## Development of Irregular-Grid Finite Difference Method (IFDM) for Governing Equations in Strong Form

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*Abstract:* - In this paper, an irregular-grid finite difference method (IFDM) with the use of Green-Gauss theorem was developed to numerically deal with problems subject to arbitrary geometrical boundaries. The focus is to elucidate the principle of IFDM and the numerical procedure to solve partial differential equations. Attention is paid to the discretization of spatial terms in partial differential format. Totally six types of discretization schemes are proposed and assessed from points of views of efficiency and accuracy. Theoretical analyses are conducted with regard to the compactness of stencil and positivity of the coefficients of supporting nodes. Upon the analyses, two schemes, II and VI, are selected for further study. Scheme II is based on one-point quadrature rule while scheme VI corresponds to 2-point quadrature rule. Numerical excises by using the two schemes are carried out to predict the solutions in a square domain that is governed by a Poisson equation. The effects of irregularity of grids are also studied. Numerical results indicate that the both schemes give satisfactory prediction. In addition, the scheme VI gives better accuracy, especially on irregular grids, but at slightly higher cost in computation. Efforts here demonstrate that the proposed IFDM method is good to be used in numerical simulations with arbitrarily geometrical bounds.

Key-Words: - IFDM, Quadrature, Gradient smoothing domain, Stencil, Grid edge, Domain face

### 1. Introduction

Apart from well-known finite element method (FEM) and finite volume method (FVM), finite difference method (FDM) is another mesh-based traditional numerical method widely adopted in numerical simulations, mainly because it is straightforward highly and efficient. In conventional FD methods, single- or multiple-block structured grids are used. The discretization of governing equations to structured grids results in a system of algebraic equations with banded matrix of coefficients. Quite a number of efficient numerical methods can be used to quickly get the solutions to such a system of algebraic equations. However, it is not trivial process to generate structured grids for arbitrary geometries, especially for the topological generation of multiple blocks [1]. This limits the FDM only for simple geometries. Besides, in conventional FDM method, the Jacobian matrix, resulting from the transformation of governing equations from physical domain to a computational domain on a curvilinear coordinate system, is needed to be predicted. This imposes additional computational cost and may give more errors in prediction. Researchers have attempted to overcome these drawbacks of FDM mentioned above. More recently, some meshfree methods, which are implemented on nodes at first place, are developed for this purpose. A survey paper written by Babuska et al [2] emphasized on the mathematical foundation of various meshfree methods. Overview of computational and implementation issues related to meshfree methods can be found in monographs about weak form [3] and strong form [4].

In general, many meshfree methods for the solution of partial differential equations in weak form are comprehensively studied When governing equations in strong form are adopted, most of these meshfree methods show notorious stability. primarily because of the sensitivity of the solution on the supporting nodes used in discretization. Besides, due to large overlap in the supporting domains discretization schemes are not conservative. This also imposes the demand of a great deal of computation.

A new and efficient generalized finite difference method, irregular-grid finite difference method (IFDM), developed for the purpose of generality and efficiency. The IFDM is derived in light of Green-Gauss theorem rather than Taylor-series expansion theorem that is usually used in any other finite difference method. In implementation, since the governing equations are directly discretized on the physical domain, the prediction for Jacobian matrix induced by coordinate transformation is avoided. In addition, the IFDM can be applied for arbitrary geometries.

In the following sections, the in-depth description of solution algorithm of IFDM is given first. The approximations to gradients (first-order derivative) and Laplace operator (second-order derivative) of a scalar are introduced with the IFDM. The focus is on the analyses of weighting coefficients on a of supporting nodes. Consequently, stencil numerical results for a square domain governed by Poisson equation are discussed а The computational efficiency and accuracy of the IFDM method are addressed. At the end, brief concluding remarks are given upon current efforts.

### 2. Solution Algorithm

### 2.1 Theoretical background

Taylor-series expansion theorem is used to discretize the derivatives in traditional FD methods. Comparatively, the IFDM method is derived on the basis of the Green-Gauss theorem.

For simplicity, let us take a 2-dimension problem as an example to illustrate the principles of IFDM method. According to Green-Gauss theorem [5], for a generic variable U, it holds

$$\int_{\Omega} \nabla U dV = \oint_{\partial \Omega} U \bar{n} ds \tag{1}$$

where  $\nabla$  is gradient operator, and *V* represents the area of gradient smoothing domain of  $\Omega$ , *ds* is the

length of domain face and  $\vec{n}$  is the unit normal vector to the domain face.



Fig. 1 Illustration of gradient smoothing domain and face vectors (pointing outward)

Mathematically, on a gradient smoothing domain (GSD) as shaded in Fig. 1, the gradients can be approximated as

$$\nabla U \approx \frac{1}{\Omega} \oint_{\partial \Omega} U \bar{n} ds \tag{2}$$

Similarly, the second-order derivatives (Laplace operator) can be approximated as

$$\nabla \bullet (\nabla U) \approx \frac{1}{\Omega} \oint_{\partial \Omega} \vec{n} \bullet \nabla U ds$$
(3)

As shown in Fig. 1, the grids are used to constitute gradient smoothing domains which are used for approximation of derivatives occurring in governing equations. In current study, two types of GSD are adopted: one is named median-based GSD adopted for the approximation of derivatives at any node of interest. It is formed by connecting relevant centroids of triangles with midpoints of relevant edges. The other is just the grid itself that is employed in some schemes for prediction of derivatives at any centroid. It is called grid-based GSD here.

### 2.2 Discretization of derivatives

Totally six schemes, as summarized in Table 1, were proposed and studied. For the three basic schemes, I, III and V, they differ with one another in the order of quadrature adopted for integral approximation and the approximation of gradients at centroids. In one-point based schemes, the integration over any domain face is approximated with rectangular rule by using the values at midpoint of any edge. In two-point based schemes, trapezoidal rule based on values at midpoints of relevant edges and centroids is adopted. Both the first- and second-order derivatives are obtained by successively applying Green-Gauss theorem to the same MGSD. In Scheme I and III, the gradients at any centroid are obtained by arithmetic averaging of gradients at the relevant grid nodes, while they are calculated by applying Green-Gauss theorem onto grid-based GSD in scheme V. Application of directional correction to these basic schemes gives another three schemes, II, IV and VI, respectively. Details about directional correction will be illustrated in the following section.

Table 1 Spatial discretization schemes

Scheme	Quadrature	Type of GSD	Directional
			correction
Ι	One-point	MGSD	no
II	One-point	MGSD	yes
III	Two-point	MGSD	no
IV	Two-point	MGSD	yes
V	Two-point	MGSD,GGSD	no
VI	Two-point	MGSD,GGSD	yes

For simplicity, the spatial discretizations based on scheme I and III are described here. In Scheme I, derivatives at node i of interest can be approximated, respectively, as

$$\frac{\partial U_i}{\partial x} \approx \frac{1}{\Omega_i} \sum_{j=1}^K \Delta S X_{ij} U_{ij}^m, \frac{\partial U_i}{\partial y} \approx \frac{1}{\Omega_i} \sum_{j=1}^K \Delta S Y_{ij} U_{ij}^m$$
(4)

and

$$\nabla \cdot (\nabla U) \approx \frac{1}{\Omega_i} \sum_{j=1}^{K} \left[ \frac{1}{2} \left( \frac{\partial U_i}{\partial x} + \frac{\partial U_j}{\partial x} \right) \Delta S X_j + \frac{1}{2} \left( \frac{\partial U_i}{\partial y} + \frac{\partial U_j}{\partial y} \right) \Delta S Y_{ij} \right]$$
(5)

where

$$\begin{split} U_{ij}^{(L)} &= U_{ij}^{(R)} = U_{ij}^{m} = \frac{1}{2} (U_{i} + U_{j}) \\ \Delta SX_{ij} &= \Delta SX_{ij}^{(L)} + \Delta SX_{ij}^{(R)}, \Delta SY_{ij} = \Delta SY_{ij}^{(L)} + \Delta SY_{ij}^{(R)} \\ \Delta SX_{ij}^{(L)} &= \Delta S_{ij}^{(L)} (n_{x})_{ij}^{(L)}, \Delta SY_{ij}^{(R)} = \Delta S_{ij}^{(R)} (n_{y})_{ij}^{(R)} \end{split}$$

Here,  $\Delta SX_{ij}$  and  $\Delta SY_{ij}$ , and  $n_x$  and  $n_y$ , are, respectively, the two components of a face vector and a unit normal vector with respect to *x* and *y* directions. They are evaluated and stored before the intensive calculation is started. *K* denotes the total number of nodes in the stencil of the node *i*.

In Scheme III, the values of functions and gradients at the centroids of grids are calculated by simple arithmetic averaging of values at constitutive nodes. Thus, the derivatives are approximated as follows:

$$\frac{\partial U_{i}}{\partial x} \approx \frac{1}{\Omega_{i}} \sum_{j=1}^{K} \left[ \frac{1}{2} \Delta S X_{ij}^{(L)} (U_{m} + U_{c}^{(L)}) + \frac{1}{2} \Delta S X_{ij}^{(R)} (U_{m} + U_{c}^{(R)}) \right]$$

$$\frac{\partial U_{i}}{\partial y} \approx \frac{1}{\Omega_{i}} \sum_{j=1}^{K} \left[ \frac{1}{2} \Delta S Y_{ij}^{(L)} (U_{m} + U_{c}^{(L)}) + \frac{1}{2} \Delta S Y_{ij}^{(R)} (U_{m} + U_{c}^{(R)}) \right]$$
(6)

$$\frac{\partial^{2}U_{i}}{\partial x^{2}} + \frac{\partial^{2}U_{i}}{\partial y^{2}} \approx \frac{1}{\Omega_{i}} \sum_{j=1}^{k} \frac{1}{2} \left[ \frac{\partial U_{m}}{\partial x} + \frac{\partial U_{i}^{(k)}}{\partial x} \right] \Delta S X_{ij}^{(k)} + \left( \frac{\partial U_{m}}{\partial y} + \frac{\partial U_{i}^{(k)}}{\partial y} \right) \Delta S Y_{ij}^{(k)}}{\left( \frac{\partial U_{m}}{\partial x} + \frac{\partial U_{i}^{(k)}}{\partial x} \right) \Delta S Y_{ij}^{(k)}} \right]$$
(7)

where

$$\begin{split} U_{m} &= \frac{U_{i} + U_{j}}{2}, U_{c}^{(L)} = \frac{U_{i} + U_{j} + U_{k}^{(L)}}{3}, U_{c}^{(R)} = \frac{U_{i} + U_{j} + U_{k}^{(R)}}{3} \\ \nabla U_{m} &= \frac{\nabla U_{i} + \nabla U_{j}}{2}, \nabla U_{c}^{(L)} = \frac{\nabla U_{i} + \nabla U_{j} + \nabla U_{k}^{(L)}}{3}, \nabla U_{c}^{(R)} = \frac{\nabla U_{i} + \nabla U_{j} + \nabla U_{k}^{(R)}}{3} \end{split}$$

In comparison to schemes based on one-point quadrature, these schemes based on two-point quadrature impose additional computational demands and storage for values at centroids and face vectors associated with their common grid edge.

The edge-based data structure is adopted in the study, together with scatter-gather approach, as described by Barth [6][7].

# **3.** Analyses of Stencil of Supporting Nodes

For convenience and simplicity, the discretizations of gradients and Laplace operator are performed onto structured quad grids and equilateral triangles, respectively. The coefficients of supporting nodes are analysed accordingly. The stencils for gradient approximation with different schemes are shown in Fig. 2.

As addressed by Barth [6], for good discretization schemes, the weighting coefficients for Laplace operator are expected to be positive and proportionally varied with distance to the node of interest. Besides, for better computational efficiency, compact stencil corresponding to supporting nodes should be created. In-depth discussion about this issue can be found in Haselbacher and Blazek [8].

As indicated in Fig. 3(a), 3(c) and 3(e), schemes I, III and V result in wide stencils with unfavorable weighting coefficients on structured quad grids. With such schemes, as addressed in Blazek [9], unexpected decoupling solutions may be produced, which will be further illustrated in the following section.

Crumpton *et al* [10] proposed to use modified gradients for the approximation of second-order derivatives, with the help of the following directional correction along grid edges:

$$\nabla \tilde{U}_{ij} = \nabla U_{ij} - \left[\nabla U_{ij} \cdot \bar{t}_{ij} - \left(\frac{\partial U}{\partial l}\right)_{ij}\right] \bar{t}_{ij}$$
(8)

where

$$\begin{split} \nabla \, \bar{U}_{ij} &= \frac{1}{2} (\nabla \bar{U}_i + \nabla \bar{U}_j), \ \left( \frac{\partial U}{\partial l} \right)_{ij} \approx \frac{U_j - U_i}{\Delta l_{ij}} \\ \bar{t}_{ij} &= \frac{\bar{t}_{ij}}{\Delta l_{ij}}, \ \bar{t}_{ij} = \mathbf{X}_j - \mathbf{X}_i, \ \Delta l_{ij} = \left| \mathbf{X}_j - \mathbf{X}_i \right| \end{split}$$

and  $X_i$  and  $X_j$  denotes the positions of node *i* and *j*, respectively.

As depicted in Fig. 3(b) and 3(e), relatively compact stencil with favorable coefficients are formed in Scheme II and VI. Scheme II has 5-point based stencil and Scheme VI corresponds to 9-node based compact stencil. However, as shown in Fig. 3(d), Scheme IV still results in unfavorable stencil. The analyses were also conducted on equilateral shows the stencils triangles. Fig. 4 and corresponding weighting coefficients of supporting nodes for a discretized Laplace operator. It is obvious that schemes II, IV, V and VI, all produce stencils with favorable coefficients on equilateral triangles, except schemes I and III. Besides, it is interesting to notice that both schemes II and VI produce identical stencil, so do schemes IV and V. With additional concerns about computational efficiency, schemes II and VI are superior to schemes IV and V, because of compactness in stencil.

In summary, upon the stencil analyses, both scheme II and scheme VI are proposed to be used in the IFDM, because both of them produce compact stencil with favorable coefficients on both types of regular grids of concern (quadrilateral and triangular).



Fig. 2 Stencils and weighting coefficients for the approximation of  $(\frac{\partial u}{\partial x}, \frac{\partial u_i}{\partial y})$  on different types of grids









(a) I and III (b) IV and V (c) II and VI Fig. 4 Stencils and weighting coefficients for the approximation of  $\frac{\partial^2 u_i}{\partial x^2} + \frac{\partial^2 u_i}{\partial y^2}$  on equilateral triangles

# 4. Application of IFDM for Solution of Poisson Equation

#### 4.1 Poisson equation and its discretization

The IFDM is used to predict the solution to Poisson equations on a square domain. In current study, the Dirichlet condition is applied to the boundaries, i.e., the values at the boundaries are prescribed.

The pseudo-transient approach is used in current study for pursuing steady-state solutions. The governing equations under investigation take the following form:

$$\frac{\partial U}{\partial t} = \frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} - f(x, y)$$

$$f(x, y, t) = 13 \exp(-2x + 3y)$$

$$U(x, y, 0) = 0$$

$$(0 \le x \le 1, 0 \le y \le 1)$$
(9)

The exact solution to this Poisson equation is

$$\hat{U}(x,y) = e^{(-2x+3y)}$$
  $(x,y) \in \Omega$  (10)

As described above, the function values at the boundaries are specified accordingly.

The spatial derivatives are discretized as shown in previous section and the temporal term is dealt with the explicit five-stage Runge-Kutta (*RK5*) method in current study.

The convergence index in the form of

error \_norm = 
$$\sqrt{\sum_{i=1}^{modes} (U_i^{(m+1)} - U_i^{(m)})^2} / \sqrt{\sum_{i=1}^{modes} (U_i^{(1)} - U_i^{(0)})^2}$$
 (11)

is evaluated at each time-step. For excluding the effect due to the temporal discretization, computations are terminated when *error\_norm* approaches machine error. In current study, numerical errors for the overall field are predicated in the form of

$$error = \sqrt{\sum_{i=1}^{nnode} (U_i - \hat{U}_i)^2} / \sqrt{\sum_{i=1}^{nnode} \hat{U}_i^2}$$
(12)

where *nnode* is the total number of nodes in the domain, and  $U_i$  and  $\hat{U}_i$  are predicted and exact function values at node *i*, respectively. The node-wise relative error is also evaluated in the fashion of

$$rerror_{i} = \left| U_{i} - \hat{U}_{i} \right| / \left| \hat{U}_{i} \right|$$
(13)

### 4.2 Results and Discussion

In current study, three types of grids, i.e. structured quadrilateral grids, unstructured right triangular and irregular triangles, are investigated, as shown in Fig. 5. The unstructured right triangles are generated by simply splitting the quad along one of its diagonals.



As shown in Fig. 6 (a), it is obvious that the decoupled solution is predicted by using Scheme I when it is applied onto structured quadrilateral grids. With the help of directional correction, this problem is overcome in Scheme II, as shown in Fig. 6(b).



(a) Scheme I (b) Scheme II Fig. 6 Contour plots of relative errors on structured quadrilateral grids (441 nodes)

Besides, with directional corrections, the overall numerical error is dramatically reduced, as shown in Table 2 below. However, with Scheme II, smaller time step is needed for stability requirement at the cost of more intensive computation in terms of the number of iterations.

Table 2 Comparison of accuracy in prediction by using Scheme I and Scheme II

No. of	Scheme I		Scheme II	
nodes	error	iteration	error	iteration
36	1.96e-2	20	5.07e-3	24
121	8.58e-3	89	1.66e-3	82
441	2.63e-3	202	4.87e-4	303
1681	7.16e-4	728	1.33e-4	1379
6561	1.86e-4	2679	3.38e-5	4299



Fig. 7 Profiles of accuracy for schemes II and VI on structured quadrilateral and right triangular grids

In general, Scheme II gives more accurate prediction than Scheme VI on structured quadrilateral grids, while the both schemes result in more accurate prediction on right triangles. More precisely, the Scheme VI gives slightly better prediction than Scheme II when right triangles are used. It implies that the scheme VI may give more accurate prediction on irregular grids. This is proved to be true, as shown in Table 3. The better accuracy may attribute to the accurate prediction of integration over domain faces.

Table 3 Overall errors predicted based on irregular triangles

No. of	Time stan	error		
nodes	Time-step	Scheme II	Scheme VI	
131	0.008	1.95e-3	1.68e-3	
478	0.001	7.02e-4	6.46e-4	
1887	0.0005	1.89e-4	1.74e-4	
7457	0.0001	4.38e-5	4.12e-5	
29629	0.00003	1.22e-5	1.11e-5	

### **5.** Conclusion

In current study, a new irregular-grid finite difference method (IFDM) for governing equations in strong form is development. The IFDM can be used for general application subjected to arbitrary geometries. In this paper, the principle of IFDM, based on Green-Gauss theorem, is introduced and the numerical procedure for predictions of spatial derivatives is elucidated. Analyses of the stencils of supporting nodes for discretized spatial derivatives. with respect to totally eight types of discretization schemes, are performed. Assessment is made upon the compactness of stencil and positivity of weighting coefficients. Two schemes with better efficiency and accuracy are selected in further study. Numerical excises by using the two schemes are carried out for solutions to a Poisson equation on a square domain. It further proves that the both schemes indeed give satisfactory prediction. Besides, the Scheme VI is superior to Scheme II in terms of accuracy, especially on irregular grids, at the cost of slightly higher computational demand.

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