Variational Iteration Method for the Time-Fractional Elastodynamics of 3D Quasicrystals

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Abstract: This paper presents the approximate analytical solutions to the time fractional differential equations of elasticity for 3D quasicrystals with initial conditions. These equations are written in the form of a vector partial differential equation of the second order. The time fractional vector partial differential equations with initial conditions are solved by variational iteration method (VIM). The fractional derivatives are described in the Caputo sense. Numerical example shows that the proposed method is quite effective and convenient for solving kinds of time fractional system of partial differential equations.

Keywords: Time fractional anisotropic dynamic elasticity(3D), Three-dimensional quasicrystals, Icosahedral quasicrystal, Variational iteration method, Caputo derivative.

1 Introduction

Fractional differential equations have been the focus of attention of researchers due to describe of many phenomena in engineering physics, chemistry, other sciences by differential equations of fractional order [Miller and Ross (1993); Samko, Kilbas, and Marichev (1993); Podlubny (1974); Iovane (2006)]. Hence, considerable attention has been given to finding the solutions of fractional differential equations. In general, there exists no method that yields an exact solution for a fractional differential equation. Only approximate solutions can be derived using the linearization or perturbation method. Recently, variational iteration method [He (1999)] has been widely applied to analytically solve fractional differential equations [Wu (2011); Wu and Lee (2010); Nawaz (2011); Molliq, Noorani, and Hashim (2009); Molliq, Noorani, Hashim, and Ahmad (2009); Khan, Faraz, Yildirim, and Wu (2011); Inc (2008); Elsaid (2010); Das (2009); Odibat and Momani (2009); Vang, Xiao,

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and Su (2010); Sakar, Erdogan, and Yildirim (In press); Song, Wang, and Zhang (2009)].

The quasicrystal as a new structure of solids was first discovered in 1984. [Shechtman, Blech, Gratias, and Cahn (1980)] found an icosahedral structure with five-fold symmetry in AlMn alloys. Three-dimensional quasicrystals, such as icosahedral quasicrystals (e.g., Al-Cu-Fe and Al-Li-Cu) are quasiperiodic in three dimensions, without periodic direction. They play a central role in the study of quasicrystalline solids. The elasticity problems of 3D quasicrystals are more complicated than those of 1D and 2D quasicrystals. It is more difficult to obtain rigorous analytic solutions. The time-dependent elastic problems in QCs have been studied in [Fan and Mai (2004); Wang (2006); Akmaz and Akinci (2009); Akmaz (2009); Yakhno and Yaslan (2011b); Yakhno and Yaslan (2011a)]. Using PS method related with polynomial presentation of data 3D elastic problems in 3D QCs have been solved in [Akmaz (2009)]. A new method for the derivation of the time-dependent fundamental solution with three space variables in 3D QCs with arbitrary system of anisotropy have been studied in [Yakhno and Yaslan (2011a)].

In this paper, time fractional differential equations of elasticity for 3D quasicrystals with initial conditions are solved by variational iteration method.

2 The basic equations for 3D QCs

Let $x = (x_1, x_2, x_3) \in \mathbb{R}^3$ be a space variable, $t \in \mathbb{R}$ be a time variable. The generalized Hooke's laws of the elasticity problem of 3D QCs are [Ding, Yang, Hu, and Wang (1993); Hu, Wang, and Ding (2000); Gao and Zhao (2006)]

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} + R_{ijkl}w_{kl}, \qquad (1)$$

$$H_{ij} = R_{klij}\varepsilon_{kl} + K_{ijkl}w_{kl}, \ i, j, k, l = 1, 2, 3,$$

$$\tag{2}$$

and the time fractional dynamic equilibrium equations are

$$\rho \frac{\partial^{\alpha} u_i(x,t)}{\partial t^{\alpha}} = \sum_{j=1}^3 \frac{\partial \sigma_{ij}(x,t)}{\partial x_j} + f_i(x,t),$$
(3)

$$\rho \frac{\partial^{\alpha} w_i(x,t)}{\partial t^{\alpha}} = \sum_{j=1}^3 \frac{\partial H_{ij}(x,t)}{\partial x_j} + g_i(x,t), \ i = 1, 2, 3, \ 1 < \alpha \le 2,$$
(4)

where $f_i(x,t)$, $g_i(x,t)$ all are continuous functions and α is a parameter describing the order of the time fractional derivative.

Besides, geometry equations are given by

$$\varepsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \ w_{ij} = \frac{\partial w_i}{\partial x_j}, \ i, j = 1, 2, 3.$$
(5)

Here u_i and w_i , i = 1, 2, 3, are the phonon and phason displacements, σ_{ij} and H_{ij} , i, j = 1, 2, 3, are phonon and phason stresses, $\varepsilon_{ij}(x,t)$, $w_{ij}(x,t)$, i, j = 1, 2, 3, are phonon and phason strains, $f_i(x,t)$ and $g_i(x,t)$, i = 1, 2, 3, are body forces for the phonon and phason displacements, respectively. And the constant $\rho > 0$ is the density.

 C_{ijkl} are the phonon elastic constants, K_{ijkl} are the phason elastic constants, R_{ijkl} are the phonon-phason coupling elastic constants. Moreover, they satisfy the following symmetric properties [Ding, Yang, Hu, and Wang (1993); Hu, Wang, and Ding (2000); Gao and Zhao (2006)]

$$C_{ijkl} = C_{jikl} = C_{ijlk} = C_{klij}, \ K_{ijkl} = K_{klij}, \ R_{ijkl} = R_{jikl}.$$
(6)

The positivity of elastic strain energy density requires that the elastic constant tensors C_{ijkl} , K_{ijkl} , R_{ijkl} must be positive definite.

In this study we consider (3) and (4) subject to initial conditions

$$u_i(x,0) = \varphi_i(x), \quad \frac{\partial u_i}{\partial t}(x,0) = \phi_i(x), \quad w_i(x,0) = \xi_i(x),$$

$$\frac{\partial w_i}{\partial t}(x,0) = \psi_i(x), \quad i = 1, 2, 3.$$
 (7)

Here $\varphi_i(x)$, $\phi_i(x)$, $\xi_i(x)$ and $\psi_i(x)$ are all continuous functions.

3 Basic definitions

We give some basic definitions and properties of the fractional calculus theory [Podlubny (1974); Oldham and Spanier (1974)] which are used in this paper.

Definition 2.1.A real function f(y), y > 0, is said to be in the space $C_{\mu}, \mu \in R$ if there exists a real number $p(>\mu)$, such that $f(y) = y^p f_1(y)$, where $f_1(y) \in C[0,\infty)$, and it is said to be in the space C_{μ}^m iff $f^{(m)} \in C_{\mu}, m \in N$.

Definition 2.2. The Riemann-Liouville fractional integral operator of order $\alpha \ge 0$, of a function $f \in C_{\mu}, \mu \ge -1$, is defined as

$$J^{\alpha}f(y) = \frac{1}{\Gamma(\alpha)} \int_{0}^{y} (y-t)^{\alpha-1} f(t) dt, \ \alpha > 0, \ y > 0,$$

$$J^{0}f(y) = f(y).$$

Definition 2.3. The fractional derivative of f(y) in Caputo sense is defined as

$$D^{\alpha}f(y) = J^{m-\alpha}D^{m}f(y) = \frac{1}{\Gamma(m)}\int_{0}^{y} (y-s)^{m-\alpha-1}f^{(m)}(s)ds,$$

for $m-1 < \alpha \le m, \ m \in N, \ y > 0, \ f \in C_{-1}^{m}.$

Definition 2.4. For *m* to be the smallest integer that exceeds α , the Caputo time-fractional derivative operator of order $\alpha > 0$ is defined as

$$D^{\alpha}u(y,t) = \begin{cases} \frac{1}{\Gamma(m-\alpha)} \int_{0}^{y} (t-\tau)^{m-\alpha-1} \frac{\partial^{m}u(y,t)}{\partial \tau^{m}} d\tau, & m-1 < \alpha < m, \\ \frac{\partial^{m}u(y,t)}{\partial t^{m}}, & \alpha = m \in N. \end{cases}$$

4 Variational iteration method

Equations (3) and (4) with together (1) and (2) can be written in the vector form [Akmaz (2009)]

$$\rho \frac{\partial^{\alpha} \mathbf{V}}{\partial t^{\alpha}} = \sum_{j,l=1}^{3} \mathbf{P}_{jl} \frac{\partial^{2} \mathbf{V}}{\partial x_{j} \partial x_{l}} + \mathbf{F}(x,t), x \in \mathbb{R}^{3}, t \in \mathbb{R}, \ 1 < \alpha \le 2,$$
(8)

where $\mathbf{V} = (u_1, u_2, u_3, w_1, w_2, w_3)$, $\mathbf{F} = (f_1, f_2, f_3, g_1, g_2, g_3)$, matrices \mathbf{P}_{jl} are

$$\begin{split} \mathbf{P}_{jl} &= \frac{1}{2} \times \\ \begin{bmatrix} C_{1j1l} + C_{1l1j} & C_{1j2l} + C_{1l2j} & C_{1j3l} + C_{1l3j} & R_{1j1l} + R_{1l1j} & R_{1j2l} + R_{1l2j} & R_{1j3l} + R_{1l3j} \\ C_{2j1l} + C_{2l1j} & C_{2j2l} + C_{2l2j} & C_{2j3l} + C_{2l3j} & R_{2j1l} + R_{2l1j} & R_{2j2l} + R_{2l2j} & R_{2j3l} + R_{2l3j} \\ C_{3j1l} + C_{3l1j} & C_{3j2l} + C_{3l2j} & C_{3j3l} + C_{3l3j} & R_{3j1l} + R_{3l1j} & R_{3j2l} + R_{3l2j} & R_{3j3l} + R_{3l3j} \\ R_{1j1l} + R_{1l1j} & R_{2j1l} + R_{2l1j} & R_{3j2l} + R_{3l2j} & R_{3j3l} + R_{3l1j} \\ R_{1j2l} + R_{1l2j} & R_{2j2l} + R_{2l2j} & R_{3j2l} + R_{3l2j} & K_{2j1l} + K_{2l1j} & K_{2j2l} + K_{2l2j} & K_{2j3l} + K_{2l3j} \\ R_{1j3l} + R_{1l3j} & R_{2j3l} + R_{2l3j} & R_{3j3l} + R_{3l3j} & K_{3j1l} + K_{3l1j} & K_{3j2l} + K_{3l2j} & K_{3j3l} + K_{3l3j} \\ \end{bmatrix} \end{split}$$

The initial conditions (7) can be written in the vector form

$$\mathbf{V}(x,0) = \mathbf{H}(x), \ \frac{\partial \mathbf{V}}{\partial t}(x,0) = \mathbf{G}(x), \tag{9}$$

where $\mathbf{H}(x) = (\varphi_1(x), \varphi_2(x), \varphi_3(x), \xi_1(x), \xi_2(x), \xi_3(x)), \mathbf{G}(x) = (\phi_1(x), \phi_2(x), \phi_3(x), \psi_1(x), \psi_2(x), \psi_3(x))$. To solve IVP (8)-(9) by means of VIM, the correction functional for system (8) can be written as follows

$$\mathbf{V}^{n+1}(x,t) = \mathbf{V}^{n}(x,t) + \int_{0}^{t} \lambda(\tau) \{ \rho \frac{\partial^{2} \mathbf{V}^{n}(x,\tau)}{\partial t^{2}} - \sum_{j,l=1}^{3} \mathbf{P}_{jl} \frac{\partial^{2} \tilde{\mathbf{V}}^{n}(x,\tau)}{\partial x_{j} \partial x_{l}} - \mathbf{F}(x,\tau) \} d\tau,$$

where λ is a general Lagrange multiplier [Inokuti, Sekine, and Mura (1978)], $\frac{\partial^2 \tilde{\mathbf{v}}^n(x,\tau)}{\partial x_j \partial x_l}$ is considered as restricted variations. Making the above functional stationary, noticing that $\delta \tilde{\mathbf{v}}^n = 0$,

$$\delta \mathbf{V}^{n+1}(x,t) = \delta \mathbf{V}^n(x,t) + \delta \int_0^t \lambda(\tau) \left\{ \rho \frac{\partial^2 \mathbf{V}^n(x,\tau)}{\partial t^2} - \mathbf{F}(x,\tau) \right\} d\tau,$$

yields the following Lagrange multiplier $\lambda(\tau) = \frac{\tau-t}{\rho}$. Therefore, the following variational iteration formula can be obtained

$$\mathbf{V}^{n+1}(x,t) = \mathbf{V}^{n}(x,t) + \frac{1}{\rho} \int_{0}^{t} (\tau - t) \{\rho \frac{\partial^{\alpha} \mathbf{V}^{n}(x,\tau)}{\partial t^{\alpha}} - \sum_{j,l=1}^{3} \mathbf{P}_{jl} \frac{\partial^{2} \mathbf{V}^{n}(x,\tau)}{\partial x_{j} \partial x_{l}} - \mathbf{F}(x,\tau) \} d\tau,$$
(10)

In this case, we begin with the initial approximation

$$\mathbf{V}^{0}(x) = \mathbf{H}(x) + t\mathbf{G}(x).$$
⁽¹¹⁾

5 Application

Example. In this example we consider icosahedral quasicrystals. For three-dimensional icosahedral quasicrystals [Ding, Yang, Hu, and Wang (1993)], C_{ijkl} has the expression

$$C_{ijkl} = \lambda \, \delta_{ij} \delta_{kl} + \mu (\delta_{jl} \delta_{ik} + \delta_{il} \delta_{jk}),$$

where λ and μ are Lame constants. The nonzero phason elastic constants are

$$\begin{split} K_{1111} &= K_{2222} = K_{1212} = K_{2121} = K_1, \\ K_{1131} &= K_{1113} = K_{2213} = K_{2312} = -K_{2231} = -K_{2321} = -K_{1232} = -K_{3221} = K_2, \\ K_{3333} &= K_1 + K_2, \ K_{2323} = K_{3131} = K_{3232} = K_{1313} = K_1 - K_2. \end{split}$$

The nonzero phonon-phason coupling elastic constants are

$$\begin{array}{rcl} R_{1111} & = & R_{1122} = R_{1133} = R_{1113} = R_{2233} = R_{2332} = R_{3111} = R_{3131} = R_{1221} = R, \\ R_{2211} & = & R_{2222} = R_{2213} = R_{2312} = R_{2321} = R_{3122} = R_{1223} = R_{1212} = -R, \\ R_{3333} & = & -2R. \end{array}$$

For our calculations we choose $\rho = 1$, $\lambda = 4.51$, $\mu = 1.25$, $K_1 = 1.35$, $K_2 = 0.4$, R = -0.57 [Akmaz (2009)]. And initial conditions and nonhomogenous terms are given as

$$\begin{aligned} \varphi_i(x) &= \xi_i(x) = (1+x_1)(2+x_2)(3+x_3), \ \phi_i(x) = \psi_i(x) = 0, \\ f_i(x,t) &= g_i(x,t) = 0, \ i = 1, 2, 3. \end{aligned}$$

Using the formula (10) with initial approximation (11) we can obtain the following approximations

$$\begin{aligned} \mathbf{V}^{0}(x,t) &= \mathbf{H}(x), \\ \mathbf{V}^{1}(x,t) &= \mathbf{H}(x) + \frac{1}{\rho} \frac{t^{2}}{2} \sum_{j,l=1}^{3} \mathbf{P}_{jl} \frac{\partial^{2} \mathbf{H}(x)}{\partial x_{j} \partial x_{l}}, \\ \mathbf{V}^{2}(x,t) &= \mathbf{H}(x) + \frac{1}{\rho} t^{2} \sum_{j,l=1}^{3} \mathbf{P}_{jl} \frac{\partial^{2} \mathbf{H}(x)}{\partial x_{j} \partial x_{l}} + \frac{1}{\rho^{2}} \sum_{j,l=1}^{3} \mathbf{P}_{jl} \frac{\partial^{2}}{\partial x_{j} \partial x_{l}} \sum_{j,l=1}^{3} \mathbf{P}_{jl} \frac{\partial^{2} \mathbf{H}(x)}{\partial x_{j} \partial x_{l}} \frac{t^{4}}{24} \\ &- \frac{1}{\rho} \sum_{j,l=1}^{3} \mathbf{P}_{jl} \frac{\partial^{2} \mathbf{H}(x)}{\partial x_{j} \partial x_{l}} \frac{t^{4-\alpha}}{\Gamma(5-\alpha)}. \end{aligned}$$

Here components of the second order approximation $\mathbf{V}^2(x,t)$ are found explicitly as follows

$$\begin{split} u_1^2(x,t) &= (1+x_1)(2+x_2)(3+x_3) + t^2(21.96 + 4.62x_3 + 4.48x_2 + 1.14x_1) \\ &- \frac{t^{4-\alpha}(21.96 + 4.62x_3 + 4.48x_2 + 1.14x_1)}{\Gamma(5-\alpha)}, \\ u_2^2(x,t) &= (1+x_1)(2+x_2)(3+x_3) + t^2(28.74 + 6.9x_3 + 1.14x_2 + 5.76x_1) \\ &- \frac{t^{4-\alpha}(28.74 + 6.9x_3 + 1.14x_2 + 5.76x_1)}{\Gamma(5-\alpha)}, \\ u_3^2(x,t) &= (1+x_1)(2+x_2)(3+x_3) + t^2(2.07 + 1.14x_3 + 5.76x_2 + 5.76x_1) \\ &- \frac{t^{4-\alpha}(2.07 + 1.14x_3 + 5.76x_2 + 5.76x_1)}{\Gamma(5-\alpha)}, \\ w_1^2(x,t) &= (1+x_1)(2+x_2)(3+x_3) + t^2(4.68 + 1.14x_3 - 0.34x_2 + 1.94x_1) \\ &- \frac{t^{4-\alpha}(4.68 + 1.14x_3 - 0.34x_2 + 1.94x_1)}{\Gamma(5-\alpha)}, \\ w_2^2(x,t) &= (1+x_1)(2+x_2)(3+x_3) + t^2(0.22 - 0.8x_3 + 0.34x_2 + 1.94x_1) \\ &- \frac{t^{4-\alpha}(0.22 - 0.8x_3 + 0.34x_2 + 1.94x_1)}{\Gamma(5-\alpha)}, \\ w_3^2(x,t) &= (1+x_1)(2+x_2)(3+x_3) + t^2(-5.82 - 0.8x_3 - 1.14x_2 - 1.14x_1) \\ &- \frac{t^{4-\alpha}(-5.82 - 0.8x_3 - 1.14x_2 - 1.14x_1)}{\Gamma(5-\alpha)}. \end{split}$$

This problem has been solved in the polynomial form explicitly [Akmaz (2009)]. In Table 1 we compare the second order approximation $V^2(x,t)$ for $\alpha = 2$ with the polynomial solution and we obtain same results. And we calculate all components

for the second order approximation $V^2(x,t)$ for $\alpha = 1.7, 1.5, 1.1$, respectively. In Table 1 we take $x_1 = 1$, $x_2 = 2$, $x_3 = 3$ and t = 5.

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Tal	ble 1: The compone	ents of	$\mathbf{V}^2(x,t)$ for x_1 =	$=1, x_2 = 2, x_3 =$	=3, t=5.
$\mathbf{V}^2(x,t)$	Polynomial solution	$\alpha = 2$	$\alpha = 1.7$	$\alpha = 1.5$	$\alpha = 1.1$
2					
$u_1^2(x,t)$	597	597	482.8651137	407.2267976	264.0288056
$u_2^2(x,t)$	766.5	766.5	617.1267472	518.1356176	330.7262238
$u_3^{\overline{2}}(x,t)$	565.5	565.5	457.9138367	386.6154239	251.6337102
$w_1^2(x,t)$	165	165	140.6761718	124.5565306	94.03892579
$w_2^2(x,t)$	53.5	53.5	52.35657218	51.59881127	50.16422301
$w_{3}^{\bar{2}}(x,t)$	-97.5	-97.5	-67.25113669	-47.20491629	-9.253535921

In Figure 1 shows the second order approximation $w_3^2(1,2,3,t)$ for values $\alpha = 2$, $\alpha = 1.7$, $\alpha = 1.5$ and $\alpha = 1.1$ for different values of t.



Figure 1: $w_3^2(1,2,3,t)$ for different values of α and t.

Conclusion 6

Variational iteration method has proven as an efficient tool to solve the time fractional equations of anisotropic elasticity for 3D quasicrystals. The method has been used in a direct way without using linearization, perturbation or restrictive assumptions. The result shows that a few iterations of the Variational iteration method recursive formula can yield a good solution. The basic idea described in this work can be employed to solve kinds of system of partial differential equations with time fractional order.

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