ANOMALOUS DIFFUSION EQUATION AND DIFFUSIVE STRESSES

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Abstract. Essentials of the Riemann-Liouville fractional calculus are recalled. Non-local generalizations of the Fourier law of the classical theory of heat conduction relating the heat flux vector to the temperature gradient and of the Fick law of the classical theory of diffusion relating the matter flux vector to the concentration gradient lead to nonclassical theories. The time-nonlocal dependence between the flux vectors and corresponding gradients with "long-tale" power kernel can be interpreted in terms of fractional integrals and derivatives and yields the time-fractional diffusion equation.

1. Essentials of the Riemann-Liouville fractional calculus

In this section we recall the main ideas of fractional calculus (see [1, 2], among others). It is common knowledge that integrating by parts n-1 times the calculation of the n-fold primitive of a function f(t) can be reduced to the calculation of a single integral of the convolution type

$$I^{n} f(t) = \frac{1}{(n-1)!} \int_{0}^{t} (t-\tau)^{n-1} f(\tau) d\tau, \tag{1}$$

where n is a positive integer.

The Riemann–Liouville fractional integral is introduced as a natural generalization of the convolution type form (1):

$$I^{\alpha}f(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t - \tau)^{\alpha - 1} f(\tau) d\tau, \qquad \alpha > 0,$$
 (2)

where $\Gamma(\alpha)$ is the gamma function.

The Riemann–Liouville derivative of the fractional order α is defined as left-inverse to I^{α}

$$D_{RL}^{\alpha}f(t) = D^{n}I^{n-\alpha}f(t) \tag{3}$$

and for its Laplace transform rule requires the knowledge of the initial values of the fractional integral $I^{n-\alpha}f(t)$ and its derivatives of the order $k=1,2,\ldots,n-1$.

An alternative definition of the fractional derivative was proposed by Caputo [3]:

$$D_C^{\alpha}f(t) = I^{n-\alpha}D^n f(t). \tag{4}$$

For its Laplace transform rule the Caputo fractional derivative requires the knowledge of the initial values of the function f(t) and its integer derivatives of order k = 1, 2, ..., n - 1.

The Caputo fractional derivative is a regularization in the time origin for the Riemann–Liouville fractional derivative by incorporating the relevant initial conditions. The major utility of Caputo fractional derivative is caused by the treatment of differential equations of fractional order for physical applications, where the initial conditions are usually expressed in terms of a given function and its derivatives of integer (not fractional) order, even if the govering equation is of fractional order [4].

2. Nonlocal generalizations of the Fick and Fourier laws

The classical theory of diffusion is based on the Fick law

$$\mathbf{J} = -\kappa \operatorname{grad} c \tag{5}$$

relating the matter flux vector \mathbf{J} to the concentration gradient, where κ is the diffusion conductivity. In combination with the balance equation for mass the Fick law leads to the classical diffusion equation

$$\frac{\partial c}{\partial t} = a \,\Delta \,c,\tag{6}$$

where a is the diffusivity coefficient.

The classical theory of heat conduction is based on the Fourier law

$$\mathbf{q} = -k \operatorname{grad} T \tag{7}$$

relating the heat flux vector \mathbf{q} to the temperature gradient, where k is the thermal conductivity of a solid. In combination with the law of conservation of energy, this equation leads to the parabolic heat conduction equation

$$\frac{\partial T}{\partial t} = a_{\rm T} \Delta T,\tag{8}$$

where $a_{\rm T}$ is the thermal diffusivity coefficient, t is time, Δ is the Laplace operator.

During the past three decades, nonclassical theories, in which the Fourier law and the Fick law as well as the heat conduction equation and the diffusion equation were replaced by more general equations, have been proposed. Some of these theories were formulated in terms of the theory of heat conduction, other in terms of the diffusion theory.

In time-nonlocal theories the Fourier law is generalized to integral dependence between the heat flux vector and the temperature gradient

$$\mathbf{q}(t) = -k \int_0^t K(t - \tau) \operatorname{grad} T(\tau) d\tau$$
 (9)

or in terms of diffusion

$$\mathbf{J}(t) = -\kappa \int_0^t K(t - \tau) \operatorname{grad} c(\tau) \, d\tau. \tag{10}$$

The time-nonlocal dependence between the flux vectors and corresponding gradients with "long-tale" power kernel can be interpreted in terms of fractional integrals and derivatives and yields the time-fractional diffusion (or heat conduction) equation

$$\frac{\partial^{\alpha} c}{\partial t^{\alpha}} = a \,\Delta \,c, \qquad 0 < \alpha < 2. \tag{11}$$

This equation is usually referred to "anomalous diffusion". Other terms used in this context are: "anomalous transport", "fractional diffusion", "paradoxal diffusion", "strange kinetics".

Various types of anomalous transport can be distinguished. The limiting case $\alpha=0$ corresponding to the Helmholtz equation is associated with localized diffusion. The slow diffusion regime is characterized by the value $0<\alpha<1$. The power-law tails make it possible to have very long waiting times, and particles move slower than in the ordinary diffusion which corresponds to $\alpha=1$. In the fast diffusion regime $(1<\alpha<2)$ it is possible to have very long jumps, and particles move faster than in the ordinary diffusion. The limiting case $\alpha=2$ corresponding to the wave equation is known as ballistic diffusion.

Equation (11) is a mathematical model of important physical phenomena ranging from amorphous, colloid, glassy and porous materials through fractals, percolation clusters, random and disordered media to comb structures, dielectrics and semiconductors, polymers and biological systems.

3. Theory of diffusive stresses based on anomalous diffusion equation

A quasi-static uncoupled theory of diffusive (or thermal) stresses based on Eq. (11) was proposed by the author [5–7]. A quasi-static uncoupled theory of diffusive stress is governed by the equilibrium equation in terms of displacements

$$\mu \Delta \mathbf{u} + (\lambda + \mu) \operatorname{grad} \operatorname{div} \mathbf{u} = \beta_c K_c \operatorname{grad} c,$$
 (12)

the stress-strain-concentration relation

$$\sigma = 2\mu \mathbf{e} + (\lambda \operatorname{tr} \mathbf{e} - \beta_c K_c c) \mathbf{I}, \tag{13}$$

and the time-fractional diffusion equation

$$\frac{\partial^{\alpha} c}{\partial t^{\alpha}} = a \,\Delta \, c + Q, \qquad 0 \le \alpha \le 2, \tag{14}$$

where **u** is the displacement vector, $\boldsymbol{\sigma}$ the stress tensor, **e** the linear strain tensor, c the concentration, Q the mass source, a the diffusivity coefficient, λ and μ are Lamé constants, $K_c = \lambda + 2\mu/3$, β_c is the diffusion coefficient of volumetric expansion, **I** denotes the unit tensor.

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