

NUMERICAL MODELLING OF TRANSIENT CONVECTION-DIFFUSION BASED ON A WEIGHTED MASS EXPLICIT SCHEME

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ABSTRACT

An explicit scheme based on a weighted mass matrix, for solving time-dependent convection-diffusion problems is studied. Convenient bounds for the time step, in terms of both the weights and the mesh step size, ensure its stability in the maximum norm, in both space and time, for piecewise linear finite element discretizations in any space dimension. Convergence results in the same sense also hold under certain conditions. The scheme is exploited numerically in order to illustrate its performance.

INTRODUCTION

This work deals with an explicit scheme introduced in [4], for the numerical time integration of the convection-diffusion equations, discretized in space by techniques based on variational formulations such as the finite element method. In this framework, since the mid-eighties, the most widespread manner to deal with dominant convection has been the use of stabilizing procedures based on the space mesh parameter, among which the streamline upwind Petrov-Galerkin (SUPG) technique introduced by Hughes and Brooks (cf. [1]) is one of the most popular.

The first and third authors together with Trales studied in [5] a contribution in this direction, based on a standard Galerkin approach, and a space discretization of the convection-diffusion equations with piecewise linear finite elements, combined with a non standard explicit forward Euler scheme for the time integration. The main theoretical result in that work, states that the numerical solution is stable in the maximum norm in both space and time, and even convergent with order $h | \ln h |$ where h is the space mesh parameter, if the mesh is of the acute type (cf. [8]), provided that roughly the time step is bounded by h^2 multiplied by a mesh-independent constant that we specify. Actually, in this paper the authors further study this scheme in the sense specified in the next section. As it should be clarified, the scheme under consideration follows similar principles to the one long exploited by Kawahara and collaborators, for simulating convection dominated phenomena (see e.g. [3],

among several other papers published by them before and later on). The originality of this contribution relies on the fact that it not only introduces a reliable scheme for any space dimension, but also exhibits rigorous conditions for it to provide converging sequences of approximations in the sense of the maximum norm. In this work, besides addressing relevant implementation aspects pertaining to the determination of the weighted mass matrix, new numerical examples are given in order to illustrate the adequacy of this approach.

An outline of the paper is as follows: In Section 2 we recall the problem to solve. In Section 3 we describe the type of discretization corresponding to the new method, and more specially the weighted manner to deal with the mass matrices on both sizes of the discrete equations. In Section 4 we recall the stability results that hold for the method being considered, in the sense of the space and time maximum norm, together with the conditions to be fulfilled by the scheme parameters in order to ensure convergence. Finally in Section 5 we study in detail a particular choice of the weights associated with the scheme, satisfying the conditions leading to both stability and convergence. Numerical results to be shown in the conference's presentation illustrate the good performance of the new scheme.

NOMENCLATURE

u	unknown field or temperature
\mathbf{a}	convective velocity
t	time variable
\mathbf{x}	space variable
Special characters	
∇	gradient operator
Δ	laplacian operator
V	diffusion coefficient or conductivity
Ω	flow domain
ω	weight lower bound
h_{min}	minimum element height
max	maximum
min	minimum
sup	supremum
$\mathbf{y} \cdot \mathbf{z}$	euclidean inner product of two vectors \mathbf{y} and \mathbf{z}

PROBLEM STATEMENT

Let us consider a time-dependent convection-diffusion problem described as follows:

Find a scalar valued function $u(\mathbf{x}, t)$ defined in $\overline{\Omega} \times [0, \infty)$, Ω being a bounded open subset of \mathbb{R}^n with boundary $\partial\Omega$, $N = 1, 2$ or 3 , such that,

$$\begin{cases} u_t + \mathbf{a} \cdot \nabla u - \nu \Delta u = f \text{ in } \Omega \times (0, \infty) \\ u = g \text{ on } \partial\Omega \times (0, \infty) \\ u = u^0 \text{ in } \Omega \text{ for } t = 0 \end{cases} \quad (1)$$

where u_t represents the first order derivative of u with respect to t , ν is a diffusivity constant and \mathbf{a} is a given solenoidal convective velocity at every time t , assumed to be uniformly bounded in $\Omega \times (0, \infty)$. The data f and g are respectively, a given forcing function bounded in $\Omega \times (0, \infty)$, and a prescribed value bounded on $\partial\Omega \times (0, \infty)$. We further assume that u^0 is bounded in Ω and that for every $\mathbf{x} \in \Omega$ $g(\mathbf{x}, \cdot)$ is of bounded variation in $(0, \infty)$.

For a normalized velocity \mathbf{a} , ν represents the inverse of the Péclet number, and the convective dominant case corresponds to a low value of ν . Whenever ν is not so small, the diffusion will influence the phenomenon being modelled practically everywhere in the domain, and convection will not be dominant.

SPACE AND TIME DISCRETIZATIONS

In all the sequel, for the sake of simplicity, and without loss of essential aspects, we assume that Ω is an interval if $N = 1$, a polygon if $N = 2$ or a polyhedron if $N = 3$. In so doing we next consider a partition \mathfrak{T}_h of Ω into N -simplices, with maximum edge length equal to h . We assume that \mathfrak{T}_h satisfies the usual compatibility conditions for finite element meshes, and that it belongs to a quasi-uniform family of partitions. We further define a second mesh parameter h_{min} as the minimum height of all the elements of \mathfrak{T}_h if $N = 2$ or 3 and the minimum length of $K \in \mathfrak{T}_h$ if $N = 1$.

Let N_h be the number of nodes (i.e. vertices) of \mathfrak{T}_h , denoted by $P_j, j=1, 2, \dots, N_h$. We assume that these are numbered in such a manner that the first I_h nodes are located in the interior of Ω and the remaining $N_h - I_h$ nodes are located on $\partial\Omega$. $u_j^n \in \mathbb{R}$ is the value of u_h^n at P_j . Now for every $K \in \mathfrak{T}_h$ we denote by $P_1(K)$ the space of polynomials of degree less than or equal to one defined in K . In so doing we introduce the following spaces or manifolds associated with \mathfrak{T}_h :

$$V_h := \{v \mid v \in C^0(\overline{\Omega}) \text{ and } v|_K \in P_1(K), \forall K \in \mathfrak{T}_h\}$$

$$V_h^0 := \{v \mid v \in V_h \text{ and } v|_{\partial\Omega} = 0\}$$

We further introduce for any function ϕ defined in $C^0(\partial\Omega)$ the following manifold of V_h :

$$V_h^\phi := \{v \in V_h \mid v(P_j) = \phi(P_j) \forall \text{ vertex } P_j \text{ of } \mathfrak{T}_h \text{ on } \partial\Omega\}$$

Now let u_h^0 be the field of $V_h^{g(\cdot, 0)}$ satisfying $u_h^0(P_j) = u^0(P_j)$ for every vertex P_j of \mathfrak{T}_h , and $\Delta t > 0$ be a given time step.

Defining g^n on $\partial\Omega$ by $g^n(\cdot) = g(\cdot, n\Delta t)$, f^n in Ω by $f^n(\cdot) = f(\cdot, n\Delta t)$ and \mathbf{a}^n in Ω by $\mathbf{a}^n(\cdot) = \mathbf{a}(\cdot, n\Delta t)$ for $n = 1, 2, \dots$, idealistically we wish to determine approximations $u_h^n(\cdot)$ of $u_h^n(\cdot, n\Delta t)$ for $n = 1, 2, \dots$, by solving the following finite element discrete problem described below, corresponding to a modification of the first order forward Euler scheme.

For n successively equal to $1, 2, \dots$, we wish to determine $u_h^n \in V_h^{g^n}$ of the form

$$u_h^n = \sum_{j=1}^{N_h} u_j^n \varphi_j$$

where φ_j is the canonical basis function of V_h associated with the j -th node of \mathfrak{T}_h , i.e. P_j , $u_j^n \in \mathbb{R}$ being the value of u_h^n at P_j . We denote by S_j the support of φ_j and by Π_j its measure.

The unknowns u_i^n for $n = 1, 2, \dots$, are recursively determined by the following expressions:

$$m_{ii}^n u_i^n = \sum_{j=1}^{N_h} [m_{ij}^n - \Delta t a_{ij}^{n-1}] u_j^{n-1} + \Delta t b_i^n, \text{ for } i = 1, \dots, I_h \quad (2)$$

where, setting $\mathbf{a}_i^n(\cdot) := \mathbf{a}^n(P_i)$ and $f_i^n(\cdot) := f^n(P_i)$, the coefficients a_{ij}^n and b_i^n are given by:

$$a_{ij}^n = \int_{\Omega} [(\mathbf{a}_i^n \cdot \nabla) \varphi_j \varphi_i + \nu \nabla \varphi_j \cdot \nabla \varphi_i] \quad (3)$$

$$b_i^n = \int_{\Omega} f_i^{n-1} \varphi_i$$

Coefficient $m_{ii}^L(\cdot)$ is the well-known lumped mass diagonal matrix [7] given by $II_i/(N+1)$. The mass matrix coefficients m_{ij}^W on the right hand side of (2) in turn are defined by a weighted quadrature formula described as follows.

Let M_i be the number of nodes different from P_i lying in the closure of S_i , i.e. \bar{S}_i , and P_{k_j} be such nodes for $j=1,2,\dots,M_i$ with $1 \leq k_j \leq N_h$. Let also W_j^i be the measure fractions associated with P_{k_j} given by:

$$W_j^i = \frac{\text{measure}(S_i \cap S_{k_j})}{N+1} \quad (4)$$

and ω_j^i be corresponding strictly positive weights satisfying,

$$\sum_{j=1}^{M_i} \omega_j^i W_j^i = \frac{NII_i}{(N+1)(N+2)} \quad (5)$$

Notice that since each N -simplex in S_i appears in exactly N measure fractions W_j^i , we necessarily have:

$$\sum_{j=1}^{M_i} W_j^i = \frac{NII_i}{(N+1)} \quad (6)$$

Now selecting the nodes P_{k_j} in \bar{S}_i different from P_i , we define,

$$m_{ik_j}^W = \frac{h_{\min}}{\nu + h_{\min}} \omega_j^i W_j^i \quad \text{for } i \neq k_j \quad (7)$$

together with

$$m_{ii}^W = \frac{\nu}{h_{\min} + \nu} m_{ii}^L + \frac{h_{\min}}{h_{\min} + \nu} m_{ii}^C \quad (8)$$

where m_{ii}^C is the i -th diagonal coefficient of the standard consistent mass matrix [7] given by $(2II_i)/[(N+1)(N+2)]$. Naturally enough, by definition, $m_{ij}^W = 0$ if P_{k_j} does not lie in \bar{S}_i .

Typically we may choose $\omega_j^i = 1/(N+2)$ for every j and for every node P_i , thereby generating a weighted combination of the lumped mass and the consistent mass matrix (cf. [7]) on the right hand side of (2), with weights equal to $\nu/(h_{\min} + \nu)$ and $h_{\min}/(h_{\min} + \nu)$, respectively. However, except for the case of uniform meshes, in principle this is not the

choice to make, if one wishes to reach the best results in terms of accuracy, as seen in the next Section.

STABILITY AND CONVERGENCE OF SCHEME

In this Section we show that, provided Δt is chosen conveniently small with respect to the space mesh parameter, the scheme (2) is stable in the sense of the maximum norm. Moreover we specify a condition under which it converges in both space and time in the same sense, as h and Δt go to zero.

First we have to define the following quantities:

$$A = \sup_{t \in (0, \infty)} \max_{1 \leq i \leq I} |a_i(t)|$$

$$\omega = \min_{1 \leq i \leq I} \min_{1 \leq j \leq M_i} \omega_j^i$$

The following theorem proved in [5] states the stability result that holds for scheme (2).

Theorem 1: If Δt fulfills the condition

$$\Delta t \leq \frac{\omega h_{\min}^3}{(\nu + h_{\min})[A h_{\min} + (N+1)\nu]} \quad (9)$$

then the finite element solution sequence $\{u_h^n\}_n$ given by

$$u_h^n = \sum_{j=1}^{N_h} u_j^n \varphi_j \quad \text{generated by (2) for } n = 1, 2, \dots \text{ satisfies the}$$

following stability result for every $m \in \mathbb{N}$, whereby $\|F\|_{\infty, D}$ denotes the maximum norm of a function F defined in an open set D of \mathbb{R}^n , and $BV[G]$ represents the standard norm of a function $G(t)$ having bounded variation for $t \in (0, \infty)$:

$$\|u_h^m\|_{\infty, \Omega} \leq \|u^0\|_{\infty, \Omega} + \max \left\{ \max_{P \in \partial \Omega} BV[g(P, \cdot)], \Delta t \sum_{n=1}^m \|f^{n-1}\|_{\infty, \Omega} \right\} \quad (10)$$

The above stability result can be refined as follows, in the particular case where the partition \mathfrak{T}_h is of the *acute type* (see e.g. [8]). In the two-dimensional case this means that no angle of the triangles of \mathfrak{T}_h is obtuse.

Theorem 2: (cf. [5]) Assume that the partition \mathfrak{T}_h is of the acute type (cf. [8]). Then if Δt satisfies the condition

$$\Delta t \leq \frac{h_{\min}^2}{(\nu + h_{\min})} \min \left[\frac{\omega}{A}, \frac{\nu(N+2) + 2h_{\min}}{\nu(N+1)(N+2)} \right] \quad (11)$$

the finite element solution sequence $\{u_h^n\}_n$ given by

$u_h^n = \sum_{j=1}^{N_h} u_j^n \varphi_j$ generated by (2) for $n = 1, 2, \dots$ satisfies the stability condition (10).

In [5] we give error estimates for the approximations of the solution of (1) generated by (2) under condition (9), provided the family of meshes in use is quasiuniform [2], and the weights ω_j^i are chosen in such a manner that they satisfy condition (5) together with condition (12) specified in **Lemma 1** below, and moreover ω is bounded below by a strictly positive constant independent of the mesh step size h . Actually it is also proven in the same paper that scheme (2) provides quasi-first order convergent approximations in the space-time maximum norm, as both h and Δt go to zero, under the assumption (11) of **Theorem 2**.

The crucial condition for all those results to hold is a suitable consistency result, which together with the stability result given in **Theorem 2** leads to convergence. Actually the consistency of our scheme is a consequence of the following lemma:

Lemma 1: (cf. [5]) Let P_i be a node of \mathfrak{T}_h , for $i \in \{1, 2, \dots, I_h\}$, and \mathbf{l}_j^i be the vector leading from P_i to its neighbor P_{k_j} , that is, the j -th node belonging to \bar{S}_j , $j = 1, 2, \dots, M_i$. Then there exists strictly positive weights ω_j^i satisfying (5) such that

$$\sum_{j=1}^{M_i} \omega_j^i W_j^i \mathbf{l}_j^i = \mathbf{0} \quad (12)$$

A CONSISTENT CHOICE OF THE WEIGHTS

In this section we describe a coherent strategy to determine a set of M_i strictly positive weights, for each mesh inner node P_i , that can be proven to be bounded below by a strictly positive constant independent of the mesh parameter h . Let us first consider the one-dimensional case. From (12) and (5) it is trivially seen that the pair of weights (ω_1^i, ω_2^i) associated with inner node P_i is uniquely defined by the equations:

$$\begin{cases} -\omega_1^i (l_1^i)^2 + \omega_2^i (l_2^i)^2 = 0 \\ \frac{l}{2} [\omega_1^i l_1^i + \omega_2^i l_2^i] = \frac{l_1^i + l_2^i}{6} \end{cases} \quad (13)$$

where l_1^i and l_2^i are the lengths of the intervals of \mathfrak{T}_h having P_i as the right and left end, respectively. This yields $\omega_1^i = l_2^i / 3l_1^i$ and $\omega_2^i = l_1^i / 3l_2^i$.

Next we switch to the case $N > 1$. In principle for $N = 2$ or $N = 3$ there are infinitely many solutions, except for the case of the least possible value of M_i , i.e. $M_i = N + 1$, in which the

solution is necessarily unique. The construction described as follows allows for the unique determination of a set of weights satisfying (12) and (5), and incidentally it applies even to the particular case where this set is unique.

Let then $E_i^+ := \{\mathbf{e}_j^i\}_{j=1}^{M_i}$ be the set of unit vectors corresponding to the vectors \mathbf{l}_j^i , that is, $\mathbf{e}_j^i = \mathbf{l}_j^i / l_j^i$, where l_j^i is the modulus of \mathbf{l}_j^i , and $E_i^- := \{-\mathbf{e}_j^i\}_{j=1}^{M_i}$.

Let us first consider the case where $E_i^- = E_i^+$. Then for every $j_1 \in \{1, \dots, M_i\}$ there is necessarily another $j_2 \in \{1, \dots, M_i\}$ such that $\mathbf{e}_{j_1}^i + \mathbf{e}_{j_2}^i = \mathbf{0}$. This implies in particular that M_i must be an even number. Hence we may choose the weights in pairs, say $(\mathbf{e}_{j_1}^i, \mathbf{e}_{j_2}^i)$, in the same way as in the one-dimensional case (cf. (13)). More specifically, we number the vectors in E_i^+ in such a manner that the first $M_i/2$ ones form a subset of E_i^+ whose vectors do not have any vector opposite to it in this subset, and from $(M_i/2) + 1$ up to M_i the vectors in the complementary subset consisting of corresponding opposite vectors. In so doing the weights satisfy:

$$\begin{cases} -\omega_{j_1}^i l_{j_1}^i W_{j_1}^i + \omega_{j_2}^i l_{j_2}^i W_{j_2}^i = 0 \\ \omega_{j_1}^i W_{j_1}^i + \omega_{j_2}^i W_{j_2}^i = \frac{W_{j_1}^i + W_{j_2}^i}{N+2} \end{cases} \quad (14)$$

for all pairs $(j_1, j_2) \in \{1, \dots, M_i/2\} \times \{M_i/2 + 1, \dots, M_i\}$, such that $\mathbf{e}_{j_1}^i + \mathbf{e}_{j_2}^i = \mathbf{0}$. Notice that the set of weights determined by solving (14) trivially satisfy both (12) and (5).

Next we assume the general case where $E_i^- \neq E_i^+$. Distinguishing eventually coincident vectors in E_i^- and E_i^+ , we put together all the vectors in both sets, thereby forming a set of exactly $2M_i$ vectors not necessarily distinct, say $\{\mathbf{e}_j^i\}_{j=1}^{2M_i}$, where the first M_i vectors are those of E_i^+ and the last M_i vectors are $\mathbf{e}_{j+M_i}^i := -\mathbf{e}_j^i$ for $j=1, \dots, M_i$.

Now let the segment $P_i Q_k^i$ be the intersection of \bar{S}_i with the half straight line with origin at P_i and oriented in the sense and direction of \mathbf{e}_k^i for $k > M_i$, Q_k^i being necessarily a point of the boundary of S_i . It follows that $P_i Q_k^i$ either coincides with an edge $P_i P_{k_j}$, where P_{k_j} is a vertex of S_i , or is contained in either a single N -simplex of S_i for $N = 2$ or $N = 3$, or yet in a common face of exactly two neighboring tetrahedra for $N = 3$. In any case, the vector leading from P_i to Q_k^i , for $k = M_i + 1, \dots, 2M_i$, still denoted by \mathbf{l}_k^i , is a non trivial

convex combination of at most N edge vectors \mathbf{I}_j^i with $1 \leq j \leq M_i$ pertaining to the same N -simplex of S_i . Let J be the number of such edge vectors, i.e., $J=1$ if Q_k^i coincides with a given vertex of S_i , $J=2$ for $N=3$ only if Q_k^i is contained in a common face of two neighboring tetrahedra of S_i , or $J=N$ for $N=2$ or $N=3$ otherwise. Let P_{k,m_l} , for $l=1, \dots, J$ with $1 \leq m_l \leq M_i$, be the vertices of S_i whose convex combination yields \mathbf{I}_k^i for $k=M_i+1, \dots, 2M_i$. Let l_k^i denote the modulus of \mathbf{I}_k^i , for $k=M_i+1, \dots, 2M_i$ too. In so doing,

$$\mathbf{I}_k^i = \sum_{l=1}^J \alpha_l^k \mathbf{I}_{m_l}^i, \quad k = M_i + 1, \dots, 2M_i \quad (15)$$

where the α_l^k 's for $l=1, \dots, J$ are coefficients of a non trivial convex combination, that is, $0 < \alpha_l^k < 1$, $l=1, \dots, J$, and $k = M_i + 1, \dots, 2M_i$, with $\sum_{l=1}^J \alpha_l^k = 1$.

Now we assign to each point Q_k^i , $k = M_i + 1, \dots, 2M_i$ the measure fraction $W_k^i = W_{k-M_i}^i$, and the weight $\tilde{\omega}_k^i = \left(l_{k-M_i}^i / l_k^i \right) \tilde{\omega}_{k-M_i}^i$, where $\tilde{\omega}_j^i$ are provisional weights respectively associated with the vertices P_{k_j} of S_i different from P_i satisfying $\tilde{\omega}_k^i + \tilde{\omega}_{k-M_i}^i = 1 / (N + 2)$. Then similarly to the case of (14), one can easily check the validity of

$$\sum_{j=1}^{2M_i} \tilde{\omega}_j^i W_j^i \mathbf{I}_j^i = \mathbf{0} \quad (16)$$

together with

$$\sum_{j=1}^{2M_i} \tilde{\omega}_j^i W_j^i = \frac{N \prod_i}{(N+1)(N+2)} \quad (17)$$

Now we replace in (16) the \mathbf{I}_k^i 's for $k = M_i + 1, \dots, 2M_i$, with the expression given by (15). Then rearranging the terms in the resulting expression, we establish that relation (12) holds for weights ω_j^i defined in the following manner:

$$\omega_j^i = C_i \left(\tilde{\omega}_j^i + \delta_j^i \right), \quad \text{for } j = 1, \dots, M_i \quad (18)$$

In (18) C_i is a normalizing constant allowing (5) to hold. Notice that, provided the weight increments δ_j^i are all non-negative, the value of C_i is strictly positive. The values of δ_j^i

in turn, simply account for the sum of the contributions of \mathbf{I}_j^i for a given $j \leq M_i$, to the vectors \mathbf{I}_k^i for $k > M_i$, expressed by (15), respectively multiplied by $\tilde{\omega}_k^i$, and the corresponding convex combination coefficient. More specifically we have,

$$\delta_j^i = \sum_{k=M_i+1}^{2M_i} \beta_j^k \tilde{\omega}_k^i \quad (19)$$

where $\beta_j^k = 0$ if Q_k^i does not belong to $S_i \cap S_{k_j}$ and $\beta_j^k = \alpha_l^k$ for the pertaining convex combination coefficients in (15), that is, all the α_l^k 's such that $m_l = j$. In view of this definition of β_j^k it is readily seen from (19) that all the weight increments δ_j^i are non-negative. Furthermore by construction (5) holds for the weights ω_j^i defined by (18)-(19).

As one can easily infer from the construction of the set of weights described in this Section, this choice gives rise to a straightforward implementation of the method.

Remark 1: A second consistent choice of weights was proposed in [6]. For both such a choice and the present one a lower bound for ω independent of h can be determined.

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