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Fractional vector calculus for fractional advection–dispersion ☆

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Abstract

We develop the basic tools of fractional vector calculus including a fractional derivative version of the gradient, divergence, and curl, and a fractional divergence theorem and Stokes theorem. These basic tools are then applied to provide a physical explanation for the fractional advection–dispersion equation for flow in heterogeneous porous media.

Keywords: Functional derivatives; Advection–dispersion equation; Porous media flow; Transport

1. Introduction

Fractional derivatives are almost as old as their more familiar integer-order counterparts [1–4]. Fractional derivatives have recently been applied to many problems in physics [5–18], finance [15,19–22], and hydrology [23–28]. Hilfer [29] collects a variety of applications to polymer physics, biophysics and thermodynamics. Zaslavsky [30] reviews the relation between fractional models and chaotic dynamics. Metzler and Klafter [31,32] survey the connections to random walks with heavy tail jumps and/or waiting times. Briefly, fractional derivatives are used to model anomalous diffusion or dispersion, where a particle plume spreads at a rate inconsistent with the classical model, and the plume may be asymmetric. Sokolov and Klafter [33] give a nice, brief overview of anomalous diffusion in physics. When a fractional derivative replaces the second derivative in the diffusion/dispersion equation, it leads to enhanced diffusion (also called super-diffusion). This super-diffusion equates to a heavy tailed random walk model for particle jumps, where occasional large jumps dominate the more common smaller jumps. A fractional time derivative leads to sub-diffusion, where a cloud of particles spreads slower than the classical $t^{1/2}$ rate. This is connected with a random walk model where the random waiting time between particle jumps has a heavy probability tail, causing a small number of very long sticking times to slow the diffusion.

In ground water, a plume of tracer particles carried along with the flow (advection) spreads out due to velocity contrasts caused by the intervening porous medium (dispersion), see for example Bear [34]. The

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classical advection–dispersion equation $\partial\rho/\partial t = -v\partial\rho/\partial x + c\partial^2\rho/\partial x^2$ for the particle density ρ at location x at time t is mathematically identical to the diffusion equation with drift, and furthermore, the same random walk model underlies them both. The mean jump size determines the velocity v of the (advective) drift, and deviations from the mean govern the spread, converging to a bell-shaped plume due to the Central Limit Theorem. This connection between diffusion and random walks is due to Einstein [35]. Random waiting times do not affect the eventual shape as long as the waiting times have a finite mean, they simply retard the average velocity by an amount equal to the mean waiting time. This is a simple consequence of the Renewal Theorem [36, Chapter XI]. Sokolov and Klafter [37] discuss Einstein's result and its limitations. When particle jumps Y have a heavy tail $P(|Y|>r) \approx r^{-\alpha}$ with $0<\alpha<2$, the central limit theorem fails because the variance of the particle jumps is infinite. In this case, an extended central limit theorem due to Lévy [38] applies to show that the resulting plume follows a stable density curve, the solution to a fractional diffusion/dispersion equation $\partial\rho/\partial t = -v\partial\rho/\partial x + c\partial^\alpha\rho/\partial x^\alpha$, see for example [8,11,39]. This plume has skewness and a power-law leading edge. In the continuous time random walk (CTRW) model, a random waiting time T precedes each particle jump. For heavy tailed waiting times $P(T>t) \approx t^{-\beta}$ with $0<\beta<1$, the mean waiting time is infinite, so the renewal theorem does not apply. The resulting sub-diffusion equation $\partial^\beta\rho/\partial t^\beta = -v\partial\rho/\partial x + c\partial^2\rho/\partial x^2$ describes a plume that spreads away from its center of mass at the rate $t^{\beta/2}$, slower than classical diffusion [14,17,40]. The sub-diffusive stochastic model involves subordination, replacing the time variable t by an inverse stable Lévy process $E(t)$ that grows more slowly [11,41].

The classical diffusion equation (or heat equation) and its Gaussian solution existed long before Einstein established a connection with random walks. Anomalous diffusion equations, on the other hand, were originally developed from stochastic random walk models. A deterministic Eulerian derivation of the scalar fractional advection–dispersion equation [27] illuminates the manner in which fractional derivatives code for power-law velocity variations, and suggests a connection with heterogeneous/random media [42]. This paper extends that approach to the vector equation. First, we develop the basic tools of fractional vector calculus including a fractional derivative version of the gradient, divergence, and curl, and a fractional divergence theorem and Stokes theorem. Then these basic tools are applied to provide an Eulerian derivation of the fractional advection–dispersion equation for flow in heterogeneous porous media.

2. Fractional advection–dispersion equation

We begin by briefly recounting the classical derivation of the advection–dispersion equation (see, e.g., Ref. [34]), to establish notation and focus the discussion. Let $\rho = \rho(\boldsymbol{x}, t)$ represent particle mass density of a contaminant in some fluid at a point $\boldsymbol{x}$ in d-dimensional space at time t. The classical dispersion equation is the result of two separate equations. Let $\boldsymbol{v}$ denote the constant average velocity of contaminant particles (which need not equal the fluid velocity). Fick's Law states that the flux

$$\boldsymbol{V} = \boldsymbol{v}\rho - Q\nabla\rho \tag{1}$$

is the vector rate at which mass is transported through a unit area ΔA. Here Q is a symmetric $d \times d$ matrix, or 2-tensor, called the dispersion tensor, which codes the ability of the contaminant to disperse through the intervening porous medium. For the purposes of this discussion, it is interesting to note that the dispersion matrix Q can be written in the form

$$Q = \int_{\|\boldsymbol{\theta}\|=1} \boldsymbol{\theta}\boldsymbol{\theta}' M(\mathrm{d}\boldsymbol{\theta}) \tag{2}$$

where $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_d)'$ is a unit column vector and $M(\mathrm{d}\boldsymbol{\theta})$ is a positive finite measure on the set of unit vectors, which we call the mixing measure. Here $\boldsymbol{\theta}\boldsymbol{\theta}'$ is the outer product, a $d \times d$ matrix, as opposed to the inner product $\boldsymbol{\theta} \cdot \boldsymbol{\theta} = \boldsymbol{\theta}'\boldsymbol{\theta}$, which is a scalar. The ij entry of the matrix Q is then given by $q_{ij} = \int \theta_i\theta_j M(\mathrm{d}\boldsymbol{\theta})$, and then the symmetry $q_{ij} = q_{ji}$ is apparent. The mixing measure $M(\mathrm{d}\boldsymbol{\theta}) = m(\boldsymbol{\theta})\,\mathrm{d}\boldsymbol{\theta}$ codes the relative strength of the dispersion in each radial direction. For a homogeneous medium, $m(\boldsymbol{\theta})$ is constant, and the matrix $Q = cI$ a scalar multiple of the identity, where $c = \int \theta_i^2 M(\mathrm{d}\boldsymbol{\theta})$. The advection–dispersion equation results from combining Fick's Law (1) with a continuity equation (conservation of mass)

$$\frac{\partial \rho}{\partial t} = -\mathrm{div}\, \boldsymbol{V} \tag{3}$$

where the divergence $\mathrm{div}\, \boldsymbol{V} = \nabla \cdot \boldsymbol{V}$ is a scalar quantity representing the net outflow of mass concentration at each point in space. Substituting (1) into (3) yields the advection–dispersion equation

$$\frac{\partial \rho}{\partial t} = -\boldsymbol{v} \cdot \nabla \rho + \nabla \cdot Q \nabla \rho \tag{4}$$

that models the flow and spread of contaminant particles carried by a fluid through a porous medium. The spreading of a contaminant plume in this model is due to mechanical dispersion, the velocity variations imposed by the tortuosity of paths the particles must take to navigate around obstacles in the porous medium.

For any scalar field $f(\boldsymbol{x})$ define the Fourier transform $\hat{f}(\boldsymbol{k}) = \int \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$ and recall that the gradient operator ∇ has Fourier symbol $(\mathrm{i}\boldsymbol{k})$, meaning that $\nabla f(\boldsymbol{x})$ has Fourier transform $(\mathrm{i}\boldsymbol{k})\hat{f}(\boldsymbol{k})$. The point source solution to (4) is computed by taking Fourier transforms to obtain

$$\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = -\boldsymbol{v} \cdot (\mathrm{i}\boldsymbol{k})\hat{\rho} + (\mathrm{i}\boldsymbol{k}) \cdot Q(\mathrm{i}\boldsymbol{k})\hat{\rho}, \quad \hat{\rho}(\boldsymbol{k}, t=0) \equiv 1 \tag{5}$$

which leads to the Fourier solution

$$\hat{\rho} = \exp(-\boldsymbol{v} \cdot (\mathrm{i}\boldsymbol{k})t + (\mathrm{i}\boldsymbol{k}) \cdot Q(\mathrm{i}\boldsymbol{k})t) \tag{6}$$

that inverts to a multivariate Gaussian density with mean $\boldsymbol{v}t$ and covariance matrix $2Qt$. The Gaussian or normal density is consistent with the random walk model for dispersion, where the sum of a large number of particle jumps converges to a normal limit in view of the central limit theorem of statistics. The dispersion matrix Q controls the shape of the evolving plume, an ellipse whose principal axes are the eigenvectors of Q. A simple scaling argument shows that the plume spreads away from its center of mass at the rate $t^{1/2}$, consistent with the fact that the variance of particle displacements grows linearly with time.

The fractional advection–dispersion equation

$$\frac{\partial \rho}{\partial t} = -\boldsymbol{v} \cdot \nabla \rho(\boldsymbol{x}, t) + c\mathbb{D}_M^\alpha \rho(\boldsymbol{x}, t) \tag{7}$$

was introduced in [43] to model anomalous dispersion in ground water flow. The diffusivity constant $c > 0$ and the fractional derivative operator $\mathbb{D}_M^\alpha \rho$ is defined in terms of its Fourier transform

$$\int \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} \mathbb{D}_M^\alpha \rho(\boldsymbol{x}, t)\,\mathrm{d}\boldsymbol{x} = \int_{\|\boldsymbol{\theta}\|=1} (\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{\theta})^\alpha \hat{\rho}(\boldsymbol{k}, t) M(\mathrm{d}\boldsymbol{\theta}) \tag{8}$$

where $1 < \alpha \leqslant 2$ and $M(\mathrm{d}\boldsymbol{\theta})$ is the mixing measure, as in Eq. (2). If $\alpha = 2$, then $\mathbb{D}_M^\alpha \rho = \nabla \cdot Q \nabla \rho$ where the matrix Q is given by (2), and if $\alpha < 2$ the point source solution to (7) is a family of multi-variable stable densities $\rho(\boldsymbol{x}, t)$ that spread away from their center of mass $\boldsymbol{v}t$ like $t^{1/\alpha}$, indicating a super-diffusion. If $M(\mathrm{d}\boldsymbol{\theta})$ is uniform over all direction vectors, then the plume is spherically symmetric, and the fractional derivative $\mathbb{D}_M^\alpha = c_1 \Delta^{\alpha/2}$ a fractional power of the Laplacian operator [43,44], also called the Riesz fractional derivative, see, for example, Samko et al. [4]. Inverting (8) reveals that

$$\mathbb{D}_M^\alpha \rho(\boldsymbol{x}, t) = \int_{\|\theta\|=1} D_{\boldsymbol{\theta}}^\alpha \rho(\boldsymbol{x}, t) M(\mathrm{d}\boldsymbol{\theta})$$

a mixture of fractional directional derivatives [45]. Here $D_{\boldsymbol{\theta}}^\alpha \rho(\boldsymbol{x}, t)$ is the inverse Fourier transform of $(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{\theta})^\alpha \hat{\rho}(\boldsymbol{k}, t)$, extending the familiar formula $(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{\theta})\hat{\rho}(\boldsymbol{k}, t)$ for the Fourier transform of the directional derivative $D_{\boldsymbol{\theta}}^1 \rho(\boldsymbol{x}, t) = \boldsymbol{\theta} \cdot \nabla \rho(\boldsymbol{x}, t)$. The fractional Laplacian is the only classically defined vector fractional derivative. The operator $\mathbb{D}_M^\alpha$ extends the definition of the fractional Laplacian by allowing asymmetric mixing measures. The physical meaning of the mixing measure will be discussed at the end of Section 4.

3. Vector fractional calculus

A physical explanation for the fractional advection–dispersion equation requires the development of a vector fractional calculus. We outline the essential ideas here. More detail will be given in Section 4, in the context of applications to porous media flow. Our basic definition is the fractional integration operator

$$J_M^{1-\beta}[\cdot] = \int_{\|\boldsymbol{\theta}\|=1} \boldsymbol{\theta} D_{\boldsymbol{\theta}}^{\beta-1} \boldsymbol{\theta}'[\cdot] M(\mathrm{d}\boldsymbol{\theta}) \tag{9}$$

for $0 < \beta \leqslant 1$, which has Fourier symbol

$$\hat{J}_M^{1-\beta} = \int_{\|\boldsymbol{\theta}\|=1} \boldsymbol{\theta}(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{\theta})^{\beta-1} \boldsymbol{\theta}' M(\mathrm{d}\boldsymbol{\theta}). \tag{10}$$

In the classical case $\beta = 1$, this operator is simply the dispersion tensor (2). In the remaining case we have $\beta - 1 < 0$, so the operator with Fourier symbol $(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{\theta})^{\beta-1}$ is a fractional integral of order $1-\beta$ in the $\boldsymbol{\theta}$ direction. Given a scalar field $f(\boldsymbol{x})$ we now define the fractional gradient

$$\begin{aligned} \nabla_M^{\beta} f(\boldsymbol{x}) = J_M^{1-\beta} \nabla f(\boldsymbol{x}) &= \int_{\|\boldsymbol{\theta}\|=1} \boldsymbol{\theta} D_{\boldsymbol{\theta}}^{\beta-1} \boldsymbol{\theta} \cdot \nabla f(\boldsymbol{x}) M(\mathrm{d}\boldsymbol{\theta}) \\ &= \int_{\|\boldsymbol{\theta}\|=1} \boldsymbol{\theta} D_{\boldsymbol{\theta}}^{\beta} f(\boldsymbol{x}) M(\mathrm{d}\boldsymbol{\theta}) \end{aligned} \tag{11}$$

using the fact that $D_{\boldsymbol{\theta}}^{\beta-1} \boldsymbol{\theta} \cdot \nabla f(\boldsymbol{x}) = D_{\boldsymbol{\theta}}^{\beta-1} D_{\boldsymbol{\theta}}^{1} f(\boldsymbol{x}) = D_{\boldsymbol{\theta}}^{\beta} f(\boldsymbol{x})$. The fractional divergence of a vector field $\boldsymbol{V} = (V_1, V_2, V_3)$ is defined as

$$\begin{aligned} \mathrm{div}_M^{\beta} \boldsymbol{V}(\boldsymbol{x}) = \nabla \cdot J_M^{1-\beta} \boldsymbol{V}(\boldsymbol{x}) &= \int_{\|\boldsymbol{\theta}\|=1} \nabla \cdot \boldsymbol{\theta} D_{\boldsymbol{\theta}}^{\beta-1} \boldsymbol{\theta} \cdot \boldsymbol{V}(\boldsymbol{x}) M(\mathrm{d}\boldsymbol{\theta}) \\ &= \int_{\|\boldsymbol{\theta}\|=1} D_{\boldsymbol{\theta}}^{\beta} \boldsymbol{V}(\boldsymbol{x}) \cdot \boldsymbol{\theta} M(\mathrm{d}\boldsymbol{\theta}), \end{aligned} \tag{12}$$

where again we have used $\nabla \cdot \boldsymbol{\theta} = D_{\boldsymbol{\theta}}^{1}$ and $D_{\boldsymbol{\theta}}^{\beta-1} D_{\boldsymbol{\theta}}^{1} = D_{\boldsymbol{\theta}}^{\beta}$. The fractional curl is

$$\mathrm{curl}_M^{\beta} \boldsymbol{V}(\boldsymbol{x}) = \nabla \times J_M^{1-\beta} \boldsymbol{V}(\boldsymbol{x}) = \int_{\|\boldsymbol{\theta}\|=1} \nabla \times \boldsymbol{\theta} D_{\boldsymbol{\theta}}^{\beta-1} \boldsymbol{\theta} \cdot \boldsymbol{V}(\boldsymbol{x}) M(\mathrm{d}\boldsymbol{\theta}). \tag{13}$$

The fractional gradient has Fourier transform

$$\int_{\|\boldsymbol{\theta}\|=1} \boldsymbol{\theta}(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{\theta})^{\beta} \hat{f}(\boldsymbol{k}) M(\mathrm{d}\boldsymbol{\theta}), \tag{14}$$

the fractional divergence has Fourier transform

$$\int_{\|\boldsymbol{\theta}\|=1} (\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{\theta})^{\beta} \hat{\boldsymbol{V}}(\boldsymbol{k}) \cdot \boldsymbol{\theta} M(\mathrm{d}\boldsymbol{\theta}), \tag{15}$$

and the fractional curl has Fourier transform

$$\int_{\|\boldsymbol{\theta}\|=1} (\mathrm{i}\boldsymbol{k} \times \boldsymbol{\theta})(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{\theta})^{\beta-1} \hat{\boldsymbol{V}}(\boldsymbol{k}) \cdot \boldsymbol{\theta} M(\mathrm{d}\boldsymbol{\theta}). \tag{16}$$

4. Derivation of the fractional ADE

A physical derivation of the scalar fractional advection–dispersion equation was developed in [27]. It combined a classical mass balance and drift with a fractional dispersive flux. Following the same outline in d dimensions, we define a fractional Fick's law

$$\boldsymbol{V} = \boldsymbol{v}\rho - c\nabla_M^{\beta} \rho \tag{17}$$

for $\beta = \alpha - 1$ and $1 < \alpha \leqslant 2$, which combines with the classical conservation of mass equation (3) to give

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\boldsymbol{v}\rho - c\nabla_M^\beta \rho) = -\nabla \cdot \boldsymbol{v}\rho + c\nabla \cdot \nabla_M^\beta \rho. \tag{18}$$

Since $\nabla \cdot \nabla_M^\beta \rho = \mathbb{D}_M^\alpha \rho$, which can easily be checked by writing down the corresponding Fourier transforms, Eq. (18) is the same as the fractional ADE in (7). The total flux $\boldsymbol{V}$ in (17) is the sum of the advective flux $\boldsymbol{V}_1 = \boldsymbol{v}\rho$ and the dispersive flux $\boldsymbol{V}_2 = -c\nabla_M^\beta \rho$.

The physical meaning of the fractional dispersive flux is revealed by decomposing the fractional gradient into its radial components. The fractional gradient is a weighted sum of the fractional directional derivatives $D_{\boldsymbol{\theta}}^\beta \rho$ of the contaminant particle density in each direction, laid out along those directions. If the mixing measure M is a point mass at each coordinate vector $\boldsymbol{e}_i$, then $D_{\boldsymbol{e}_1}^\beta \rho = \partial^\beta \rho / \partial x_i^\beta$ for $i = 1, \ldots, d$, and then we get a simplified form of the fractional gradient in explicit coordinate form

$$\nabla_M^\beta \rho = \frac{\partial^\beta \rho}{\partial x_1^\beta} \boldsymbol{e}_1 + \cdots + \frac{\partial^\beta \rho}{\partial x_d^\beta} \boldsymbol{e}_d \tag{19}$$

that reduces to the usual gradient when $\beta = 1$. The fractional derivative [4,46]

$$\frac{\mathrm{d}^\beta g(t)}{\mathrm{d}t^\beta} = \lim_{h \to 0} h^{-\beta} \sum_{j=0}^{\infty} w_\beta(j) g(t - jh) \tag{20}$$

employs a discrete convolution with weights $w_\beta(0) = 1$, $w_\beta(1) = -\beta$, $w_\beta(2) = \beta(\beta - 1)/2!$ and generally

$$w_\alpha(j) = (-1)^j \binom{\beta}{j} = \frac{\Gamma(j - \beta)}{\Gamma(-\beta)\Gamma(j + 1)}.$$

When β is a positive integer this reduces to the usual one-sided finite difference formula. When $0 < \beta < 1$ we have $w_\beta(j) < 0$ for $j = 1, 2, 3, \ldots$ and $w_\beta(0) + w_\beta(1) + w_\beta(2) \cdots = 0$, the latter resulting from the classical binomial formula

$$(1 + z)^\beta = \sum_{j=0}^{\infty} \binom{\beta}{j} z^j \tag{21}$$

for any complex $|z| \leqslant 1$ and any $\beta > 0$, take $z = -1$ in (21).

Subdivide the domain into a grid of mesh h so that the grid points are the corners of d-dimensional rectangles of length h. Use (20) to write

$$\frac{\partial^\beta \rho}{\partial x_i^\beta} \approx h^{-\beta} \sum_{j=0}^{\infty} w_\beta(j) \rho(x_1, \ldots, x_i - jh, \ldots, x_d). \tag{22}$$

This formula represents a weighted average of the particle densities at rectangles located at grid points extending in the negative ith coordinate direction. Then the fractional flux in this case

$$\boldsymbol{V}_2 \approx -ch^{-\beta} \sum_{i=1}^{d} \sum_{j=0}^{\infty} w_\beta(j) \rho(x - jh\boldsymbol{e}_i) \boldsymbol{e}_i$$

takes a proportion $cw_\beta(j)$ of the particles in the rectangle at grid point $x - jh\boldsymbol{e}_i$ and moves them into the rectangle at grid point $\boldsymbol{x}$, while it moves a proportion c of the particles at grid point $\boldsymbol{x}$ out (recall that $w_\beta(0) = -1$) into other rectangles in the positive ith coordinate direction. Since $\sum_j w_\beta(j) = 0$ this redistribution is mass-preserving. Since the weights $w_\beta(j)$ fall off like $j^{-\beta-1}$ (see, e.g., Ref. [46]), the fractional flux represents the result of a velocity distribution that falls off like a power-law, which is characteristic of heterogeneous porous media. The fractional model recognizes that microscopic particle velocities cannot be resolved to a single number or vector at any scale, because in a fractal porous medium there will be a wide power-law distribution of particle velocities observed at every scale.

The general form of the fractional dispersive flux

$$\boldsymbol{V}_2 = -c\nabla_M^\beta \rho(\boldsymbol{x},t) = -c\int_{\|\boldsymbol{\theta}\|=1} \boldsymbol{\theta} D_{\boldsymbol{\theta}}^\beta \rho(\boldsymbol{x},t) M(\mathrm{d}\boldsymbol{\theta}) \tag{23}$$

accommodates particle flux in every radial direction. The term

$$D_{\boldsymbol{\theta}}^\beta \rho(\boldsymbol{x},t) \approx h^{-\beta}\sum_{j=0}^{\infty} w_\beta(j)\rho(\boldsymbol{x}-jh\boldsymbol{\theta},t)$$

relates to the fractional flux in the $\boldsymbol{\theta}$ direction. The integral in (23) represents a weighted average of the fractional flux terms in each radial direction, and the mixing measure $M(\mathrm{d}\boldsymbol{\theta})$ governs the relative strength of the particle flux in different radial directions. In a homogeneous medium, the mixing measure is uniform to reflect the same diffusive effect in every radial direction. In a heterogeneous medium, the mixing measure gives greater weight to preferential pathways laid out in the direction of mean flow. In fractured rock, the mixing measure places all the weight on a discrete set of fracture directions [28].

5. Alternative derivation of the fractional ADE

An alternative derivation of the fractional advection–dispersion equation relates to the moving coordinate system $\boldsymbol{x}+\boldsymbol{v}t$ at the center of mass of the plume. In these coordinates, combine the dispersive flux equation $\boldsymbol{V} = -c\nabla\rho$ with a fractional conservation of mass equation

$$\frac{\partial\rho}{\partial t} = -\mathrm{div}_M^\beta \boldsymbol{V} = -\nabla_M^\beta \cdot \boldsymbol{V} \tag{24}$$

with $\beta = \alpha - 1$ (note $0<\beta\leqslant 1$) to obtain

$$\frac{\partial\rho}{\partial t} = -\mathrm{div}_M^\beta(-c\nabla\rho) = c\mathbb{D}_M^\alpha \rho(\boldsymbol{x},t)\,, \tag{25}$$

where the last equality follows by comparing the corresponding Fourier transforms

$$-\int_{\|\boldsymbol{\theta}\|=1} (\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\theta})^\beta(-c(\mathrm{i}\boldsymbol{k})\hat{\rho}(\boldsymbol{k},t))\cdot\boldsymbol{\theta}M(\mathrm{d}\boldsymbol{\theta}) = c\int_{\|\boldsymbol{\theta}\|=1} (\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\theta})^{\beta+1}\hat{\rho}(\boldsymbol{k},t)M(\mathrm{d}\boldsymbol{\theta}). \tag{26}$$

The fractional advection–dispersion equation (7) can be recovered from (25) by subtracting an advective drift term on the right-hand side, to adjust for the moving coordinate system.

The physical meaning of the fractional conservation of mass equation is revealed by decomposing the fractional divergence into its radial components. Suppose that $d = 3$ and write $(x_1,x_2,x_3)' = (x,y,z)'$. Use (20) to write in explicit coordinate form

$$\frac{\partial^\beta V_1}{\partial x^\beta} \approx \Delta x^{-\beta}\sum_{j=0}^{\infty} w_\beta(j) V_1(x-j\Delta x,y,z) \tag{27}$$

and similarly for the y and z terms. Recall that V_1 represents the x component of the vector field $\boldsymbol{V}$, the rate at which mass density is transported through the area element $\Delta A = \Delta y\Delta z$. In the classical divergence the net outflow of mass in the x direction

$$V_1(x+\Delta x,y,z)\Delta A - V_1(x,y,z)\Delta A \approx \frac{\partial V_1}{\partial x}\Delta x\Delta y\Delta z$$

is combined with similar y and z terms to give the rate $\mathrm{div}\,\boldsymbol{V}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$ at which mass is lost at the point (x,y,z). In the fractional divergence, the anomalous dispersion of mass spreads over a wide range of velocities due to the intervening porous medium. In (27) the $j = 0$ term $V_1(x,y,z)$ represents the rate at which concentration at the point (x,y,z) is diminishing due to mass leaving the volume $\Delta x\Delta y\Delta z$, and each remaining term $w_\beta(j)V_1(x-j\Delta x,y,z)$ in (27) represents the rate at which mass from a volume element j steps to the left is leaping into (recall that $w_\beta(j)<0$ for $j>0$) the volume element at location (x,y,z). The fact that $\sum_j w_\beta(j) = 0$ ensures conservation of mass, just as in the integer case $\beta = 1$.

The general form of the fractional divergence (12) accommodates concentration flux in all directions. The integrand

$$D_{\boldsymbol{\theta}}^{\beta} \boldsymbol{V}(\boldsymbol{x}) \cdot \boldsymbol{\theta} \approx h^{-\beta} \sum_{j=0}^{\infty} w_{\beta}(j) \boldsymbol{V}(\boldsymbol{x} - jh\boldsymbol{\theta}) \cdot \boldsymbol{\theta} \tag{28}$$

in (12) is a fractional mass balance in the $\boldsymbol{\theta}$ direction. The first term $\boldsymbol{V}(\boldsymbol{x}) \cdot \boldsymbol{\theta}$ is the flux component in the $\boldsymbol{\theta}$ direction at the point $\boldsymbol{x}$, representing the rate at which mass density is transported through the area element perpendicular to $\boldsymbol{\theta}$, and the remaining terms $\boldsymbol{V}(\boldsymbol{x} - jh\boldsymbol{\theta}) \cdot \boldsymbol{\theta}$ represent the rate at which mass from a volume element j units away along the $-\boldsymbol{\theta}$ direction is leaping into the volume element at location $\boldsymbol{x}$.

The fractional conservation of mass formula (24) is a mass balance that recognizes the possibility of velocity contrast at every scale. The fractional model recognizes that microscopic particle velocities cannot be resolved to a single number or vector at any scale, because in a fractal porous medium there will be a wide power-law distribution of particle velocities observed at every scale. This is why modern constructions often treat the velocity parameter in the diffusion equation as a random quantity. The fractional model embodies the same physical idea while avoiding the complexity of stochastic partial differential equations. Even in the classical diffusion equation with drift $\partial\rho/\partial t = -\boldsymbol{v} \cdot \nabla\rho + \nabla \cdot A\nabla\rho$ the velocity $\boldsymbol{v}$ is only an average drift. The Brownian particle paths do not have a well-defined infinitesimal velocity, since these fractal paths have infinite total length (unbounded variation) over any time interval.

6. Unified derivation of the fractional ADE

The first derivation of the fractional ADE given in this paper combines a fractional Fick's Law for flux with a classical mass balance. The second combines a fractional mass balance with a classical Fickian flux. There is actually no disagreement between these two derivations, because they both reduce to a third derivation that clarifies and unifies the first two. In this derivation we emphasize that, even in the classical ADE (4), there are three operators in the dispersion term that are applied sequentially. First we take the gradient $\nabla\rho$ of the concentration density, then we apply the dispersion tensor Q, and lastly we take the divergence of this quantity. The fractional ADE simply replaces the dispersion tensor in the second step by the fractional operator $cJ_M^{1-\beta}$ introduced in (9) as the basic building block of the vector fractional calculus. We have already noted that

$$\mathbb{D}_M^{\alpha}\rho = \operatorname{div}_M^{\beta}(\nabla\rho) = \nabla \cdot J_M^{1-\beta}\nabla\rho = \operatorname{div}(\nabla_M^{\beta}\rho)$$

and hence the first (fractional flux) derivation lumps the $J_M^{1-\beta}$ term into the Fick's Law while the second lumps it into the conservation of mass equation. Ultimately, it does not make any difference which point of view we choose, as all are equally valid. The fundamental idea is that fractional integration is applied to represent the effect of power-law variations in the velocity field, leading to enhanced dispersion.

7. Theorems of vector fractional calculus

As another application of the fractional vector calculus, we develop and interpret a fractional divergence theorem. Recall that the fractional divergence of a vector field $\boldsymbol{V}(\boldsymbol{x})$ was defined in (12) by $\operatorname{div}_M^{\beta}\boldsymbol{V}(\boldsymbol{x}) = \nabla \cdot J_M^{1-\beta}\boldsymbol{V}(\boldsymbol{x})$, so that the fractional divergence is just the classical divergence of the fractionally integrated vector field. Given a closed and bounded manifold Ω with boundary $\partial\Omega$ we can now apply the classical divergence theorem to conclude that

$$\int_{\Omega} \operatorname{div}_M^{\beta}\boldsymbol{V}(\boldsymbol{x})\,\mathrm{d}V = \int_{\Omega} \nabla \cdot J_M^{1-\beta}\boldsymbol{V}(\boldsymbol{x})\,\mathrm{d}V = \int_{\partial\Omega} J_M^{1-\beta}\boldsymbol{V}(\boldsymbol{x}) \cdot \boldsymbol{n}\,\mathrm{d}S, \tag{29}$$

where $\boldsymbol{n}$ is the unit outer normal vector. In more detailed form, using the definitions (9) and (12), the fractional divergence theorem (29) becomes

$$\int_{\Omega}\int_{\|\boldsymbol{\theta}\|=1} D_{\boldsymbol{\theta}}^{\beta}(\boldsymbol{V}(\boldsymbol{x}) \cdot \boldsymbol{\theta})M(\mathrm{d}\boldsymbol{\theta})\,\mathrm{d}V = \int_{\partial\Omega}\int_{\|\boldsymbol{\theta}\|=1} (D_{\boldsymbol{\theta}}^{\beta-1}(\boldsymbol{\theta} \cdot \boldsymbol{V}(\boldsymbol{x})))(\boldsymbol{\theta} \cdot \boldsymbol{n})M(\mathrm{d}\boldsymbol{\theta})\,\mathrm{d}S. \tag{30}$$

If the vector field $\boldsymbol{V} = \rho \boldsymbol{v}$ is the advective flux, then the fractional divergence theorem equates the rate at which mass leaves the region Ω with the mass flux through the boundary $\partial\Omega$. The difference in the fractional case is that the mass can jump with widely varying velocities from any point. The term $D_{\boldsymbol{\theta}}^{\beta}(\boldsymbol{V}(\boldsymbol{x}) \cdot \boldsymbol{\theta})$ on the left-hand side of (30) represents the fractional flux (of order β) in the $\boldsymbol{\theta}$ direction as in (28), the inner integral on the left adds up the flux in each radial direction, and the outer integral is the accumulation of the net flux from every point in the region. In the integral on the right, the term

$$D_{\boldsymbol{\theta}}^{\beta-1}(\boldsymbol{\theta} \cdot \boldsymbol{V}(\boldsymbol{x})) \approx h^{1-\beta} \sum_{j=0}^{\infty} w_{\beta-1}(j) \boldsymbol{V}(\boldsymbol{x} - jh\boldsymbol{\theta}) \cdot \boldsymbol{\theta} \tag{31}$$

represents a fractional integral (since $\beta - 1 < 0$) of the flux in the $\boldsymbol{\theta}$ direction. In this case all the Grünwald weights $w_{\beta-1}(j)$ are positive, and $w_{\beta-1}(j) \sim j^{-\beta}$ for j large. Hence the integrand adds up the mass flux through the boundary at the point $\boldsymbol{x}$ in the unit outer normal direction depending on the values of $\boldsymbol{V}$ at all the points on the ray $\boldsymbol{x} - t\boldsymbol{\theta}$. The inner integral adds up the contributions from every direction $\boldsymbol{\theta}$, and the outer integral is the accumulation of the flux at every point on the boundary.

A fractional Stokes Theorem can also be obtained in a similar manner. Using the definition $\operatorname{curl}_M^{\beta} \boldsymbol{V}(\boldsymbol{x}) = \nabla \times J_M^{1-\beta} \boldsymbol{V}(\boldsymbol{x})$ from (13) the classical Stokes Theorem yields

$$\int_S \operatorname{curl}_M^{\beta} \boldsymbol{V}(\boldsymbol{x}) \cdot \boldsymbol{n} \, \mathrm{d}A = \int_S \nabla \times J_M^{1-\beta} \boldsymbol{V}(\boldsymbol{x}) \cdot \boldsymbol{n} \, \mathrm{d}A = \oint_C J_M^{1-\beta} \boldsymbol{V}(\boldsymbol{x}) \cdot \mathrm{d}\boldsymbol{r}, \tag{32}$$

where C is the simple closed curve that bounds the oriented surface S, and $\boldsymbol{n}$ is the unit outer normal vector. In more detailed form, using the definitions (9) and (13), the fractional Stokes theorem (32) becomes

$$\int_{\|\boldsymbol{\theta}\|=1} \int_S \nabla \times (\boldsymbol{\theta} D_{\boldsymbol{\theta}}^{\beta-1}(\boldsymbol{V}(\boldsymbol{x}) \cdot \boldsymbol{\theta})) \cdot \boldsymbol{n} \, \mathrm{d}A M(\mathrm{d}\boldsymbol{\theta}) = \int_{\|\boldsymbol{\theta}\|=1} \oint_C (D_{\boldsymbol{\theta}}^{\beta-1}(\boldsymbol{V}(\boldsymbol{x}) \cdot \boldsymbol{\theta}))\boldsymbol{\theta} \cdot \mathrm{d}\boldsymbol{r} M(\mathrm{d}\boldsymbol{\theta}). \tag{33}$$

Since the fractional Stokes theorem is merely the classical Stokes theorem applied to the fractionally integrated field $J_M^{1-\beta} \boldsymbol{V}(\boldsymbol{x})$, it has a similar interpretation. The term $D_{\boldsymbol{\theta}}^{\beta-1}(\boldsymbol{V}(\boldsymbol{x}) \cdot \boldsymbol{\theta})$ in the integral on the right-hand side is the fractionally integrated flux (31) in the $\boldsymbol{\theta}$ direction, so the inner integral is the circulation of this field, and the outer integral adds up the circulation from each $\boldsymbol{\theta}$ component. The term $\nabla \times \boldsymbol{\theta} D_{\boldsymbol{\theta}}^{\beta-1} \boldsymbol{V}(\boldsymbol{x}) \cdot \boldsymbol{\theta}$ in the integral on the left-hand side is the curl of the fractionally integrated flux (31) in the $\boldsymbol{\theta}$ direction, the inner integral adds up the curl at every point on the surface, and the outer integral adds up the contributions for each $\boldsymbol{\theta}$.

Finally, since the fractional divergence and curl of a field $\boldsymbol{V}(\boldsymbol{x})$ are nothing more than the classical divergence and curl of the fractionally integrated field $J_M^{1-\beta} \boldsymbol{V}(\boldsymbol{x})$, all of the remaining basic results of vector calculus have straightforward extensions. If $\operatorname{curl}_M^{\beta} \boldsymbol{V}(\boldsymbol{x}) = 0$ at every point we say that $\boldsymbol{V}(\boldsymbol{x})$ is fractionally irrotational, and it follows that $J_M^{1-\beta} \boldsymbol{V}(\boldsymbol{x}) = \nabla W(\boldsymbol{x})$ for some scalar field $W(\boldsymbol{x})$ which can be called a fractional scalar potential. If $\operatorname{div}_M^{\beta} \boldsymbol{V}(\boldsymbol{x}) = 0$ at every point we say that $\boldsymbol{V}(\boldsymbol{x})$ is fractionally solenoidal, and it follows that $J_M^{1-\beta} \boldsymbol{V}(\boldsymbol{x}) = \nabla \times \boldsymbol{A}(\boldsymbol{x})$ for some vector field $\boldsymbol{A}(\boldsymbol{x})$ which can be called a fractional vector potential.

8. Conclusions

A fractional vector calculus has been developed that extends the usual vector calculus by describing the fractional derivative versions of the gradient, divergence, and curl. The fractional advection–dispersion equation for flow and transport of contaminants in heterogeneous porous media has been derived from first principles using the fractional vector calculus. A fractional version of Stokes theorem and the divergence theorem have been laid out, the novel feature of the fractional versions being the nonlocal effect of power-law velocity distributions at every scale in a fractal porous medium. Since scalar fractional derivative models are now widely used in many areas of physics, it is likely that the constructions here will also find further applications in other areas.

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