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FE Simulation of Viscoplastic Consistency Model

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Finite element (FE) simulations provides an inexpensive alternative for material testing of new metal alloys. Carrying out experimental testing is expensive. Nanoindentation is particularly costly due to the equipment needed to work on such a scale. FE simulations provide an inexpensive means of material testing if accurately carried out. This paper will demonstrate the applicability and accuracy of using FE modelling for basic material tests and will propose that the viscoplastic model may be used for nanoindentation testing. The simulations will test the Young's modulus of materials during analysis when an Abaqus VUMAT is used. The viscoplastic model is incorporated into a subroutine and is tested at the macroscopic scale against previous published results.

Nomenclature

Symbols

ϵ strain

λ^{vp} viscoplastic multiplier defining magnitude of viscoplastic strain

\mathbf{E} elasticity matrix

q_1, q_2 fitting constants which provide profile of energy barrier

β_2, \bar{B} material parameters defined in terms of microstructural quantities

Y_a athermal yield stress

\hat{Y} threshold stress at which dislocations can overcome barriers without assistance of thermal activation

h, θ, y hardening modulus, softening parameter and strain-rate sensitivity parameter

Symbols

$()_n, ()_{n+1}$ previous and new step time

$()_i, ()_{i+1}$ previous and new iteration

I. Introduction

Niobium, tantalum, vanadium and titanium are important metallic chemical elements widely used in alloys.¹⁻⁵ These materials are used for a range of applications today including the aerospace and medical industry.¹⁻⁵ Under such conditions the materials will be subject to a variation of environmental and loading conditions hence thorough testing is required. Experimental work is used to test material properties to ensure that loading requirements are met however this is expensive. Nanoindentation is one such experimental method used to measure mechanical and tribological material properties however the cost of the equipment required to measure properties on a nanoscale is prohibitive. To reduce the need for experimental testing, numerical simulations have been established as an alternative method for testing materials. One such method is Molecular Dynamics (MD) where the crystal structure of the metal is numerical modelled via the energy potential and forces acting between particles. This method however is computationally expensive and an alternative computational method is desirable.

Rather than modelling the individual particles during a simulation a FE analysis will treat materials as homogeneous. However, in order to carry out accurate FE simulations, correct constitutive material models

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are needed. Constitutive material models describe the behaviour of a material under a load. Metallic material behaviour may be considered as a combination of linear and non-linear behaviour. The linear behaviour is described by Hooke's Law which is the most common material constitutive model used for mechanical loading. Hooke's law describes the relationship between stress and strain through a linear equation where the relationship is defined by the elastic modulus. The deformation undergone during elasticity is reversible. Non-linear material behaviour of metal is known as plasticity where irreversible material deformation occurs once the material has yielded. FE modelling of nanoindentation has been carried out however the material models used have been either elastic or some basic plasticity models.⁶⁻⁹ They do not capture the physical events occurring in the material during nanoindentation.

The current work will carries out elastic analysis on the three materials previously mentioned to demonstrate that simulations accurately model the elastic response of metals in this region. A viscoplastic model is proposed for nanoindentation modelling. To validate viscoplastic model a macroscopic simulation is carried out and compared with previous published data.

II. User-defined elasticity analysis

Before non-linear behaviour is considered, confidence in FE modelling of the materials is necessary. Testing of the material elasticity is necessary to ensure that FE analysis can model the material behaviour as defined by the user. The more complex material models described later must be modelled through user-defined subroutine rather than by the CAE environment therefore, although elasticity may be defined through the CAE interface in Abaqus, in this case it will be user-defined.

In this analysis the elastic modulus of different materials, niobium, tantalum and vanadium, are tested in a simple uniaxial tension problem where the material is subject to a $25ms^{-1}$ velocity. The material sample is 20mm x 20mm however due to symmetry of the plate only a quarter is modelled. The test is carried out on a single 2D axisymmetric element, using Abaqus CAX4R element, where the velocity is defined along one edge of the plate, the opposite edge is simply supported and the centreline is also simply supported. All analysis are carried out in Abaqus Explicit due to the large strain rate. Abaqus Explicit uses explicit integration algorithms and is used for dynamic problems occurring over short timescales as is the case in this analysis. The elastic constitutive equations are modelled in a user-defined subroutine, VUMAT. Figure II shows the elastic stress strain curve for niobium, tantalum and vanadium during the FE analysis. The gradient between the first and last points were found to match the inputted elastic moduli of the materials exactly.

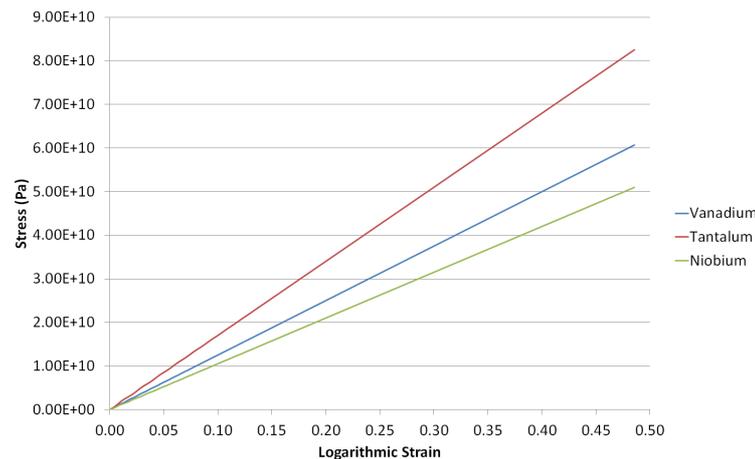


Figure 1. Elastic stress-strain curve for niobium, tantalum and vanadium agrees well with inputted Young's modulus

III. Viscoplasticity Model Proposal

Plastic deformation at the molecular (nano) scale is dependent on crystal structure of the material. The material behaviour is also dependent on the rate of deformation and temperature. Rate or time-dependent

behaviour is known as viscosity. At low rates of deformation the heat produced by dissipation of mechanical energy in the system will dissipate immediately due to heat flow and radiation. However at higher rates of loading, the mechanical energy produced in the system cannot dissipate due to the short time scale of the loading. It is obvious then that there is coupling between rate of deformation and temperature in a system at large loading rates however viscoplastic models, such as the Johnson-Cook model, which do not provide coupling between these parameters have been used thus far in microindentation and nanoindentation FE models.⁶ The classic constitutive models for viscoplasticity rely on yield functions to define when plastic flow occurs. The consistency model is used in this paper to include coupling effects of strain rate and temperature. This occurs through introducing a time-dependency into the yield function which together with a consistency parameter which obeys the classical Kuhn-Tucker relations. Therefore a time-derivative of the rate-dependent yield surface governs irreversible, viscous deformation behaviour.

IV. Viscoplasticity Theory

In small strain theory, the total strain rate $\dot{\epsilon}$ in an elasto-viscoplastic material may be additively decomposed into an elastic $\dot{\epsilon}^{el}$ and viscoplastic component $\dot{\epsilon}^{vp}$

$$\dot{\epsilon} = \dot{\epsilon}^{el} + \dot{\epsilon}^{vp} \quad (1)$$

where the superimposed dot denotes the time derivative. The stress and back stress are written as

$$\dot{\sigma} = \mathbf{E} : (\dot{\epsilon} - \dot{\epsilon}^{vp}) \quad (2)$$

$$\dot{\mathbf{X}} = \frac{2}{3}C\dot{\epsilon}^{vp} - \gamma\dot{\lambda}^{vp}\mathbf{X} \quad (3)$$

where γ and C are material constants and (\cdot) denotes tensor contraction ($e : \epsilon = E_{ijkl}\epsilon_{kl}$). The evolution of the viscoplastic strain rate tensor is defined by the viscoplastic flow rule;

$$\dot{\epsilon}^{vp} = \dot{\lambda}^{vp} \frac{\partial f}{\partial \sigma} = \dot{\lambda}^{vp} \mathbf{N} \quad (4)$$

where $\dot{\lambda}^{vp}$ is known as the consistency parameter.¹⁰ This parameter specifies the magnitude of the viscoplastic strain, $\dot{\epsilon}^{vp}$, while \mathbf{N} is the unit normal to the yield surface pointing out of the direction of the viscoplastic strain thus determining the direction of $\dot{\epsilon}^{vp}$. It is written as

$$\mathbf{N} = \frac{3}{2\sigma_{eq}}(\boldsymbol{\tau} - \mathbf{X}) \quad (5)$$

where $\boldsymbol{\tau}$ is the deviatoric component of the Cauchy stress tensor $\boldsymbol{\sigma}$ ($\tau_{ij} = \sigma_{ij} - \frac{1}{3}\sigma_{mm}\delta_{ij}$), \mathbf{X} is the back-stress tensor or the kinematic hardening conjugate force, and σ_{eq} is known as the equivalent stress defined in deviatoric space as

$$\sigma_{eq} = \sqrt{\frac{3}{2}(\boldsymbol{\tau} - \mathbf{X}) : (\boldsymbol{\tau} - \mathbf{X})} \quad (6)$$

To solve this problem, the above equations must be discretised. This is achieved by dividing the load history into a number of sub-intervals thus we begin with a known converged state at time step n ($\sigma_n, X_n, R_n, T_n, \epsilon_n^{vp} \dots$) to calculate the corresponding values after a time increment, Δt , at time step $n+1$. An implicit backward-Euler scheme is applied to such that discrete equations may be found as given in Appendix VI.

In this strain-driven process, the value of the strain-increment, ϵ_{n+1} is known however the unknowns are $\sigma_{n+1}, X_{n+1}, R_{n+1}, T_{n+1}, \epsilon_{n+1}^{vp} \dots$ which are driven by the viscoplastic multiplier, λ^{vp} . Calculation of the viscoplastic multiplier however requires some of the unknown variables. This problem is addressed through the introduction of a trial elastic state where the superscript $*$ indicates a trial state i.e. $\sigma_{n+1}^*, X_{n+1}^*, R_{n+1}^*, T_{n+1}^* \dots$. The trial values may be used to determine whether the trial elastic stress state lies outside the yield surface. If the stress state is beyond the yield surface then the trial values are taken as an initial condition for calculation of the viscoplastic multiplier. Iterations of the trial values and the viscoplastic multiplier take place to return the stresses to the yield surface. Iterations are performed using the Newton-Raphson method.

In the Perzyna model, the magnitude of the viscoplastic flow as characterised by the viscoplastic multiplier, $\dot{\lambda}^{vp}$, is proportional to or a nonlinear function of the overstress. With the consistency model the

ratio of the overstress and the viscosity defines the viscoplastic multiplier. The dynamic yield surface in the Consistency model is defined as (reference)

$$f_d = \sigma_{eq} - Y_a - R - \hat{Y} \left(1 - (-\beta_2 T \ln(\eta_o^{vp} \dot{p}))^{1/q_1} \right)^{1/q_2} \quad (7)$$

where η^{vp} is the relaxation time(the viscosity parameter). When $f_d = 0$, viscoplastic loading begins to occur while the material response is elastic only for $f_d < 0$. The viscoplastic consistency condition yields

$$\dot{f}_d = \frac{\partial f_d}{\partial \sigma_{ij}} \dot{\sigma}_{ij} + \frac{\partial f_d}{\partial X_{ij}} \dot{X}_{ij} + \frac{\partial f_d}{\partial p} \dot{p} + \frac{\partial f_d}{\partial T} \dot{T} + \frac{\partial f_d}{\partial \dot{p}} \ddot{p} = 0 \quad (8)$$

A more convenient form of Equation 8 is used so that the viscoplastic multiplier may be obtained

$$\dot{f}_d = N_{ij} \dot{\sigma}_{ij} - (h_1 + h_2 + \theta) \dot{\lambda}^{vp} - y \ddot{\lambda}^{vp} \quad (9)$$

For bcc metals the scalar parameters h , θ and y are defined as

$$h = -\frac{\partial f_d}{\partial R} \frac{\partial R}{\partial p} = \frac{\partial R}{\partial p} = \dot{R} = \dot{\lambda}^{vp} \frac{k}{2R} (\bar{B}^2 - R^2) \text{ for } R = \bar{B}(1 - e^{-kp})^{1/2} \quad (10)$$

$$\theta = -\frac{\partial f_d}{\partial T} = -\frac{\partial f_d}{\partial T} \frac{\Delta T}{\Delta \lambda^{vp}} z \hat{Y} \zeta \ln \left(\eta_o^{vp} \frac{\Delta \lambda^{vp}}{\Delta t} \right) \quad (11)$$

$$y = \frac{\partial f_d}{\partial \dot{p}} = \Delta t \hat{Y} T \zeta / \Delta \lambda^{vp} \quad (12)$$

where h is equal to the evolution of the hardening rule. The strain hardening rule, R , considers the plastic strain evolution of the forest dislocation density through the Taylor dislocation. \bar{B} , k , and m represent hardening parameters and ζ is

$$\zeta = \frac{\beta_2}{q_1 q_2} \left(1 - \left(-\beta_2 T \ln \left(\eta_o^{vp} \frac{\Delta \lambda^{vp}}{\Delta t} \right) \right)^{1/q_1} \right)^{\frac{1}{q_2} - 1} \left(-\beta_2 T \ln \left(\eta_o^{vp} \frac{\Delta \lambda^{vp}}{\Delta t} \right) \right)^{\frac{1}{q_1} - 1} \quad (13)$$

The radial return mapping method can then be used to solve $\Delta \lambda^{vp}$ by reducing it to a non-linear scalar equation in deviatoric stress space. In deviatoric stress space, the von Mises criteria is circular and therefore the normal, \mathbf{N} , to the yield surface is radial. The return mapping algorithm can then return the trial stress to the yield surface radially in deviatoric stress space hence \mathbf{N} remains radial and unchanged throughout the viscoplastic corrector phase of the algorithm. The nonlinear scalar relation that determines the consistency parameter, $\Delta \lambda^{vp}$, is

$$r(\Delta \lambda^{vp}) = \sigma_{n+1}^{eq} - Y_a - R_{n+1} - \hat{Y} \left(1 - \left(-\beta_2 T_{n+1} \ln \left(\eta_o^{vp} \frac{\Delta \lambda^{vp}}{\Delta t} \right) \right)^{1/q_1} \right)^{1/q_2} \quad (14)$$

where

$$\sigma_{n+1}^{eq} = \sigma_{n+1}^{eq*} - \Delta \lambda^{vp} (3\mu + aC) \quad (15)$$

σ_{n+1}^{eq*} is the trial equivalent stress for the new time increment $n + 1$. Equation, 14, is the key equation for the numerical method as it represents the equivalent algorithm of the consistency condition for the considered state variables. It can be solved using the Newton-Raphson method the general form of which is given below,

$$x^{i+1} = x^i - \mathbf{J}(x^i) \mathbf{r}(x^i) \quad (16)$$

where the superscript i and $i + 1$ refer to the previous iteration and the current iteration respectively.

$$\mathbf{J}(x^i) = \left(\frac{\partial r_{n+1}^i}{\partial x_{n+1}^i} \right)^{-1} \mathbf{1} \quad (17)$$

$$(\lambda^{vp})^{i+1} = (\lambda^{vp})^i - (J(\lambda^{vp}))^i (r(\lambda^{vp}))^i \quad (18)$$

The Jacobian is a scalar quantity given as

$$(J(\lambda^{vp})) = \left(\frac{\partial \lambda^{vp}}{\partial \lambda^{vp}} \right)^{-1} \quad (19)$$

where

$$\frac{\partial \lambda^{vp}}{\partial \lambda^{vp}} = \frac{\partial \sigma_{n+1}^{eq*}}{\partial \lambda^{vp}} + \lambda^{vp} \gamma C a_{n+1}^2 - a_{n+1}^2 C - -3\mu - h_{n+1} - \theta_{n+1} - \frac{y_{n+1}}{\Delta t} \quad (20)$$

$$\frac{\partial \sigma_{n+1}^{eq*}}{\partial \lambda^{vp}} = \frac{3\gamma a_{n+1}^2}{\sigma_{n+1}^{eq*}} \boldsymbol{\xi}_{n+1}^* : \mathbf{X}_n \quad (21)$$

The viscoplastic multiplier is then used to update the dynamic yield condition, where if the prescribed tolerance is met, the multiplier is also used to update viscoplastic strain and hence the new stress. More comprehensive review of this model is found in.¹⁰⁻¹²

V. Thermal Effect on stress-strain curve

The viscoplastic model has been incorporated into a VUMAT and the FE analysis described earlier has been carried out using the viscoplastic model. Materials parameters used for these materials may be found in.¹¹ This analysis was then run for a range of temperatures. Fig 2 compares the stress history with respect to time for these simulations with Abed's FE results.¹¹ Experimental results have shown that there is a significant difference in stress history curves when the materials are subjected to varying temperatures.¹¹ At higher temperatures the material has greater thermal energy to overcome the barriers preventing dislocations in the metal. The variation in temperature is also captured in the FE analysis carried out. Initial yield point does not change for higher temperatures however the stress values in the viscoplastic region compare well with experimental results at low temperatures. At high temperatures convergence of the stress curves should occur as the thermal stress approaches zero and at this point an athermal condition in the material is reached where its behaviour is no longer dependent on temperature. This is not the case here.

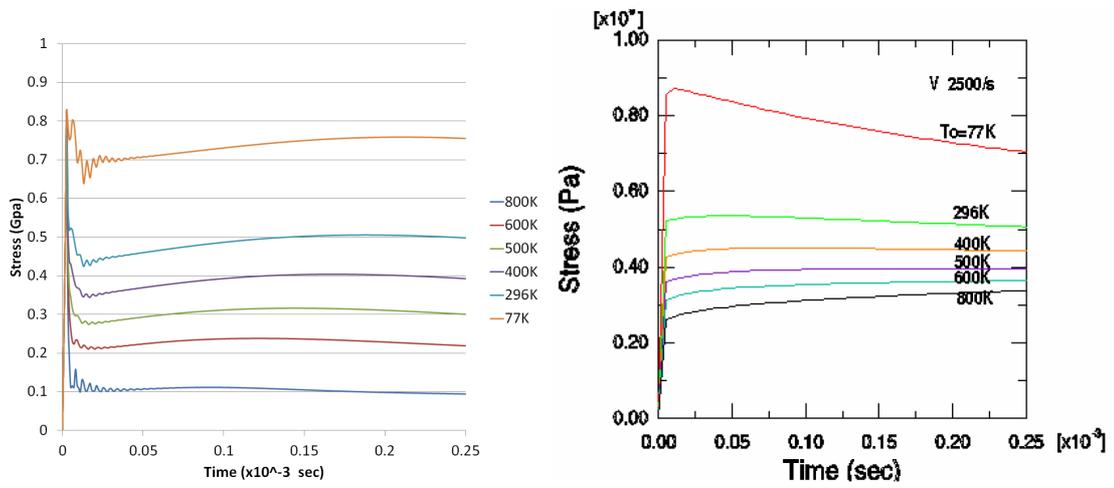
As can be seen in the initial yield point in this work's simulations is the same for all temperatures. This is because temperature dependence only occurs when there is viscoplastic strain therefore the initial yield is not affected by temperature. The stress oscillates somewhat after initial yield as the temperature begins to effect yield as viscoplastic flow is occurring. Abed's results demonstrate that at low temperatures significant strain softening occurs during loading whereas at higher temperatures a small amount of strain hardening occurs before levelling off. These results differ from Abed's as a strain hardening occurs at 77K and a small amount of strain softening occurs at high temperatures.

Further investigation of the constitutive model is required to identify the differences and improve the current viscoplastic model. Initial yield condition should be temperature dependent by introducing total strain into yield condition rather than the viscoplastic multiplier.

Once the viscoplastic subroutine is corrected and validated against Abed's results indentation analysis will be carried out. This will begin with indentation on a micrometre scale and validating results against published experimental data before investigating the use of this model for nanoindentation.

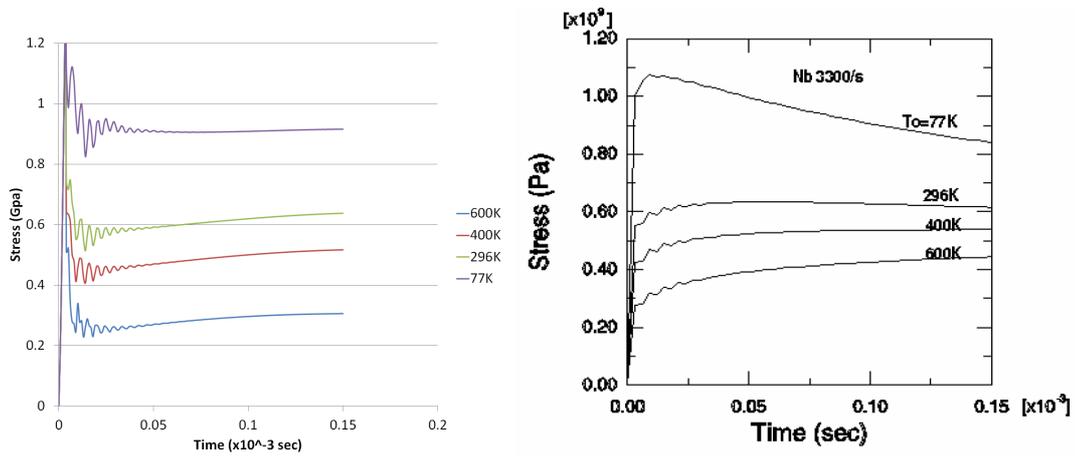
VI. Conclusions

- This paper demonstrates the use of FE modelling as an inexpensive alternative for material testing.
- Analysis has shown that the simulations can successfully model material elasticity during analysis through a VUMAT subroutine.
- The Consistency viscoplastic model has been proposed based on micromechanical behaviour which couples strain-rate dependence and temperature. This model is being incorporated in a subroutine and validated against published numerical results. Results demonstrate the effect of temperature on viscoplastic flow in metals.
- Further work on the viscoplastic model is needed to simulate viscoplastic flow more accurately during loading.
- It is proposed that the viscoplastic model is used for FE analysis of nanoindentation.



(a) Current simulation of vanadium for a load velocity of $25ms^{-1}$ (strain rate= $2500s^{-1}$)

(b) Abed's simulation of vanadium for a load velocity of $25ms^{-1}$ (strain rate= $2500s^{-1}$)



(c) Current simulation of niobium for a load velocity of $33ms^{-1}$ (strain rate= $3300s^{-1}$)

(d) Abed's simulation of vanadium for a load velocity of $33ms^{-1}$ (strain rate= $3300s^{-1}$)

Figure 2. Comparison of current work with published numerical results

Appendix A

The Consistency model computational steps are given below. It should be noted that as kinematic hardening has not been computed in this analysis, the kinematic parameters, γ and C , and hence the backstress X are

zero.

$$\begin{aligned}\sigma_{n+1}^* &= \sigma_n + \mathbf{E} : \Delta \epsilon \\ \boldsymbol{\tau}_{n+1}^* &= \sigma_{n+1}^* - \frac{1}{3} \text{tr}(\sigma_{n+1}^*) \boldsymbol{\delta}_{ij} \\ f_{n+1}^{d*} &= \sqrt{\frac{3}{2} (\boldsymbol{\tau}_{n+1}^* - \mathbf{X}_{n+1}) : (\boldsymbol{\tau}_{n+1}^* - \mathbf{X}_{n+1}) - Y_a - R_n - \hat{Y} \left(1 - \left(-\beta_2 T_n \ln \left(\eta_o^{vp} \frac{\Delta \lambda^{vp}}{\Delta t} \right) \right)^{1/q_1} \right)^{1/q_2}}\end{aligned}$$

Calculation of the $\Delta \lambda^{vp}$ using the Newton-Raphson method as described in Section

$$\begin{aligned}\boldsymbol{\xi}_{n+1}^* &= \boldsymbol{\tau}_{n+1}^* - a \mathbf{X}_n \\ \mathbf{N}_{n+1} &= \frac{3}{2 \sigma_{n+1}^{eq*}} \boldsymbol{\xi}_{n+1}^* \\ \boldsymbol{\xi}_{n+1} &= \boldsymbol{\xi}_{n+1}^* - \Delta \lambda^{vp} \left(2\mu + \frac{2}{3} aC \right) \mathbf{N}_{n+1} \\ R_{n+1} &= R_n + \Delta \lambda^{vp} \frac{k}{2R} (\bar{B}^2 - R^2) \\ \sigma_{n+1}^{eq} &= \sqrt{\frac{3}{2} \boldsymbol{\xi}_{n+1} : \boldsymbol{\xi}_{n+1}} \\ z_{n+1} &= \frac{1}{\rho c_p} \left(\sigma_{n+1}^{eq} - \frac{3\gamma}{2C} \mathbf{X}_{n+1} : \mathbf{X}_{n+1} - R_{n+1} \right) \\ T_{n+1} &= T_n + \Delta \lambda^{vp} z_{n+1} \\ \Delta \epsilon &= \Delta \lambda^{vp} \mathbf{N}_{n+1} \\ \boldsymbol{\epsilon}_{n+1}^{vp} &= \boldsymbol{\epsilon}_n^{vp} + \Delta \boldsymbol{\epsilon}^{vp} \\ f_{n+1}^d &= \sigma_{n+1}^{eq} - Y_a - R_{n+1} - \hat{Y} \left(1 - \left(-\beta_2 T_{n+1} \ln \left(\eta_o^{vp} \frac{\Delta \lambda^{vp}}{\Delta t} \right) \right)^{1/q_1} \right)^{1/q_2} \\ \sigma_{n+1} &= \sigma_n + \Delta \sigma = \mathbf{E} : (\boldsymbol{\epsilon}_{n+1} - \boldsymbol{\epsilon}_{n+1}^{vp})\end{aligned}$$

Acknowledgments

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