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Visualizing the Energy of Scattered Data by Using Cubic Timmer Triangular Patches

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Abstract. This paper discusses the application of the new cubic Timmer triangular patches constructed by Ali et al. [1] to interpolate the irregularly scattered data with C^1 continuity. In order to apply the cubic Timmer triangular patches for scattered data interpolation, the data is first triangulated by using the Delaunay algorithm, and then the sufficient condition for C^1 continuity is derived along the adjacent triangles. Two methods will be used to calculate the cubic Timmer ordinates on each triangle. The convex combination between three local schemes $T_i, i = 1,2,3$ will be used to produce the C^1 surface everywhere. The proposed scheme will be tested to visualize one energy data set with irregular shape properties. Numerical and graphical results are presented by using MATLAB. Comparisons between the proposed scheme and existing schemes such as cubic Ball and cubic Bézier triangular patches are also carried out. The results indicate that the surface produced by cubic Timmer triangular patch is better than surface produced using cubic Ball and cubic Bezier triangular patches with overall coefficient of determination R^2 value obtained to be larger than 0.9234.

1. Introduction

Computer Aided Geometric Design (CAGD) is a field initially developed to introduce computer-based applications to industries such as automotive, aerospace and shipbuilding. The term CAGD was proposed by Barnhill and Riesenfeld in 1974. This term was coined during a conference on the CAGD organized by them at the University of Utah, U.S.A [8]. CAGD deals mainly with the mathematical aspects of computer aided design such as the construction of the curves and surfaces [20].

In the early 1980s, Harry Timmer proposed the Timmer method which is a variation of the Bèzier method [8]. Although Timmer curve does not obey the convex hull property, it is more useful and easier to use in the designing of objects compared to the Bèzier method. The curve produced is nearer to its control polygon. Timmer curve may have the weakness of not obeying the convex hull property, but it is the best method for manipulating the curve [23]. Timmer curve has the special property where the curve meets the midpoint of the line segment.

Scattered data can be used to visualize the non-uniform distribution of data points and it encountered in many areas of scientific applications such as in meteorology (for example, the amount of rainfall) and geology (such as the depths of underground formations). Researches on scattered data interpolation as well as shape preserving interpolation and range restricted interpolation can be found in [14-18, 20-22, 25, 26].

Many researchers investigated surface interpolation based on triangulations for scattered data. The construction of scattered data interpolation using Bézier triangular patches can be described as follows:

(a) Triangulate the domain by using Delaunay triangulation,
(b) Specify the derivatives at the data points, and then assign Bézier ordinate values for each triangular patch,
(c) Generate the triangular patches of the surfaces, and finally,
(d) Apply spatial data interpolation to estimate the missing value.

Scattered data technique is important to visualize the geochemical images of the surface data. In Karim and Saaban [15], they visualized terrain data by using the cubic Ball triangular patches. They claimed that the cubic Ball triangular can reconstruct the surface with good approximation properties. Wu et al. [26] proposed a new approach to construct shape preserving interpolating curves. This new approach is based on the use of a class of multiquadric quasi-interpolation operator and supported radial basis functions.

Several type of surfaces are concerned with nonnegativity preserving interpolation on rectangular surfaces such as the study in Peng et al. [21]. In their study, rational splines are used to construct the nonnegativity preserving interpolant of the data. Ramli and Ali [23] extended the Timmer function to higher order Timmer blending functions which are quartic and quantic functions. The quintic Timmer function is used because the higher order basis function will make them control the curve easier.

Shape preserving scattered data interpolation is useful in geometric modelling and visualization. Ordinary interpolation methods do not preserve the data shape. In Hussain et al [14], they developed a method to preserve the shapes of scattered data when it is convex. Convexity is useful in shape property and its applications example are in telecommunication system design and approximation theory. Feng and Zhang [10] discussed a piecewise bivariate Hermite interpolation function in order to approximate three-dimensional scattered data sets.

Surface reconstruction is the process of generating three dimensional surfaces from a point cloud of data of the real object. This method was significant in the area of computer animation and industrial manufacturing. In Awang et al. [6], six different test functions were used in reconstructing the surface of scattered data points. Their research aims were to test the accuracy of Delaunay triangulation in generating different surface when the points were removed. Awang and Rahmat [4] focused on developing a smooth surface using the cubic Bèzier triangular patch. The Delaunay triangulation process was chosen as the method did not require the deletion of the sample data points. Thus, it could preserve the original surface topology. The Graphical User Interface (GUI) function is applied to represent the results and the comparison of the interpolation surface generated by 6 test functions are discussed.

Luo and Peng [17] described the rational spline as a piecewise rational convex combination of three cubic Bézier triangular patches that share the same boundary Bézier ordinates. The sufficient conditions for non-negativity were derived on the boundary Bézier ordinates of adjacent triangle and the normal derivatives at the data sites. Thus, their main scheme also requires the modification of the first order partial and normal derivatives.

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Saaban et al. [24] described the positivity preserving property by using quintic triangular Bézier patches. The surface is constructed by using convex combination of quintic triangular Bézier patches. They used the real data collected from rainfall at various stations in West Peninsular Malaysia. Goodman et al. [10] described the local derivative estimation for scattered data interpolation. Amidor [4] and Lodha and Franke [17] provided a good survey on scattered data interpolation techniques with applications in surface reconstruction and electronic imaging systems. Hussain et al. [14] described the convexity-preserving property to preserve the shape of the scattered data arranged over a triangular grid. Bernstein-Bézier quartic function was used for interpolation.

In Karim et al. [16], Cubic Bèzier triangular patches used to estimate the unknown value of rainfall at spatial localization. Three different scattered data interpolation methods for positivity preserving interpolation are discussed. Saaban [46] scheme is used to estimate the unknown value of rainfall. Awang and Rahmat [5] focused on the developing a smooth surface using two processes which are the derivative estimation and the surface interpolation using the cubic Bèzier triangular patch. The estimation of the second order partial derivatives is constructed using the least squares minimization method. Chua and Kong [7] described rational blend of quartic Bèzier triangles is derived for a constrained C^1 scattered data interpolation. The derivation of sufficient range restriction conditions on the Bèzier ordinates is done to make sure the quartic Bèzier triangular patch lies on one side of the given constraint surface. In Ping and Pang [22], a composite surface interpolation is considered in order to triangulate 3D data. A surface is constructed over each triangle of the data mesh by using the point-normal interpolation technique. This method is local and it is applied to scattered data interpolation. The comparison described in Saaban et al. [25] generalized positivity-preserving schemes for triangular Bèzier patches of C^1 and C^2 scattered data interpolants are presented. Three methods of C^1 schemes using cubic Bèzier triangular patches and one C^2 scheme using quantic Bèzier triangular patches is compared.

2. Background of Study

2.1. Cubic Timmer Triangular Patches

Given three vertices V_1, V_2, V_3 of a triangle and the barycentric coordinates u, v, w. At any point of triangle V can be determined as

$$V = uV_1 + vV_2 + wV_3, u + v + w = 1 \tag{1}$$

A cubic Timmer triangular patch is defined by

$$T(u, v, w) = \sum_{i+j+k=3} a_{ijk} T_{ijk}^3(u, v, w) \tag{2}$$

$$\begin{aligned} T(u, v, w) = {} & u^2(2u-1)a_{3,0,0} + 4u^2va_{2,1,0} + 4u^2wa_{2,0,1} + v^2(2v-1)a_{0,3,0} + 4v^2ua_{1,2,0} + \\ & 4v^2wa_{0,2,1} + w^2(2w-1)a_{0,0,3} + 4w^2ua_{1,0,2} + 4w^2va_{0,1,2} + 6uvwa_{1,1,1} \end{aligned}$$

where a_{ijk} is the control point of the Timmer triangular patch as shown in figure 1. Meanwhile $T_{ijk}^n(u, v, w)$ is the cubic Timmer basis function as shown in figure 2.

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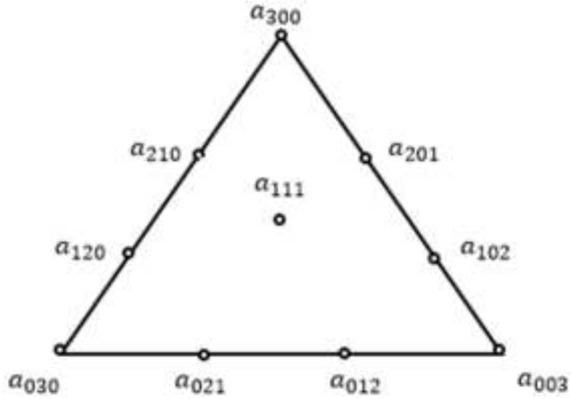

Figure 1. Control points of Timmer triangular patch.

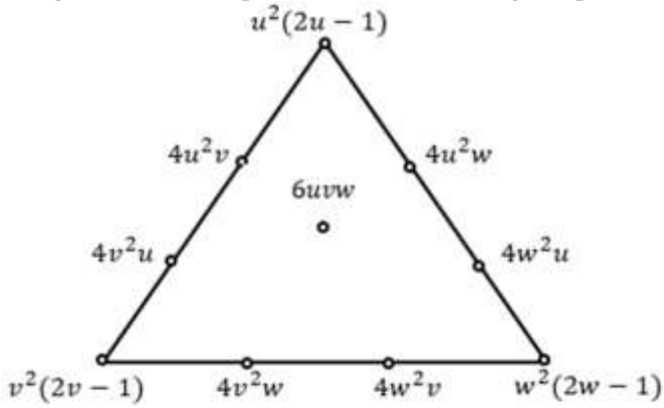

Figure 2. Cubic Timmer basis functions.

Figure 3 shows the example of one patch cubic Timmer triangular.

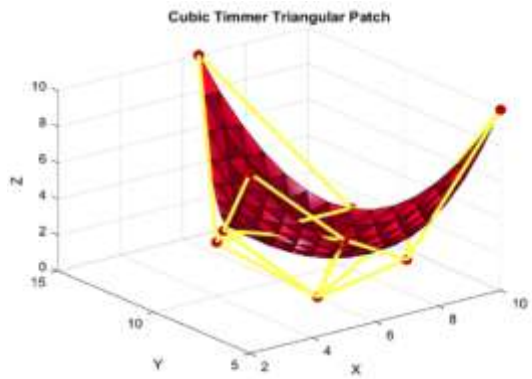

Figure 3. Cubic Timmer triangular patch.

The derivative of T with respect to the direction $z = (z_1, z_2, z_3) = z_1V_1 + z_2V_2 + z_3V_3, z_1 + z_2 + z_3 = 0$ is given by:

$$D_zT(u,v,w) = z_1\frac{\partial T}{\partial u} + z_2\frac{\partial T}{\partial v} + z_3\frac{\partial T}{\partial w} \tag{3}$$

From (2), it can be shown that

$$\begin{aligned} \frac{\partial T}{\partial u} &= 4v^2a_{120} + 4w^2a_{102} + 6vwa_{111}^1 \\ \frac{\partial T}{\partial v} &= (6v^2 - 2v)a_{030} + 8vwa_{021} + 4w^2a_{012} \end{aligned} \tag{4}$$

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$$\frac{\partial T}{\partial w} = (6w_2 - 2w)a_{003} + 4v^2 a_{021} + 8vwa_{012}$$

For further details of the Timmer triangular patch can be found in Ali et. al. [2].

2.2. Local Scheme for Scattered Data Interpolation

The problem that are concerned in this study is the interpolation of scattered data. This problem usually occurs in many practical conditions where the data are obtained experimentally or from the simulation of the studies. There is a few approaches to this problem such as uses the idea of "meshless" surface and triangulates the data points. The problem of scattered data can be defined as follows: given functional of scattered data

$$(x_i, y_i, z_i), i = 1,2, \dots, N \tag{5}$$

We wish to construct a C^1 surface $z = T(x, y)$ such that

$$z_i = T(x_i, y_i), i = 1,2, \dots, N \tag{6}$$

where N is the total number of the scattered data points.

To apply cubic Timmer triangular patches for scattered data interpolation, we construct a convex combination of three local schemes defined as

$$T(u, v, w) = \frac{vwT_1 + uwT_2 + uvT_3}{vw + uw + uv} \tag{7}$$

where the local scheme $T_i, i = 1,2,3$ is obtained by replacing the inner ordinates $a_{111}^i, i = 1,2,3$ to the cubic Timmer triangular patches defined in (1). There are two methods of convex combination proposed by Barnhill et al. [7] and Nielson [17]. Details comparison with this established scattered data interpolation schemes can be found in Ali et al. [3]. The main idea is we need to calculate the boundary ordinates by using Goodman and Said's method [13] as well as the inner ordinates by using Foley and Opitz [11] methods. The derivations are well described in the following paragraphs:

Let $e_1 = (0, -1, 1), e_2 = (1, 0, -1)$ and $e_3 = (0, 0, 1)$ be the direction vectors on edges e_1, e_2 and e_3, respectively. Let n_1 be the inward normal direction to the line segment U_2U_3 which is e_1 as shown in figure 4 where

$$n_1 = -e_3 + \frac{e_3 . e_1}{|e_1|^2} e_1 \tag{8}$$

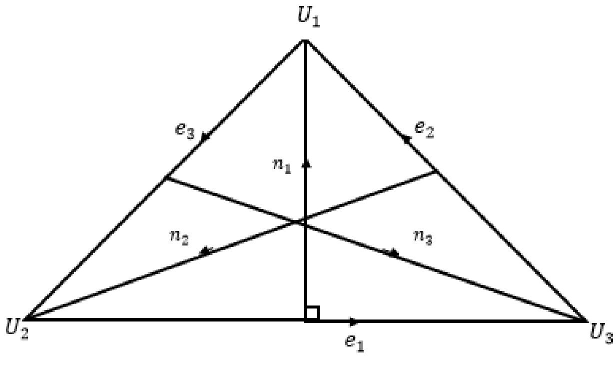

Figure 4. Inward normal direction n_1, n_2, n_3 to the edges.

Meanwhile, the normal derivative of local scheme T_1 given along inward normal direction n_1 is given as

$$D_{n_1}T_1 = (4a_{120} - 2a_{021} - 3a_{030})v^2 + (4a_{102} - 2a_{012} - 3a_{003})w^2 + 2(3a_{111}^1 - 2a_{021} - 2a_{012})vw + va_{030} + wa_{003} \tag{9}$$

Next, consider n_2 and n_3 by using the same technique as n_1.

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2.3. Determination of Timmer Ordinates

Let the data $F(U_i)$ and its first partial derivatives $F_x U_i$ and $F_y U_i$ for $i = 1,2,3$ be given at the vertices. The Timmer ordinates that lies at the edge of the triangle b_{210} and b_{201} are determined as follows. Let the directional derivatives along e_3 and e_2 at W_1 be

$$\begin{aligned}\frac{\partial F}{\partial e_3} &= D_{e_3}T(1,0,0)\\ &= \left(\frac{\partial x}{\partial v} - \frac{\partial x}{\partial u}\right)F_x(U_1) + \left(\frac{\partial y}{\partial v} - \frac{\partial y}{\partial u}\right)F_y(U_1)\\ &= (x_2 - x_1)F_x(U_1) + (y_2 - y_1)F_y(U_1) \qquad (10)\end{aligned}$$

and

$$\begin{aligned}\frac{\partial F}{\partial e_2} &= D_{e_2}T(1,0,0)\\ &= \left(\frac{\partial x}{\partial v} - \frac{\partial x}{\partial u}\right)F_x(U_1) + \left(\frac{\partial y}{\partial v} - \frac{\partial y}{\partial u}\right)F_y(U_1)\\ &= (x_1 - x_3)F_x(U_1) + (y_1 - y_3)F_y(U_1) \qquad (11)\end{aligned}$$

Next we apply the derivatives of Timmer triangular patches as follows. For the given direction shown by the vector $\hat{s} = (\hat{s}_1, \hat{s}_2, \hat{s}_3)$, with $\hat{s}_1 + \hat{s}_2 + \hat{s}_3 = 0$, the directional derivative

$$D_{\hat{s}}T(r,s,t) = \hat{s}_1\frac{\partial T}{\partial \hat{s}} + \hat{s}_2\frac{\partial T}{\partial \hat{s}} + \hat{s}_3\frac{\partial T}{\partial \hat{s}}$$

After applying (10) and (11) on cubic Timmer triangular patches, we get

$$D_{e_3}T(1,0,0) = 4(-a_{300} + a_{210}) \qquad (12)$$

$$D_{e_3}T(1,0,0) = 4(a_{300} - a_{201}) \qquad (13)$$

Therefore, from (12) and (13),

$$a_{210} = a_{300} + \frac{1}{4}[(x_2 - x_1)F_x(U_1) + (y_2 - y_1)F_y(U_1)]$$

and

$$a_{201} = a_{300} + \frac{1}{4}[(x_1 - x_3)F_x(U_1) + (y_1 - y_3)F_y(U_1)\ ]$$

Similarly, we obtain the remaining boundary cubic Timmer ordinates:

$$a_{012} = a_{030} + \frac{1}{4}[(x_3 - x_2)F_x(U_2) + (y_3 - y_2)F_y(U_2)]$$

$$a_{120} = a_{030} + \frac{1}{4}[(x_2 - x_1)F_x(U_2) + (y_2 - y_1)F_y(U_2)]$$

$$a_{102} = a_{003} + \frac{1}{4}[(x_1 - x_3)F_x(U_3) + (y_1 - y_3)F_y(U_3)]$$

and

$$a_{012} = a_{003} + \frac{1}{4}\left[(x_3 - x_2)F_x(U_3) + (y_3 - y_2)F_y(U_3)\right] \qquad (14)$$

Now we need only to determine the inner ordinates for each local scheme. There are two methods that can be used to calculate the inner ordinates which are Goodman and Said [13] method and Foley and Opitz [11] method. Further explanation of this two methods can be referred in Ali et. al. [2].

2.4. Final Scheme for Scattered Data Interpolation

The final scheme of the scattered data interpolation can be written as follows:

$$T(u,v,,w) = \frac{vwT_1 + uwT_2 + uvT_3}{vw + uw + uv}$$

which can be simplified to

$$T(u,v,w) = c_1\,T_1\,(u,v,w) + c_2\,T_2\,(u,v,w) + c_3\,T_3\,(u,v,w)$$

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where

$$c_1 = \frac{vw}{vw + uv + uw}, c_2 = \frac{uw}{vw + uv + uw},$$
$$c_3 = \frac{uv}{vw + uv + uw}$$

Or, in much simpler form, as

$$T(u,v,w) = \sum_{\substack{i+j+k=3, \\ i\neq 1, j\neq 1, k\neq 1,}} a_{i,j,k} T_{ijk}^3(u,v,w) + 6uvw(c_1 a_{111}^1 + c_2 a_{111}^2 + c_3 a_{111}^3). \tag{15}$$

3. Results and Discussion

To test the capability of the proposed scheme for scattered data interpolation, we choose one type of energy data set. The data samples are irregular since in many applications the collected data are irregular i.e. not in uniform sampling or regular. To measure the effectiveness on the scheme, we calculate root mean square error (RMSE), maximum error and coefficient of determination (R^2). The comparison has been made between the cubic Timmer triangular patches and the cubic Ball and cubic Bezier triangular patches based on two different methods to calculate the inner ordinates i.e. Goodman and Said [13] and Foley and Opitz [11] methods. The function of kinetic energy is obtained from Gilat [12].

Consider the scenario where one container contains a lot of molecules of a gas moving around at different speeds. Maxwell's speed distribution law gives the probability distribution $P(v)$ as a function of speed and temperature as stated below:

$$P(v) = 4\pi \left(\frac{M}{2\pi RT}\right)^{3/2} v^2 e^{(-Mv^2)/(2RT)} \tag{16}$$

where $M = 0.032$ kg/mol is denoted as the molar mass of the gas, $R = \text{J}/(\text{K}\cdot\text{mol})$ is the gas constant, $70 \leq T \leq 320\ K$ is the temperature and $0 \leq v \leq 1000\ m/s$ is the speed of the molecules.

To apply cubic Timmer triangular patches, we sample it into 36 irregular data sets as given in the following table 1.

Table 1. 36 irregular data sets.

No	v	T	P(v)	No	v	T	P(v)
1	0	70	0.000000	21	700	180	2.05E-04
2	0	100	0.000000	22	700	250	0.000543
3	0	180	0.000000	23	700	280	0.000686
4	0	250	0.000000	24	700	320	0.000856
5	0	280	0.000000	25	850	70	5.51E-10
6	0	320	0.000000	26	850	100	1.25E-07
7	250	70	0.003647	27	850	180	2.51E-05
8	250	100	0.003577	28	850	250	1.34E-04
9	250	180	0.002529	29	850	280	2.05E-04
10	250	250	0.001863	30	850	320	0.000311
11	250	280	0.001655	31	1000	70	3.69E-13
12	250	320	0.001429	32	1000	100	8.29E-10
13	500	70	8.40E-05	33	1000	180	1.79E-06
14	500	100	0.000387	34	1000	250	2.18E-05
15	500	180	0.001361	35	1000	280	4.20E-05
16	500	250	0.001758	36	1000	320	8.12E-05

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17	500	280	0.001823
18	500	320	0.00185
19	700	70	2.24E-07
20	700	100	7.47E-06

Figure 5 shows the Delaunay triangulation for the irregular data. Figure 6 shows the 3D visualization of the irregular data sets and the surface interpolation for data sets in table 1 is shown in figure 7.

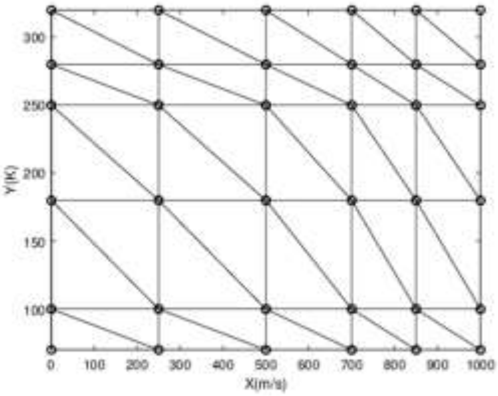


Figure 5. Delaunay triangulation for data in Table 1.

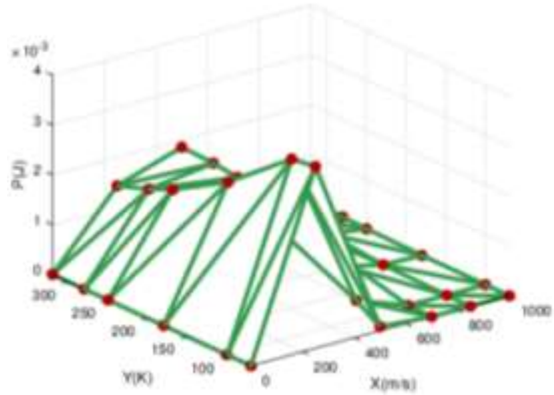
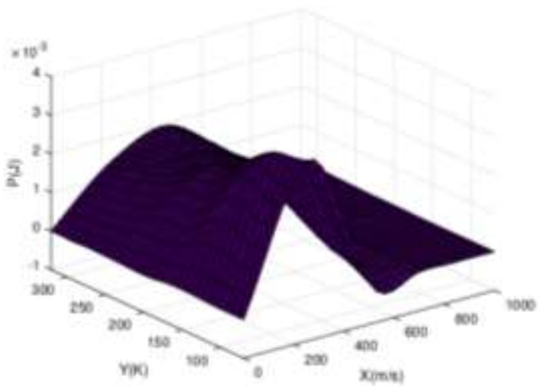
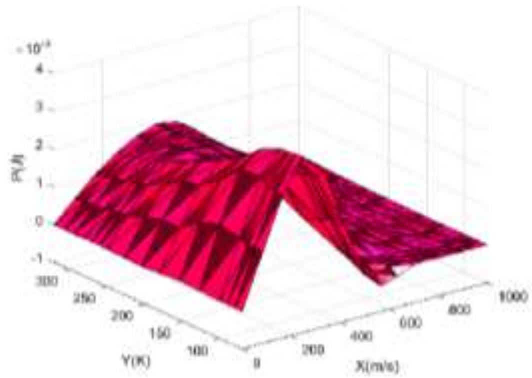


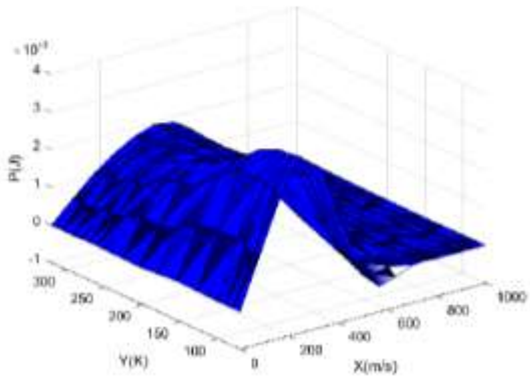
Figure 6. 3D linear interpolant.



(a)



(b)



(c)

Figure 7. Scattered data interpolation; (a) True solution, (b) Cubic Timmer triangular using Goodman and Said, (c) Cubic Timmer triangular using Foley and Opitz.

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Table 2. Error using Goodman and Said.

Error	Bezier	Ball	Timmer
RMSE	2.78E-04	2.78E-04	2.78E-04
Max Error	1.49E-03	1.49E-03	1.49E-03
$\boldsymbol{R^2}$	0.9234	0.9234	0.9234

Table 3. Error using Foley and Opitz.

Error	Bezier	Ball	Timmer
RMSE	2.76E-04	2.78E-04	2.72E-04
Max Error	1.48E-03	1.48E-03	1.48E-03
$\boldsymbol{R^2}$	0.9246	0.9199	0.9266

From the numerical results stated in table 2 and table 3, we found that when Foley and Opitz's [11] method is used to calculate the inner ordinates for each local schemes, we obtained smaller RMSE and Maximum error as compared to Goodman and Said's [13] method. Besides that, we can see that, the cubic Timmer gives higher R^2 value compared to cubic Ball and cubic Bezier. Overall, the cubic Timmer triangular patches give the results on par with the established schemes.

Finally, we can use the proposed scheme in this study to predict the amount of the energy. For this we consider the Goodman and Said scheme only. Supply any value of *x*-*y* plane that is located in the given domain. We take the values of selected data points v and T as shown in table 4. Then calculate the value of the kinetic energy is calculated as follows:

$$P(v) = 4\pi \left(\frac{0.032}{2\pi 3T}\right)^{3/2} v^2 e^{(-0.032v^2)/(6T)} \tag{17}$$

Table 4. Selected points.

$\boldsymbol{v}$	$\boldsymbol{T}$	Actual $\boldsymbol{P}$
0	70	0
83.33	90	1.34E-03
83.33	180	5.09E-04
83.33	226.67	3.66E-04
166.67	80	3.79E-03
566.67	226.67	1.17E-03
566.67	250	1.30E-03
700	180	2.05E-04
1000	226.67	1.14E-05
1000	203.33	5.08E-06

Figure 8 shows the location of the selected data points in the Delaunay triangulation.

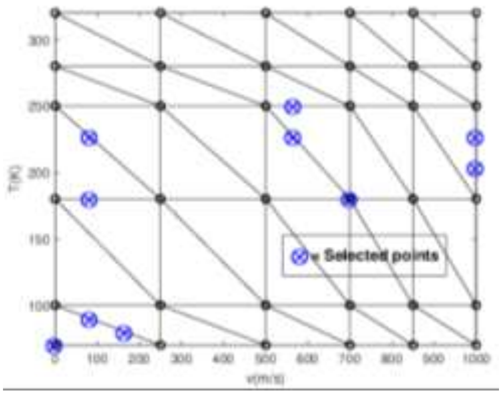

Figure 8. Delaunay triangulation with the location of the selected data points.

Then, the energy (V) located at selected point can be predicted by using the cubic Timmer triangular patches. The energy prediction data points are given in table 5.

Table 5. Energy prediction with absolute error.

$\boldsymbol{v}$	$\boldsymbol{T}$	Actual $\boldsymbol{P}$	Prediction $\boldsymbol{P_p}$	Absolute Error $\lvert\boldsymbol{P-P_p}\rvert$
0	70	0	0	0
83.33	90	1.34E-03	1.40E-03	6.00E-05
83.33	180	5.09E-04	1.06E-03	5.51E-04
83.33	226.67	3.66E-04	9.16E-04	5.50E-04
166.67	80	3.79E-03	2.79E-03	1.00E-03
566.67	226.67	1.17E-03	1.32E-03	1.50E-04
566.67	250	1.30E-03	1.42E-03	1.20E-04
700	180	2.05E-04	2.05E-04	0
1000	226.67	1.14E-05	1.02E-05	1.20E-06
1000	203.33	5.08E-06	8.75E-06	3.67E-06

Table 5 shows the absolute error for the prediction at selected locations. We can see that, some of the energy prediction is similar to the energy values from the true function and hence, the absolute error is equal to zero. This is due to the properties of cubic Timmer triangular patch that interpolates end points. Overall, the cubic Timmer triangular patches can be used to predict the kinetic energy for the data that lies inside the Delaunay triangulation.

4. Conclusion

In this study, the cubic Timmer triangular patches constructed in Ali et al. [1] is applied to reconstruct the surface coming from irregular scattered data. Two methods are discussed to calculate the inner ordinates for each local scheme i.e. Goodman and Said [13] and Foley and Opitz [11]. Both methods will produce C^1 surface everywhere in the given domain. The proposed scheme is used to visualize the kinetic energy of molecules of gas moving in a container as well as to predict the energy for some selected data points. From the prediction, the cubic Timmer triangular patches give quite good results since the prediction values are almost similar to the actual values provided in table 5. Future works are underway to study the application of the cubic Timmer triangular for shape preserving scattered data interpolation.

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