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Numerical Solution of Gas Solution in a Fluid: Fractional Derivative Model

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ABSTRACT

A computational technique for solution of mathematical model of gas solution in a fluid is presented. This model describes the change of mass of the gas volume due to diffusion through the contact surface. An appropriate representation of the solution based on the Müntz polynomials reduces its numerical treatment to the solution of a linear system of algebraic equations. Numerical examples are given and discussed to illustrate the effectiveness of the proposed approach.

1. INTRODUCTION

A number of examples in nature can illustrate the capability of liquids to dissolve gases; in fact, human life would not be feasible if blood cannot dissolve oxygen, nor marine life is likely to happen if oxygen did not dissolve in water. The solubility anticipation of oxygen gas in the liquid is important as it can be used in aquaculture and biological issues such as oxygen uptake in lungs and its dissolution in the blood. The prediction of CO_2 gas solubility in water can be used for growing plants and in the production of carbonated drinks [24]. Such interesting natural phenomena are described by differential equations.

This paper is concerned with providing good quality algorithm for the numerical solution of the three–term fractional differential equations of the form

$$p'(t) + F(t)D^{1/2}p(t) + G(t)p(t) = H(t), \qquad (1.1)$$

combined with the suitable initial condition $p(0) = p_0$. This equation describes the change of mass of the gas volume due to diffusion through the contact surface [2]. Here, $D^{1/2}p(t)$

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denotes the fractional derivative $D_*^{1/2}p(t)$ in the Caputo version [7] and the Riemann–Liouville fractional derivative ${}^{RL}_{0}D_t^{1/2}p(t)$, defined by

$$D_*^{1/2}p(t) = \frac{1}{\sqrt{\pi}}\int_0^t \frac{p'(s)}{\sqrt{t-s}}ds, \tag{1.2}$$

$${}^{RL}_{0}D_t^{\frac{1}{2}}p(t) = \frac{1}{\sqrt{\pi}}\frac{d}{dt}\int_0^t \frac{p(s)}{\sqrt{t-s}}ds, \tag{1.3}$$

respectively [9,23]. It is well-known that the fractional derivative of Riemann–Liouville and Caputo type are closely linked by the following relationship:

$$D_*^{1/2}p(t) = {}^{RL}_{0}D_t^{1/2}[p(t)-p(0)]. \tag{1.4}$$

Fractional calculus, including the operators of fractional order integration and differentiation, is known to provide an excellent setting for capturing in a model framework concerned with real–world problems in a variety of disciplines from physics, chemistry, biology and engineering [1, 4, 17, 23]. In order to approximate fractional derivatives, a number of methods have been proposed [4, 6, 11]. Since few of the fractional differential equations can be solved explicitly, it is necessary to employ numerical techniques to find the approximate solution. Especially, numerical schemes for the multi–term fractional differential equations have been developed in the past ten to fifteen years and have been studied in numerous papers [4, 9, 10, 22].

As a fractional derivative is a non–local operator, it is very natural to consider a global method like the spectral method for its numerical solution. Spectral collocation methods are efficient and highly accurate techniques for numerical solution of differential equations [13, 25]. The basic idea of the spectral collocation method is to assume that the unknown solution$p(t)$can be approximated by a linear combination of some basis functions, called the trial functions, such as orthogonal polynomials.

Whereas the classical orthogonal polynomials work well for numerical solution of conventional differential equations, their application for the fractional differential equations implies at least two difficulties in connection with the collocation method. First, according to Theorems 4.1 in [16], the solutions of the problem (1.1) can contain some fractional–power terms with which the classical orthogonal polynomials cannot match. In this case, the rate of convergence of the numerical approximations is not reasonable when the classical polynomial bases are used. Second, to apply a collocation method, it is required that the derivatives of any trial function can be expressed in terms of the same trial bases. However, the fractional derivatives of a classical polynomial are not polynomials. Therefore, roughly speaking, a good approximation for the fractional derivatives via the classical orthogonal polynomials is not hoped to be obtained.

In the present article, the Müntz–Legendre polynomials are used, which are a family of generalized orthogonal polynomials. These polynomials were introduced and investigated in [5, 18]. A fractional derivative of a Müntz–Legendre polynomial is again a

Müntz–Legendre polynomial. This is a crucial feature of these bases for using them in the collocation method for the numerical solution of the fractional differential equations.

The structure of the paper is as follows. In the next section, the derivation of mathematical model of gas solution in a fluid is briefly recalled. Then, to construct a numerical algorithm, this equation as a three–term fractional differential equation is reformulated. In Section 3, the Müntz–Legendre polynomials and related topics are introduced. A description of the proposed numerical scheme is provided in Section 4. Some details concerning the practical implementation are discussed in Section 5. Finally, the numerical results to demonstrate the efficiency of the proposed method are given in Section 6.

2. PROBLEM STATEMENT

The mathematical model of the process of solution of a compressible gas volume in a fluid, when there are no convection currents, is described by the system [2, 23]

$$\frac{d}{d\tau}\left(V_0 f\left(\frac{\tau}{\theta}\right) P(0,\tau)\frac{M}{RT}\right) = SK\left.\frac{\partial C}{\partial x}\right|_{x=0}, \qquad 0 < \tau < \theta, \tag{2.1}$$

$$-\sqrt{K}\left.\frac{\partial C}{\partial x}\right|_{x=0} = {}^{RL}_{0}D_{\tau}^{1/2}[C(0,\tau) - C(x,0)], \tag{2.2}$$

$$P(0,\tau) = \kappa C(0,\tau), \qquad P(x,0) = \kappa C(x,0), \tag{2.3}$$

where V_0 is the initial gas volume, θ is the time of the gas compression to zero volume, f is a function describing a change of the gas volume, such that $f(0) = 1$ and $f(1) = 0$, M is the molecular weight of the gas, R is the molar gas constant, K is the gas diffusion coefficient in the fluid, S is the contact surface between the gas and the fluid, κ is the Henry's constant, $C(x,\tau)$ is the gas concentration, and $P(x,\tau)$ is the unknown gas pressure (Figure 1).

The gas pressure near the contact surface $P(0,\tau)$ is to be found. The x–axis goes down from the contact surface, for which $x = 0$. The gas temperature T is assumed to be constant, which implies the gas compression is slow enough. If necessary, a weak nonisothermality can be accounted by making a correction to the function $f(\tau/\theta)$. The depth of the fluid is taken infinite [2, 23].

The change of the gas volume mass due to diffusion through the contact surface is described by (2.1). The mass change depends on the change of the gas concentration near the contact surface, which is given by (2.2). Taking into account the condition (2.3), makes the consideration of mass transfer process for $x > 0$ unnecessary.

The problem (2.1)–(2.3) for determining the dimensionless gas pressure

$$p(\tau) = \frac{P(0,\tau)}{P(x,0)} = \frac{C(0,\tau)}{C(x,0)},$$

near the constant surface can be written as [23]

$$p'(t) + F(t)D_*^{1/2}p(t) + G(t)p(t) = 0, \qquad p(0) = 1, \tag{2.4}$$

where

$$t = \frac{\tau}{\theta} \in (0,1], \quad F(t) = \frac{\lambda}{f(t)}, \quad G(t) = \frac{f'(t)}{f(t)}, \quad \lambda = \frac{RTS\sqrt{K\theta}}{\kappa M V_0}.$$

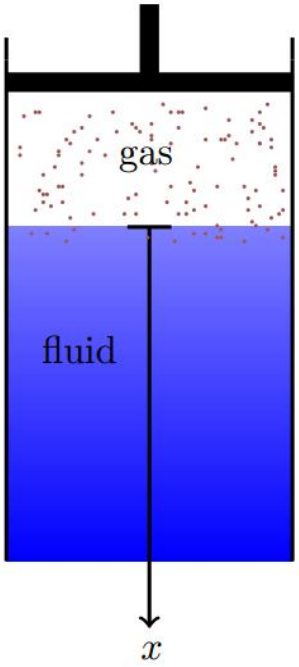

Figure 1. Solution of a gas in a fluid [23].

3. MÜNTZ–LEGENDRE POLYNOMIALS

Let the complex numbers from the set $\Lambda_n = \{\lambda_0, \dots, \lambda_n\}$ satisfy the condition $\Re(\lambda_k) > -\frac{1}{2}$ and $\lambda_k \neq \lambda_j$, $k \neq j$. Then, for every $n = 0,1,2, \dots$, the Müntz–Legendre polynomials on the interval $[0,1]$ are defined by [5, 18]

$$L_n(\Lambda_n; x) = \sum_{k=0}^{n} c_{nk} x^{\lambda_k}, \qquad c_{nk} = \frac{\prod_{\nu=0}^{n-1}(\lambda_k + \bar{\lambda}_\nu + 1)}{\prod_{\nu=0,\nu\neq k}^{n}(\lambda_k - \lambda_\nu)}. \tag{3.1}$$

For the Müntz–Legendre polynomials (3.1), the orthogonality relation

$$\int_0^1 L_n(\Lambda_n; x)\bar{L}_m(\Lambda_m; x)\,dx = \frac{\delta_{nm}}{\lambda_n + \bar{\lambda}_m + 1},$$

holds for every $m, n = 0,1,2, \dots$ [5].

In this paper, the case when the powers of the Müntz basis elements build an arithmetic progression is considered [12, 20]. In other words, we assume that $\lambda_k = k/2$. In this case, the Müntz–Legendre polynomials on the interval $[0,1]$ are represented by the formula

$$L_n(t) = \sum_{k=0}^{n} c_{nk} t^{k/2}\ , \qquad c_{nk} = \frac{(-1)^{n-k}}{k!\,(n-k)!} \prod_{\nu=0}^{n-1} (k+\nu+2)\ . \tag{3.2}$$

The functions $L_k(t)$, $k = 0,1,\dots,n$ form an orthogonal basis for $\mathbb{M}_n$, where

$$\mathbb{M}_n = \operatorname{span}\{1, t^{1/2}, t, t^{3/2}, \dots, t^{n/2}\}.$$

The denseness of $\mathbb{M}_n$ in $C[0,1]$, the set of continuous functions on the interval $[0,1]$, in the uniform norm is characterized by $\sum_{k=1}^{\infty} 1/k = \infty$ [5].

4. MÜNTZ–LEGENDRE COLLOCATION METHOD

In this section, the collocation method based on Müntz–Legendre polynomials is applied for solving an initial value problem of the form

$$p'(t) + F(t) D_*^{1/2} p(t) + G(t) p(t) = H(t), \tag{4.1}$$

$$p(0) = p_0\ . \tag{4.2}$$

Under certain conditions on the functions$F$, G and H, the initial value problem (4.1)–(4.2) possesses unique solution$p$ in an appropriate space of functions [9, 16]. As a generally applicable method to determine the exact solution of initial value problem (4.1)–(4.2) is not readily accessible, some numerically computed approximate solutions are inevitable. Numerical evaluation of this solution is the aim of this section. At first, the solution p is approximated by $p_n \in \mathbb{M}_n$ as the finite sum

$$p_n(t) = \sum_{k=0}^{n} a_k L_k(t), \tag{4.3}$$

where a_k are unknown coefficients. It is worthwhile to note that if $p_n \in \mathbb{M}_n$, then $D_*^{1/2} p_n$ belongs to $\mathbb{M}_n$, too. This key property is crucial for application of the collocation method to the initial value problem (4.1)–(4.2).

The unknown coefficients a_k in approximation (4.3) are obtained from the initial condition

$$p_n(0) = p_0\ , \tag{4.4}$$

and the fact that $p_n(t)$ should satisfy the fractional differential equation in some suitably chosen collocation points ξ_j, $j = 1,2,\dots,n$. More precisely, the relation holds as follows:

$$p'(\xi_j) + F(\xi_j) D_*^{1/2} p(\xi_j) + G(\xi_j) p(\xi_j) = H(\xi_j). \tag{4.5}$$

Substituting (4.3) into (4.4), the equation

$$\sum_{k=0}^{n} a_k g_{k0} = p_0, \tag{4.6}$$

with $g_{k0} = L_k(0)$ is obtained. In its turn, equation (4.5) can be presented in form of n algebraic equations

$$\sum_{k=0}^{n} a_k g_{kj} = H(\xi_j), \quad j = 1,2,\dots,n, \tag{4.7}$$

where

$$g_{kj} = L_k'(\xi_j) + F(\xi_j) D_*^{1/2} L_k(\xi_j) + G(\xi_j) L_k(\xi_j).$$

Note that $L_k'(\xi_j)$ and $D_*^{1/2} L_k(\xi_j)$ in (4.7) can be computed by using the subsequent stable methods (5.3) and (5.8), respectively. The equations (4.6) and (4.7) are nothing else but a linear system of $n+1$ equations for the $n+1$ unknown coefficients a_k that can be solved by one of the known methods. Substituting the coefficients a_k into (4.3) leads to an approximated solution of the fractional initial value problem (4.1)–(4.2).

It should be noted that, the error analysis of the collocation method based on nonclassical polynomials is very complicated and is beyond the scope of this paper.

5. IMPLEMENTATION ISSUES

In this section, some details to provide additional insight on this new method are presented.

5.1. NUMERICAL EVALUATION OF $L_n(t)$ AND $D^{1/2}L_n(t)$

A direct evaluation of Müntz–Legendre polynomials in the form (3.1) can be problematic in finite arithmetic, especially when n is a large number and$x$ is close to 1. These problems have been addressed by Milovanović in [18]. He stated that the coefficients c_{nk} become very large when n increases, but their sums are always equal to 1.

Here, a stable method for evaluating the Müntz–Legendre polynomials defined by (3.2) is presented. The proposed technique is based on a three–term recurrence relation induced from the following theorem.

Proposition 5.1. ([12]) Let $L_n(t)$ be Müntz–Legendre polynomial defined by (3.2) and $t \in [0,1]$. Then

$$L_n(t) = P_n^{(0,1)}(2\sqrt{t} - 1), \tag{5.1}$$

holds true, where $P_n^{(0,1)}$ is a Jacobi polynomial.

Hence, in view of [21, (18.9.2)], the Müntz–Legendre polynomials $L_n(t)$ can be evaluated by means of the three–term recursion

$$b_{1n}L_{n+1}(t) = b_{2n}(t)L_n(t) - b_{3n}L_{n-1}(t), \qquad n \geq 1, \tag{5.2}$$

where $L_0(t) \equiv 1$, $L_1(t) = 3\sqrt{t} - 2$, and

$$b_{1n} = 2(n+1)(n+2)(2n+1),$$
$$b_{2n}(t) = 2(n+1)\big[(2n+1)(2n+3)\big(2\sqrt{t}-1\big) - 1\big],$$
$$b_{3n} = 2n(n+1)(2n+3).$$

Another result of Proposition 5.1 is a formula for evaluating $L_n'(t)$. More precisely, by means of [21, (18.9.15)] the first derivative of $L_n(t)$ is given by

$$L_n'(t) = \frac{n+2}{2\sqrt{t}} P_{n-1}^{(1,2)}\big(2\sqrt{t}-1\big). \tag{5.3}$$

Proposition 5.2. ([12]) Let $L_n(t)$ be Müntz–Legendre polynomial defined by (3.2) and $t \in [0,1]$. Then

$$D_*^{1/2}L_n(t) = \frac{n+2}{\sqrt{\pi}} \int_0^1 (1-x^2)^{-1/2} P_{n-1}^{(1,2)}\big(2x\sqrt{t}-1\big)dx, \tag{5.4}$$

holds true.

5.2. GAUSS–TYPE QUADRATURE RULES

An n–point quadrature rule for the weight function w is called a formula of the type

$$\int_a^b w(x)f(x)dx = \sum_{k=1}^{n} w_k f(x_k) + R_n[f], \tag{5.5}$$

where the sum on the right–hand side of the equation provides an approximation to the integral and R_n is the error. The numbers x_k, $k = 1, \dots, n$ are called *nodes* and w_k are called *weights* of the quadrature rule. Among all quadrature rules of the form (5.5) those of the Gaussian type have the best performance. More precisely, if nodes x_k and weights w_k are chosen in the way that quadrature rule (5.5) becomes exact for polynomials of degree at most $2n-1$, then this quadrature rule is called a Gauss–type quadrature rule. It can be proved that the nodes x_k in a Gaussian quadrature are the roots of the orthogonal polynomial $\pi(t;w)$ associated with the weight function and the weights w_k can be obtained from the following system of linear equations:

$$\sum_{k=1}^{n} w_k x_k^j = \int_a^b x^j w(x)dx, \qquad j = 0,1,\dots,2n-1. \tag{5.6}$$

As n increases, finding roots of $\pi(t;w)$ and solving the linear system (5.6) become an ill–conditioned and time consuming problem. Alternatively, the Golub–Welsch

algorithm to determine the nodes and the weights of a Gaussian quadrature can be used [15].

The construction of the Gaussian quadrature (5.5) for an arbitrary$n \geq 1$ can be realized very easy by MATHEMATICA package `OrthogonalPolynomials`[8,19]. Alternatively, for this purpose, there is also Gautschi's package `OPQ` written in MATLAB [14]. These packages provide many other calculations with orthogonal polynomials and different quadrature rules, and they are downloadable from Web Sites: `www.mi.sanu.ac.rs/~gvm/` and `www.cs.purdue.edu/archives/`, respectively.

To calculate the integral on the right–hand side of (5.4), N–point Gaussian quadrature rule

$$\int_0^1 (1-x^2)^{-1/2} f(x)dx = \sum_{k=1}^{N} w_k f(x_k), \quad f \in \mathbb{P}_{2N-1}, \tag{5.7}$$

is used. The weight function $w(x) = (1-x^2)^{-1/2}$ is a nonclassical one and no explicit formulae are known for x_k and w_k. However, the Chebyshev and Golub–Welsch algorithms to calculate the nodes and weights in (5.7) can be used [14, 15]. The quadrature rule (5.7) with $N = \lceil n/2 \rceil$ becomes exact for computing the integral in (5.4). The nodes and weights in the generalized Gaussian quadrature rule (5.7) are reported in Table 1.

Table 1: Nodes and weights in 10–point Gaussian quadrature rule (5.7).

Nodes x_k	Weights w_k
0.013428248384359	0.034319541263749
0.165229282898357	0.077205134746572
0.165088161001579	0.114617582317493
0.292182309608721	0.145264568917587
0.438817309663802	0.169221867374936
0.591551320859218	0.187274168806872
0.736030889552124	0.200396120129594
0.858545000002092	0.209464924712622
0.947393707327565	0.215148632394853
0.994059476652251	0.217883786130620

After obtaining the nodes x_k and weights w_k, the fractional derivative $D_*^{1/2} L_n(t)$ can be computed by using the formula

$$D_*^{1/2} L_n(t) = \frac{n+2}{\sqrt{\pi}} \sum_{k=1}^{\lceil n/2 \rceil} w_k \, P_{n-1}^{(1,2)}\left(2x_k\sqrt{t} - 1\right). \tag{5.8}$$

This section ends with a brief discussion of collocation points. Grid points for orthogonal collocation method should lie approximately in a minimal–energy configuration associated with inverse linear repulsion between points. Hence, a proper choice of collocation points is crucial for the accuracy of the numerical solution and for its computational stability [13, 25]. In the proposed case, a particularly convenient choice for the collocation points ξ_j is $\xi_j = t_j^2$, $j = 1, \dots, n$ where t_j are Chebyshev points associated with the interval $[0,1]$, i.e.,

$$t_j = \frac{1}{2}\left(1 - \cos\frac{\pi j}{n}\right), \quad j = 0,1, \dots, n .$$

6. NUMERICAL EXPERIMENTS

In this section, some numerical studies are presented to illustrate and test the behavior of the approach described in the Section 4. As is common, there is no comparison to other known methods. The main reason for this is that the numerical solution for this problem comes only in [23] and has a slow convergence. The following numerical experiments were implemented through MATHEMATICA and MATLAB.

Example 1. As the first experiment, given $\lambda = 8/(3\sqrt{\pi})$ and the change of gas volume $f(t) = 1 - \sqrt{t}$, then the initial value problem (2.4) has the analytical solution

$$p(t) = 1 + \sqrt{t} - \frac{1}{3}t + \left(\frac{32}{27\pi} - \frac{1}{3}\right)t\sqrt{t} .$$

The analytical and numerical solutions of this problem are plotted in Figure 2. Furthermore, to explore the dependence of errors on the discretization parameter n, the error in the ∞–norm is used. As it is seen, the presented method provides accurate results even with a few number of nodes.

Example 2. Consider the initial value problem (2.4) with $f(t) = 1 - t$. In this case, it is hard to find a closed form solution of (2.4). However, thanks to the work of Babenko [3, (7.25)], if the compression is slow ($\lambda \gg 1$), the following asymptotic representation for $p(t)$ is obtained:

$$p(t) = 1 + \frac{2\sqrt{t}}{\sqrt{\pi}}\frac{1}{\lambda} + \left(\frac{3}{2}t - 1\right)\frac{1}{\lambda^2} + \mathcal{O}\left(\frac{1}{\sqrt{t}\lambda^3}\right), \quad t > 0 . \tag{6.1}$$

Moreover, in the case of rapid compression ($\lambda \ll 1$), a similar expression in powers of λ can be obtained [3, (7.26)] as follows:

$$p(t) = \frac{1}{1-t} + \frac{2}{\sqrt{\pi}}\left(\frac{\sqrt{t}}{1-t} - \frac{\sin^{-1}\sqrt{t}}{(1-t)^{3/2}}\right)\lambda + \mathcal{O}\left(\frac{\lambda^2}{(1-t)^2}\right), \quad t < 1 . \tag{6.2}$$

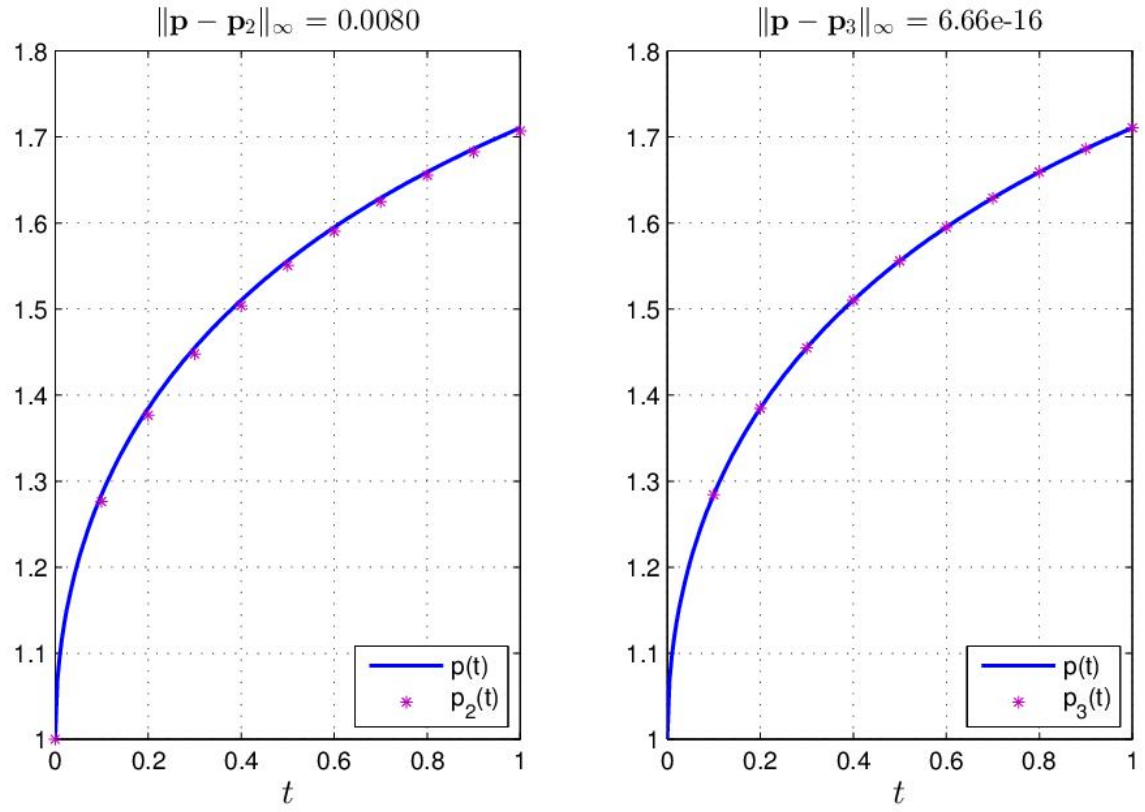

Figure 2: Analytical and numerical solutions of problem (2.4) (Example 1).

In Figure 3, the numerical and asymptotic solutions of problem (2.4) are illustrated. These results indicate that the approximate solutions of the present method are in agreement with asymptotic solutions. It can be shown that the maximum pressure, p_{max}, occurs at $t = 1$. On the other hand, from (6.1), the following asymptotic expression is obtained

$$p(t) \approx 1 + \frac{2}{\sqrt{\pi}}\frac{1}{\lambda} + \frac{1}{2}\frac{1}{\lambda^2} + \mathcal{O}(1)\frac{1}{\lambda^3}, \quad \lambda \to \infty . \tag{6.3}$$

The numerical solutions for various values of n are reported in Table 2. As tabulated, the asymptotic expression (6.3) as a reference "exact" solution is used. It can be seen that the presented method provides accurate results and indicate an exponential decay.

Table 2: Numerical solutions at $t = 1$ and related errors with $\lambda = 5$ (Example 2).

n	5	10	15	20	25	30
$p_n(1)$	1.2457842	1.2456764	1.2456758	1.2456758	1.2456758	1.2456758
Error	1.08(–04)	5.93(–07)	2.19(–09)	5.89(–12)	1.24(–14)	2.22(–16)

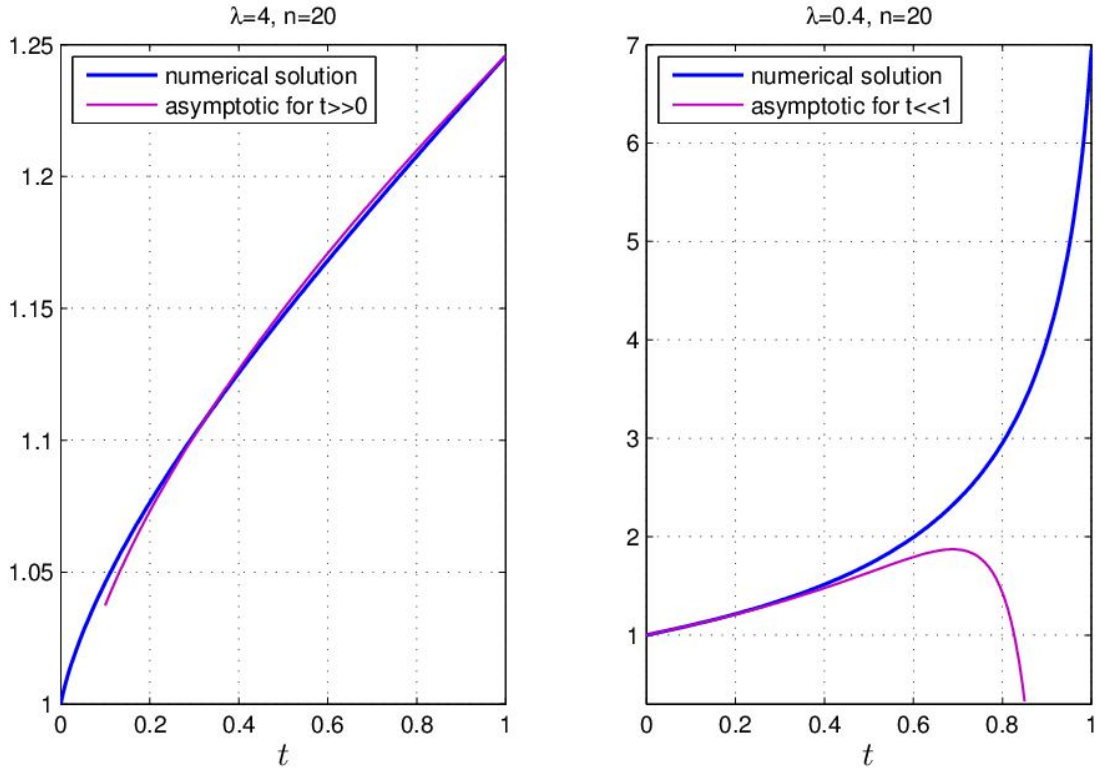

Figure 3. Numerical and asymptotic solutions of problem (2.4): slow compression (left) and rapid compression (right) (Example 2).

7. CONCLUSION

In this paper, a computational technique based on the Müntz polynomials for solution of mathematical model of gas solution in a fluid is presented. The exact solution of this problem can contain some fractional–power terms with which the Müntz polynomials can match. An appropriate representation of the solution based on the Müntz polynomials reduces its numerical treatment to the solution of a linear system of algebraic equations. The numerical results obtained by the new method indicated the effectiveness of the proposed approach.

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Numerical Solution of Gas Solution in a Fluid: Fractional Derivative Model

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حل عددی مسألهٔ محلول گاز در یک سیال: مدل مشتق کسری

ادیتور رابط : علیرضا اشرفی

چکیده

یک روش محاسباتی برای حل مدل ریاضی محلول گاز در یک سیال ارائه می‌شود. این مدل، تغییر جرم حجمی گاز انتشاریافته بر اثر تماس با سطح سیال را توصیف می‌کند. یک نمایش مناسب از جواب بر پایهٔ چندجمله‌ایهای مونتس، حل عددی مسأله را به حل یک دستگاه خطی از معادله‌های جبری تبدیل می‌کند. چند مثال عددی نیز برای تأیید دقت و کارایی این روش ارائه شده است.

لغات کلیدی: مشتق‌های کسری، محلول گاز، چندجمله‌ایهای مونتس، چهارگوشهٔ گاوسی، روش هم‌مکانی