Evaluation of high order versions of the diffuse approximate meshless method

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Abstract

A high order version of a diffuse approximate meshless method has been implemented and tested on two problems, namely diffusion and transport diffusion two-dimensional equations. It is shown that the fourth-order approximation greatly improves the numerical solution.

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1. Introduction

Meshless methods have been developed in the last decade as an alternative approach for solving many engineering problems \([1–13]\) due to their advantage of avoiding finite element meshing. Among them, the moving least squares based collocation method has been successfully used to solve fluid flow, heat transfer and phase change problems \([14–17]\). Up to now, this method has been implemented by using a second-order approximation. For some applications however, like it is the case in the direct numerical simulation of Navier–Stokes equation or in computational aeroacoustics, interpolations of higher order are necessary to reach the requirements of accurate solutions. The main goal of this paper is therefore to demonstrate that higher-order approximations can be easily implemented and lead to more accurate solutions. In the following sections, the meshless method and the moving least squares approximations are first described. Two numerical examples with localized sharp gradients are then presented to illustrate the improvement in accuracy. The refinement of the nodal discretization is also examined.

2. Moving least squares based meshless method

The moving least square or diffuse approximation based meshless method uses multi-dimensional Taylor series expansions to construct the approximation of the derivatives of unknown functions. The reconstructed
values of a field and its derivatives at a certain location are obtained using the information from neighboring nodes and weightings that are functions of distances between nodes, with no reference to any mesh-based data structure. At each point of the discretization, the derivatives appearing in the equation to be solved are replaced by their diffuse approximation thus leading to an algebraic system which is solved by the BICGSTAB method with ILUT preconditioning after the introduction of the boundary conditions.

The MLS approximation \( u^h(x) \) of a continuous function \( u \) at a given point of coordinates \( x = [x, y, z]^T \) in the domain \( \Omega \) is defined as

\[
    u^h(x) = \sum_{i=1}^{m} p_i(x) a_i(x) = p(x)^T a(x),
\]

where \( p(x) = [p_1(x), p_2(x), \ldots, p_m(x)] \) is a basis of \( m \) dimensions and \( a(x) \) is a vector containing coefficients \( a(x) \), \( i = 1, 2, \ldots, m \), which are determined by minimizing the error in the weighted least-squares sense for the following quadratic form:

\[
    J = \sum_{i=1}^{n} \omega(x, x_i) [u(x_i) - p(x_i)^T a(x)]^2,
\]

where \( \omega(x, x_i) \), \( i = 1, 2, \ldots, n \), are the weights associated with node I which should be among the number of the \( n \) selected points in the neighborhood of \( x \) for which the weight function \( \omega(x, x_i) > 0 \). \( u(x_i) \) is the value of \( u \) at this node.

In our precedent studies [6–9], the following radial gaussian weighting windows have been used:

\[
    \omega(x, x_i) = \begin{cases} 
        10^{-wp} \left( \frac{|x-x_i|}{\sigma} \right)^2, \\
        0 \quad \text{if} \quad (x-x_i)^2 > \sigma^2,
    \end{cases}
\]

where \( \sigma \) is the size defining the limits of the support domain with \( \omega = 10^{-wp} \) (Fig. 1). In this work, the value \( wp \) is set to 6.

After minimization the unknown coefficient \( a(x) \) are given by the following relation:

\[
    A(x) a(x) = B(x) u,
\]

where

\[
    A(x) = \sum_{i=1}^{n} \omega(x, x_i) p(x_i) p(x_i)^T,
\]

\[
    B(x) = [\omega(x, x_1) p(x_1), \omega(x, x_2) p(x_2), \ldots, \omega(x, x_n) p(x_n)],
\]

\[
    u^T = [u_1, u_2, \ldots, u_n].
\]

Diffuse derivatives are obtained by choosing polynomial and locally defined basis,

\[
    p^T(x, x) = [1, x_i - x, y_i - y, 1/2(x_i - x)^2, (x_i - x)(y_i - y), 1/2(y_i - y)^2].
\]

This choice allows to consider \( u^h(x, x) \) as two-dimensional Taylor expansion limited to second order in space. Three-dimensional and higher orders are also possible.

In this paper, two-dimensional examples are treated by employing third- and fourth-order approximations with the following polynomials basis:

\[
    p^T(x, x) = [1, x_i - x, y_i - y, 1/2(x_i - x)^2, (x_i - x)(y_i - y), 1/2(y_i - y)^2, 1/6(x_i - x)^3, \\
    1/2(x_i - x)^2(y_i - y), 1/2(x_i - x)(y_i - y)^2, 1/6(y_i - y)^3],
\]

and

\[
    p^T(x, x) = [1, x_i - x, y_i - y, 1/2(x_i - x)^2, (x_i - x)(y_i - y), 1/2(y_i - y)^2, (x_i - x)^3, 1/2(x_i - x)^2(y_i - y), \\
    1/2(x_i - x)(y_i - y)^2, 1/6(y_i - y)^3, 1/24(x_i - x)^4, 1/6(x_i - x)^3(y_i - y), 1/4(x_i - x)^2(y_i - y)^2, \\
    1/6(x_i - x)(y_i - y)^3, 1/24(y_i - y)^4].
\]
An estimation of successive derivatives can be obtained by identification with the unknown coefficient $a(x)$. The inversion of system (4) gives then algebraic expressions of these successive estimated derivatives $[Du]$ which can be directly used for the discretization of partial derivative equations if evaluation point $x$ and nodal point are collocated

$$[Du]^T = A(x)^{-1} \cdot \sum_{i=1}^{n} \omega(x, x_i) p(x_i, x) \cdot u_i,$$

where

$$[Du] \equiv \left[ \begin{array}{cccc} \frac{\partial u}{\partial x}, & \frac{\partial u}{\partial y}, & \frac{\partial^2 u}{\partial x^2}, & \frac{\partial^2 u}{\partial x \partial y}, & \frac{\partial^2 u}{\partial y^2} \end{array} \right]_x$$

for second order of approximation,

$$[Du] \equiv \left[ \begin{array}{cccccc} \frac{\partial u}{\partial x}, & \frac{\partial u}{\partial y}, & \frac{\partial^2 u}{\partial x^2}, & \frac{\partial^2 u}{\partial x \partial y}, & \frac{\partial^2 u}{\partial y^2}, & \frac{\partial^3 u}{\partial x^3} \end{array} \right]_x$$

for third order of approximation

$$[Du] \equiv \left[ \begin{array}{cccccccc} \frac{\partial u}{\partial x}, & \frac{\partial u}{\partial y}, & \frac{\partial^2 u}{\partial x^3}, & \frac{\partial^2 u}{\partial x \partial y^2}, & \frac{\partial^2 u}{\partial x^2 \partial y}, & \frac{\partial^2 u}{\partial y^3}, & \frac{\partial^3 u}{\partial x^3 \partial y}, & \frac{\partial^3 u}{\partial x^2 \partial y^2}, & \frac{\partial^3 u}{\partial x \partial y^3}, & \frac{\partial^3 u}{\partial y^4} \end{array} \right]_x$$

for fourth order of approximation.

### 2.1. Computational aspects

The evaluation of the derivatives at a given point involves the inversion of the moment matrix $A(x)$, whose size is $m \times m$, where $m$ is the dimension of the basis $p(x)$. For the fourth-order basis, for instance, $m = 5$, $m = 15$ and $m = 21$ in one, two and three dimensions, respectively. Note that the size of $A(x)$ does not depend on the number of neighbors included in the computation.

In order to prevent the matrix $A(x)$ from being singular or ill-conditioned, the cloud of selected neighbors should fulfill certain requirements.
Thus, the number of neighbors must be greater than \( m \) (the number of functions in the basis), \( A(x) \). Severely ill-conditioned matrix can also be avoided when selecting a number of neighbors greater than the minimum, and with a repartition covering as many directions as possible.

Several strategies have been proposed in order to avoid the singularity of the moment matrix. Liu and Gu [11] proposed a moving node method to slightly change the coordinates of nodes randomly before computation. Changing basis function through the transformation of the local coordinate has also proven to be an effective method [13].

Fig. 2. Analytical field for the conduction problem.

Fig. 3. Spatial convergence for conduction patch test.
Fig. 4. (21 * 21) grid refined (a) once and (b) twice.
Using scaled monomials in the basis improves advantageously the conditioning of the moment matrix $A(x)$. In this case, the basis would be of the form $p(x_i/h, x/h)$ were $h$ is chosen as a local characteristic length like the size of the support domain around the considered point or in this work as the minimum distance to selected nodes. With this transformation, the expressions to approximate the field and the derivatives are now obtained by the relations

$$
\begin{bmatrix}
  u, h \frac{\partial u}{\partial x}, h \frac{\partial u}{\partial y}, h^2 \frac{\partial^2 u}{\partial x^2}, h^2 \frac{\partial^2 u}{\partial x \partial y}, h^2 \frac{\partial^2 u}{\partial y^2}
\end{bmatrix}^T_x \equiv A(x)^{-1} \cdot \sum_{i=1}^{n} \omega(x, x_i)p(x_i/h, x/h) \cdot u_i.
$$

(11)

Fig. 5. Absolute error with regular (41 * 41) grid and (21 * 21) refined once.
Fig. 6. Fourth-order absolute error with regular (81 * 81) grid and (21 * 21) refined twice.
3. Numerical tests

The preceding developments are illustrated here by considering two examples whose analytical solution is known. The first one is a problem of diffusion presenting a narrow zone with very strong gradient. The spatial convergence is investigated for second, third and fourth order of the approximation. The ability in employing several levels of refinement according to the stiffness of the solution is shown.

The second example is a 2D transport-diffusion which requires a higher level resolution in one area of the domain as it can be encountered in many problems in the field of computational fluid dynamics.

Fig. 7. Solution of transport-diffusion problem $Re = 1000$: (a) with $\mu = 10^3$ and (b) $\mu = 10^4$. 
3.1. Diffusion problem

We consider on a unit square domain the following diffusion problem:

\[
\frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} = S(x, y),
\]

where

\[
S(x, y) = 5 \times 10^4 \cdot \{100 \cdot ((1 - x)^2 + y^2) - 2\} \cdot \exp\{-50[(1 - x)^2 + y^2]\}
\]

and where boundary conditions are written as

\[
\Phi(1, y) = 100 \cdot (1 - y) + 500 \cdot \exp\{-50 \cdot y^2\}, \quad \Phi(0, y) = 500 \cdot \exp\{-50 \cdot (y^2 + 1)\},
\]

\[
\Phi(x, 0) = 100 \cdot x + 500 \cdot \exp\{-50 \cdot (1 - x)^2\}, \quad \Phi(x, 1) = 500 \cdot \exp\{-50 \cdot ((1 - x)^2 + 1)\}.
\]

The analytical solution of this problem writes

\[
\Phi(x, y) = 500 \cdot \exp\{-50 \cdot ((1 - x)^2 + y^2)\} + 100 \cdot (1 - y) \cdot x.
\]

As shown in Fig. 2, it presents a sharp shape in one corner \((x = 1, y = 0)\).

This problem is solved by using second-order, third-order and fourth-order approximations. Nodes are regularly distributed on the domain with the same regular step in \(x\)- and \(y\)-directions. In fact this regular distribution of nodes is not the better repartition to cover as many directions as possible in a nodal star. The minimal number of selected nodes in a star around each nodal point is respectively 9, 17 and 26 nodes, for second, third and fourth order of discretization. On the graph of Fig. 3 which presents the mean absolute error \(\varepsilon\) defined by \(\sum|\Phi^{\text{calc}} - \Phi^{\text{exact}}|/(n - 1)^2\), it can be seen that the numerical solutions converge when the spatial step \(dx\) is diminishing as expected. Second- and third-order solutions show the same slope even if third order is
more accurate. Fourth-order approximations ameliorate strongly the solution and the rate of convergence is really better.

Fig. 9. Spatial convergence ($Re = 1000$, $\mu = 1000$). (a) Regular grids, (b) perturbed grids.

Table 1

<table>
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<th>$32 \times 32$</th>
<th>$64 \times 64$</th>
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<tr>
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<td></td>
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<tr>
<td>$Re = 1000$, $\mu = 10000$</td>
<td>Zhang [18]</td>
<td>78.1</td>
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<tr>
<td></td>
<td>Present</td>
<td>14.31</td>
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</tbody>
</table>
Refined distributions of nodes are also possible with fourth-order simulations at it was done for second-order simulation [15]. As a matter of example, a refined distribution of nodes is used on regular grid by employing half space step in the area of sharp gradient (Fig. 4a); the solution shows the same order of accuracy than the regular mesh corresponding to the finest grid dimension as it can been seen in Fig. 5a and b for a regular 41 * 41 grid and for a regular 21 refined once. A particular treatment was employed for the nodes in the vicinity of the frontier between refined and sparse area; the opening of the weighting window in a node close to this frontier should include the neighboring nodes situated in the coarse region. These neighbors are thus chosen first and the set of selected points is completed by the selection of nearest nodes in the fine grid region. Experiment was also made for a grid refined twice (Fig. 4b). Results show that there is not a prohibitive error in the vicinity of the frontier of sparse and coarse grid and the comparison of error with corresponding regular grids show quite the same local error (Fig. 6a and b).

3.2. Transport-diffusion problem

The transport phenomena in computational fluid dynamics are described by the convection diffusion equation which can be written for 2D problems with the Dirichlet boundary condition,

\[
- \frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} + p(x, y) \frac{\partial u}{\partial x} + q(x, y) \frac{\partial u}{\partial y} = f(x, y), \quad (x, y) \in \Omega,
\]

\[
u(x, y) = g(x, y), \quad (x, y) \in \partial \Omega,
\]

where \( \Omega \) is a domain in \( \mathbb{R}^2 \). Even for sufficiently smooth convection coefficients \( p(x, y) \) and \( q(x, y) \), the solution function \( u(x, y) \) and the forcing function \( f(x, y) \) can show local singularity as it is the case on boundary layers.

We consider here Eq. (11) with \( p(x, y) = Re \cdot x(x - 1)(1 - 2y) \) and \( q(x, y) = Re \cdot y \cdot (y - 1) \cdot (1 - 2x) \); Re being the Reynolds number reflecting the strength of the convection.

![Fig. 10. Example of perturbed grid.](image-url)
The exact solution given in [17] is \( u(x, y) = \exp(-\mu x - 0.5)^2 - y^2 \). As it can be seen, this solution sketched in Fig. 7 for with \( \mu = 10^3 \) and \( 10^6 \) presents a singularity along the line \( x = 1/2 \).

This problem has been solved first on regular meshes with second, third and fourth orders of discretizations. The numerical fields and the mean absolute errors for a regular \( 41 \times 41 \) grid are given in Fig. 8 for \( \mu = 1000 \). It can be seen that the accuracy is improved when higher-order approximations are employed. The spatial convergence given in Fig. 9a shows the expected trend and rate of convergence. The fourth-order version of the present method leads to a maximum value of absolute error comparable with those obtained by Zhang et al. [18] with a fourth-order compact finite difference scheme (Table 1). The convergences on irregular grids, generated by using a perturbation of regular grids coordinates with the addition of a normalized random process of 20% of the initial spatial step, have also been tested. An example of such irregular nodal repartition is given in Fig. 10. With the given problem of sharp gradient, the evolution of error is not so linear when irregular distributions of nodes are employed but Fig. 9b shows that second- and fourth-order solutions follow the same trend of convergence as with regular grids.

When the position of the singularity is known or can be determined, it is judicious to concentrate the nodes in the identified region, (along the line \( x = 1/2 \) here) and this is generally done by stretching techniques. This can be obtained for example by using the following transformation of regular \( x \) coordinates:

\[
\begin{align*}
  x &= 1 + \frac{\tanh(k \cdot (2x_r - 2))}{2 \cdot \tanh(k)} \quad \text{for } x > 0.5 \\
  x &= \frac{\tanh(2kx_r)}{2 \cdot \tanh k} \quad \text{for } x < 0.5,
\end{align*}
\]

where \( x_r \) are the coordinates on the uniform grid, and \( k \) a transformation coefficient.

In its configuration presenting a strong singularity (\( \mu = 10^4 \)), the solution has been calculated by starting with a regular grid (\( 21 \times 21 \)) and by combining a local refinement in the area close to the position \( x = 1/2 \) (grid step is divided by three), followed by a stretching transformation with \( k = 1.5 \) (Fig. 11). Results which were
obtained with at least 26 neighboring nodes except for the points lying near the upper and lower parts of the boundary where we used 36 neighbors are presented in Fig. 12. As it can be seen, the solution is correctly predicted and the absolute error remains small (lower than 2% in the singular area).

4. Conclusion

The implementation of third- and fourth-order approximations for solving conduction and transport diffusion problems with localized singularities by a meshless method has been tested. It has been shown that the rates of convergence follow the expected trend. Local refinement or stretching can be easily implemented and lead to accurate results. Further work is still needed to fully access this accuracy improvement when dealing with fluid flow equations.
References


