NUMERICAL SIMULATION OF 3-D FRACTIONAL-ORDER CONVECTION-DIFFUSION PDE BY A LOCAL MESHLESS METHOD

by

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In this article, we present an efficient local meshless method for the numerical treatment of 3-D convection-diffusion PDE. The demand of meshless techniques increment because of its meshless nature and simplicity of usage in higher dimensions. This technique approximates the solution on set of uniform and scattered nodes. The space derivatives of the models are discretized by the proposed meshless procedure though the time fractional part is discretized by Liouville-Caputo fractional derivative. Some test problems on regular and irregular computational domains are presented to verify the validity, efficiency, and accuracy of the method.

Key words: Liouville-Caputo derivative, meshless method, radial basis function, convection-diffusion equation, irregular domain

Introduction

Fractional calculus has attracted significant interests in the field of engineering and applied sciences in the last few years. The elementary knowledge of fractional calculus can be found in [1, 2]. Fractional differential equations contain derivatives of any complex or real order, being considered as general form of differential equations. The comprehensive applications in real world problems are described by fractional PDE and it is found to be an effective tool in interpretation and modeling of numerous problems appear in physics and applied mathematics [3-8].

Recently, a great effort has been expended to develop the exact and approximate behavior of fractional PDE. In this effort several enthusiastic methods have been applied for the solution of fractional PDE such as homotopy analysis method [9, 10], expansion methods [11, * Corresponding author, e-mail: harimsri@uvic.ca
12], homotopy analysis transform method [13], fractional difference method [14], operational method [15], variational iteration method [5, 16-18], homotopy perturbation method [19], direct approach [20, 21], Lie symmetry analysis [22], differential transform method [23], reproducing kernel method [24], extended differential transform [25], local fractional Riccati differential equation method [26], meshless methods [27, 28] and Chebychev spectral method [29].

Different types of meshless techniques have been got expansive consideration for tackling diverse kind of PDE model arises in almost all disciplines of engineering. Especially the radial basis functions (RBF) based meshless methods are one of the most popular type among these methods. The meshless methods, consider a set of scattered and uniform data points on the domain in contrast to some classical mesh-based techniques such as finite difference and finite element methods. Therefore these processes do not require to mesh the domain. Moreover, the uses of RBF [30] increase advantages and preferences of technique due to this property that the RBF only depend on the Euclidian distance between two points of the spatial domain. According to these facts, meshless methods are known as very flexible and useful mathematical tools which can be applied to high dimensional models with irregular and complicated domains. Meshless collocation technique based on the RBF is one of the very popular strong-form meshless methods which is widely employed to many practical problems [31, 32]. Although the classical meshless collocation method based on the globally supported RBF is known as a very efficient computational technique to deal with complicated and high dimensional PDE, but the method leads to an ill-conditioned and dense system of algebraic equations. In the global meshless method, the RBF are used to obtain the coefficients, so that the derivatives of a function \( f(x) \) can be written as a linear combination of the functional values at the predetermined nodes. This numerical scheme is simple and effective. However, the approximation can become unstable as the number of collocation points become large resulting in dense matrices. This leads to ill-conditioning and sensitivity to the shape parameters in the RBF formulation. Unfortunately, this ill-conditioning and computational cost of implementation of the technique will increase dramatically by increasing number of the scattered data points. To ward off these deficiencies, the researchers suggested local meshless method (LMM) [33, 34].

The LMM use only neighboring collocation points and it does not have the typical ill-conditioning that comes with large dense matrix systems. Additionally, in such RBF based meshless techniques, the proper selection of RBF as well as shape parameter value play a crucial rule in the convergence. Among these RBF, the multiquadric (MQ) is perhaps the most popular that is used in applications. This is due to its high convergence rate and accuracy. Perhaps a disadvantage that the MQ RBF has as compared to the polyharmonic splines is that the accuracy depends on the correct choice of the shape parameter. The same disadvantage applies to the inverse multiquadric (IMQ) and the Gaussian (GA) RBF as well. Finding the appropriate shape parameter is an ongoing research problem. In local methods, the shape parameter does not vary much, which is beneficial in choosing a good value. Another advantage of the local technique is that the accuracy is not compromised by the computational efficiency. Unlike the global approach where it is required to work with a dense matrix, the local technique results in a sparse matrix which can be solved accurately and efficiently.

In the recent literature, LMM are used for better numerical approximation of complex PDE models [35, 36]. Meshless techniques using RBF are viable alternate numerical mechanisms used for solutions of different types of complicated linear, non-linear, integer and fractional order PDE arising in science and engineering. Different variants of meshless procedures are reported in the literature. Some of the reported work include Mohebbi et al. [37] time fractional non-linear Schrodinger equation, Piret and Hanert [38] fractional diffusion equations,
Mohebbi et al. [39] 2-D modified anomalous fractional sub-diffusion equation, Hosseini et al. [40] fractional telegraph equation, Wei et al. [41] 2-D time fractional diffusion equations, Ghehsareh et al. [42] 2-D fractional evolution equation, Aslefallah and Shivanian [43] non-linear time-fractional integro-differential reaction-diffusion equation, Kumar et al. [44] time fractional diffusion wave equation. Current research work is devoted to use the LMM for the numerical investigation of 3-D time-fractional convection-diffusion and Burgers’ equations. The space derivatives are approximated by the local meshless procedure using the inverse quadratic (IQ), MQ, and the GA radial basis functions whereas time fractional part is approximated by using Liouville-Caputo definition. Both rectangular and non-rectangular geometries are considered in numerical experiments.

Consider the unsteady time fractional linear convection-diffusion PDE:

\[
\frac{\partial^\alpha W(\bar{z},t)}{\partial t^\alpha} = \beta V W(\bar{z},t) + \gamma \Delta W(\bar{z},t) + F(\bar{z},t) = LW(\bar{z},t), \quad \bar{z} \in \Omega, \quad 0 < \alpha \leq 1, t > 0
\]  

(1)

with the following initial-boundary conditions:

\[
W(\bar{z},0) = W_0
\]  

(2)

\[
\frac{\partial \xi(\bar{z},t)}{\partial t} = g_1(\bar{z},t), \quad \bar{z} \in \partial \Omega
\]  

(3)

where \( \beta \) is the diffusion coefficient, and \( \gamma \) the real constants.

Similarly, the time fractional Burgers’ equation:

\[
\frac{\partial^\alpha W(\bar{z},t)}{\partial t^\alpha} = \beta V W(\bar{z},t) - \frac{1}{2} \frac{\partial W^2(\bar{z},t)}{\partial x} - \frac{\partial}{\partial x} \left[ \frac{3}{2} W(\bar{z},t) - \frac{1}{2} \frac{\partial W^2(\bar{z},t)}{\partial y} \right] - \frac{\partial}{\partial z} \left[ \frac{3}{2} W(\bar{z},t) - \frac{1}{2} \frac{\partial W^2(\bar{z},t)}{\partial z} \right] \quad \bar{z} \in \Omega, \quad 0 < \alpha \leq 1, t > 0
\]  

(4)

with the following initial-boundary conditions:

\[
W(\bar{z},0) = W_0
\]  

(5)

\[
\frac{\partial \xi(\bar{z},t)}{\partial t} = g_2(\bar{z},t), \quad \bar{z} \in \partial \Omega
\]  

(6)

where \( \beta \) is a diffusion coefficient.

**Scheme of the LMM**

The LMM [33] is extended to the time fractional convection-diffusion models. The derivatives of \( W(\bar{z},t) \) are approximated at the centers \( \bar{z}_h \) by the neighborhood of \( \bar{z}_h \), \( \{\bar{z}_h, \bar{z}_{h+1}, \bar{z}_h+1, ..., \bar{z}_{h+n} \} \subset \{\bar{z}_1, \bar{z}_2, ..., \bar{z}_n \} \), \( n_h \ll N^n \), where \( h = 1, 2, ..., N^n \). In case of 1-D, \( \bar{z} = x \), and for 2-D, \( \bar{z} = (x, y) \) and for 3-D case, \( \bar{z} = (x, y, z) \). Now, in 1-D case, we have:
By substituting RBF $\psi(\|x - x_p\|)$ in eq. (7), we have:

$$
\psi^{(m)}(\|x - x_p\|) = \sum_{k=1}^{n_h} \lambda_k^{(m)} \psi(\|x_{hk} - x_p\|), \quad p = h_1, h_2, \ldots, h_{n_h} \tag{8}
$$

where

$$
\psi(\|x_{hk} - x_p\|) = \exp(-\|x_{hk} - x_p\|^2 / \sigma^2), \quad \psi(\|x_{hk} - x_p\|) = [1 + (c \|x_{hk} - x_p\|^2)]^{-1}, \text{ and}
$$

$$
\psi(\|x_{hk} - x_p\|) = \sqrt{1 + (c \|x_{hk} - x_p\|^2)}
$$
in case of GA, IQ, and MQ RBF, respectively.

Matrix form of eq. (8) is:

$$
\mathbf{\psi}_m = \mathbf{A}_n \mathbf{\lambda}_n^{(m)}
$$

where $\psi_p(x_k) = \psi(\|x_k - x_p\|), p = h_1, h_2, \ldots, h_{n_h}$, for each $k = h_1, h_2, \ldots, h_{n_h}$. Equation (9) can be written:

$$
\mathbf{\psi}_m = \mathbf{A}_n \mathbf{\lambda}_n^{(m)} \tag{10}
$$

From eq. (10), we obtain:

$$
\mathbf{\lambda}_n^{(m)} = \mathbf{A}_n^{-1} \mathbf{\psi}_m \tag{11}
$$

Equations (7) and (11) imply:

$$
W^{(m)}(x_h) = [\mathbf{\lambda}_n^{(m)}]^{T} \mathbf{W}_n
$$

where

$$
\mathbf{W}_n = [W(x_{h1}), W(x_{h2}), \ldots, W(x_{h_{n_h}})]^{T}
$$

In case of 2-D, the derivatives of $W(x, y, t)$ regarding $x$ and $y$ are approximated in the comparative manner:

$$
W^{(m)}_x(x_h, y_h) = \sum_{k=1}^{n_h} \lambda_k^{(m)} W(x_{hk}, y_{hk}), \quad h = 1, 2, \ldots, N^2 \tag{12}
$$

$$
W^{(m)}_y(x_h, y_h) = \sum_{k=1}^{n_h} \lambda_k^{(m)} W(x_{hk}, y_{hk}), \quad h = 1, 2, \ldots, N^2 \tag{13}
$$
To find out the relating coefficients $\gamma_k^{(m)}$ and $\eta_k^{(m)}$ ($k = 1, 2, \ldots, n_h$), we continue:

$$
\gamma_k^{(m)} = A_{n_h}^{-1} \Phi_k^{(m)} \\
\eta_k^{(m)} = A_{n_h}^{-1} \Phi_k^{(m)}
$$

(14)

(15)

The previous technique can be rehashed for 3-D case, etc.

In 3-D geometries the local central stencils are developed around each center $z_h$ whose schematic is appeared in fig. 1.

**Discretization of time derivatives**

The time derivative $[\partial^\alpha W(z,t)]/\partial t^\alpha$ is discretized by using Liouville-Caputo derivative [48]. The Liouville-Caputo fractional derivative for $\alpha \in (0,1)$ is:

$$
\frac{\partial^\alpha W(z,t)}{\partial t^\alpha} = \left\{ \begin{array}{ll}
\frac{1}{\Gamma(1-\alpha)} \int_0^t \partial W(z,\vartheta) (t-\vartheta)^{-\alpha} \, d\vartheta, & 0 < \alpha < 1 \\
\frac{\partial W(z,t)}{\partial t} & \alpha = 1
\end{array} \right.
$$

For the interval $[0,t]$, $Q + 1$ is considered as equally spaced time intervals $t_0, t_1, \ldots, t_Q$, such that $t_q = qt$, $n = 0, 1, 2, \ldots, Q$, $\tau$ is the time step and to approximate the first-order derivative involved in the time fractional term, finite difference scheme is used:

$$
\frac{\partial^\alpha W(z,t_{q+1})}{\partial t^\alpha} = \frac{1}{\Gamma(1-\alpha)} \int_0^{t_{q+1}} \partial W(z,A)/(t_{q+1}-\vartheta)^{-\alpha} \, d\vartheta
$$

$$
= \frac{1}{\Gamma(1-\alpha)} \sum_{s=0}^{q} \int_{st}^{(s+1)t} \partial W(z,A)/(t_{s+1}-\vartheta)^{-\alpha} \, d\vartheta
$$

$$
= \frac{1}{\Gamma(1-\alpha)} \sum_{s=0}^{q} \int_{st}^{(s+1)t} \partial W(z,A)/(t_{s+1}-\vartheta)^{-\alpha} \, d\vartheta
$$

The term $[\partial W(z,\vartheta)]/\partial \vartheta$ is approximated:

$$
\frac{\partial W(z,\vartheta)}{\partial \vartheta} = \frac{W(z,\vartheta_{s+1}) - W(z,\vartheta_s)}{\vartheta} + \mathcal{O}(\tau)
$$

Then
\[
\frac{\partial^\alpha W(\bar{z}, t_{q+1})}{\partial t^\alpha} \approx \frac{1}{\Gamma(1-\alpha)} \sum_{s=0}^{q} \frac{W(\bar{z}, t_{s+1}) - W(\bar{z}, t_s)}{\tau} \int_{s}^{(s+1)\tau} (t_{s+1} - \theta)^{-\alpha} \, d\theta \\
= \frac{1}{\Gamma(1-\alpha)} \sum_{s=0}^{q} \frac{W(\bar{z}, t_{q+1-s}) - W(\bar{z}, t_{q-s})}{\tau} \int_{s}^{(s+1)\tau} (t_{s+1} - \theta)^{-\alpha} \, d\theta \\
= \left( \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} (W^{q+1} - W^q) + \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \sum_{s=1}^{q} (W^{q+1-s} - W^{q-s}) [(s + 1)^{1-\alpha} - s^{1-\alpha}] \right), \quad q \geq 1 \\
= \left( \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} (W^1 - W^0) \right), \quad q = 0
\]

Letting \( a_0 = \tau^{-\alpha}/[\Gamma(2-\alpha)] \) and \( b_s = (s + 1)^{1-\alpha} - s^{1-\alpha}, \ s = 0, 1, \ldots, q \), we can write the above equation in more precise form:

\[
\frac{\partial^\alpha W(\bar{z}, t_{q+1})}{\partial t^\alpha} \approx \begin{cases} 
  a_0(W^{q+1} - W^q) + a_0 \sum_{s=1}^{q} b_s (W^{q+1-s} - W^{q-s}), & q \geq 1 \\
  a_0(W^1 - W^0), & q = 0
\end{cases}
\]

**Numerical results**

In this section, the numerical results of the 3-D time fraction convection-diffusion model equations using the proposed LMM. The GA, IQ, and MQ RBF are used for space discretization in all numerical simulation. All numerical experiments are performed using local supported domain \( n_i = 7 \). All the computations are performed on HP (ProBook) PC Laptop with an Intel(R) Core(TM) i5-4210M CPU 2.60 GHz, 2.60 GHz 4 GB RAM. The accuracy is measure through \( |\varepsilon| \), \( \max(\varepsilon) \), and \( \varepsilon \) norms which are define:

\[
|\varepsilon| = |\hat{W} - W|, \\
\max(\varepsilon) = \max(|\varepsilon|), \\
\varepsilon = \sqrt{\frac{\sum_{i=1}^{N} (\hat{W}_i - W_i)^2}{\sum_{i=1}^{N} (\hat{W}_i)^2}}
\]

where \( \hat{W} \) is exact solution and \( W \) is the approximate solution.

**Test problem 1.** Consider eq. (1) as 3-D unsteady convection-diffusion having exact solution for \( \alpha = 1 \):

\[
W(\bar{z}, t) = e^{(Dt-E(x+y+z))}, \quad t \geq 0, \quad (x, y, z) \in [-1,1]^3
\]

where \( E = \sqrt{(D/6)} \), \( D = 1/10 \), \( F(\bar{z}, t) = 0 \), and \( \gamma = (-E, -E, -E) \).

The numerical results for Test problem 1 are obtained by the LMM in explicit form and are shown in tab. 1. Three different RBF (GA, IQ, and MQ) with shape parameter value
$c = 100$, are used. The error is measured in terms of $\max(\varepsilon)$ and $\varepsilon$ for this test problem by taking different nodes $N$, time step size $\tau = 0.002$ and final time $t = 1$. This shows that the suggested method gives good accuracy and also we can observe that the accuracy of mentioned RBF are all most the same. A comparison of exact and numerical results are shown in fig. 2(a), while in fig. 2(b) for different values of $\alpha$ the results are shown for $x = y = z$.

Table 1. Numerical results of convection-diffusion equation for Test problem 1

<table>
<thead>
<tr>
<th>RBF</th>
<th>$N = 125$</th>
<th>$N = 512$</th>
<th>$N = 1331$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\max(\varepsilon)$</td>
<td>$\varepsilon$</td>
<td>$\max(\varepsilon)$</td>
</tr>
<tr>
<td>GA</td>
<td>$1.0325 \cdot 10^{-5}$</td>
<td>$1.3020 \cdot 10^{-6}$</td>
<td>$2.0926 \cdot 10^{-7}$</td>
</tr>
<tr>
<td>IQ</td>
<td>$1.1047 \cdot 10^{-5}$</td>
<td>$1.3935 \cdot 10^{-6}$</td>
<td>$2.2963 \cdot 10^{-7}$</td>
</tr>
<tr>
<td>MQ</td>
<td>$1.0109 \cdot 10^{-5}$</td>
<td>$1.2746 \cdot 10^{-6}$</td>
<td>$1.9962 \cdot 10^{-7}$</td>
</tr>
</tbody>
</table>

Figure 2. Numerical solution of the LMM using GA RBF at $t = 1$ for Test problem 1

Test problem 2. Consider eq. (1) with $\gamma = 0$, having exact solution for $\alpha = 0.9$ is given:

$$W(x, y, z, t) = t^2 e^{(x+y+z)} , \quad t \geq 0, \quad (x, y, z) \in [0,1]^3$$

and the source term is:

$$F(x, y, z, t) = \frac{\Gamma(3)}{\Gamma(2.1)} t^{1.1} e^{(x+y+z)} - 3t^2 e^{(x+y+z)}$$

The numerical results for the Test problem 2 using GA RBF in terms of $\max(\varepsilon)$ and $\varepsilon$ norms, are described in tab. 2 for shape parameter value $c = 10$ and $t = 1$. It can be seen in this test problem as well that the LMM gives accurate results.

Table 2. Simulation results of the LMM for Test problem 2

<table>
<thead>
<tr>
<th>RBF</th>
<th>$N = 125$</th>
<th>$N = 216$</th>
<th>$N = 512$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\max(\varepsilon)$</td>
<td>$\varepsilon$</td>
<td>$\max(\varepsilon)$</td>
</tr>
<tr>
<td>GA</td>
<td>$8.5305 \cdot 10^{-4}$</td>
<td>$9.3340 \cdot 10^{-5}$</td>
<td>$6.0538 \cdot 10^{-4}$</td>
</tr>
</tbody>
</table>
A comparison of exact and numerical results using GA RBF for \( N = 125 \) at \( t = 0.5 \), and taking the values of \( z = 0, 0.25, 0.5, 0.75, \) and 1 are shown in fig. 3. This figure is also the evidence of the proposed method for better accuracy. The error, \( |\varepsilon| \), are also shown in fig. 4 using \( N = 729 \) and \( T = 0.5 \). The LMM is testified on irregular domain with non-uniform nodes as shown in fig. 5. The numerical results are shown in tab. 3 for different final time. It is clear from the table that the LMM gives good numerical results irrespective of the domain and node points.

**Figure 3.** Numerical solution of the LMM using GA RBF taking \( N = 125 \) and \( z = 0, 0.25, 0.5, 0.75, \) and 1 for Test problem 2

**Figure 4.** Error in term of \( |\varepsilon| \) of the LMM using IQ (a) and MQ (b) at \( z = 0.5 \) for Test problem 2

**Test problem 3.** Consider the 3-D Burgers’ eq. (4). For \( \alpha = 1 \) the exact solutions is:

\[
W(\bar{z},t) = 1 - \frac{1}{2} \left[ 1 + \exp \left( \frac{-3t - x + y + z}{4\beta} \right) \right]^{-1}, \quad t \geq 0, \quad (x, y, z) \in [0,1]^3
\]  

(19)

Figure 6 shows \( |\varepsilon| \) error norm of the LMM by taking \( N = 1331 \) and \( \beta = 1 \) for Test problem 3. The figure shows that the proposed LMM gives good results in this test problem as well for all the three RBF. The numerical results for computational domain given in fig. 5 in terms of \( \max(\varepsilon) \) and \( \varepsilon \) error norms for Test problem 3 are given in tab. 4 with \( \beta = 1 \) and
$N = 2046$. Figure 7 shows the exact vs. numerical solution of the LMM which is self explanatory. The numerical results for $N = 9261$, $\beta = 0.02$, $\alpha = 0.8$, and $\alpha = 0.9$ are shown in fig. 8 at different values of $z = 0, 0.2, 0.4, 0.6, 0.8, \text{ and } 1$.

Table 3. Numerical results on computational domain in fig. 5 for Test problem 2

<table>
<thead>
<tr>
<th>RBF</th>
<th>$T = 0.1$</th>
<th>$T = 0.5$</th>
<th>$T = 1$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\varepsilon$</td>
<td>$\varepsilon$</td>
<td>$\varepsilon$</td>
</tr>
<tr>
<td>GA</td>
<td>$1.1749 \cdot 10^{-4}$</td>
<td>$3.914 \cdot 10^{-3}$</td>
<td>$4.5966 \cdot 10^{-4}$</td>
</tr>
<tr>
<td></td>
<td>$2.6781 \cdot 10^{-4}$</td>
<td>$4.5966 \cdot 10^{-4}$</td>
<td>$1.4041 \cdot 10^{-2}$</td>
</tr>
</tbody>
</table>

Table 4. Simulation results on computational domain in fig. 5 for Test problem 3

<table>
<thead>
<tr>
<th>RBF</th>
<th>$T = 0.1$</th>
<th>$T = 0.5$</th>
<th>$T = 1$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\varepsilon$</td>
<td>$\varepsilon$</td>
<td>$\varepsilon$</td>
</tr>
<tr>
<td>MQ</td>
<td>$6.8692 \cdot 10^{-5}$</td>
<td>$1.5408 \cdot 10^{-5}$</td>
<td>$3.4544 \cdot 10^{-4}$</td>
</tr>
<tr>
<td></td>
<td>$1.4177 \cdot 10^{-5}$</td>
<td>$7.5077 \cdot 10^{-5}$</td>
<td>$1.6527 \cdot 10^{-4}$</td>
</tr>
</tbody>
</table>

Figure 5. Computational domain with non-uniform nodes [34]

Figure 6. Error in term of $|\varepsilon|$ at $x = y = z$ for Test problem 3

Figure 7. Exact vs. numerical solutions with $\beta = 0.02$ at $z = 0.5$ for Test problem 3
Conclusion

In this work, we have applied a local meshless method based on RBF as a modern powerful numerical method to investigate 3-D time dependent fractional convection-diffusion PDE models. The time derivative part is defined and simplified in Liouville-Caputo sense and the scheme is constructed for $0 < \alpha < 1$. Various test problems have been considered on regular and irregular domains to check the accuracy of the proposed scheme. The numerical results are the evidence that the suggested LMM is a flexible interpolation method as it produce the coefficient matrix well-conditioned. In light of the current work we can say that the proposed technique is powerful and effective to find the numerical solutions of 3-D time dependent fractional PDE, so it can be also applied to a wide range of complex problems that occur in natural sciences and engineering.

References


