A least-squares spectral collocation formulation for solving PDEs on complex geometry domains

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Abstract:
A least squares collocation scheme is used to solve PDEs defined on a complex geometry domain. Triangular finite elements are used to build a macro-mesh of the whole domain and Fekete points are used as collocation points. We combine together the standard least squares method and spectral method to compute the global solution. The assembling process of local solutions is explained through an algorithm. The success of this method is studied throughout a test problem. Numerical results prove the accuracy of the method which takes into account the boundary conditions.

Keywords: Least-squares formulation, Spectral elements, Fekete points, differentiation matrices.

1 Introduction

Computing solutions of partial differential equations (PDEs) on complex geometry domains is one of the important challenges in numerical analysis. Many classical numerical schemes suffer on the fact they do not take into account the complexity of the domain geometry.

It is well known that the finite element method (FEM) in its different variants is one of the most frequently used techniques to approximate the solutions of PDEs. The FEM is become more popular since the middle of the twentieth century mainly because of its applications by engineers to structural mechanics such that the analysis of pollutant transport in a fluid [3], [21], [30], the estimation of crustal deformation fields from GPS measurements [12], [15], [25], [26] and more generally some numerical solutions of Navier-Stokes equations [4], [13], [23]. One of the variant of the FEM is the Least-squares Finite Element Method (LSFEM) that gives accuracy solutions in the case of elliptic problems. But this method is not efficient for solving non linear and parabolic problems [5]. Alternatively to the LSFM the Least Squares Spectral Collocation Method (LSSCM) was developed for solving some non linear PDEs. These methods have become an attractive class of methods for the numerical solutions of PDEs. LSSCM is particularly well suitable for solving problems that require coordinate transformations or tracking [22], [24], [29], [36]. However, it seems to require more computational effort and higher order continuity basis functions and more work in the matrix assembly. An other variant is the hp-Finite Element
Method (hp-FEM). This version has been developed to take into account the boundary layers and the singularity of the solutions [16], [34], [37]. This method presents best abilities. For example the hp-FEM automatically refines the grid around the singularity and increases the polynomial order of approximation in regions where the solutions are smooth. The overall convergence of the method is very fast (exponential convergence).

Because the problem domain needs to be discretized into a mesh, these FEM versions suffer from drawbacks such as tedious meshing and re-meshing. The meshless method [2], [31], [32], [33], [42] has been proposed for the problem of computational mechanics in order to avoid the tedious meshing and re-meshing. The meshless method is used to establish a system of algebraic equations for the whole problem domain without the use of a predefined mesh.

Taking into account the problems met by the previous methods, FEMs has been developed in [40]. The domain is meshed by using a hybrid discretization consisting of triangular and quadrilateral sub-domains in order to provide great flexibility in refinement and unrefinement techniques. The spectral method is used over each finite element, in which the weak formulation of Galerkin is used to discretize the equations. An assembled matrix is easily defined but the difficulties for applying this method lies in the choice of suitable basis functions to interpolate the solutions.

In this paper we develop a scheme that combines LSCMs, [11], [22], [29] and Spectral collocation finite elements methods [14], [17], [18], [35]. Collocation points over an arbitrary triangle are generated using Fekete points [38].

We should also note that a lot of research for the LSSCM is done for Stokes and Navier-Stokes equations as well as for singular perturbation problems. The most important papers where LSSCM has been developed in different directions are given in [20], [27], [28]. For a general overview for spectral methods we should refer to [9]. Furthermore an adaptive LSSCM on triangular elements is presented in [19].

The paper is organized as follows. In Section 2 we describe the generating collocation points into a triangular element. In Section 3, we introduce the pseudospectral differentiation. The least squares collocation method is presented in section 4. The section 5 is devoted to numerical experiments and we conclude the paper with some remarks in section 6.

2 Triangular-collocation points

In this paper the whole domain is meshed by triangular elements. In this section we define collocation points in an arbitrary triangle by using Fekete points.

Let us define the standard triangle by

\[ \hat{T} = \{(r, s), -1 \leq r, s \leq 1; r + s \leq 0\} \]  

and let us consider the Dubiner basis functions [14]

\[ \phi_{ij}(r, s) = \left(1 - \frac{s}{2}\right)^i \times p_{i}^{0,0}(\frac{2r + s + 1}{1 - s}) \times p_{j}^{2i+1,0}(s) \]

where the \( p_{j}^{\alpha,\beta}(s) \) are the \((\alpha, \beta)\)-order Jacobi polynomials of degree \( j \) [1]. It is well known that the set of functions \( \phi_{ij}, 0 \leq i, j \leq N \) and \( i + j \leq N \) is an orthogonal basis of \( P_N(\hat{T}) \), the space of polynomial of degree less than \( N \). In all the following of this paper we shall write \( \phi_k \) instead of \( \phi_{ij}, 1 \leq k \leq (N + 1)(N + 2)/2 \) for any arbitrary bijection \( k \equiv k(i, j) \). Let us now consider the generalized Vandermonde matrix \( V \) whose components are \( V_{ij} = \phi_j(z_i) \) for arbitrary points \( z_k \in \hat{T}, k = 1, ..., \eta \), where we have set \( \eta = (N + 1)(N + 2)/2 \). Fekete points are the points \( \hat{z}_i, i = 1, ..., \eta \) that maximize the determinant of \( V \):

\[ \max_{\{z_i\} \in \hat{T}} |V(z_1, z_2, ..., z_N)| \]

\[ d \]

\[ \hat{d} \]
In the framework of this paper Fekete points will be generate into an arbitrary triangular element using appropriate transformation map.

Figure 1: The Lobatto triangle nodes (+) and associated Fekete nodes (o) over the reference triangle $\tilde{T}$ for $N = 10$.

Figure 2: Distribution of Fekete points from reference triangle (left) to arbitrary triangle (right) for $N = 10$.

Fekete points are alternative collocation points to Gauss-Lobatto quadrature points. Clearly in the case of tensor-product domains such as lines or quadrangles, the Gauss-Lobatto quadrature points are well suitable for spectral approximation [7],[8]. However, in the case of the triangular domains, the Fekete points are commonly used in numerical methods to achieve both accurate high-order polynomial interpolation and quadrature properties [11],[38]. One can notice that the Fekete points are independent of the chosen basis but since we must compute numerically the inverse, it is important for the matrix to be well-conditioned.

3 Pseudo spectral Differentiation

Solving PDEs requires accurate approximation of derivatives. We want to provide a discrete differentiation matrix associated with Fekete collocation points on arbitrary triangles. We refer to [39]
in the case of one dimension and the standard quadrangle. In the case of triangular domains, singularities often arise near edges. Therefore both suitable collocation points and accurate numerical methods are required.

### 3.1 Differentiation over the reference triangle

For any continuous function \( u(r, s) \) on the reference triangle \( \hat{T} \) we can write its spectral approximation in the space \( P_N \) by

\[
 u^N(r, s) = \sum_{k=1}^{\eta} U_k \phi_k(r, s) \tag{3.1}
\]

where \( \eta = (N + 1)(N + 2)/2 \), and where the coefficients \( U_k \) are obtained by using collocation equations at Fekete points \( \hat{z}_m \)

\[
 u(\hat{z}_m) = \sum_{k=1}^{\eta} U_k \phi_k(\hat{z}_m), \quad m = 1, 2, ..., \eta \tag{3.2}
\]

Setting \( U = (u(\hat{z}_1), u(\hat{z}_2), ..., u(\hat{z}_\eta))^T \) and \( C = (U_1, U_2, ..., U_\eta)^T \) the coefficients vector, we obtain

\[
 C = V^{-1} \times U \tag{3.3}
\]

where \( V \) is the Vandermonde matrix for the Fekete points. According to (3.1), the derivatives in \( s \) and in \( r \) directions at Fekete collocation points \( \hat{z}_m \) are given by

\[
 \partial_r u^N(\hat{z}_m) = \sum_{k=1}^{\eta} U_k \times \partial_r \phi_k(\hat{z}_m)
\]

and

\[
 \partial_s u^N(\hat{z}_m) = \sum_{k=1}^{\eta} U_k \times \partial_s \phi_k(\hat{z}_m)
\]

respectively. We introduce two differentiation matrices \( V^r, V^s \), of size \( \eta \times \eta \) in \( r \)-direction respectively in \( s \)-direction whose components are \( V^r_{ij} = \partial_r \phi_j(\hat{z}_i) \) and \( V^s_{ij} = \partial_s \phi_j(\hat{z}_i) \). Denoting \( U_r \) respectively \( U_s \) the vector values of the differential approximation respectively in \( r \) and \( s \) directions at Fekete collocation points, we obtain

\[
 U_r = D^r \times U \quad \text{and} \quad U_s = D^s \times U \tag{3.4}
\]

with

\[
 D^r = V^r \times V^{-1} \quad \text{and} \quad D^s = V^s \times V^{-1} \tag{3.5}
\]

We deduce the second order differentiation matrices over the reference triangle from (3.4) and (3.5)

\[
 D^{rr} = V^{rr} \times V^{-1}, \quad D^{ss} = V^{ss} \times V^{-1}, \quad D^{rs} = V^{rs} \times V^{-1} \tag{3.6}
\]

where

\[
 V^{rr} = \partial_r V^r, \quad V^{ss} = \partial_s V^s, \quad V^{rs} = \partial_r V^s
\]

### 3.2 Differentiation over an arbitrary triangle

Any derivative over an arbitrary triangle is derived from the reference triangle according to the bijective transformation such that:

\[
 u(r, s) = u(x_1(r, s), x_2(r, s)) \tag{3.7}
\]
Applying the derivative rule in $r$ (respectively $s$) direction, we have

\[
\begin{align*}
\partial_r u &= (\partial_r x_1) \partial_{x_1} u + (\partial_r x_2) \partial_{x_2} u \\
\partial_s u &= (\partial_s x_1) \partial_{x_1} u + (\partial_s x_2) \partial_{x_2} u
\end{align*}
\]  

(3.8)

Let us denote by $U_{x_1}$ and $U_{x_2}$ the vector values of the differential approximation respectively in $x_1$ and $x_2$ directions at Fekete collocation points. Then, from (3.5) and (3.8) we deduce

\[
\begin{pmatrix}
U_{x_1} \\
U_{x_2}
\end{pmatrix} = G^{-1} \times \begin{pmatrix}
D^r \\
D^s
\end{pmatrix} \times U
\]

(3.9)

where the matrix $G$ is associated to the system (3.8) over Fekete collocation points. Setting $\mathbb{D} = G^{-1} \times \begin{pmatrix} D^r \end{pmatrix}$ then the differentiation matrices over an arbitrary triangle in $x$–direction, and $y$–direction are given by

\[D^x = \mathbb{D}(1 : \eta, : ) \quad \text{and} \quad D^y = \mathbb{D}(\eta + 1 : 2\eta, : )\]

(3.10)

respectively. Second order differentiation matrices on an arbitrary triangle are derived from (3.6) and (3.8). Thus, there exists a matrix $Q$ of size $3 \times 3$, obtained from the derivative of (3.8), such that

\[
\begin{pmatrix}
D^{xx} \\
D^{xy} \\
D^{yy}
\end{pmatrix} = Q \times \begin{pmatrix}
D^{rr} \\
D^{rs} \\
D^{ss}
\end{pmatrix}
\]

(3.11)

4 Least Squares spectral elements formulation

Collocation least squares methods (CLSM) also known as point least-squares or overdetermined collocation methods, have got a great success in elliptic equations solving [5],[6]. In this section we present them as an alternative method of standard Least Squares method applied to spectral collocation methods (LSSCM). The CLSM carried also a numerical contribution for solving some hyperbolic equations [10], [29], [41]. The parabolic problem case is not enough developed to our knowledge so we propose in this section the achievement on a test problem over a complex domain. The Fekete points have been used as collocation points over triangles.

4.1 The test problem

As a test problem, we consider the following parabolic equation

\[
\begin{align*}
\Delta u + 2\pi^2 \times u &= f \quad \text{in} \ \Omega \\
u_{\Gamma} &= g \quad \text{on} \ \Gamma = \partial \Omega
\end{align*}
\]

(4.1)

where $\Omega$ is a plane domain that contains an obstacle taking into account the complexity of the domain geometry (see Fig. 3).

4.2 Triangulation and global assembling procedure

The differentiation procedure using finite element over a non standard domain requires the subdivision of the whole domain into finite elements (quadrilaterals, triangles) [40]. We have studied in the previous section the differentiation operators (the gradient and the Laplacian) over elementary triangles. We present now the procedure to assemble these elementary operators into a global operator by means of an operator that assembles the local coefficients into the global coefficients and ensure $C^0$ continuity.

Our numerical scheme is based on computing a local solution $u_{\text{loc}}$ over each elementary triangles and then the global solution is obtained using an assembly procedure. To illustrate this global
assembly procedure, we consider a global domain made up of two triangles as shown in the figure below.

The figure (4) illustrates the local and global numbering of a domain containing two triangular elements. For example we have taken $N = 3$ for the expansion order. This technique will allows us to avoid the repeated collocations points in global assembly. In the examples above, the total number of freedom in local numbering is $N_{Loc} = 12$ and the global numbering is $N_{glob} = 9$. Let $u$ be a continuous function defined over such a domain and $\hat{u}_g$ the global vector value of $u$ calculated over the global collocation points

$$\hat{u}_g = \left( \hat{u}^1_g, \hat{u}^2_g, ..., \hat{u}^9_g \right)^T$$  \hspace{1cm} (4.2)

and $\hat{u}_1$ and $\hat{u}_2$ respectively the vector value of $u$ over the first (respectively the second) triangular element

$$\hat{u}_1 = \left( \hat{u}^1_1, \hat{u}^2_1, ..., \hat{u}^6_1 \right)^T \quad \text{and} \quad \hat{u}_2 = \left( \hat{u}^1_2, \hat{u}^2_2, ..., \hat{u}^6_2 \right)^T$$  \hspace{1cm} (4.3)

In this case the global assembled matrix $A$ is a $(12 \times 9)$ matrix such that

$$\begin{bmatrix} \hat{u}_1 & \hat{u}_2 \end{bmatrix} = A \times \hat{u}_g$$  \hspace{1cm} (4.4)

The mesh of the domain above can be done by the program "dismesh_2d" available in Matlab software, this returns the matrix of $p$ coordinates of each edge and the matrix of numbering of triangulation. Let us consider an elementary triangle $k$ in $\Omega$, the problem (4.1) is linear so there exists a matrix $H^k$ such that

$$H^k \times U^k + 2\pi^2 U^k = f^k$$  \hspace{1cm} (4.5)

for $1 \leq k \leq n_t$, where $n_t$ is the total number of triangles in $\Omega$. We deduce the system

$$\begin{pmatrix} H^1 & \vdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \ddots & H^{n_t} \end{pmatrix} \times \begin{pmatrix} U^1 \\ \vdots \\ U^{n_t} \end{pmatrix} + 2\pi^2 \times \begin{pmatrix} U^1 \\ \vdots \\ U^{n_t} \end{pmatrix} = \begin{pmatrix} f^1 \\ \vdots \\ f^{n_t} \end{pmatrix}$$  \hspace{1cm} (4.6)
Let us denote by

$$
H = \begin{pmatrix}
H^1 & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & H^{n_t}
\end{pmatrix}
$$

and

$$
U_{Loc} = (U^1, \ldots, U^{n_t})^T
$$

$$
F_{Loc} = (f^1, \ldots, f^{n_t})^T
$$

According to the relation (4.4), there exists an assembled matrix $Z$ such that:

$$
U_{Loc} = Z \times U_{glob}
$$

Then, the relation (4.6) becomes

$$
H \times Z \times U_{glob} + 2\pi^2 \times Z \times U_{glob} = F_{Loc}
$$

Hence, for simplicity, we deduce from (4.11) a differentiation matrix $D$ such that:

$$
D \times U_{glob} + 2\pi^2 \times U_{glob} = F_{glob}
$$

where we have set

$$
D = \text{inv}(Z^T \times Z) \times Z^T \times H \times Z
$$

It is important to note that the definition of $D$ is justified by the fact that the matrix $Z$ is not square. For boundary conditions, there exists a matrix $B$ such that

$$
B \times U_{glob} = G_{glob}
$$

The operator of least squares method is then derived from (4.11 and 4.13)

$$
\mathcal{L}(U) = \alpha \left\| D \times U + 2\pi^2 \times U - F_{glob} \right\|^2_{\mathbb{R}^{n_p}} + \beta \left\| B \times U - G_{glob} \right\|^2_{\mathbb{R}^{n_b}}
$$

where the weights $\beta$ and $\alpha$ can be used to adjust the relative importance of the terms in the functional. Here $\| \cdot \|^2_{\mathbb{R}^{n_p}}$ and $\| \cdot \|^2_{\mathbb{R}^{n_b}}$ denote $l^2$-norm respectively over $\mathbb{R}^{n_p}$ and $\mathbb{R}^{n_b}$. The integers
\( n_p \) and \( n_b \) represent the number of collocation points on the whole domain and the number of boundary collocation points. Finally, one obtains the numerical solution of the problem (4.1) by solving the following problem
\[
\min_{U \in \mathbb{R}^{n_p}} \mathcal{L}(U) \tag{4.15}
\]
We summarize the algorithmic scheme in (Fig.5).

<table>
<thead>
<tr>
<th>(1)</th>
<th>Read the parameters:</th>
</tr>
</thead>
<tbody>
<tr>
<td>- ( n ) : Mesh parameter.</td>
<td></td>
</tr>
<tr>
<td>- ( N ) : degree of interpolation polynomials.</td>
<td></td>
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<table>
<thead>
<tr>
<th>(2)</th>
<th>Compute the vectors and matrices associated to the meshing:</th>
</tr>
</thead>
<tbody>
<tr>
<td>- ( \mathcal{B} ) : Matrix which selects the boundary points, computed according to (eq.26).</td>
<td></td>
</tr>
<tr>
<td>- ( \mathbb{D} ) : Discret differential operator, computed as (eq.25).</td>
<td></td>
</tr>
<tr>
<td>- ( x_{loc} ) : Vector of local collocation points, obtained according to (eq.2).</td>
<td></td>
</tr>
<tr>
<td>- ( x_{glob} = Z \times x_{loc} ) : Vector of global collocation points</td>
<td></td>
</tr>
<tr>
<td>- ( x_{bord} = D_{bord} \times x_{glob} ) : Vector of boundary points</td>
<td></td>
</tr>
<tr>
<td>- ( \hat{g} ) : Boundary values computed using (eq.29) evaluated at each point of ( x_{bord} ).</td>
<td></td>
</tr>
</tbody>
</table>

| (3) | Define the coefficients \( \hat{\beta} \) and \( \hat{\alpha} \), |

| (4) | Define the least squares operator (eq.27): |
\[
\mathcal{L}(U; g) = \hat{\alpha} \left\| \mathbb{D} \times U + 2\pi^2 \times U \right\|_{R^{n_p}}^2 + \hat{\beta} \left\| \mathcal{B} \times U - \hat{g} \right\|_{R^{n_p}}^2 \tag{26}
\]

| (5) | Choose an arbitrary value \( U_0 \) for iterative process |

| (6) | Compute by an iterative method the \( R^{N_p} \) minimizing problem |
\[
\mathcal{L}(U^*; g) = \min_{U \in \mathbb{R}^{n_p}} \mathcal{L}(U; g)
\]

Figure 5: *Algorithm for the Least Squares Spectral Elements Method.*

### 5 Computational Experiments

For our numerical experiment we consider the test problem (4.1) from which the exact solution is
\[
u_e = \sin(\pi x) \sin(\pi y) \tag{5.1}\]
when we have taken \( f = 0 \) and the data of the function \( g \) called \( G_{glob} \) in (4.14) are available by computing the value of (5.1) at boundaries points. All calculations are performed with a fixed mesh size by varying the degree \( N \) of the interpolation polynomial. The aim of this experience is to analyze the efficiency of the algorithmic scheme (Fig.5).
Figures 7, 8 and 9 illustrate the solution of problem (4.1) for \( N = 2, 4 \) and 6 respectively. These graphics show the convergence process of approached solutions toward the exact solution and take better account of boundary conditions. The gradient field in figures (10-12) shows the convergence of the solution in regions with high concentration gradient. In figures (13-15), we evaluate the absolute error committed when approximating first and second order partial derivatives. Thus, it is clear that these errors become as small as the number \( N \) of collocation points increases. Starting from \( N = 4 \), the approached solution is very close to the exact one.

Figure 7: Numerical solution for \( N = 2 \), and \( \hat{\alpha} = \hat{\beta} = 1 \).

6 Concluding remarks

A least squares collocation scheme for solving PDEs over a complex domain is presented. Using triangular finite elements and Fekete points, the assembling process of global solution has been quite easy. The macro-mesh of complex domain by triangles has enabled to take into account the boundary conditions. Numerical simulations on a test problem have confirmed the high accuracy of our spectral least-squares scheme.
Figure 8: Numerical solution for $N = 4$, and $\hat{\alpha} = \hat{\beta} = 1$.

Figure 9: Numerical solution of (4.1) with $N = 6$, and $\hat{\alpha} = \hat{\beta} = 1$.

References


Figure 10: Gradient of solution through the domain for $N = 2$, and $\hat{\alpha} = \hat{\beta} = 1$.

Figure 11: Gradient of solution through the domain for $N = 4$, and $\hat{\alpha} = \hat{\beta} = 1$.


Figure 12: Gradient of solution through the domain for $N = 6$, $\hat{\alpha} = \hat{\beta} = 1$.

Figure 13: Distribution of absolute error for $N = 2$, and $\hat{\alpha} = \hat{\beta} = 1$.


Figure 14: Distribution of absolute error for $N = 4$, and $\hat{\alpha} = \hat{\beta} = 1$.

Figure 15: Distribution of absolute error for $N = 6$, and $\hat{\alpha} = \hat{\beta} = 1$.


