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Dedicated to Academician S.K. Godunov on the occasion of his 90th birthday

Thermodynamic Consistency and Mathematical Well-Posedness in the Theory of Elastoplastic, Granular, and Porous Materials

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Abstract—Mathematical models of the dynamics of elastoplastic, granular, and porous media are reduced to variational inequalities for hyperbolic differential operators that are thermodynamically consistent in the sense of Godunov. On this basis, the concept of weak solutions with dissipative shock waves is introduced and a priori estimates of smooth solutions in characteristic conoids of operators are constructed, which suggest the well-posedness of the formulation of the Cauchy problem and boundary value problems with dissipative boundary conditions. Additionally, efficient shock-capturing methods adapted to solution discontinuities are designed.

Keywords: dynamics, shock wave, elasticity, plasticity, granular medium, porous medium, thermodynamic consistency, variational inequality, shock-capturing method

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1. INTRODUCTION

Special formulations of nonstationary equations of continuum mechanics in the form of thermodynamically consistent systems of conservation laws were previously studied by Godunov and his colleagues and students [1–4]. Such formulations were obtained for gas dynamics equations, elasticity theory, magnetohydrodynamics, electrodynamics, etc., and were found useful in the study of well-posedness of boundary value problems with initial and boundary conditions, in the analysis of discontinuous solutions with shock waves, and in the construction of finite-difference and finite-volume schemes for the numerical solution of boundary value problems.

Given a continuous medium with an m-dimensional vector $U(t,x)$ of state functions, the governing equations for $U(t,x)$ in the form of a thermodynamically consistent system of conservation laws are formulated using generating potentials $\Phi(U)$ and $\Psi_i(U)$, ($i = 1,\dots,n$; n is the spatial dimension of the model). The equations are written as

$$\mathcal{D}\langle U\rangle = g(U), \tag{1.1}$$

where g is a given m-dimensional right-hand side vector and $\mathcal{D}$ is a first-order quasilinear differential operator (the angle brackets indicate a functional dependence):

$$\mathcal{D}\langle U\rangle = \frac{\partial \varphi(U)}{\partial t} - \sum_{i=1}^{n}\frac{\partial \psi_i(U)}{\partial x_i}, \quad \varphi(U) = \frac{\partial \Phi}{\partial U}, \quad \psi_i(U) = \frac{\partial \Psi_i}{\partial U}.$$

Generally speaking, the vector $g(U)$ depends on the variables t, x. The generating potentials can also depend on t and x regarded as parameters if the medium is inhomogeneous or its properties vary with time. However, these arguments are omitted in what follows to simplify the formulas.

The system of thus written equations involves an additional equation in divergent form,

$$\frac{\partial}{\partial t}(U\cdot\varphi(U) - \Phi(U)) = \sum_{i=1}^{n}\frac{\partial}{\partial x_i}(U\cdot\psi_i(U) - \Psi_i(U)) + U\cdot g(U), \tag{1.2}$$

and has a corresponding integral conservation law, which is consistent with the conservation laws of the basic system (1.1) for smooth solutions, but may contradict them in the case of strong discontinuities, namely, shock waves. In solid mechanics models, Eq. (1.2) represents the energy conservation law written in differential form. The generating potential $\Phi(U)$ usually depends on an additional parameter (temperature or entropy) that remains constant in the domain of smoothness of the solution and suffers a jump across the discontinuity surfaces, thus ensuring the fulfillment of this law. However, if the additional parameter is not taken into account in specific models (e.g., in the case of isothermal or isentropic processes), then the violation of the law across the discontinuities is justified, since there has to be an outflow of energy behind the shock front to ensure the isothermal or isentropic property of the flow.

Assuming that the generating potentials are continuously differentiable, the equations of the basic system are transformed into a nonconservative matrix form

$$A(U)\frac{\partial U}{\partial t} = \sum_{i=1}^{n} B^i(U)\frac{\partial U}{\partial x_i} + g(U), \quad A(U) = \frac{\partial \varphi}{\partial U}, \quad B^i(U) = \frac{\partial \psi_i}{\partial U}, \tag{1.3}$$

with symmetric matrix coefficients A and B^i. If the matrix $A(U)$ is positive definite, which holds in the case of a strongly convex generating potential $\Phi(U)$, then the system under consideration is t-hyperbolic in the sense of Friedrichs [5]. In some sense, hyperbolicity guarantees the well-posedness of the mathematical model and makes it possible to analyze it by applying well-developed numerical methods and techniques.

The main goal of this paper is to generalize the given approach to models of dynamics of deformable elastoplastic, granular, and porous materials. Such models are used to describe thermodynamically irreversible processes and are formulated in the form of variational inequalities following directly from the fundamental principles of nonequilibrium thermodynamics.

2. VARIATIONAL INEQUALITIES

As a generalization of system (1.1), we consider the variational inequality

$$(\tilde{U} - U) \cdot (\mathcal{D}\langle U \rangle - g(U)) \geq 0, \quad U, \tilde{U} \in F. \tag{2.1}$$

Here, F is the set of admissible variations of the vector U (F is assumed to be convex and closed in the m-dimensional arithmetic space and, generally speaking, depends parametrically on t and x) and $\tilde{U}$ is an arbitrary element of F. In mechanics of elastoplastic media, the variational inequality represents a formulation of the von Mises maximum principle, according to which, for a given rate of plastic deformation, the dissipation rate takes a maximum value under actual stresses. The boundary of F in the stress space is a yield surface in the material. If the vector U lies inside F, then, since the variation is arbitrary, (2.1) yields system (1.1) describing an elastic process. If U is a boundary point, then the associated law of plastic flow holds, according to which the vector of the plastic strain rate equal to the difference $g(U) - \mathcal{D}\langle U \rangle$ is directed along the outward normal to the boundary of F.

An important feature of the model formulation in the form of variational inequality (2.1) is that it, as well as numerical algorithms relying on it, automatically takes into account the elastic unloading condition. If unloading occurs after an irreversible deformation at some point of the medium, i.e., if the vector U in the phase space moves from the boundary to the inside of F, then the system of elasticity equations (1.1) holds at this point.

The generalization of the von Mises maximum principle to arbitrary thermodynamically irreversible processes known as the fundamental principle of Ziegler plays an extremely important role in physics, chemistry, and biology (see [6]). It can also be used to model conditions at solution discontinuities in nonequilibrium thermodynamics.

Below, we give examples of solid mechanics models admitting formulation (2.1).

2.1. Theory of the Prandtl–Reuss Elastoplastic Flow

In this theory, the variational inequality is written for the velocity vector v and the symmetric stress tensor σ [7]:

$$(\tilde{v} - v) \cdot (\rho \dot{v} - \nabla \cdot \sigma - \rho g) + (\tilde{\sigma} - \sigma) : (a : \dot{\sigma} - \nabla v) \geq 0, \quad \sigma, \tilde{\sigma} \in F.$$

Here, ρ is the density of the medium and a is the fourth-order tensor of elastic compliance moduli, which is positive definite and has a special symmetry. We use the standard notation and tensor analysis operations.

Since the velocity variation is arbitrary, the above inequality yields a system of equations of motion. The condition that the term with the stress tensor variation is nonnegative, which follows from this inequality at $\tilde{v} = v$, is in total agreement with the formulation of the von Mises principle. The components of the vector U in the transition to variational inequality (2.1) are the components of velocity and the stress tensor in Cartesian coordinates written in a column. The generating potentials are defined as the following quadratic functions (the subscript denotes the projection of a vector onto a coordinate axis):

$$\Phi(U) = \frac{1}{2}(\rho v^2 + \sigma : a : \sigma), \quad \Psi_i(U) = (\sigma \cdot v)_i. \tag{2.2}$$

In this example, $\mathcal{D}\langle U \rangle$ is a linear differential operator with constant coefficients.

A similar inequality describes dynamic processes in structurally inhomogeneous materials within the theory of the Cosserat continuum, which takes into account the rotational degrees of freedom of microstructure particles. The corresponding vector U consists of the components of the linear velocity vector, the nonsymmetric stress tensor, the angular velocity vector, and the couple stress tensor, which is also nonsymmetric (see [8]). A more general variational inequality for a nonlinear operator appears in the theory of hardening elastoplastic media. In this case, in addition to the velocity and stress components, the vector U contains the components of the tensor parameter of translational hardening and the scalar parameter of isotropic hardening [7].

2.2. Model of an Elastoplastic Granular Material

In the case of a granular material, whose behavior under tension and compression differs significantly, constitutive equations for describing material deformations are derived using the generalized rheological method [9]. The mathematical model of an ideal medium with elastoplastic particles is brought to the variational inequality

$$(\tilde{v} - v) \cdot (\rho \dot{v} - \nabla \cdot \sigma - \rho g) + (\tilde{\sigma} - \sigma) : (a : \dot{s} - \nabla v) \geq 0,$$
$$\sigma, \tilde{\sigma} \in F, \quad \sigma = \pi_K(s).$$

Here, s is a symmetric tensor of conditional stresses and π_K is the projector onto the convex closed cone K with vertex at the origin that contains all possible admissible stress tensors corresponding to a compression state. The projection onto the cone is calculated with respect to the Euclidean norm $|\sigma|_a = \sqrt{\sigma : a : \sigma}$.

In an ideal granular material, there are no couplings between the particles, so there are no stressed states other than compressions. This property is described by a closure equation for determining the tensor σ in terms of s.

Let U and V denote vectors with components v, s and components v, σ, respectively. In this notation, the variational inequality of the model is transformed into matrix form:

$$(\tilde{V} - V) \cdot \left(A \frac{\partial U}{\partial t} - \sum_{i=1}^{n} B^i \frac{\partial V}{\partial x_i} \right) \geq 0, \quad V, \tilde{V} \in F, \quad V = \pi_K(U), \tag{2.3}$$

where A and B^i are symmetric matrices with constant coefficients, which can be obtained by differentiating the elastoplastic quadratic potentials (2.2) twice with respect to U, and π_K is the projector onto the cone K with respect to the norm of the positive definite matrix A.

However, for granular materials, it seems that formulation (2.3) is not reduced to (2.1), i.e., corresponding generating potentials cannot be constructed. Let us show how this can be done for a regularized model that takes into account a weak elastic coupling between the particles under tension.

Following the regularization procedure, the closure equation in (2.3) is replaced by an equation with a small parameter $\varepsilon > 0$ (elastic modulus of the coupling):

$$V = \varepsilon U + (1 - \varepsilon)\pi_K(U).$$

Since the projection onto the convex cone with the vertex at the origin has the property $\pi_K(V) = \pi_K(U)$ (see, e.g., [9, Chapter 2]), the above equation can be inverted so that

$$U = \frac{1}{\varepsilon}V - \frac{1-\varepsilon}{\varepsilon}\pi_K(V).$$

By setting

$$\Phi(V) = \frac{1}{2\varepsilon}(V \cdot AV - (1-\varepsilon)\pi_K(V) \cdot A\pi_K(V)), \quad \Psi_i(V) = \frac{1}{2}V \cdot B^i V, \tag{2.4}$$

the model is reduced to variational inequality (2.1) for the vector function $V(t, x)$.

Indeed, by using the properties of the projection onto the cone established in [9], we can prove that the generating potential Φ is a continuously differentiable function such that

$$\frac{\partial \Phi}{\partial V} = \frac{1}{\varepsilon}AV - \frac{1-\varepsilon}{\varepsilon}A\pi_K(V) = AU.$$

Moreover, since the projection onto cone with the vertex at the origin taken with respect to the norm $|V|_A = \sqrt{V \cdot AV}$ satisfies the equation $\pi_K(V) \cdot A(V - \pi_K(V)) = 0$, we have the continued equality

$$\begin{aligned} V \cdot AV + \frac{1-\varepsilon}{\varepsilon}(V \cdot AV - \pi_K(V) \cdot A\pi_K(V)) &= |V|_A^2 + \frac{1-\varepsilon}{\varepsilon}(V + \pi_K(V)) \cdot A(V - \pi_K(V)) \\ = |V|_A^2 + \frac{1-\varepsilon}{\varepsilon}\left(|V - \pi_K(V)|_A^2 + 2\pi_K(V) \cdot A(V - \pi_K(V))\right) &= |V|_A^2 + \frac{1-\varepsilon}{\varepsilon}|V - \pi_K(V)|_A^2, \end{aligned}$$

which implies that $\Phi(V)$ is a strongly convex function for $\varepsilon \le 1$. This guarantees the hyperbolicity of the differential operator $\mathcal{D}\langle V \rangle$.

2.3. Model of a Porous Medium

In contrast to usual elastoplastic materials (metals and their alloys), porous media have different mechanical characteristics before and after the collapse of the pores when influenced by external dynamic or static loads. The pore collapse leads to an increased stiffness of the material. This behavior is taken into account in the mathematical model of [10], which is also constructed using the generalized rheological method. The variational inequality for this model has the form

$$\begin{gathered} (\tilde{v} - v) \cdot (\rho\dot{v} - \nabla \cdot \sigma - \rho g) + (\tilde{s} - s) : (a : \dot{s} - \nabla v) + (\tilde{q} - \pi_K(q)) : (b : \dot{q} - \nabla v) \ge 0, \\ s, \tilde{s} \in F, \quad \sigma = s + \pi_K(q). \end{gathered}$$

Here, a is a symmetric positive definite fourth-order tensor of elastic compliance moduli of the porous skeleton; b is a tensor with the same properties characterizing an increase in the material stiffness under the pore collapse; and s and q are symmetric stress tensors, which determine the actual stress tensor σ and describe the skeleton's stress state and its variation due to the contact interaction of the skeleton walls after the pore collapse.

Depending on the porosity of the medium, plasticity can arise before the pore collapse (as a rule, in high-porosity materials) or after it. As in the previous models, the transition to plasticity is described using a convex closed subset F of the stress space bounded by the yield surface of the material. Initial porosity, which is, in the general case, inhomogeneously distributed over the medium, is taken into account in specifying initial data.

The vector U is made up of the velocity components and the components of the stress tensors s and q, while, in the vector V, the tensor q is replaced by its projection $\pi_K(q)$ onto the cone K. Then these vectors are related by the equation $V = \pi_K(U)$, and the variational inequality of the model is written in the form of (2.3) with matrix coefficients of suitable dimension. Thus, in the general notation, the considered model of a porous medium is entirely similar to the model of an ideal granular medium. Therefore, after passing to a regularized closure equation with a small parameter $\varepsilon > 0$, namely, to

$$\sigma = s + \varepsilon q + (1-\varepsilon)\pi_K(q),$$

the model can be reduced to variational inequality (2.1) with generating potentials (2.4).

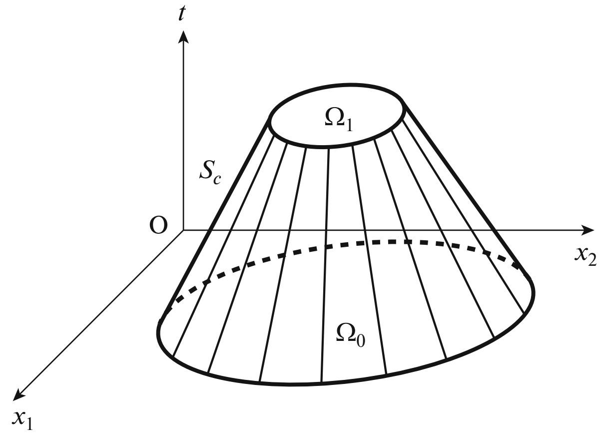

Fig. 1. Truncated conoid for estimating solutions.

Note that, if the above models take into account the rotational motion of the particles, then one can obtain new refined mathematical models of structurally inhomogeneous granular and porous materials in the form of (2.1).

3. INTEGRAL ESTIMATES

Below, we consider some general properties of solutions to variational inequality (2.1). Let $U(t, x)$ and $U'(t, x)$ be continuously differentiable solutions determined in a closed domain G. In what follows, we assume that the generating potentials $\Phi(U)$ and $\Psi_i(U)$ are three times continuously differentiable functions and the vector function $g(U)$ satisfies the Lipschitz condition with respect to U.

Setting $\tilde{U} = U' \in F$ in (2.1) and $\tilde{U} = U \in F$ in the variational inequality characterizing the solution U', after summing the results, we obtain

$$(U' - U) \cdot \left(\mathcal{D}\langle U'\rangle - \mathcal{D}\langle U\rangle\right) \leq (U' - U) \cdot (g'(U') - g(U)). \tag{3.1}$$

To estimate the influence exerted by the right-hand side vector on the solution, we consider the general case when the vector function g' involved in the variational inequality for U' differs from the vector function g in (2.1) and both depend on t and x.

An inequality similar to (3.1) is the starting point for deriving a priori estimates for the integral norm of the difference between solutions of the hyperbolic system of quasilinear equations (1.3) in characteristic conoids of the differential operator. Such estimates were obtained, for example, in [2, 11, 12], and they have the same form for solutions of the variational inequality.

Consider a truncated conoid G in the space of variables (t, x) with bases lying in the hyperplanes $t = t_0$ and $t = t_1$ (Fig. 1) and with a lateral surface S_c described by an equation of the form $h(t, x) = 0$. Assume that G satisfies the Hamilton–Jacobi inequality for the operator $\mathcal{D}\langle U\rangle$:

$$\dot{h} + H(\nabla h) \geq 0.$$

Here, $H(\nu)$ is the smallest among the m real roots $c = H_k(\nu)$ $(k = 1, \ldots, m)$ of the characteristic equation

$$\det D(c, \nu) = 0, \qquad D(c, \nu) = cA(U) + \sum_{i=1}^{n} \nu_i B^i(U).$$

An important property of the Hamilton–Jacobi inequality is that the matrix $D(\dot{h}, -\nabla h)$ is positive semidefinite at points of the thus constructed conic surface S_c. Since the matrix $A(U)$ is positive definite, the above property holds if and only if all roots of the following polynomial in λ are nonnegative:

$$\det(D(\dot{h}, -\nabla h) - \lambda A(U)) = \det D(\dot{h} - \lambda, -\nabla h).$$

Taking into account the accepted notation, the roots of this polynomial easily are computed:

$$\lambda_k = \dot{h} - H_k(-\nabla h) = \dot{h} + H_k(\nabla h), \quad k = 1,\dots,m,$$

and the positive semidefiniteness condition takes the form of the Hamilton–Jacobi inequality.

Based on the method of characteristics for the Hamilton–Jacobi equation, a method for constructing a conic domain G with such properties in an arbitrary neighborhood within the solution domain is described in detail in [2, pp. 162–180].

The norm of the difference of solutions is defined as the integral of a quadratic form over the section $\Omega(t)$ of the domain G by the hyperplane $t = \text{const}$:

$$\|U' - U\|^2(t) = \int_{\Omega(t)} (U' - U) \cdot A(U)(U' - U)\, d\Omega.$$

To obtain an estimate, the left-hand side of (3.1) is transformed into

$$\frac{1}{2}\frac{\partial}{\partial t}((U' - U) \cdot A(U)(U' - U)) - \frac{1}{2}\frac{\partial}{\partial x_i}\sum_{i=1}^{n}((U' - U) \cdot B^i(U)(U' - U)) - (U' - U) \cdot \mathcal{N}\langle U', U\rangle,$$

where, for brevity, we introduced the notation

$$\mathcal{N}\langle U', U\rangle = \frac{1}{2}\left(\frac{\partial}{\partial t}A(U) - \sum_{i=1}^{n}\frac{\partial}{\partial x_i}B^i(U)\right)(U' - U) - (A(U') - A(U))\frac{\partial U'}{\partial t} + \sum_{i=1}^{n}(B^i(U') - B^i(U))\frac{\partial U'}{\partial x_i}.$$

After these transformations, we integrate both sides of the inequality over G, applying the Green formula to the conservative terms. As a result,

$$\|U' - U\|^2(t_1) - \|U' - U\|^2(t_0) - \int_{S_c}(U' - U) \cdot D(c, \nu)(U' - U)\frac{dS}{\sqrt{1 + c^2}}$$
$$\leq 2\iint_G (U' - U) \cdot (\mathcal{N}\langle U', U\rangle + g'(U') - g(U))\, d\Omega\, dt.$$

Here, $c = -\dot{h}/|\nabla h|$ is the velocity of motion of the boundary of $\Omega(t)$ in the direction of the normal $\nu = \nabla h/|\nabla h|$. The unit vector with components $(-c, \nu)/\sqrt{1 + c^2}$ is an outward normal (with respect to G) to the conic surface S_c in the space of variables t, x.

The right-hand side of the resulting inequality is represented in the form of a sum of terms by setting

$$g'(U') - g(U) = (g'(U') - g'(U)) + (g'(U) - g(U)).$$

Next, the difference in the first bracket is estimated using the Lipschitz condition, while the second bracket remains intact, since it characterizes the variation in g. By using the Cauchy–Schwarz inequality, the integral on the right-hand side is estimated by

$$\int_{t_0}^{t_1}\left(a\|U' - U\|^2 + b\|g'(U') - g(U')\|\|U' - U\|\right)(t)\,dt$$

with positive constants a and b that depend, generally speaking, on both solutions, their first derivatives with respect to t and x_i, and the Lipschitz constant for the vector function $g(U)$. As a result, since the integrand in the integral over S_c is nonpositive, we obtain the inequality

$$\|U' - U\|^2(t_1) \leq \|U' - U\|^2(t_0) + 2a\int_{t_0}^{t_1}\|U' - U\|^2(t)\,dt + 2b\int_{t_0}^{t_1}(\|g'(U') - g(U')\|\|U' - U\|)(t)\,dt.$$

This inequality remains valid if t_0 and t_1 are replaced by arbitrary moments of time $t' < t$ belonging to the interval (t_0, t_1). As t' tends to t, the resulting inequality simplifies to

$$\frac{d}{dt}\|U' - U\|(t) \leq a\|U' - U\|(t) + b\|g'(U') - g(U')\|(t)$$

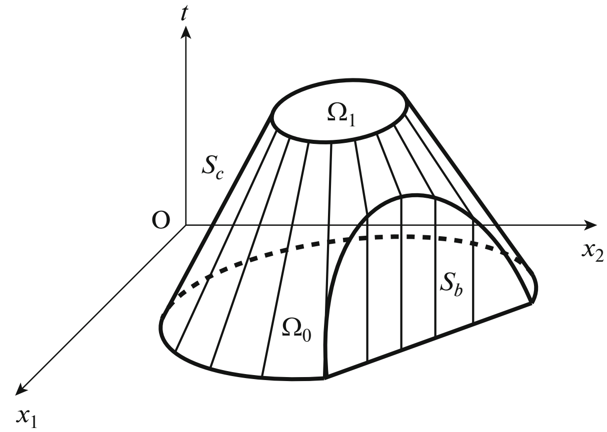

Fig. 2. Truncated conoid resting on the boundary of the domain.

or

$$e^{at}\frac{d}{dt}\left(e^{-at}\left\|U' - U\right\|(t)\right) \le b\left\|g'(U') - g(U')\right\|(t),$$

from which, after integration with respect to t from t_0 to t_1, we obtain the final estimate

$$\left\|U' - U\right\|(t_1) \le \left\|U' - U\right\|(t_0)e^{a(t_1 - t_0)} + b\int_{t_0}^{t_1}\left\|g'(U') - g(U')\right\|(t)e^{a(t_1 - t)}dt. \quad (3.2)$$

Estimate (3.2) implies that the solution of the Cauchy problem is unique and depends continuously on the initial data

$$U|_{t=0} = U_0(x) \in F.$$

Indeed, if the Cauchy problem has a solution $U(t,x)$, then, by virtue of (3.2), any other solution $U'(t,x)$ of this problem coincides with the former one in any truncated conoid with a lateral surface satisfying the Hamilton–Jacobi inequality. Moreover, a small variation in the vector function $U_0(x)$, as well as a small variation in the vector function $g(U)$, leads to a small variation in the solution in any section $\Omega(t)$ of the domain G by the hyperplane $t = \text{const}$.

By using (3.2), we can also prove that the perturbations have a finite velocity of propagation (the domains of dependence and influence of solutions are bounded).

A similar estimate can be obtained in a neighborhood of the stationary hypersurface S_b with dissipative boundary conditions specified on it, i.e., with general conditions the fulfillment of which for the vector functions U and U' ensures that the inequality

$$(U' - U)\cdot\sum_{i=1}^{n}\nu_i B^i(U)(U' - U) \le 0$$

holds at points of S_b; here, ν is the outward normal (with respect to the solution domain of the problem) to the section of S_b by the hyperplane $t = \text{const}$. In deriving the estimate, the domain G is specified as the part of the truncated conoid resting on S_b (see Fig. 2).

4. DISCONTINUOUS SOLUTIONS

Variational inequality (2.1) written in conservative form can be used to construct weak (discontinuous) solutions:

$$\tilde{U}\cdot\mathcal{D}\langle U\rangle - (\tilde{U} - U)\cdot g(U) \ge \frac{\partial}{\partial t}(U\cdot\varphi(U) - \Phi(U)) - \sum_{i=1}^{n}\frac{\partial}{\partial x_i}(U\cdot\psi_i(U) - \Psi_i(U)),$$

and, thus, has an integral generalization equivalent to it for smooth solutions:

$$\begin{aligned}&\iint_G \left(-\frac{\partial(\chi\tilde{U})}{\partial t}\cdot\varphi(U)+\sum_{i=1}^{n}\frac{\partial(\chi\tilde{U})}{\partial x_i}\cdot\psi_i(U)-\chi(\tilde{U}-U)\cdot g(U)\right)d\Omega dt\\&\geq\iint_G\left(-\frac{\partial\chi}{\partial t}(U\cdot\varphi(U)-\Phi(U))+\sum_{i=1}^{n}\frac{\partial\chi}{\partial x_i}(U\cdot\psi_i(U)-\Psi_i(U))\right)d\Omega dt.\end{aligned}\tag{4.1}$$

The integral generalization is derived by multiplying both sides of the conservative inequality by an arbitrary compactly supported (in G) nonnegative function $\chi\in C^{\infty}(G)$ and by integrating the result over G with the Green formula applied to all terms involving the derivatives of the solution with respect to time and space variables. It is assumed that the "test" vector function $\tilde{U}(t,x)$ in inequality (4.1) is continuously differentiable in G and the constraint $\tilde{U}\in F$ is satisfied in a pointwise manner.

In a natural way, the integral inequality determines a class of weak solutions. This class contains vector functions $U\in L_1(G)$ satisfying (4.1) for all admissible $\tilde{U}$ for which the integrals involved in this inequality are defined in the sense of Lebesgue. Specifically, this class includes solutions with a strong discontinuity, i.e., having a discontinuity of the first kind on some hypersurface $S_0\subset G$ and continuously differentiable in the rest of G.

After applying the Green formula to integrals over subdomains of continuity of such a solution, inequality (4.1) yields a system of relations satisfied at points of S_0. Moreover, the integrals in (4.1) that involve derivatives with respect to time and space variables, namely,

$$\iint_{G^{\pm}}\frac{\partial(\chi\tilde{U})}{\partial t}\cdot\varphi(U)d\Omega dt,\qquad\iint_{G^{\pm}}\frac{\partial(\chi\tilde{U})}{\partial x_i}\cdot\psi_i(U)d\Omega dt,$$

are transformed into

$$\mp\int_{S_0}c\tilde{U}\cdot\varphi(U)\frac{\chi dS}{\sqrt{1+c^2}}-\iint_{G^{\pm}}\tilde{U}\cdot\frac{\partial\varphi}{\partial t}\chi d\Omega dt,\qquad\pm\int_{S_0}\nu_i\tilde{U}\cdot\psi_i(U)\frac{\chi dS}{\sqrt{1+c^2}}-\iint_{G^{\pm}}\tilde{U}\cdot\frac{\partial\psi_i(U)}{\partial x_i}\chi d\Omega dt.$$

The other integrals are transformed in a similar manner. Adding the integrals over the subdomains G^{+} and G^{-}, we obtain the inequality

$$\begin{aligned}&\int_{S_0}\tilde{U}\cdot\Big(c\varphi(U)+\sum_{i=1}^{n}\nu_i\psi_i(U)\Big)\frac{\chi dS}{\sqrt{1+c^2}}+\iint_{G^+\cup G^-}\tilde{U}\cdot\left(\frac{\partial\varphi(U)}{\partial t}-\sum_{i=1}^{n}\frac{\partial\psi_i(U)}{\partial x_i}\right)\chi d\Omega dt\\&-\iint_G(\tilde{U}-U)\cdot g(U)\chi d\Omega dt\geq\int_{S_0}\left(c[U\cdot\varphi(U)-\Phi(U)]+\sum_{i=1}^{n}\nu_i[U\cdot\psi_i(U)-\Psi_i(U)]\right)\frac{\chi dS}{\sqrt{1+c^2}}\\&+\iint_{G^+\cup G^-}\left(\frac{\partial(U\cdot\varphi(U)-\Phi(U))}{\partial t}-\sum_{i=1}^{n}\frac{\partial(U\cdot\psi_i(U)-\Psi_i(U))}{\partial x_i}\right)\chi d\Omega dt.\end{aligned}$$

Here, square brackets denote the jump in a function at a discontinuity: $[a]=a^{+}-a^{-}$, where $a^{\pm}$ are the one-sided limits at S_0 on the side of G^{+} and G^{-}, respectively.

Let $(t_0,x^0)\in G$ be a point at which the solution $U(t,x)$ is continuous. Then there exists a neighborhood of this point that does not intersect S_0. For any admissible test function $\chi(t,x)$ supported in this neighborhood, the integrals over S_0 in the resulting inequality vanish; therefore,

$$\iint_G(\tilde{U}-U)\cdot(\mathcal{D}\langle U\rangle-g(U))\chi d\Omega dt\geq 0.$$

If $(t_0, x^0) \in S_0$, then, for $\chi(t, x)$ supported in a neighborhood of this point, we have

$$\int_{S_0} \Big(\tilde{U}\big(c\varphi(U) + \sum_{i=1}^{n} \nu_i \psi_i(U)\big) - c[U \cdot \varphi(U) - \Phi(U)] - \sum_{i=1}^{n} \nu_i [U \cdot \psi_s(U) - \Psi_i(U)]\Big) \frac{\chi dS}{\sqrt{1 + c^2}}$$
$$\geq - \iint_{G^+ \cup G^-} (\tilde{U} - U) \cdot (\mathcal{D}\langle U \rangle - g(U)) \chi d\Omega dt.$$

Since the function $\chi \geq 0$ is arbitrary and the considered neighborhood can be reduced unboundedly, these two inequalities imply that variational inequality (2.1) holds in the open subdomains $G^{\pm}$, where the solution is sufficiently smooth, while, on S_0, it is true that

$$\tilde{U} \cdot [r(U)] \geq c[U \cdot \varphi(U) - \Phi(U)] + \sum_{i=1}^{n} \nu_i [U \cdot \psi_i(U) - \Psi_i(U)], \quad r(U) = c\varphi(U) + \sum_{i=1}^{n} \nu_i \psi_i(U),$$

where $c > 0$ is the velocity of the shock front representing the section of S_0 by the hyperplane $t = \text{const}$ in the direction of the outward normal ν with respect to G^+.

With the help of simple transformations relying heavily on the identity

$$a^+ b^+ - a^- b^- = (a^+ - a^-) \frac{b^+ + b^-}{2} + \frac{a^+ + a^-}{2} (b^+ - b^-),$$

the inequality at points of the solution discontinuity hypersurface is rewritten equivalently as

$$(\tilde{U} - U^0)[r(U)] \geq -d(U) = c([U] \cdot \varphi^0(U) - [\Phi(U)]) + \sum_{i=1}^{n} \nu_i ([U] \cdot \psi_i^0(U) - [\Psi_i(U)]), \tag{4.2}$$

where $U^0 = (U^+ + U^-)/2$ and the quantities $\varphi^0(U)$ and $\psi_i^0(U)$ are defined in a similar fashion.

Setting $\tilde{U} = U^0 \in F$ in (4.2), we can obtain a condition for the existence of a discontinuity, namely, $d(U) \geq 0$. The same condition arises in analyzing discontinuous solutions of system (1.1), which is a special case of variational inequality (2.1) with the set F coinciding with the entire space. In models of solid mechanics, $d(U)$ is the portion of energy released at the shock front due to elastic deformation. The left-hand side of (4.2) characterizes energy released due to plasticity. In view of the hypothesis that thermodynamically reversible and irreversible processes are independent, inequality (4.2) on the discontinuity hypersurface is replaced by the stronger inequality

$$(\tilde{U} - U^0)[r(U)] \geq 0, \quad U^{\pm}, \tilde{U} \in F. \tag{4.3}$$

In fact, this inequality corresponds to the Ziegler principle formulated for the thermodynamically irreversible transition of the medium from the state ahead of the shock front to the state behind it, in which U^0 and $[r(U)]$ play the role of a thermodynamic flux vector and a vector of thermodynamic forces, respectively. From this point of view, the variational inequality (4.2) is a mathematical model of a strong discontinuity treated as an independent phenomenon.

The following assertion is true: under condition (4.3) at the solution discontinuity front, for any $\alpha : |\alpha| \leq 1$, we have a more general variational inequality:

$$(\tilde{U} - U^{\alpha})[r(U)] \geq 0, \quad U^{\alpha} = \frac{1 + \alpha}{2} U^+ + \frac{1 - \alpha}{2} U^-, \quad \tilde{U} \in F. \tag{4.4}$$

Indeed, by virtue of (4.3), this inequality holds for $\alpha = 0$. Using, as $\tilde{U} \in F$, the vector U^+ and then U^- and summing the resulting inequalities, we can show that $[U] \cdot [r(U)] = 0$. Combining this relation with the formula $U^{\alpha} = U^0 + \alpha[U]/2$, we conclude that inequality (4.4) holds for any α.

The proved assertion has the following geometric interpretation. If some point U^{α} of the interval with endpoints U^- and U^+ in the m-dimensional space lies strictly inside the set F, then, since the variation $\tilde{U} - U^{\alpha}$ in (4.4) is arbitrary, the vector $[r(U)]$ vanishes. If the entire interval belongs to the boundary of the convex set F, then this vector is directed along the inward normal to the boundary; moreover, the normal direction does not change in passing to another point of the interval.

Thus, weak solutions in the mechanics of elastoplastic media can contain discontinuities of two types: neutral (elastic) waves determined by the system of equations $[r(U)] = 0$ and dissipative (plastic) waves corresponding to the gradient condition with respect to the yield surface; in this case, the interval with the endpoints at U^+ and U^- belongs to the yield surface.

Note that, in the geometrically linear theory of elastic-ideally plastic media, the generating potentials $\Phi(U)$ and $\Psi_i(U)$ are quadratic functions, so $d(U)$ is identically zero. Therefore, inequality (4.3) follows from (4.2) without using any additional hypotheses or assumptions.

The method described above was used to obtain a complete system of relations for a strong discontinuity in the theory of elastic-ideally plastic flow [13]. Earlier, it was shown in [14] that the system of equations of this theory based on the associated plasticity law cannot be reduced to a conservative form. Therefore, it cannot be generalized in the form of a complete system of integral conservation laws. The velocities of plastic shock waves were first determined in [15] by applying the auxiliary hypothesis that energy dissipation is maximal at a discontinuity. In [16] the method described above was applied to the model of linear isotropic and translational hardening, in which case the generating potentials are also quadratic. A qualitative analysis of discontinuous solutions within this model was performed in [17]. In [18, 19] discontinuous solutions in the theory of granular materials were investigated taking into account that the material has a different resistance to tension and compression.

5. NUMERICAL ALGORITHMS

The general approach for constructing numerical methods for problems admitting formulations in the form of variational inequalities is reduced to two stages: an approximation of the differential operator of the problem and an approximation of the constraint determining the set of admissible variations of the solution. As usual, the operator is approximated by its discrete analogue $\mathcal{D}_h\langle U_h\rangle$ (h is the characteristic parameter of a space-time grid). The approximation of the constraint, in fact, indicates the sense in which the sought discrete solution U_h is included in the set F. Next, inequality (2.1) is approximated by the discrete variational inequality

$$(\tilde{U}_h - \hat{U}_h)\cdot(\mathcal{D}_h\langle U_h\rangle - g(U_h)) \ge 0, \quad \hat{U}_h = \mathcal{I}_h\langle U_h\rangle, \quad \tilde{U}_h \in F, \tag{5.1}$$

where $\mathcal{I}_h\langle U_h\rangle$ is the difference operator approximating the constraint.

Let $\mathcal{D}_h\langle U_h\rangle$ be a nonconservative difference operator of the form

$$\mathcal{D}_h\langle U_h\rangle = A(U^{k-1})\frac{U^k - U^{k-1}}{\Delta t} - \sum_{i=1}^{n} B^i(U^{k-1})\mathcal{L}_i\left\langle U^{k-1}\right\rangle - g(U^{k-1}).$$

Here, $\mathcal{L}_i\left\langle U^{k-1}\right\rangle$ is a time-explicit difference approximation of the spatial derivative, the superscripts indicate the time level index, and the index h in the expanded form is omitted for notational brevity.

This approximation yields low-cost difference schemes with computational costs proportional to the number of grid nodes.

Let $\bar{U}_h$ be an auxiliary grid vector function that solves the following difference scheme for the system of quasilinear equations $\mathcal{D}\langle U\rangle = g(U)$:

$$A(U^{k-1})\frac{\bar{U}^k - U^{k-1}}{\Delta t} = \sum_{i=1}^{n} B^i(U^{k-1})\mathcal{L}_i\left\langle U^{k-1}\right\rangle + g(U^{k-1}). \tag{5.2}$$

Then the discrete variational inequality (5.1) at each grid node is written as

$$(\tilde{U} - \hat{U}^k)\cdot A(U^{k-1})(U^k - \bar{U}^k) \ge 0, \quad \hat{U}^k, \tilde{U} \in F. \tag{5.3}$$

Since the relationship between the node values $\hat{U}_h$ and U_h can be specified in an arbitrary manner, it is possible to construct various correcting algorithms for computing the solution U^k of variational inequality (5.1) in terms of the solution $\bar{U}^k$ of system (5.2). In the simplest case, when $\hat{U}^k = U^k$, solving (5.3) is equivalent to minimizing, on the set F, the quadratic function $(U^k - \bar{U}^k)\cdot A(U^{k-1})(U^k - \bar{U}^k)$, which defines the squared norm associated with the symmetric positive definite matrix $A(U^{k-1})$ or, equivalently, to finding the vector U^k as the projection of $\pi_{k-1}(\bar{U}^k)$ onto the set F with respect to this norm. In the case of an isotropic elastic-ideally plastic medium with the von Mises yield criterion, this algorithm is known as the Wilkins stress correction [20].

Specifying the above-mentioned relationship by the formula $2\hat{U}^k = (1+\alpha)U^k + (1-\alpha)\bar{U}^k$, we can derive from (5.3) a more general version of correction depending on the parameter α. In this case,

$$U^k = \frac{2}{1+\alpha}\hat{U}^k - \frac{1-\alpha}{1+\alpha}\bar{U}^k, \quad \hat{U}^k = \pi_{k-1}(\bar{U}^k). \tag{5.4}$$

The numerical stability of this algorithm can be analyzed using variational inequality (5.3). Let $\delta\bar{U}^k$ be a perturbation of the auxiliary solution $\bar{U}^k$ caused by roundoff errors. By setting $\tilde{U} = \hat{U}^k + \delta\hat{U}^k$ in (5.3) and $\tilde{U} = \hat{U}^k$ in a similar inequality written for the perturbed solution $U^k + \delta U^k$ and summing the results, it can be shown that

$$\delta\hat{U}^k \cdot A(U^{k-1})(\delta U^k - \delta\bar{U}^k) \le 0.$$

Computing the variation $\hat{U}^k$ in terms of the variations U^k and $\bar{U}^k$ yields the inequality

$$|\delta U^k|^2_{k-1} + \alpha|\delta U^k - \delta\bar{U}^k|^2_{k-1} \le |\delta\bar{U}^k|^2_{k-1}$$

(here, vertical bars denote the associated vector norm). For $\alpha \ge 0$, this inequality leads to the condition that the norm of the perturbation at the correction stage does not increase. The value $\alpha = 0$ corresponds to a zero additional numerical energy dissipation, for which the second term on the left-hand side of the inequality is responsible. This choice of the parameter is most preferable. On the other hand, by varying the value of α, we can suppress undesirable effects of the numerical solution, such as oscillations at the fronts of dissipative shock waves.

Given a relation between the space-time step sizes, if the difference scheme (5.2), together with the necessary boundary conditions of the problem, satisfies the stability condition for the transition from one time level to another, i.e., if

$$\left\|\delta\bar{U}^k\right\|_{k-1} \le \left\|\delta U^{k-1}\right\|_{k-2}(1 + C\Delta t), \quad C = \text{const} \ge 0,$$

and, additionally, the discrete norm is consistent with the associated vector norm, then

$$\left\|\delta U^k\right\|_{k-1} \le \left\|\delta U^1\right\|_0 \exp(Ck\Delta t),$$

which guarantees that the solution of the discrete variational inequality is stable with respect to the initial data. Thus, the application of correction procedure (5.4) as a stage in solving the problem for $\alpha \ge 0$ does not lead to the instability of the computations.

The method described can be improved by applying a two-step solution procedure with the first step coinciding with algorithm (5.2), (5.3) and with the second step being the same algorithm with the matrices $A(U^{k-1})$, $B^i(U^{k-1})$ and the vector $g(U^{k-1})$ replaced by

$$A\left(\frac{U^k + U^{k-1}}{2}\right), \quad B^i\left(\frac{U^k + U^{k-1}}{2}\right), \quad g\left(t^{k-1} + \frac{\Delta t}{2}, x, \frac{U^k + U^{k-1}}{2}\right).$$

The idea of this improvement is used in the second-order accurate two-step Euler method as applied to systems of ordinary differential equations. The resulting improvement in the accuracy of the solution can be demonstrated on test examples.

A more complicated procedure for the numerical implementation of the variational inequality is obtained in the case of a conservative approximation of the differential operator, which is convenient, for example, in computing weak solutions with strong discontinuities. Now let $\bar{U}_h$ be the solution of the following conservative difference scheme for the system of quasilinear equations $\mathcal{D}\langle U\rangle = g(U)$:

$$\frac{\varphi(\bar{U}^k) - \varphi(U^{k-1})}{\Delta t} = \sum_{i=1}^{n} \mathcal{L}_i\left\langle \psi_i(U^{k-1})\right\rangle + g(U^{k-1}). \tag{5.5}$$

Then the corresponding discrete inequality can be written as

$$(\tilde{U} - \hat{U}^k)\cdot(\varphi(U^k) - \varphi(\bar{U}^k)) \ge 0, \quad \hat{U}^k, \tilde{U} \in F. \tag{5.6}$$

Setting $\hat{U}^k = U^k$ and taking into account the criterion for the convexity of the generating potential $\Phi(U)$, according to which

$$\Phi(\tilde{U}) - \Phi(U^k) \geq (\tilde{U} - U^k) \cdot \varphi(U^k),$$

we see that the sought vector U^k is the solution of the constrained minimization problem

$$\min\{\Phi(\tilde{U}) - \tilde{U} \cdot \varphi(\bar{U}^k) \,|\, \tilde{U} \in F\}, \tag{5.7}$$

which generalizes the problem of finding the projection onto the set F in the numerical implementation of variational inequality (5.3). The converse is also true: a unique minimizer of the above-defined strongly convex function under the constraint $\tilde{U} \in F$ is a solution of inequality (5.6).

In the case of a conservative approximation of the operator, the application of the above-described correction procedure with parameter α is not reasonable. Generally speaking, the stability of this procedure and a reduction in numerical energy dissipation with decreasing α fail to be established. Moreover, numerical experiments for test problems show that the resulting difference scheme loses accuracy in the presence of strong discontinuity surfaces.

As a generalization, we consider the correction procedure [21]

$$\varphi(U^k) = \frac{2}{1+\alpha}\varphi(\hat{U}^k) - \frac{1-\alpha}{1+\alpha}\varphi(\bar{U}^k). \tag{5.8}$$

With this choice of the relationship between the grid functions $\hat{U}_h$ and U_h, variational inequality (5.6) is reduced to the form

$$(\tilde{U} - \hat{U}^k) \cdot (\varphi(\hat{U}^k) - \varphi(\bar{U}^k)) \geq 0.$$

Therefore, the vector $\hat{U}^k$ is also a solution of the convex programming problem (5.7) and the vector U^k is determined by solving the systems of nonlinear equations (5.8).

For small perturbations of the solution, in this case,

$$\delta\hat{U}^k \cdot (\delta\varphi(U^k) - \delta\varphi(\hat{U}^k)) \leq 0, \quad 2A(\hat{U}^k)\delta\hat{U}^k = (1+\alpha)\delta\varphi(U^k) + (1-\alpha)\delta\varphi(\bar{U}^k).$$

After eliminating the vector $\delta\hat{U}^k$, we obtain the estimate

$$|\delta\varphi(U^k)|_k^2 + \alpha|\delta\varphi(U^k) - \delta\varphi(\bar{U}^k)|_k^2 \leq |\delta\varphi(\bar{U}^k)|_k^2.$$

Here, $|U|_k = \sqrt{U \cdot A(\hat{U}^k)^{-1}U}$ is the norm associated with the inverse of the matrix $A(\hat{U}^k)$. Thus, for $\alpha \geq 0$, the correction procedure ensures the stability of the computations if scheme (5.5) is stable with respect to the corresponding discrete norm.

Let us discuss the numerical implementation of the correction procedure in the form of (5.3) and in a more general form related to problem (5.6). In solving the variational inequality, the correction stage is applied repeatedly (at each time level and at each spatial grid node), so the efficiency of the algorithm as a whole is determined by the performance at this stage. In the simplest situation, when the matrix $A(U^{k-1})$ and the structure of the constraints specified by the set of admissible variations F are such that the projector $\pi_{k-1}(U)$ can be written in closed form, the correction procedure is implemented directly using formulas (5.3) after computing $\bar{U}^k$ from system (5.2). This situation occurs in most applications concerning isotropic elastoplastic materials and the classical von Mises and Tresca–Saint-Venant yield criteria [7].

In the case of a conservative approximation of the differential operator, equivalent to (5.7), problem (5.6) can be solved by iteration in which every step involves solving the linearized inequality

$$(\tilde{U} - \hat{U}^{k}) \cdot (A(\hat{U}^k)(\hat{U}^{k} - \hat{U}^k) + \omega(\varphi(\hat{U}^k) - \varphi(\bar{U}^k))) \geq 0, \quad \hat{U}^{k}, \tilde{U} \in F. \tag{5.9}$$

Here, $A(\hat{U}^k)$ is a matrix computed at the first iteration and $\omega > 0$ is an iteration parameter, its initial value $\omega = 1$ is halved every time the sequence of approximations is not a relaxation one. The new approximation $\hat{U}^{k}$ in this inequality is found in terms of the preceding approximation $\hat{U}^k$ by applying algorithm (5.4) for solving variational inequality (5.3).

The convergence rate of iterations (5.9) depends, generally speaking, on the initial approximation, which is should be specified as $\hat{U}^k = U^{k-1}$. To accelerate the algorithm, after a certain number of steps, the matrix $A(\hat{U}^k)$ can be updated with reconstructing $\omega = 1$. The convergence of a similar iterative process in a somewhat different interpretation was studied in [22, p. 209].

When the algorithm is implemented with the parameter $\alpha = 1$, there is no need to subsequently solve system (5.8), since $U_h = \hat{U}_h$. In the general case, the solution can be computed by applying the Newton–Raphson method.

In the case of anisotropic materials satisfying special plasticity conditions for which the projector cannot be written in closed form, a fairly efficient approach might be to solve a convex programming problem by applying an augmented Lagrangian (see [23]). If the set F can be parametrized in the form

$$F = \{U \mid f_j(U) \le 0,\ j = 1,\dots,l\},$$

where $f_j(U)$ is a system of convex functions, then the augmented Lagrangian is defined by

$$\Lambda^k(U,\gamma) = \Phi(U) - U \cdot \varphi(\bar{U}^k) + \frac{1}{2\kappa}\sum_{j=1}^{l}(\max{}^2\{0, \gamma_j + \kappa f_j(U)\} - \gamma_j^2).$$

Here, $\kappa > 0$ is a parameter of the method and γ is the dual vector. Equivalent to (5.7), the problem of finding a saddle point of the Lagrangian

$$\Lambda^k(U^k,\gamma^k) = \min_{\tilde{U}} \max_{\tilde{\gamma}} \Lambda^k(\tilde{U},\tilde{\gamma})$$

is solved using the iterative process

$$A^k(U^k)(U'^k - U^k) = -\omega\frac{\partial\Lambda^k(U^k,\gamma^k)}{\partial U}, \quad \gamma'^k - \gamma^k = \lambda\frac{\partial\Lambda^k(U^k,\gamma^k)}{\partial\gamma}.$$

The iteration parameters $\omega > 0$ and $\lambda > 0$ are initially set to unity and are then chosen by applying a bisection procedure such that the sequence of approximations for U^k and γ^k is a relaxation one.

To conclude, we note that mathematical models for elastoplastic, granular, and porous materials formulated in the form of variational inequality (2.1) can be used to design universal shock-capturing algorithms that are stable with respect to roundoff errors and are adapted for computing discontinuous solutions in the case of a suitable approximation of the differential operator involved in the inequality.

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