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Mathematical modeling of growth processes in nature and engineering: A variational approach

A. V. Manzhirov¹ and S. A. Lychev¹

1Ishlinsky Institute for Problems in Mechanics of the Russian Academy of Sciences, Vernadsky Ave 101 Bldg 1, Moscow, 119526, Russian Federation
E-mail: manzh@ipmnet.ru

Abstract. We present a variational approach to the mathematical theory of accreted solids. One main point in this approach is that the operator of the accretion problem proves to be self-adjoint with respect to an appropriately modified convolution bilinear form, and it is this linear form that we use in the construction of the variational functional.

Our growing solid model can be efficiently applied to describe processes such as concreting, pyrolytic deposition, laser spraying, electrolytic deposition, polymerization, solidification of melts, crystal growth, glacier and ice cover freezing, sedimentary and volcanic rock forming, and biological tissue growth. These applications will be considered elsewhere.

1. Introduction

Deformation processes in a solid whose composition, mass, or volume varies in a piecewise continuous manner owing to accretion—the addition of new material to the body outer surface—were studied in [1–12]. The solid mechanics problems arising in the modeling of such processes are completely new and constitute a separate field of research, known as mechanics of accreted solids. Its importance is due to the fact that the manufacturing of virtually all objects considered in solid mechanics (buildings, structures, structural components, machine parts, etc.) involves accretion. (Specific examples include continuous concrete structure erection, metal solidification, spray deposition of semiconducting films, and crystal growth—one could easily continue the list.)

We consider the variational statement of the piecewise continuous accretion problem and suggest a method for solving the resulting variational problem.

The following main stages of deformation clearly manifest themselves in a piecewise continuous accretion process:

(i) The initial stage occurring prior to accretion.
(ii) The continuous accretion stage.
(iii) The deformation stage occurring after accretion (or growth) stops.

Stages (ii) and (iii) alternate, and each of the stages is naturally characterized by its start time and termination time. For stage (i), these are the times at which the load is applied to the solid and then growth starts; for stage (ii), the times at which growth starts and then stops; and for stage (iii), conversely, the times at which growth stops and then starts. After a number of alternations, the process is usually finished at the third stage, for which the termination time is taken to be arbitrarily large. The original solid occurring at the initial stage will also be called
the basic solid. The rest of the solid at any given time is called the additional solid; it may have a complex structure and consists of the collection of solids formed on different time intervals of continuous accretion [stage (ii)]. We refer to these as sub-solids, so that the additional solid is the union of sub-solids. The domains occupied by the former and latter can be disconnected. The whole solid, which is the union of the basic and additional solids, will be called the accreted (or growing) solid. Note that accretion may well occur without the basic solid, starting from an infinitesimal material element.

The part of the surface where infinitesimal pieces of the material are deposited at the current time is called the accretion (or growth) surface. The growth surface may be disconnected in general. In particular, it can be the entire surface of the solid. Finally, the part of the surface of the original or growing solid that coincides with the growth surface at the growth start time will be called the base surface. The base surface is clearly the part of the surface of the solid on which material will be deposited during the next stage of continuous accretion. At various stages, it usually coincides with the surface between the basic solid and the additional solid or with a surface between sub-solids.

To study the stress-strain state of the accreted solid, one should know the deformation laws

- Of the basic body from the time at which the load is applied until the time at which accretion starts.
- Of the deposited material from the time at which the load is applied to this material until the time of its deposition on the accreted solid.

While the state of the original body is determined from the solution of the problem at the stage preceding accretion, the previous history of the strain tensor of the infinitesimally thin continuously deposited material is assumed to be known.

Prior to stating the problem considered in the present paper, we point out that the growth problem for a solid differs dramatically from a problem involving the removal of material. The latter is solely characterized by the fact that the domain occupied by the body is reduced, subject to the standard equations and boundary conditions.

2. Main results

The aim of this section is to obtain the variational statement of the problems under consideration. This permits us to apply direct variational methods for numerical simulation and furthermore define correct boundary and initial conditions in the above-mentioned applied initial–boundary value problems.

Let us obtain kinematic relations and use material coordinates that specify unique material particles. The positions of these particles in Euclidian space can be characterized by the spatial coordinates $\chi(x; t)$. We denote the time variable by $t$. We assume that the accretion scenario is known; i.e. the accretion time $\tau^*(x)$ is prescribed for each particle $x$. Suppose that annihilation of material particles does not occur. Thus, the function $\chi(x; t)$ is well defined for each $x$ in the corresponding interval $(\tau^*(x), \infty)$. The set $\mathcal{B}$ of accreted material particles is assumed to be a simply connected domain in the topological space. The boundary $\partial\mathcal{B}$ of $\mathcal{B}$ is assumed to be regular. For simplicity, we suppose that the accreted material is in natural state at the accretion or deposition time $\tau^*(x)$. All these assumptions permit us to determine the displacements as follows:

$$ u(x; t) = \int_{\tau^*(x)}^{t} v(x; \tau) \, d\tau, $$

where $v(x; t)$ is the velocity of the particle with material coordinate $x$,

$$ v(x; t) = \frac{\partial \chi(x; t)}{\partial t}. $$
Note that the displacement defined in such a way is the *displacement of a particle with respect to its position at the accretion time*. Hence we have a well-defined vector field $u$ in $\mathcal{B}$, and it is reasonable to define the deformation gradient in the interior of $\mathcal{B}$ by the formula

$$ F = \nabla \otimes u = \nabla \otimes \int_{\tau^*(x)}^{t} v(x; \tau) d\tau. $$

We point out that, in contrast with conventional elasticity [13], the Hamiltonian operator and the definite integral over time do not commute, because the lower integration limit $\tau^*(x)$ depends on the material variables. Indeed,

$$ F = \int_{\tau^*(x)}^{t} \nabla \otimes v(x; \tau) d\tau - \nabla \tau^*(x) \otimes v(x; \tau^*(x)). \quad (2) $$

Now we introduce the velocity gradient in the classical context,

$$ D = \nabla \otimes v(x; \tau). $$

It is easily seen that

$$ D = \dot{F}, $$

where the dot stands for differentiation with respect to $t$, but at the same time it follows from Eq. (2) that

$$ F = \int_{\tau^*(x)}^{t} D d\tau + \Omega. $$

Here we have used the notation

$$ \Omega = - \nabla \tau^*(x) \otimes v(x; \tau^*(x)). $$

Recall that $v(x; \tau^*(x))$ is the material particle velocity at the accretion time.

Consider the tensor field

$$ \tilde{F} = \int_{\tau^*(x)}^{t} D d\tau, $$

similar to the deformation gradient. This tensor field can be referred to as a primitive of the velocity gradient. Obviously,

$$ \nabla \times F = 0, \quad \nabla \times \tilde{F} = \nabla \times \Omega \neq 0. $$

This means that, in general, $F$ satisfies the compatibility conditions, while $\tilde{F}$ still does not. Indeed,

$$ \nabla \times \Omega = - \nabla \tau^*(x) \otimes \nabla \times v^*(x). $$

Therefore, if the initial velocity field $v^*(x)$ is not potential, then the tensor field $\tilde{F}$ does not satisfy the compatibility conditions. Of course, the difference disappears if we use the derivatives of the above-mentioned tensor fields. This leads to the statement of the problem in terms of velocities.

Now we construct the variational statement of the problems under consideration with the use of the following well-known assertion: if a linear operator $A$ with domain $\mathcal{D}$ is self-adjoint with respect to a symmetric bilinear form $(.,.)$ and if this bilinear form is nondegenerate, i.e., satisfies the condition

$$ (\forall u \in \mathcal{D} \ (u, v) = 0) \Rightarrow v = 0, $$


then the stationary points of the quadratic functional

\[ J[u] = \frac{1}{2} \langle u, A[u] \rangle \]

defined on the same domain \( \mathcal{D} \) are exactly the solutions of the equation

\[ A[u] = 0. \]

This statement is obvious. Nevertheless, except in trivial cases, the operators that arise in continuum mechanics are not self-adjoint with respect to classical bilinear forms, which usually coincide with the standard inner products in the corresponding function spaces. The problems concerning the variational statement of dynamic elasticity by Hamilton’s principle are well known. That is, the extension of variational formalism to novel problems depends on an appropriate definition of nonclassical bilinear forms. Noticeable progress in this field was obtained by Gurtin [14], Tonzi [15], and Belli and Morosi [16]. They proposed the use of the convolution as a bilinear form. In particular, this permits one to obtain a well-defined variational statement for linear dynamic elasticity and thermoelasticity.

In what follows, we use a modification of the convolution bilinear form adapted to growing elastic solids. We assume that accretion of additional material takes place only on the boundary and that the classical conservation laws hold in the interior parts of the body. Thus, we can expect that the variational principles for elastic and thermoelastic growing solids and the principles recently proposed by Gurtin and Tonzi differ in the boundary terms and function domains.

Consider an elastic accreted solid. It follows from the conservation of momentum that in an open neighborhood \( \mathcal{N}_x \) of an arbitrary interior point \( x \) one has

\[ \nabla \cdot [E : \nabla \otimes u] + \rho \dot{f} - \rho \ddot{u} = 0, \]

where \( \rho \) is the mass density, \( f \) is the body force per unit mass, and \( E \) is the elasticity tensor. We use this notation for brevity; in conventional linear elasticity, the symmetric part of the deformation gradient is customarily used.

Consider the class \( \mathcal{A} \) of smooth compactly supported functions defined in \( \mathcal{N}_x \times (\tau^*, t) \). Thus, the functions belonging to \( \mathcal{A} \), together with their all derivatives, are zero in the complement of the set \( \mathcal{N}_x \times (\tau^*, t) \). On the class \( \mathcal{A} \), we introduce the differential operator

\[ A[u] = \nabla \cdot [E : \nabla \otimes u] - \rho \ddot{u} \]

and the bilinear form

\[ \langle u, v \rangle = \int_{\mathcal{N}_x} \int_{\tau^*(x)}^{t} u(x; t + \tau^* - \tau) \cdot v(x; \tau) \, d\tau \, dV. \tag{3} \]

A straightforward computation readily shows that this form is symmetric,

\[ \forall u, v \in \mathcal{A} \quad \langle u, v \rangle = \langle v, u \rangle, \]

and nondegenerate. The latter assertion is a consequence of well-known functional properties of the convolution.

The Gauss divergence theorem with respect to material variables, the rule of integration by parts with respect to time \( t \), and the assumption

\[ E = E^{(3412)} \tag{4} \]
(where \( E^{(3412)} \) is the tensorial isomer with dyadic permutation 3412) give the following relation for arbitrary elements of \( \mathcal{A} \):

\[
\langle A[u], v \rangle = \langle u, A[v] \rangle.
\]

In other words, the operator \( A \) is self-adjoint with respect to the bilinear form (3). Note that assumption (4) always holds in the framework of classical hyperelasticity and corresponds to the existence of an elastic potential.

Now we are in a position to construct a variational statement for the problem without body forces for functions of the class \( \mathcal{A} \) as follows:

\[
I[u] = \frac{1}{2} \langle u \cdot A[u] \rangle, \quad \delta I[u] = 0.
\] (5)

If the tensor \( E \) is positive definite, then problem (5) has only the trivial solution. It follows from this remark that the properties of elastic bodies manufactured by accretion in the absence of body forces and with trivial initial conditions are identical to those of classical elastic bodies.

Taking into account the body forces, we obtain

\[
I[u] = \frac{1}{2} \langle u \cdot A[u] \rangle + \mathcal{R}_1,
\]

where the additional operator \( \mathcal{R}_1 \) depends on the prescribed body force distribution \( f = f(x; t) \),

\[
\mathcal{R}_1 = \langle u, \rho f \rangle.
\]

Now let us expand the domain \( N_A \) as much as possible. This possibility is limited to the current body boundary corresponding to time \( t \). The above-mentioned expansion involves additional terms in the definition of the functional,

\[
I[u] = \frac{1}{2} \langle u \cdot A[u] \rangle + \mathcal{R}_1 + \mathcal{R}_2 + \mathcal{R}_3,
\]

The term \( \mathcal{R}_2 \) depends on the prescribed initial velocity distribution \( v^*(x) = v(x; \tau^*(x)) \),

\[
\mathcal{R}_2 = -\frac{1}{2} \int_B v^*(x) \rho v(x; t) \, dV,
\]

and the term \( \mathcal{R}_3 \) depends on prescribed traction distribution \( p = p(x; t) \big|_{\partial B} \) on the current body boundary,

\[
\mathcal{R}_3 = \frac{1}{2} \int_{\partial B} \int_{\tau^*(x)}^t p(x; t + \tau - \tau^*) \cdot v(x; \tau) \, d\tau \, dV.
\]

Note that now the bilinear form is defined in the entire material region \( B \),

\[
\langle u, v \rangle = \int_B \int_{\tau^*(x)}^t u(x; t + \tau - \tau^*) \cdot v(x; \tau) \, d\tau \, dV,
\]

and the function class \( \mathcal{A} \) is expanded to the class \( \mathcal{D} \) of twice differentiable functions that satisfy the above-mentioned boundary and initial conditions. Therefore, we obtain the variational principle that can be stated as follows:

\[
2I[u] = \int_B \int_{\tau^*(x)}^t u(x; t + \tau - \tau^*) \cdot \{ \nabla \cdot [E(x) \cdot \nabla \odot u(x; \tau)] - \rho \ddot{u}(x; \tau) + 2\rho f(x; \tau) \} \, d\tau \, dV
\]

\[
+ \int_{\partial B} \int_{\tau^*(x)}^t p(x; t + \tau - \tau^*) \cdot u(x; t) \, d\tau \, dV - \int_B v^*(x) \cdot \rho \ddot{u}(x; t) \, dV, \quad u \in \mathcal{D}, \quad \delta I = 0.
\]
To prove the well-posedness of this variational statement, let us compute the variation of the functional $J[u]$. We have

$$2 \delta J = \langle \delta u \cdot A[u] \rangle + \langle u \cdot A[\delta u] \rangle + 2 \delta R_1 + \delta R_2 + \delta R_3. $$

It follows from the Gauss divergence theorem and the rule of integration by parts with respect to $t$ that

$$\langle u \cdot A[\delta u] \rangle = \langle A[u] \cdot \delta u \rangle + \int_{\partial B} n \cdot \int_{\tau^*(x)} [u(x; t + \tau^* - \tau) \cdot E(x) \cdot \nabla \otimes \delta u(x; \tau) - \nabla \otimes u(x; t + \tau^* - \tau) : E(x) \cdot \delta u(x; \tau)] d\tau dA$$

$$+ \int_{\partial B} [\hat{u}(x; \tau^* ) \delta u(x; t) - \hat{u}(x; t) \delta u(x; \tau^* ) - u(x; \tau^* ) \delta \hat{u}(x; t) + u(x; t) \delta \hat{u}(x; \tau^* )] \rho dV,$$

where $n$ is the outward unit normal to the current material boundary $\partial B$. Moreover,

$$\delta R_1 = \langle \delta u, \rho f \rangle, \quad \delta R_2 = -\int_B v^*(x) \rho \delta v(x; t) dV, \quad \delta R_3 = \int_{\partial B} \int_{\tau^*(x)} p(x; t + \tau^* - \tau) \delta v(x; t) d\tau dA.$$

Since the traction on the boundary and the initial velocities are prescribed and the initial displacements are always zero by virtue of (1), we have

$$E(x) \cdot \nabla \otimes \delta u(x; \tau) = 0, \quad \delta u(x; \tau^*) = \delta \hat{u}(x; \tau^*) = u(x; \tau^*) = 0.$$

Hence, we finally obtain

$$\delta J = \langle \delta u \cdot (A[u] + \rho f) \rangle + \frac{1}{2} \int_B [\hat{u}^*(x; \tau^*) - v^*(x)] \rho \delta v(x; t) dV +$$

$$+ \frac{1}{2} \int_{\partial B} \int_{\tau^*(x)} [p(x; t + \tau^* - \tau) - n \cdot (\nabla \otimes u(x; t + \tau^* - \tau) : E(x))] \cdot \delta v(x; \tau) d\tau dA.$$

By using the fundamental lemma of calculus of variations, we obtain the Euler–Lagrange equations

$$A[u] + \rho f = 0, \quad \text{i.e.} \quad \nabla \cdot [E \cdot \nabla \otimes u] + \rho f - \rho \dot{u} = 0,$$

the natural boundary conditions

$$p(x; \tau) \bigg|_{\partial B} = n \cdot (\nabla \otimes u(x; \tau) : E(x)) \bigg|_{\partial B},$$

and the natural initial conditions

$$\hat{u}^*(x; \tau^*) = v^*(x).$$

Recall that the initial displacements are always zero by virtue of (1).

Certainly, we could use the velocity $v(x; t) = \hat{u}(x; t)$ instead of the displacement as a basic variable in the variational statement. This brings about some inessential transformations of the variational principle and the Euler–Lagrange equations; for example, the equation of motion becomes\(^1\)

$$\nabla \cdot \left[ E \cdot \nabla \otimes \int_{\tau^*}^{t} v(\tau) d\tau \right] + \rho f - \rho \dot{v} = 0.$$

\(^1\) The following form of the equation of motion is also used:

$$\nabla \cdot \left[ E \cdot \int_{\tau^*}^{\tau} \nabla \otimes v(\tau) d\tau \right] + \rho f - \rho \dot{v} = 0.$$

It is clear that these forms are different. But if we compute the derivatives of the left- and right-hand sides of both equations, they become identical. For this reason, the equations in terms of velocities are often considered.
The generalization of the variational principle to the nonlinear case is based on the Vainberg theorem [17]. Let $A[u]$ be a nonlinear operator. By the Vainberg theorem, the assertion that the variation of the functional

$$J[u] = \langle u, \int_0^1 A[\lambda u] d\lambda \rangle$$

is zero if and only if $u$ satisfies the equation

$$A[u] = 0$$

holds provided that the Fréchet derivative is self-adjoint.

In the nonlinear case, the momentum balance law implies that

$$\nabla \cdot \rho \frac{\partial \Psi}{\partial (\nabla \otimes u)} + \rho f - \rho \ddot{u} = 0,$$

where $\Psi(x, \nabla \otimes u)$ is the elastic potential. The corresponding nonlinear differential operator is

$$A[u] = \nabla \cdot \rho \frac{\partial \Psi}{\partial (\nabla \otimes u)} - \rho \ddot{u}. \tag{6}$$

One can readily show that if the condition

$$E = E^{(3412)}, \quad E = \rho \frac{\partial^2 \Psi}{\partial (\nabla \otimes u)(\partial \nabla \otimes u)}$$

holds, then the Fréchet derivative of the operator (6) is self-adjoint with respect to the convolution bilinear form. Note that this condition is equivalent to the condition that $\Psi$ is two times differentiable and is usually accepted in continuum mechanics. Thus, one can obtain the functional in the form

$$J[u] = \langle u, \int_0^1 A[\lambda u] d\lambda \rangle + R_1 + R_2 + R_3,$$

or, in expanded form,

$$J[u] = \int_B \int_{\tau^*(x)} \int_0^t u(x; t + \tau^* - \tau) \left[ \int_0^1 \nabla \cdot \rho \frac{\partial \Psi(x, \lambda \nabla \otimes u(x; \tau))}{\lambda \partial (\nabla \otimes u)} d\lambda - \frac{\rho}{2} \ddot{u}(x; \tau) + \rho f(x; \tau) \right] d\tau dV + \frac{1}{2} \int_{\partial B} \int_{\tau^*(x)} p(x; t + \tau^* - \tau) \cdot u(x; t) d\tau dV - \frac{1}{2} \int_B \nu^*(x) \cdot \rho \ddot{u}(x; t) dV.$$

3. Conclusion

Thus, we have described the variational statement of the accretion problem. The further development of the present theory is based on the refinement of the boundary and initial operators $R_2$ and $R_3$. That permits one to take into account specific features of the accretion process such as the initial tension, phase transitions, etc. In conclusion, note that the same procedure allows us to obtain the variational statements of dynamic problems for growing thermoelastic bodies in linear and nonlinear approaches. This topic will be considered elsewhere.

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