Influence of the discrete on mathematical models for continuous mechanics and rarefied gas for great gradients

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Abstract

This paper presents a sample of the deep and multiple interplay between discrete and continuous behaviors and corresponding models in mechanics. There are influence of an angular momentum in classical and quantum cases, non-local and non-space mechanics, the conditions of their application. Influence of an angular momentum received from Boltzmann equation and phenomenological, for solid is from another interpretation of classical theory. The non-local effects are investigated by the distribution function in classical case and one-particle matrix of density in quantum case. Peculiarities of these processes were analysed for gas and solids.

Keywords: angular momentum, conservation laws, nonsymmetrical stress tensor, Boltzmann equations, Chapman-Enskog method, conjugate problem the Navie-Stokes, the molecular dynamics method.

1 Introduction

There are several theories that clarify the classical conservation laws of continuum mechanics and kinetic theory. The paper considers two types of effects: nonlocal effects and dispersion, ie examines the impact of non-locality in time and space and the influence of angular momentum. Influence of sampling difference equations representation is not considered. Each effect is considered separately. On the role of the latter in the solid indicate the experimental data obtained in Tomsk (V.E. Panin Group) and Perm (group V.P. Matveenko) [1, 2], experiments with nanofilms, in liquid – study of a plume current in a gas – observation astrophysicists.

Previously, the role of angular momentum indicated L.L. Landau, S. de Groot, P. Mazur, I. Dyarmati, I. Prigogine, L.I. Sedov, V.V. Struminskii, A.A. Ilyushin, A.Y. Ishlinsky, D.D. Ivlev et al. Most developed in this direction moment theory of elasticity (R.D. Mindlin, V.A. Palma, A.G. Gorshkov, E.I. Starovoytov, A.V. Yarovoy, V. Levin, S.E. Kanaun, E.L. Aero, P.A. Zhilin etc.). It was assumed that these effects can be important for the structural particles. Delay observed in experiments with shock waves in a gas (rarefied gas). Discussion of the role of delay in the theory was performed in [3, 4]. Now the angular momentum of inclusion in the theory is achieved by selecting an additional term proportional to the square of the length (similar theories brothers E. Cosserat, F. Cosserat). Typically, the contribution angular momentum is ignored on the grounds that the bulk order of magnitude smaller surface. Due to significant complications equations describing these processes, it is necessary to know the possibilities of application of each of the models. Currently flows in the elementary volume considered normal to the surface, thus only the movement along the stream, although the volume element may be involved in a circular motion. Not considered contribution to the density of self-diffusion, thermal diffusion, pressure diffusion. By rotation of the elementary volume flow density across the border changes by $\frac{d(\rho u)}{dr} \cdot (r' - r) + \cdots$. The contribution of other components is small, taking into account the smallness of the volume and the absence of rotation axis. In constructing the theory is now implicitly assumed that the axis of inertia always passes through the point of elementary volume. In the second transition to the classical theory of conservation laws is accomplished by using the density sum of delta functions on the difference $(x_i - x)$, similar to line up for the conservation laws of momentum and energy. For a point of inertia axis selection is not important as for the elementary volume is essential. Thus, the transition from a discrete medium and back is carried out without taking into account the spatial distribution of physical quantities, static point. Classical and quantum theory built on a single algorithm. Partially these issues are discussed in B.N. Chetverushkin, T.G. Elizarova [5, 6] and other modern continuum mechanics takes as its basis the conditions of equilibrium of forces. This leads to the symmetry of the stress tensor and disruption "continuity" of the environment. After we have received clarification unbalanced stress tensor. Degree of asymmetry of the tensor is determined from the law of conservation of angular forces derived from the law of conservation of angular momentum. In this approach does not require a new permanent. All parameters are already present in the equations. Equations for gas found from the modified Boltzmann equation and of the phenomenological theory. New equations with the inclusion of angular momentum and cross streams contain only two dimensionless parameters: Reynolds and Prandtl number. Additional issues arise when writing communication tensors stress and strain rate. The usual assumption of proportionality becomes invalid because of the asymmetry of the stress tensor. The basic direction relations are preserved (τ_{xy}), the second direction are required additives. Under the hypothesis of proportionality τ_{yx} velocity component $\tau_{yx} = \frac{\partial \nu}{\partial x}(y' - y)$; estimates and because of the small sensitivity of the experimental data to the form closing relations, you can leave the old closure relations. Thus, in this paper we propose one of the possible closure relations. Established causes of delay and the need for the equations of motion, based on estimates of the time derivatives and coordinate with the definitions of derivatives and the mean free path of the molecules, the time between collisions. Set process priorities in different situations. We begin with a discussion of our modified equations, we give a new interpretation of the classical equations of a continuous medium. Accounting for a continuous medium angular momentum and giving some examples were made [7, 9].

2 Analysis of mathematical models

Consider the results of the analysis of mathematical models used in continuum mechanics and quantum mechanics to derive the equations of a continuous medium. Traditional models based on the record describing the conservation laws in the form of integral conservation laws for the elementary volume and subsequent aspiration volume size to zero. Replacement extended volume distribution of points leads to the neglect of all its twists and turns, since by definition Material point (particle) – simple physical models in mechanics – the ideal body size, and rotation may be neglected. You can also body sizes considered infinitely small compared with other dimensions or distances within the assumptions of the problem considered. A material point in space is defined as the position of the geometric point. Almost at the material point understand having a mass body size, shape and rotation may be neglected when solving this problem [10, 11]. Weight material point assumed to be constant in time and independent of any features of its movement and interaction with other bodies. $n * (x) = \sum_i \delta(x_i(t) - x)$, whence $\frac{\partial n(x)}{\partial t} = \sum_i \dot{\delta}(x_i(t) - x) = \sum_i \dot{x} \cdot \bigtriangledown_i \delta(x_i(t) - x)$, $\frac{\partial n(x)}{\partial t} = -\operatorname{div}\mathbf{j}(\mathbf{x})$. Here x, t – coordinate and time, $\mathbf{j}(x)$ – flow, $\mathbf{p}(x)$ – pressure,

$\mathbf{j}(x) = \sum_i \frac{\mathbf{p_i}}{m}\delta(x_i - x)$, $\mathbf{p}(x) = m\mathbf{j}(x) = \sum_i \mathbf{p_i}\delta(x_i - x)$, $\int \mathbf{p}(x)\,dx = \sum \mathbf{p_i} = \mathbf{P}$. In quantum theory, particles are also treated with both points. In the study are restricted to closed systems. Mainly considered pairwise interactions or system of noninteracting particles. When considering several particles simultaneously additive extensive values limited quantities if no charged particles. In fact, each particle is far enough away from each other, the field within the range of the interaction of molecules uniform. In the analysis of the interaction of charged particles the presence of all the particles is taken into account through the potential to include the interaction of electrons and ions or through a hypothetical distribution function or solution of the Poisson equation with the charge distribution around the core particles (computational methods particle-particle, particle mesh) [12]. In turn, this implies a violation of symmetry.

In Newton's second law are all the forces acting on the body. In fact, very important characteristics are the nature and arrangement of the particles associated action angular momentum particularly important action is the moment at large gradients in the presence of charged particles. Action points clearly evident when considering the process of interaction between two particles in classical mechanics. In quantum mechanics separately makrolaw conservation of angular momentum is not issued. It is obtained by multiplying the vector equation for the amount of traffic on the vector r [13].

$$\frac{dJ_0}{dt} = -\nabla \cdot L, \text{ but this is not true,since } \quad \frac{d(r \times \nu)}{dt} \neq r \times \frac{d\nu}{dt}.$$

Partially account angular momentum of occurs in solving the molecular dynamics method. Causality principle and the principle of the finite velocity of propagation of interactions require that the differential equations describing the fundamental fields belonged to the hyperbolic type, but for the wave function, we have an equation of first order in time. Newton's equation is an equation of the second order. Based on the Hamiltonian formalism, we obtain the Newton equation and the quantum and classical cases. In quantum mechanics, we postulate as a particular solution of the wave function, which can only make sense for very high frequencies, as this energy is ignored in the mass of the particle ($E = h\nu$) [14, 15].

$i\frac{d\Psi}{dt} = \hat{L}\Psi$, $h\hat{L}$ – the Hamiltonian function or $i\, h\frac{d\Psi}{dt} = \hat{H}\ \Psi$, operator of density is $\rho(x', x) = \int \Psi^*(q, x')\Psi(q, x)\,dq$, the Wigner function of distribution

$$f_{lm,lm'}(r,p,t) = \frac{1}{(\pi h)^3}\int \exp\frac{2i\mathbf{p}\cdot R}{h}\rho\left(\begin{matrix} lm \\ r+R \end{matrix}\middle|\begin{matrix} lm' \\ r-R \end{matrix}\right) d^3R.$$

In continuum mechanics equations were derived previously given angular momentum [14]. From this consideration the need to consider the time and quantum mechanics [16, 18].

To do this, add the term corresponding to the operator instead of the moment $\xi_i \cdot \frac{\partial}{\partial x_i}\left(x_j\frac{\partial f_N}{\partial t}\right)$.

3 Interrupt of interaction for particles

All interactions occur at a finite rate. Consider the action of a finite values of the propagation velocity of the interacting particles in the kinetic theory.The mean free path of the molecules i-th group of molecules with respect to the j-th group is in classical mechanics $\lambda_{ij} = \frac{\xi_i}{\sigma_{ij} n_j g_{ij}}$,

$\bar{\lambda} = \frac{\sum_i^k \xi_i n_i}{\frac{1}{2}\sum_{i,j=1}^k \sigma_{ij} n_i n_j g_{ij}}$ – mean free path of the molecules,

$\bar{g} = \frac{1}{2n^2}\sum_{i,j=1}^k n_i n_j g_{ij}$ – the average velocity of the molecules. Mean time $\bar{\tau} = \frac{\bar{\lambda}}{\bar{g}}$.

With that said, the Boltzmann equation can be written as

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \mathbf{c}_i \cdot [\frac{\partial f}{\partial \underline{r}_i}] + \mathbf{c}_i \cdot \frac{\partial}{\partial \mathbf{r}_i}[r_{ij}\frac{\partial f}{\partial r_{ij}}] - \frac{F}{m}\frac{\partial f}{\partial \mathbf{c}_i} = I,$$

$$\Delta^- = dt\, d\underline{x}\, d\underline{\xi}\, f(t,\underline{x},\underline{\xi}) \int \left[f_1(t,\underline{x},\underline{\xi}) + O\left(\Delta t \underline{\xi} \frac{\partial f_1}{\partial x}\right)\right] gb\, db\varepsilon\, d\underline{\xi_1},$$

$$\Delta^+ = dt\, d\underline{x}\, d\underline{\xi}' \int \left[f(t,\underline{x},\underline{\xi}')f(t,\underline{x},\underline{\xi_1}') + O\left(\Delta t \underline{\xi} \frac{\partial f}{\partial x}\right)\right] g'b'\, db'\, d\varepsilon'\, d\underline{\xi_1},$$

$$I = \Delta^- - \Delta^+.$$

In the case of a finite path length

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \bar{\tau}\frac{\partial^2 f}{\partial^2 t} + \mathbf{c}_i \cdot \frac{\partial f}{\partial \mathbf{r}_i} + \mathbf{c}_i \cdot \frac{\partial}{\partial \mathbf{r}_i} r_{ij} \frac{\partial f}{\partial \mathbf{r}_{ij}} - \frac{\mathbf{F}}{m}\frac{\partial f}{\partial \mathbf{c}_i} = I.$$

Here are without the angular momentum

$$\frac{\partial f}{\partial t} \leftrightarrow \frac{\partial f}{\partial t} + \bar{\tau}\frac{\partial^2 f}{\partial^2 t},$$

$$f'(t,x,\xi') \leftrightarrow f'(t,x,\xi'),$$

$$f(t,x,\xi) \leftrightarrow f(t+\bar{\tau}, x+\bar{\lambda}, \xi) \leftrightarrow f(t,x,\xi) + \bar{\tau}\frac{\partial f}{\partial t} + \bar{\lambda}\frac{\partial f}{\partial x} + \cdots,$$

$$f_1(t,x,\xi_1) \leftrightarrow f_1(t+\bar{\tau}, x+\bar{\lambda}, \xi_1) \leftrightarrow f_1(t,x,\xi_1) + \bar{\tau}\frac{\partial f_1}{\partial t} + \bar{\lambda}\frac{\partial f_1}{\partial x} + \cdots.$$

Then we have

$$f'f_1' - ff_1 \leftrightarrow f'f_1' - ff_1 + \tau\left(\frac{\partial f}{\partial t} f_1 + f\frac{\partial f_1}{\partial t}\right) + \bar{\lambda}(\ldots).$$

We can only build new makroequations. However, it should be noted that the collision integral terms give new value of the first order, which leads to the magnitude of the second order overall. It seems that in numerical calculations at each step is better to use the current speed.

4 Conclusion

Accounting for the time lag and the law of conservation of angular momentum conservation allows to specify makrolaws continuum mechanics, to calculate the contribution of these effects, and track their impact.

References

[1] *V.E. Panin, U.V. Grinyaev, A.A. Panin,* Actual problems of solid mechanics. Physical Mesomechanics. Vol.10, N. 5, 2007. P. 5-10.

[2] *V.V. Korepanov, M.A. Kuleshov, V.P. Matveenko, I.N. Shardanov,* Analytical and numerical solutions of static and dynamic problems of asymmetric elasticity. Vol.10, N. 5, 2007. P. 77-90.

[3] *D.N. Zubarev,* Nonequilibrium statistical thermodynamics, Moscow: Nauka, 1971. 414 p.

[4] *B.V. Alekseev,* Mathematical kinetics reacting gases. Nauka, 1982. 420 p.

[5] *B.N. Chetverushkin,* Kinetic schemes and quasi-gasdynamic system of equations. M. MAKSPress, 2004. 332 p.

[6] *T.G. Elizarova,* Quasi-gasdynamic equations and methods for viscous flow. M: Science mir. 2007. P. 352.

[7] *E.V. Prozorova,* The effect of dispersion in nonequilibrium continuum mechanics problems environment, Moscow State University, Electronic Journal "Physico-chemical kinetics in gas dynamics", 2012. T. 13,URL: http://www.chemphys.edu.ru/pdf/2012-10-30-001.pdf

[8] *Evelina V. Prozorova, Aleksandr Shadrin* Influence dispersion in gas and solid for moving body. 5th European Conference for Aeronautics and Space Sciences 1-5 July 2013 / Holiday Inn Munich City Centre, Munich, Germany.

[9] *E.V.Prozorova,* About models of continuum mechanics. International Scientific IFNA-ANS Journal "Problems of nonlinear analysis in engineering systems", N. 1 (39), v.19, 2013. P. 45-57.

[10] *L.D. Landau, E.M. Lifshitz,* Theory of Fields. - 8th Edition, stereotypical. - M.: Fizmatlit, 2001. - 534 p. - ("Theoretical Physics", Volume II). - ISBN 5-9221-0056-4

[11] *V.P. Pavlov,* FIELD PHYSICAL // Physical encyclopedia / D.M. Alekseev, A.M. Baldin, A.M. Bonch, Borovik- Romanov, B.K. Vainshtein, S.V. Vonsovskii, A.V.Gaponov - Sin, S.S. Gerstein, Gurevich, A.A. Gusev, M.A. El'yashevich, M.E. Jabotinsky, Zubarev, B.B. Kadomtsev, Shapiro, D. Shirkov, under Society. Ed. Prokhorov - Moscow: Soviet Encyclopedia, 1994. - T. 4. - 704 p. - 40 000 copies.

[12] *X.W. Zhou a, H.N.G. Wadleyb, D.X. Wang,* Transient hole formation during the growth of thin metal oxide layers. Computational Materials Science 39, 2007. P. 794-802.

[13] *Fertsiger J., G. Kaper,* Mathematical theory of transport processes in gases. Verlag, 1976. 554 p.

[14] *Enrico Fermi,* Notes on quantum mechanics. The University of Chicago, 1960.

[15] *Eugene P. Wigner,* Symmetries and reflections. Indiana university press Bloomington-London, 1970.

[16] *C. Cercignani,* Mathematical methods in kinetic theory Macmillan, 1969. 254 p.

[17] *J.O. Hirschfelder, C.F. Curtiss, R.B. Bird,* The molecular theory of gases and liquids. New-York, 1954.

[18] *M.N. Kogan,* The dynamics of a dilute gas. Nauka, 1967. 440 p.

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