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A positivity-preserving method for matrix-valued solution of the diffusion equation on deformed meshes

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Abstract

This work proposes a method to solve the diffusion equation with a matrix-valued unknown. A maximum principle can be proved for this equation and the solution is expected to be positive definite-valued if the initial data is also positive definite-valued. Reproducing such a positivity principle at the discrete level for a deformed mesh is a challenge. The method we present satisfies this property, is consistent and conservative in a sense we make precise.

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1 Introduction

In this work, we focus on the diffusion equation for a matrix-valued variable:

$$\forall(k, l) \in [1, m]^2, \partial_t E_{k,l} - \kappa \Delta E_{k,l} = 0, \tag{1}$$

where the unknown $E = (E_{k,l}(t, \mathbf{x}))_{1 \leq k, l \leq m}$ is a symmetric matrix of size $m \in \mathbb{N}^*$. The computational domain Ω is a cube of \mathbb{R}^d , where d is the space dimension.

The diffusion coefficient κ is positive. For simplicity, we assume periodic boundary conditions for (1), together with a suitable initial condition

$$E(0, \mathbf{x}) = E^0(\mathbf{x}), \tag{2}$$

where $E^0(\mathbf{x})$ is a symmetric matrix depending on the space variable \mathbf{x} . It is well known that Equation (1) is well-posed (see [RB17] for instance). Moreover, we have a maximum principle:

Proposition 1.1 (Maximum principle for a matrix-valued solution). *Assume that $E^0(\mathbf{x})$ is positive definite for all $(t, \mathbf{x}) \in \mathbb{R}_+ \times \Omega$, and that $\kappa > 0$. Consider a solution $E(t, \mathbf{x})$ to (1)-(2). Then, for all $(t, \mathbf{x}) \in \mathbb{R}_+ \times \Omega$, $E(t, \mathbf{x})$ is positive definite.*

Proof. Equation (1) being linear, we have, for any $\xi \in \mathbb{R}^m \setminus \{0\}$:

$$\partial_t \langle E\xi, \xi \rangle - \kappa \Delta (\langle E\xi, \xi \rangle) = 0.$$

Therefore, if $E(t = 0, \mathbf{x})$ is positive definite for all $\mathbf{x} \in \Omega$, the maximum principle for the scalar diffusion equation (see [Eva10] for instance) implies that $\langle E(t, \mathbf{x})\xi, \xi \rangle > 0$ for any $t \geq 0$, any $\mathbf{x} \in \Omega$ and any $\xi \in \mathbb{R}^m \setminus \{0\}$. This gives the desired result. \square

The present work proposes a numerical method that discretises Equation (1) while satisfying Proposition 1.1 at the discrete level.

Another important property for the applications we have in mind is conservation. Indeed, if $\Omega = \mathbb{R}^d$ or if periodic boundary conditions are imposed then a simple integration of (1) over the computation domain gives:

$$\frac{d}{dt} \int_{\Omega} E(t, \mathbf{x}) d\mathbf{x} = 0. \tag{3}$$

Our aim is thus to derive a consistent scheme for (1), that satisfies both Proposition 1.1 and (3) on deformed meshes. As we will see, we are only able to reproduce (3) for diagonal entries. We explain below why this is nevertheless a good point, both from a physical and a numerical viewpoint.

Equation (1) appears naturally in the simulation of mixing-induced turbulent flows (see for instance [BCD⁺21] and the references therein). Such a phenomenon is important for instance in the development of hydrodynamical instabilities in inertial confinement fusion experiments [MP20].

In such models, the tensor E may be either the Reynolds stress tensor or a correlation tensor. In both cases, the original equation satisfied by E actually includes transport and possibly reaction terms. However, dealing with such additional terms is already well documented: the upwind scheme is consistent, positivity preserving and conservative [EGH10], and many high-order extensions have been proposed that satisfy these properties [CDL11, HL14, ZS16].

In contrast, the diffusion part of the equation is more challenging. Since the turbulence model is usually coupled with Lagrangian or ALE hydrodynamics, we need the scheme to be valid on deformed meshes. In such a situation, a standard two-point flux scheme is positivity-preserving, but is not consistent [EGG⁺14], except on cartesian grids. Several strategies have been developed to design consistent finite volume schemes on deformed meshes, see for instance [Ker81, Per81, CVV99, DEGH10, Her00, BLS05, BBL09, EGH10, AEK⁺07, BM07], among other works. Unfortunately, all these schemes are non-positive on deformed meshes. Several works have addressed the question of positivity. The first we know of are those of J. Droniou and Ch. Le Potier (see for instance [LP09, DLP11]), based on ideas of [BM05]. It has been followed by many others [SYY09, SY16, YSGN22, LSSV07, LSV10, GW15, GYWH20, ZSW17]. All these schemes have the nice properties of being consistent, conservative, and positive. This comes at the price of making the scheme nonlinear.

The above-mentioned works deal with scalar-valued unknowns only, and have never been adapted to matrix-valued problems of the type (1), so far as we know. In order to design such a scheme, we are going to use as a starting point any of the above positivity-preserving schemes, and apply it to each diagonal term of the matrix E . Then, we apply the scheme to each unknown of the form

$$E_{k,k} + E_{l,l} + 2E_{k,l}, \quad 1 \leq k, l, \leq m,$$

which is positive since the matrix E is positive-definite. This allows to compute the off-diagonal term $E_{k,l}$ in a consistent way. However, this does not ensure positivity of the matrix E , so we apply a limitation procedure to recover this property. As we will see, this method is consistent, positive, and conservative for the diagonal terms. This is a good point as, for instance, when E is a Reynolds stress tensor, it is fundamental for the scheme to be conservative for the turbulent kinetic energy, that is, the trace of E .

We emphasize that our methodology is also valid for the anisotropic diffusion equation with a source term. In fact it can be applied to any linear equation which admits a positivity principle. Besides, it can be applied in any space dimension $d \in \mathbb{N}^*$. We choose here to set $d = 2$ for simplicity.

It should be also noted that the above strategy applies to any positive scalar scheme. Here, we choose to use the scheme defined in [BHL23], inspired from ideas of [BD06, BD03], and [BDF12a, FBD11] (see also [Fra12, Chapitre 6]).

The present article is organized as follows: in Section 2, we set the notations. In Section 3 we explain our method in detail and prove that it is positive in the sense of symmetric matrices. We present a numerical result in Section 4 that confirms the properties of the scheme.

2 Notations

We present here the notations that we use in the rest of the paper:

- \mathcal{T} a mesh,
- J the number of cells,
- in the following, Ω_j is a cell, $j < J$ is its index and we write $j \in \mathcal{T}$,
- \mathbf{x}_j is its center,
- V_j is its volume,
- $\sum_{j \in \mathcal{T}}$ is the sum over all the cells of the mesh,
- Δx is the maximum edge length.

We denote by $f : \mathbb{R}^J \rightarrow \mathbb{R}^J$ a scalar numerical scheme that is consistent in L^∞ -norm with orders q in time and q' in space ; that is to say, for any scalar-valued smooth function u satisfying:

$$\partial_t u - \kappa \Delta u = 0, \quad (4)$$

we have, for any cell j :

$$u_j(t^{n+1}) - (\mathcal{U}^{n+1})_j = O(\Delta t^q + \Delta x^{q'}), \quad \mathcal{U}^{n+1} = f\left((u_j(t^n))_{j \in \mathcal{T}}\right), \quad (5)$$

and where $u_j(t^n)$ is the exact value of the solution in cell j , which may be given by:

$$u_j(t^n) = \frac{1}{V_j} \int_{\Omega_j} u(t^n, \mathbf{x}) d\mathbf{x}. \quad (6)$$

More precisely, we have:

$$\max_{j \in \mathcal{T}} \left| u_j(t^{n+1}) - (\mathcal{U}^{n+1})_j \right| \leq C(\Delta t^q + \Delta x^{q'}), \quad (7)$$

where the constant $C > 0$ may depend on the derivatives of u . The choice of the L^∞ -norm is explained in Section 3.1. Moreover, we assume that the scheme f is positive (possibly under some stability condition): for any $g \in \mathbb{R}^J$,

$$\text{if: } \forall 1 \leq j \leq J, \quad g_j > 0, \quad \text{then: } \forall 1 \leq j \leq J, \quad [f(g)]_j > 0. \quad (8)$$

3 Method

We denote by:

- $E^n = (E_{k,l}^n)_{1 \leq k,l \leq m}$ the value of the unknown at iteration $n \in \mathbb{N}$,
- $(E_{k,l}^n)_j$ the value of the (k,l) coefficient of the unknown at iteration n and in cell j ,
- $E_{k,l}^n = \left((E_{k,l}^n)_j \right)_{j \in \mathcal{T}} \in \mathbb{R}^J$ the vector of the values of the (k,l) coefficient.

We first compute the diagonal terms using the scheme f :

$$\forall k \leq m, \quad E_{k,k}^{n+1} = f(E_{k,k}^n). \quad (9)$$

Then we compute a first approximation of the off diagonal terms using:

$$\forall k \leq m, \quad \forall l \neq k, \quad \tilde{E}_{k,l} = \frac{1}{2} \left(f(E_{k,k}^n + 2E_{k,l}^n + E_{l,l}^n) - E_{l,l}^{n+1} - E_{k,k}^{n+1} \right). \quad (10)$$

We choose to use Formula (10) instead of directly computing $\tilde{E}_{k,l} = f(E_{k,l}^n)$ for the following reason. The diffusion scheme f may be defined only for positive data. Besides, the matrix $(E_{k,l}^n)_{1 \leq k,l \leq m}$ being positive, the quantity $E_{k,k}^n + 2E_{k,l}^n + E_{l,l}^n$ is positive. In addition, using Assumption (5), the quantity $\tilde{E}_{k,l}$ computed with (10) may be proved to be a consistent approximation of $E_{k,l}(t^{n+1})$.

Let j be the index of a cell of the mesh \mathcal{T} . We define the matrix $E_j^{n+1/2}$ by:

$$E_j^{n+1/2} = \begin{pmatrix} (E_{1,1}^{n+1})_j & (\tilde{E}_{1,2})_j & \cdots & (\tilde{E}_{1,m})_j \\ (\tilde{E}_{1,2})_j & \ddots & \cdots & \vdots \\ \vdots & \ddots & \cdots & (\tilde{E}_{m-1,m})_j \\ (\tilde{E}_{1,m})_j & \cdots & (\tilde{E}_{m-1,m})_j & (E_{m,m}^{n+1})_j \end{pmatrix}. \quad (11)$$

There is no reason so far for this matrix (11) to be positive definite. To recover this condition, we locally modify the off diagonal terms. We already know that the diagonal terms of the matrix (11) are positive:

$$\forall k \leq m, \quad \left(E_{k,k}^{n+1} \right)_j > 0. \quad (12)$$

Let $\lambda \in [0, 1]$, we define:

$$\tilde{E}_j(\lambda) = \begin{pmatrix} (E_{1,1}^{n+1})_j & \lambda (\tilde{E}_{1,2})_j & \dots & \lambda (\tilde{E}_{1,m})_j \\ \lambda (\tilde{E}_{1,2})_j & \ddots & \dots & \vdots \\ \vdots & \ddots & \dots & \lambda (\tilde{E}_{m-1,m})_j \\ \lambda (\tilde{E}_{1,m})_j & \dots & \lambda (\tilde{E}_{m-1,m})_j & (E_{m,m}^{n+1})_j \end{pmatrix}.$$

We choose $\lambda_j \geq 0$ such that $\tilde{E}_j(\lambda_j)$ is positive definite. More precisely, E_j^{n+1} is given by:

$$E_j^{n+1} = \tilde{E}_j(\lambda_j^*), \quad \lambda_j^* = \sup \{ \lambda \in [0, 1] \mid \tilde{E}_j(\lambda) \text{ is positive definite} \}. \quad (13)$$

The quantity λ_j^* is well defined because:

$$0 \in \{ \lambda \in [0, 1] \mid \tilde{E}_j(\lambda) \text{ is positive definite} \}.$$

thanks to Equation (12). We also have the following result.

Proposition 3.1. *Under Assumption (8), the matrix $\tilde{E}_j(\lambda)$ is positive definite for any $\lambda \in [0, \lambda_j^*]$.*

Proof. Owing to Assumption (8), we know that the diagonal matrix $\tilde{E}_j(0)$ is positive definite. Moreover, we have, any $\lambda \in [0, \lambda_j^*]$:

$$\tilde{E}_j(\lambda) = \underbrace{\left(1 - \frac{\lambda}{\lambda_j^*} \right)}_{>0} \underbrace{\tilde{E}_j(0)}_{\text{positive definite}} + \frac{\lambda}{\lambda_j^*} \underbrace{\tilde{E}_j(\lambda_j^*)}_{\text{non-negative}},$$

thus $\tilde{E}_j(\lambda)$ is positive definite. □

However, if $\lambda_j^* < 1$, then the matrix $\tilde{E}_j(\lambda_j^*)$ is only non-negative. We overcome this difficulty by choosing: $E_j^{n+1} = \tilde{E}_j(\lambda_j^* - \delta)$ with $\delta = 10^{-12}$. In practice, λ_j^* is computed using a bisection algorithm. We emphasize that the computation of λ_j^* is local and that it requires only the quantities in the cell j . That is why the (λ_j^*) can be easily computed in parallel.

Remark 1. *The principle of the truncation (13) is to use the fact that the set*

$$\left\{ (X_{k,l})_{k < l} \in \mathbb{R}^{m(m-1)/2} \mid \begin{pmatrix} (E_{1,1}^{n+1})_j & X_{1,2} & \dots & X_{1,m} \\ X_{1,2} & \ddots & \dots & \vdots \\ \vdots & \ddots & \dots & X_{m-1,m} \\ X_{1,m} & \dots & X_{m-1,m} & (E_{m,m}^{n+1})_j \end{pmatrix} \text{ is positive definite} \right\}$$

is convex and contains 0. The idea originates from the Minkowski functional (or gauge function, see [Bou87] for instance).

3.1 Properties

Proposition 3.2 (Consistency of the method). *We assume that the scheme f is consistent in L^∞ norm with the diffusion equation with order q in time and q' in space (Assumptions (4) (5)). Then the scheme (9) (10) (13) is also consistent in L^∞ norm with the same orders:*

$$E(t^{n+1}) - E^{n+1} = O(\Delta t^q + \Delta x^{q'})$$

Proof. Using (4) (5), we easily have, for any cell j :

$$\tilde{E}_j(1) = E_j(t^{n+1}) + O(\Delta t^q + \Delta x^{q'}). \quad (14)$$

The scheme f being consistent in L^∞ norm (Assumption (7)), we can write more precisely:

$$\max_{j \in \mathcal{T}} \|\tilde{E}_j(1) - E_j(t^{n+1})\| \leq C(\Delta t^q + \Delta x^{q'}), \quad (15)$$

and the constant C may depend on the derivatives of the exact solution $E(t, \mathbf{x})$ but not on Δt nor on Δx . Moreover, $E_j(t^{n+1})$ is positive definite for any $j \in \mathcal{T}$, hence $\tilde{E}_j(1)$ is also positive definite for $\Delta t^q + \Delta x^{q'}$ small enough. Therefore $\lambda_j^* = 1$ for all j and:

$$E^{n+1} = \tilde{E}(1) = E(t^{n+1}) + O(\Delta t^q + \Delta x^{q'}). \quad \square$$

The scheme f is said to be conservative if for all $g \in \mathbb{R}^J$:

$$\sum_{j \in \mathcal{T}} V_j [f(g)]_j = \sum_{j \in \mathcal{T}} V_j g_j. \quad (16)$$

Proposition 3.3 (Conservation). *If the scheme f is conservative (see Equation (16)) then the diagonal coefficients are conserved.*

Proof. Using (9) and (16), we easily have:

$$\forall k \leq m, \quad \sum_{j \in \mathcal{T}} V_j \left(E_{k,k}^{n+1} \right)_j = \sum_{j \in \mathcal{T}} V_j \left(E_{k,k}^n \right)_j.$$

□

Remark 2. A priori, the extra-diagonal coefficients are not conserved. Indeed, using (10) (13), we have, for $k \leq m$ and $l \neq k$:

$$\sum_{j \in \mathcal{T}} V_j \left(E_{k,l}^{n+1} \right)_j = \sum_{j \in \mathcal{T}} V_j \left(\tilde{E}_{k,l}^n \right)_j = \sum_{j \in \mathcal{T}} V_j \lambda_j^* \left(E_{k,l}^n \right)_j.$$

A priori $\lambda_j^* \neq 1$, therefore:

$$\forall k \leq m, \quad \forall l \neq k, \quad \sum_{j \in \mathcal{T}} V_j \left(E_{k,l}^{n+1} \right)_j \neq \sum_{j \in \mathcal{T}} V_j \left(E_{k,l}^n \right)_j.$$

3.2 A finite volume scheme for the scalar diffusion equation

In this Section we present the scheme we use to discretise the scalar diffusion equation:

$$\partial_t u - \kappa \Delta u = 0. \quad (17)$$

We use the second order finite volume scheme from [BHL23] with $\theta = 1/2$. The scheme is non-linear, conservative, explicit and second order consistent in space and first order in time. It also preserves the positivity of the numerical solution under a following parabolic CFL condition: $\Delta t \leq C \Delta x^2 / \kappa$, where $C > 0$ is a constant that depends on the connectivity of the mesh.

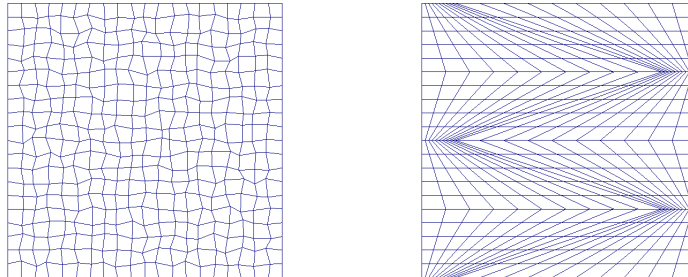


Figure 1: Random mesh (left) and Kershaw type mesh (right) of size 20×20 .

Remark 3. We use this scheme here, but our strategy applies to any consistent and positive scheme. In particular those from [LP09, LMS14, YSGN22, SY16, SYY09, AN21, WPL⁺22, NSL22, BL16, BHLP23] would fit in the present framework.

4 Numerical results

In this Section, we propose a numerical example so as to compare our method *with correction* (9) (10) (13) and the method *without correction* (9) (10). We choose $\kappa = 1/3$. The computational domain is $\Omega = [0, 2]^2$. The exact solution reads as:

$$E = R^T \begin{pmatrix} u_1 & 0 & 0 \\ 0 & u_1 & 0 \\ 0 & 0 & u_2 \end{pmatrix} R, \quad R = \begin{pmatrix} 1 & 0 & 0 \\ 0 & a & b \\ 0 & -b & a \end{pmatrix}, \quad b = \sqrt{1 - a^2}.$$

where $a = 0.4$ and u_1, u_2 are solution of (17) with $\kappa = 1/3$. They are given by:

$$u_1(t, \mathbf{x}) = \frac{3}{4\pi(t + t_0)} \exp\left(-3 \frac{\|\mathbf{x} - \mathbf{x}_0\|^2}{4(t + t_0)}\right) + \varepsilon, \quad \mathbf{x}_0 = (1, 1), \quad t_0 = 0.01.$$

and:

$$u_2(t, x, y) = \frac{1 - \varepsilon}{2} \left(\operatorname{erf}\left(\frac{x - 0.4}{\sqrt{4t}} \sqrt{3}\right) - \operatorname{erf}\left(\frac{x - 0.6}{\sqrt{4t}} \sqrt{3}\right) \right) + \varepsilon,$$

The matrix R is a rotation matrix and $\varepsilon = 10^{-15}$. Periodic boundary conditions are imposed (u_1 is almost constant on the boundary of the domain, while u_2 is constant on the $x = 0$ and $x = 2$ boundaries and does not depend on the y variable). The final time is $T = 0.03$. We perform convergence analysis on cartesian meshes, random meshes and Kershaw type meshes, see Figure 1. The time step is given by $\Delta t = \Delta x^2$ for cartesian and random meshes. We had to choose a smaller constant on Kershaw type meshes, namely $\Delta t = \Delta x^2/100$, because of the strong deformation of the meshes.

We use the Sylvester criterion \mathcal{S} to check that the matrices are positive definite (see Appendix 5). Tables 1 show the number of cells N^- where the solution is not positive definite and the minimum of the Sylvester criterion \mathcal{S} for the scheme *without correction* (9) (10). Figure 2 shows that the scheme *with correction* (9) (10) (13) is indeed second order accurate as expected. We noticed that the value of λ^* (defined in (13)) varies significantly with the geometry. We observed the following values for the meshes of sizes 160×160 . For the cartesian mesh, it is always equal to 1. For the random mesh, it may decrease up to 0.9. For the Kershaw type mesh it can be of order 10^{-2} . We emphasize that this does not create consistency issues.

Eventually, we tested our method with the diffusion scheme from [BDF12b]. This scheme being linear, the step (10) is equivalent to directly iterating every coefficient. We present in Table 2 the results *without*

N_x	N^-	min
5	1	-1×10^{-13}
10	0	1×10^{-45}
20	16	-4×10^{-23}
40	20	-3×10^{-27}
80	0	4×10^{-33}
160	0	9×10^{-33}

N_x	N^-	min
5	4	-0.002
10	3	-9×10^{-6}
20	21	-3×10^{-23}
40	19	-6×10^{-20}
80	0	3×10^{-33}
160	0	8×10^{-33}

N_x	N^-	min
5	4	-9×10^{-6}
10	10	-0.003
20	60	-0.0008
40	236	-6×10^{-5}
80	532	-3×10^{-10}
160	94	-8×10^{-14}

Table 1: Values of N^- and minimum values of \mathcal{S} on cartesian (left), random (center) and Kershaw type meshes (right) for the scheme *without correction* (9) (10).

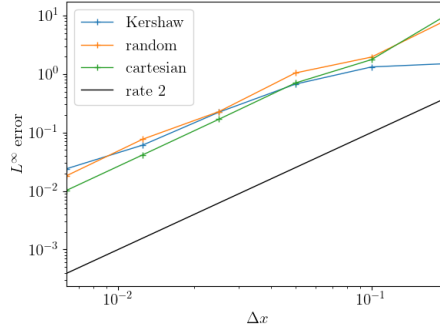


Figure 2: L^∞ errors at $t = 0.03$ for for the scheme *with correction* (9) (10) (13) on cartesian, random type meshes and Kershaw type meshes.

correction. This scheme is not positive so we can not use the correction step (13) here. We see that the method does produces negative values.

5 Appendix: The Sylvester criterion for positive definite matrices

Let $A \in \mathbb{R}^{m \times m}$ be symmetric and $1 \leq l \leq m$. The l^{th} leading principal minor $\mathcal{M}_l(A)$ is defined by: $\mathcal{M}_l(A) = \det \left((A_{k,k'})_{k,k' \leq l} \right)$. We also define: $\mathcal{S}(A) = \min_{1 \leq l \leq m} \mathcal{M}_l(A)$. Note that \mathcal{S} is a continuous mapping.

Theorem 5.1 (Sylvester condition). *Let $A \in \mathbb{R}^{m \times m}$ be symmetric. Then A is positive definite if and only if: $\mathcal{S}(A) > 0$.*

Proof. The proof can be found in [HJ85], Theorem 7.2.5. □

N_x	N^-	min
5	0	8×10^{-37}
10	0	1×10^{-45}
20	0	1×10^{-45}
40	0	3×10^{-42}
80	0	8×10^{-33}
160	0	1×10^{-32}

N_x	N^-	min
5	7	-0.1
10	1	-0.0007
20	0	1×10^{-45}
40	0	4×10^{-42}
80	0	9×10^{-33}
160	0	1×10^{-32}

N_x	N^-	min
5	4	-0.02
10	26	-0.7
20	68	-1
40	440	-0.2
80	1088	-0.004
160	1418	-0.0007

Table 2: Values of N^- and minimum values of \mathcal{S} on cartesian (left), random (center) and Kershaw type meshes (right) for the P_1 diffusion scheme [BDF12b].

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