COMPUTATIONAL CONTINUUM MECHANICS

ВЫЧИСЛИТЕЛЬНАЯ МЕХАНИКА СЛОШНЫХ СРЕД

Computational Continuum Mechanics. 2021. Vol. 14. No. 1. pp. 61-76 DOI: 10.7242/1999-6691/2021.14.1.6

AN APPROACH TO NUMERICAL ESTIMATING THE STABILITY OF MULTILEVEL CONSTITUTIVE MODELS

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Multilevel constitutive models of materials give the possibility to explicitly describe the mechanisms of inelastic deformation, the material structure evolution and changes in the physical and mechanical properties of materials determined by their chemical composition and their internal structure. Therefore, these models seem to be very effective for improving metal processing and forming techniques. A study of the solutions (response change histories) obtained using constitutive models under perturbation of input data (influence history and initial conditions) and model operator is actual due to the fact that the material mechanical characteristics (including the lower scale level properties), physical processes occurring during deformation (for example, acts of interaction of defect structures at the microscale level) and the resulting influences (produced by stochastic boundary conditions) are stochastic in nature. Finding the solution to this problem is particularly important when researchers need to justify the use of new constitutive models for describing modern technological processes of thermomechanical treatment, in particular, those focused on creation of functional materials. The disadvantages of traditional analytical approaches (Lyapunov methods) taken to analyze the stability of multilevel material models have been briefly discussed. The definition of the solution stability is introduced; in contrast to the traditional definition, it takes into account the parametric perturbation of operators and the perturbation of the history of influences, which determine the right-hand side of the system of equations. A procedure for the model stability numerical assessment includes consideration of solutions stability for various values of the parameters that determine the operator and input data. The description of the program of computational experiments for the implementation of the proposed approach is presented. This program can be used to study various perturbations of initial conditions, the influence history, the operator, as well as to analyze the norms of their deviations and the integral norm of deviation of perturbed solutions from the base ones obtained in calculations with unperturbed parameters.

Key words: multilevel constitutive model, mathematical model stability, perturbation sensitivity

1. Introduction

It is known that an arbitrary mathematical model can be represented as an operator that allows one to find the output dataset (solution) input data which contains, in the general case, time-varying influences on the object under consideration and initial conditions [1]. An essential attribute of the analysis of complex models is examining the stability of solutions with respect to input and operator perturbations.

Rigorous mathematical stability analysis for nonlinear operators (in particular, algorithmic operators based on the principles of cellular automata) is difficult to implement analytically. In order to evaluate the features of the model, the stability of some model parameters or their aggregates under input disturbances are usually assessed numerically [2–6]. In a broad sense, the term “parameters” means the material functions and constants included in a model operator and an input dataset (initial conditions and influences). For this purpose, the sensitivity of the model to parameter perturbations - relationship between output data and parameter variations - is commonly analyzed. The variation of parameters takes place only at the initial moment of time, hence, the parameters included in the model operator are known as constants. Similar studies on the sensitivity of nonlinear models are carried out in such areas of science as oceanology [7], chemistry [8], population dynamics [9], ecology (determining the state of river basins [10, 11]), etc. For instance, in the framework of solid mechanics, the sensitivity of models has been investigated in relation to changes in the influences parameters and characteristics of the material. The analysis was frequently carried out using the approach suggesting that response derivatives can be explicitly found from parameters [12–15]. In this case, along with the factors of stress, functions taking into account the safety factor and the cost of the structure can be considered as the response parameters [12].

The constitutive relations, or constitutive models (CMs), used to describe the behavior of materials, are the most important components of the models. In solid mechanics, these models are employed to study the manufacturing features of metal products and their application. In recent

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decades, significant progress has been made in the development of multilevel CMs able to describe the material structure evolution and changes in the effective physical and mechanical properties of the material determined by its structure [16–19]. Due to the introduction of a sufficient number of internal variables [19–22], complex integral operators need not be used to take into account the memory of the material represented by the internal variables**,** to study the state of the structure and to implement the deformation mechanisms in terms of the CM of this type. Thus, in the general case, the multilevel CMs can be taken as the algorithmic operator equations containing the systems of differential and/or tensor-algebraic equations.

In [23], the sensitivity of the multilevel CMs to parameter (the numerical values of the operator constants) perturbations was evaluated using a technique that is based on the integral correlation of response histories for several types of loading; the models include perturbed and unperturbed parameters. The application of this technique to the two- and three-level CMs was discussed. The relevance of the study stems from the need to use (new) multilevel models of materials in describing the technological processes of thermomechanical treatment. In these processes, the mechanical properties of the structure (including the lower scale level properties) and the influences, produced by the stochastic boundary conditions specified for the entire billet, on its separate representative volumes are stochastic in nature. From the above reasoning, it is clear that the CMs meant for evaluating real technological processes should be resistant to corresponding perturbations. What is more, stability analysis is useful for the CM identification procedure [24–27]. If the model exhibits high sensitivity to material parameters (weakly perturbed at the values established during the identification procedure), then the domain of their definition seems to be revised with regard to physical considerations.

It is worth noting here that, in [23] and in other studies known to the authors, the sensitivity of the model to operator parameter perturbations implemented in an initial (unloading) configuration was investigated, and these values of material constants were assumed to remain unchanged in each process. For a more complete stability analysis, it is essential to identify the model responses to other types of an operator and input perturbations, especially those occurred at various instants of time during the entire process. In this paper, we explore the problems related to application of traditional analytical approaches to the stability analysis of multilevel CMs and discuss the ways to solve them. For this purpose, we propose a numerical method for assessing the stability of multilevel material models. This method makes it possible to extend the numerical procedure previously proposed in [23] to the cases of input and operator perturbations at different instants of time.

In section 2, the mathematical structure of multilevel CMs is given. A primary concern of our study is to analyze the features of CMs essential for describing the behavior of a representative macrovolume of the material; the applicability of CMs to solving boundary value problems is not considered. Section 3 contains a brief description of the traditional approaches to the study of the stability of mathematical models; the limitations of Lyapunov's methods are analyzed. At the end of the section, a detailed definition of stability is given which takes into account (in contrast to the traditional one) perturbations of the history of influences (right-hand side of differential equations) and parametric perturbations of the operator.Section 4 describes a computer program (software) for numerical implementation of the approach; particular attention is given to studying various perturbations of initial conditions, influences histories, and operators, as well as to evaluating the norms of their deviations and the integral norm of deviation of the perturbed solutions from the base ones obtained in the calculations with unperturbed parameters.

Due to the limited volume of the journal article, the capabilities of the proposed approach have been demonstrated in other separate publications of the authors.

2. Mathematical structure of multilevel constitutive models

Nowadays, for research and improvement of materials processing technologies, as well as for solving problems related to the development of new functional materials, a multilevel approach to the construction of CMs appears to offer the most promise. This approach is based on the introduction of internal variables and physical theories of plasticity [16–19, 28–31]. Internal variables (IVs) characterize material structure and deformation mechanisms at different scale levels; some IVs are explicitly involved in constitutive relations. CMs can include additional (hidden) IVs so that kinetic equations can be formulated for explicit IVs [19–22]. The physical and mechanical properties of the material at the macroscale level are determined by the state of the material structure. The structure of materials is known to vary significantly under large inelastic deformations (in particular, texture formation and refinement of the grain structure) [19]. Therefore, the use of a multilevel approach with a sufficient set of IVs is more preferable compared to the macrophenomenological relations, at least, for modeling complex thermomechanical loadings that are typical of technological processing techniques.

The main advantages of multilevel CMs are as follows. They can be used to describe the evolution of the material structure and, accordingly, material’s physicomechanical macroproperties (including the anisotropic ones). In the case of CMs models, the number of experiments is less in comparison with those required to determine the material functions of the macrophenomenological models which implicitly take into account structural rearrangements. In order to find macrophenomenological models that best suited to modeling machining processes, the experiments must be carried out under complex loading conditions. However, such experiments can be performed only in a three-dimensional subspace of the six-dimensional combined stress–strain space; another limitation being small deformations, compared with real technological processes, due to the early loss of stability of tubular specimens during torsion [32–34]. Generally speaking, multilevel models can be identified without any experiments on complex loading at the macroscale level [19].

The experimentally observed property of the memory of inelastically deformed solids [35, 36] was taken into account in the multilevel models due to the IVs, and therefore complex integral operators need not be introduced in these models. In the general case, multilevel CMs are the algorithmic operator equations that involve the systems of relatively simple mathematical relationships (differential and/or tensor-algebraic equations) [19–22, 37–41]. For example, the mesolevel elastoplastic submodel implies an algorithmic determination of active intragranular slip systems and a solution of the system of equations to find shear rates [42]. Multilevel CMs are very versatile, and therefore they can be applied to a wide class of materials and influences (including complex loadings), provided that the material structure, the basic deformation mechanisms, and the interactions between them are properly taken into account. The need to introduce a large number of IVs and kinetic equations (as a rule, the nonlinear ones) to describe changes in CMs is the price for the versatility. At the same time, the peculiarities of this approach make it promising for constructing mathematical models for complex systems and processes in various fields. Using this approach, the system is decomposed into constituent elements, and the relationships are formulated for its separate elements with subsequent aggregation. This makes the structure of the model transparent and applicable to many related systems and processes, which allows direct and indirect verification based on the experimental results for the processes occurred at the lowest scale levels. The specified features of the approach to the construction of CMs are consistent with the system analysis methodology [43].

One part of the IVs directly appears in the constitutive relations between response and influence; these variables are called the internal explicit variables and are denoted as $\mathbf{J}^{e}_{\beta},\ \beta=\overline{1,B^{e}}$. Another part of the IVs (the majority of these variables relate to deeper structural-scale levels), denoted as $\mathbf{J}^{i}_{\beta},\ \beta=\overline{1,B^{i}}$, is necessary to construct physically justified relations for describing the evolution of the explicit IVs; the variables of this group are called implicit variables. Thus, the full set of internal variables can be represented as $\left\{\mathbf{J}_{\beta}\right\}=\left\{\mathbf{J}^{e}_{\gamma},\mathbf{J}^{i}_{\delta}\right\}$, $\beta=\overline{1,B}$, $\gamma=\overline{1,B^{e}}$, $\delta=\overline{1,B^{i}}$, $B=B^{e}+B^{i}$. We consider CMs that can be written at the macroscale level as the following system of equations [21]:

$$
\begin{aligned}
\boldsymbol{\Sigma}^{(\mathrm{r})} &= \mathbf{F}_{(\mathrm{r})}\left(\boldsymbol{\Sigma}, \mathbf{P}_{\alpha}, \mathbf{J}^{\mathrm{e}}_{\gamma}\right), \\
\mathbf{J}^{\mathrm{e}\,(\mathrm{r})}_{\gamma} &= \mathbf{C}_{(\mathrm{r})\,\gamma}\left(\mathbf{J}^{\mathrm{e}}_{\gamma}, \mathbf{P}_{\alpha}, \mathbf{J}^{\mathrm{i}}_{\delta}\right), \\
\mathbf{J}^{\mathrm{i}\,(\mathrm{r})}_{\delta} &= \mathbf{R}_{(\mathrm{r})\,\delta}\left(\mathbf{J}^{\mathrm{i}}_{\delta}, \mathbf{P}_{\alpha}, \mathbf{J}^{\mathrm{i}}_{\kappa}\right),
\end{aligned}
\tag{1}
$$

where $\boldsymbol{\Sigma}$ is the stress state measure (response), $\mathbf{P}_{\alpha}$, $\alpha = \overline{1, \mathrm{A}}$ are the parameters describing the influences of thermomechanical (e.g., temperature and deformed state measure) and non-thermomechanical (e.g., irradiation, chemical effects) character , $\kappa = \overline{1, \mathrm{B}^{\mathrm{i}}}$. The right-hand side of (1) is represented by the tensor-valued functions of tensor arguments. In the left-hand side of this equation, one can see the index (r) which denotes the derivatives (most often, the corotational ones) independent of a choice of the coordinate system [44–46]. The question of how to find the derivative of a specified type for the geometrically nonlinear CR remains one of the most acute problems of continuum mechanics. The results of the studies performed by the authors in this research direction and the resulting formulations, which involve a corotational derivative that takes into account the symmetry properties of the material, are given in [19, 47–49]. Note that the algorithmic operator equations of CMs can be represented in form (1). To this end, the right-hand side of the relations must be set in a proper way, for example, using the conditional functions such as a Heaviside function.

The system of equations (1) can be transformed to the form:

$$
\begin{aligned}
\dot{\boldsymbol{\Sigma}} &= \mathbf{F}\,(\boldsymbol{\Sigma}, \mathbf{P}_{\alpha}, \mathbf{J}^{\mathrm{e}}_{\gamma}), \\
\dot{\mathbf{J}}^{\mathrm{e}}_{\gamma} &= \mathbf{C}_{\gamma}(\mathbf{J}^{\mathrm{e}}_{\gamma}, \mathbf{P}_{\alpha}, \mathbf{J}^{\mathrm{i}}_{\delta}), \\
\dot{\mathbf{J}}^{\mathrm{i}}_{\delta} &= \mathbf{F}_{\delta}(\mathbf{J}^{\mathrm{i}}_{\delta}, \mathbf{P}_{\alpha}, \mathbf{J}^{\mathrm{i}}_{\kappa}),
\end{aligned}
\tag{2}
$$

where the material time derivatives are on the left. The spin of the moving macrolevel coordinate system, which is used to specify the corotational derivative in (1), must be added to a set of explicit internal variables. The effective elastic property tensors and the inelastic and thermal strain rate tensors act as other explicit IVs at a macrolevel. The characteristics of individual crystallites (material property, spin, inelastic and thermal strain rate tensors) serve as implicit IVs at a macrolevel. In the two-level formulation, the last variables are also the explicit IVs at a mesoscale. They are used to determine stresses, and kinetic equations for these variables are written with additional implicit mesoscale IVs (slip rates, critical shear stresses, etc.) [19, 50]. For these IVs, $\mathbf{j}^{\mathrm{i\,mezo}}_{\eta}$, $\eta = \overline{1, \mathrm{B}^{\mathrm{i\,mezo}}}$, and thus the relations of the two-level model can be written as

$$
\begin{aligned}
\dot{\boldsymbol{\Sigma}} &= \mathbf{F}\,(\boldsymbol{\Sigma}, \mathbf{P}_{\alpha}, \mathbf{J}^{\mathrm{e}}_{\gamma}), \\
\dot{\mathbf{J}}^{\mathrm{e}}_{\gamma} &= \mathbf{C}_{\gamma}(\mathbf{J}^{\mathrm{e}}_{\gamma}, \mathbf{P}_{\alpha}, \mathbf{J}^{\mathrm{i}}_{\delta}), \\
\dot{\mathbf{J}}^{\mathrm{i}}_{\delta} &= \mathbf{R}_{\delta}(\mathbf{J}^{\mathrm{i}}_{\delta}, \mathbf{P}_{\alpha}, \mathbf{J}^{\mathrm{i}}_{\kappa}, \mathbf{j}^{\mathrm{i\,mezo}}_{\eta}), \\
\dot{\mathbf{j}}^{\mathrm{i\,mezo}}_{\eta} &= \mathbf{G}_{\eta}(\mathbf{J}^{\mathrm{i\,mezo}}_{\eta}, \mathbf{J}^{\mathrm{i}}_{\delta}, \mathbf{P}_{\alpha}, \mathbf{J}^{\mathrm{i}}_{\kappa}, \mathbf{j}^{\mathrm{i\,mezo}}_{\lambda}),
\end{aligned}
\tag{3}
$$

where $\lambda = \overline{1, \mathrm{B}^{\mathrm{i\,mezo}}}$. In the three-level (in terms of the scales) models, there occurs another group of variables and kinetic equations appears, and so happens at each new scale. For any element at every level, the stress-strain state (SSS) and IVs are assumed to be homogeneous. Therefore, spatial coordinates are not explicitly included in the arguments in (3). At the same time, all the parameters at a mesoscale (or at the lowest of the levels entering the model), including the IVs, are “assigned” to the same crystallites throughout the entire process.

Note that our study is focused on analyzing the properties of the models describing the representative macrovolume behavior of the material, i.e. the multilevel statistical CMs. These models do not consider any solutions to boundary value problems with inhomogeneous SSS fields. Moreover, in contrast to the commonly used statistical models, which are based on crystal plasticity (see [51, 52] and others and ignore any grain interactions, the generalized statistical models proposed by the authors can partially take into account the grain structure topology – the mutual arrangement of crystallites in space [19]. This feature of the model is necessary to describe grain boundary hardening and grain boundary sliding, and it can be implemented in an efficient way, without considering the spatial configurations of individual grains (only the grain packing is analyzed). The proposed mathematical apparatus can also be applied to direct crystal plasticity models [17, 53, etc.]. In these models, the inhomogeneous fields of SSS and IVs at a mesoscale are investigated using the finite element method, and the perturbations must be consistent in this case with the relationships of the mathematical model (boundary value problem).

The main output data of the CM are the macrostress tensor components, which are usually determined in a fixed laboratory coordinate system. In order to formulate some particular problems, the output data are supplemented with the additional variables related to the IVs which reflect the material structure conditions. These variables involve, e.g., the macroscale components of the effective physical and mechanical property tensors, the crystallite orientation distribution function, the average intragranular shear rates, the temperature source intensity under inelastic deformations, the mesostress distribution of (at zero macrostresses, these are residual mesostresses), and some others. In the terminology of a classical stability problem, an output data set can be called a "solution" to the specific problem. For clarity of presentation, all the output data are combined into a common vector of the decision variables $\mathbf{Y}(t)$, $t\in[0,T]$, where T is the end deformation moment. The output data set (the solution), obtained in terms of the CM, is represented as the vector-function $\mathbf{Y}_{t\in[0,T]} \in A_{t\in[0,T]} \subset \mathrm{C}^n_{\mathrm{L}^2}$, where $\mathrm{C}^n_{\mathrm{L}^2}$ is the space of n-dimensional continuous vector functions (at $t\in[0,T]$) with a norm set by the Riemann integral $\left\|\mathbf{Y}_{t\in[0,T]}\right\|_{\mathrm{C}^n_{L^2}} = \left(\int\limits_0^T \sum\limits_{i=1}^m \left(Y_i\left(t\right)\right)^2 dt\right)^{1/2}$ [54], where $A_{t\in[0,T]}$ is the range of the values defined by the CM operator.

The CM input data are the parameters of the kinematic and temperature influences, which, in the general case, vary with time, and the initial conditions. The initial conditions include the initial stress values (there may be nonzero residual stresses at different levels, coordinated through averaging) and the initial IVs values, which correspond to the initial state of the material structure. Using the IVs, the initial effective physical and properties are established at a macrolevel. For instance, the sampling of the initial crystallite orientations and material constants at a mesoscale makes it possible to determine the initial physical and mechanical (elastic, temperature) properties at a macroscale. Note that the assignment of the initial IVs values to the input data implies the knowledge of the form of the model operator (as a result, the IVs gain an appropriate physical meaning), which is typical for the "white box" models [1].

Let us combine all the kinematic and temperature influences $\mathbf{P}_\alpha(t)$ into the influence vector $\mathbf{X}(t)$, $t\in[0,T]$. Hence, the influences occurred during the process can be represented as $\mathbf{X}_{t\in[0,T]} \in DX_{t\in[0,T]} \subset Q_2^m[0,T]$, where $Q_2^m{}_{t\in[0,T]}$ is the space of m-dimensional piecewise continuous vector functions (at $t\in[0,T]$) with a norm set by the Riemann integral $\left\|\mathbf{X}_{t\in[0,T]}\right\|_{Q_2^m} = \left(\int\limits_0^T \sum\limits_{i=1}^m \left(X_i\left(t\right)\right)^2 dt\right)^{1/2}$ [54], where $DX_{t\in[0,T]}$ is the domain of the (permissible) influences, limited by the ranges of influences (for example, in terms of strain rate and temperature) for which the CM is applicable. We note that, these functions are considered to be the same; they only differ in a finite number of points. In the context of a physico-mechanical model, this is similar to disregarding the instantaneous (in terms of infinitesimal periods of time) fluctuations of influences. Hence, we assume that they can be neglected, since the periods of process realization in solids are finite, and the material does not have time to respond to these fluctuations.

Similarly, all the components of the tensor IVs are inserted in the vector $\mathbf{Z}(t)$, $t\in[0,T]$, $\mathbf{Z}(t)\in DZ(t)\subset l_2^k$, where l_2^k is the R^k space with a norm $\|\mathbf{Z}(t)\|_{l_2^k}=\left(\sum_{i=1}^{n}\left(Z_i(t)\right)^2\right)^{1/2}$ (this happens at a certain instant of time $t\in[0,T]$), where $DZ(t)$ is the IVs domain (at t) defined by the model operator. Since IVs are related to structure elements and deformation mechanisms, their values must fall into the physically realizable ranges. The difference of the IVs norm from the integral norms introduced above for the response and influences is due to the fact that there is no need to consider the history of changes in IVs. This norm is used to establish the deviations of the initial conditions for IVs. As it has been already noted, the additional response variables can be introduced into the CM via linking them with IVs, which, if necessary, offers an opportunity to analyze the IVs evolution.

Then, formally, the multilevel CM (3) can be written as

$$\begin{aligned}
&\dot{\mathbf{Y}}(t)=\mathbf{f}\left(\mathbf{X}(t),\mathbf{Y}(t),\mathbf{Z}(t)\right), && 1\\
&\dot{\mathbf{Z}}(t)=\mathbf{g}\left(\mathbf{X}(t),\mathbf{Y}(t),\mathbf{Z}(t)\right), && 2\\
&\mathbf{Y}\big|_{t=0}=\mathbf{Y}_0, && 3\\
&\mathbf{Z}\big|_{t=0}=\mathbf{Z}_0. && 4
\end{aligned} \tag{4}$$

The input data of the model include the history of influences $\mathbf{X}_{t\in[0,T]}$, and the initial conditions for output variables $\mathbf{Y}_0$ (4_3) and for initial conditions for internal variables $\mathbf{Z}_0$ (4_4). The nonlinear functions $\mathbf{f}$, $\mathbf{g}$ define the composite operator of the model $\mathbf{f}(t)$: $R^m\times R^n\times R^k\to R^n$, $\mathbf{g}(t)$: $R^m\times R^n\times R^k\to R^k$, which contains a set of tensor differential and algebraic relationships between the response (macrostresses), influences and internal variables. Note that the definition of $\mathbf{f}$ and $\mathbf{g}$ is a complex procedure. Thus, for elastoplastic and rigid-plastic models, an algorithmic procedure is required to establish slip systems that are active at the considered instant of time in each crystallite and to formulate a system of relations for defining shear rates [42]. In the case of elastoviscoplastic models, there is no need for such a procedure, however, the right-hand side of the equation includes the Heaviside functions of the difference between shear and critical stresses on slip systems [19].

Based on the input data $\left\{\mathbf{X}_{t\in[0,T]},\mathbf{Y}_0,\mathbf{Z}_0\right\}$, the constitutive model (4) enables finding the solution $\mathbf{Y}_{t\in[0,T]}$ which can be considered as a composite operator Φ [1]: $\mathbf{Y}_{t\in[0,T]}=\Phi\left(\mathbf{X}_{t\in[0,T]},\mathbf{Y}_0,\mathbf{Z}_0\right)$. Note that the class of examined problems (finding a relationship between input and output data) is classified as ill-posed in the sense of Hadamard [55]; for any input data, there are no proofs of the existence and uniqueness of a solution to these problems. The possibility of establishing the response of the material based the history of influences (existence of a solution for a correct CM) provides in continuum mechanics axiomatically (the principle of determinism by W. Noll [35] or essentially equivalent A.A. Ilyushin's postulate of macrophysical determinability [56]) and has been confirmed experimentally. Moreover, the experimental data for both homogeneously and inhomogeneously deformed samples demonstrate that the instability (non-uniqueness) of SSS at a macrolevel manifests itself only occasionally, i.e, when the influences are chosen for some specific states of the material structure specially (similar to a special choice of input data for the mathematical model). This has been confirmed by the experience of many researchers who worked with multilevel material models (an extensive review of these studies is presented in [19]). Thus, following the indicated physical considerations, the problem of establishing the response of a material to the prescribed influences can be considered correct according to Tikhonov [55]. In this case, the subproblem of identifying an operator definition subdomain, where a solution to problem (4) is unique (stable), is very important. In particular, in order to justify the use of constitutive models (first of all, new models) for describing the technological processes of thermomechanical treatment, it is essential to study characteristic loading modes, in other words, to find solutions at certain input data. Therefore, at the initial stage of the subproblem solution, it is advisable to perform the local stability analysis (in the vicinity of suchsolutions).

The parameters of the CM operator include constants (coefficients in the equations formulated to describe the main deformation mechanisms) that characterize the properties of the materials at different scale levels. Certainly, possible perturbations of the operator are not limited to the cases of perturbations of these parameters, which, for instance, can arise due to the perturbation of the IVs value at different times. Indeed, according to the representation of the mathematical model as an operator connecting the input and output data [1], the IVs and the equations for them are the elements of a composite operator. Therefore, the perturbation of the IVs values at the instants of time different from the initial one (initially, they correspond to the perturbation of initial conditions), is interpreted as a parametric perturbation of the operator. The authors have previously considered some particular problems of the stability analysis for multilevel models. As a parametric perturbation of the operator through a change in the corresponding IVs, one can interpret the use of various formulations of elastic mesolevel relationships [57, 58] and various formulations for establishing the spin of the moving coordinate system at a mesolevel [59]. In [23], the sensitivity of a mesolevel model to the values of the constants (parametric perturbations of the operator) was estimated in the above sense. However, the authors of the cited works did not explicitly use the mathematical concept of the multilevel model stability, though it must be introduced for a more complete analysis, including analysis of a wide range of input and operator perturbations during the process. The mathematical definitions and methods for studying the stability proposed by A.M. Lyapunov are of utmost importance for modeling the systems and processes on the basis of differential equations. We will consider further the possibility of their application to the analysis of stability of CM materials.

3. Basic concepts and definitions in assessment of multilevel constitutive model stability: application of traditional approaches for studying the stability of solutions of a system of differential equations

Traditional mathematical studies on the differential equations of the (DE)/DE systems consider the conditions for stability (instability) of solutions in relation to the changes in the initial conditions (Lyapunov's stability) [60–66]. If, for any small deviations in the initial conditions, the obtained solution is close to the solution without perturbations, then the corresponding basic solution is said to be Lyapunov stable (if, in addition to this, the perturbed solution at infinity approaches the basic one, then the basic solution is said to be asymptotically Lyapunov stable). Otherwise, in the presence of at least one small perturbation of the input data, leading to a significant deviation of the solution from the base one, the base solution is believed to be Lyapunov unstable. Using a specific form of the operator and, for example, the Lyapunov methods, conditions are formulated to be imposed on model coefficients and on initial conditions that ensure the stability of the solution. To study the behavior of a solution, it is also possible to analyze the proximity of the solutions - the base solution and that determined in the presence of initial condition perturbations - in the phase space. When the trajectories are close, we speak about the orbital stability - Poincaré stability (Poincaré stability follows from Lyapunov stability, but not vice versa). Note that the approach based on the analysis of the evolution of the perturbed solution is widely used to study the stability of the solution of boundary value problems, e.g., in hydrodynamics [64, 67, 68]. It is assumed that the perturbations depend on both time and coordinates and satisfy the boundary value problem constraints. In these cases, numerical methods are extended to the solution;

the influences are usually introduced into spatial problems through boundary conditions, and therefore the problem considering the stability of solutions in relation to boundary conditions is identified in research.

By *the model stability assessment procedure,* we mean the analysis of stability of the solutions obtained by the examined model for different values of parameters that determine the operator and input data (initial conditions and influences), i.e., the consideration of various problems of assessing the local stability of the model [69, 70].

At certain parameters and input data, the nonlinear mathematical models give unstable solutions. If the instability of solution can be explained from the physical viewpoint (e.g., for models from other research areas - sociological, economic, etc.) and has been confirmed experimentally, then it can be termed *"physically induced instability"*. The domain of definition of the parameters and input data of the model, at which it occurs, is called the domain of physically induced instability. As a classical example, we can mention the compression induced rod-shaped instability described by Euler's formulas [71]. The instability of all solutions obtained using the mathematical model is termed *"mathematically induced instability"* and, accordingly, the domain of this instability is introduced. The coincidence of subdomains of the domains of mathematically and physically induced instabilities provides evidence for the correctness of the mathematical model in this range of parameters and input data. If some part of the domain of the mathematically induced instability does not fall into the region of physically induced instability, then there arises a need to limit the region of applicability of the model by excluding the corresponding ranges.

The method of Lyapunov functions (the second Lyapunov method, i.e. direct Lyapunov method) [63, 72, 73] offers a rigorous solution to the problem of stability of solutions to the systems of nonlinear differential equations. To the best of our knowledge, there are examples of its effective application to various particular problems [74–77], however an adequate universal procedure for its use in arbitrary complex nonlinear DE systems has not been yet proposed. Therefore, in the general case, it is possible to use only approximate methods for assessing the stability of solutions.

The complexity of the problem of studying the stability of systems of type (4) equations is due to the nonlinearity of an operator. For the bounded nonlinear operators $\mathbf{f}$, $\mathbf{g}$, one can speak about the existence of an exact upper boundary for the ratio of the norm of the output data to the norm of the argument (over a small vicinity in the input data space around the base solution). Unfortunately, there are no methods for finding this boundary. Indeed, the maximum for a certain countable set of input data can be found, but this value can be exceeded with increasing number of the input variants. Strictly speaking, clarification is the endless process. Therefore, when studying nonlinear operators, we usually consider their changes in the specific small vicinity of the arguments, analyzing the Gateaux derivative or, for linear operator approximation, the Frechet derivative [54, 78]. In assessing the stability of the nonlinear DE systems, this is reflected in the fact that the linear approximations of such systems are the first to be analyzed [60–62]. Note that the approach based on the linearization of the operator of the boundary value problem is often used in the studies on stability of mechanical systems. For instance, in the problems of hydrodynamic stability, the equations are linearized with respect to small perturbations of the base solutions [68]. It is interesting to note that, in these statements, the perturbations of the operator itself are absent.

Let us now consider the possibility of applying the first Lyapunov method to (4) by analyzing the stability in the first approximation [62]. To this end, we analyze the spectrum of the first approximation matrix determined from the derivatives of the components (for example, in a fixed laboratory coordinate system) present on the right-hand side of system (4) in terms of the components $\mathbf{Y}(t), \mathbf{Z}(t)$. It is known that the necessary and sufficient condition for the asymptotic stability in the first approximation is that the eigenvalues of the matrix of the first approximation have negative real parts. It is obvious that the application of the first approximation method to multilevel CMs is associated with some difficulties. First, the method is approximate. Second, for some CMs, e.g., those involving the algorithmic definition of the operator on the right-hand side of (4), the analytical expression for the first approximation matrix may not exist under certain conditions. Third, due to the multiplicity of IVs in the multilevel CMs (at least, several tens of thousands), the matrix will be a high dimensional matrix. The analytical finding of eigenvalues is impossible, but numerical methods do not guarantee the finding of all the roots of a nonlinear equation, and analysis of the nonlinearity and high dimension of the matrix necessitates large computational resources. This can also be observed when we assess the negativity of the real parts of all roots, for example, the Hurwitz or Mikhailov criteria [63]. Besides, when numerical methods are used to calculate the determinants of high-dimensional matrices, computational errors can accumulate. To estimate the spectrum of the first approximation matrix, one can use the Gershgorin theorems [79]stating that: if the right boundary of the range of the real part of the eigenvalues determined by the theorem is located on the negative semi-axis, then all the eigenvalues will have negative real parts (which corresponds to asymptotic stability), if the left side of the range is found on the right semi-axis, then the real parts of all eigenvalues will be positive (which means instability), but if the left boundary of the range is located on the negative semi-axis and the right boundary on the positive semi-axis, then in the general case it will be unclear whether there are eigenvalues with a positive real part (that is, it is impossible to judge the stability).

Thus, the application of the Lyapunov methods for studying the CMs stability is hampered by the fact that they have significant nonlinearity and high dimensionality, and thus their use does not provide a comprehensive answer to the problem of stability and additionally requires extremely large computational resources. Moreover, these methods do not comprise the analysis of influences and operator perturbations at arbitrary times. Obviously, nowadays, an analytical apparatus for the general case of perturbations cannot be developed. However, because of the topicality of the problem specified in Section 2, it seems reasonable to propose a methodology to estimate numerically the local stability of the solutions obtained using CMs.

The difference between the perturbed history of influences and the history of influences, at which the basic solution has been found, can be obtained by applying the integral norm introduced above. However, in order to estimate the deviation of the operator, we have to introduce an approximation because of the just mentioned lack of a rigorous definition for the norm of a nonlinear operator. We assume that, in the case of stability of the solution to operator perturbation, the difference between the effects of the perturbed Φ^* and unperturbed operator on any argument $\mathcal{X}^*$ in a small vicinity of the input data $\mathcal{X}=\left\{\mathbf{X}_{t\in[0,T]},\mathbf{Y}_0,\mathbf{Z}_0\right\}$ is represented through the effect of a specified linear operator A on it: $\Phi^*\left(\mathcal{X}^*\right)-\Phi\left(\mathcal{X}^*\right) = \mathrm{A}\left(\mathcal{X}^*\right)$. Then, we can formally introduce a norm for the deviation of the operator $\left\|\Phi-\Phi^*\right\|_{o\left(\left\{\mathbf{X}_{t\in[0,T]},\mathbf{Y}_0,\mathbf{Z}_0\right\}\right)}$, which will be equal to the norm of the linear operator A, confining possible arguments to the small neighborhood $o(\mathcal{X})=o(\left\{\mathbf{X}_{t\in[0,T]},\mathbf{Y}_0,\mathbf{Z}_0\right\})$. This assumption implies that the nonlinear operators are sufficiently smooth. The indicated norm is used for introducing the definition of stability of a solution in such a way that we can consider a small vicinity of the solution. In virtue of significant nonlinearity and high dimensionality of CMs, this norm cannot be found analytically and the methods for its numerical calculation are unknown; if such a method exists, then its implementation would be a real challenge due to the enormous resource intensity. Therefore, the numerical procedure proposed here for estimating stability in the presence of parametric operator perturbations involves a norm for the deviation of the operator parameters. This norm serves to calculate the operator deviation norm. Description of the assessment procedure is given below.

Using $(\ )^*$ for the perturbed characteristics of the model, we formulate the definition of *stability of the solution* obtained with CMs as follows. If, for any number $\varepsilon>0$ there are such positive numbers, there are $\delta_{Y_0}(\varepsilon)<\infty$, $\delta_{Z_0}(\varepsilon)<\infty$, $\delta_X(\varepsilon)<\infty$, $\delta_\Phi(\varepsilon)<\infty$, at which, for any acceptable perturbations of influences $\mathbf{X}^*_{t\in[0,T]}$, initial conditions $\mathbf{Y}_0^*$, $\mathbf{Z}_0^*$, operator Φ^* satisfying the following set of equations

$$\left\|\mathbf{Y}_0^*-\mathbf{Y}_0\right\|_{l_2^n}<\delta_{Y_0}(\varepsilon), \tag{5}$$

$$\left\| \mathbf{Z}_0^{*} - \mathbf{Z}_0 \right\|_{l_2^k} < \delta_{Z_0}\left(\varepsilon\right), \tag{6}$$

$$\left\| \mathbf{X}^*_{t\in[0,T]} - \mathbf{X}_{t\in[0,T]} \right\|_{Q_2^m} < \delta_X\left(\varepsilon\right), \tag{7}$$

$$\left\| \Phi^* - \Phi \right\|_{o(\{\mathbf{X}_{t\in[0,T]},\, \mathbf{Y}_0,\, \mathbf{Z}_0\})} < \delta_\Phi\left(\varepsilon\right), \tag{8}$$

the inequality

$$\left\| \mathbf{Y}^*_{t\in[0,T]} - \mathbf{Y}_{t\in[0,T]} \right\|_{C^n_{L^2}} < \varepsilon, \tag{9}$$

is fulfilled, then the base solution $\mathbf{Y}_{t\in[0,T]} = \Phi\left(\mathbf{X}_{t\in[0,T]}, \mathbf{Y}_0, \mathbf{Z}_0\right)$, obtained through the operator Φ for the input data $\mathbf{X}_{t\in[0,T]}$, $\mathbf{Y}_0$, $\mathbf{Z}_0$, is *stable.*

If we, instead of the time integral response norm, use the norm of tensor value at each instant of time (e.g., $\| \cdot \|_{l_2^n}$) and consider only the initial condition perturbations (ignoring influences and operator perturbations), then for $T \to \infty$ we get the classical definition of stability of a solution according to Lyapunov [60–63]. Note that, in order to analyze CMs, it is essential to investigate not only the influence of perturbations $\mathbf{X}^*(0)$ at the initial instant of time but also the influence of the perturbed influences history $\mathbf{X}^*_{t\in[0,T]}$, $t \in [0,T]$. This is of particular importance because, in real deformation processes, the perturbations of influences are realized at all instants of time due to the stochastic kinematic and temperature boundary conditions (perturbation of the history of influences causes the right-hand part of (4) to change). The need to consider the initial condition perturbations $\mathbf{Y}_0^*, \mathbf{Z}_0^*$ is generated by fact that the representative volume may contain the residual (initial) stresses ($\mathbf{Y}_0^*$), and the initial physico-mechanical properties determined by the initial IVs values $\mathbf{Z}_0^*$ are stochastic in character. The relevance of analysis of the influence of operator perturbations Φ^* on the solution is related to the fact that some physical processes (taken into account in the deterministic CM) actually have a probabilistic nature. We can note such processes as the microscale defect interactions, which efficiently described by applying mesoscale ratios for critical shear stresses along the dislocation intragranular slip systems [19]. During deformation, the scenarios for defect substructure interactions can differ significantly. To assess the possible influence of this fact on the response, we will consider further the parametric operator perturbation by analyzing changes in internal variables.

It should be noted that, for stochastic models, the definition of stability can be applied in a probabilistic sense [80]. However, in our study only deterministic CMs are analyzed, and therefore this option is dropped from the consideration – there are stochastic perturbations of parameters, but, for each variant of the implementation of these parameter perturbations, the fulfillment of the above strictly stability criterion is verified.

As noted above, in the case of an adequate CM with some input data and parameters, unstable solutions are feasible and hence it is desirable that these situations will be interpreted physically. The use of the crystal plasticity in studying a single crystal with kinematic effects led to the conclusion [81] that an unstable solution appears due to the outlet of the point representing the stress state (in stress space) perpendicularly to the face of the yield surface determined by the Schmid criterion. This takes place because, at various small initial orientation perturbations but at the same influence, this point moves to different vertices of this face (depending on the specified deviation from the basic orientation). For a substantially textured polycrystal at a macrolevel, under some influences, a similar behavior (unstable in the above sense) will appear. The situations described correspond to the physically induced instability. By changing the process control, we can eliminate this instability; the stresses are accepted as the influences, and the deformation characteristics - as the response.

At the same time, it goes without saying that the multilevel CMs describing polycrystal deformation in the presence of a great majority of variants of influences and initial conditions (in particular, the initially non-textured polycrystals with a uniform distribution function of crystallite orientations) should give stable solutions, as evidenced by the experiments on the homogeneously and inhomogeneously deformed samples. The instability of the SSS established in the macrolevel experiments occurs extremely rare (if the final stage of deformation with necking is excluded from consideration).

The practical application of the proposed definition of stability has revealed challenges related to calculating the deviation norm of operator (8), which arise due to the essential nonlinearity and large dimension of the CM. Analytical determination of this norm is impossible and numerical methods for its finding are absent; if the method existed, its implementation would be quite difficult due huge resource intensity. To assess the stability of a solution with respect to the model operator, computational experiments with a parametric specification of the (small) deviation of the perturbed operator from the base one are proposed. The analysis of the operation of multilevel models shows that in most cases a small perturbation of the parameters composed the right-hand sides of (4) leads to a small change in the response [23]. In connection with the above, the numerical stability assessment procedure will include, instead of the formally indicated condition (8), a norm for the deviation of the operator parameters. Thus, we have

$$\left\| \boldsymbol{\Lambda}^{*}_{t\in[0,T]} - \boldsymbol{\Lambda}_{t\in[0,T]} \right\|_{Q_2^S} < \delta_{\Phi}(\varepsilon), \tag{10}$$

where the vectors of operator parameters $\boldsymbol{\Lambda}^{*}_{t\in[0,T]}, \boldsymbol{\Lambda}_{t\in[0,T]}$, which vary with time $t \in [0,T]$, have the dimension S corresponding to the number of CM operator parameters, the perturbations of which are considered. The components $\boldsymbol{\Lambda}_{t\in[0,T]}$ at $t \in [0,T]$ refer to the parameters defining at this instant of time the operator of the model for finding an unperturbed solution, and $\boldsymbol{\Lambda}^{*}_{t\in[0,T]}$ - a perturbed solution. The norm is set by Riemann integral $\left\| \mathbf{K}_{t\in[0,T]} \right\|_{Q_2^S} = \left(\int\limits_0^T \sum\limits_{i=1}^{S} \left(K_i(t)\right)^2 dt \right)^{1/2}$ [54].

As stated earlier, the procedure to assess the stability of a model includes solution stability analysis carried out for various CM operator parameters and input data, which were derived from the domain of their definition, the analysis implying consideration of various problems related to the evaluation of the local stability of a model. For the nonlinear CM with a set of IVs, all the solutions and any possible perturbations cannot be checked. That is why we have developed a numerical procedure, in the framework of which, in order to simplify the problem by analyzing basic physical properties, significant solutions are identified and these solutions are investigated only under specified physically permissible perturbations. We believe that the proposed procedure holds promise for assessing the stability of any model that can be reduced to (4).

4. Description of the numerical algorithm for the stability assessment of a multilevel constitutive material model

The approach proposed in this study involves the following steps:

Step 1. Creation of an array of basic solutions for some input data (initial conditions and influences) and operator parameters. It is reasonable to consider the solutions obtained in the presence of the influences and initial states typical for the analyzed technological processes of thermomechanical treatment. If there is only one solution, then this algorithm can be interpreted as an algorithm for assessing its stability.

Step 2. Identification of the part of the CM parameters (initial conditions, influences, perturbed parameters of the operator), the perturbations of which are physically justified.

Step 3. Development of a program (a set of variants) for numerical experiments to study the behavior of basic solutions (Step 1) in the presence of perturbations of certain sets of CM parameters (Step 2): separate and different sets.

Step 4. Multiple realizations for each step in the experimental plan (Step 3) in the presence of the corresponding perturbations of CM parameters and calculation, for each realization, the norms of perturbations of initial conditions (5) and (6), influences (7), response (9), as well as the norm for deviation of operator parameters (10).

Step 5. Verification of the correctness of the definition of stability formulated in Step 3 by analyzing the totality of the calculated data obtained in Step 4.

Step 6. Physical assessment (provided that an unstable solution, i.e., the mathematically induced instability, has been revealed in Step 5) to find out whether the mathematically identified instability is a physically induced instability. If an acceptable physical justification is lacking, then arises a need to carefully check the applicability of the CM. If no unjustified unstable solutions were found, then? at a large number of different variants of numerical experiments, this would serve as an indirect evidence of the adequacy of the CM as a whole (subject to compliance with field experiments).

5. Conclusion

We have analyzed the stability of the solutions obtained using the constitutive models of materials (the history of response changes) in relation to small finite perturbations of the input data and the model operator. The topicality of our study is determined by the probabilistic nature of the initial physical and mechanical characteristics of the material (including those obtained at the lower structural-scale levels), the physical processes occurring during deformation (for example, interactions of defective structures at a microscale level), and the influences produced by the stochastic boundary conditions on the representative volumes inside the product.

We have formulated the definition of stability of the solution, which, unlike the traditional one, takes into account the parametric perturbation of the operator and the perturbation of the history of influences (determining the right-hand side of the system of differential equations).

A program of computational experiments has been developed to implement the proposed approach. It includes consideration of various perturbations of the initial conditions, the history of influences, the operator, and the analysis of the norms of their deviations, as well as the integral norm of deviation of the perturbed solutions from the basic ones (obtained in calculations with unperturbed parameters).

Examples illustrating the application of the proposed approach and the algorithm based on it to the study of multilevel constitutive models of polycrystalline metals are presented by the authors in separate publications.

This work was supported by the Russian Science Foundation (grant No. 17-19-01292).

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The authors declare no conflict of interests.

The paper was received on 12.03.2021.
The paper was accepted for publication on 22.03.2021.