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New implementation of the Tau method for PDEs

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Abstract

In this work we propose an extension of the algebraic formulation for the Tau method for the numerical solution of partial differential problems set on domains in $\mathbb{R}^n$, $n > 2$. This extension is based on an appropriate choice of a basis for the space of polynomials in $\mathbb{R}^n$ and on the construction of the algebraic equivalent representation of the problem. Another feature of this implementation is related to the solution procedure for the necessarily large dimensional linear systems involved. We developed for this purpose an adapted LU factorization with a special pivoting strategy to build approximants in the sense of Tau method and to allow the solution of large problems.

Numerical results for differential problems in 2D and 4D will be shown.

Keywords: Tau method; Polynomial approximation; n-dimensional PDE

1. Introduction

The Tau method originally proposed by Lanczos [4,5] for ordinary differential equations has been extended by Ortiz [6], and formulations for partial differential equations have been studied by Ortiz et al. [1,8]. Most of these formulations are based on an algebraic representation of the differential problem. On the literature all the problems treated by this approach were for dimension $n = 2$, and the algorithms were developed with that in mind. In fact, most of the algorithmic approaches are not generalizable. This may be an important limitation for the application of the method to real life

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problems. It is relevant to stress that recently there has been work on applications of the Tau method published in literature, for instance [2,3,9], for dimension $n \leqslant 2$.

In this work, we present an extension of the algebraic formulation, given in [8] and further developed in [1,7], that allows the generalization to partial differential problems set on domains on $\mathbb{R}^n$. With this new approach, real life problems of dimension higher than two can be solved using Tau approximation.

This paper is organized as follows. In Section 2, we briefly review the classical description of the Tau method. In Section 3, we will describe the extension of the algebraic formulation of the Tau method to problems in $\mathbb{R}^n$. This will be done also for the case $n=2$ to be more easily understood and the generalization for greater dimensions is straightforward. In Section 4, the algorithm and the details of the pivoting strategy will be given and finally in Section 5, we will present some numerical results for problems with domains in $\mathbb{R}^2$ and $\mathbb{R}^4$.

2. The classical formulation

The Tau method for the solution of the partial differential problem

$$
\begin{aligned}
&Dy(x) = f(x), \quad x \in \Omega \subset \mathbb{R}^n,\\
&D_j y(x) = \sigma_j(x), \quad j = 1,\ldots,J,
\end{aligned}
\tag{1}
$$

in a rectangular domain Ω, where D is a linear partial differential operator, consists of the construction on a polynomial approximation $\hat{y}$ to y such that $\hat{y}$ satisfies the supplementary (boundary, initial or mixed) conditions and $D\hat{y}$ agrees with D applied to the series expansion of y, as far as possible or, equivalently, $\hat{y}$ satisfies exactly a perturbed equation $Dy(x) = f(x) + \tau(x)$, where τ is a polynomial perturbation term.

In [1,8], the authors represent, for $n=2$, $y(x_1,x_2)=X_1^{\mathrm{T}}AX_2$ with $X_j=(1,x_j,x_j^2,\ldots)^{\mathrm{T}}$, $j=1,2$, where A is the coefficient matrix of the series expansion, and the algebraic representation of the differential operator is given by $Dy(x_1,x_2) = X_1^{\mathrm{T}}D(A)X_2$. Such representation is not suitable to generalize to higher dimension since the action of each basis is taken on both sides of matrix $D(A)$.

3. Extension to $\mathbb{R}^n$

The idea is to consider the action of the basis in one-side of the matrix representation of the operator. In [8] a technique is presented, called stringing, but, although it is not restricted to $n=2$, the authors did not present any implementation of it. In [7] the one-sided approach is used but only for bidimensional (nonlinear) PDEs. In [10] the authors presented a systematic way to construct the action of the basis in one-side for the bidimensional case. Here we extend this idea to n-dimensional case and in the next section we present a numerical implementation that allows the automatic resolution of the problem (1) and the use of high degrees in the Tau approximants.

3.1. Algebraic representation of the differential problem

We begin by defining the convenient basis for $\mathbb{R}^n$. Let $i=(i_1,\ldots,i_n)\in\mathbb{R}^n$ be a multiindex in $\mathbb{N}_0^n$, $i_j\in\mathbb{N}_0$, $j=1,\ldots,n$. By definition $|i|=i_1+\cdots+i_n$. For $x=(x_1,\ldots,x_n)\in\mathbb{R}^n$ the associated monomial to i is $x^i=x_1^{i_1}\cdots x_n^{i_n}$.

Let $X=X_n\otimes X_{n-1}\otimes\cdots\otimes X_1$ be the Kronecker product of the power basis $X_j=(1,x_j,x_j^2,\ldots)$, $j=1,\ldots,n$. $X=(x^i)_{i=0}^{\infty}$ defines a basis for the space of algebraic polynomials in the variables $x_1,\ldots,x_n$ and induces a natural ordering in the multiindexes set $\mathbb{N}_0^n$. With this ordering we can write, at least formally,

$$y=a(x)=\sum_{i=0}^{\infty}a_ix^i,$$

as a power series expansion

$$a(x)=a\cdot X,$$

where $a=(a_i)_{i=0}^{\infty}$ is the coefficient vector of that representation.

Let D be a linear differential operator with polynomial coefficients $p_i(x)$, of order v_j in each of the variables x_j,

$$D\equiv\sum_{i=0}^{v}p_i(x)\,\frac{\partial^{|i|}}{\partial x^i},\tag{2}$$

where $v=(v_1,\ldots,v_n)$ is a multiindex on $\mathbb{N}_0^n$. The effect of the action of the operator D on the coefficients of $a(x)$ is given [11] by

$$Da(x)=a\cdot\Pi_x\cdot X,$$

where $\Pi_x=((\Pi_{ij}))_{i,j=0}^{\infty}$ is a band infinite matrix and Π_{ij} is the coefficient of x^j in the polynomial Dx^i. The number of upper diagonals in the matrix Π_x is equal to $h=(h_1,\ldots,h_n)$, the height of the differential operator.

If $W_j=V_j\cdot X_j$ is an orthogonal polynomial basis for the space of polynomials in the variable x_j, defined by the lower triangular matrix V_j, then $V=V_n\otimes\cdots\otimes V_1$ defines a basis

$$W=V\cdot X=(w_i)_{i=0}^{\infty},\quad w_i=V\cdot x^i\tag{3}$$

for the space of polynomials in n variables.

Let

$$y=\alpha(w)=\sum_{i=0}^{\infty}\alpha_iw_i=\alpha\cdot W,$$

where $\alpha=a\cdot V^{-1}$ is the projection onto the basis W of the series expansion of the function y. Then

$$Dy=\alpha\cdot\Pi_w\cdot W,$$

where $\Pi_w=V\cdot\Pi_x\cdot V^{-1}$ is the trapezoidal infinite matrix representing the action of the operator D on the elements of the basis W.

The differential equation of (1)

$$Dy = f(x), \quad x \in \Omega \subset \mathbb{R}^n \tag{4}$$

with D as in (2) and $f(x)$ an algebraic polynomial, can be written as an infinite linear matrix equation

$$a \cdot \Pi_x = f_x,$$

where $f(x) = f_x \cdot X$ is the representation of $f(x)$ in the basis X. If $f_w = f_x \cdot V^{-1}$ is the projection of f_x on the orthogonal basis $W = V \cdot X$ that equation can be written as

$$\alpha \cdot \Pi_w = f_w.$$

The supplementary conditions of (1)

$$D_j y \equiv \sum_i g_{j,i}(x) \left.\frac{\partial^{|i|}}{\partial x^i} a(x)\right|_{x_l = k_j} = \sigma_j(x), \; j = 1, \ldots, J, \tag{5}$$

where $\sigma_j(x)$ and $g_{j,i}(x)$ are polynomials and $x_l = k_j$ are conditions related to different sections of the domain Ω, can be treated in similar way as we did with the differential equation. In fact, let B_j be the matrix representing the action of D_j on X and σ_j the vector representing $\sigma_j(x) = \sigma_j \cdot X$. Then Eq. (5) can be written in the matrix form

$$a \cdot B^{(j)} = \sigma_j, \quad j = 1, \ldots, J$$

or, in the basis W,

$$\alpha \cdot B_w^{(j)} = \sigma_j, \quad j = 1, \ldots, J,$$

where $B_w^{(j)} = V \cdot B_j, \quad j = 1, \ldots, J$.

We conclude that, at least formally, the differential problem (1) is equivalent to the algebraic problem

$$\alpha \cdot \Pi_w = f_w,$$

$$\alpha \cdot B_w^{(j)} = \sigma_j, \quad j = 1, \ldots, J.$$

3.2. Dimension 2

For the case $n = 2$ we have shown in [10] that if the solution of (4) admits the representation

$$y = a(x_1, x_2) = \alpha(w_1, w_2) = \alpha \cdot (w_2 \otimes w_1),$$

then $\alpha(w_1, w_2)$ satisfies

$$\alpha \cdot \Pi_w = f_w$$

and the supplementary conditions (5), for some $P \cdot Q$ such that $P + Q = J$, can be expressed as

$$\alpha \cdot B_p = \sigma_p, \quad p = 1, \ldots, P$$

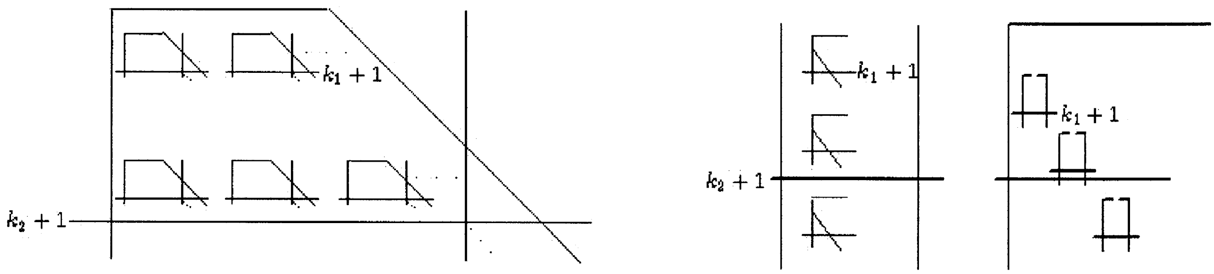

Fig. 1. Structures of Π_w, B_p and B_q in dimension 2.

and

$$\alpha \cdot B_q = \sigma_q, \quad q = 1, \dots, Q.$$

In this case the structure of the matrices Π_w, B_p and B_q is shown in Fig. 1.

To obtain a Tau approximation $\alpha^{(k_1,k_2)}(w_1,w_2)$ of degree at most k_1 in w_1 and k_2 in w_2 we truncate the vector α and the columns of Π_w, B_p and B_q to its first k_2+1 row blocks, each of them truncated to its first k_1+1 rows. This operation results in rectangular matrices with k_2+h_2+1 column blocks each of them with k_1+h_1+1 columns, where for $i=1,2$, $h_i = \max\{h_{ij}, j=0,\dots,J\}$, h_{i0} is the height of D in x_i and h_{ij} is the height of D_j in x_i.

3.3. Dimensions higher than 2

If y admits the representation

$$y = a(x) = \alpha(w) = \alpha \cdot (w_n \otimes \cdots \otimes w_1),$$

then we can use exactly the same procedure that we have for dimension 2 for the construction of a Tau approximation of the solution of the differential problem. For dimension n the structure in the matrices can be defined, like we did for dimension 2, as being recursively the "Kronecker product" of the matrices for the case of dimension $n-1$ and for the case of dimension 1.

To obtain a Tau approximation $\alpha^{(k)}$ of degree at most

$$k = (k_1, \dots, k_n), \tag{6}$$

in $w=(w_1,\dots,w_n)$ we truncate the vector α and the matrices Π_w and $B_w^{(j)}$ to its first k_i+1 blocks in each of the levels $i, i=1,\dots,n$ of their structures. This approximation $\hat{y} = a^{(k)}(x) = \alpha^{(k)} \cdot W$ is a Tau approximation of the solution of the problem since

$$D_j \hat{y} = \sigma_j, \; j = 1, \dots, J$$

and

$$D\hat{y} = f(x) + \tau^{(k)}(x), \tag{7}$$

where $\tau^{(k)}$ is a polynomial. In fact $\hat{y}$ satisfies the given differential equation with a polynomial perturbation, following the formulation of Lanczos and Ortiz, and $D\hat{y}(x)$ agrees with Dy as far as possible, following the alternative formulation of da Silva [12,13] for the Tau method.

4. Numerical computation of the Tau approximation

As explained in the previous section in order to get a Tau approximation $\alpha^{(k)}$ of degree at most k (6) in $w=(w_1,\dots,w_n)$, we construct a linear system

$$Az=b, \tag{8}$$

where $A=[B_w^{(1)}\cdots B_w^{(J)}\Pi_w]^{\mathrm{T}}$ of dimension $nr\times nc$, $b=[\sigma_1\cdots\sigma_J f_w]^{\mathrm{T}}$, $z^{\mathrm{T}}=\alpha^{(k)}$,

$$nc=\prod_{i=1}^{n}(k_i+h_i+1) \quad \text{and} \quad nr=(J+1)\prod_{i=1}^{n}(k_i+1),$$

with $h_i=\max\{h_{ij}, j=0,\dots,J\}$, h_{i0} the height of D in x_i and h_{ij} the height of D_j in x_i, for $i=1,\dots,n$.

The structure of the coefficient matrix is divided in $J+1$ row blocks, where the first J blocks correspond to the supplementary conditions and the last one to the differential operator. On Figs. 2 and 3, we can see the block structure of the coefficient matrices for the examples (with two different basis) given in Section 5.

To solve the linear system (8) we need to take into account the fact that the supplementary conditions must be satisfied which implies that the equations of the first J blocks are to be preferred to the operator equations in the last one. A special LU factorization can be developed to integrate this requirement by inducing a special row ordering within the partial pivoting. The need of introducing that special row ordering justifies the impossibility to solve the rectangular linear system by means of least-squares methods or iterative methods.

To obtain a rectangular LU factorization of A, where the lower triangular factor L has dimension $nr\times nc$ and the upper factor U is $nc\times nc$, Gaussian elimination is used over the total rectangular system with a special pivoting strategy. This strategy must be developed in order to preserve the stability of LU factorization and, at the same time, to ensure that the supplementary conditions are satisfied. The approach followed consists on using partial pivoting in the first J blocks, and just allowing interchanges between equation ℓ with one equation from the last block (related to the operator) in case of unsuccessful pivoting—a null pivot in step ℓ.

After the process we obtain a L factor matrix divided in 2 blocks. The first one, $\hat{L}$, of dimension $nc\times nc$ corresponds to linearly independent supplementary conditions and linearly independent operator equations. The remaining block, R, of dimension $(nr-nc)\times nc$ contains the redundant supplementary and operator equations, and the inconsistent operator equations.

From the linear system (8) we solve $\hat{L}Uz=\hat{b}$ with $b=(\hat{b},r)^{\mathrm{T}}$, where $\hat{b}$ represents the permuted right-hand side b associated with the rows of $\hat{L}$. The R block is related to the polynomial $\tau^{(k)}$ (7) by $\tau^{(k)}=(r-Rz)^{\mathrm{T}}W$. Empirically a "good" Tau approximation $\hat{y}$ of y is obtained whenever $\|r-Rz\|_\infty$ is "small".

The main steps of our procedure are summarized in the following algorithm:

(1) Given Ω, D, D_j, $f(x), \sigma_j(x)$ (as defined in (4), (5)), W (like in (3)) and k (like in (6)).
(2) Build (truncated to k) $\Pi_w, B_w^{(j)}, f_w, \sigma_j$.

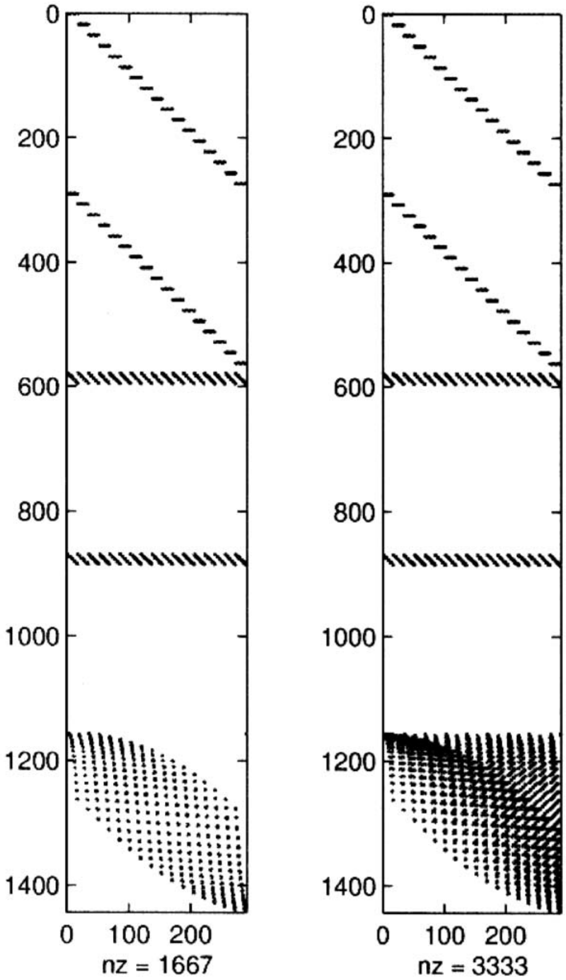

Fig. 2. Sparsity pattern of the coefficient matrices for Example 1, using, respectively the canonical and the Chebyshev basis. Matrices of size 1442×290 with nz nonzero elements.

(3) Compute LU factorization with special pivoting strategy
for $\ell = 1, nc$,
   (a) find a non null pivot over the rows from ℓ to $J * \prod_{i=1}^{n}(k_i + 1)$,
   (b) if (a) fails (only null pivots on the supplementary conditions blocks) then find a non null pivot over the rows from $J * \prod_{i=1}^{n}(k_i + 1) + 1$ to nr (operator block),
   (c) if (a) and (b) fails then there is no solution,
   (d) interchange row ℓ with selected pivot row,
   (e) form column ℓ of $\hat{L}$ and row ℓ of U.

(4) Solve $\hat{L}U_z = \hat{b}$, where $\hat{b}$ represents the permuted right-hand side b associated with the rows of $\hat{L}$.
(5) Compute $\hat{y} = z^{\mathrm{T}} W$.

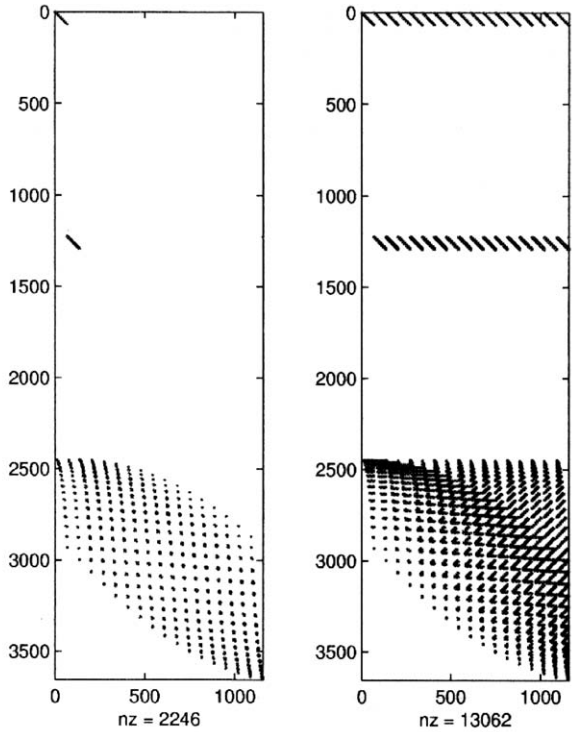

Fig. 3. Sparsity pattern of the coefficient matrices for Example 2, using, respectively the canonical and the Chebyshev basis. Matrices of size 3248×1025 with nz nonzero elements.

Steps 1 and 2 of this algorithm were implemented using exact arithmetic in MATHEMATICA [2] in order to take advantage of its algebraic manipulation capacities. Due to memory limitations for high dimensional problems and/or high degree of polynomial approximations the following steps were implemented using floating point arithmetic in Fortran. Finally MATLAB [3] was used to integrate both software packages allowing to profit from its pos-processing facilities.

5. Numerical results

The previous algorithm was applied to two test problems.

Example 1 is the Saint–Venant's torsion problem for a prismatic bar [14], solved by the Tau method in [8] and Example 2 is a four-dimensional wave equation [15]. In Example 1, we want to compare the results from our approach with those of [8]. In Example 2, we test our algorithm to a higher dimensional problem.

[2] MATHEMATICA is a registered trademark of Wolfram Research, Inc.
[3] MATLAB is a registered trademark of The MathWorks, Inc.

Table 1
$\|y-\hat{y}^{(k)}\|_\infty$ for Example 1

k	$W=C,C$
(4,4)	1.8×10^{-2}
(8,8)	1.1×10^{-3}
(16,16)	5.3×10^{-5}

In each example the figures display the error surfaces $y-\hat{y}^{(k)}$ choosing degrees k_i and basis W_i, in the variable $x_i, i=1,\dots,n$. On the examples, $W_i=C$ stands for the Chebyshev basis and $W_i=I$ for the canonical one.

Example 1. *Problem*:

$$\frac{\partial^2}{\partial x_1^2}a(x_1,x_2)+\frac{\partial^2}{\partial x_2^2}a(x_1,x_2)=-2,\quad (x_1,x_2)\in(-1,1)\times(-1,1)$$

$$a(\pm 1,x_2)=a(x_1,\pm 1)=0.$$

Exact solution:

$$y=a(x_1,x_2)=\frac{32}{\pi^3}\sum_{n=1,3,5,\dots}^{\infty}\frac{(-1)^{(n-1)/2}}{n^3}\left[1-\frac{\cosh(nx_2\pi/2)}{\cosh(n\pi/2)}\right]\cos(nx_1\pi/2).$$

In Table 1, we show the ∞-*norm* of the error $y-\hat{y}$ obtained for several polynomial degrees and using the canonical and the Chebyshev basis.

Our algorithm reproduces the results presented in [8] with $k=(4,4)$ and $k=(8,8)$ for $W=C,C$ (the only two cases treated). As expected, in this example by increasing the degree of the polynomial approximants we get a gain in the accuracy of the approximation.

In Fig. 4, we plot the error surface for the Chebyshev basis with $k=(16,16)$. In this particular example, and as for other choices of symmetric degrees, the error surface shows a balancing behavior that was also observed in [1].

Example 2. *Problem*:

$$\frac{\partial^2}{\partial x_1^2}a(x)+\frac{\partial^2}{\partial x_2^2}a(x)+\frac{\partial^2}{\partial x_3^2}a(x)=\frac{\partial^2}{\partial x_4^2}a(x),\quad x\in\Omega,$$

$$a(x_1,x_2,x_3,0)=0,$$

$$(x_3+3)\frac{\partial}{\partial x_4}a(x_1,x_2,x_3,0)=x_1+x_2,$$

where $\Omega=\{x=(x_1,x_2,x_3,x_4): -1<x_1<1, -1<x_2<1, -1<x_3<1, x_4>0\}$.

Exact solution:

$$a(x_1,x_2,x_3,x_4)=\frac{1}{2}(x_1+x_2)\ln\frac{3+x_3+x_4}{3+x_3-x_4}.$$

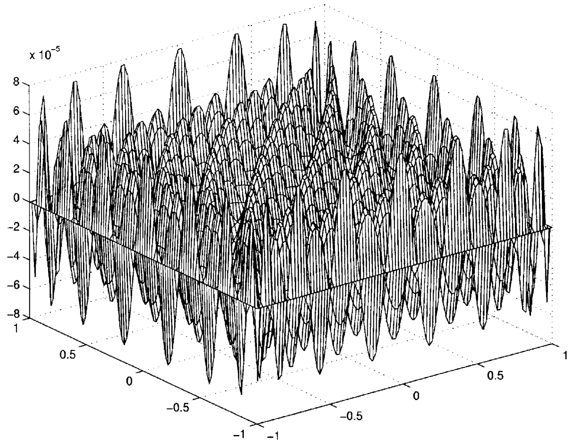

Fig. 4. Error surface $y-\hat{y}^{(16,16)}$ in Example 1 for the Chebyshev basis.

Table 2
$\|y-\hat{y}^{(k)}\|_\infty$ for Example 2

k	$W = I,I,I,I$	$W = I,I,C,C$
(1,1,4,4)	3.0×10^{-2}	2.5×10^{-2}
(1,1,8,8)	4.5×10^{-3}	2.7×10^{-3}
(1,1,12,12)	6.5×10^{-4}	1.3×10^{-4}
(1,1,16,16)	1.0×10^{-4}	4.5×10^{-5}

In this example we recover an important feature of the Tau method: if the solution is polynomial in any variable then the Tau approximation of appropriate degree reproduces that polynomial. The polynomial (x_1+x_2) is preserved as the degrees of the approximation in variables x_1 and x_2 increase. With this example we get

$$\hat{y}^{(1,1,1,1)} = \frac{1}{9}(x_1+x_2)(3-x_3)x_4,$$

$$\hat{y}^{(2,2,2,2)} = \frac{1}{27}(x_1+x_2)(9-3x_3+x_3^2)x_4,$$

$$\hat{y}^{(3,3,3,3)} = \frac{1}{81}(x_1+x_2)(27-9x_3+3x_3^2-x_3^3+x_4^2-x_3x_4^2)x_4,$$

$$\hat{y}^{(4,4,4,4)} = \frac{1}{243}(x_1+x_2)(81-27x_3+9x_3^2-3x_3^3+x_3^4+3x_4^2-3x_3x_4^2+2x_3^2x_4^2)x_4,$$

in the canonical basis.

In Table 2, we show the ∞-*norm* of the error $y-\hat{y}$ obtained for several polynomial degrees. Since the exact and the Tau solution are both linear in variables x_1 and x_2, we worked with degree 1 in these variables. By the same reason, there was no need to choose an orthogonal basis for these

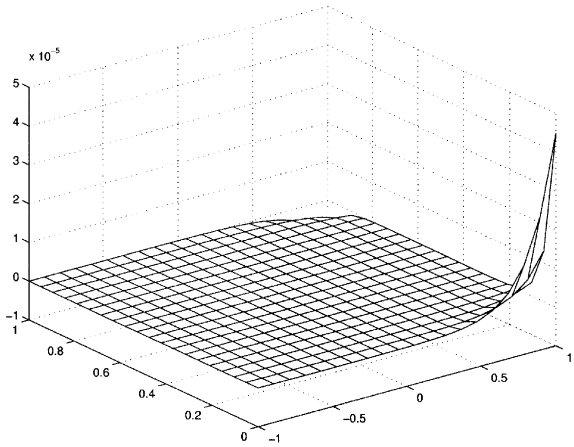

Fig. 5. Error surface $y - \hat{y}^{(1,1,16,16)}$ for approximants in Example 2, with degrees 1 in x_1 and x_2 variables (canonical basis) and degrees 16 in x_3 and x_4 (Chebyshev basis).

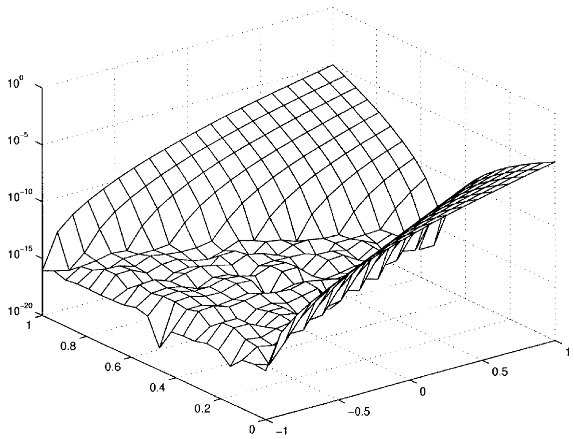

Fig. 6. Absolute error surface $|y - \hat{y}^{(1,1,16,16)}|$, in logarithmic scale, obtained from that on Fig. 5.

two variables. The ability of consider distinct basis for each variable is another feature of the Tau method.

We also see in this example, that by increasing the polynomial degree of the approximants smaller error norms are obtained. For the case $W = I, I, C, C$ and $k = (1, 1, 16, 16)$ our method produced an analytical solution with a precision of 5 decimal digits all over the domain.

In Fig. 5, we plot the error surface restricted to $x_1 = x_2 = 1$, with $k = (1, 1, 16, 16)$ for $W = I, I, I, I$ and $W = I, I, C, C$. The Tau method produces, on a significative part of the domain, an approximate solution with error in the order of the machine precision used (10^{-16}); this is clear from Fig. 6. This is a four-dimensional problem solved in the Tau sense.

6. Conclusions

We developed an extension of an approach of the Tau method for linear PDEs with domains in $\mathbb{R}^n$. Other current implementations only covered the case $n = 2$.

With this implementation it is possible to obtain approximate analytical solutions of linear n-dimensional PDEs. This is important because recently there have been several application problems for $n \leqslant 2$ using the Tau method, some of them cited in Section 1.

We developed a special pivoting strategy for the LU factorization to solve the overdeterminated truncated linear system involved in the algebraic formulation of the Tau method. This approach allowed us to solve larger problems than with symbolic computation.

We tested this approach with 2D and 4D examples. For both we could achieve a precision of 10^{-5} for the Tau approximation, although better precisions are achieved for most part of the points in the domain.

This implementation preserves the characteristics of Tau method, namely it can deal with several boundary type conditions (initial or multipoint).

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