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An Heuristic Finite Difference Scheme on Irregular Plane Regions

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Abstract

In this paper, we present an heuristic finite difference scheme for the second-order linear operator, which is derived from an unconstrained least squares problem defined by the consistency condition on the residuals of order one, two and three in the Taylor expansion of the local truncation error. It is based on a non-iterative calculation of the difference coefficients and can be used to solve efficiently Poisson-like equations on non-rectangular domains which are approximated by structured convex grids.

Mathematics Subject Classification: 65M06, 65M50

Keywords: finite differences, Poisson-like equations, irregular regions, convex structured grids

1 Introduction

A very important problem in scientific computing is the numerical solution of Poisson-like problems. It is a well studied problem when the domain has a simple geometry; unfortunately, in some specific real-world settings, the

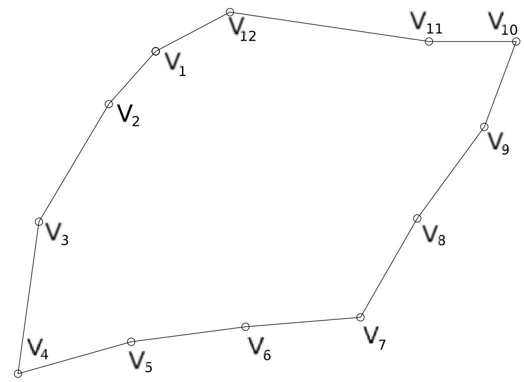


Figure 1: Example of a typical domain when $m = n = 4$.

domain is irregular and very non-symmetric, and in this case the classical finite difference formulas do not produce accurate results. As a matter of fact, there are rather few reliable finite difference schemes which can be successfully applied on irregular domains. In the following sections we present a sound heuristic scheme based on a least squares problem for this case.
The domains of interest here are simply connected polygonal domains -mostly irregular- which can not be decomposed into rectangles. For such domains, it is possible to generate suitable convex structured grids using the direct optimization method, as discussed in detail in [3, 10, 12, 13, 16].
To introduce the required notation for the grids, let m and n be the number of "vertical" and "horizontal" numbers of nodes on the "sides" of a typical domain boundary; the latter is the positively oriented polygonal Jordan curve γ of vertices

$$V = \{v_1, \cdots, v_{2(m+n-2)}\},$$

and it defines the typical domain $\Omega \in I\!R^2$. An example can be seen in figure 1.

A set

$$G = \{P_{i,j} | 1 \leq i \leq \ m, 1 \leq j \leq n\}$$

of points of the plane with the fixed boundary positions given by V is a structured grid with quadrilateral elements for Ω, of order $m \times n$; a grid G is convex if and only if each one of the $(m-1)(n-1)$ quadrilaterals (or cells) $c_{i,j}$ of vertices $\{P_{i,j}, P_{i+1,j}, P_{i,j+1}, P_{i+1,j+1}\}$, $1 \leq i < m$, $1 \leq j < n$, is convex and non-degenerate (Fig. 2).

The functional which was minimized to generate the convex structured grids of the numerical tests for this paper, as implemented in UNAMALLA [4], was

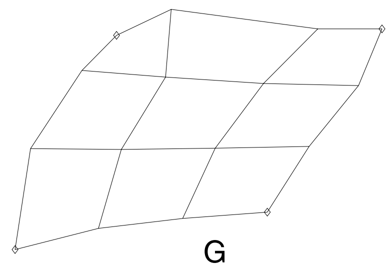


Figure 2: Example of a typical grid G with 4 points per side for the boundary shown in figure 1.

the convex linear combination of the area functional $S_\omega(G)$ and length $L(G)$ with weight $\sigma = 0.5$ (See [11] for details).

2 Finite difference schemes for linear operators

Let us consider the second order linear operator

$$Lu = Au_{xx} + Bu_{xy} + Cu_{yy} + Du_x + Eu_y + Fu \tag{1}$$

where A, B, C, D, E and F are smooth functions defined on an open set containing Ω; general finite difference schemes can be obtained by considering a finite set of nodes $p_0 = (x_0, y_0)$,..., $p_k = (x_k, y_k)$, for which it is required to find coefficients $\Gamma_0, \Gamma_1, \Gamma_2, ..., \Gamma_k$ such that

$$\sum_{i=0}^{k} \Gamma_i u(p_i) \approx \left[Au_{xx} + Bu_{xy} + Cu_{yy} + Du_x + Eu_y + Fu\right]_{p_0}. \tag{2}$$

It is important to emphasize that there are few efficient finite difference schemes for numerical solution of partial differential equations on non-rectangular regions using finite differences [1, 2, 5, 6, 7, 9, 14].

The limit value in (2) is given by the weak consistency condition [15]

$$\sum_{i=0}^{k} \Gamma_i u(p_i) - \left[Au_{xx} + Bu_{xy} + Cu_{yy} + Du_x + Eu_y + Fu\right]_{p_0} \to 0, \quad \text{as} \quad p_1, ...p_q \to p_0,$$

whose Taylor expansion up to third order yields

$$
\begin{aligned}
\left[Au_{xx}+Bu_{xy}+Cu_{yy}+Du_x+Eu_y+Fu\right]_{p_0}-\sum_{i=0}^{k}\Gamma_i u(p_i) &= \\
\left(F(p_0)-\sum_{i=0}^{k}\Gamma_i\right)u(p_0)+\left(D(p_0)-\sum_{i=1}^{k}\Gamma_i\Delta x_i\right)u_x(p_0) &+ \\
\left(E(p_0)-\sum_{i=1}^{k}\Gamma_i\Delta y_i\right)u_y(p_0)+\left(A(p_0)-\sum_{i=1}^{k}\frac{\Gamma_i(\Delta x_i)^2}{2}\right)u_{xx}(p_0) &+ \\
\left(B(p_0)-\sum_{i=1}^{k}\Gamma_i\Delta x_i\Delta y_i\right)u_{xy}(p_0)+\left(C(p_0)-\sum_{i=1}^{k}\frac{\Gamma_i(\Delta y_i)^2}{2}\right)u_{yy}(p_0) &+ \\
\left(-\sum_{i=1}^{k}\frac{\Gamma_i(\Delta x_i)^3}{3!}\right)u_{xxx}(p_0)+\left(-\sum_{i=1}^{k}\frac{\Gamma_i(\Delta x_i)^2\Delta y_i}{2}\right)u_{xxy}(p_0) &+ \\
\left(-\sum_{i=1}^{k}\frac{\Gamma_i\Delta x_i(\Delta y_i)^2}{2}\right)u_{xyy}(p_0)+\left(-\sum_{i=1}^{k}\Gamma_i\frac{\Gamma_i(\Delta y_i)^3}{3!}\right)u_{yyy}(p_0) &+ \\
\mathcal{O}\left(\max\{\Delta x_i,\Delta y_i\}\right)^4 &
\end{aligned}
$$

where $\Delta x_i = x_i - x_0, \quad \Delta y_i = y_i - y_0,\ 1 \le i \le k.$

In the case of the 3×3 grid defined by $p_0, p_1, ..., p_8$, the consistency condition up to third order defines the linear system

$$
\begin{pmatrix}
1 & 1 & ... & 1\\
0 & \Delta x_1 & ... & \Delta x_8\\
0 & \Delta y_1 & ... & \Delta y_8\\
0 & (\Delta x_1)^2 & ... & (\Delta x_8)^2\\
0 & \Delta x_1\Delta y_1 & ... & \Delta x_8\Delta y_8\\
0 & (\Delta y_1)^2 & ... & (\Delta y_8)^2\\
0 & (\Delta x_1)^3 & ... & (\Delta x_8)^3\\
0 & (\Delta x_1)^2\Delta y_1 & ... & (\Delta x_8)^2\Delta y_8\\
0 & (\Delta y_1)^2\Delta x_1 & ... & (\Delta y_8)^2\Delta x_8\\
0 & (\Delta y_1)^3 & ... & (\Delta y_8)^3
\end{pmatrix}
\begin{pmatrix}
\Gamma_0\\ \Gamma_1\\ \Gamma_2\\ .\\ .\\ .\\ \Gamma_8
\end{pmatrix}
=
\begin{pmatrix}
F(p_0)\\ D(p_0)\\ E(p_0)\\ 2A(p_0)\\ B(p_0)\\ 2C(p_0)\\ 0\\ 0\\ 0\\ 0
\end{pmatrix}
\tag{3}
$$

which must be satisfied by the Γ_i coefficients.
One must note that, in general, this system is not well-determined. Hence, the main question is how to produce a solution of (3) which provides a consistent scheme.
In [8], in order to get a second order scheme, we proposed to calculate the coefficients $\Gamma_0, \Gamma_1, ..., \Gamma_8$ by solving the constrained optimization problem

$$
\begin{array}{cr}
\min & z = R_6^2 + R_7^2 + R_8^2 + R_9^2,\\
\text{subject to} & R_i = 0,\ i = 0, ..., 5.
\end{array}
\tag{4}
$$

where

$$\begin{array}{ll} R_0 = \sum_{i=0}^{8} \Gamma_i - F, & R_3 = \sum_{i=1}^{8} \Gamma_i (\Delta x_i)^2 - 2A, \\ R_1 = \sum_{i=1}^{8} \Gamma_i (\Delta x_i) - D, & R_4 = \sum_{i=1}^{8} \Gamma_i (\Delta x_i)(\Delta y_i) - B, \\ R_2 = \sum_{i=1}^{8} \Gamma_i (\Delta y_i) - E, & R_5 = \sum_{i=1}^{8} \Gamma_i (\Delta y_i)^2 - 2C, \end{array} \quad (5)$$

$$\begin{array}{l} R_6 = \sum_{i=1}^{8} \Gamma_i (\Delta x_i)^3 \\ R_7 = \sum_{i=1}^{8} \Gamma_i (\Delta x_i)^2 (\Delta y_i) \\ R_8 = \sum_{i=1}^{8} \Gamma_i (\Delta x_i)(\Delta y_i)^2 \\ R_9 = \sum_{i=1}^{8} \Gamma_i (\Delta y_i)^3. \end{array} \quad (6)$$

Problem (4) must be solved iteratively for the 3×3 structured subgrid around every inner grid node $P_{i,j}$ defined by G to provide the optimal local approximation to the differential operator (1).
Very satisfactory results obtained with this scheme were reported in [8]. In this paper, we propose an alternative heuristic scheme based on an unconstrained optimization problem which is closely related to the constrained one. First, we separate the first equation of the matrix system (3)

$$\sum_{i=1}^{8} \Gamma_i - F = 0 \quad (7)$$

and then we solve the least squares problem defined by

$$\begin{pmatrix} \Delta x_1 & ... & \Delta x_8 \\ \Delta y_1 & ... & \Delta y_8 \\ (\Delta x_1)^2 & ... & (\Delta x_8)^2 \\ \Delta x_1 \Delta y_1 & ... & \Delta x_8 \Delta y_8 \\ (\Delta y_1)^2 & ... & (\Delta y_8)^2 \end{pmatrix} \begin{pmatrix} \Gamma_1 \\ \Gamma_2 \\ . \\ . \\ . \\ \Gamma_8 \end{pmatrix} = \begin{pmatrix} D(p_0) \\ E(p_0) \\ 2A(p_0) \\ B(p_0) \\ 2C(p_0) \end{pmatrix}. \quad (8)$$

through the Cholesky factorization of its normal equations

$$M^T M \ \Gamma = M^T \beta, \quad (9)$$

where

$$M = \begin{pmatrix} \Delta x_1 & ... & \Delta x_8 \\ \Delta y_1 & ... & \Delta y_8 \\ (\Delta x_1)^2 & ... & (\Delta x_8)^2 \\ \Delta x_1 \Delta y_1 & ... & \Delta x_8 \Delta y_8 \\ (\Delta y_1)^2 & ... & (\Delta y_8)^2 \end{pmatrix} \qquad \Gamma = \begin{pmatrix} \Gamma_1 \\ \Gamma_2 \\ . \\ . \\ . \\ \Gamma_8 \end{pmatrix}, \qquad \beta = \begin{pmatrix} D(p_0) \\ E(p_0) \\ 2A(p_0) \\ B(p_0) \\ 2C(p_0) \end{pmatrix}.$$

Next, Γ_0 is obtained from (7).
One must note that, due to the lack of restrictions, this scheme is indeed less

restrictive than the previous one, and that in some very irregular grids, the residuals of order one and two might not be equal to zero; however, in spite of these facts, a large amount of numerical experiments led us to conclude that the proposed scheme is accurate enough.
In a similar manner to the rectangular case, the approximation to the differential operator at every inner grid point produces a linear equation whose coefficients are given by the Γ_i values, and the set of all these equations can be rearranged into a sparse matrix-vector algebraic system of equations whose solution approximates the solution of (1).

3 Numerical Test

For the numerical tests, we have selected 4 polygonal domains which resemble geographical regions: Great Britain (ENG), Havana bay (HAB), Michoacán (MIC) and Ucha (UCH). Using these boundaries, we considered two sets of tests:

a) Convex grids with 21 points per side were generated in UNAMALLA by minimizing the functional [4]

$$1/2(S_\omega(G) + L(G)),$$

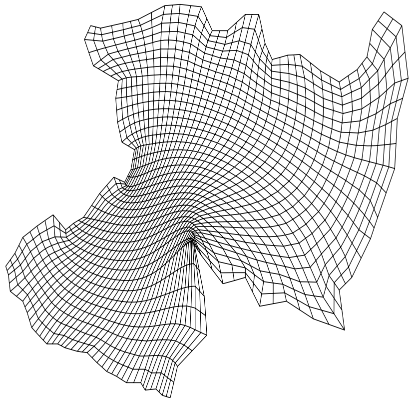
these grids were lated uniformly refined in order to generate grids with 41 and 81 points per side.
The refined grids with 41 points per side for these regions are shown in figure 3.

b) Convex grids with 21, 41 and 81 points per side were generated in UNAMALLA by minimizing the same functional.
The optimal grids with 41 points per side for these regions are shown in figure 4.

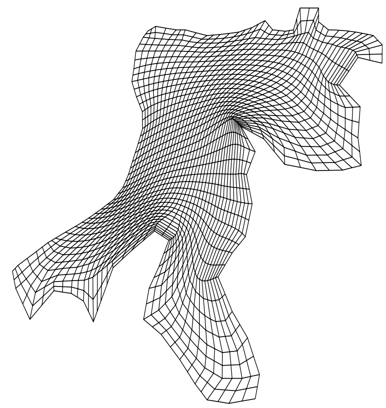
The resulting structured grids were used to calculate the Γ_i coefficients for the schemes described in the previous section. In all cases, the algebraic systems obtained from (1) were assembled and later solved using a sparse Gaussian Elimination routine in MATLAB 7.2 in a personal computer with Intel Pentium processor B970@2.30 GHz and 6Gb of RAM memory.
To test the performance of the new scheme in the solution to the Poisson problem $-\nabla(K\nabla u) = f$, the following values for K and u were selected [5]:

1. First problem.

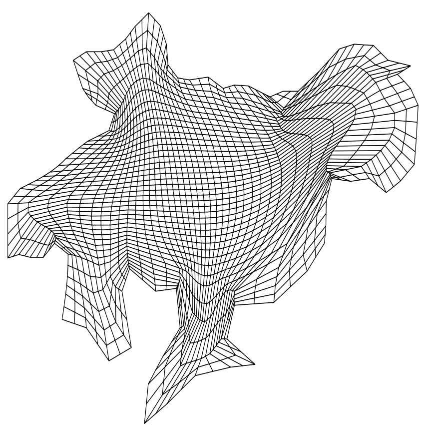
$$K(x,y) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad u = 2\exp(2x + y).$$



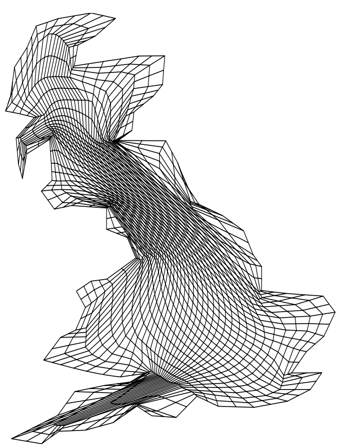
Michoacán.



Havana Bay.

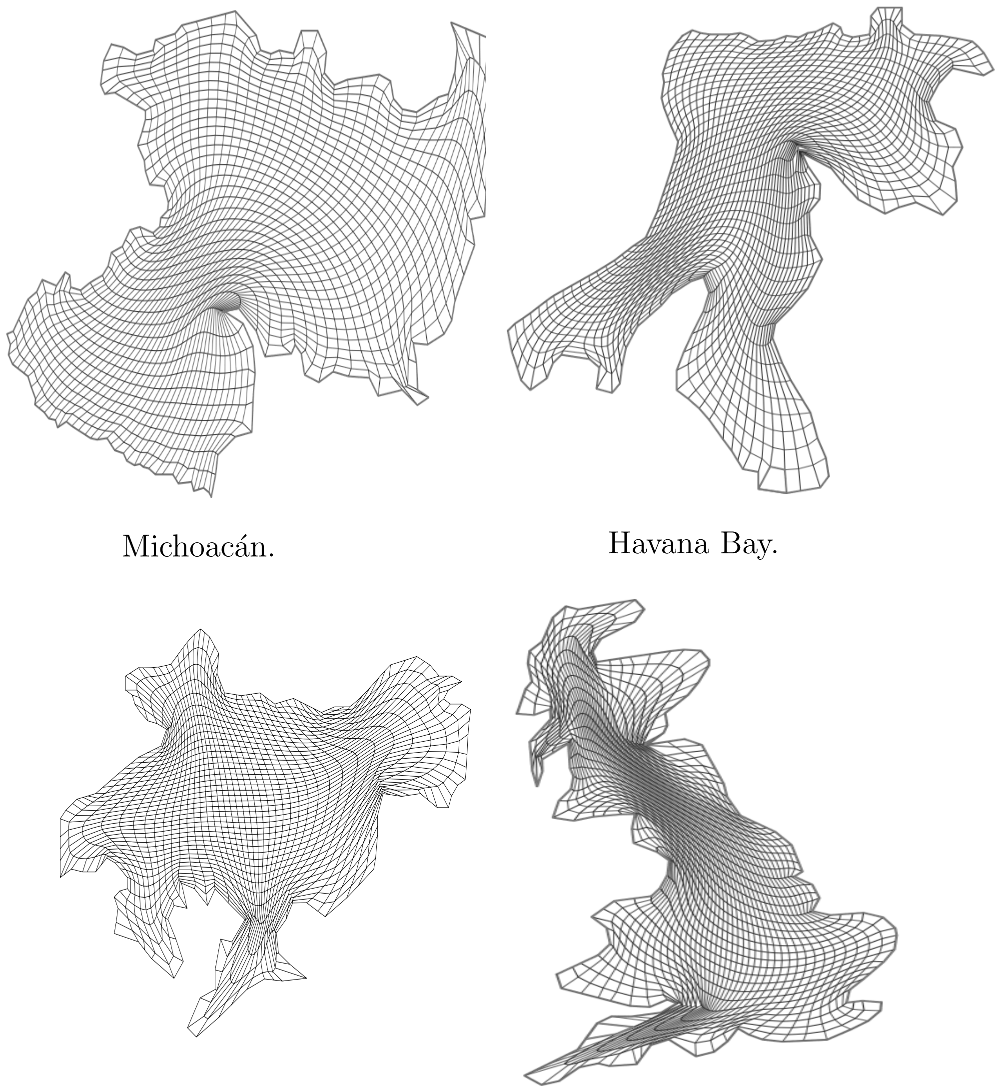


Ucha.



Great Britain.

Figure 3: Refined grids with 41 points per side.



Michoacán. Havana Bay.

Ucha. Great Britain.

Figure 4: Optimal grids with 41 points per side.

2. Second problem.

$$K(x,y) = P^T D P,$$

with

$$P = \begin{pmatrix} cos(\frac{\pi}{8}) & sin(\frac{\pi}{8}) \\ -sin(\frac{\pi}{8}) & cos(\frac{\pi}{8}) \end{pmatrix}$$

and

$$D = \begin{pmatrix} 1 + 2x^2 + y^2 & 0 \\ 0 & 1 + x^2 + 2y^2 \end{pmatrix},$$

$$u = \sin(\pi x)\sin(\pi y).$$

Function f inside the domain was chosen in such a way that u was the exact solution in both cases. Moreover, for the boundary, the function u was selected as the Dirichlet condition.

The tests results are summarized in tables 1 and 2 for the tests set a, and in tables 3 and 4 for the test set b.

In all the tables, the values of the quadratic error norm is calculated as the grid function

$$\|u - U\|_2 = \sqrt{\sum_{i,j} (u_{i,j} - U_{i,j})^2 \mathcal{A}_{i,j}} \quad ,$$

where U and u are the approximated and the exact solution calculated at the i, j^{th} grid point $P_{i,j} = (x_{i,j}, y_{i,j})$ respectively, and $\mathcal{A}_{i,j}$ is the area of the i, j^{th}-element, calculated as the area of the polygon defined by $\{P_{i+1,j}, P_{i,j+1}, P_{i-1,j}, P_{i,j-1}\}$; e_k and $\hat{e}_k$ are the errors for the unconstrained and the constrained scheme, respectively. In an analogous way, t_k and $\hat{t}_k$ are the CPU times for the unconstrained and the constrained scheme.

The empirical order is calculated as $\left(\frac{\log e_{k-1}}{\log e_k}\right) \Big/ \left(\frac{\log N_k}{\log N_{k-1}}\right)$, where e_k and N_k denote the quadratic error and number of points per side, which are calculated for a given grid and the coarser one for the same region.

The examination of the empirical errors shows that both schemes produce numerical solutions which are very close, despite one of them, the heuristic, was defined by an unconstrained problem. However, the algebraic systems assembled for the heuristic scheme are solved faster in all the tests. Another important issue is that the presence of strong non convexities in the boundaries causes the generation of elongated grids cells which affect the accuracy of the numerical solution for both schemes, although the unconstrained heuristic scheme turns out to be more robust than the constrained one in most of the numerical tests (and always more robust in the case of the refined grids of the test set a). Nevertheless, in a similar way to the case of finite elements on very elongated triangles, convergence is expected to be achieved [17].

Grid	N_k	e_k	Order	$\hat{e}_k$	Order	t_k	$\hat{t}_k$
	21	4.0978E-03		7.2750E-02		0.5148	1.7784
ENG	41	1.0457E-03	2.04	2.2820E-03	5.17	1.0764	3.6972
	81	2.9498E-04	1.86	2.2796E-01	-6.76	5.4912	16.801
	21	2.4566E-02		2.4486E-02		0.2028	0.8112
HAB	41	3.3506E-03	2.98	2.8796E-03	3.20	0.9984	3.5412
	81	9.5978E-04	1.84	2.9990E-03	-0.06	5.5068	17.191
	21	3.2036E-03		2.4260E-03		0.2496	0.8268
MIC	41	8.2957E-04	2.02	6.8105E-04	1.90	0.9360	3.6972
	81	2.0733E-04	2.04	2.1665E-04	1.68	5.5692	17.113
	21	1.7855E-02		1.4069E-02		0.2184	0.8268
UCH	41	4.6341E-03	2.02	1.6251E-01	-3.66	0.9516	3.6036
	81	1.2982E-03	1.87	1.4109E-02	3.59	5.4756	17.362

Table 1: Problem 1 data. Test set a.

Grid	N_k	e_k	Order	$\hat{e}_k$	Order	t_k	$\hat{t}_k$
	21	2.3268E-03		1.1946E-01		0.4368	0.9048
ENG	41	7.8006E-04	1.63	2.5912E-02	2.28	1.1700	3.8376
	81	2.5829E-04	1.62	3.1582E-02	-0.29	6.1464	17.643
	21	1.1520E-03		7.9012E-04		0.2340	0.8736
HAB	41	2.2112E-04	2.47	4.7134E-03	-2.67	1.3572	3.9468
	81	5.8999E-05	1.94	6.6787E-04	2.87	5.9592	18.018
	21	6.1494E-04		5.5369E-04		0.2184	0.8736
MIC	41	1.5843E-04	2.03	4.9182E-04	0.18	1.2012	3.7284
	81	3.9553E-05	2.04	4.7460E-04	0.05	6.0528	18.142
	21	3.6074E-03		2.7881E-03		0.2028	0.8580
UCH	41	8.0719E-04	2.24	2.4089E-02	-3.22	1.2480	3.8064
	81	2.0597E-04	2.01	5.3070E-03	2.22	5.9436	17.924

Table 2: Problem 2 data. Test set a.

Grid	N_k	e_k	Order	$\hat{e}_k$	Order	t_k	$\hat{t}_k$
	21	7.7271E-02		7.2750E-02		0.1560	1.0608
ENG	41	8.8895E-04	6.67	8.8152E-04	6.60	0.5148	2.4180
	81	2.7676E-02	-5.05	1.0990E-02	-3.71	4.2120	11.1541
	21	2.4494E-02		2.4486E-02		0.2496	0.6396
HAB	41	2.6795E-03	3.31	2.6794E-03	3.31	1.0920	2.5584
	81	1.4604E-03	0.89	1.5902E-03	0.77	5.5848	12.0277
	21	2.4260E-03		2.4260E-03		0.2652	0.6552
MIC	41	2.1554E-03	0.18	2.1534E-03	0.18	0.9984	2.6208
	81	1.9383E-04	3.54	1.8933E-04	3.57	5.6316	11.7781
	21	1.4072E-02		1.4069E-02		0.2340	0.5616
UCH	41	5.6130E-03	1.37	5.6093E-03	1.37	0.9672	2.4648
	81	1.6973E-03	1.76	1.6968E-03	1.76	5.3820	11.5285

Table 3: Problem 1 data. Test set b.

Grid	N_k	e_k	Order	$\hat{e}_k$	Order	t_k	$\hat{t}_k$
	21	9.6602E-02		1.1946E-01		0.1872	0.6396
ENG	41	1.0796E-03	6.72	1.3285E-03	6.72	0.6708	2.6520
	81	6.5654E-03	-2.65	5.8604E-03	-2.18	5.9904	12.0589
	21	7.9066E-04		7.9012E-04		0.2652	0.6552
HAB	41	1.7011E-04	2.30	1.6983E-04	2.30	1.0608	2.8392
	81	4.5272E-04	-1.44	7.8058E-04	-2.24	6.0372	12.6361
	21	5.5356E-04		5.5369E-04		0.2496	0.6240
MIC	41	2.0389E-04	1.49	2.0414E-04	1.49	1.2324	2.8548
	81	3.2880E-05	2.68	3.2882E-05	2.68	5.6628	12.1525
	21	2.7874E-03		2.7881E-03		0.2496	0.6240
UCH	41	6.2938E-04	2.22	6.2963E-04	2.22	1.1700	2.7456
	81	6.5345E-04	-0.06	8.1611E-04	-0.38	5.5848	12.3241

Table 4: Problem 2 data. Test set b.

4 Conclusion

As follows from the numerical tests, the proposed heuristic scheme produces satisfactory results and, even though it might be in theory slightly less accurate than the scheme addressed in [8], it was as robust as the scheme defined by a local constrained optimization problem 4. In addition, in all the tests, it was notably faster due to the lack of constraints. This leds to conclude that it can be used with ease in order to get reliable approximations to the solution of linear second-order partial equations in irregular regions. Besides, its implementation can be made in a very simple direct way.

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