Abstracts

Numerical solution of generalized mechanics based on a variational formulation

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(joint work with Wolfgang H. Müller)

A beam of a length in micrometer range shows a phenomenon called *size effect* that is well-observed in experiments. Classical mechanics fails to describe this phenomenon accurately. Various proposals in the literature are called with different names, viz., strain gradient theory, micropolar theory, micromorphic theory. They all have higher gradients in space, which play a role in the formulation of the theory. For the case of elasticity we present the variational formulation including second gradients in space and obtain the weak form necessary for performing numerical simulations.

1. Principle of least action in generalized mechanics

In order to obtain the weak form there are different possible approaches used in the literature. A usual way is to start with balance equations and determine the field equations describing the system. In case of classical mechanics, where we ignore electric charge and any deviation from the reference temperature, we employ the balance of linear momentum in order to calculate displacements. In this approach the balance of linear momentum is the axiom; we just start with it.

Another approach is to start axiomatically with a Lagrangean density, $\mathcal{L}$. For example, in case of classical mechanics,

$$\mathcal{L} = \mathcal{L}\big(x_\mu, \phi_A, \phi_{A,\mu}\big) \ , \tag{1}$$

states that there is a function capable of describing the system. This Lagrangean density depends on any number of coordinates, x_μ, on some primitive variables, ϕ_A, and on its first gradients, $\phi_{A,\mu}$. The generalization is now obvious: In case of generalized mechanics we include at least one more gradient of the primitive variables such that Lagrangean density in generalized mechanics becomes

$$\mathcal{L} = \mathcal{L}\big(x_\mu, \phi_A, \phi_{A,\mu}, \phi_{A,\mu\nu}\big) \ . \tag{2}$$

For orthonormal coordinates we can introduce an action functional:

$$\mathcal{A} = \int_\Omega \mathcal{L} \, \mathrm{d}\Sigma \ , \quad \mathrm{d}\Sigma = \mathrm{d}x_1 \, \mathrm{d}x_2 \ldots \mathrm{d}x_m \ . \tag{3}$$

The principle of least action asserts that this action is an invariant under a transformation of primitive variables and its derivatives. In other words, the value of action

remains the same if we apply an arbitrary transformation in $\{\phi_A, \phi_{A,\mu}, \phi_{A,\mu\nu}\}$ as $\{\phi'_A, \phi'_{A,\mu}, \phi'_{A,\mu\nu}\}$ such that

$$\begin{aligned} \delta\mathcal{A} &= 0 \ , \\ \delta\mathcal{A} &= \int_\Omega \mathcal{L}' \,\mathrm{d}\Sigma - \int_\Omega \mathcal{L} \,\mathrm{d}\Sigma \ . \end{aligned} \tag{4}$$

The prime of LAGRANGEan density has the following meaning:

$$\begin{gathered} \mathcal{L}' = \mathcal{L}\big(x_\mu, \phi'_A, \phi'_{A,\mu}, \phi'_{A,\mu\nu}\big) \ , \\ \phi'_A = \phi_A + \varepsilon\delta\phi_A \ , \quad \phi'_{A,\mu} = \phi_{A,\mu} + \varepsilon\delta\phi_{A,\mu} \ , \quad \phi'_{A,\mu\nu} = \phi_{A,\mu\nu} + \varepsilon\delta\phi_{A,\mu\nu} \ , \end{gathered} \tag{5}$$

with a small number ε the so-called *test* functions, $\delta\phi_A$, are arbitrary. We can now expand $\mathcal{L}'$,

$$\mathcal{L}' = \mathcal{L} + \frac{\partial\mathcal{L}}{\partial\phi_A}\varepsilon\delta\phi_A + \frac{\partial\mathcal{L}}{\partial\phi_{A,\mu}}\varepsilon\delta\phi_{A,\mu} + \frac{\partial\mathcal{L}}{\partial\phi_{A,\mu\nu}}\varepsilon\delta\phi_{A,\mu\nu} \ , \tag{6}$$

and obtain out of the principle of least action by dividing by the constant ε,

$$\int_\Omega \left(\frac{\partial\mathcal{L}}{\partial\phi_A}\delta\phi_A + \frac{\partial\mathcal{L}}{\partial\phi_{A,\mu}}\delta\phi_{A,\mu} + \frac{\partial\mathcal{L}}{\partial\phi_{A,\mu\nu}}\delta\phi_{A,\mu\nu}\right)\mathrm{d}\Sigma = 0 \ . \tag{7}$$

The coordinates are space, $X_i \in \mathcal{B}_0$, denoting to particles; and time, $t \in \tau$, such that the latter variational form reads

$$\begin{aligned} \int_\tau \int_{\mathcal{B}_0} \Big(&\frac{\partial\mathcal{L}}{\partial\phi_A}\delta\phi_A + \frac{\partial\mathcal{L}}{\partial\dot{\phi}_A}\delta\dot{\phi}_A + \frac{\partial\mathcal{L}}{\partial\phi_{A,i}}\delta\phi_{A,i} + \\ &+\frac{\partial\mathcal{L}}{\partial\ddot{\phi}_A}\delta\ddot{\phi}_A + \frac{\partial\mathcal{L}}{\partial\dot{\phi}_{A,i}}\delta\dot{\phi}_{A,i} + \frac{\partial\mathcal{L}}{\partial\phi_{A,ij}}\delta\phi_{A,ij}\Big)\,\mathrm{d}V\,\mathrm{d}t = 0 \ . \end{aligned} \tag{8}$$

Furthermore, for addressing boundary terms we need the redefine the action functional:

$$\mathcal{A} = \int_\tau \int_{\mathcal{B}_0} \mathcal{L}\,\mathrm{d}V\,\mathrm{d}t + \int_\tau \int_{\partial\mathcal{B}_0} W_\mathrm{s}\,\mathrm{d}A\,\mathrm{d}t + \int_\tau \int_{\partial\partial\mathcal{B}_0} W_\mathrm{e}\,\mathrm{d}\ell\,\mathrm{d}t, \tag{9}$$

since we have second gradients in primitive variables, $\partial\partial\mathcal{B}_0$ is admissible, where $\mathrm{d}\ell$ denotes a line element. We assume that W_s and W_e depend only on primitive variables in order to have a physical interpretation of the boundary terms.

2. Generating the weak form

For a numerical calculation such as by using finite element method, we necessitate the weak form following naturally from Eq. (8) after integrating by parts all the terms with a time rate in the test functions,

$$\begin{aligned} \int_{\mathcal{B}_0} \Big(&\frac{\partial\mathcal{L}}{\partial\phi_A}\delta\phi_A - \Big(\frac{\partial\mathcal{L}}{\partial\dot{\phi}_A}\Big)^{\cdot}\delta\phi_A + \frac{\partial\mathcal{L}}{\partial\phi_{A,i}}\delta\phi_{A,i} + \\ &+\Big(\frac{\partial\mathcal{L}}{\partial\ddot{\phi}_A}\Big)^{\cdot\cdot}\delta\phi_A - \Big(\frac{\partial\mathcal{L}}{\partial\dot{\phi}_{A,i}}\Big)^{\cdot}\delta\phi_{A,i} + \frac{\partial\mathcal{L}}{\partial\phi_{A,ij}}\delta\phi_{A,ij}\Big)\,\mathrm{d}V + \\ &+\int_{\partial\mathcal{B}_0} \frac{\partial W_\mathrm{s}}{\partial\phi_A}\delta\phi_A\,\mathrm{d}A + \int_{\partial\partial\mathcal{B}_0} \frac{\partial W_\mathrm{e}}{\partial\phi_A}\delta\phi_A\,\mathrm{d}\ell \ , \end{aligned} \tag{10}$$

where the boundary (in time) terms vanish. This fact can be seen as prescribing ϕ_A and $\phi^{\bullet}_A$ in the initial time, we know the values in the last two time steps by considering in a discrete in time fashion. Since we know the values the test function vanishes on the (time) boundaries. The latter integral form in Eq. (10) is called the *weak form*.

In mechanics the only primitive variable is the displacement:

$$\phi_A = u_i \ , \quad u_i = x_i - X_i \ , \tag{11}$$

which indicates the difference between the current position, x_i, and the reference position, X_i, denoting the particles. For the LAGRANGEan energy density we can employ the following function:

$$\mathcal{L} = \frac{1}{2}\rho_0 u^{\bullet}_i u^{\bullet}_i - w + \rho_0(f_i u_i + l_{ij}u_{j,i}) \ , \tag{12}$$

where the first term addresses the kinetic energy density, w is the stored energy density, the last term creates volumetric change in the displacement and its gradient. For the energy densities on the boundaries we may choose a simple approach: The energy density on the surface, $W_{\mathrm{s}} = \hat{t}_i u_i$, gets use of a traction vector, $\hat{t}_i$, as the force per area; since a physical interpretation is difficult we may set the energy on the line as being zero, $W_{\mathrm{e}} = 0$. Now by inserting the energies on the boundary and lines into the weak form and after using EULER backwards time discretization with a finite element method in space, the weak form for generalized mechanics reads

$$\begin{aligned}\mathrm{Form} = \sum_{n=1}^{\mathrm{ele.}} \int_{E^n} \Big(&\rho_0 f_i \delta u_i - \rho_0 \frac{u_i - 2u_i^0 + u_i^{00}}{\Delta t \Delta t}\delta u_i - \frac{\partial w}{\partial u_{i,j}}\delta u_{i,j} + \rho_0 l_{ji}\delta u_{i,j} - \\ &- \frac{1}{\Delta t \Delta t}\Big(\frac{\partial w}{\partial u_{i,j}} - 2\frac{\partial w^0}{\partial u^0_{i,j}} + \frac{\partial w^{00}}{\partial u^{00}_{i,j}}\Big)\delta u_{i,j} - \frac{\partial w}{\partial u_{i,jk}}\delta u_{i,jk}\Big) \,\mathrm{d}V + \int_{\partial \mathcal{B}_0} \hat{t}_i \delta u_i \,\mathrm{d}A \ ,\end{aligned} \tag{13}$$

with

$$\begin{aligned} w^0 = w(E^0_{ij}, E^0_{ij,k}) \ , \quad w^{00} = w(E^{00}_{ij}, E^{00}_{ij,k}) \ , \\ E^0_{ij} = \frac{1}{2}u^0_{k,i}u^0_{k,j} + u^0_{(i,j)} \ , \quad E^{00}_{ij} = \frac{1}{2}u^{00}_{k,i}u^{00}_{k,j} + u^{00}_{(i,j)} \ . \end{aligned} \tag{14}$$

For a successful implementation we only need an adequate definition of the stored energy density. Depending on this energy definition one can construct different theories existing in the literature. The simplest choice is quadratic in strain and strain gradients:

$$w = w(E_{ij}, E_{ij,k}) = E_{ij}C_{ijkl}E_{kl} + E_{ij,k}D_{ijklmn}E_{lm,n} + E_{ij}G_{ijklm}E_{kl,m} \ , \tag{15}$$

for a homogeneous material, where the strain can be a nonlinear measure:

$$E_{ij} = \frac{1}{2}u_{k,i}u_{k,j} + u_{(i,j)} \ . \tag{16}$$

We refer to [1] or [2] for a concrete representation of the coefficients, C_{ijkl}, D_{ijklmn}, G_{ijklm}, for isotropic materials.

By using the weak form in Eq. (13) we can implement and solve any particular problem with strain gradient elasticity. We recall that the weak form has been taken out from a variational formulation. This formulation seems to be more beneficial for a generalization since the only way to generalize the LAGRANGEan density relies on adding one more gradients of primitive variables.

References

[1] F. dell'Isola, G. Sciarra, S. Vidoli, *Generalized Hooke's law for isotropic second gradient materials*, Proceedings of the Royal Society A: Mathematical, Physical and Engineering Science, **465** (2009), 2177–2196.

[2] B. E. Abali, W. H. Müller, V. A. Eremeyev, *Strain gradient elasticity with geometric nonlinearities and its computational evaluation*, Mechanics of Advanced Materials and Modern Processes, **1**(1) (2015), 1–11.

Calculation of stress field of a disconnection

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(joint work with Chiqun Zhang)

We demonstrate a method for mathematically representing a disconnection defect in a grain boundary

(1) as a composite of a disclination dipole and a slip dislocation and
(2) by a dislocation whose Burgers vector is the sum of the effective Burgers vector of the disclination dipole and the slip dislocation.

We then compute the stress and energy density fields of these two configurations and compare them. The calculations are done by a finite element implementation of a novel theory of combined dislocations and generalized disclination defects [1].

References

[1] A. Acharya, C. Fressengeas, *Continuum mechanics of the interaction of phase boundaries and dislocations in solids*, G.-Q.G. Chen et al. (eds.), Differential Geometry and Continuum Mechanics, Springer Proceedings in Mathematics and Statistics, **137** (2015), 123–164.

Line defect dynamics and solid mechanics

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(joint work with Chiqun Zhang, Xiaohan Zhang)

We describe a model of dislocation dynamics in a Pde-setting capable of representing motion of individual dislocations in the presence of inertia and finite deformation effects. We compare our results with molecular dynamic simulations showing supersonic dislocation motion. Our careful computations show an apparent Peierls stress effect in a translationally-invariant Pde-model that demands analytical substantiation or falsification. We also demonstrate calculations of coupled dislocation and disclination fields representing penta-twin configurations observed in nano-crystalline materials (wires).