

# Consistency in solving the inverse problem of the Voce-Chaboche constitutive model for plastic straining

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## ABSTRACT

This paper focuses on an inverse problem involving a commonly used material model in structural steel applications - the Voce-Chaboche model. In particular, this paper proposes an approach focused on obtaining a consistent set of material parameters that accurately represents a wide range of mechanical uniaxial cyclic load histories. The main focus of the methodology presented in this manuscript is its application to structural steels in the field of earthquake engineering. A set of load protocols representative of seismic loading are proposed for this purpose. It is shown that the calibration procedure optimally leverages Voce-Chaboche's ability to describe the material response to an arbitrary load history. Parameters for prevailing American, European and Japanese structural steels are also proposed.

**Keywords:** Inverse problem, Structural steel, Chaboche, Material modeling, Earthquake loading

## INTRODUCTION

Representative modeling of the behavior of structural systems at large deformations associated with collapse depends crucially on two features: material and geometric nonlinearities. Behavior is often governed by a composition of these two phenomena and, as such, greater

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20 accuracy in modeling each of these traits will improve simulating the dynamics of their in-  
21 teraction. In structural steel applications this is of particular consequence in estimating  
22 member and local buckling and their performance in the post-buckling regime, which are  
23 essential in assessing behavior to collapse. This paper focuses on the material nonlinearity  
24 side of the issue.

25 Experimental observations of cyclically loaded structural steels show a combination of dis-  
26 tinctive features. Chiefly among them are strain hardening, the *Bauschinger effect* (Bauschinger  
27 1874), and ratcheting (Hassan and Kyriakides 1992). Strain hardening encapsulates the find-  
28 ing that the stress carried after some amount of irreversible deformation has a tendency to  
29 increase due to the built up resistance to the movement of dislocations caused by phenomena  
30 such as interactions with dislocations forests and dislocation pile-ups - *c.f.* Nabarro et al.  
31 (1964) for a classic review of the fundamental mechanisms. The Bauschinger effect captures  
32 the observation that an increase in the flow stress in a particular direction lowers the yield  
33 stress when loading is exacted in the opposite direction. This is mainly attributed to dislo-  
34 cation pile-ups and stress accumulation in the original load direction that when it's reversed  
35 assist the movement of the dislocations in the inverse path. Lastly, under constant stress  
36 amplitude and nonzero mean stress cyclic tests an accumulation of plastic strain with each  
37 cycle in the direction of the average stress is typically observed. This phenomenon is termed  
38 ratcheting or cyclic creep - *c.f.* Hassan and Kyriakides (1992) for an overview of relevant  
39 experimental results.

40 Modeling the aforementioned material behaviors is typically done within the  $J_2$  plasticity  
41 framework (von Mises 1928) and literature on the subject is vast. Some focus is demanded  
42 and therefore this paper concerns itself solely with time-independent uniaxial material re-  
43 sponses - *c.f.* Chaboche (2008) for a thorougher review. Time-independent material models  
44 are usually employed unless the application at hand strictly mandates a material-transient  
45 analysis. To date, structural analyses of steel buildings specific to seismic seldom consider  
46 material transient effects. Simulation strategies frequently address the aforementioned issues

47 by assigning evolution laws to the yield function and the plastic potential (associative plas-  
48 ticity). The surfaces either change in size (isotropic hardening - Hill 1950) and/or translate  
49 in stress space (kinematic hardening - Prager 1956) in order to capture work hardening.  
50 The kinematic approach has the added feature of capturing the Bauschinger effect and as a  
51 consequence is used ubiquitously in cyclic loading. The introduction of material nonlinearity  
52 in the models can be achieved in a variety of ways: analytically, by specifying the evolu-  
53 tion of a surface as power laws or saturating exponentials (*e.g.* the Ludwik 1909 or Voce  
54 (1948) expressions for isotropic hardening, respectively); a combination of linear-hardening  
55 surfaces (Hodge 1956 for isotropic and Mróz 1967 for kinematic hardening); or by stipulating  
56 growth rates as a function of the distance of the current surface to a limit surface (Dafalias  
57 and Popov 1975 and Dafalias 1986 for kinematic hardening). A significant contribution in  
58 modeling nonlinear kinematic hardening was made by Armstrong and Fredrick (1966). The  
59 simplicity in their approach in combination with its ability to simulate ratcheting has made  
60 its use widespread. Later, Chaboche et al. (1979) suggested using an additive decomposition  
61 of that rule to improve its performance. After, Dafalias et al. (2008) introduced the concept  
62 of multiplicative Armstrong-Fredrick (AF) hardening to further enhance Chaboche’s model.  
63 Although AF-type laws perform well in uniaxial loading one of its main criticisms is the  
64 overestimation of ratcheting strains in multiaxial settings as shown, *e.g.*, in Ohno and Wang  
65 (1993).

66 Caution should, nonetheless, be exercised when considering those criticisms as analyses  
67 are arguably only as good as the input model parameters used in performing them. As  
68 pointed out by Rezaiee-Pajand and Sinaie (2009), too often are trial-and-error approaches  
69 used to approximate a response to subjective levels of accuracy, whereas using a systematic  
70 methodology to calibrate the Chaboche model parameters can be shown to improve their  
71 behavior when compared to values previously reported in literature. Nonunique solutions is  
72 the issue at hand. Distinct parameter sets can have very similar error levels in one situation,  
73 but very disparate ones in other circumstances - *c.f.*, *e.g.*, Cooke and Kanvinde (2015). An

74 essential part in facing this problem is, therefore, finding sufficiently differentiating conditions  
75 and minimizing the lack-of-fit of the models to the experiments. Using a diverse collection  
76 of load protocols is a valuable tool in this regard.

77 Past experimental studies (e.g., Krawinkler et al. 1983; Lignos et al. 2011; Suzuki and  
78 Lignos 2015) have underscored the sensitivity of structural component deterioration to the  
79 imposed loading history. Systematic load protocols have been developed for structural testing  
80 to depict the strength and stiffness deterioration of a component under seismic loading  
81 depending on the performance level of interest (e.g., Krawinkler 1996; Suzuki and Lignos  
82 2019 ). However, there seems to be a lack of systematic protocols at a macroscopic material  
83 scale to manifest reliable material parameters (e.g., cyclic hardening) that could be used  
84 for constitutive material model input parameter calibrations to reliably prognosticate the  
85 behavior of steel structural components under seismic loading. Past experimental studies and  
86 standards (ASTM 2012; ASTM 2013; ISO 2016) have mainly focused on the identification  
87 of typical mechanical properties of structural steels under tensile loading as well as various  
88 types of fatigue applications involving constant, step-wise increasing or variable amplitude  
89 material testing (Miller and Amin 1975; Krawinkler et al. 1983; Kaufmann et al. 2001;  
90 Braconi et al. 2013; Dehghani et al. 2017) .

91 Methods to solve inverse problems are not straightforward and a number of suggestions  
92 to address them can be found in literature. There exist analytical procedures that are model-  
93 specific, like the ones suggested by Rezaiee-Pajand and Sinaie (2009) or, more recently, Koo  
94 et al. (2019) which are relevant for the material model in question. Their application is  
95 however focused more on ratcheting behavior and less so on more comprehensive hysteretic  
96 responses under different load conditions. More general methodologies can be found in the  
97 context of mathematical optimization. There, one tries to minimize a well-defined objective  
98 function that describes how a material model approximates the experimental data. There  
99 are established and powerful tools under this framework for least square fitting of nonlinear  
100 functions - see *e.g.* Bierlaire (2015). Unconstrained gradient-based minimization methods

101 like the Gauss-Newton method and its damped version, the Levenberg-Marquardt algorithm  
102 (Levenberg 1944, Marquadt 1963), are among the state of the art in inverse problems with  
103 applications in hyperelastic (Gendy and Saleeb 2000, Holzapfel et al. 2000), nonlinear het-  
104 erogeneous with a prescribed stress-strain curve (Bickel et al. 2009), plastic, viscoplastic  
105 and damaged materials (Bruhns and Anding 1999, Andrade-Campos et al. 2007, Lemaitre  
106 and Desmorat 2005). A different class of methods known as randomized search algorithms  
107 can also be found in literature for the calibration of material properties, such as simulated  
108 annealing (Kirkpatrick et al. 1983), genetic and evolutionary algorithms (Pal et al. 1996,  
109 Furukawa and Yagawa 1997), and swarm algorithms (Smith et al. 2017). Although an anal-  
110 ysis between the two approaches is beyond the scope of this paper, the reader is nonetheless  
111 referred to Andrade-Campos et al. (2007) for an interesting discussion of the topic. The  
112 scheme used in this paper is gradient-based, comparable to the Levenberg-Marquadt algo-  
113 rithm but formulated within a Newton Trust-Region (NTR) framework (Conn et al. 2000).  
114 Essential details on its implementation are given in the methodology section.

115 This paper proposes a methodology comprising (a) experimental and (b) optimization  
116 procedures in order to solve, implement, and obtain calibrated input model parameters.  
117 The material model herein consists of a nonlinear isotropic and kinematic hardening model,  
118 following the Voce and Chaboche rules, respectively. Subsequently, the results of the appli-  
119 cation of these techniques to a set European, American and Japanese structural steels will  
120 be presented, followed by a section discussing those results. The paper will finish with a  
121 brief conclusion section summarizing the main observations of this research study.

## 122 **METHODOLOGY**

123 This section presents the proposed methodology used in the inverse problem approach.  
124 It is organized into five subsections, starting with the definition materials and testing pro-  
125 cedures, followed by selection of load protocols, a presentation on the material model, the  
126 inverse problem definition, and, finally, the recommended optimization scheme. The method-  
127 ology focuses on model behavior under uniaxial load and uses this fact to simplify the evalu-

128 ation procedure. The approach is based on the integration of the analytic uniaxial version of  
129 the Voce-Chaboche (VC) hardening model. The integration of the response along the strain  
130 path is conducted numerically by using discrete true-strain steps following the load protocols.  
131 It is recommended that responses be obtained from engineering metrics of uniaxial coupon  
132 tests. This approach is in contrast to procedures that explicitly model coupons in Finite  
133 Element analyses and obtain their responses by imposing displacement boundary conditions  
134 at their ends. Furthermore, this approach distinguishes itself from calibration methods that  
135 are based in far-field measurements, such as member moment-rotation responses (*c.f.*, *e.g.*  
136 Araújo et al. 2017). It is believed that characterizing the response of coupon-scale specimens  
137 is a more apt descriptor of material behavior since the problem is more bounded. Member  
138 responses often carry confounding factors that are geometry-specific, such as the assumed  
139 imperfections for the member, or plastic hinge length effects that are influenced by both the  
140 cross-section geometry and material hardening (Elkady and Lignos 2018). On the contrary,  
141 tests conducted on round coupons with local strain measurements allow these problems to  
142 be significantly mitigated.

## 143 **Materials and testing procedures**

144 A number of structural steels of different grades and producers are studied in this paper  
145 - *c.f.* Table 1 for a summary of their tensile properties. The data analyzed herein were  
146 sourced from Grigoriou and Lignos (2017) and in-house experiments, for European steels  
147 (S355J2+N, S355J2, S460NL and S690QL) and Suzuki (2018) for typical American (A992  
148 Gr. 50 and A500 Gr. B) and Japanese steels (BCP325, BCR295 and HYP400). Specimens  
149 were obtained from different structural elements such as plates, web and flange of I-shape  
150 sections, and the walls of square hollow sections. All specimens are uniaxially loaded. Alas,  
151 not all load protocols are available for each material type. A summary table with the material  
152 parameters is provided in the results section (*cf.* Table 5) and the load protocols to which  
153 they were calibrated are noted explicitly. For the sake of simplicity, the analysis presented  
154 in the result section on the optimization algorithm is conducted with a standard material,

155 an S355J2+N steel (nominal yield stress of 355MPa, minimum Charpy V-notch test of 27  
156 Joules at -20°C and with a normalized heat treatment) whose round coupons are extracted  
157 from 50mm thick plates. The main observations, however, can be taken to hold for the whole  
158 dataset.

159 Testing procedures for metallic materials subject to uniaxial tensile loading at ambient  
160 temperatures have long been the subject of standardization.- *c.f. e.g.* ASTM (2013) and  
161 ISO (2016). Useful guiding standards for cyclic strain-controlled tests can also be - *c.f.*,  
162 *e.g.*, ASTM (2012). Two fundamental variables used extensively throughout this paper  
163 have to be defined: uniaxial true stress ( $\sigma$ ) and uniaxial true strain ( $\varepsilon$ ). Starting with the  
164 measured variables force ( $F$ ) and displacement in extensometer ( $\Delta L$ , with  $L$  being the gauge  
165 length  $\Delta L$  is the change in the initial gauge length), one defines the stress in the reference  
166 configuration as the engineering stress ( $\sigma_{eng} = F/A_0$ , with  $A_0$  the initial cross-sectional  
167 area of the specimen) and the strain in the reference configuration as the engineering strain  
168 ( $\varepsilon_{eng} = (L - L_0)/L_0$ ). True stress and true strain are stresses and strains in the deformed  
169 configuration, which in uniaxial loading can be shown to be equal to Eq. 1 and 2, respectively  
170 - *c.f., e.g.* (Lubliner 2008).

$$171 \quad \sigma = \sigma_{eng} (1 + \varepsilon_{eng}) = \frac{F}{A_0} \left( 1 + \frac{L - L_0}{L_0} \right) \quad (1)$$

$$172 \quad \varepsilon = \ln(1 + \varepsilon_{eng}) = \ln \left( 1 + \frac{L - L_0}{L_0} \right) \quad (2)$$

173 Challenges pertinent to the uniaxial cyclic coupon testing relate to (a) the type of test-  
174 setup grip (ASTM 2012), (b) specimen buckling, and (c) the stiffness of the test apparatus  
175 not to compound on those nonlinear geometric effects - *cf. e.g.* Dehghani et al. (2017).

## 176 Selection of load protocols

177 The uniaxial strain-based protocols are developed based on nonlinear response history  
178 analyses of more than 80 capacity-designed steel moment-resisting frames (MRFs) ranging

179 from two to 12 stories. The steel MRFs comprise columns with hollow square sections (HSS)  
180 and I-shape steel beams with fully restrained beam-to-column connections. The steel MRFs  
181 are modeled in 2-dimensions (2D) in the open system for earthquake engineering simulation  
182 platform (OpenSees) (McKenna 1997). Local demand parameters (e.g., stress-strain field)  
183 is of particular interest for the load protocol development. Therefore, the use of distributed  
184 plasticity frame elements is imperative. Particularly, steel beams and columns are modeled  
185 with a force-based formulation (Spacone et al. 1996) with five integration points along their  
186 length. A fiber-based approach is employed to represent the HSS cross-section, which is dis-  
187 cretized based on recommendations by Kostic and Filippou (2012) . A uniaxial stress-strain  
188 formulation is assigned to each one of the fiber elements based on the Menegotto-Pinto uni-  
189 axial formulation (Menegotto and Pinto 1973). The input model parameters are calibrated  
190 to available test data (Lignos and Krawinkler 2013). The component modeling does not con-  
191 sider the effects of strength and stiffness deterioration on the structural response. Arguably,  
192 component deterioration is likely to dominate the steel MRF response at large inelastic drift  
193 demands (Zareian et al. 2010). However, this is not expected to be the case at modest drift  
194 demands associated with design-basis seismic events with a probability of exceedance of 10%  
195 in 50 years or in cases that P-Delta effects dominate the structural response prior to collapse  
196 (Adam and Jäger 2012). Therefore, the modeling approach is justified. Second order effects  
197 are considered with the P-Delta transformation in OpenSees. Damping is simulated with  
198 the Rayleigh model according to the recommendations of Zareian and Medina (2010). A  
199 two percent (2%) viscous damping ratio is considered for the fundamental period,  $T_1$  of each  
200 frame and for that corresponding to  $20\%T_1$  as suggested in PEER (2010). The steel MRFs  
201 are subjected to suites of 40 ground motions. Each of which representing near-fault, long  
202 duration (from subduction interfaces) and ordinary seismic records based on the conditional  
203 mean spectrum (Baker 2011). Specifics to the ground motion selection are discussed in  
204 Suzuki and Lignos (2019). While seismic response at design-basis earthquakes is of interest,  
205 the ordinary ground motion set is scaled incrementally till collapse occurs only steel MRFs



206 vulnerable to P-Delta (i.e., above 8-stories) in an attempt to get a sense of column strain  
207 demands through collapse, acknowledging the limitations of the employed numerical models.

208 The simulation results of interest feature uniaxial strain histories extracted from the  
209 outer extremity of the flat part of the first-story end (exterior) column of a steel MRF in  
210 the principal direction of earthquake loading. Results indicate that for ordinary and long-  
211 duration records, mean effects are negligible. Therefore, representative strain-based load  
212 protocols are developed based on standard rainflow-counting with zero mean effects (ASTM  
213 2011). In near fault records, two distinct types of strain responses are dominant. Those  
214 that a member exhibits a full-cycle of a certain strain amplitude followed by monotonic  
215 drifting in one loading direction prior to collapse due to P-Delta effects (i.e., typical in steel  
216 MRFs above 8-stories) as well as cases that while collapse does not occur mean effects are  
217 appreciable. These two types are treated separately. In the former, the absolute peak strain  
218 demand prior to collapse is identified for steel MRFs with 8 or more stories. In the latter,  
219 rainflow-counting is conducted two times. The first one is up to the absolute peak strain  
220 demand, whereas the second one is conducted in the post-peak strain response up to rest.  
221 Conservatively, the 90th percentile of the cumulative frequency distribution of the acquired  
222 strain demands is utilized in all cases to establish the strain-based load protocols. This is  
223 consistent with the methodology presented in Krawinkler et al. (1983).

## 224 **Material model**

225 This subsection presents a nonlinear isotropic and kinematic hardening model within the  
226 framework of  $J_2$  plasticity. The essential features of its integration procedure can be readily  
227 consulted in its open-access implementation *RESSPyLab* (de Castro e Sousa et al. 2019). For  
228 a thorougher discussion on the implementation of inelastic materials the reader is referred  
229 to Simo and Hughes (1998).

230 From the  $\pi$ -plane perspective the threshold for plasticity, as defined by the Von Mises  
231 yield criterion, can be seen as a circle and isotropic hardening can be interpreted as an  
232 increase of the radius of the circle, and kinematic hardening a translation movement of the

233 center of that circle.

234 Dictating how this circle enlarges and moves as function of the loading is commensurate  
235 to defining material hardening laws. Finding appropriate parameters for those rules is the  
236 subject of this paper. Henceforth the uniaxial version of the problem will be presented since  
237 the analysis of test-data will be solely unidirectional. Consider the isotropic and kinematic  
238 hardening laws in Eq. 3, 4 and 5.

239 *Isotropic hardening (Voce 1948)*

$$240 \quad \sigma_y = \sigma_{y,0} + Q_\infty \left(1 - e^{-b\varepsilon_{eq}^p}\right) \quad (3)$$

241 *Kinematic hardening (Chaboche et al. 1979)*

$$242 \quad \dot{\alpha}_k = \text{sign}(\sigma - \alpha) C_k \dot{\varepsilon}_{eq}^p - \gamma_k \alpha_k \dot{\varepsilon}_{eq}^p \quad (4)$$

$$243 \quad \alpha = \sum_{k=1}^{nBack} \alpha_k \quad (5)$$

244 where  $\varepsilon_{eq}^p$  is the equivalent plastic strain whose definition for uniaxial loading can be  
245 expressed as in Eq. 6.

$$246 \quad \dot{\varepsilon}_{eq}^p = |\dot{\varepsilon}^p| \quad (6)$$

247 Equation 3 is an exponentially saturating isotropic hardening law, *i.e.* as plastic strain  
248 is accumulated the increase in stress will tend to the maximum saturated value  $Q_\infty$  above  
249 yield. It will do so governed by the exponential term at a rate defined by the term  $b$ .

250 Equation 4 is a kinematic hardening rule defined in rate form. There are two notable  
251 terms: (1) the term with the parameter  $C_k$  if it existed by itself would lead to a simple  
252 linear kinematic hardening model and (2) the term with  $\gamma_k$  is negatively proportional to  
253 the backstress itself and, thus, leads to a nonlinear exponentially saturating behavior. The

254 introduction of the  $\gamma_k$  term was suggested by Armstrong and Fredrick (1966) and so this  
 255 rule bears their name. For monotonic loading Eq. 4 has essentially the same form of Eq. 3  
 256 where the saturation term is  $C_k/\gamma_k$  and the rate term is  $\gamma_k$ . After Armstrong and Fredrick  
 257 (1966), Chaboche et al. (1979) suggested the use of multiple backstresses (*c.f.* Eq. 5) to the  
 258 define a more robust rule.

259 With the material parameters discussed above, one can give the formal definition of the  
 260 uniaxial Von Mises yield criteria used to solve the inverse problem in Eq. 7, in which  $\boldsymbol{\theta}$  is a  
 261 vector containing all the model parameters.

$$262 \quad \phi^{VM}(\sigma, \alpha, \sigma_y; \boldsymbol{\theta}) = \phi^{VM}(\sigma, \alpha, \sigma_y; E, \sigma_{y,0}, Q_\infty, b, C_1, \gamma_1, \dots, C_k, \gamma_k) = (\sigma - \alpha)^2 - \sigma_y^2 \leq 0 \quad (7)$$

### 263 Inverse problem definition

264 All optimization procedures operate on an objective function to be minimized. In the  
 265 particular case of inverse problems, a measure of fitness between a model and an experimental  
 266 result is sought after. For classic plasticity problems a number of different objective functions  
 267 have been used for this purpose - *c.f.* Pal et al. (1996) and Smith et al. (2017). What follows  
 268 presents and discusses what is believed to be a robust alternative to those sources.

269 Consider the definition of the accumulated true strain in Eq. 8, which expresses the sum  
 270 of the absolute values of the strain increments for a given load protocol. The purpose of this  
 271 variable is to be able, for each protocol, to define a loading function in a strict sense where  
 272 one input ( $\varepsilon^*$ ) has a unique corresponding output ( $\sigma$ ). Referring to Fig. 1, or cyclic loading,  
 273 this is equivalent to "unpacking" the hysteretic true-stress-true-strain curve.

$$274 \quad \varepsilon^* = \int_0^t |\dot{\varepsilon}| d\tau \quad (8)$$

275 Equation 9 presents the error function to be minimized in the inverse problems. The  
 276 *i-th* load protocol is expressed by the variable  $\varepsilon_i^*$  of a load protocol set of  $n_{Tests}$  number of

277 tests. The numerator consists of the sum over all experimental results (*e.g.* whose main  
278 variable is ) of the integral of the square difference between the model and experimental true  
279 stress over the accumulated true strain. This is tantamount to the square of the grey shaded  
280 area in Fig. 1b. The denominator is an averaging term to provide an error per unit strain  
281 increment. Nonlinear least squares is akin to this approach in that it is a discrete sum of  
282 square differences. Here, however, a continuous representation is used with an integral along  
283 the loading path, albeit in practice it is numerically integrated with the trapezoidal rule.  
284 Another possibility would be to use the Least Absolute Deviation (LAD). This approach is  
285 sometimes used because it is both computationally efficient and is known to be less sensitive  
286 to outliers (Wilson 1978). However, since differentiability near the solution is a desirable  
287 feature in methodologies that rely on gradient computations and since a procedure of this  
288 class is used herein, the squared difference is used.

$$289 \quad \varphi(\varepsilon_i^*; \boldsymbol{\theta}) = \sum_i \frac{\int_0^{\varepsilon_i^*} (\sigma_{model}(\varepsilon_i^*; \boldsymbol{\theta}) - \sigma_{Test})^2 d\varepsilon^*}{\int_0^{\varepsilon_i^*} d\varepsilon^*}, \quad i \in \{1, \dots, n_{Test}\} \quad (9)$$

290 To avoid negative solutions an additional reciprocal barrier equal to  $1/\theta_i^2$  is added to  $\varphi$ ,  
291 with  $\boldsymbol{\theta}$  the model parameters and steps are restricted to within  $\forall i, \theta_i \geq 1e - 4$ .

292 The error function in Eq. 9 can be challenging to interpret (units of  $MPa^2$ ) and so a  
293 normalized error function in Eq. 10 will be used to facilitate the discussion of the results.  
294 It represents the square root of the ratio between the integral of squared difference and just  
295 the squared area underneath the test.

$$296 \quad \bar{\varphi} = \sqrt{\varphi / \left\{ \sum_i \frac{\int_0^{\varepsilon_i^*} (\sigma_{Test})^2 d\varepsilon^*}{\int_0^{\varepsilon_i^*} d\varepsilon^*} \right\}} \quad (10)$$

## 297 Optimization procedure

298 The algorithm is implemented in the Python package *RESSPyLab* (de Castro e Sousa  
299 et al. 2019) for solving the inverse problem in present paper.

300 To illustrate the methodology, consider the second-order Taylor approximation  $m$  of some

301 function  $f$  ( $f : \mathfrak{R}^2 \rightarrow \mathfrak{R}$ , whose level curves are represented in Fig. 2a) about a point at the  
 302  $k$ -th iteration ( $\mathbf{x}_k$ ) in Eq. 11, with  $\mathbf{d}$  the difference between the point at the next step and  
 303 the current one ( $\mathbf{d} = \mathbf{x}_{k+1} - \mathbf{x}_k$ ),  $\nabla_{\mathbf{x}}f$  the gradient of  $f$ , and  $\nabla_{\mathbf{xx}}f$  the Hessian of  $f$ .

$$304 \quad f(\mathbf{x}_{k+1}) \approx m(\mathbf{x}_{k+1}) = m(\mathbf{x}_k + \mathbf{d}) = f(\mathbf{x}_k) + \nabla_{\mathbf{x}}f(\mathbf{x}_k)^T \mathbf{d} + \frac{1}{2} \mathbf{d}^T \nabla_{\mathbf{xx}}f(\mathbf{x}_k) \mathbf{d} \quad (11)$$

305 If one were to simply apply Newton's method into finding the minimum of  $m$ , one would  
 306 look for the step  $\mathbf{d}$  that would yield  $\nabla_{\mathbf{d}}m = 0$ . From Eq. 11, this results in Eq. 12, which  
 307 finds the minimum of  $m$  for positive-definite Hessians in a single step.

$$308 \quad \nabla_{\mathbf{d}}m = \nabla_{\mathbf{x}}f(\mathbf{x}_k) + \nabla_{\mathbf{xx}}f(\mathbf{x}_k)\mathbf{d} = 0 \Rightarrow \mathbf{d} = -\nabla_{\mathbf{xx}}f(\mathbf{x}_k)^{-1} \nabla_{\mathbf{x}}f(\mathbf{x}_k) \quad (12)$$

309 The problem with taking this step is that far from  $\mathbf{x}_i$  the quadratic approximation might  
 310 not at all be representative of  $f$ . To illustrate this point consider the search direction  
 311 delineated in dashed stroke in Fig. 2a and 2b, which is depicted in Fig. 3a. To prevent  
 312 this, the size of step  $\mathbf{d}$  is restricted to a certain magnitude ( $\Delta$ ) of a specified  $l$ -norm ( $\|\mathbf{x}\|_l =$   
 313  $\sqrt[l]{\sum_j |x_j|^l}$ ; cf. Fig. 3b ) where one is confident that  $f \approx m$  - the *Trust-Region*.

314 The next step in the methodology is how to find the step  $\mathbf{d}$  that minimizes  $m$  such that  
 315  $\|\mathbf{d}\|_l \leq \Delta$  - the trust-region *sub-problem*. This is formalized by the optimization problem 13,  
 316 with constraints 14.

$$317 \quad \text{minimize } m(\mathbf{x}_k + \mathbf{d}) \quad (13)$$

$$318 \quad \text{subject to } \|\mathbf{d}\|_l \leq \Delta \quad (14)$$

319 The analyses conducted in this article will use the 2-norm with the Steihaug-Toint trun-  
 320 cated conjugate gradient method (Bierlaire 2015).

321 To assess how much the path should be restricted, a metric on the quality of the second-  
 322 order approximation is usually employed. The ratio between the change in the value of the  
 323 function and the approximation due to the step  $\mathbf{d}$  is often used for this purpose - *c.f.* Eq.  
 324 15.

$$325 \quad \rho = \frac{f(\mathbf{x}_k) - f(\mathbf{x}_k + \mathbf{d})}{m(\mathbf{x}_k) - m(\mathbf{x}_k + \mathbf{d})} \quad (15)$$

326 Ideally this assessment should be revised as the search space is traversed. A two parameter  
 327 criterion ( $\eta_1$  and  $\eta_2$ ) is usually employed to judge the update of the step size  $\Delta$ . If  $\rho \geq \eta_1$   
 328 then  $\Delta$  is increased, whereas if  $\rho \leq \eta_2$  then  $\Delta$  is decreased. Between these two values  $\Delta$   
 329 remains unchanged. Take, for instance,  $\eta_1 = 0.9$  and  $\eta_2 = 0.01$ , this means that if the  
 330 approximation fits upwards of 90% the function value, then it is deemed to be sufficiently  
 331 good so that the restriction on the step size is relaxed. The converse happens when it fits  
 332 to less than 1% of the function value (Conn et al. 2000, Bierlaire 2015).

333 One important detail about the Steihaug-Toint truncated conjugate gradient procedure  
 334 is that in the event of an indefinite Hessian, it leverages valuable properties of the method  
 335 by conducting Hessian-orthogonal steps in descent directions. Since they are bounded by  
 336 the trust region one does not risk an unbounded search and, by always checking the quality  
 337 of solution with Eq. 15, it provides a reliable criterion for effectively canvassing the objective  
 338 function's landscape. Additionally, it is worth noting that the presence of indefinite Hessians  
 339 usually points to the existence of multiple local minima. One possible strategy to further  
 340 explore the variable space in the search for a global minimum is to keep track of the points  
 341 where negative eigenvalues occur and generate search paths on opposite senses of the negative  
 342 eigenvector - *c.f.* Wales (2003).

343 A potential problem in the convergence rate of the algorithm happens when the condition  
 344 number of the Hessian  $\nabla_{\mathbf{xx}}f(\mathbf{x}_k)$  is large. A solution to mitigate this issue is to solve a  
 345 preconditioned sub-problem. The idea is not to restrict step  $\mathbf{d}$  to some magnitude, but  
 346 apply that constraint on a distorted version of  $\mathbf{d}$  (defined as  $\mathbf{w}$ ), which is carefully chosen

347 to follow the local curvature of the quadratic model. This is more formally expressed in Eq.  
 348 16, where  $\mathbf{S}$ , to follow the curvature, should precondition as much as possible the Hessian of  
 349 the model. An illuminating discussion of this topic can be found in Conn et al. (2000) under  
 350 the rubric of *Trust-Region Scaling*.

$$351 \quad \mathbf{S}_k \mathbf{w} = \mathbf{d} \quad (16)$$

352 From Eq. 16, one can thus define a preconditioned model of  $f$  around  $\mathbf{x}_k$  as  $m^P$  as shown  
 353 in Eq. 17

$$354 \quad f(\mathbf{x}_k + \mathbf{d}) = f(\mathbf{x}_k + \mathbf{S}\mathbf{w}) \approx m(\mathbf{x}_k + \mathbf{d}) = m^P(\mathbf{x}_k + \mathbf{w}) \quad (17)$$

355 Which from Eq. 11 and 16 yields Eq. 18.

$$356 \quad m^P(\mathbf{x}_k + \mathbf{w}) = f(\mathbf{x}_k) + (g_k^P)^T \mathbf{w} + \frac{1}{2} \mathbf{w}^T \mathbf{H}_k^P \mathbf{w} \quad (18)$$

357 with,

$$358 \quad g_k^P = \mathbf{S}_k^T \nabla_{\mathbf{x}} f(\mathbf{x}_k) \quad (19)$$

$$359 \quad \mathbf{H}_k^P = \mathbf{S}_k^T \nabla_{\mathbf{xx}} f(\mathbf{x}_k) \mathbf{S}_k \quad (20)$$

360 Thus, given a certain preconditioner  $\mathbf{S}_k$ , one can now solve the equivalent sub-problem  
 361 in Eq. 21 for  $\mathbf{w}$ .

$$362 \quad \begin{aligned} & \text{minimize} && m^P(\mathbf{x}_k + \mathbf{w}) \\ & \text{subject to} && \|\mathbf{w}\|_l \leq \Delta \end{aligned} \quad (21)$$

364 To guide the choice of a proper preconditioner, it is often helpful to think of performing  
 365 the change of variables geometrically, where it would be natural to state that one would wish  
 366 to work on a model where its eigenvalues have equal magnitude. The clearest way to achieve  
 367 this would be to impose the Hessian of the scaled model to be equal to the identity matrix  
 368 - Eq. 22.

$$369 \quad \mathbf{I} = \mathbf{H}_k^P = \mathbf{S}_k^T \nabla_{\mathbf{xx}} f(\mathbf{x}_k) \mathbf{S}_k \Leftrightarrow \nabla_{\mathbf{xx}} f(\mathbf{x}_k) = (\mathbf{S}_k \mathbf{S}_k^T)^{-1} \quad (22)$$

370 If the Hessian of  $f$  is locally symmetric positive-definite, a natural method for computing  
 371  $\mathbf{S}_k$  would be to use the Cholesky decomposition as it is commonly done in the preconditioned  
 372 conjugate gradient method - *c.f.* Bierlaire (2015). A more general approach would be to  
 373 impose that  $\mathbf{S}_k$  is itself symmetric, which would yield Eq. 23.

$$374 \quad \nabla_{\mathbf{xx}} f(\mathbf{x}_k) = (\mathbf{S}_k \mathbf{S}_k^T)^{-1} = (\mathbf{S}_k^2)^{-1} \Leftrightarrow \mathbf{S}_k = (\nabla_{\mathbf{xx}} f(\mathbf{x}_k))^{-\frac{1}{2}} \quad (23)$$

375 Computing  $\mathbf{S}_k$  in Eq. 23 can then be done, similarly to the calculation of Moore-Penrose  
 376 pseudoinverses, with the Singular Value Decomposition (SVD) of the Hessian of  $f$  - *c.f.* Eq.  
 377 24.

$$378 \quad \mathbf{S}_k^{SVD} = (\nabla_{\mathbf{xx}} f(\mathbf{x}_k))^{-\frac{1}{2}} = (\mathbf{U}_k \mathbf{\Sigma}_k \mathbf{V}_k^T)^{-\frac{1}{2}} = \mathbf{V}_k \mathbf{\Sigma}_k^{-\frac{1}{2}} \mathbf{U}_k^T \quad (24)$$

379 where  $\mathbf{U}_k$  and  $\mathbf{V}_k$  are matrices that store the left and right singular vectors, respectively,  
 380 and the matrix  $\mathbf{\Sigma}_k$  stores the singular values along its diagonal.

381 The disadvantage of using this approach is the additional computational cost involved  
 382 in computing the SVD of the Hessian, which may or may not be make up for itself in an  
 383 increased rate of convergence of the overall algorithm.

384 Performing an SVD is an ideal situation, an upper bound, so to speak, for the precondi-  
 385 tioner  $\mathbf{S}_k$ . The converse would be a transformation that leaves everything unchanged with  
 386  $\mathbf{S}_k = \mathbf{I}$  so that  $m^p = m$ . In between there could be any number of preconditioners, which



387 will approximate the Hessian to greater or lesser degrees in the sense of Eq. 22.

388 One commonly used, and computationally cheap, way of approximating the Hessian  
389 is the so called *Jacobi* preconditioner (*cf.* Eq. 25). This method considers that the diagonal  
390 elements of the Hessian provides a sufficiently accurate approximation of this matrix, while  
391 being easily invertable.

$$392 \quad \mathbf{S}_k^{Jacobi} = \text{diag}(\nabla_{\mathbf{xx}} f(\mathbf{x}_k))^{-\frac{1}{2}} \quad (25)$$

393 By taking only the diagonal elements of the Hessian it is assumed they are representative  
394 of most of the magnitude of the eigenvalues, as such this preconditioner could be more aptly  
395 described as a scaling transformation.

396 As can be seen in Eq. 11, the NTR method relies heavily on the ability to compute the  
397 gradient and the Hessian of the objective function. When it comes to the class of inverse  
398 problems, which is the focus of this report, derivatives have to be computed on the integration  
399 scheme over the parameters of the model. This can be quite challenging and one will perform  
400 analyses using two methodologies on the objective function: (1) numerical differentiation  
401 (ND) with central differences and (2) algorithmic (or automated) differentiation (AD). The  
402 former approach is quite standard, but is known to be handicapped by truncation and  
403 rounding errors depending on the step size. The ND analyses presented herein were made  
404 using the central difference method with a fixed step size of  $1e-6$ . The AD approach is the  
405 result of the systematic application of chain rule over the graph of a user-defined computer  
406 function, which returns derivatives with a high level of accuracy - *cf.* Griewank and Walther  
407 (2008). A Python package called *numdifftools* (Brodtkorb 2017) was used that implements  
408 both approaches. This package is based on the *Matlab* program written by D’Errico (2006)  
409 and also wraps around the package *AlgoPy* (Walter and Lehmann 2013) for algorithmic  
410 differentiation.

411 The results shown in the following section are a direct application of this methodology  
412 to the minimization procedure of the inverse problem expressed in Eq. 9 with respect to

413 parameter vector  $\theta$ . The choice of the initial starting point for the NTR algorithm can have a  
 414 significant influence on the solution. In this report, the criterion for the starting point (S.P.)  
 415 in most NTR optimizations was chosen so as to have an elastic-perfectly-plastic model with  
 416 the yield stress equal to the nominal yield value of the steel  $\hat{\sigma}_{y,0}$  and with the nominal elastic  
 417 modulus  $\hat{E}$ . All other parameters were set to a residual value of  $1e - 1$ , which has minimal  
 418 impact both on the perfectly-plastic assumption and on the barrier added to  $\varphi$ . The results  
 419 for other starting points is presented in sub-section 3. One of these solution points is the  
 420 extreme case where very little except the nominal value of modulus of elasticity is known,  
 421 *i.e.*  $\sigma_{y,0} \approx 0$ . In addition, results for an intermediate starting point at  $\sigma_{y,0} = 0.5\hat{\sigma}_{y,0}$  are also  
 422 presented.

### 423 **Load protocol sampling**

424 Since the model should ideally capture material response irrespective of the imposed  
 425 history, the question naturally follows of how sensitive is the calibration when using a different  
 426 load protocol set. To address this question, one needs to define a metric that distinguishes  
 427 two solutions with respect to each other. It is also useful to define a base case to which  
 428 all comparisons are made. The base case chosen for all analyses is the maximum number  
 429 of available load protocols since it contains the maximum amount of information on the  
 430 problem. Other cases will be samples of that set. Due to the inordinate number of possible  
 431 sample sets for only 10 total load protocols, a small number of sets (50) were selected with  
 432 the guiding principle of (1) having a low number of load protocols and (2) having distinct  
 433 groups of load protocols of small and large amplitude histories. The first focuses on the desire  
 434 to know what is the minimum number of load protocols necessary to achieve an acceptable  
 435 accuracy, and the second on the influence of the amplitude magnitude on the error function.

436 Equations 26 and 27 represent in a sense two different metrics to evaluate a distance  
 437 between two points.  $\xi_1$  is the most intuitive choice as it is merely the root of the sum of  
 438 the relative errors squared of each of the model parameters.  $\xi_2$  is less obvious and is best  
 439 understood in conjunction with Eqs.10 and 12. From Eq. 12, the numerator within the

440 root of Eq. 27 represents the increase in the quadratic approximation of the error function  
 441 from the base point. The denominator in Eq. 27 is used for the same reason as in Eq.  
 442 10, *i.e.* to provide a normalizing term. Now since at the base point we have a positive-  
 443 definite Hessian, any deviation from  $\boldsymbol{\theta}_{base}$  will increase monotonically and, therefore, the  
 444 distance to any minima obtained with a different protocol set is a positive metric weighed  
 445 by the objective function itself. The usefulness of  $\xi_2$  will become apparent in the discussion  
 446 section, particularly while analyzing solutions with a large number of backstresses where the  
 447 positive-definite condition is technically satisfied albeit with very small eigenvalues. In such  
 448 situations there are solutions which maybe far from each other in the  $\xi_1$  sense but which do  
 449 not have a significant impact in evaluating the error function with respect to the base case.  
 450 When this happens the two solution points are said to be consistent with each other.

$$451 \quad \xi_1 = \sqrt{\sum_i \left( \frac{\theta_i - \theta_{i,base}}{\theta_{i,base}} \right)^2} \quad (26)$$

$$452 \quad \xi_2 = \sqrt{(\boldsymbol{\theta} - \boldsymbol{\theta}_{base})^T \nabla_{\boldsymbol{\theta}\boldsymbol{\theta}} \varphi_{base} (\boldsymbol{\theta} - \boldsymbol{\theta}_{base}) / \sum_i \left( \frac{\int_0^{\epsilon_i^*} \sigma_{Test} d\epsilon^*}{\int_0^{\epsilon_i^*} d\epsilon^*} \right)^2} \quad (27)$$

## 453 RESULTS

### 454 Load protocols

455 Figure 4 shows the derived strain protocols for macroscopic material evaluation of struc-  
 456 tural steels for cyclic loading representative of seismic applications. The reference protocols  
 457 are complemented by monotonic one (see Figure 4a) conducted according to ASTM spec-  
 458 ifications. The test should be carried out to fracture of the specimen. Figure 4b depicts  
 459 representative strain protocols with monotonic tension after a full cycle of cyclic inelastic  
 460 straining. Low-rise steel MRFs subjected to near-fault records are likely to experience a large  
 461 pulse prior to drifting in one loading direction. The strain range in HSS columns in this case  
 462 is  $\Delta\epsilon=10\%$  whereas the equivalent one in high-rise steel HSS columns is  $\Delta\epsilon=2\%$  prior to  
 463 the monotonic tensile push to fracture. Figure 4e shows a second protocol corresponding

464 to strain demands representative of near-fault records when collapse does not occur. The  
465 rupture directivity, characteristic of near-fault records, is depicted by the impulsive double-  
466 sided strain cycle with 3% amplitude. In long duration records, it is found that constant  
467 strain amplitude tests of at least 20 full cycles represent fairly well the seismic demands in  
468 HSS columns in steel MRFs. Particularly, strain amplitudes of 1% and 2% are found to rep-  
469 resent, on average, strain demands in mid-to-high-rise and low-rise steel MRFs, respectively,  
470 subjected to subduction zone seismic events as depicted in Figure 4c. During these tests, the  
471 material is expected to reach a steady state response, thereby exhibiting stress saturation.  
472 Incremental load protocols up to a 2% uniaxial strain demand (i.e., strain range  $\Delta\varepsilon=4\%$ ) are  
473 deemed reasonable to represent, on average, seismic demands in steel HSS columns during  
474 design-basis earthquakes. To consider the influence of a steel MRF's height (i.e., predomi-  
475 nant period) on the developed protocols, rain-flow counting is benchmarked to the results of  
476 the 2- 6- and 12-story steel MRFs. Figure 4d shows the derived protocols. Strain demands  
477 above 2% until failure (i.e., buckling or fracture) is an arbitrary decision in case the material  
478 may reach stress saturation. Referring to Fig. 4f, a protocol representative of column strain  
479 demands prior to steel MRF collapse is shown. While non-symmetric strain demands are  
480 evident, which is a characteristic of response histories prior to earthquake-induced collapse  
481 (Lignos et al. 2011) , the small strain reversals are not expected to shift a material's behavior  
482 that much from a conventional monotonic tensile test.

### 483 **Optimization algorithm performance**

484 All analyses in this subsection are demonstrated using an S355J2+N steel sampled from  
485 50 mm thick plates. The full collection of load protocols (LP) introduced in the previous  
486 section are used in solving the inverse problem (1 to 10).

#### 487 *Numerical and Algorithmic Differentiation in NTR*

488 Figure 5 shows a comparison between ND and AD for a Jacobian-preconditioned algo-  
489 rithm (J) with one backstress. Both analyses use as a starting point an elastic-perfectly  
490 plastic model, plateauing at the steel's nominal yield stress. Here, the imprecision associ-

491 ated with ND in combination with scaling that happens during preconditioning, can lead the  
492 algorithm to get locked in to searching for solutions in directions where  $\varphi$  decreases at a very  
493 slow rate. This underlines the importance in securing an accurate derivative estimation, for  
494 which AD is a useful tool.

495 Hence, all results in subsequent analyses will use algorithmic differentiation.

#### 496 *Preconditioning in NTR*

497 Figure 6 shows a comparison between no preconditioning, Jacobi (J) and singular value  
498 decomposition (SVD) preconditioning of the NTR Steihaug-Toint sub-problem for a 2 back-  
499 stress model. Here, again, the analyses use as a starting point an approximately elastic-  
500 perfectly plastic model, plateauing at the steel’s nominal yield stress. As can be seen, the  
501 cost of not using a preconditioner can be prohibitively high. This is more noticeable the more  
502 backstresses are used in the calibration. Also, the Jacobi and SVD preconditioning yield sim-  
503 ilar convergence rates although, from experience, the SVD is more stable numerically near  
504 the solution.

#### 505 *Different starting points and number of backstresses*

506 All previous analyses were conducted with the starting point of an approximately elastic-  
507 perfectly plastic material with nominal yield stress and elastic modulus. In this sub-section  
508 two other starting points are investigated, for a total of three starting values:

- 509 • Starting point 1 (S.P. 1):  $\sigma_{y,0} = \hat{\sigma}_{y,0} = 355MPa$
- 510 • Starting point 2 (S.P. 2):  $\sigma_{y,0} = 0.5\hat{\sigma}_{y,0} \approx 178MPa$
- 511 • Starting point 3 (S.P. 3):  $\sigma_{y,0} = 1e - 1 \approx 0MPa$

512 The algorithm used for the optimization procedure in all cases was the NTR with AD, Ja-  
513 cobi and SVD preconditioning. Results for 2 backstresses are presented terms of the solution  
514 path and final true stress-true strain curves for all load protocols in Figs. 7 and 8, respec-  
515 tively. Tables 2 and 3 present a summary of the algorithm’s performance and its solution  
516 point at convergence. Since the results for both J and SVD preconditioning are the same,

517 the table is condensed to include solely the SVD results. Furthermore, a comparison between  
518 experimental and model true-stress-true-strain responses with the parameter solution for 2  
519 backstresses is given in Fig. 8.

520 Referring to Fig. 7 and Table 3, it can be readily observed that for one, two, and three  
521 backstresses that same solution(model parameters) is reached regardless of the starting point.  
522 For four backstresses, for virtually the same accuracy in the error function, two different  
523 solution points were retrieved, confirming the nonuniqueness issue often debated in inverse  
524 problems (Cooke and Kanvinde 2015).

525 It was also found that the relative decrease in error using more backstresses, even for  
526 the wide variety of load protocols involved, is negligible after a certain point. The er-  
527 ror associated with two backstresses was found to be virtually the same as three and four  
528 backstresses.

### 529 **Load protocol sampling**

530 Table 4 shows results for the calibration S355J2+N steel Voce-Chaboche material param-  
531 eters for different samples from the full set of 10 load protocols (Set 1) with two backstresses.  
532 The parameters obtained are compared to the normalized error( $\bar{\varphi}$ ) computed with the full  
533 set of protocols to judge their relative impact. The results are ordered in ascending order of  
534 this metric. Also shown in Table 4 are the distances  $\xi_1$  and  $\xi_2$  defined in Eqs. 26 and 27,  
535 respectively, with respect to the base parameters of Set 1.

### 536 **Summary of results for different structural steel materials**

537 The results presented previously were obtained for an S355J2+N steel. Notwithstanding,  
538 the same methodology was applied to a a broad range of European, American and Japanese  
539 steels with the objective of obtaining material parameters for reference and comparison  
540 purposes. For context, a summary of the tensile properties for those materials is given in  
541 Table 1, and Table 5 catalogs the acquired results for the Voce-Chaboche model with 2  
542 backstresses. The implications of the obtained parameters are expounded in the Discussion  
543 section.

## DISCUSSION

### Algorithm performance

In order to achieve acceptable convergence rates there are two important factors that should be fulfilled in order to use NTR with the Steihaug-Toint method: (1) accurate derivative estimates and (2) hessian preconditioning. The first point can be clearly inferred from Fig. 5 where algorithmic differentiation is compared with the more imprecise approach of a fixed step central difference numerical differentiation. Although the convergence rate could be improved by using an adaptive step size, the computational cost associated with this option is high and, therefore, does not justify itself over the use of algorithmic differentiation. In addition, algorithmic differentiation has the benefit of being generally applicable to different hardening laws. Consequently, instead of painstakingly calculating derivatives that result from the integration algorithm of a specific material law, algorithmic differentiation achieves high accuracy levels with minimal implementation effort at a reasonable computational cost and is, thus, a valuable tool to employ. With respect to the second point, greater rates of convergence are achieved using a preconditioned hessian (*c.f.* Fig. 6) in large part due to the use of the conjugate gradient method in the Steihaug-Toint procedure (Conn et al. 2000). This effect is evermore present the greater the condition number of the hessian of the problem - *i.e.* the ratio of its highest to lowest eigenvalues. In this particular inverse problem, this observation is more noticeable the higher the number of backstresses used. As for the preconditioner itself, the two options presented in this study (Jacobi and SVD) have similar convergence rates. Both are presented because while the SVD is more stable numerically, its computational cost can be prohibitive for models with a higher number of parameters. In these cases the Jacobi preconditioner can be a useful alternative.

### Nonuniqueness and consistency

The suitability of working with the NTR method in solving the VC inverse problem should also be evaluated with respect to the possibility of retrieving multiple solutions in the parameter space, as observed in the results presented in Table 2. This possibility depends

571 both on the nonlinearity of the underlying material model and on the error function 's  
572 definition. Due to the multi-dimensional nature of the problem, it is challenging to provide  
573 a geometric depiction of the error function's landscape. One can, nonetheless, have an idea  
574 of the nonlinear nature of the problem by tracking the evolution of its eigenvalues. More  
575 concretely, if one inquires into the sign of the minimum eigenvalue of the Hessian, one can  
576 immediately get the sense if locally along the path to the minimum one encounters what  
577 resembles hyperbolic paraboloids (saddle points). Figure 9 shows that evolution for one and  
578 four backstresses at two different starting points. It can be seen that hyperbolic paraboloids  
579 are indeed encountered in the NTR path. This type of nonlinearity is particularly salient  
580 in the four backstress model where the Hessian switches from positive-definite to indefinite  
581 multiple times. Naturally, all models finish with a positive-definite Hessian thus ensuring,  
582 along with a strict tolerance on the gradient (e.g.  $\|\nabla \varphi\| < 1e - 10$ ), a proper minimum.  
583 Although the presence of negative eigenvalues is suggestive of multiple minima, it does  
584 not necessarily imply nonunique solutions since a number of nonconvex examples can be  
585 produced that possess solely one global and local minimum. General statements regarding  
586 solution uniqueness of the VC inverse problem, therefore, cannot be made.

587 From the discussion in the previous paragraph, one hopes that the nonlinear nature of  
588 the problem is clear to the reader. In light of this fact it is quite astonishing to find that the  
589 solutions retrieved with NTR are generally close to each other, although the path they take  
590 to reach their values are significantly different. The results presented in Fig. 7 illustrates this  
591 fact, as shown in the evolution of the parameters with respect to the algorithms' iterations.  
592 Though anecdotal in context, it underscores the robustness of the proposed methodology.

593 The impossibility to make general statements regarding nonuniqueness notwithstanding,  
594 one can deploy other metrics to evaluate the consistency of the solutions. Specifically, one  
595 can compare the cases relative to each other using the metrics  $\xi_1$  and  $\xi_2$  described in the  
596 Methodology section. Take, for example, the four backstresses cases where three different  
597 starting points yielded three different solutions amid keeping the normalized error function



598 values essentially the same - *c.f.* Table 2. The solutions are appreciably different particularly  
 599 in terms of the magnitude of their  $C_k$  parameters. In this case one can, in fact, use the error  
 600 metrics introduced in Eqs. 26 and 27 to quantify objectively the differences between the  
 601 solutions. For this purpose let starting point 1 serve as the base case.  $\xi_1$  for starting points  
 602 2 and 3 is  $\approx 22.71\%$  and  $\approx 5.75\%$  respectively, while  $\xi_2$  is  $\approx 1e - 6 \%$  for both cases. These  
 603 results have important implications in interpreting different calibrations. Whereas,  $\xi_1$  shows  
 604 a noticeable difference between parameters,  $\xi_2$  suggests that those differences are small when  
 605 assessing the error function with respect to the base case. It is crucial here to recall that the  
 606  $\xi_2$  metric increases monotonically from the minimum if the Hessian is positive-definite. Such  
 607 small values as  $1e - 6$  for  $\xi_2$  essentially implies that, although numerically the Hessian might  
 608 be positive-definite, the relative direction between the two solutions lies close to what can  
 609 practically be described as the null-space of the Hessian. Now, choosing solutions that locally  
 610 around the base case (in the  $\xi_2$  sense) do not significantly increase the error function implies  
 611 that those points predict behavior similarly and, for this reason, are said to be consistent  
 612 with each other. A more debatable issue is defining an acceptable threshold value for the  
 613 local increase in the error function. More on this topic is discussed in the load protocol  
 614 sampling section.

### 615 **Load protocol sampling**

616 Table 4 shows results for analyses conducted with samples from a set 10 load protocols  
 617 ordered by the relative error  $\bar{\varphi}$  that the parameters of the subset have when considering  
 618 all the load protocols. In conjunction with  $\xi_1$  and  $\xi_2$ , one can also evaluate their level of  
 619 nonuniqueness and consistency.

620 With respect to  $\bar{\varphi}$ , most of the solutions of the sampling sets have errors that are close  
 621 to full set. Notable among them are sets 45 and 18, whose solutions provide essentially the  
 622 same  $\bar{\varphi}$  but with three load protocols as opposed to 10. Equally interesting is that the load  
 623 protocols in these sets do not include constant amplitude or incrementally increasing tests  
 624 which are considered standard in evaluating material model parameters in cyclic loading.

625 Other noteworthy observations are that sets with smaller amplitudes generally lead to worst  
626 calibrations (*c.f.*, *e.g.* set 19 vs. 28) and that the inclusion of a monotonic test is not  
627 necessarily essential to obtaining good parameter estimates as the results from set 45 imply.  
628 Furthermore, one can observe that testing using a random load protocol with non-zero mean  
629 strain (LP9) is important for the calibration procedure because it is present in almost all  
630 sets with a low number of protocols.

631 As to the nonuniqueness of the parameters,  $\xi_1$  shows that the solutions are at least 40%  
632 different from each other. However, when one looks at what is the impact of that distance  
633 on the error function as evaluated by  $\xi_2$ , the effects are much more limited. Deciding on an  
634 acceptable level of  $\xi_2$  is inherently linked to the acceptable difference in our error estimate  
635 from the base case. Although debatable, a value of  $\xi_2 \leq 5\%$  seems small enough to be  
636 a suitable definition for consistency. Nevertheless,  $\xi_2$  seems to indicate that most of the  
637 solutions obtained by the NTR algorithm are consistent with the base load protocol case,  
638 except for a few cases. Consider, for example, set 51 that has a relatively low  $\bar{\varphi}$  value  
639 compared with set 2 which has the highest  $\bar{\varphi}$ . Here, set 51 is twice as far as set 2 in terms of  
640  $\xi_2$ . This implies that set 51, which is conducted with four load protocols, is farther from the  
641 base case than a solution arrived at with only a simple monotonic test. Set 51, therefore, is  
642 a truly inconsistent result.

643 Solution consistency can be further analyzed by a thorough sensitivity assessment of the  
644 parameters. However, this would have to be performed at the solution point of each load  
645 protocol set, since they can have different sensitivities. This is recommended for further  
646 investigation, but preliminary findings show that the initial yield stress in the VC model has  
647 the most weight in the error of the model.

## 648 **Proposed material parameters for structural steels**

649 There are a few noteworthy comments to be made with respect to the material param-  
650 eters. First and most conspicuous is the Young's modulus, which in Tables 2 and 5 is  
651 persistently lower than habitual values of  $\approx 200 - 210\text{GPa}$  for mild steels. Interestingly,

652 if only the monotonic test is used for the calibration the modulus is indeed close to the  
653 expected value. It is only with the addition of more load protocols, with higher accumulated  
654 plastic strains and the inclusion of load reversals, that on average the Young's modulus tends  
655 to drop.

656 Another puzzling result is that the estimation of initial yield stresses ( $\sigma_{y,0}$ ) is also re-  
657 liably lower than the yield plateau of the monotonic tests. This observation is associated  
658 with the fact that after the accumulated plastic strain passes the Lüders strain, the plateau  
659 phenomenon ceases to be present (Hall 1970). Upon load reversals, a smooth yielding phe-  
660 nomenon takes its place and starts at a lower yield level. Since most of the duration of the  
661 load protocols are spent in the smooth yielding range, what results from the optimization  
662 procedure is the incursion of a larger error at first yield in order to have smaller errors when  
663 reversals are made. It should be underscored that this is a limitation of the material model  
664 itself. Its impact could be felt in cases where the initial stress is paramount in determining  
665 structural behavior. Foremost among these are situations where geometric and material non-  
666 linearities strongly interact (Hartloper et al. 2019). The discontinuous yielding phenomenon  
667 in mild steels makes it one of the most sensitive type of structural steels to this issue.

668 From Table 2, an important conclusion can be made as to the number of backstresses  
669 necessary to accurately capture material response. The gains in terms of  $\bar{\varphi}$  are negligible  
670 after 2 backstresses are used. After this number, solution points can be consistent in the  $\xi_2$   
671 sense but do not bring any added value to the response. These results, therefore, suggest that  
672 2 backstresses suffice in the description of the material response for earthquake situations.

673 Consistency in the solution points allows one to make meaningful qualitatively asser-  
674 tions about the parameter sets, and several examples can be produced from Table 5. For  
675 instance, one can readily identify materials of similar grades as illustrated by the similari-  
676 ties between the parameters of two different thickness plates of the same material grade, an  
677 S355J2+N. Their parameters are also close to those obtained for a nominally identical steel  
678 grade (S355J2) from wide-flange hot-rolled structural profiles (an HEB500 in the present

679 case). Furthermore, it can also be stated that the higher the steel grade the lower the level  
680 of isotropic hardening, as shown by the decreasing values of  $Q_\infty$ . In fact, if one takes to  
681 evaluate the contribution of isotropic hardening in the total hardening behavior of the VC  
682 model at saturation, it can be seen that mild steels frequently present on the order of 25%  
683 of isotropic hardening whereas high strength steel (*e.g.* S690QL) is mostly kinematic. This  
684 observation is valid even between mild steels of different origin, such as the European S355  
685 and the American A992 Gr. 50 steels. When viewed in the light of the classic Hall-Petch  
686 relationship that correlates increasing yield strength with decreasing grain size (Hall 1951,  
687 Petch 1953), the parameters obtained by this methodology seem to suggest that the amount  
688 of isotropic versus kinematic hardening in a material can also be linked to microstructural  
689 grounds. In this respect, however, it should also be pointed out that the manufacturing  
690 process (and, therefore, the material's grain size) need not be the only microstructural vari-  
691 able responsible for isotropic/kinematic ratio. Indeed, if one focuses on the Japanese steel  
692 BCR295, a lower grade steel (nominal yield stress of 295MPa) with presumably larger av-  
693 erage grain size, a low level of isotropic hardening can be observed on the derived material  
694 parameters. Yet, the test specimens for this steel were sampled from the corner of a hollow  
695 square section (HSS), which implies that the material around this area had been cold-worked.  
696 Consequently, it can also be stated that previous work-hardening of the material can also  
697 have a significant impact on the proportion of isotropic to kinematic hardening.

698 On a separate note, comparisons between parameters found in literature and those pro-  
699 posed herein should be made with some care. There are two main sources of uncertainties  
700 in the determination of model parameters: (1) the inverse problem methodology and (2)  
701 inherent variations in the material properties from the manufacturing process. This paper  
702 addresses solely the first point. A lengthy comparison of the parameters proposed herein to  
703 those reported in literature would, therefore, be hard to parse out and is not attempted. It  
704 can be stated, nonetheless, that significant differences in terms of model performance can be  
705 found using literature parameters for the same material, but the source of that discrepancy

706 still needs further investigation with larger datasets.

## 707 **CONCLUSION**

708 This paper presented an approach to solve an inverse problem on a classic metal plas-  
709 ticity, rate-independent, material model using a combined nonlinear isotropic and kinematic  
710 hardening according to the Voce and Chaboche rules (VC). The approach is based on the  
711 Newton Trust-Region methodology which was introduced and its implementation was dis-  
712 cussed. An implementation of the procedure in the Python programming language is made  
713 freely available in de Castro e Sousa et al. (2019).

714 The methodology was applied to a wide variety of European, American and Japanese  
715 structural steels that are commonly used in steel construction worldwide and the resulting  
716 parameters are provided for reference.

717 The following overarching conclusions can be drawn for this work:

- 718 • Accurate derivative estimates and hessian preconditioning play a significant role in  
719 the convergence rate of the NTR method. Both Jacobi and SVD preconditioning  
720 work well in the present study;
- 721 • Solution points obtained with the NTR method for different starting points are close  
722 even in cases where the starting point is far away from the solution, *e.g.*  $\bar{\varphi} \approx 100\%$   
723 where there is virtually no information on where the solution might lay, illustrating  
724 the robustness of the algorithm;
- 725 • Two backstresses in the Chaboche kinematic hardening rule seem sufficient to char-  
726 acterize material response for earthquake loading;
- 727 • Accuracy in cyclic loading is usually achieved at the noticeable expense of underesti-  
728 mating the initial yield stress with the Voce-Chaboche model;
- 729 • Nonuniqueness and consistency were analyzed and discussed. Their importance moti-  
730 vates the introduction of two metrics to quantify them. Load protocol sampling leads  
731 in large to consistent solutions using this approach;

- 732           • The use of only three load protocols (LP2, LP3, and LP9) yield acceptable parameter  
733 estimates. These load protocols are different from the standard ones routinely used  
734 in material characterization in cyclic loading for seismic applications;

## 735 **DATA AVAILABILITY**

736           Some or all data, models, or code generated or used during the study are available in  
737 a repository or online in accordance with funder data retention policies. Some or all data,  
738 models, or code that support the findings of this study are available from the corresponding  
739 author upon reasonable request.

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## NOTATION

*The following symbols are used in this paper:*

- $\sigma$  = uniaxial true stress (Pa);
- $\varepsilon$  = uniaxial true strain;
- $\sigma_{eng}$  = uniaxial engineering stress (Pa);
- $\varepsilon_{eng}$  = uniaxial engineering strain;
- $F$  = actuator force through uniaxial specimen (N);
- $L$  = gage length (m);
- $A$  = uniaxial specimen's cross section area ( $m^2$ );
- $J_2$  = second invariant of the deviatoric stress tensor;
- $\phi^{VM}$  = Von Mises yield criterion;
- $E$  = Young's modulus;
- $\sigma_y$  = current yield stress (Pa);
- $\sigma_{y,0}$  = initial yield stress (Pa);
- $\Delta\sigma_y$  = difference between current and initial yield stress (Pa);
- $Q_\infty$  = isotropic differential stress at saturation (Pa);
- $b$  = isotropic saturation rate parameter;
- $C_k$  = kinematic stress parameter for the  $k$ -th backstress (Pa);
- $\gamma_k$  = kinematic saturation rate parameter for the  $k$ -th backstress;
- $\boldsymbol{\theta}$  = vector of all material parameters;
- $\dot{\varepsilon}_{eq}^p$  = equivalent plastic strain;
- $\varepsilon^*$  = error-metric strain;
- $\varphi$  = error function;
- $\bar{\varphi}$  = normalized error function;
- $m$  = local quadratic approximation model of a function;
- $\nabla_{\mathbf{x}}f$  = gradient of function  $f$  with respect to vector variable  $\mathbf{x}$ ;
- $\nabla_{\mathbf{xx}}f$  = hessian of function  $f$  with respect to vector variable  $\mathbf{x}$ ;

- $\|\mathbf{x}\|_l$  =  $l$ -norm of vector  $\mathbf{x}$ ;
- $\mathbf{d}$  = step vector;
- $\Delta$  = step magnitude limit;
- $\rho$  = model fitness metric;
- $\eta_1$  = lower bound on model fitness quality;
- $\eta_2$  = upper bound on model fitness quality;
- $\mathbf{w}$  = scaled step vector;
- $\mathbf{S}$  = hessian preconditioner;
- $\mathbf{H}$  = preconditioned hessian;
- $\xi_1$  = uniqueness distance metric;
- $\xi_2$  = consistency distance metric;

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TABLE 1: Summary of tensile properties for materials under study.

Material	$E$ ( $GPa$ )	$\sigma_y/\sigma_y^{nominal}$ ( $MPa$ )	$\sigma_{0.2p}$ ( $MPa$ )	$\sigma_u$ <sup>b</sup> ( $MPa$ )	$\varepsilon_u$ <sup>c</sup>
S355J2+N (Plt. <sup>a</sup> - 50mm)	204	350/355	-	537	0.171
S355J2+N (Plt. <sup>a</sup> - 25mm)	214	350/355	-	543	0.176
S355J2 (Flange <sup>e</sup> )	219	325/355	-	NA <sup>d</sup>	NA <sup>d</sup>
S355J2 (Web <sup>e</sup> )	206	320/355	-	NA <sup>d</sup>	NA <sup>d</sup>
S460NL (Plt. <sup>a</sup> - 25mm)	203	460/460	-	643	0.166
S690QL (Plt. <sup>a</sup> - 25mm)	210	-/690	712	797	0.078
A992 Gr.50 (Web <sup>f</sup> )	200	375/345	-	504	0.183
A992 Gr.50 (Flange <sup>f</sup> )	204	360/345	-	515	0.174
A500 Gr. B (HSS305x16)	185	-/315	373	439	0.184
BCP325 (Plt. <sup>a</sup> - 22mm)	212	380/325	-	522	0.218
BCR295 (HSS350x22)	187	-/295	437	455	0.107
HYP400 (Plt. <sup>a</sup> - 27mm)	227	355/400	-	535	0.209

<sup>a</sup> Plate; <sup>b</sup> ultimate engineering stress;  
<sup>c</sup> the engineering strain at  $\sigma_u$ ; <sup>d</sup> not available;  
<sup>e</sup> specimens sampled from a HEB500 section;  
<sup>f</sup> specimens sampled from a W14x82 section

TABLE 2: Summary of NTR with SVD's performance and solution for different starting points and number of backstresses (S355J2+N - t=50mm) - 1/2

S.P. <sup>a</sup>	N.B. <sup>b</sup>	$\varphi(MPa^2)$	$\bar{\varphi}$ (%)	$\ \varphi\ _2$	It. <sup>c</sup>	$E(GPa)$	$\sigma_{y,0}(MPa)$	$Q_\infty(MPa)$	$b$
1	1	14925.68	8.21	3.1e-12	34	177.54	296.62	123.26	7.17
2	1	14925.68	8.21	2.5e-12	39	177.54	296.62	123.26	7.17
3	1	14925.68	8.21	3.3e-12	41	177.54	296.62	123.26	7.17
1	2	8980.48	6.37	5.8e-12	48	184.98	270.96	107.22	5.97
2	2	8980.48	6.37	4.6e-12	48	184.98	270.96	107.22	5.97
3	2	8980.48	6.37	2.3e-12	53	184.98	270.96	107.22	5.97
1	3	8931.03	6.35	5.5e-12	81	185.32	269.22	107.01	6.00
2	3	8931.03	6.35	4.6e-12	71	185.32	269.22	107.01	6.00
3	3	8931.03	6.35	5.0e-12	68	185.32	269.22	107.01	6.00
1	4	8931.03	6.35	6.7e-12	84	185.32	269.22	107.01	6.00
2	4	8931.03	6.35	3.4e-12	87	185.32	269.22	107.01	6.00
3	4	8931.03	6.35	9.5e-12	92	185.32	269.22	107.01	6.00

<sup>a</sup> starting point;

<sup>b</sup> number of backstresses;

<sup>c</sup> iterations;

TABLE 3: Summary of NTR with SVD's performance and solution for different starting points and number of backstresses (S355J2+N - t=50mm)- 2/2

S.P. <sup>a</sup>	N.B. <sup>b</sup>	$C_1(MPa)$	$\gamma_1$	$C_2(MPa)$	$\gamma_2$	$C_3(MPa)$	$\gamma_3$	$C_4(MPa)$	$\gamma_4$
1	1	6501.83	27.90	-	-	-	-	-	-
2	1	6501.83	27.90	-	-	-	-	-	-
3	1	6501.83	27.90	-	-	-	-	-	-
1	2	14327.30	115.12	1771.06	7.56	-	-	-	-
2	2	14327.30	115.12	1771.06	7.56	-	-	-	-
3	2	14327.30	115.12	1771.06	7.56	-	-	-	-
1	3	12659.43	150.94	3226.07	51.55	1345.22	5.54	-	-
2	3	12659.43	150.94	3226.07	51.55	1345.22	5.54	-	-
3	3	12659.43	150.94	3226.07	51.55	1345.22	5.54	-	-
1	4	7290.78	150.94	5368.66	150.94	3226.07	51.55	1345.22	5.54
2	4	6595.56	150.94	6063.88	150.94	3226.07	51.55	1345.22	5.54
3	4	6359.00	150.94	6300.42	150.94	3226.07	51.55	1345.22	5.54

<sup>a</sup> starting point;

<sup>b</sup> number of backstresses;

TABLE 4: Summary of normalized error metric for subset sampling. The analyses were conducted with 2 backstresses and the SVD preconditioning with starting point 1.

Set	# LP <sup>a</sup>	LP <sup>b</sup>	$\bar{\varphi}$	$\xi_1$	$\xi_2$	Set	# LP <sup>a</sup>	LP <sup>b</sup>	$\bar{\varphi}$	$\xi_1$	$\xi_2$
1	10	1, 2, 3,	6.37	0.0	0.00	36	6	1, 3, 6,	6.87	52.0	4.30
		4, 5, 6,				7, 9, 10					
		7, 8, 9,				10					
44	8	1, 2, 4,	6.46	42.0	1.62	19	4	1, 3, 5, 9	6.88	139.0	5.41
		5, 6, 7,				9, 10					
26	5	1, 5, 6,	6.53	58.0	2.62	40	5	1, 2, 6,	6.90	71.0	4.30
		8, 9				8, 10					
45	3	2, 3, 9	6.55	83.0	3.43	16	4	1, 5, 6, 7	6.90	88.0	4.88
34	6	1, 3, 5,	6.55	70.0	2.72	31	3	1, 3, 10	6.95	76.0	4.98
		7, 9, 10				10					
18	3	1, 3, 9	6.55	92.0	3.25	32	4	1, 3, 5,	6.95	152.0	7.00
		1, 5, 6,				10					
42	6	8, 9, 10	6.57	57.0	3.14	51	4	2, 4, 6, 9	7.02	394.0	79.79
		1, 5, 6,				6, 9					
25	5	7, 9	6.57	64.0	2.79	9	2	1, 6	7.16	124.0	11.92
		1, 3, 5,				1, 3, 5, 8					
20	5	7, 9	6.58	79.0	2.83	14	4	1, 3, 5, 8	7.23	170.0	8.27
		1, 4, 6,				1, 3, 5					
43	6	8, 9, 10	6.61	69.0	5.22	8	3	1, 2, 4, 6	7.28	197.0	9.64
		2, 3, 6,				1, 2, 4, 6					
49	4	9	6.65	57.0	3.97	12	4	1, 5	7.33	395.0	79.23
		1, 3, 6,				1, 2, 9					
21	4	9	6.65	57.0	3.69	6	2	1, 5	7.33	182.0	7.75
		1, 3, 5,				1, 2, 9					
33	5	7, 10	6.70	94.0	3.88	27	3	1, 2, 9	7.38	127.0	5.69
		1, 4, 6,				1, 9					
23	5	7, 9	6.74	105.0	10.89	17	2	1, 9	7.54	126.0	5.44
		1, 4, 6,				1, 7					
24	5	8, 9	6.75	112.0	14.78	10	2	1, 7	7.71	77.0	5.96
		1, 2, 6,				1, 8					
41	6	8, 9, 10	6.80	73.0	4.22	11	2	1, 8	7.74	129.0	7.79
		1, 3, 6,				1, 2, 10					
22	5	7, 9	6.81	48.0	3.99	38	3	1, 2, 10	7.80	224.0	9.49
		1, 3, 5,				1, 10					
15	4	8	6.83	82.0	4.38	37	2	1, 10	7.90	219.0	9.67
		2, 3, 6,				1, 10					
46	3	2, 6, 9	6.87	99.0	9.78	30	2	1, 10	7.90	219.0	9.67
		1, 4, 6,				1, 2, 4,					
						39	4	10	8.31	142.0	7.76
						3	2	1, 2	8.45	113.0	9.82
						47	3	2, 4, 9	9.04	258.0	14.47
						28	4	1, 2, 4, 9	9.12	253.0	13.32
						4	2	1, 3	9.32	164.0	14.21
						7	3	1, 2, 4	10.65	290.0	15.84
						5	2	1, 4	10.99	263.0	13.19
						48	3	4, 6, 9	13.62	450.0	72.53
						2	1	1	21.15	324.0	38.92

<sup>a</sup> number of load protocol samples;

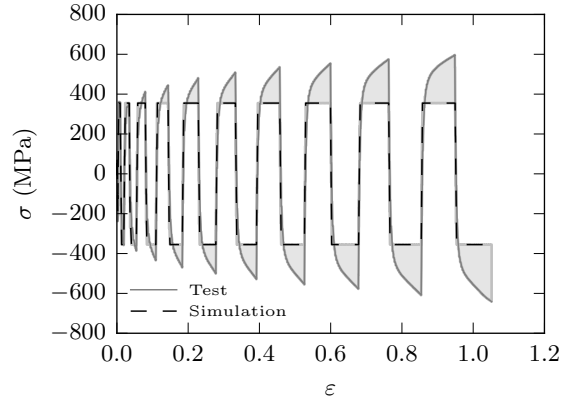
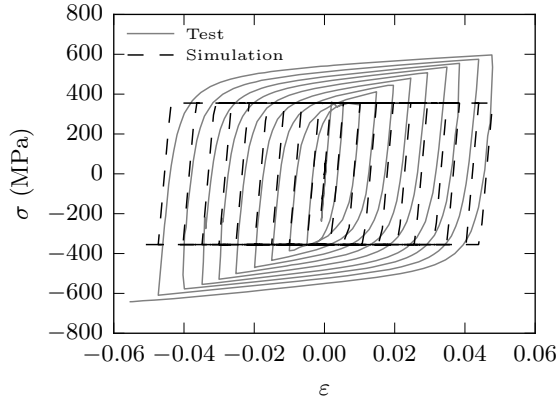
<sup>b</sup> load protocol;

TABLE 5: Results from NTR-SVD for different materials with 2 backstresses

Material	$\bar{\varphi}$ (%)	LP <sup>a</sup>	$E$ (GPa)	$\sigma_{y,0}$ (MPa)	$Q_\infty$ (MPa)	$b$	$C_1$ (MPa)	$\gamma_1$	$C_2$ (MPa)	$\gamma_2$
S355J2+N (Plt. <sup>b</sup> - 50mm)	6.37	1 to 10	185	271	107	5.97	14330	115	1771.06	7.56
S355J2+N (Plt. <sup>b</sup> - 25mm)	6.70	1 to 10	192	265	104	11.63	13000	100	1560.41	7.35
S355J2 (Flange <sup>d</sup> )	4.63	1, 2, 5, 6, 9	192	246	120	8.67	14020	205	1247.05	4.45
S355J2 (Web <sup>d</sup> )	6.16	1-3, 5-9	198	252	118	10.85	17876	236	2582.61	24.01
S460NL (Plt. <sup>b</sup> - 25mm)	6.32	1,2,4,5, 6,7,9,10	186	359	68	10.01	14202	104	2259.11	8.01
S690QL (Plt. <sup>b</sup> - 25mm)	7.95	1,2,4,5, 6,7,9,10	184	603	0.48	0.54	15938	78.8	988.77	6.57
A992 Gr.50 (Web <sup>c</sup> )	7.01	1,5,6,8,9	183	339.18	78	9.29	8716	118	1182	5.22
A992 Gr.50 (Flange <sup>c</sup> )	7.31	1,5,6,8,9	180	318.47	101	8.00	11608	145.22	1026	4.68
A500 Gr. B (HSS305x16)	6.86	1,5,6,8,9	171	301.26	130	82.2	9752	151.55	1613	8.21
BCP325 (Plt. <sup>b</sup> - 22mm)	5.05	1,5,6,8,9	178	306.09	94	5.81	11613	122.00	1744	8.29
BCR295 (HSS350x22)	8.38	1,5,6,8,9	173	346.42	0.56	0.60	9746	197.67	1852	12.84
HYP400 (Plt. <sup>b</sup> - 27mm)	5.31	1,5,6,8,9	189	376.22	29	6.41	13712	139.70	1147	4.59

<sup>a</sup> load protocols used in calibration; <sup>b</sup> Plate; <sup>c</sup> specimens sampled from a W14x82 section; <sup>d</sup> specimens sampled from an HEB500 section

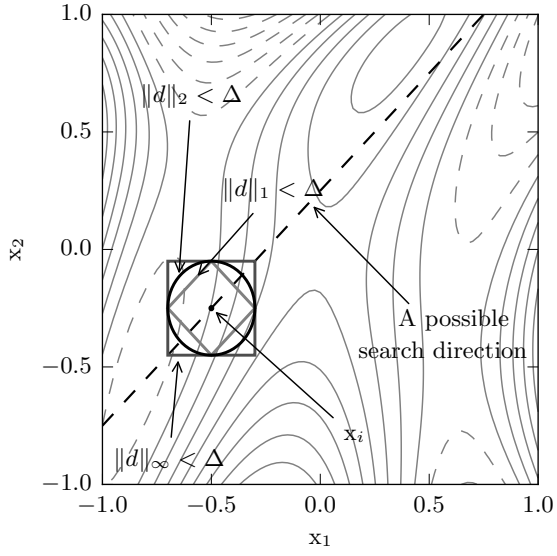
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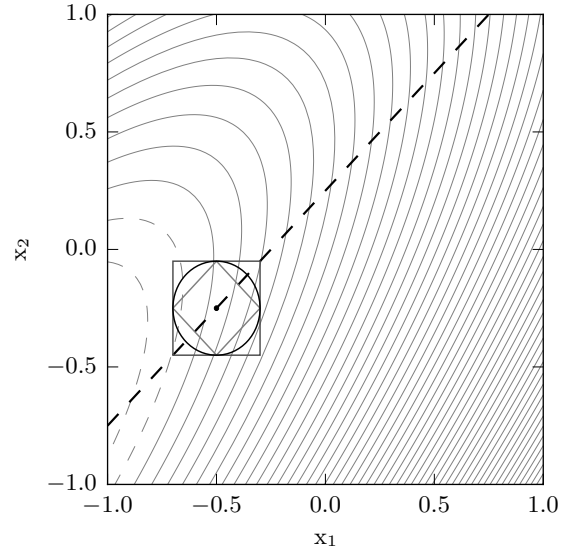
(a) Stress-strain relation of an example load protocol and corresponding estimate of an elastic-perfectly plastic model

(b) Unpacked load protocol and shaded area as a metric for the error in the elastic-perfectly plastic model

FIG. 1: Graphical representation of the error function  $\varphi$  as the square of the shaded area in  $\varepsilon^*$



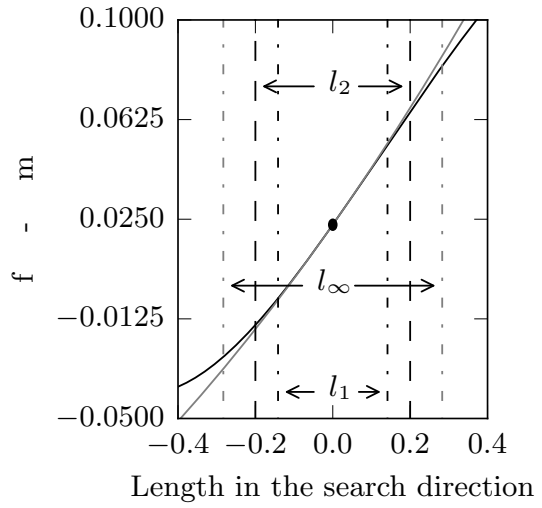
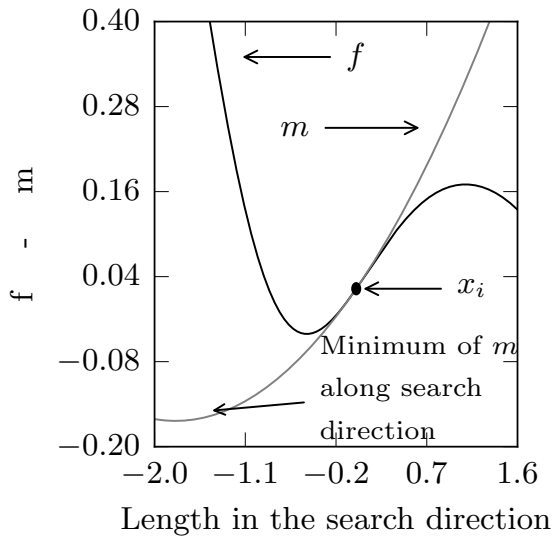
(a) Function  $f$



(b) Taylor approximation  $m$  centered on  $\mathbf{x}_i$

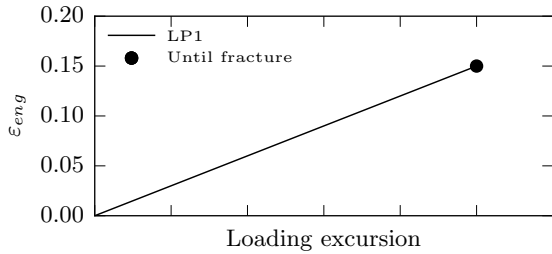
FIG. 2: Level curves of function  $f$ , Taylor approximation  $m$ , and illustration of step size according to different  $l$ -norms



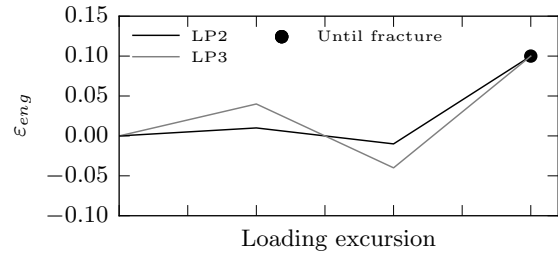


(a) Mismatch between  $f$  and  $m$  away from  $x_i$  (b) Step size restrictions according to different  $l$ -norms

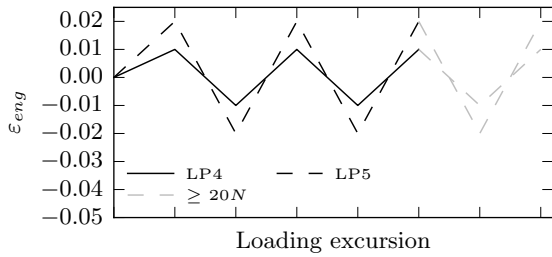
FIG. 3: Function and model values along the search direction in Fig. 2a and 2b



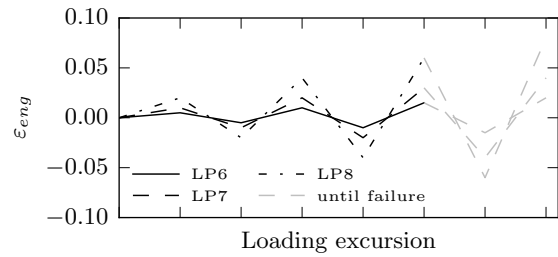
(a) Loading protocol # 1 - monotonic tensile test



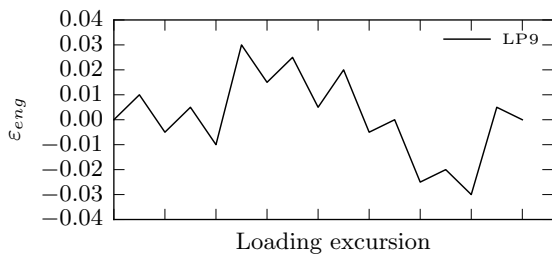
(b) Loading protocol # 2 & 3 - One cycle at 1% and 4% to fracture, respectively



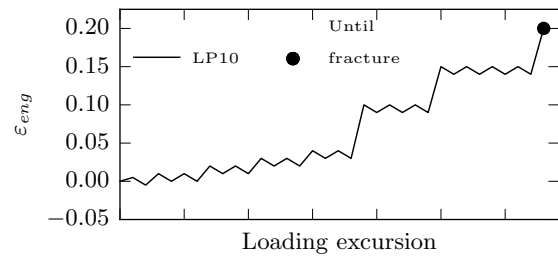
(c) Loading protocol # 4 & 5 - constant amplitude in ranges of 2% and 4% with zero mean strain, respectively



(d) Loading protocol # 6, 7 & 8 - incrementally increasing ranges of 1%, 2% and 4%, respectively, until specimen failure



(e) Loading protocol # 9 - variable amplitude



(f) Loading protocol # 10 - asymmetric

FIG. 4: Loading protocols under investigation; the loading excursion axis is schematic

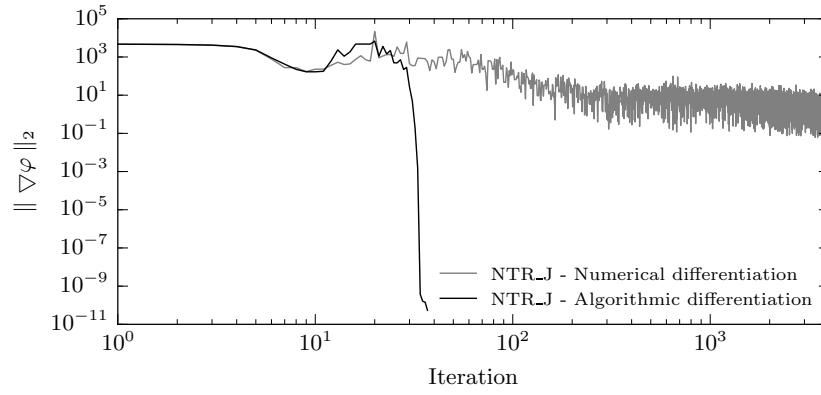


FIG. 5: Performance of the NTR algorithm with Jacobian preconditioning with respect to the use of numerical vs. algorithmic differentiation

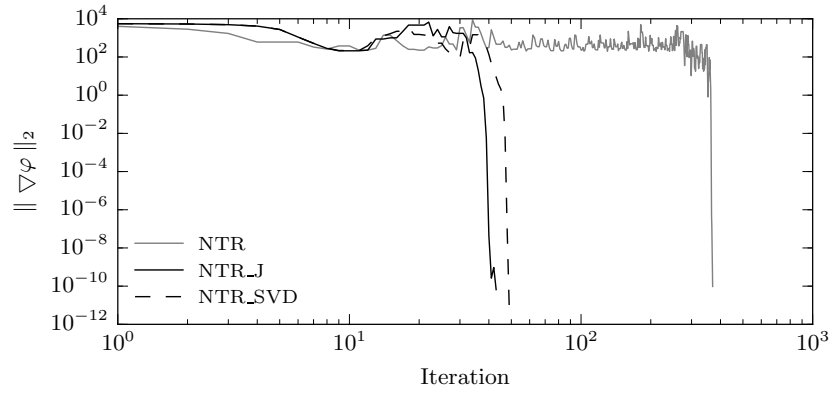
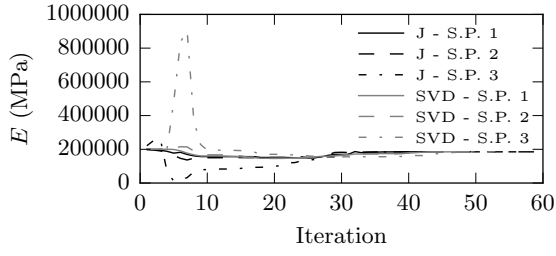
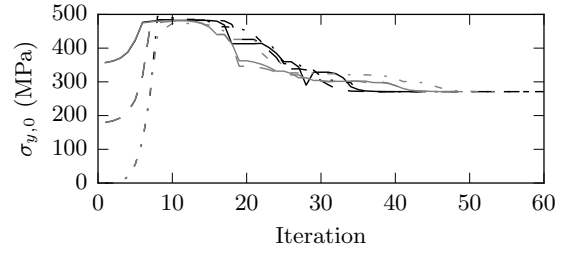


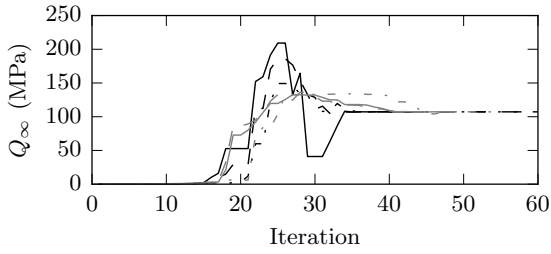
FIG. 6: Evolution of the gradient for a two backstress model for NTR with: no preconditioning(NTR), Jacobi (NTR\_J) and SVD preconditioning(NTR\_SVD)



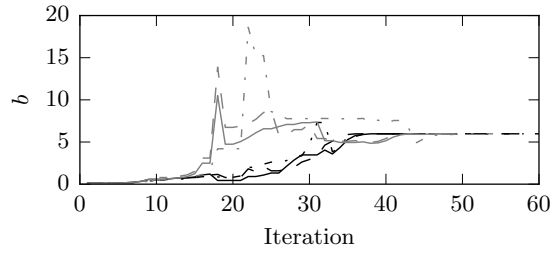
(a) Elastic modulus



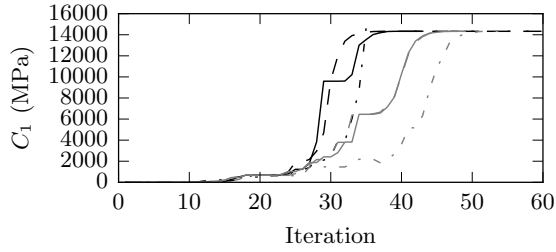
(b) Initial yield stress



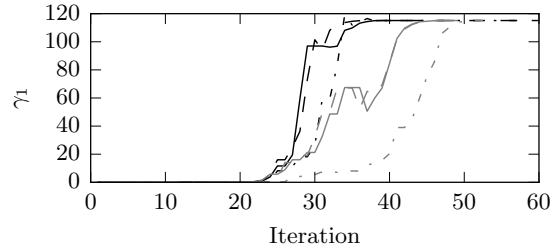
(c) Isotropic hardening parameter



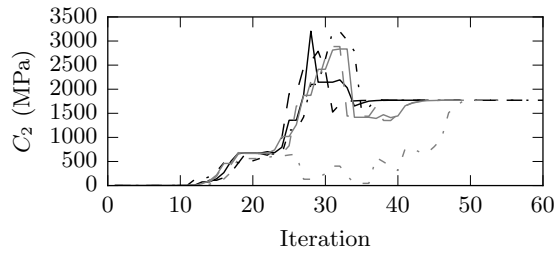
(d) Isotropic decay parameter



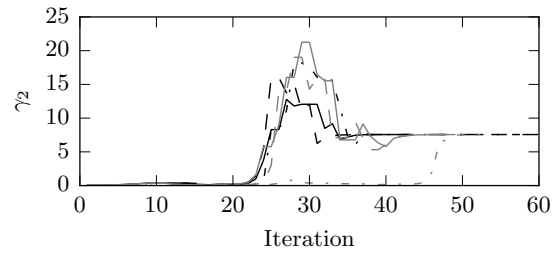
(e) 1<sup>st</sup> Kinematic hardening parameter - 1st backstress



(f) 1<sup>st</sup> Kinematic decay parameter - 1st backstress

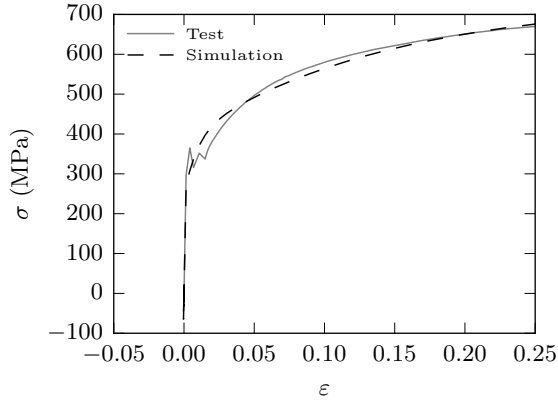


(g) 1<sup>st</sup> Kinematic hardening parameter - 2nd backstress

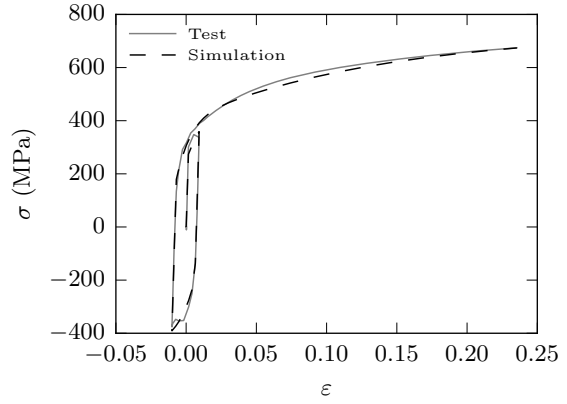


(h) 1<sup>st</sup> Kinematic decay parameter- 2nd backstress

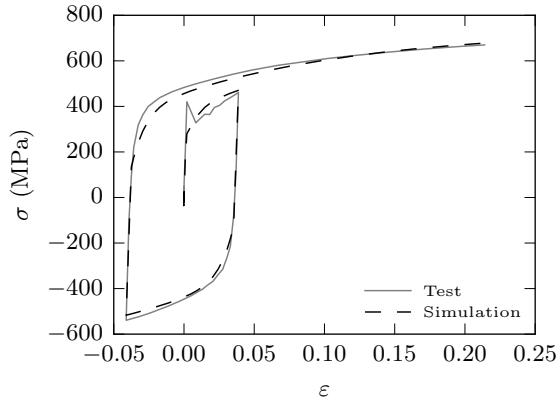
FIG. 7: Two backstress model parameter evolution for the preconditioned Newton Trust-Region algorithm at three different starting points - (J) Jacobi preconditioning; (SVD) Singular value decomposition preconditioning.



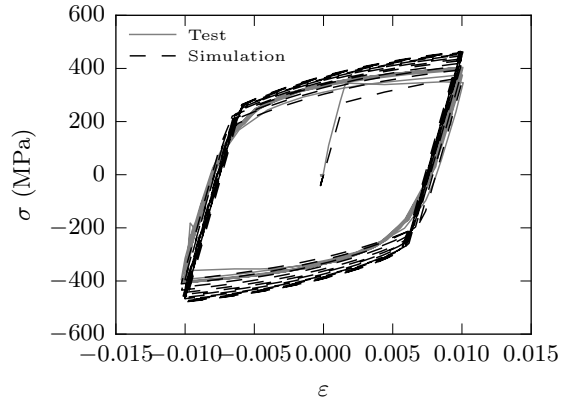
(a) Load protocol # 1



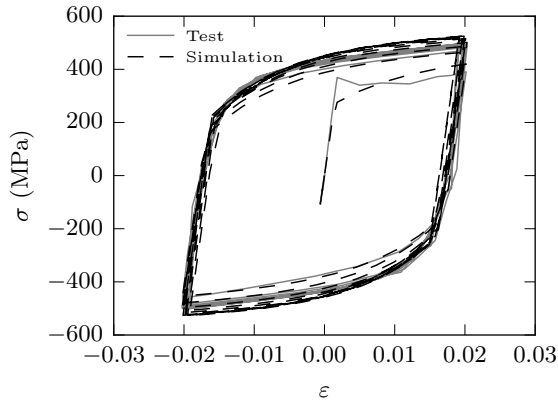
(b) Load protocol # 2



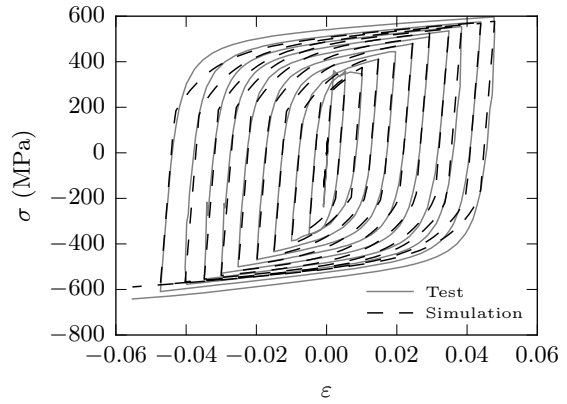
(c) Load protocol # 3



(d) Load protocol # 4

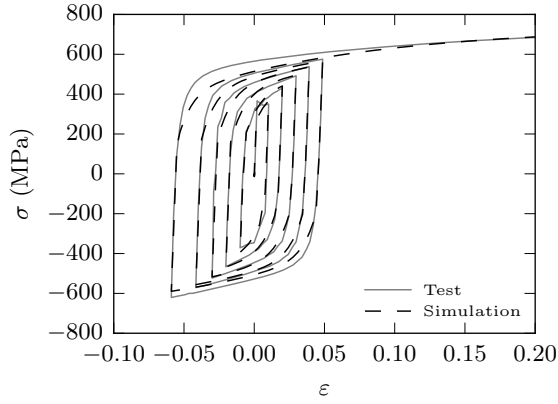


(e) Load protocol # 5

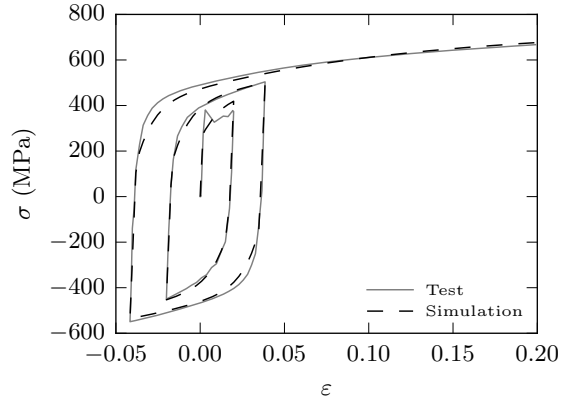


(f) Load protocol # 6

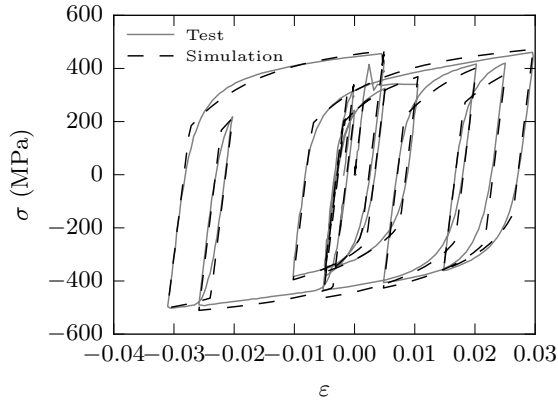
FIG. 8: Comparison of test results and the combined Voce and Chaboche model with two backstresses with parameters estimated with NTR (J) for S355J2+N ( $t=50\text{mm}$ ) steel



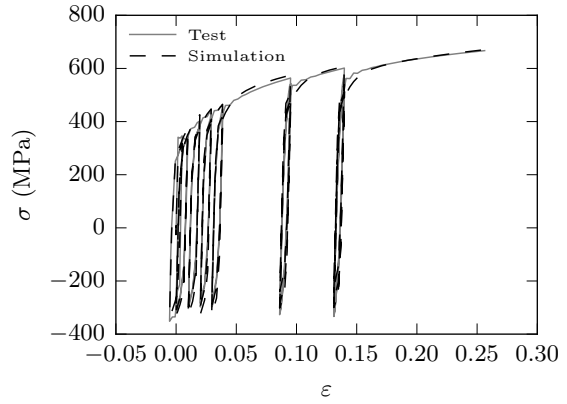
(g) Load protocol # 7



(h) Load protocol # 8

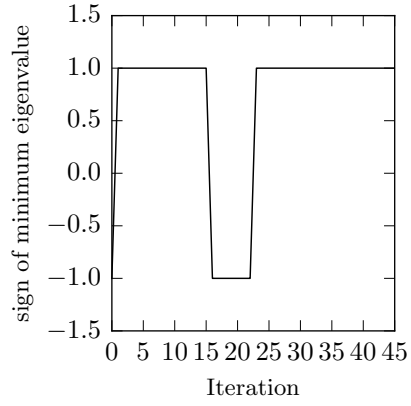
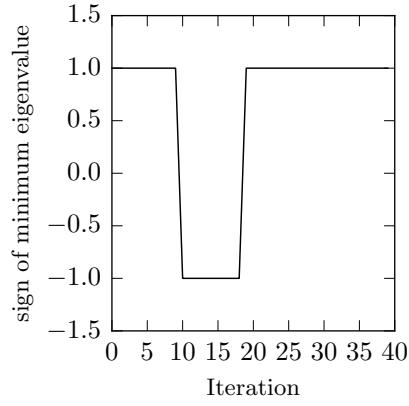


(i) Load protocol # 9

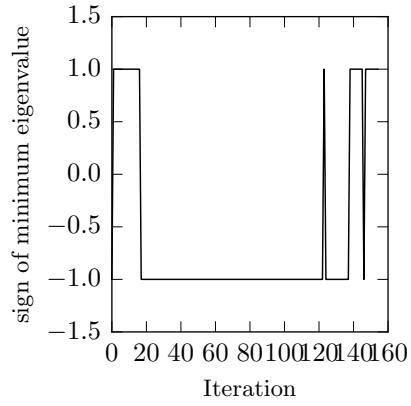
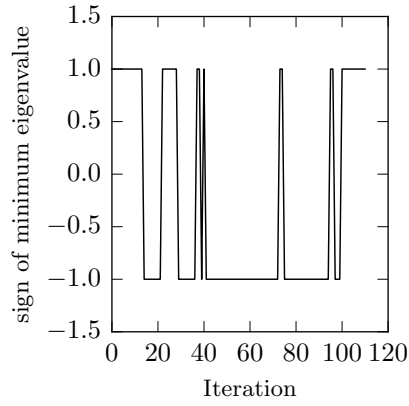


(j) Load protocol # 10

FIG. 8: (Cont.) Comparison of test results and the combined Voce and Chaboche model with two backstresses estimated with NTR (J) for S355J2+N ( $t=50\text{mm}$ ) steel



(a) 1 backstress at starting point 1 (b) 1 backstress at starting point 3



(c) 4 backstresses at starting point 1 (d) 4 backstress at starting point 3

FIG. 9: Evolution of the minimum eigenvalue sign of the Hessians in the NTR with SVD preconditioning method for different starting points and number of backstresses