Computational Materials Science 152 (2018) 268–290

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Parameter covariance and non-uniqueness in material model calibration using the Virtual Fields Method

E.M.C. Jones*, J.D. Carroll, K.N. Karlson, S.L.B. Kramer, R.B. Lehoucq, P.L. Reu, D.Z. Turner

Sandia National Laboratories, United States

ARTICLE INFO

Keywords:
Material identification
Virtual Fields Method (VFM)
304L stainless steel
Bammann-Chiesa-Johnson (BCJ) material model
Viscoplasticity
Digital Image Correlation (DIC)

ABSTRACT

Traditionally, material identification is performed using global load and displacement data from simple boundary-value problems such as uni-axial tensile and simple shear tests. More recently, however, inverse techniques such as the Virtual Fields Method (VFM) that capitalize on heterogeneous, full-field deformation data have gained popularity. In this work, we have written a VFM code in a finite-deformation framework for calibration of a viscoplastic (i.e. strain-rate dependent) material model for 304L stainless steel. Using simulated experimental data generated via finite-element analysis (FEA), we verified our VFM code and compared the identified parameters with the reference parameters input into the FEA. The identified material model parameters had surprisingly large error compared to the reference parameters, which was traced to parameter covariance and the existence of many essentially equivalent parameter sets. This parameter non-uniqueness and its implications for FEA predictions is discussed in detail. Finally, we present two strategies to reduce parameter covariance – reduced parametrization of the material model and increased richness of the calibration data – which allow for the recovery of a unique solution.

1. Introduction

Modeling material and component behavior using finite-element analysis (FEA) is critical for modern engineering. One critical – yet often under-appreciated – input into FEA is a material model, which describes the constitutive relationship between the stress induced in a specimen as a function of loading conditions (such as elastic strain, plastic strain, strain rate, and temperature), as well as material properties (such as Young's modulus, Poisson's ratio, yield stress, and hardening). While often called "material properties", these quantities are actually better designated as model parameters. Depending on the type of material model utilized, the model parameters may or may not have physical meaning. Even in physics-inspired models, the parameters in the end are not actually material properties, but simply fitting parameters for the model that approximate the material behavior. The process of identifying model parameters is also called model calibration, material identification or material characterization.

Historically, experimental data of material behavior was limited to global measurements, such as applied load and extension. As a result, test specimens for model calibration typically had simple geometries such as tensile dog bones or torsion cylinders that are statically determined with homogeneous stress states. These simple experiments have the benefit of being relatively easy to perform, and trends in the data are often easy to identify manually. A main disadvantage, though, is that uni-axial stress states do not reflect real-world loading conditions; models calibrated using simplistic, uni-axial data are routinely extrapolated and expected to predict material behavior in complex, multi-axial loading conditions. Additionally, to calibrate a complex material model, many experiments are required at different strain rates, temperatures, orientations, etc. making model calibration time-consuming and expensive.

The development and maturity of full-field diagnostics, such as Digital Image Correlation (DIC), however, have opened the door to more sophisticated methods of material model calibration. The availability of rich, full-field deformation data allows specimen geometries to be complex, inducing heterogeneous stress states and a range of loading conditions (e.g. a range of strain-rates) in a single specimen. Thus, material models can be calibrated using data that more closely resembles the complex loading conditions a component of interest might experience. Additionally, by inducing a range of loading conditions in a single test, the number of tests required to calibrate complex material models is reduced.

There are many inverse techniques that capitalize on full-field deformation data for model calibration, such as the finite element model updating method, the constitutive equation gap method, the virtual fields method, the equilibrium gap method, and the reciprocity gap

* Corresponding author.
E-mail address: emjones@sandia.gov (E.M.C. Jones).

https://doi.org/10.1016/j.commatsci.2018.05.037
Received 22 March 2018; Received in revised form 17 May 2018; Accepted 18 May 2018

method [1]. This work focuses on the virtual fields method (VFM), which is based on the principle of virtual work [2]. Since its original development for linear elastic material models, VFM has been expanded to nonlinear plasticity models for metals [3–9], with many works focusing on identifying anisotropic plasticity models [10–12] or viscoplastic (i.e. rate-dependent) models [13–15]. One main benefit of VFM over the finite element model updating method (FEMU) is that VFM is significantly more computationally efficient than FEMU. However, a significant drawback is that VFM requires deformation measurements throughout the entire volume of the test specimen, whereas FEMU accepts deformation measurements on a subset of the test specimen (e.g. on the surface of a specimen); this point will be discussed in more detail throughout this article.

As computing resources become more powerful and engineers seek to design more complex components with reduced performance margins, high-fidelity models (both in terms of the material model and the finite-element model) become more critical. However, increased complexity of the material model makes calibration difficult as model parameters are often no longer independent [16]. For instance, Salehghaffari et al. [17] describe a physics-based approach to calibrating the Bammann-Chiesa-Johnson (BCJ) viscoplastic model in order to lock down one parameter at a time in a sequential manner, thus leading to a unique solution. Notta-Cuvier et al. [15] observed parameter covariance in the Johnson-Cook material model when using VFM to calibrate the model. Grama et al. [14] discussed in detail difficulties of finding a unique set of parameters due to insensitivity of the cost function to each of the parameters. Ogden et al. [18] found that different sets of model parameters obtained from different initial guesses led to significant differences in the solutions of a boundary-value problem using the different identified parameter sets.

This work focuses on identifying model parameters for a viscoplastic material model for 304L stainless steel using VFM and discusses parameter covariance and non-uniqueness in depth. The basic steps in VFM are outlined in Section 2.1, while details of the kinematics calculations, stress reconstruction algorithms, and VFM implementation in a finite-deformation framework are reserved for Appendices A–C. The material model and specimen geometry are described in Sections 2.2 and 3.1 respectively. Synthetic experimental data was generated using Finite Element Analysis (FEA) as described in Sections 3.2 and 3.3, and this data was used to verify the VFM algorithms in Section 3.4. Sections 4.1 and 4.2 contain information on the optimization process while the identified parameters are presented in Section 4.3. Covariance and non-uniqueness of the parameters are discussed in Section 5, while strategies to reduce parameter covariance are identified in Section 6. Lastly, the article concludes in Section 7 with some ideas for improving material models and model calibrations.

2. Background

2.1. Virtual Fields Method (VFM)

The original motivation for this work was to explore the potential of using a single specimen of unique geometry, in which a range of strain rates is induced in a single test, to calibrate a viscoplastic material model. We selected VFM as our technique for model calibration amongst other techniques that capitalize on full-field data because it is less computationally expensive than finite-element updating, and because we had prior experience with VFM. For nonlinear material models, the basic steps of VFM are outlined below, while specifics are contained throughout this article.

1. Select a material model (Section 2.2) and specimen geometry (Section 3.1).
2. Measure specimen deformation and applied load during testing (Section 3.2).
3. Compute kinematic quantities (i.e. deformation gradient and rate of deformation) from the full-field deformation measurements (Appendix A).
4. Reconstruct the stresses according to the selected material model, using an initial guess of model parameters, and the kinematic quantities (Appendix B):

$$\boldsymbol{\sigma} = \mathbf{g}_1(\sigma_f(\boldsymbol{\xi}),\boldsymbol{F},t) \tag{1}$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor, σ_f is the flow stress from the viscoplastic material model, $\boldsymbol{\xi}$ is a vector representing the material model parameters, $\boldsymbol{F}$ is the deformation gradient tensor, and t is time.
5. Select one or more kinematically-admissible virtual velocity fields (Appendix C.2).
6. Calculate the internal and external virtual power, P_{int} and P_{ext} respectively, as a function of time (Appendix C):

$$P_{int} = \int_{V_o} ((\det\boldsymbol{F})\boldsymbol{\sigma}\boldsymbol{F}^{-T}): \dot{\boldsymbol{F}}^* \, dV \tag{2a}$$

$$P_{ext} = \boldsymbol{f}\cdot\overline{\boldsymbol{v}^*} \tag{2b}$$

where V_o is the volume of the specimen in the reference configuration, $\boldsymbol{f}$ is the measured resultant load, $\overline{\boldsymbol{v}^*}$ is the virtual velocity field (chosen to be constant over the traction boundaries), and $\dot{\boldsymbol{F}}^*$ is the virtual velocity gradient derived from the virtual velocity field. In Eq. (2), the experimentally measured quantities are the deformation gradient and the applied load, in the internal and external power respectively; the material model (and thus the model parameters) enters through the Cauchy stress.
7. Integrate the virtual powers over time and compute a cost function, Φ, based on the balance of internal and external virtual work, W_{int} and W_{ext} (Appendix C):

$$W_{int} = \int P_{int}\, dt \tag{3a}$$

$$W_{ext} = \int P_{ext}\, dt \tag{3b}$$

$$\Phi = (W_{int} - W_{ext})^2 \tag{3c}$$

8. Iterate on the model parameters until the cost function is minimized.

While the details of nonlinear VFM can be complex and are reserved for the appendices, the key point is that the material model parameters are embedded into the cost function through a series of cascading relationships. The cost function is based on the internal virtual work, which is computed from the reconstructed stresses, which are determined in part through the flow stress, which is a function of the material model parameters:

$$\Phi = g_2(W_{int}(\boldsymbol{\sigma}(\sigma_f(\boldsymbol{\xi})))) \tag{4}$$

Therefore, by measuring the specimen deformation (over the volume of the specimen) and applied load during an experiment, one is able to use VFM to identify the material model parameters by minimizing the cost function and balancing internal and external virtual work.

2.2. Viscoplastic material model

There are many possible material models to describe the viscoplastic behavior of steel, such as the empirical Johnson-Cook model or the physics-based Bammann-Chiesa-Johnson (BCJ) to name two options. For simulations where material history is important, such as simulations with varying temperature and load, an internal state variable model such as BCJ can more accurately predict material behavior. Since