Simulation of the Dynamics of Blocky Media Based on the Cosserat Continuum Theory Using High-Performance Computations

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Plastification by high pressure torsion



Experiments on joint compression and torsion of samples show the existence of two mechanisms of plastic deformation. The first of them is associated with the formation of Chernov–Luders bands at the macro level, and the second one is realized at the mesoscale due to the rotation of grains (blocks) of a structurally inhomogeneous material.

In this presentation we simulate this process based on the equations of a multi-blocky medium with compliant interlayers and on the basis of Cosserat equations.



Schemes of two experiments - on compression and on high pressure torsion

Panin V.E., Surikov N.S., Smirnova A.S., Pochivalov Yu.I. Mesoscopic structural states in plastically deformed nanostructured metal materials. Fizicheskaya Mesomekhanika. 2018. 21(3): 12–17. [in Russian] DOI: 10.24411/1683-805X-2018-13002 http://www.ispms.ru/ru/journals/455/2540/

Sadovskii V.M., Guzev M.A., Sadovskaya O.V., Qi Ch. Modeling of plastic deformation based on the theory of an orthotropic Cosserat continuum. Fizicheskaya Mesomekhanika. 2019. 22(2): 59–66. [in Russian] DOI 10.24411/1683-805X-2019-12005 http://www.ispms.ru/ru/journals/465/2657/

Elastic interlayers

Elastic blocks and elastic interlayers



Scheme of a blocky medium

A motion of each block is defined by the system of equations of a homogeneous isotropic elastic medium:

$$\begin{aligned} \rho \,\dot{v}_1 &= \sigma_{11,1} + \sigma_{12,2} \\ \rho \,\dot{v}_2 &= \sigma_{12,1} + \sigma_{22,2} \\ \dot{\sigma}_{11} &= \rho \,c_1^2 \left(v_{1,1} + v_{2,2} \right) - 2 \,\rho \,c_2^2 \,v_{2,2} \\ \dot{\sigma}_{22} &= \rho \,c_1^2 \left(v_{1,1} + v_{2,2} \right) - 2 \,\rho \,c_2^2 \,v_{1,1} \\ \dot{\sigma}_{12} &= \rho \,c_2^2 \left(v_{2,1} + v_{1,2} \right) \end{aligned}$$

Elastic interlayer between the horizontally located nearby blocks is described by the system of equations:

$$\rho' \frac{\dot{v}_1^+ + \dot{v}_1^-}{2} = \frac{\sigma_{11}^+ - \sigma_{11}^-}{\delta_1}, \quad \frac{\dot{\sigma}_{11}^+ + \dot{\sigma}_{11}^-}{2} = \rho' c_1'^2 \frac{v_1^+ - v_1^-}{\delta_1}; \quad \rho' \frac{\dot{v}_2^+ + \dot{v}_2^-}{2} = \frac{\sigma_{12}^+ - \sigma_{12}^-}{\delta_1}, \quad \frac{\dot{\sigma}_{12}^+ + \dot{\sigma}_{12}^-}{2} = \rho' c_2'^2 \frac{v_2^+ - v_2^-}{\delta_1}$$

Elastic interlayer between the vertically located nearby blocks is modeled using similar system:

$$\rho' \frac{\dot{v}_2^+ + \dot{v}_2^-}{2} = \frac{\sigma_{22}^+ - \sigma_{22}^-}{\delta_2}, \quad \frac{\dot{\sigma}_{22}^+ + \dot{\sigma}_{22}^-}{2} = \rho' c_1'^2 \frac{v_2^+ - v_2^-}{\delta_2}; \quad \rho' \frac{\dot{v}_1^+ + \dot{v}_1^-}{2} = \frac{\sigma_{12}^+ - \sigma_{12}^-}{\delta_2}, \quad \frac{\dot{\sigma}_{12}^+ + \dot{\sigma}_{12}^-}{2} = \rho' c_2'^2 \frac{v_1^+ - v_1^-}{\delta_2}$$



Elastic-plastic interlayers



To take into account the plasticity, constitutive equations of the vertical elastic interlayer are replaced by the variational inequality:

$$(\delta\sigma_{11}^{+} + \delta\sigma_{11}^{-})\dot{\varepsilon}_{11}^{p} + (\delta\sigma_{12}^{+} + \delta\sigma_{12}^{-})\dot{\varepsilon}_{12}^{p} \leqslant 0$$

$$\begin{split} &\delta\sigma_{jk}^{\,\pm} = \tilde{\sigma}_{jk}^{\,\pm} - \sigma_{jk}^{\,\pm} - \text{variations of stresses} \\ &\dot{\varepsilon}_{11}^{\,p} = \frac{v_1^+ - v_1^-}{\delta_1} - \frac{\dot{\sigma}_{11}^{\,+} + \dot{\sigma}_{11}^-}{2\,\rho' c_1'^{\,2}}, \quad \dot{\varepsilon}_{12}^{\,p} = \frac{v_2^+ - v_2^-}{\delta_1} - \frac{\dot{\sigma}_{12}^+ + \dot{\sigma}_{12}^-}{2\,\rho' c_2'^{\,2}} - \text{plastic strain rates} \end{split}$$

The actual stresses σ_{jk}^{\pm} and variable stresses $\tilde{\sigma}_{jk}^{\pm}$ are subjected to the constraint in the form:

$$f\left(\frac{\tilde{\sigma}_{11}^+ + \tilde{\sigma}_{11}^-}{2}, \frac{\tilde{\sigma}_{12}^+ + \tilde{\sigma}_{12}^-}{2}\right) \leqslant \tau(\chi)$$

 τ – material yield point of interlayers, χ – a material parameter (or set of parameters) of hardening $f(\sigma_n, \sigma_{\tau})$ – equivalent stress function, in which arguments are normal and tangential stresses

The simplest form of the constraint for a microfractured medium is as follows:

$$|\sigma_{ au}| \leqslant au_s - k_s \, \sigma_n$$
 (au_s and k_s – material parameters)

Constitutive equations of the horizontal elastic-plastic interlayer are formulated in a similar way

Poynting-Thomson's viscoelastic model

and the power of the viscous energy dissipation



To describe the viscous dissipative effects in the interlayers under shear stresses, the Poynting–Thomson model of a viscoelastic medium is used.



Poynting-Thomson's rheological scheme

Hooke's law for elastic element: $\varepsilon_{12}' = a_0 (\sigma_{12}^+ + \sigma_{12}^-)/2, \quad \varepsilon_{12}'' = a_1 s_{12}$

Newton's law for viscous element: $\eta \dot{\varepsilon}_{12}'' = (\sigma_{12}^+ + \sigma_{12}^-)/2 - s_{12}$ Total strain: $\varepsilon_{12} = \varepsilon_{12}' + \varepsilon_{12}''$

Constitutive equations of the interlayer: $a_0 \frac{\dot{\sigma}_{12}^+ + \dot{\sigma}_{12}^-}{2} + a_1 \dot{s}_{12} = \frac{v_2^+ - v_2^-}{\delta_1}, \quad \frac{\sigma_{12}^+ + \sigma_{12}^-}{2} = s_{12} + \eta \, a_1 \, \dot{s}_{12}$ Energy balance equation: $\frac{\sigma_{12}^+ + \sigma_{12}^-}{2} \frac{v_2^+ - v_2^-}{\delta_1} = \dot{W} + \eta \, a_1^2 \, \dot{s}_{12}^2, \quad 2W = a_0 \frac{(\sigma_{12}^+ + \sigma_{12}^-)^2}{4} + a_1 \, s_{12}^2$ according to which the power of internal stresses in the interlayer is the sum of the reversible elastic strain power



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Model of separation cracks



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Rheological scheme of contact interaction of crack edges

Conditions of contact interaction of the crack edges are formulated as a variational inequality:

$$\delta\sigma_{11}\left(\frac{1}{\rho'c_1'^2}\,\sigma_{11}-\varepsilon_{11}\right) \ge 0, \quad \dot{\varepsilon}_{11}=\frac{v_1^+-v_1^-}{\delta_1}$$

The algorithm of numerical implementation in a mesh of a grid is based on the equations

$$\hat{\varepsilon}_{11} = \varepsilon_{11} + \frac{v_1^+ - v_1^-}{\delta_1} \tau, \quad z_1 v_1^+ + \sigma_{11}^+ = R_1^+, \qquad z_1 v_1^- - \sigma_{11}^- = R_1^-$$

and the closing equation $\hat{\sigma}_{11} + \sigma_{11} = \sigma_{11}^+ + \sigma_{11}^-$, guaranteeing the absence of artificial dissipation of energy,

which gives the procedure of stress correction:
$$\hat{\sigma}_{11} = \frac{1}{\kappa} \pi_{-} \left(\varepsilon_{11} + \frac{R_1^+ - R_1^- - \sigma_{11}}{z_1 \delta_1} \tau \right), \qquad \kappa = \frac{1}{\rho' c_1'^2} + \frac{\tau}{\rho c_1 \delta_1}$$

Model of porous interlayers



The longitudinal deformation of the interlayers is described on the basis of a complicated version of the porous elastic model, which takes into account the nonlinear threshold behavior of a material with the strength increasing during the collapse of pores.



Rheological scheme of a porous interlayer

Total strain: $\varepsilon_{11} = \sigma'_{11}/b_1 + \theta_1 - \theta_0$

 $\sigma'_{11}\leqslant 0$ – stress in a rigid contact, $\theta_0>0$ and $\theta_1\geqslant 0$ – initial and current porosity values

 $\text{Governing relationships of a rigid contact:} \quad (\tilde{\sigma}_{11} - \sigma'_{11}) \, \theta_1 \leqslant 0, \quad \tilde{\sigma}_{11}, \, \sigma'_{11} \leqslant 0$

 $\sigma_{11}'=b_1\,\pi(\theta_0+\varepsilon_{11}),\ \pi(\theta)=\min(\theta,0) \text{ - projection onto the non-positive semi-axis}$

Constitutive equations of the interlayer including the equation for porosity:

$$\dot{\varepsilon}_{11} = \frac{v_1^+ - v_1^-}{\delta_1}, \quad \frac{\sigma_{11}^+ + \sigma_{11}^-}{2} = b_0 \,\varepsilon_{11} + b_1 \,\pi(\theta_0 + \varepsilon_{11}), \quad \theta_1 = \theta_0 + \varepsilon_{11} - \pi(\theta_0 + \varepsilon_{11})$$

The energy balance equation:
$$\frac{\sigma_{11}^+ + \sigma_{11}^-}{2} \,\dot{\varepsilon}_{11} = \dot{W}, \quad 2W = b_0 \,\varepsilon_{11}^2 + b_1 \,\pi^2(\theta_0 + \varepsilon_{11})$$



Two-cyclic splitting



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We developed parallel computational algorithm for supercomputers of the cluster architecture based on a two-cyclic method of splitting, which has high accuracy and permits the efficient parallelization of computations.

Governing equations in blocks and interlayers are represented in the form of symbolic evolution equation:

 $\dot{U} = A_1(U) + A_2(U)$

- A_1 and A_2 nonlinear differential-difference operators, simulating 1D motion of a blocky medium in the direction of the coordinate axes x_1 and x_2
- $U\,$ vector–function of unknown quantities, which includes the projection of the velocity vector and the stress tensor in blocks and interlayers

The method of splitting on the time interval $(t_0, t_0 + \Delta t)$ includes 4 steps:

- 1) the step of solving 1D equation in the x_1 direction on the interval $(t_0, t_0 + \Delta t/2)$
- 2) a similar step of solving the equation in the x_2 direction
- 3) the step of recomputation in the x_2 direction on the interval $(t_0 + \Delta t/2, t_0 + \Delta t)$
- 4) the step of recomputation in the x_1 direction on the same time interval

$$\begin{split} \dot{U}^{(1)} &= A_1(U^{(1)}), \quad U^{(1)}(t_0) = U(t_0) \\ \dot{U}^{(2)} &= A_2(U^{(2)}), \quad U^{(2)}(t_0) = U^{(1)}(t_0 + \Delta t/2) \\ \dot{U}^{(3)} &= A_2(U^{(3)}), \quad U^{(3)}(t_0 + \Delta t/2) = U^{(2)}(t_0 + \Delta t/2) \\ \dot{U}^{(4)} &= A_1(U^{(4)}), \quad U^{(4)}(t_0 + \Delta t/2) = U^{(3)}(t_0 + \Delta t) \end{split}$$

The solution at the time instant $t_0 + \Delta t$ equals to $U(t_0 + \Delta t) = U^{(4)}(t_0 + \Delta t)$

Efficiency of parallelization



Computational algorithm is implemented as the parallel program for analysis of the waves propagation processes in blocky media under external dynamic loads. The parallelization is performed on the basis of domain decomposition – each processor of a cluster expects a separate chain of blocks including the boundary interlayers in the horizontal direction.

The programming language is Fortran, and the message passing interface (MPI) library is used.



Dependence of the runtime T on the linear dimension N of a grid in blocks (circle points – actual computational time, solid line – semi-theoretical computational time)



Instant rotation of the central block in the rock mass



The case of porous interlayers: intensive load (with pore collapse)

 $\delta = 0.1 \, \mathrm{mm}$

 $\delta = 1 \,\mathrm{mm}$

 $\delta = 5 \,\mathrm{mm}$



Level curves of the fluid circulation around blocks depending on the thickness of interlayers

Rock massif consists of 100 \times 100 blocks, size of each block is 50 mm \times 50 mm

Sadovskii V.M., Sadovskaya O.V. Modeling of elastic waves in a blocky medium based on equations of the Cosserat continuum. Wave Motion. 2015. **52**: 138–150. https://doi.org/10.1016/j.wavemoti.2014.09.008

Sadovskii V.M., Sadovskaya O.V., Lukyanov A.A. Modeling of wave processes in blocky media with porous and fluid-saturated interlayers. Journal of Computational Physics. 2017. **345**: 834–855. https://doi.org/10.1016/j.jcp.2017.06.001



Crack propagation in a blocky medium



 Π -shaped smoothed pulse load

The action of load on a part of the upper boundary of a blocky massif

 $\Pi\text{-shaped}$ pulse load



Orthotropic elastic Cosserat continuum

For plane strain, the equations of the Cosserat elastic continuum:

$$\begin{aligned} \rho_0 \, \dot{v}_1 &= \sigma_{11,1} + \sigma_{12,2}, & \rho_0 \, \dot{v}_2 &= \sigma_{21,1} + \sigma_{22,2} \\ J_0 \, \dot{\omega}_3 &= \mu_{31,1} + \mu_{32,2} + \sigma_{21} - \sigma_{12} \\ a_1 \, \dot{\sigma}_{11} - b_1 \, \dot{\sigma}_{22} &= v_{1,1}, & a_1 \, \dot{\sigma}_{22} - b_1 \, \dot{\sigma}_{11} &= v_{2,2} \\ a_2 \, \dot{\sigma}_{21} - b_2 \, \dot{\sigma}_{12} &= v_{2,1} - \omega_3 \\ a_2 \, \dot{\sigma}_{12} - b_2 \, \dot{\sigma}_{21} &= v_{1,2} + \omega_3 \\ \dot{\mu}_{31} &= \alpha_2 \, \omega_{3,1}, & \dot{\mu}_{32} &= \alpha_2 \, \omega_{3,2} \end{aligned}$$

written in Cartesian coordinates relative to the linear velocities v_1, v_2 , angular velocity ω_3 , stresses σ_{jk} and couple stresses μ_{jk} can be represented in the matrix form:

$$A\frac{\partial U}{\partial t} = B^1 \frac{\partial U}{\partial x_1} + B^2 \frac{\partial U}{\partial x_2} + QU, \qquad U = \left(v_1, v_2, \omega_3, \sigma_{11}, \sigma_{22}, \sigma_{21}, \sigma_{12}, \mu_{31}, \mu_{32}\right)$$

with symmetric matrix-coefficients A, B^1 , B^2 and antisymmetric matrix Q.

This system belongs to the class of symmetric t-hyperbolic systems by Friedrichs and systems of thermodynamically consistent conservation laws by Godunov.





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Accounting for plasticity

Elastic-plastic Cosserat continuum



It is possible to construct a model of elastic-plastic Cosserat continuum on the basis of the system of equations of the theory of elasticity. Such a model is formulated as a variational inequality:

$$(\tilde{U}-U)\cdot\left(A\,\frac{\partial U}{\partial t}-B^1\,\frac{\partial U}{\partial x_1}-B^2\,\frac{\partial U}{\partial x_2}-Q\,U\right)\geqslant 0,\qquad \tilde{U},\,U\in F$$

F – set of admissible variations of vector $U;\,\tilde{U}$ – an arbitrary element of F

This variational inequality is a formulation of von Mises principle of maximum power of plastic dissipation. The boundary of F in the space of stress and couple stress tensors is the yield surface of a material, which is equivalent to the system of constitutive equations of plasticity in the form of associative flow rule.

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Sadovskaya O., Sadovskii V. Mathematical Modeling in Mechanics of Granular Materials.
 Ser.: Advanced Structured Materials, Vol. 21. Springer, Heidelberg – New York – Dordrecht – London, 2012. 390 p. http://link.springer.com/book/10.1007/978-3-642-29053-4



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Plasticity in interlayers



Since the behavior of continuum is completely determined by the deformation properties of the weakened interlayers of blocky structure, the yield criterion is used in the form:

$$\begin{split} |\sigma_{21}| &\leqslant \tau_0 - \kappa_\tau \, \sigma_{11}, \qquad |\sigma_{12}| \leqslant \tau_0 - \kappa_\tau \, \sigma_{22} \\ |\mu_{31}| &\leqslant \mu_0 - \kappa_\mu \, \sigma_{11}, \qquad |\mu_{32}| \leqslant \mu_0 - \kappa_\mu \, \sigma_{22} \end{split}$$

It limits the tangential stresses, which characterize shifts along the interlayers, and couple stresses, the attainment of which limit values lead to an irreversible change in the curvature.





Selection of the parameters



Cosserat continuum parameters for a masonry with elastic blocks of $0.1 \text{ m} \times 0.1 \text{ m}$ and elastic-plastic interblocks of thickness δ .

δ,	$ ho_0$,	J_0 ,	a_1 ,	b_1 ,	a_2 ,	b_2 ,	α_2 ,
mm	kg/m^3	kg/m	GPa	GPa	GPa	GPa	MN
0.1	3690	6.15	44.5	19.1	14.8	6.77	22.2
1.0	3650	6.05	38.6	16.5	6.46	4.05	9.60
5.0	3470	5.59	23.8	10.2	2.33	0.53	3.39

Mechanical parameters of the orthotropic Cosserat continuum

The yield strengths of the seams during shear τ_0 and bending μ_0 were taken equal to 0.86 MPa and 8.8 kPa \cdot m, respectively. Material hardening due to compression was not taken into account. To analyze the influence on the process of deformation of various factors – shear and curvature deformations – one of the two yield strengths was assigned a value exceeding the stress level in the problem with elastic interlayers.

 Sadovskii V.M., Sadovskaya O.V. Supercomputer Modeling of Wave Propagation in Blocky Media Accounting Fractures of Interlayers. In: Nonlinear Wave Dynamics of Materials and Structures (Eds.: Altenbach H., Eremeyev V.A., Pavlov I.S., Porubov A.V.). Ser.: Advanced Structured Materials, Vol. 122. Springer, Cham, 2020. P. 379–398.

https://link.springer.com/chapter/10.1007/978-3-030-38708-2_22



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0.800

0.592

0.490

0 386 0.28

0.180

0.026

0 33 0.438 0.644

U-shaped pulse without fracture



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Level curves of tangential stress σ_{12}





Level curves of normal stress σ_{22}

Image: A mathematical states and a mathem



U-shaped pulse loading: Cosserat model





Level curves of tangential stress σ_{12}



σ	11 [MPa]
	84.55
	62.73
	51.82
	40.91
	19.09
	- 2.73
	- 13.64
	- 24.55
	- 46.36
	- 57.27
	- 79.09
	- 90.00

Level curves of normal stress σ_{22}



U-shaped pulse loading



without fracture



Configuration of plastic zones

Cosserat model



Level curves of plastic energy dissipation





Vladimir M. Sadovskii (ICM SB RAS, Krasnoyarsk) Dynamics of Blocky Media - Cosserat Continuum Model NP 7.1 EGU 2020-2741 19/24 07.05.2020

Numerical results

Squeezing of a medium by rotating plate





Scheme of a medium loading by a rotating plate

The solution under high shear plasticity, when $\tau_0 \to 0$ and μ_0 is sufficiently high:

$$\sigma_{21} = \sigma_{12} = 0, \quad \sigma_{11,1} = \sigma_{22,2} = 0$$
$$\mu_{31,1} + \mu_{32,2} = 0$$
$$\mu_{31} = \alpha_2 \varphi_{3,1}, \quad \mu_{32} = \alpha_2 \varphi_{3,2}$$

Hence, $\sigma_{22} = -\gamma x_1$, $\sigma_{11} = 0$, and the angle of rotation φ_3 is a harmonic function (it satisfies the Laplace equation): $\varphi_3 = -x_2 \varepsilon_0 t_0^2/(2h)$

$$u_1 = \frac{\gamma}{2} \left(b_1 \, x_1^2 + a_1 \, x_2^2 \right), \quad u_2 = -\gamma \, a_1 \, x_1 \, x_2, \quad \gamma = \frac{\varepsilon_0 \, t_0^2}{2 \, a_1 h}$$



Results of computations



In the case of high bending plasticity $\mu_0 \rightarrow 0$ and τ_0 is sufficiently high. Then the equations of plane problem of static elasticity are fulfilled with $\varphi_3 = (u_{2,1} - u_{1,2})/2$.

Numerical solution of the problem with sufficiently low yield strengths repeats the qualitative features of these solutions.



Level curves of displacement u_1



Level curves of displacement u_2





Numerical results

Results of computations



thin interlayers ($\delta = 0.1 \text{ mm}$)



thick interlayers ($\delta = 5 \text{ mm}$)



Level curves of the energy of plastic dissipation





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Level curves of the energy of plastic dissipation due to irreversible changes in curvature



Numerical results

Results of computations



thin interlayers ($\delta = 0.1 \text{ mm}$)



thick interlayers $(\delta = 5 \text{ mm})$



Level curves of couple stress μ_{31}





Level curves of couple stress μ_{32}



Conclusions



- To study wave processes in structurally inhomogeneous media, a discrete-continuous model of a blocky structure composed of elastic blocks is proposed, accounting irreversible deformation and fracture of weakened interlayers.
- An alternative approach is developed based on the Cosserat model of the orthotropic continuum, taking into account the plastic deformation of a material. Comparative analysis showed that by appropriate choosing the mechanical parameters of the Cosserat continuum, it is possible to achieve agreement on the results both on a qualitative and quantitative levels.
- The hypothesis, that the plasticization of a structurally inhomogeneous material in the whole volume at the meso-level is due to the rotations of particles is confirmed in the problem of slow squeezing of a blocky medium by a rotating plate.
- The developed computational algorithms and software can be used to test the adequacy of the formulas for calculating the parameters of the Cosserat continuum of blocky-layered structures obtained as a result of homogenization procedures.

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Many thanks for your attention and for your interest !!!

