



Research Paper

The generalized moving least squares technique combined with a Householder transformation for computing the first derivatives on the sphere

Vahid Mohammadi*

Department of Mathematics, Faculty of Science, Shahid Rajaee Teacher Training University, Tehran, 16785-163, I. R. Iran

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Abstract. We present a new and simple direct approach based on generalized moving least squares (GMLS) for computing the first derivatives of the functions defined on the sphere. The novel method utilizes a Householder transformation (reflection) and a projection onto the tangent plane to compute the first derivatives at the original point on the sphere. The main benefit of this algorithm is that there is no need to use the spherical harmonics for constructing the approximation of the first derivatives. An example of the approximation has been tested to show the ability of the developed method. Moreover, this method has been applied to solve the transport equation in one example.

Keywords: generalized moving least squares approximation, a Householder reflection transport equation

Mathematics Subject Classification (2010): 33E30.

1 Introduction

One of the most important meshless techniques (e.g. [8–11, 26]) is the GMLS approximation (or called a direct approximation) [18], which it is applied for solving partial differential equation (PDE)

*Email address: vahid.mohammadi@sru.ac.ir

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problems arising in branches of the applied science in recent years. This method was first introduced by Mirzaei and his co-authors in 2012 for approximating the real-valued functions defined in $\Omega \subset \mathbb{R}^d$ ($d \geq 1$) [17]. To find the approximate value of the real-valued functions defined on S^2 , this method has been developed by Mirzaei in 2017 [18]. This approach is called *generalized finite difference scheme* such that it can be implemented for scattered data points on each local sub-domain [18, 22]. There are different mathematical models formulated on the sphere, which have important applications in geophysics. For example, the transport equation on S^2 has many applications, which can be found in [1–3, 12, 13, 16, 21]. Over the past two decades, there are diverse numerical methods for finding the numerical solution of the PDE problems on the sphere in both Cartesian and spherical coordinates such as *continuous and discontinuous Galerkin (DG) methods* [24], *radial basis functions (RBFs)* [5], a type of semi-Lagrangian scheme [14], stabilized RBF-generated finite difference (RBF-FD) technique [6], semi-Lagrangian idea applied in three types of RBFs method [23], the GMLS approximation [19] and spline-based RBF-FD with polynomials [7].

In this investigation, we employ a new approach based on a recent work in [7] for computing the first derivatives of the function on S^2 via the GMLS approximation. Unlike the radial basis functions (RBFs) interpolation, the GMLS technique does not depend on the constant parameter, namely *shape parameter* that affects both the *stability* and *accuracy* of the approximation (cf. [4, 25]). Besides, the novel method overcomes some difficulties of employing the original GMLS technique on the sphere [18]. First, the computational cost can be reduced in approximating the first derivatives of a given function defined on the sphere. Of course, we do not report here for brevity. Second, there is no need to use *the spherical harmonics* to construct the approximation.

The rest of this paper is organized as follows. In Section 2, a brief discussion of the GMLS approximation in \mathbb{R}^2 proposed in [17] is given. The novel method is discussed in Section 3. In Section 4, some numerical results are presented to show the ability of the developed numerical method. This paper is ended with a conclusion given in Section 5.

2 The GMLS approximation in two-dimensional space

Here, we briefly review the GMLS approximation, which was introduced in [17]. To seek more details on this subject, the interested reader can refer to [17]. Suppose that $u \in C^{k+1}(\Omega)$ for some $k \geq 0$, where $\Omega \subset \mathbb{R}^2$. Also, $\lambda \in C^{k+1*}(\Omega)$ is assumed to be a linear functional, in which $C^{k+1*}(\Omega)$ represents the dual space of $C^{k+1}(\Omega)$. The main idea of the GMLS is to approximate λu by $\widehat{\lambda u}$ at each point $\mathbf{x} \in \Omega$ via the function values $u(\mathbf{x}_1), u(\mathbf{x}_2), \dots, u(\mathbf{x}_N)$ computed at a set of N points $X = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\}$, which is a *quasi-uniform* nodes set on Ω (cf. [25]). Hence, we have [17]

$$\lambda u(\mathbf{x}) \approx \widehat{\lambda u}(\mathbf{x}) = \sum_{j \in I(\mathbf{x})} a_{j,\lambda}(\mathbf{x}) u(\mathbf{x}_j) = \mathbf{a}_{\lambda}^T(\mathbf{x}) \mathbf{u}_X. \quad (1)$$

In (1), $I(\mathbf{x}, \delta, X) \equiv I(\mathbf{x}) := \left\{ j \in \{1, 2, \dots, N\} : \|\mathbf{x} - \mathbf{x}_j\|_2 \leq \delta \right\}$ is defined as a set of indices around point \mathbf{x} , where δ is the radius of supporting \mathbf{x} . Also, $\mathbf{u}_X =: [u(\mathbf{x}_j)]_{1 \leq j \leq N}$, and the vector $\mathbf{a}_{\lambda}^T(\mathbf{x})$ is given by the following representation (see [17] for more details)

$$\mathbf{a}_{\lambda}^T(\mathbf{x}) = \lambda(\mathbf{p}(\mathbf{x}))^T (P^T W P)^{-1} P^T W, \quad (2)$$

in which $\lambda(\mathbf{p}(\mathbf{x})) = [\lambda(p_1(\mathbf{x})), \lambda(p_2(\mathbf{x})), \dots, \lambda(p_Q(\mathbf{x}))]^T$, $p_i(\mathbf{x}), i = 1, \dots, Q$ with $Q = \binom{k+2}{2}$, where k is the most degree of the basis polynomial functions. Besides, in Eq. (2)

$$\begin{aligned}\mathbf{p}(\mathbf{x})^T &= [p_1(\mathbf{x}), p_2(\mathbf{x}), \dots, p_Q(\mathbf{x})], \quad P = P(\mathbf{x}) = (p_k(\mathbf{x}_j)) \in \mathbb{R}^{|I(\mathbf{x})| \times Q}, \\ W &= W(\mathbf{x}) = \text{diag}\{w(\mathbf{x}, \mathbf{x}_j)\} \in \mathbb{R}^{|I(\mathbf{x})| \times |I(\mathbf{x})|}, \quad A(\mathbf{x}) := P^T WP,\end{aligned}\quad (3)$$

In (3), the weight function, i.e., w is defined as follows

$$w(\mathbf{x}, \mathbf{x}_j) = \phi\left(\frac{\|\mathbf{x} - \mathbf{x}_j\|_2}{\delta}\right), \quad (4)$$

where ϕ is a radial function with $r := \frac{\|\mathbf{x} - \mathbf{x}_j\|_2}{\delta}$ and compactly supported in $[0, 1]$ (cf. [25, Chapter 9]). In this article, we consider $\phi(r) := r^{-2}$, which gives an interpolant form of the GMLS technique [15]. Now, in order to compute the approximation values of $\frac{\partial u}{\partial x}$ and $\frac{\partial u}{\partial y}$ at point $\mathbf{x} \in \Omega$ using Eq. (1), we have

$$\widehat{\frac{\partial u(\mathbf{x})}{\partial x}} = \sum_{j \in I(\mathbf{x})} \frac{\partial a_j(\mathbf{x})}{\partial x} u(\mathbf{x}_j) = \frac{\partial \mathbf{a}^T(\mathbf{x})}{\partial x} \mathbf{u}_X = \frac{\partial \mathbf{p}^T(\mathbf{x})}{\partial x} (P^T WP)^{-1} P^T W \mathbf{u}_X, \quad (5)$$

and

$$\widehat{\frac{\partial u(\mathbf{x})}{\partial y}} = \sum_{j \in I(\mathbf{x})} \frac{\partial a_j(\mathbf{x})}{\partial y} u(\mathbf{x}_j) = \frac{\partial \mathbf{a}^T(\mathbf{x})}{\partial y} \mathbf{u}_X = \frac{\partial \mathbf{p}^T(\mathbf{x})}{\partial y} (P^T WP)^{-1} P^T W \mathbf{u}_X,$$

where $\mathbf{x} \in \Omega$. Note that, the above procedure for computing the first derivatives is called the direct approximations because the linear operators such as $\frac{\partial}{\partial x}$ and $\frac{\partial}{\partial y}$ act only on the polynomial basis functions [17].

3 The novel approach

Assume that $u : \mathbb{S}^2 \rightarrow \mathbb{R}$ is a $C^1(\mathbb{S}^2)$ function. Also, a set of points $X = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\}$ is scattered on \mathbb{S}^2 . Our goal is to approximate $\frac{\partial u(\mathbf{x})}{\partial x}$, $\frac{\partial u(\mathbf{x})}{\partial y}$ and $\frac{\partial u(\mathbf{x})}{\partial z}$ at the point $\mathbf{x} = \mathbf{x}_1 \in \mathbb{S}^2$, where $\frac{\partial}{\partial x}$, $\frac{\partial}{\partial y}$ and $\frac{\partial}{\partial z}$ are restricted to \mathbb{S}^2 . In [18], these derivatives have been obtained through the GMLS approximation on \mathbb{S}^2 . However, here we apply a new approach based on *Householder reflections*, where the GMLS approximation in two dimensions presented in the previous section is utilized. We now give the details of the algorithm in the following four steps.

- The first step is to find n nearest points to \mathbf{x}_1 . This can be done by a kd-tree search [7] (Step 1 of Figure 1.). To do so, we use MATLAB software with the function `knnsearch`. This is done as pre-processing step with costing $\mathcal{O}(N \log N)$ for all points \mathbf{x}_i , $i = 1, 2, \dots, N$, where N is the number of points on \mathbb{S}^2 .
- The second step is to apply a Householder transformation on each point (for the original stencil). Here, it is defined by a unitary matrix Q with size 3×3 , which makes the point $\mathbf{x}_1 = (x_1, y_1, z_1)^T$ transforms to $(1, 0, 0)$ (Step 2 of Figure 1.).

- The third step is as follows. The obtained x -coordinates should be ignored. This is considered as a stencil in the y, z -plane. With this, for each stencil (here, we only consider a stencil related to the point $\mathbf{x}_1 = (x_1, y_1, z_1)^T$), $\frac{\partial \mathbf{a}^T(\mathbf{x})}{\partial y}$ and $\frac{\partial \mathbf{a}^T(\mathbf{x})}{\partial z}$ will be computed at point $(1, 0, 0)$ due to the GMLS approximation defined in two-dimensional space.
- At the last step, we must compute $\frac{\partial \mathbf{a}^T(\mathbf{x})}{\partial x}$, $\frac{\partial \mathbf{a}^T(\mathbf{x})}{\partial y}$ and $\frac{\partial \mathbf{a}^T(\mathbf{x})}{\partial z}$ at the original sphere position of the stencil, i.e., $\mathbf{x} = \mathbf{x}_1$. These three column vectors can be computed by considering two vectors obtained in the previous step. This is done as follows. We get the two vectors computed in Step 3 into a vector, namely V with size $n \times 2$. It transforms to original stencil by $V = VQ(2 : 3, :)$, where $Q(2 : 3, :)$ is the matrix Q with size 2×3 , in which the first row is eliminated. This gives a vector with size $n \times 3$, where the first column is $\frac{\partial \mathbf{a}^T(\mathbf{x}_1)}{\partial x}$, the second column is $\frac{\partial \mathbf{a}^T(\mathbf{x}_1)}{\partial y}$, and the third column is $\frac{\partial \mathbf{a}^T(\mathbf{x}_1)}{\partial z}$.

The above four steps can be repeated for points \mathbf{x}_i , $i = 2, \dots, N$, which create the sparse differentiation matrices related to the first derivatives, which are called A_x , A_y and A_z with size $N \times N$, respectively.

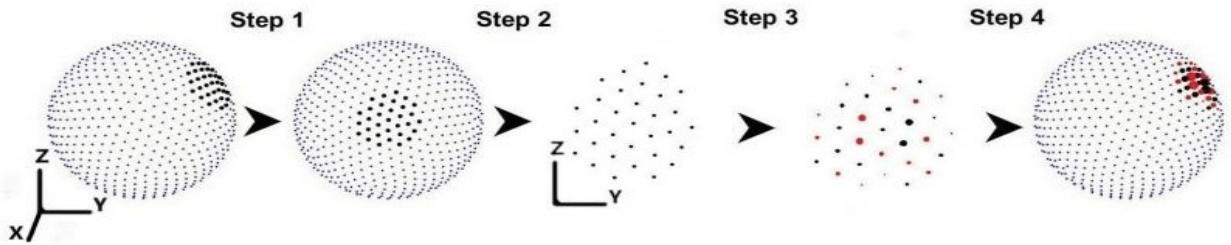


Figure 1. Steps of the new method for finding $\frac{\partial u}{\partial x}$, $\frac{\partial u}{\partial y}$ and $\frac{\partial u}{\partial z}$ of a given function u (this picture is taken from [7]).

4 Results

In this section, we demonstrate the performance of the developed numerical method in some tests. The first test is an example of approximation, and the second one is a well-known test in transport equation on S^2 , namely *vortex roll-up* [5, 6, 20]. The *quasi-uniform* points on S^2 , i.e., the *phyllotaxis spiral* (PTS) and the minimum energy (ME) have been used (cf. [5, 23]). We fix the number of points in each support domain, i.e., $|I(\mathbf{x})| := n$ to be 10 (it is possible to increase its value, but we do not report their results here). Besides, the basis polynomial functions (the shifted and scaled version, see [17]) with degree $k = 2$ is used in GMLS approximation in two-dimensional space. Also, to measure the accuracy of the developed numerical algorithm, we have computed $\ell_\infty(X)$ errors, where X is a set of ME or PTS points on S^2 .

In addition, the rate of convergence of the method presented here has been computed by the following formula:

$$\frac{\log \left(\frac{e_{\text{old}}}{e_{\text{new}}} \right)}{\log \left(\frac{h_{\text{old}}}{h_{\text{new}}} \right)}, \quad (6)$$

where e and h show the numerical $\ell_\infty(X)$ -error and the fill distance of a set of points X (see [25,

N	PTS points		ME points	
	ℓ_∞	orders	ℓ_∞	orders
121	1.90 – 1	—	1.94 – 1	—
484	5.62 – 2	1.76	5.66 – 2	1.78
1936	1.49 – 2	1.92	1.50 – 2	1.92
7744	3.45 – 3	2.11	3.78 – 3	1.99

Table 1. ℓ_∞ -errors of the first derivative with respect to x .

N	PTS points		ME points	
	ℓ_∞	orders	ℓ_∞	orders
121	1.61 – 1	—	2.05 – 1	—
484	5.50 – 2	1.55	5.23 – 2	1.97
1936	1.44 – 2	1.93	1.55 – 2	1.75
7744	3.50 – 3	2.04	3.90 – 3	1.99

Table 2. ℓ_∞ -errors of the first derivative with respect to y .

Definition 1.4]), respectively. Moreover, e_{old} and e_{new} represent the errors computed on the set of points X_{old} and X_{new} with the fill distances h_{old} and h_{new} , respectively.

4.1 Test 1

As the first test, we consider the following function.

$$u(x, y, z) = \sinh(x + y + z), \quad (x, y, z) \in \mathbb{S}^2. \quad (7)$$

The results with the order of convergence are presented in Tables 1.-3.. We can see that the order of convergence of the proposed technique is the same with the original GMLS approximation on the sphere [18].

N	PTS points		ME points	
	ℓ_∞	orders	ℓ_∞	orders
121	1.67 – 1	—	1.87 – 1	—
484	4.94 – 2	1.76	6.07 – 2	1.62
1936	1.16 – 2	2.09	1.48 – 2	2.04
7744	3.30 – 3	1.81	3.91 – 3	1.92

Table 3. ℓ_∞ -errors of the first derivative with respect to z .

N	PTS points		ME points	
	ℓ_2	orders	ℓ_2	orders
121	2.90 – 2	—	2.92 – 2	—
484	1.92 – 2	0.59	1.81 – 2	0.69
1936	8.23 – 3	1.22	8.11 – 3	1.16
7744	2.66 – 3	1.63	3.33 – 3	1.28

Table 4. The normalized ℓ_2 -errors of vortex roll-up test.

4.2 Test 2

The second test is to find the numerical solution of the transport equation on the sphere (in *spherical coordinates*) as follows [5,6,20]

$$\frac{\partial q}{\partial t} + \mathbf{v} \cdot \nabla q = 0, \quad (8)$$

where $q := q(\lambda, \theta, t)$ is the transport variable. Also, $\mathbf{v} := \mathbf{v}(\lambda, \theta, t) = (v_1(\lambda, \theta, t), v_2(\lambda, \theta, t))^T$ is the velocity field, and $\nabla := (\frac{1}{\cos(\theta)} \frac{\partial}{\partial \lambda}, \frac{\partial}{\partial \theta})^T$ is the surface gradient. Since the proposed method works for *Cartesian coordinates*, we use the following chain rule [7]

$$\frac{\partial}{\partial \lambda} = -\frac{zx}{x^2 + y^2} \frac{\partial}{\partial x} - \frac{zy}{x^2 + y^2} \frac{\partial}{\partial y} + (x^2 + y^2) \frac{\partial}{\partial z}, \quad \frac{\partial}{\partial \theta} = -y \frac{\partial}{\partial x} + x \frac{\partial}{\partial y}.$$

Besides, $v_1(\lambda, \theta) = \omega(\theta) \cos(\theta)$, $v_2(\lambda, \theta) = 0$, where

$$\omega(\theta) = \begin{cases} \frac{3\sqrt{3}}{2\rho(\theta)} \operatorname{sech}^2(\rho(\theta)) \tanh(\rho(\theta)), & \rho(\theta) \neq 0, \\ 0, & \rho(\theta) = 0, \end{cases}$$

in which $\rho(\theta) = \rho_0 \cos(\theta)$ is the radial distance of the vortex. The exact solution of this problem is $q(\lambda, \theta, t) = 1 - \tanh\left(\frac{\rho(\theta)}{\zeta} \sin(\lambda - \omega(\theta)t)\right)$, $t \geq 0$ with $\rho_0 = 3$ and $\zeta = 5$. The proposed method is applied to discretize Eq. (8) due to the space variables, and to deal with the time variable, we apply the second-order time discretization proposed in [19] with the time step $\Delta t = 1 \times 10^{-3}$ (see [19] to find more details), which is omitted here for brevity. The obtained fully discrete scheme of Eq. (8) that is a linear system of algebraic equations per time step is solved via an iterative algorithm, i.e., the biconjugate gradient stabilized (BiCGSTAB) algorithm with a zero-fill incomplete lower-upper (ILU) preconditioner. In this test, the normalized ℓ_2 error (cf. [23]) with the order of convergence are presented in Table 4. at $t = 3$.

5 Conclusion

In this manuscript, a new method based on the GMLS technique combined with a Householder reflection has been developed to approximate the first derivatives of function on the sphere. The main benefit of this idea is that there is no need to use the spherical harmonics for constructing the approximation, where the GMLS approximation is only used in two-dimensional space. Besides, the computational cost could be reduced in comparison with the original GMLS technique on the sphere.

The proposed algorithm is simple such that it needs to define a 3×3 Householder matrix for each point on the sphere. This matrix projects a point onto the sphere to y,z – plane (x,y – and x,z – planes can also be considered), and so the approximate derivatives are computed via the GMLS technique in two dimensions. Then, these derivatives are computed at the original position on the sphere using the last step of the algorithm. Finally, we test the accuracy of the developed algorithm by getting an example, and also a test problem related to the transport equation.

References

- [1] M. Afenyo, F. Khan, B. Veitch, M. Yang, Modeling oil weathering and transport in sea ice, *Mar. Pollut. Bull.* 107(1) (2016) 206–215.
- [2] L. C. Bender, Modification of the physics and numerics in a third-generation ocean wave model, *J. Atoms Ocean. Tech.* 13(3) (1996) 726–750.
- [3] C. J. Cotter, J. Shipton, Mixed finite elements for numerical weather prediction, *J. Comput. Phys.* 231(21) (2012) 7076–7091.
- [4] G. E. Fasshauer, *Meshfree Approximation Methods with MATLAB*, World Scientific: USA, 2007.
- [5] N. Flyer, G. B. Wright, Transport schemes on a sphere using radial basis functions, *J. Comput. Phys.* 226(1) (2007) 1059–1084.
- [6] B. Fornberg, E. Lehto, Stabilization of RBF-generated finite difference methods for convective PDEs, *J. Comput. Phys.* 230(6) (2011) 2270–2285.
- [7] D. Gundersen, N. Flyer, B. Fornberg, Transport schemes in spherical geometries using spline-based RBF-FD with polynomials, *J. Comput. Phys.* 408 (2020) 109–256.
- [8] A. Hamed, M. Tadi, A numerical method for inverse source problems for Poisson and Helmholtz equations, *Phys. Lett. A.* 380(44) (2016) 3707–3716.
- [9] Y. C. Hon, R. Schaback, Solving the 3D Laplace equation by meshless collocation via harmonic kernels, *Adv. Comput. Math.* 38 (2013) 1–19.
- [10] Y. C. Hon, R. Schaback, M. Zhong, The meshless Kernel-based method of lines for parabolic equations, *Comput. Math. Appl.* 68(12) (2014) 2057–2067.
- [11] Y. C. Hon, R. Schaback, Direct meshless kernel techniques for time-dependent equations, *Appl. Math. Comput.* 258 (2015) 220–226.
- [12] A. Khodadadian, C. Heitzinger, A transport equation for confined structures applied to the OprP, Gramicidin A, and KcsA channels, *J. Comput. Electron.* 14(2) (2015) 524–532.
- [13] M. Krems, The boltzmann transport equation: Theory and applications, Website, December 2007.
- [14] P. H. Lauritzen, W. C. Skamarock, M. Prather, M. Taylor, A standard test case suite for two-dimensional linear transport on the sphere, *Geosci. Model Dev.* 5(3) (2012) 887–901.
- [15] D. Levin, The approximation power of moving least-squares, *Math. Comput.* 67(224) (1998) 1517–1531.
- [16] J. MacLaren, L. Malkinski, J. Wang, First principles based solution to the boltzmann transport equation for co/cu/co spin valves, *Mater. Res. Soc. Symp. Proc.* 614 (2000).
- [17] D. Mirzaei, R. Schaback, M. Dehghan, On generalized moving least squares and diffuse derivatives, *IMA J. Numer. Anal.* 32 (2012) 983–1000.
- [18] D. Mirzaei, Direct approximation on spheres using generalized moving least squares, *BIT Numer. Math.* 57(4) (2017) 1041–1063.
- [19] V. Mohammadi, M. Dehghan, A. Khodadadian, T. Wick, Numerical investigation on the transport equation in spherical coordinates via generalized moving least squares and moving kriging least squares approximations, *Eng. Comput.* 37 (2021) 1231–1249.
- [20] R. D. Nair, J. Côté, A. Staniforth, Cascade interpolation for semi-Lagrangian advection over the sphere, *Q. J. Roy. Meteor. Soc.* 125(556) (1999) 1445–1486.
- [21] R. D. Nair, P. H. Lauritzen, A class of deformational flow test cases for linear transport problems on the sphere, *J. Comput. Phys.* 229(23) (2010) 8868–8887.
- [22] R. Schaback, Error analysis of nodal meshless methods, in: *Meshfree Methods for Partial Differential Equations VIII*, Springer, 2017, 117–143.

- [23] V. Shankar, G. B. Wright, Mesh-free semi-Lagrangian methods for transport on a sphere using radial basis functions, *J. Comput. Phys.* 366 (2018) 170–190.
- [24] M. Taylor, J. Edwards, S. Thomas, R. D. Nair, A mass and energy conserving spectral element atmospheric dynamical core on the cubed-sphere grid, *J. Phys.: Conf. Ser.* 78 (2007) 012074.
- [25] H. Wendland, Scattered Data Approximation, in: Cambridge Monograph on Applied and Computational Mathematics, Cambridge University Press, 2005.
- [26] L. Zhang, J. Ouyang, X. Zhang, The two-level element free Galerkin method for MHD flow at high Hartmann numbers, *Phys. Lett. A.* 372 (2008) 5625–5638.

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