delta \phi_{n+1} + \frac{\overline{G}\Delta \phi_{n+1}K_{n+1}^{*}c_{1}}{2q_{n+1}^{1+\mu}\Gamma(1-\mu)} \right) + K_{n+1}^{*}c_{1} \right] / b \\ b_{2} = -\left(2a_{8}b_{3}\overline{G}\frac{\partial f_{4}}{\partial f} \right) / b \\ b_{3} = \sqrt{6}\frac{q}{N^{2}} + \sqrt{\frac{3}{2}}K_{n+1}^{*} \left[\left(2p_{n+1} - p_{c,n+1} \right)a_{3} - p_{n+1}a_{6} \right] \\ b_{4} = a_{1}a_{7}a_{9}\Delta \phi_{n+1} + a_{2}a_{7}a_{9}b_{1}\Delta \phi_{n+1} + a_{7}b_{1}\overline{G} + \frac{\overline{G}\Delta \phi_{n+1}K_{n+1}^{*}(c_{1} + b_{1}c_{2})}{2q_{n+1}^{1+\mu}\Gamma(1-\mu)} \\ b_{5} = a_{2}a_{7}a_{9}\Delta \phi_{n+1} + a_{7}\overline{G} + \frac{\overline{G}\Delta \phi_{n+1}K_{n+1}^{*}c_{2}}{2q_{n+1}^{1+\mu}\Gamma(1-\mu)} \end{cases}$$
(38)

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256

Substituting Eqs. (34) and (35) into Eq. (27), the consistent tangent operator is obtained analytically as follows:

$$\frac{\partial \mathbf{\sigma}_{n+1}}{\partial \mathbf{\varepsilon}_{n+1}} = (a_1 + a_2 b_1) K_{n+1}^* \mathbf{1} \otimes \mathbf{1} + (a_2 b_2 + \sqrt{6} a_3 a_8 \overline{G}) K_{n+1}^* \mathbf{1} \otimes \tilde{\mathbf{n}} : \mathbf{R} : \mathbf{P} + \sqrt{6} a_3 a_8 a_9 (a_1 + a_2 b_1) K_{n+1}^* \mathbf{1} \otimes \tilde{\mathbf{n}} : \mathbf{R} : \Delta \gamma_{n+1} \otimes \mathbf{1}$$

$$257 + \sqrt{6} a_2 a_3 a_8 a_9 b_2 K_{n+1}^* \mathbf{1} \otimes \tilde{\mathbf{n}} : \mathbf{R} : \Delta \gamma_{n+1} \otimes \tilde{\mathbf{n}} : \mathbf{R} : \mathbf{P} - 6 a_3 a_8 b_4 q_{n+1} K_{n+1}^* \mathbf{1} \otimes \tilde{\mathbf{n}} : \mathbf{R} : \tilde{\mathbf{n}} \otimes \mathbf{1} - 6 a_3 a_8 b_2 b_5 q_{n+1} K_{n+1}^* \mathbf{1} \otimes \tilde{\mathbf{n}} : \mathbf{R} : \tilde{\mathbf{n}} \otimes \tilde{\mathbf{n}} : \mathbf{R} : \mathbf{P}$$

$$+ 2 \overline{G} a_8 \mathbf{R} : \mathbf{P} + 2 a_8 a_9 (a_1 + a_2 b_1) \mathbf{R} : \Delta \gamma_{n+1} \otimes \mathbf{1} + 2 a_2 a_8 a_9 b_2 \mathbf{R} : \Delta \gamma_{n+1} \otimes \tilde{\mathbf{n}} : \mathbf{R} : \mathbf{P} - 6 \sqrt{\frac{2}{3}} a_8 b_4 q_{n+1} \mathbf{R} : \hat{\mathbf{n}} \otimes \mathbf{1} - 6 \sqrt{\frac{2}{3}} a_8 b_2 b_5 q_{n+1} \mathbf{R} : \hat{\mathbf{n}} \otimes \tilde{\mathbf{n}} : \mathbf{R} : \mathbf{P}$$

$$(39)$$

258 where $\frac{\partial \sigma_{n+1}}{\partial \varepsilon_{n+1}}$ will degenerate into that of the MCC model presented in the literature ¹⁹ in the case of $\mu = 1$.

259 4.2 Numerical evaluation

Section 4.1 has provided the analytic consistent tangent operator. It can be observed that it is a cumbersome task to derive analytically the consistent tangent operator for the elastoplastic model with highly nonlinear characteristics. The verbose and complex expressions also make programming and code debugging more difficult. Therefore, the numerical evaluation is recommended from the perspective of implementation difficulty. In what follow, the CSDA is used to evaluate the derivatives of stress integral equations. As a comparison, the central difference method (CDM) and forward difference method (FDM) are also presented. In the FDM, the derivative of f(x) at the interesting point x is obtained by the Taylor expansion of f(x+h)

267 on the real number axis:

275

268
$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)h^2}{2!} + \frac{f'''(x)h^3}{3!} + \dots$$
(40)

where *h* denotes a smaller perturbation value. Assuming the truncation error terms can be neglected, one can yield:

270
$$f'(x) = \frac{f(x+h) - f(x)}{h} + O(h)$$
(41)

271 where O(h) indicates that the FDM has first-order accuracy. Following a similar procedure. The Taylor expansion

272 of f(x-h) on the real number axis can yield:

273
$$f(x-h) = f(x) - f'(x)h + \frac{f''(x)h^2}{2!} - \frac{f'''(x)h^3}{3!} + \dots$$
(42)

From Eqs. (40) and (42), the approximation of f'(x) based on the CDM is obtained by:

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + O(h^2)$$
(43)

There are two numerical errors in Eqs. (41) and (43). One is the truncation error which decreases with the decrease of *h*. The other is the rounding off error caused by representing real numbers with floating-point numbers of finite digits. It is worth emphasizing that the subtraction operation of two very close numbers will cause a significant subtractive cancellation error which is a special case of rounding off error and increases with the decrease of *h*. The error distribution of the finite difference method with the perturbation is shown in Fig. 7 (a). In the CSDA⁴⁷, the Taylor series expansion is conducted on both the real number and imaginary number axes:

282
$$f(x+h) = f(x) + f'(x) \lambda h - \frac{f''(x)h^2}{2!} - \frac{f'''(x)\lambda h^3}{3!} + \dots$$
(44)

where λ denotes the imaginary number ($\lambda^2 = -1$). The approximation formula of f'(x) with second-order accuracy can be obtained by the division operation of the imaginary part of Eq. (44) as follows:

285
$$f'(x) = \frac{I\left[f\left(x + \lambda h\right)\right]}{h} + O\left(h^2\right)$$
(45)

where I [·] is used to extract the imaginary part of the argument. The approximation formula in Eq. (45) can be easily extended to multi-dimensional cases as follows:

288
$$\frac{\partial f}{\partial x_i} = \frac{I \left[f\left(\mathbf{x} + \lambda h_i \mathbf{e}_i\right) \right]}{h_i} + O\left(h_i^2\right)$$
(46)

where x_i denotes *i*th component of **x**. \mathbf{e}_i and h_i denote *i*th unit vector and the perturbation value in *i*th direction. It can be found that there is no subtraction operation in the CSDA. Therefore, there is no subtraction cancellation error and the rounding off error is bounded. On the other hand, the truncation error can be reduced by decreasing the perturbation value. In theory, there is no lower bound for the perturbation value in the CSDA³¹. Fig. 7 (b) demonstrates the error distribution of CSDA with the perturbation.



Fig. 7 Errors change with the perturbation h: (a) FDM/CDM; (b) CSDA..

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The derivative of $f(x) = \cos(x)/[1 + \sin^2(x)]$ at $x = \pi/3$ is calculated as an example to further demonstrate 295 296 the characteristics of three numerical schemes. The numerical examples are run on MATLAB 2020a. The range of the 297 perturbation value h is $[10^{-16}, 10^{-1}]$. Fig. 8 (a) shows the change of relative total error with the perturbation value, in 298 which the double-precision computation is conducted and the lower limit of relative total error is set to eps = 2.2204e-299 16 (double floating-point relative accuracy). It is clear that, at the beginning of decreasing perturbation, the decline rate of the relative total error of CSDA and CDM is approximately the same and faster than that of FDM since CSDA 300 301 and CDM are second-order accuracy schemes while FDM is first-order accuracy scheme. With the further decrease of 302 perturbation, the relative total errors of CDM and FDM begin to increase due to the presence of subtractive cancellation error while in the CSDA any perturbation value lower than 10⁻⁸ gives rise to a relative error near eps. A clearer contrast 303 304 can be found in Fig. 8 (b), in which the precision of the variables is set to 100 bits. Therefore, it can be approximately 305 considered that there is no rounding off error in the calculation results and the total error equals the truncation error.

The results depicted in Fig. 8 (b) show the decline rate of the relative truncation error of the three schemes is completely consistent with their accuracy orders of the numerical differentiation method. By subtracting the truncation error from the total error, one can obtain the change of the rounding off error dominated by the subtractive cancellation error with the perturbation, as shown in Fig. 8 (c). It is clear that the relative rounding off error of CSDA is maintained near *eps* owing to the lack of the subtractive cancellation error but the relative rounding off errors of CDM and FDM increase with decreasing perturbation. The CSDA provides a more robust numerical derivation scheme than the finite difference methods.



313 Fig. 8 Change of relative errors with the perturbation value: (a) relative total error; (b) relative truncation error; (c)

relative rounding off error.

Based on the presented CSDA, the numerical Jacobian matrix of Eq. (20) can be easily obtained without cumbersome derivation. To numerically calculate the consistency tangent operator, however, the non-orthogonal stress

317 integral equations usually need to be expressed in the following more general form:

318
$$\begin{cases} f_{\sigma} \\ f_{p_{c}} \\ f_{\Delta\phi} \end{cases} = \begin{cases} \sigma_{n+1} - \sigma_{n} - \overline{\mathbf{D}} : \left(\Delta \varepsilon_{n+1} - \Delta \varepsilon_{n+1}^{p}\right) \\ p_{c,n+1} - p_{c,n} \exp\left[c_{p}\Delta \varepsilon_{v,n+1}^{p}\right] \\ \sqrt{\left(c_{d}\Delta \phi_{n+1}\right)^{2} + f_{n+1}^{2} + 2\beta} - c_{d}\Delta \phi_{n+1} + f_{n+1}} \end{cases} = \begin{cases} \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{cases}$$
(47)

319 Taking the total differential of Eq. (47) with independent variables $\mathbf{\sigma}_{n+1}$, $\mathbf{\epsilon}_{n+1}$, $p_{c,n+1}$, and $\Delta \phi_{n+1}$, one can yield:

320
$$\begin{bmatrix}
\frac{\partial f_{\sigma}}{\partial \sigma} & \frac{\partial f_{\sigma}}{\partial \rho_{c}} & \frac{\partial f_{\sigma}}{\partial \Delta \phi} \\
\frac{\partial f_{p_{c}}}{\partial \sigma} & \frac{\partial f_{p_{c}}}{\partial \rho_{c}} & \frac{\partial f_{p_{c}}}{\partial \Delta \phi} \\
\frac{\partial f_{\Delta \phi}}{\partial \sigma} & \frac{\partial f_{\Delta \phi}}{\partial \rho_{c}} & \frac{\partial f_{\Delta \phi}}{\partial \Delta \phi}
\end{bmatrix}_{n+1} + \begin{bmatrix}
\frac{\partial f_{\sigma}}{\partial \varepsilon} & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix} \begin{bmatrix}
d\varepsilon \\
0 \\
0
\end{bmatrix}_{n+1} = \begin{bmatrix}
0 \\
0 \\
0
\end{bmatrix}$$
(48)

321 where the Jacobian matrix of Eq. (47) can be solved by the numerical evaluation. After transposition and matrix

322 inversion operations, one can obtain:

323
$$\begin{cases} d\boldsymbol{\sigma} \\ d\boldsymbol{p}_{c} \\ d\Delta\boldsymbol{\phi} \end{pmatrix}_{n+1} = -\begin{bmatrix} \frac{\partial f_{\boldsymbol{\sigma}}}{\partial \boldsymbol{\sigma}} & \frac{\partial f_{\boldsymbol{\sigma}}}{\partial p_{c}} & \frac{\partial f_{\boldsymbol{\sigma}}}{\partial \Delta \boldsymbol{\phi}} \\ \frac{\partial f_{p_{c}}}{\partial \boldsymbol{\sigma}} & \frac{\partial f_{p_{c}}}{\partial p_{c}} & \frac{\partial f_{p_{c}}}{\partial \Delta \boldsymbol{\phi}} \\ \frac{\partial f_{\Delta\phi}}{\partial \boldsymbol{\sigma}} & \frac{\partial f_{\Delta\phi}}{\partial p_{c}} & \frac{\partial f_{\Delta\phi}}{\partial \Delta \boldsymbol{\phi}} \end{bmatrix}_{n+1}^{-1} \begin{bmatrix} \partial f_{\boldsymbol{\sigma}}/\partial \boldsymbol{\epsilon} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} d\boldsymbol{\epsilon} \\ 0 \\ 0 \end{bmatrix}_{n+1} = \begin{bmatrix} \mathbf{A} \end{bmatrix} \begin{bmatrix} d\boldsymbol{\epsilon} \\ 0 \\ 0 \end{bmatrix}_{n+1}$$
(49)

324 where the consistent tangent operator is determined by extracting 6×6 upper-left block matrix of [A].

325 5. NUMERICAL VALIDATION

The NEP clay model can degenerate into the MCC model under the condition of $\mu = 1.0$. In this case, the accuracy of model implementation can be validated by the analytical solutions of the MCC model in a cylindrical cavity expansion problem. The robustness of model implementation can be also assessed by comparison with the MCC model that is available in the ABAQUS software. In what follows, the accuracy and performance of the presented model implementation are validated and evaluated. The influence of perturbation value on the numerical stability is also investigated. In particular, the ability of the model implementation to address the coupling geotechnical problem is also assessed by a pile foundation bearing capacity test under the undrained condition. These computations were made on Intel[®] Core(TM) i5-6200U processor 2.3 GHz processor running on a 64-bit Windows 10 operating system.

334 **5.1 Cylindrical cavity expansion**

335 The cylindrical cavity expansion is a typical axisymmetric problem, as shown in Fig. 9(a), and thus its mathematical description can be transformed into ODEs, which makes it possible to obtain the analytical solution to 336 337 the problem. With the aid of scientific computing software Mathematica, Chen and Abousleiman have given the 338 undrained⁴⁹ and drained⁴⁹ exact solutions of the MCC model in the case of cylindrical cavity expansion, which provides 339 a valuable benchmark for the verification of the stress update results of the critical state models. Fig. 9(b) shows the 340 simplified finite element model where the eight-node axisymmetric elements (CAX8) and the corresponding pore 341 pressure elements (CAX8P) are employed respectively for the drained and undrained cases. It should be noted that the 342 displacement of the right boundary in 1-direction is constrained in the undrained case and is free in the drained case. The initial state of soil and model parameters⁴⁸ are presented in Table 3 and Table 5. In particular, the permeability of 343 soil and water weight are set to 2.3×10^{-3} m/s and 10 kN/m^{3 50} for the undrained case, respectively. The total 344 345 analysis time of 0.001 s is used to approximate undrained loading conditions. Fig. 10 shows the calculation results 346 of the cylindrical cavity expansion problem under drained and undrained conditions, respectively. The over 347 consolidation ratios (OCR) of examples is set to 10. It is clear that the numerical solution from the model 348 implementation is in good agreement with the analytical solution.

349

Table 3 Initial state of soil in the cylindrical cavity expansion problem

10 144 144 72 120 72 0.90	OCR	σ_{r0}'	$\sigma_{\scriptscriptstyle heta 0}^{\prime}$	σ_{z0}'	p_0'	q_0'	e_0
	10	144	144	72	120	72	0.802

Undrained case: permeability: 2.3×10^{-3} m/s, water weight: 10 kN/m³.



351

(b)

352 Fig. 9 Cylindrical cavity expansion example: (a) problem schematic; (b) simplified finite element model and mesh.



Fig. 10 Comparison between analytical and numerical solutions: (a) undrained condition; (b) drained condition.

355 **5.2** Conventional triaxial compression test

356 From the analysis results of Section 3.2, the computational accuracy of numerical differentiation methods depends heavily on the perturbation value. The inappropriate perturbation value may destroy the quadratic convergence when 357 358 the consistent tangent operator is evaluated by numerical differentiation. In this subsection, the influence of 359 perturbation value on the performance of numerical consistent tangent operator is assessed by an example of 360 conventional triaxial compression demonstrated in Fig. 11. The model parameters of soil are tabulated in Table 5. The initial stress state of $\sigma_1 = \sigma_2 = \sigma_3 = 100$ kPa is employed. The vertical displacement of 0.7m is loaded on the top 361 362 surface of cylinder with 14 equal incremental steps to ensure that the soil can reach the critical state. The generalized shear stress vs. axial strain and the stress path of the examples are depicted in Fig. 12, where $\mu = 1.0$ is considered. 363



Fig. 11 Summary of conventional triaxial compression test: (a) problem schematic; (b) finite element mesh.

(b)



Fig. 12 Simulation result of conventional triaxial compression test: (a) stress path; (b) generalized shear stress *vs.* axial
 strain.

Table 4 reports the total number of global iterations for the 14 steps and CPU time required by the numerical 367 368 consistent tangent operator with the different perturbations. It is worth emphasizing that the CPU time and global iterations are 38.1s and 39 for the analytical derivation case. In the case of $h \ge 10^{-2}$, the numerical consistent tangent 369 370 operators obtained by three numerical methods require more global iteration steps than the analytical consistent tangent 371 operator or have encountered failure in the global iteration, which shows that the truncation error caused by too large perturbation value has seriously distorted the numerical solution. In the case of $10^{-10} \le h \le 10^{-3}$, the analytical 372 373 derivation and numerical differentiation schemes both have about the same amount of global iterations, which indicates 374 that the numerical consistent tangent operator obtained by FDM, CDM, and CSDA all achieve quadratic convergence. 375 With the further decrease of h, the CSDA still remains convergent, the global iterations of the other two difference methods increase again, and even the global calculation encounter failure when $h \le 10^{-12}$ for the FDM and $h \le 10^{-13}$ 376 377 for CDM. The reason is that the increasing subtractive cancellation error caused by the decrease of h has resulted in 378 the distortion of the numerical consistent tangent operator again, which further spoils the convergence of global 379 iteration. From the results presented in Table 4, it is observed that CSDA is superior to other numerical differentiation 380 methods in numerical stability. Finally, an additional case denoted by full CSDA is also presented in Table 4, where 381 both the consistent tangent operator and the Jacobian matrix are evaluated by the CSDA.

1	Number	of global i	terations	CPU time / s				
n	FDM	CDM	CSDA	Full CSDA	FDM	CDM	CSDA	Full CSAD
100	failure	failure	failure	failure	failure	failure	failure	failure
10-1	56	56	failure	failure	98.3	100.1	failure	failure
10-2	55	47	47	failure	95.4	86.4	84.3	failure
10-3	36	38	39	failure	69.4	73.5	72.4	failure
10-4	38	40	39	42	72.1	76.1	72.0	194.7
10-5	39	39	39	40	73.0	74.9	71.9	166.0
10-6	40	39	40	40	74.4	75.6	73.5	162.2
10-7	40	39	42	39	74.4	75.5	76.8	159.9
10-8	40	39	39	42	75.0	74.4	72.1	169.8
10-9	39	40	39	41	73.8	75.8	72.2	165.0
10-10	39	43	42	40	72.8	80.6	76.4	162.1
10-11	47	42	40	39	86.6	79.4	74.4	159.5
10-12	failure	58	39	40	failure	103.0	71.6	161.0
10-13	failure	failure	39	40	failure	failure	71.9	161.9
10-14	failure	failure	41	40	failure	failure	74.6	160.2
10-15	failure	failure	40	39	failure	failure	73.8	156.6
10-16	failure	failure	39	39	failure	failure	71.3	157.5

Table 4 Computational overhead of different numerical schemes

It can be found that the full CSDA consumes more CPU time than CSDA because the full CSDA involves more numerical evaluation of derivatives. In addition, the convergence of full CSDA is worse than that of CSDA when the perturbation value is large. The reason is that the truncation error of the numerical solution obtained by the full CSDA will not only influence the convergence of the global solution but also influence the convergence of local iteration by the Jacobian matrix. Whereas, the full CSDA will make the model implementation extremely simple because there is no need for any analytical derivative evaluation for both the consistent tangent operator and Jacobian matrix. In the practical application, the simple derivative terms in the two can be analytically derived to reduce the computationaloverhead.

In what follows, the convergence behaviour of the proposed algorithm on the global level is investigated in the cases of $\mu = 1.0$ and 0.9. Fig. 13 shows the changing law of logarithm normalized largest residual force with the global iteration number, where the numerical consistent tangent operator obtained by the CSDA and the analytical consistent tangent operator are compared. The global iterations number of each load step is almost less than 4 due to the global quadratic convergence of consistent tangent operator. In addition, the convergence behaviours of the numerical consistent tangent operator is almost the same as that of the analytical one, which shows that the proposed algorithm based on the CSDA can avoid tedious derivative operation while ensuring the global quadratic convergence.



398

Fig. 13 Convergence behaviour at the global equilibrium iteration: (a) $\mu = 1.0$; (b) $\mu = 0.9$.

399

5.3 Strip foundation under inclined load

In what follows, the convergence of the model implementation under large load increment input is investigated by comparing it with the default MCC model of ABAQUS. The analytical Jacobian matrix and consistent tangent operator are used to objectively evaluate the gain from the line search method on the algorithm's convergence. The target example is a strip foundation under an inclined load. Fig. 14 presents boundary conditions and finite element mesh of example. The elastic model and NEP clay model are adopted for the strip foundation and soil, respectively.

405 E = 20 MPa and v = 0.3 are chosen for the elastic model. The total weight of soil is set to 19 kN/m³. The material 406 parameters of NEP clay model⁵¹ are presented in Table 5. The preload of top surface is 9kPa at the geostatic step. Then, 407 the top surface of foundation is subjected to an inclined displacement load ($U_1 = -0.8$ m and $U_1 = -0.2$ m). The total 408 analysis time of 1 s and the initial time increment size of 0.01 s are chosen. The size of subsequent time increments 409 is determined by the ABAQUS default step control strategy.





Fig. 14 Strip foundation: (a) model geometry; (b) finite element mesh.



almost the same. The reason is that the line search method has a stronger convergence than the Newton method.Therefore, a larger load step input is allowed for the presented model implementation than the ABAQUS default



417



416 Fig. 15 Comparison between ABAQUS default algorithm and the presented numerical implementation with

 $\mu = 1.0$: (a) reaction force vs. displacement; (b) change in time increment.

Furthermore, the influence of fractional order μ on the mechanical response of strip foundation example are 418 419 investigated, where the cases of $\mu = 0.3, 0.6, 1.0, 1.4$, and 1.7 are considered, as shown in Fig. 16. During the initial 420 loading period, the reaction force-displacement curves with the different μ -values almost coincide. With the increase 421 of displacement load, the reaction force of the foundation top surface is smaller with a higher μ -value due to that the 422 stiffness of clay decreases as μ increases. This means that the NEP clay model may provide an effective tool for 423 numerical analysis of geotechnical problems of clay with different stiffness. On the other hand, the calculation results 424 with the different μ -values also demonstrate that the proposed algorithm is not only applicable to MCC model (μ = 1.0), but also NEP clay model ($\mu \neq 1.0$). 425



Fig. 16 Influence of parameter μ on simulation results

427 **5.4 Pile foundation bearing capacity test**

426

428 The last boundary problem is a pile load capacity in the undrained clay subsoil. In view of the symmetry of the 429 problem, a quarter model as shown in Fig. 17 (a) is established to further explore the ability of the presented model 430 implementation to address the 3D coupled problem. The bottom boundary of the analysis area is 1 times the pile 431 diameter from the pile bottom, and the horizontal range is 20 times the pile diameter. The pile-soil interface is modelled by the frictional contact with a frictional coefficient of 0.25. The parameters of NEP clay model are presented in Table 432 433 5. The pile employs the linear elastic model with E = 20 GPa and v = 0.2. The 8 nodes brick pore pressure elements 434 (C3D8P) is used to capture the pore pressure response of soil during pile penetration. The effective weight of soil $8 \text{ kN} / \text{m}^3$ and permeability $3.6 \times 10^{-4} \text{ m/h}$ are used. The numerical simulation contains two analysis steps, i.e., the 435 436 geostatic equilibrium and loading analysis steps. The vertical displacement of 0.05 m is loaded on the pile top. The 437 initial time increment, maximum time increment, and total analysis time are set to 500 s, 50 s, and 3600 s, 438 respectively. Fig. 17 (b) depicts the pore pressure distribution result.



those of ABAQUS, which again verifies the current algorithm's correctness. The results under different μ -values are also presented in Fig. 18 (b). The difference of simulation results with different μ -values is very small. For the pile foundation problem, its bearing capacity mainly depends on the friction effect between the pile and soil and the undrained shear strength of soil. The change of parameter μ will not affect these two.





Fig. 17 Pile foundation: (a) model geometry; (b) simulation results.



446 Fig. 18 Reaction force-displacement curves of pile foundation: (a) comparison between ABAQUS and UMAT; (b)

influence of parameter μ on simulation results.

Boundary value problems	М	λ	К	ν	<i>e</i> ₁	μ
Cylindrical cavity expansion ⁴⁸	1.2	0.15	0.03	0.278	1.823	1.0
Conventional triaxial compression test	1.0	0.25	0.05	0.3	1.825	0.9/1.0
Square/Strip foundations ⁵¹	0.898	0.25	0.05	0.3	1.6	0.3~1.7
Pile foundation ²⁰	1.2	0.2	0.04	0.35	2.0	0.3~1.7

Table 5 Material parameters of NEP clay model used for boundary value problems

449

450 6. CONCLUSION

This paper has proposed a robust and concise implicit stress update algorithm through the combination of smooth function, line search method, and CSDA to implement the NEP clay model. In the model implementation, the smooth function replaces inequality constraints of stress integral equations to eliminate the non-smoothness. The use of the line search method makes the proposed algorithm have a better convergence in large step calculation, even for strong nonlinear cases. The CSDA was used to numerically evaluate the Jacobian matrix used in the local iteration of the model and the consistent tangent operator used in the global iteration to provide quadratic convergence. The NEP clay model has been implemented into the ABAQUS through the new algorithm.

For the validation purpose, the performance of model implementation was assessed by four boundary value problems. In the cylindrical cavity expansion examples, the numerical predictions with the UMAT were in good agreement with the analytical solution, which verified the accuracy of the model implementation. Conventional triaxial compression examples under different perturbation values show that the CSDA has a better numerical robustness than the FDM and the CDM because it has no subtraction cancellation error. The strip foundation example under inclined load also indicated that the proposed algorithm has better convergence than the ABAQUS default algorithm and allows

464 large step load calculation. As a potential application, the model implementation based on the proposed algorithm was 465 used for the analysis of bearing capacity of the pile in the undrained clay subsoil, where the consistency of the results 466 from the UMAT and the ABAQUS further verify the effectiveness of the model implementation in dealing with 467 geotechnical problems.

The proposed algorithm is extremely attractive for the implicit implementation of the complex elastoplastic model since there is no need for cumbersome derivative evaluation and loading/unloading estimation. Users are only required to pay attention to the construction of implicit stress integral equations. Although the numerical differentiation requires more computational overhead than the analytical derivation for the determination of the Jacobian matrix and consistent tangent operator, this additional time consumption can be reduced by using the analytical derivation to obtain simple

473 derivative terms.

474 CREDIT AUTHORSHIP CONTRIBUTION STATEMENT

Dechun Lu: Conceptualization, Methodology, Supervision, Project administration, Writing - Original draft
preparation. Yaning Zhang: Data curation, Writing - Original draft preparation, Writing - Review & Editing,
Visualization, Software, Formal analysis. Xin Zhou: Writing - Original draft preparation, Software, Writing - Review
& Editing, Formal analysis, Supervision. Cancan Su: Conceptualization, Methodology, Formal analysis. Zhiwei Gao:
Conceptualization, Methodology. Xiuli Du: Conceptualization, Methodology.

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483 DATA AVAILABILITY STATEMENT

484 The source codes of this study are available from https://github.com/zhouxin615.

APPENDIX A. DETAILS OF JACOBIAN MATRIX: 485

$$\begin{cases} f_{1,1} = 1 + \Delta \phi_{n+1} K_{n+1}^* \left(\frac{2p_{n+1}^{1-\mu}}{\Gamma(2-\mu)} - \frac{\mu q_{n+1}^2}{N^2 p_{n+1}^{1+\mu} \Gamma(1-\mu)} - \frac{p_{c,n+1}}{p_{n+1}^{\mu} \Gamma(1-\mu)} \right) \\ f_{1,2} = \frac{2q_{n+1} \Delta \phi_{n+1} K_{n+1}^*}{N^2 p_{n+1}^{\mu} \Gamma(1-\mu)} \\ f_{1,3} = -\frac{p_{n+1}^{1-\mu} \Delta \phi_{n+1} K_{n+1}^*}{\Gamma(2-\mu)} \\ f_{1,4} = K_{n+1}^* \left(\frac{q_{n+1}^2}{p_{n+1}^{\mu} N^2 \Gamma(1-\mu)} + \frac{2p_{n+1}^{2-\mu}}{\Gamma(3-\mu)} - \frac{p_{c,n+1} p_{n+1}^{1-\mu}}{\Gamma(2-\mu)} \right) \end{cases}$$
(A1)

$$487 \qquad \begin{cases} f_{2,1} = -\sqrt{\frac{3}{2}}a_{8}\left\{2a_{9}\frac{\partial\Delta\varepsilon_{v,n+1}^{e}}{\partial p_{n+1}}\hat{\mathbf{n}}:\Delta\gamma_{n+1} - 6a_{8}\Delta\phi_{n+1}\|\mathbf{s}_{n} + 2\bar{G}\Delta\gamma_{n+1}\|\left[a_{9}\frac{\partial\Delta\varepsilon_{v,n+1}^{e}}{\partial p_{n+1}}\left[\frac{q_{n+1}^{l-\mu}}{N^{2}\Gamma(3-\mu)} + \frac{p_{n+1}(p_{n+1}-p_{c,n+1})}{2q_{n+1}^{l+\mu}\Gamma(1-\mu)}\right] + \bar{G}\frac{(2p_{n+1}-p_{c,n+1})}{2q_{n+1}^{l+\mu}\Gamma(1-\mu)}\right]\right\} \\ f_{2,2} = 1 - \sqrt{\frac{3}{2}}a_{8}\left\{2a_{9}\frac{\partial\Delta\varepsilon_{v,n+1}^{e}}{\partial q_{n+1}}\hat{\mathbf{n}}:\Delta\gamma_{n+1} - 6a_{8}\Delta\phi_{n+1}\|\mathbf{s}_{n} + 2\bar{G}\Delta\gamma_{n+1}\|\left[a_{9}\frac{\partial\Delta\varepsilon_{v,n+1}}{\partial q_{n+1}}\left[\frac{q_{n+1}^{l-\mu}}{N^{2}\Gamma(3-\mu)} + \frac{p_{n+1}(p_{n+1}-p_{c,n+1})}{2q_{n+1}^{l+\mu}\Gamma(1-\mu)}\right] + \bar{G}[\frac{1-\mu}{N^{2}q_{n+1}^{\mu}\Gamma(3-\mu)} + \frac{p_{n+1}(-\mu-1)(p_{n+1}-p_{c,n+1})}{2q_{n+1}^{l+\mu}\Gamma(1-\mu)}]\right]\right\} \\ f_{2,3} = -\sqrt{\frac{3}{2}}a_{8}\left\{2a_{9}\frac{\partial\Delta\varepsilon_{v,n+1}}{\partial p_{c,n+1}}\hat{\mathbf{n}}:\Delta\gamma_{n+1} - 6a_{8}\Delta\phi_{n+1}\|\mathbf{s}_{n} + 2\bar{G}\Delta\gamma_{n+1}\|\left[a_{9}[\frac{q_{n+1}^{l-\mu}}{N^{2}\Gamma(3-\mu)} + \frac{p_{n+1}(p_{n+1}-p_{c,n+1})}{2q_{n+1}^{\mu+1}\Gamma(1-\mu)}\right]\frac{\partial\Delta\varepsilon_{v,n+1}}{\partial p_{c,n+1}} - \frac{\bar{G}p_{n+1}}{2q_{n+1}^{\mu+1}\Gamma(1-\mu)}\right]\right\}$$
(A2)

488 where
$$\hat{\mathbf{n}} = \frac{\mathbf{s}_{n+1}}{\|\mathbf{s}_{n+1}\|}$$
, $\overline{G} = \overline{K}r = r \frac{p_n}{\Delta \varepsilon_{v,n+1}^e} \Big[\exp(c_\kappa \Delta \varepsilon_{v,n+1}^e) - 1 \Big]$.

$$\begin{cases} f_{3,1} = -c_p \Delta \phi_{n+1} p_c^* \Big[\frac{2p_{n+1}^{1-\mu}}{\Gamma(2-\mu)} - \frac{\mu q^2}{p_{n+1}^{1+\mu} N^2 \Gamma(1-\mu)} - \frac{p_{c,n+1}}{p_{n+1}^{\mu} \Gamma(1-\mu)} \Big] \\ f_{3,2} = -\frac{2p_c^* c_p \Delta \phi_{n+1} q_{n+1}}{p_{n+1}^{\mu} N^2 \Gamma(1-\mu)} \\ f_{3,3} = 1 + \frac{p_c^* c_p \Delta \phi_{n+1} p_{n+1}^{1-\mu}}{\Gamma(2-\mu)} \\ f_{3,4} = p_c^* c_p \Big[\frac{p_{c,n+1} p_{n+1}^{1-\mu}}{\Gamma(2-\mu)} - \frac{q_{n+1}^2}{N^2 p_{n+1}^{\mu} \Gamma(1-\mu)} - \frac{2p_{n+1}^{2-\mu}}{\Gamma(3-\mu)} \Big] \end{cases}$$
(A3)

where $p_{c}^{*} = (p_{c})_{n} \exp\left(c_{p}\Delta\phi_{n+1}\frac{\partial^{\mu}f_{n+1}}{\partial p_{n+1}^{\mu}}\right)$ 490

491

$$\begin{cases}
f_{4,1} = \frac{\partial f_4}{\partial p_{n+1}} = \chi_0 \left(2 p_{n+1} - p_{c, n+1} \right) \\
f_{4,2} = \frac{\partial f_4}{\partial q_{n+1}} = \chi_0 \frac{2q_{n+1}}{N^2} \\
f_{4,3} = \frac{\partial f_4}{\partial p_{c, n+1}} = -\chi_0 p_{n+1} \\
f_{4,4} = \frac{\partial f_4}{\partial \Delta \phi_{n+1}} = \chi_1
\end{cases}$$
(A4)

492 where
$$\chi_0 = \frac{\partial f_4}{\partial f_{n+1}} = \frac{f_{n+1}}{\sqrt{(c_d \Delta \phi_{n+1})^2 + f_{n+1}^2 + 2\beta}} + 1$$
 and $\chi_1 = \frac{\partial f_4}{\partial \Delta \phi_{n+1}} = \frac{c_d^2 \Delta \phi_{n+1}}{\sqrt{(c_d \Delta \phi_{n+1})^2 + f_{n+1}^2 + 2\beta}} - c_d$.

493 APPENDIX B. MATRIX REPRESENTATION OF TENSORS:

494 The matrix representation of second order includes:

 $\mathbf{1} = \delta_{ij} \mathbf{e}_i \otimes \mathbf{e}_j$, where \mathbf{e}_i and \mathbf{e}_j denote the orthonormal bases of second-order tensor. The Kronecker delta δ_{ij}

496 can be expressed by:

$$\delta_{ii} = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \end{bmatrix}^T \tag{B1}$$

 $\partial f / \partial \boldsymbol{\sigma} = \partial f / \partial \sigma_{ij} \, \mathbf{e}_i \otimes \mathbf{e}_j$, where $\partial f / \partial \sigma_{ij}$ is expressed by:

499
$$\frac{\partial f}{\partial \sigma_{ij}} = \begin{bmatrix} \partial f / \partial \sigma_{11} & \partial f / \partial \sigma_{22} & \partial f / \partial \sigma_{33} & 2 \partial f / \partial \sigma_{12} & 2 \partial f / \partial \sigma_{23} & 2 \partial f / \partial \sigma_{13} \end{bmatrix}^T$$
(B2)

 $\Delta \boldsymbol{\sigma} = \Delta \sigma_{ij} \mathbf{e}_i \otimes \mathbf{e}_j$, where $\Delta \sigma_{ij}$ can be expressed by:

501
$$\Delta \sigma_{ij} = \begin{bmatrix} \Delta \sigma_{11} & \Delta \sigma_{22} & \Delta \sigma_{33} & \Delta \sigma_{12} & \Delta \sigma_{23} & \Delta \sigma_{13} \end{bmatrix}^T$$
(B3)

 $\Delta \boldsymbol{\varepsilon}_{n+1} = \Delta \boldsymbol{\varepsilon}_{ij} \boldsymbol{e}_i \otimes \boldsymbol{e}_j$, where $\Delta \boldsymbol{\varepsilon}_{ij}$ can be expressed by:

$$\Delta \varepsilon_{ij} = \begin{bmatrix} \Delta \varepsilon_{11} & \Delta \varepsilon_{22} & \Delta \varepsilon_{33} & \Delta \varepsilon_{12} & \Delta \varepsilon_{23} & \Delta \varepsilon_{13} \end{bmatrix}^T$$
(B4)

 $\Delta \mathbf{\gamma}_{n+1} = \Delta \gamma_{ij} \mathbf{e}_i \otimes \mathbf{e}_j$, where $\Delta \gamma_{ij} = \Delta \varepsilon_{ij} - \delta_{ij} \Delta \varepsilon_v / 3$ can be expressed by:

505
$$\Delta \gamma_{ij} = \begin{bmatrix} \Delta \gamma_{11} & \Delta \gamma_{22} & \Delta \gamma_{33} & \Delta \gamma_{12} & \Delta \gamma_{23} & \Delta \gamma_{13} \end{bmatrix}^T$$
(B5)

 $\hat{\mathbf{n}} = \hat{n}_{ij} \mathbf{e}_i \otimes \mathbf{e}_j$, where \hat{n}_{ij} can be expressed by:

507
$$\hat{n}_{ij} = \begin{bmatrix} \hat{n}_{11} & \hat{n}_{22} & \hat{n}_{33} & \hat{n}_{12} & \hat{n}_{23} & \hat{n}_{13} \end{bmatrix}^T = \frac{1}{\|\mathbf{s}\|} \begin{bmatrix} s_{11} & s_{22} & s_{33} & s_{12} & s_{23} & s_{13} \end{bmatrix}^T$$
 (B6)

 $\tilde{\mathbf{n}} = \tilde{n}_{ij} \mathbf{e}_i \otimes \mathbf{e}_j$, where \tilde{n}_{ij} can be expressed by:

509
$$\tilde{n}_{ij} = \begin{bmatrix} \hat{n}_{11} & \hat{n}_{22} & \hat{n}_{33} & 2\hat{n}_{12} & 2\hat{n}_{23} & 2\hat{n}_{13} \end{bmatrix}^T$$
 (B7)

510 The matrix representation of fourth order includes:

511
$$\mathbf{I} = \mathbf{I} \otimes \mathbf{I} = \delta_{ij} \delta_{kl} \mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l$$
, where \mathbf{e}_i , \mathbf{e}_j , \mathbf{e}_k , and \mathbf{e}_l are the orthonormal bases of fourth-order tensor

512 and $\delta_{ij}\delta_{kl}$ can be expressed by:

 $\mathbf{I}^{\text{vol}} = \frac{1}{3} \mathbf{1} \otimes \mathbf{1} = \frac{1}{3} \delta_{ij} \delta_{kl} \mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l$, where $\frac{1}{3} \delta_{ij} \delta_{kl}$ can be expressed by:

516
$$\mathbf{I}^{\text{sym}} = \frac{1}{2} \left(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) \mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l \text{, where } \frac{1}{2} \left(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) \text{ can be expressed by:}$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \end{bmatrix}$$

517
$$\frac{1}{2} \left(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/2 \end{bmatrix}$$
(B10)

518
$$\overline{\mathbf{D}} = 3\mathbf{I}^{\text{vol}}\left(\overline{K} - \frac{2}{3}\overline{G}\right) + 2\mathbf{I}^{\text{sym}}\overline{G} = \overline{D}_{ijkl}\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l \text{, where } \overline{D}_{ijkl} \text{ can be expressed by:}$$

519
$$\overline{D}_{ijkl} = \delta_{ij}\delta_{kl}\overline{K}\left(1 - \frac{2}{3}r\right) + \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right)\overline{K}r = \overline{K}\begin{bmatrix} 1 + \frac{1}{3}r & 1 - \frac{2}{3}r & 0 & 0 & 0\\ 1 - \frac{2}{3}r & 1 + \frac{1}{3}r & 1 - \frac{2}{3}r & 0 & 0 & 0\\ 1 - \frac{2}{3}r & 1 - \frac{2}{3}r & 1 + \frac{1}{3}r & 0 & 0 & 0\\ 0 & 0 & 0 & r & 0 & 0\\ 0 & 0 & 0 & 0 & r & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & r & 0\\ 0 & 0 & 0 & 0 & 0 & r & 0 \end{bmatrix}$$
(B11)

520
$$\mathbf{P} = \left(\delta_{ik}\delta_{jl} - \frac{1}{3}\delta_{ij}\delta_{kl}\right)\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l \text{ where } \delta_{ik}\delta_{jl} - \frac{1}{3}\delta_{ij}\delta_{kl} \text{ can be expressed by:}$$

521
$$\overline{D}_{ijkl} = \delta_{ij} \delta_{kl} \overline{K} \left(1 - \frac{2}{3}r \right) + \left(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) \overline{K}r = \overline{K} \begin{bmatrix} 1 + \frac{1}{3}r & 1 - \frac{2}{3}r & 1 - \frac{2}{3}r & 0 & 0 & 0 \\ 1 - \frac{2}{3}r & 1 + \frac{1}{3}r & 1 - \frac{2}{3}r & 0 & 0 & 0 \\ 1 - \frac{2}{3}r & 1 - \frac{2}{3}r & 1 + \frac{1}{3}r & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & r & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & r & 0 \\ 0 & 0 & 0 & 0 & 0 & r & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & r \end{bmatrix}$$
(B12)
522
$$\delta_{ik} \delta_{jl} - \frac{1}{3} \delta_{ij} \delta_{kl} = \begin{bmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} & 0 & 0 & 0 \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & 0 & 0 & 0 \\ -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \end{bmatrix}$$
(B13)

523

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