

Monotone schemes for a class of nonlinear elliptic and parabolic problems¹

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Abstract

We construct monotone numerical schemes for a class of nonlinear PDE for elliptic and initial value problems for parabolic problems. The elliptic part is closely connected to a linear elliptic operator, which we discretize by monotone schemes, and solve the nonlinear problem by iteration. We assume that the elliptic differential operator is in the divergence form, with measurable coefficients satisfying the strict ellipticity condition, and that the right hand side is a positive Radon measure. The numerical schemes are not derived from finite difference operators approximating differential operators, but rather from a general principle which ensures the convergence of approximate solutions. The main feature of these schemes is that they possess stencils stretching far from basic grid-rectangles, thus leading to system matrices which are related to M-matrices.

Key words: homogenization, elliptic operator, nonlinear parabolic PDE, divergence form, monotone scheme.

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1 INTRODUCTION

There is a number of interesting phenomena in engineering problems that lead to equations of the form $\partial_i u - \sum_{ij} \partial_i a_{ij} u \partial_j u = \mu$, where a_{ij} define a diffusion tensor with a general structure, mostly degenerate. These problems range from laminated plates, composite materials, polymer production and

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porous media to electrochemistry and, recently, mathematical biology. It is common for most of them that they originate from the method of homogenization, frequently involving non-smooth diffusion tensor, and sometimes right hand sides which are only measures. To mention just a few interesting problems to which the method can be applied, let us mention diffusion of gases in polymers [12], diffusion of ions through solution of charged molecules [5], advection-diffusion problems arising in deterministic approach to aggregating populations in mathematical biology [11] or anisotropic diffusion in image processing [14]. Finally, the classic problem of dispersion of pollutants in the sea and lakes, where diffusion tensor can be evaluated from measured components of velocity of the fluid is also in the same class, though in this case the operator is linear. In what follows, we propose a new numerical scheme for such problems with a desirable property of yielding a positive approximation to solution for which the right hand side may be as weak as a positive Radon measure.

In Section 2 we define the abstract setting for the problem in question, functional spaces needed, and a specific discretization on a numerical grid. In Section 3 we briefly describe basic properties of the linear elliptic problem and its parabolic counterpart. These are followed by an explicit construction of the system matrix for discretized problem in Section 4, and results on convergence can be found in Section 5. Finally, two examples with nonlinear PDE, one elliptic and one parabolic, illustrate the efficiency of the proposed numerical scheme.

2 DEFINITION OF THE PROBLEM

Let $\mathbb{1}_S$ be the *indicator* of $S \subset \mathbb{R}^d$, i.e. $\mathbb{1}_S(\mathbf{x}) = 1$ for $\mathbf{x} \in S$, and zero otherwise. We say that f on \mathbb{R}^d is *piecewise continuous* if $f = \sum_{j=1}^L f_j \mathbb{1}_{D_j}$, where D_j are measurable and mutually disjoint, and f_j are bounded, uniformly continuous functions on \mathbb{R}^d . A bounded domain $D \subset \mathbb{R}^d$ is called a Lipschitz domain if D is an open set and its boundary ∂D is a Lipschitz boundary [10]. Although our interest is in Lipschitz domains, often we express results for the case of the whole Euclidean space \mathbb{R}^d , whence we write $D = \mathbb{R}^d$. The closure of a set S is denoted by \bar{S} or $\text{cls}(S)$.

Banach spaces of functions $C^{(k)}(\mathbb{R}^d)$, $C^{(k)}(\bar{D})$ are defined as usual. The closure of functions with compact supports in $C^{(k)}(\mathbb{R}^d)$ determines the subspace $C_0^{(k)}(\mathbb{R}^d)$. The closure of functions in $C(\bar{D})$ with supports in D determines the subspace $\dot{C}(\bar{D})$, and then $\dot{C}^{(1)}(\bar{D}) = C^{(1)}(\bar{D}) \cap \dot{C}(\bar{D})$. The L_p -spaces, as well as Sobolev W_p^1 -spaces, are defined in a standard way [10,13], their norms being $\|\cdot\|_p$ and $\|\cdot\|_{p,1}$, respectively. The completion in the norm of $W_p^1(D)$ of functions in $\dot{C}^{(1)}(\bar{D})$ is denoted by $\dot{W}_p^1(D)$. Let X be a Banach space and X^\dagger its dual.

Then the value of $f \in X^\dagger$ at $u \in X$ is denoted by $\langle f|u \rangle$. Let $\mathcal{R}(D)$ be the convex set of positive Radon measures μ on $\mathfrak{B}(D)$. Then $\langle v|\mu \rangle = \int_D v(\mathbf{x})\mu(d\mathbf{x})$ is well defined for $v \in \dot{W}_\infty^1(D)$. We say that a sequence of $\mu_n \in \mathcal{R}(D)$ converges weakly to $\mu \in \mathcal{R}(D)$ if $\lim_n \langle v|\mu_n \rangle = \langle v|\mu \rangle$ for each $v \in \dot{C}(\bar{D})$.

Nonlinear elliptic and parabolic problems for which we construct monotone schemes are defined in terms of the linear 2nd-order elliptic operator on \mathbb{R}^d ,

$$A(\mathbf{x}) = - \sum_{i,j=1}^d \partial_i a_{ij}(\mathbf{x}) \partial_j + \sum_{j=1}^d b_j(\mathbf{x}) \partial_j + c(\mathbf{x}), \quad (1)$$

where $a_{ij} = a_{ji}$, b_i , ($i, j = 1, 2, \dots, d$) and c are piecewise continuous on \mathbb{R}^d , $c \geq 0$, and $a_{ij}(\mathbf{x})$ must converge to constant values as $|\mathbf{x}|$ increases. We also require strict ellipticity, *i.e.* that there exist positive numbers $0 < \underline{M} \leq \bar{M}$, such that $\underline{M}|\mathbf{x}|^2 \leq \sum_{i,j=1}^d a_{ij}(\mathbf{x}) z_i \bar{z}_j \leq \bar{M}|\mathbf{x}|^2$. In addition, $\operatorname{div} \mathbf{b} = 0$ in the generalized sense. The differential operator $A_0(\mathbf{x}) = - \sum_{i,j=1}^d \partial_i a_{ij}(\mathbf{x}) \partial_j$ is called the *main part* of $A(\mathbf{x})$. Then $A(\mathbf{x}) = A_0(\mathbf{x}) + L(\mathbf{x})$, where $L(\mathbf{x})$ is a lower order differential operator. A real bilinear form on $W_q^1(D) \times W_p^1(D)$, $1/p + 1/q = 1$, defined by $a(v, u) = \sum_{i,j=1}^d \int_D a_{ij}(\mathbf{x}) \partial_i v(\mathbf{x}) \partial_j u(\mathbf{x}) d\mathbf{x} + \langle v|Lu \rangle$ is associated with (1). For each pair $v \in \dot{W}_q^1(D)$, $u \in \dot{W}_p^1(D) \cap \{Au \in (\dot{W}_q^1(D))^\dagger\}$, $1 < p < \infty$, we have $a(v, u) = \langle v|Au \rangle$, this also being true for each pair $v \in \dot{W}_\infty^1(D)$, $u \in \dot{W}_1^1(D) \cap \{Au \in \mathcal{R}(D)\}$.

We consider a class of nonlinear operators defined by $(\mathbf{x}, u(\mathbf{x})) \mapsto A(\mathbf{x}, u(\mathbf{x})) = - \sum_{i,j} \partial_i a_{ij}(\mathbf{x}) u(\mathbf{x})^\alpha \partial_j + L(\mathbf{x})u(\mathbf{x})$, $\alpha > 0$, so that $A(\mathbf{x}, 1)$ coincides with (1). The corresponding analogue of the bilinear form $a(\cdot, \cdot)$ is

$$a(u; v, u) = \sum_{i,j=1}^d \int_D a_{ij}(\mathbf{x}) u(\mathbf{x})^\alpha \partial_i v(\mathbf{x}) \partial_j u(\mathbf{x}) d\mathbf{x} + \langle v|Lu \rangle. \quad (2)$$

In this work we study numerical methods for BVPs and IVPs for the second order parabolic linear and nonlinear PDE. Results for linear BVPs are expressed in terms of properties of solutions of the variational formulation for a solution $u \in \dot{W}_p^1(D)$:

$$\lambda \langle v|u \rangle + a(v, u) = \langle v|\mu \rangle, \quad \text{for any } v \in \dot{W}_\infty^1(D), \quad (3)$$

where $\lambda \geq 0$, and the inhomogeneous term μ is a positive Radon measure. For $D = \mathbb{R}^d$ we replace $v \in \dot{W}_\infty^1(D)$ with $v \in \dot{W}_\infty^1(\mathbb{R}^d) \cap C_0(\mathbb{R}^d)$. Nonlinear BVPs are also formulated by using a variational formulation:

$$\lambda \langle v|u \rangle + a(u; v, u) = \langle v|\mu \rangle, \quad \text{for any } v \in \dot{W}_\infty^1(D). \quad (4)$$

The aim is to study discrete approximations to the solution $u \in C(\mathbb{R}_+, \dot{W}_p^1(D))$ of IVP's which are defined in terms of the variational equalities:

$$\begin{aligned} & \langle v(t) | u(t) \rangle - \langle v(0) | u(0) \rangle - \int_0^t ds \langle \partial_s v(s) | u(s) \rangle \\ & + \int_0^t ds a(u(s); v(s), u(s)) = \langle \int_0^t v(s) ds | \mu \rangle, \quad t > 0, \end{aligned} \quad (5)$$

for any $v \in \dot{C}^{(1)}(\mathbb{R}_+, \dot{W}_\infty^1(D))$,

where μ is a positive Radon measure and the initial condition $u_0 \in \dot{W}_p^1(D)$. Problem (3) is called auxiliary to the problem (4). The Euler–Lagrange equations of (3), (4) or (5) are called *formal linear (nonlinear) elliptic and parabolic problems*, respectively.

The orthogonal coordinate system in \mathbb{R}^d is determined by unit vectors \mathbf{e}_i . Discretizations of \mathbb{R}^d are defined by the grids $G_n := \{\mathbf{x} = h(n) \sum_{l=1}^d k_l \mathbf{e}_l : k_l \in \mathbb{Z}\}$, where $h(n) = 2^{-n}$ is the *grid-step*, usually denoted by h , and the elements of G_n are *grid-knots*. The subgrids $G_n(D) = G_n \cap D$ are *discretizations* of D . The index set of grid-knots $\mathbf{x} \in G_n(D)$ is $J_n(D)$.

A mapping from G_n or $G_n(D) \rightarrow \mathbb{R}$ is called a *grid function*, and the linear space of grid functions on G_n or $G_n(D)$ is denoted by $l(G_n(D))$ or $l(G_n)$. The initial condition and measure in Problems (4), (5), are discretized by grid-functions $\mathbf{u}_{0n}, \boldsymbol{\mu}_n$, respectively, The differential operator (1) is discretized by a matrix A_n with the index set $J_n(D) \times J_n(D)$; such a matrix A_n obtained from discretization is called the *system matrix*.

The discretizations of Problem (4) have the following forms:

$$(\lambda I + A_n(\mathbf{u}_n))\mathbf{u}_n = \boldsymbol{\mu}_n. \quad (6)$$

Similarly, discretizations of Problem (5) have the form:

$$\dot{\mathbf{u}}_n(t) + A_n(\mathbf{u}_n(t))\mathbf{u}_n(t) = \boldsymbol{\mu}_n, \quad \mathbf{u}_n(0) = \mathbf{u}_{0n}. \quad (7)$$

Apparently, Problems (6) are algebraic linear or nonlinear systems, while Problems (7) are IVP for systems of linear or nonlinear ODE. We say that Problems (6) and (7) define monotone schemes of the original problems (4) and (5) if the matrices $A_n = A_n(\mathbf{u}_n(t)), t \geq 0$ have the following structure:

$$\begin{aligned} (A_n)_{ii} &> 0, \text{ for } i \in J_n(D) \\ (A_n)_{ij} &\leq 0, \text{ for } i \neq j, \end{aligned} \quad \sum_{i \in J_n(D)} (A_n)_{ij} \geq 0 \text{ for } j \in J_n(D).$$

We say that a matrix A_n with such properties has the *compartmental structure*. Naturally, the system matrices A_n with the compartmental structure are the main object in this work. Let us mention that the transpose A^T of a compartmental matrix is a M-matrix if A^{-1} exists.

An element (column) $\mathbf{u}_n \in l(G_n)$ can be associated with a continuous function on \mathbb{R}^d in various ways. Here we utilize a mapping $l(G_n) \mapsto C(\mathbb{R}^d)$ defined in terms of hat functions. Let χ be the canonical hat function on \mathbb{R} , centered at the origin and having the support $[-1, 1]$. Then $z \mapsto \phi(h, x, z) = \chi(h^{-1}(z - hx))$ is the hat function on \mathbb{R} , centered at $x \in \mathbb{R}$ with support $[x - h, x + h]$. The functions $\mathbf{z} \mapsto \phi_{\mathbf{k}}(\mathbf{z}) = \prod_{i=1}^d \phi(h, x_i, z_i)$, $x_i = hk_i$, define d -dimensional hat functions with supports $S_n(\mathbf{1}, \mathbf{x}) = \prod_i [x_i - h, x_i + h]$. The functions $\phi_{\mathbf{k}}(\cdot) \in G_n$, span a linear space, denoted by $E_n(\mathbb{R}^d)$. Let $\mathbf{u}_n \in l(G_n)$ have the entries $u_{n\mathbf{k}} = (\mathbf{u}_n)_{\mathbf{k}}$. Then the function $u(n) = \sum_{\mathbf{k} \in I_n} u_{n\mathbf{k}} \phi_{\mathbf{k}}$ belongs to $E_n(\mathbb{R}^d)$ and defines an imbedding of grid-functions into the space of continuous functions. We denote the corresponding mapping by $\Phi_n : l(G_n) \mapsto E_n(\mathbb{R}^d)$. Obviously, there exists $\Phi_n^{-1} : E_n(\mathbb{R}^d) \mapsto l(G_n)$ and the spaces $l(G_n)$ and $E_n(\mathbb{R}^d)$ are isomorphic with respect to the pair of mappings Φ_n, Φ_n^{-1} . It is clear that $E_n(\mathbb{R}^d) \subset E_{n+1}(\mathbb{R}^d)$ and the space of functions $\cup_n E_n(\mathbb{R}^d)$ is dense in $L_p(\mathbb{R}^d)$, $p \in [1, \infty)$, as well as in $\dot{C}(\mathbb{R}^d)$. Let us mention that $\sum_{\mathbf{k}} \phi_{\mathbf{k}} = 1$ on \mathbb{R}^d .

Grid-solutions $\mathbf{u}_n(t), \mathbf{u}_n$ of (7) and (6) are imbedded into the space of hat functions and the functions $u(n, t) = \Phi_n \mathbf{u}_n(t), u(n) = \Phi_n \mathbf{u}_n$ in $E_n(D)$ are called the approximate solutions of respective Problems (7) and (6).

3 GROUND FOR NUMERICAL APPROACH

Let us start with a description of certain properties of the linear operator $A(\mathbf{x})$ and the corresponding problem (3). The inverse of the differential operator $\lambda I + A(\mathbf{x})$ on \mathbb{R}^d , as well as the inverse of this operator on a Lipschitz domain with the homogeneous boundary conditions on ∂D , are denoted by $T(\lambda, A)$ and $T(\lambda, A_D)$, respectively. We say that the operator $T(\lambda, A)$ exists if the differential equation $(\lambda + A(\mathbf{x}))u(\mathbf{x}) = f(\mathbf{x})$ has a unique solution $u \in L_{1,loc}(\mathbb{R}^d)$ for any $f \in C_0(\mathbb{R}^d)$. We say that the operator $T(\lambda, A_D)$ exists if the BVP (3) has a unique solution $u \in L_1(D)$. By using the defined objects we can prove the following theorem [2,6]:

THEOREM 3.1 *Let D be a bounded domain with a Lipschitz boundary, $\mu \in \mathcal{R}(D)$ and $T(\lambda, A)$ exist. Let a sequence of functions $\mathfrak{U} = \{u(n) : n \in \mathbb{N}\} \subset L_1(D)$ converge to μ weakly. Then the sequence of functions $\mathfrak{V} = \{v(n) : n \in \mathbb{N}\} \subset \dot{W}_p^1(D)$, where $v(n) = T(\lambda, A)u(n)$, converges strongly in $\dot{W}_p^1(D)$ to $T(\lambda, A)\mu$ for each $p < 1 + 1/(d - 1)$.*

A numerical approach to the linear problem (3) on D with a Radon measure on right hand side is based on Theorem 3.1. The method is described in [7,8]. In addition, this result satisfies our needs for theoretical grounds of nonlinear BVPs to be studied in Sections 5, 6. Defined nonlinear BVPs on D of mentioned sections are transformed to equivalent nonlinear BVPs of the form $A_0(\mathbf{x})u(\mathbf{x}) + L(u(\mathbf{x})) = \mu(\mathbf{x})$ with the corresponding boundary conditions, where $u \mapsto L(u)$ is a simple nonlinear operator.

Nonlinear IVPs (5) cannot be transformed to equivalent nonlinear IVPs with a linear term involving the second order derivatives. Thus a linear IVP representing a counterpart of (5) is omitted from our analysis. For nonlinear IVP (5) a general result can be used [9], Section 12. of Chpt. 1. and Section 3. of Chpt. 2.:

THEOREM 3.2 *Let $u_0 \in W_2^{-1}(D)$ and $\mu \in W_q^{-1}(D)$ where $q = (2 + \alpha)/(1 + \alpha)$, $\alpha > 0$. Then there exists a unique solution $u \in L^{2+\alpha}((0, t_b) \times D)$, $t_b > 0$, to the problem (5) in which $a(u(s); v(s), u(s))$ is replaced with $a(|u(s)|; v(s), u(s))$.*

If stronger conditions are imposed, for instance, $u_0 \in L_2(D)$ and $\mu \in L_q(D)$, $\mu > 0$, then a smoother solution to the problem (5) exists: $u \in L_\infty((0, T), L_2(D))$, $u^{\alpha/2} \in L_2((0, T), \dot{W}_2^1(D))$ and $du/dt \in L_q((0, T), W_q^{-1}(D))$ [3,9]. In the case of $q > d/2$ we can use an iterative process for the construction of solution to (5), as proposed in [1].

4 CONSTRUCTION OF THE SYSTEM MATRIX

Discretized nonlinear problems (6) and (7) are numerically solved by iterations. In each iteration a linear problem is solved for which the system matrix must have the compartmental structure. Therefore, in this section we describe constructions of matrices A_n discretizing the linear differential operator (1).

Construction of discretizations in this section is possible if certain conditions on a_{ij} are fulfilled. The required conditions are stronger than the assumed ones in Section 2. By relaxing them gradually as $n \rightarrow \infty$ we obtain discretizations for a general $A(\mathbf{x})$ which is defined in Section 2. In order to make our presentation brief, we assume that $\mathbf{x} \mapsto a(\mathbf{x})$ is a continuous tensor valued function on \mathbb{R}^d .

To a given diffusion tensor $a = \{a_{ij}\}_{11}^{dd}$ we associate an auxiliary tensor \hat{a} defined by the components $\hat{a}_{ii} = a_{ii}$, $\hat{a}_{ij} = -|a_{ij}|$, $i \neq j$. Also, we need sets $S(\mathbf{q}, \mathbf{x}) = \prod_{i=1}^d [x_i - hq_i, x_i + hq_i]$.

Assumption 4.1 *The auxiliary diffusion tensor \hat{a} is strictly positive definite*

on \mathbb{R}^d . There exists $\mathbf{q} \in \mathbb{N}^d$ such that for each $\mathbf{x} \in G_n$ there is a parameter $\mathbf{r}(\mathbf{x}) \in \mathbb{N}^d$ satisfying:

$$\inf_n \min_i \inf_{\mathbf{x}} \left\{ \frac{1}{r_i(\mathbf{x})} \inf_{\mathbf{z} \in S(\mathbf{q}, \mathbf{x})} a_{ii}(\mathbf{z}) - \sum_{m \neq i} \frac{1}{r_m(\mathbf{x})} \sup_{\mathbf{z} \in S(\mathbf{q}, \mathbf{x})} |a_{im}(\mathbf{z})| \right\} > 0.$$

This Assumption is crucial in the construction of discretizations A_n possessing the compartmental structure. For two-dimensional problems it always holds, but for a dimension $d \geq 3$ it is not fulfilled in all the cases, thus limiting the proposed numerical scheme. The scheme can be extended to a larger class of diffusion tensors $a = \{a_{ij}\}_{11}^{dd}$ after performing rotation of coordinate axes.

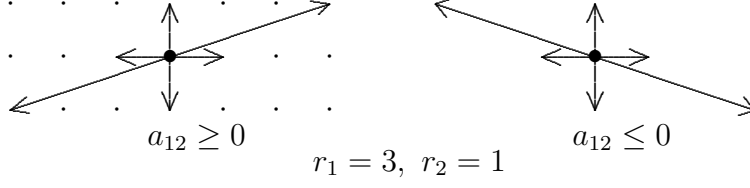
Contrary to the standard approach in developing discretizations of $A_0(\mathbf{x})$, we construct methods based on the general principle which is not *a priori* related to the forward/backward finite difference formulæ. One such method is described here, which follows from basic principles discussed in [7].

Discretizations A_n are defined in terms of its matrix entries $(A_n)_{\mathbf{k}\mathbf{l}}$, where $h\mathbf{k}, h\mathbf{l} \in G_n$. For a fixed $\mathbf{x} = h\mathbf{k} \in G_n$ the set of all the grid-knots $\mathbf{y} = h\mathbf{l}$ such that $(A_n)_{\mathbf{k}\mathbf{l}} \neq 0$ is denoted by $\mathcal{N}(\mathbf{x})$ and called the *numerical neighbourhood* of A_n at $\mathbf{x} \in G_n$. A set $\mathcal{N}(\mathbf{x})$ contains always a "cross" consisting of \mathbf{x} and $2d$ elements $\pm hr_i \mathbf{e}_i$. Additional elements of $\mathcal{N}(\mathbf{x})$ depend on the sign of $a_{ij}, i \neq j$.

Let us consider the two-dimensional case and assume a possibility of a partition of \mathbb{R}^2 as described in the following. There exists a finite index set \mathcal{L} and a partition $\mathbb{R}^d = \cup_l D_l$. The set \mathcal{L} is split into the subsets \mathcal{L}_{\mp} , where $l \in \mathcal{L}_-$ means that $a_{ij} \leq 0$ on D_l and $l \in \mathcal{L}_+$ means $a_{ij} \geq 0$ on D_l . To each D_l there is associated a parameter $\mathbf{r}(l) \in \mathbb{N}^2$. Now we define $D_n(-) = \cup_{l \in \mathcal{L}_-} D_l$ and $D_n(+) = D_n(-)^c$. The subgrids $G_n(\mp)$ are defined by $G_n(-) = G_n \cap D_n(-)$ and $G_n(+) = G_n \cap \text{cls}(D_n(+))$. The convex set $\{t\mathbf{x} + (1-t)\mathbf{y} : t \in [0, 1]\}$ is called segment. The subgrids $G_n(+)$ are characterized by the following property. Let $\mathbf{x} \in \text{cls}(D_l)$, $\mathbf{y} = \mathbf{x} + h(n)r_1(l)\mathbf{e}_1$ and $I(\mathbf{x}, \mathbf{y})$ be the corresponding segment. Then $\mathbf{x} \in G_n(+)$ if $I(\mathbf{x}, \mathbf{y}) \subset \text{cls}(D_n(+))$. It follows that each $\mathbf{x} \in G_n$ must be contained in one of sets $G_n(\mp)$ and each of segments $I_i(\mathbf{x}, \mathbf{y}), \mathbf{y} = \mathbf{x} + h(n)r_i(l)\mathbf{e}_i, i = 1, 2$ must have both of its end points \mathbf{x}, \mathbf{y} in some $G_n(\mp)$. Some grid-knots and some segments are contained in both sets, $G_n(\mp)$ and $\text{cls}(D_n(\mp))$, respectively. The subgrids $G_n(l, \mp) = G_n(\mp) \cap D_l$ cover G_n and some of them may have common grid-knots. For measurable functions a_{ij} on \mathbb{R}^2 which have constant values outside a bounded set the described decomposition is possible after smoothing the functions a_{ij} with a sequence of mollifiers as described in [8].

In order to write down the entries of A_n we need the abbreviations:

Fig. 1. Numerical neighbourhoods



$$\begin{aligned}
 a_{ij}^{\pm+}(\mathbf{r}) &= a_{ij}\left(\mathbf{x} + \frac{h}{2}(\pm r_1 \mathbf{e}_1 + r_2 \mathbf{e}_2)\right), & a_{ij}^{\pm-}(\mathbf{r}) &= a_{ij}\left(\mathbf{x} + \frac{h}{2}(\pm r_1 \mathbf{e}_1 - r_2 \mathbf{e}_2)\right), \\
 \hat{a}_{12}^{(-+)}(\mathbf{r}) &= a_{12}\left(\mathbf{x} + \frac{h}{2}(r_1 \mathbf{e}_1 + r_2 \mathbf{e}_2) - h \mathbf{e}_1\right), & \hat{a}_{12}^{(++)}(\mathbf{r}) &= a_{12}^{(++)}(\mathbf{r}), \\
 \hat{a}_{12}^{(+-)}(\mathbf{r}) &= a_{12}\left(\mathbf{x} + \frac{h}{2}(r_1 \mathbf{e}_1 + r_2 \mathbf{e}_2) - h \mathbf{e}_2\right), & \hat{a}_{12}^{(--)}(\mathbf{r}) &= a_{12}^{(--)}(\mathbf{r}).
 \end{aligned}$$

For each $\mathbf{x} \in G_n \cap \text{int}(D_l)$ nontrivial off-diagonal entries of A_n have a simple structure. The entries on the "cross" are:

$$\begin{aligned}
 (A_n)_{\mathbf{k}\mathbf{k}\pm\mathbf{e}_1} &= -\frac{1}{h^2} \begin{cases} a_{11}^{(\pm+)}(\mathbf{1}) - \frac{r_1(l)}{r_2(l)} |\hat{a}_{12}^{(\pm+)}(\mathbf{r}(l))| \text{ for } a_{12} \leq 0, \\ a_{11}^{(\pm-)}(\mathbf{1}) - \frac{r_1(l)}{r_2(l)} |\hat{a}_{12}^{(\pm-)}(\mathbf{r}(l))| \text{ for } a_{12} \geq 0 \end{cases} \quad (8) \\
 (A_n)_{\mathbf{k}\mathbf{k}\pm\mathbf{e}_2} &= -\frac{1}{h^2} \left[a_{22}^{(\pm\pm)}(\mathbf{1}) - \frac{r_2(l)}{r_1(l)} |\hat{a}_{12}^{(\pm\pm)}(\mathbf{r}(l))| \right],
 \end{aligned}$$

while the entries in the directions $\mathbf{w}^{(\pm)}(l) = r_i(l)\mathbf{e}_i \pm r_j(l)\mathbf{e}_j$ are:

$$\begin{aligned}
 (A_n)_{\mathbf{k}\mathbf{k}\pm\mathbf{w}^{(-)}(l)} &= -\frac{1}{h^2 r_1(l) r_2(l)} |a_{12}^{(\pm\mp)}(\mathbf{r}(l))| \quad \text{for } a_{12} \leq 0 \text{ on } D_l, \\
 (A_n)_{\mathbf{k}\mathbf{k}\pm\mathbf{w}^{(+)}(l)} &= -\frac{1}{h^2 r_1(l) r_2(l)} |a_{12}^{(\pm\pm)}(\mathbf{r}(l))| \quad \text{for } a_{12} \geq 0 \text{ on } D_l.
 \end{aligned} \quad (9)$$

For grid-knots $\mathbf{x} = h\mathbf{k} \in D_l$ such that the numerical neighborhood $\mathcal{N}(\mathbf{x})$ has points outside of $\text{cls}(D_l)$ the entries have a complex structure. Their structure follows from the corresponding discretized forms [7,8]. The diagonal entries are the negative sums of off-diagonal entries. The numerical neighbourhoods of discretizations A_n defined by (8), (9) are illustrated in Fig. 1. The quantities $\hat{a}_{ij}^{(\alpha\beta)}$ in (8) can be replaced with $a_{ij}^{(\alpha\beta)}$. However, the quantities $a_{ij}^{(\alpha\beta)}$ should not be replaced with $a_{ij}(h\mathbf{k})$ since the resulting $(A_n)_{\mathbf{k}\mathbf{l}}$ would be discretizations of $\sum_{ij} a_{ij} \partial_i \partial_j$.

Discretizations A_n of (8) and (9) are obtained by applying the variational calculus to certain bilinear forms $(\mathbf{v}_n, \mathbf{u}_n) \mapsto a_n(\mathbf{v}_n, \mathbf{u}_n)$ which discretize the original bilinear form $a(1; \cdot, \cdot)$ [7,8]. These forms can be expressed as the sums of backward/forward finite difference formulæ with various step sizes.

Construction of discretizations A_n with the compartmental structure for $d \geq 3$ is based on the reduction to two-dimensional problems, and one can prove [7,8]:

THEOREM 4.1 *Let Assumption 4.1 be valid. There exists $n_0 \in \mathbb{N}$ such that for $n \geq n_0$ the discretizations A_n are symmetric matrices having the compartmental structure.*

The differential operator $L(\mathbf{x}) = \sum b_i(\mathbf{x})\partial_i$ is discretized on G_n by matrices L_n which are obtained by applying the standard upwind scheme to each grid-knot $\mathbf{x} \in G_n$. If the functions b_i are constant, then the obtained discretizations $A_n + L_n$ have the compartmental structure. For a general vector valued function \mathbf{b} the matrices $A_n + L_n$ do not have the compartmental structure. In this article $\operatorname{div} \mathbf{b} = 0$, so that the column sums of $A_n + L_n$ can have negative values converging to zero as $n \rightarrow \infty$. If A_n^{-1} exists, then the transpose $A_n^T + L_n^T$ is an M -matrix, implying $A_n^{-1} \geq 0$.

5 CONVERGENCE OF APPROXIMATE SOLUTIONS

Let $\lambda = 0$, and let the linear boundary value problem (3) be discretized by systems (6), $A_n \mathbf{u}_n = \boldsymbol{\mu}_n$, where A_n have the compartmental structure. The discretizations $\boldsymbol{\mu}_n \in l(G_n(D))$ of a measure $\mu \in \mathcal{R}(D)$ are defined by $\mu_{\mathbf{k}} = \|\phi_{\mathbf{k}}\|_1^{-1} \langle \phi_{\mathbf{k}} | \mu \rangle \phi_{\mathbf{k}}$. The following result holds [7,8]:

THEOREM 5.1 *Let $D \subset \mathbb{R}^d$ be a bounded domain with a Lipschitz boundary, and let $\mathfrak{U} = \{u(n) : n \in \mathbb{N}\} \subset E_n(D)$ be a sequence of approximate solutions, $u(n) = \Phi_n \mathbf{u}_n$, where \mathbf{u}_n are grid-solutions to Problem (6). For each $p \in [1, d/(d-1))$ there exists a subset $J(p) \subset \mathbb{N}$ such that $\mathfrak{U}' = \{u(n) : n \in J(p)\}$ converges to the unique solution of (3), strongly in $L_p(D)$ and weakly in $\dot{W}_p^1(D)$.*

Here we consider nonlinear BVPs for which $b_i = 0, i = 1, 2, \dots, d$ on D . We do not know results on the existence of solutions to (4) with non-trivial functions b_i and a Radon measure on the right hand side. In the case of $b_i = 0$ nonlinear problems (4) can be rewritten by using an equivalent formulation for which the main part of differential operator is u -independent. The transformation is realized by using the substitution $w = u^{1+\alpha}$ and formulating the problem for w . The new form $(v, u) \mapsto a(u; v, u)$ is now defined by $a(u; v, u) = (1 + \alpha)^{-1} \langle v | A_0 u \rangle + \langle v | L u^{1/(1+\alpha)} \rangle$ and the new problem (4) has a simpler expression. It is discretized by systems $A_n(\mathbf{u}_n) \mathbf{u}_n = \boldsymbol{\mu}_n$ for which the system matrix is such that discretizations of $A_0(\mathbf{x})$ have the form $D_n - B_n$, where D_n are positive diagonal matrices and B_n are non-negative off-diagonal matrices defined by (8) and (9). The lower order differential operator is discretized by a nonlinear function of \mathbf{u}_n resulting in a non-negative diagonal

matrix $L(\mathbf{u}_n)$. Then the systems $A_n(\mathbf{u}_n)\mathbf{u}_n = \boldsymbol{\mu}_n$ are solved by iterations:

$$\left(D_n + L_n(\mathbf{u}_n(k))\right) \mathbf{u}_n(k+1) = B_n \mathbf{u}_n(k) + \boldsymbol{\mu}_n, \quad (10)$$

where the initial iteration $\mathbf{u}_n(0) \geq \mathbf{0}$ is known in advance. This implies $\mathbf{u}_n(k) > 0$ on $G_n(D)$.

THEOREM 5.2 *Let D be a bounded domain with a Lipschitz boundary and $\boldsymbol{\mu}_n$ be discretizations of a positive Radon measure with the support in D . For each $p \in (1, d/(d-1))$ there exists a constant $\rho(p)$ such that the approximate solutions $u(n) = \Phi_n \mathbf{u}_n$ have the property $\|u(n)\|_{p,1} \leq \rho(p)$. The sequence $\mathfrak{U} = \{u(n) : n \in \mathbb{N}\} \subset E_n(D)$ has a subsequence \mathfrak{U}' converging to a solution of (4), strongly in $L_p(D)$ and weakly in $\dot{W}_p^1(D)$.*

PROOF: In the first step of proof we derive the inequality $\|u(n)\|_{p,1} \leq \rho(p)$ implying the existence of a weakly convergent subsequence \mathfrak{U}' . In the second step we demonstrate that the weak limit of \mathfrak{U}' is a weak solution to (4).

A bound on $\|\mathbf{u}_n\|_p$ is derived from the representation of grid solution $\mathbf{u}_n = A_n^{-1}\boldsymbol{\mu}_n - A_n^{-1}L_n(\mathbf{u}_n)$ which follows directly from (6). From this representation we have

$$\langle \mathbf{v}_n | \mathbf{u}_n \rangle = \langle \mathbf{v}_n | A_n^{-1} \boldsymbol{\mu}_n \rangle - \langle \mathbf{v}_n | A_n^{-1} L_n(\mathbf{u}_n) \rangle. \quad (11)$$

Due to $\boldsymbol{\mu}_n \geq \mathbf{0}$ on $G_n(D)$ we have also $\mathbf{u}_n \geq \mathbf{0}$. Let us consider the grid-function \mathbf{v}_n defined by values at grid-knots as follows: $v_{\mathbf{k}} = h^{-d/q} u_{\mathbf{k}}^{p-1} / \|\mathbf{u}_n\|_p^{p-1}$, where $1/p + 1/q = 1$. Then $h^d \|\mathbf{v}_n\|_q^q = 1$ and $\langle \mathbf{v}_n | \mathbf{u}_n \rangle = h^{-d/q} \|\mathbf{u}_n\|_p$. In order to estimate two terms on the right hand side of (11) we need a bound of $\|A_n^{-1} \mathbf{v}_n\|_\infty$. From Corollary 6.1 in [8] we have the following result. For $q > d$ the grid-functions $\mathbf{w}_n = A_n^{-1} \mathbf{v}_n$ are bounded on G_n uniformly with respect to n , i.e. $\|\mathbf{w}_n\|_\infty \leq \beta$ where β is a positive number which does not depend on n . An immediate consequence of this result is $\langle \mathbf{v}_n | A_n^{-1} \boldsymbol{\mu}_n \rangle \leq \beta \|\boldsymbol{\mu}_n\|_1$. Similarly we have $|\langle \mathbf{v}_n | A_n^{-1} L_n(\mathbf{u}_n) \rangle| \leq \beta \|L_n(\mathbf{u}_n)\|_1$ and we must find out an upper bound on $\|L_n(\mathbf{u}_n)\|_1$. Let \bar{c} be the supremum of values $c(\mathbf{x})$ in (1). Then $\|L_n(\mathbf{u}_n)\|_1 \leq \bar{c} \sqrt{\|\mathbf{u}_n\|_1}$. By using the Hölder inequality we get $\|\sqrt{\|\mathbf{u}_n\|_1}\|_1 \leq \|\mathbf{u}_n\|_p^{1/2} N^{(2p-1)/(2p)}$, where N is the number of grid-knots in $G_n(D)$. From $h^d N < |D|$ we get a desired bound $|\langle \mathbf{v}_n | A_n^{-1} L_n(\mathbf{u}_n) \rangle| \leq \bar{c} \beta h^{-d(2p-1)/(2p)} |D|^{(2p-1)/(2p)} \|\mathbf{u}_n\|_p^{1/2}$. After inserting the obtained bounds into (11) we get the inequality:

$$h^{-d/q} \|\mathbf{u}_n\|_p \leq \beta \|\boldsymbol{\mu}_n\|_1 + \bar{c} \beta h^{-d(2p-1)/(2p)} |D|^{(2p-1)/(2p)} \|\mathbf{u}_n\|_p^{1/2}.$$

This inequality must be multiplied by h^d in order to get $h^{d/p} \|\mathbf{u}_n\|_p < \rho(p)$ where $\rho(p)$ depends on $p, |D|, \mu(D)$ and \bar{c} . To finish the proof on the boundedness of $u(n) = \Phi_n \mathbf{u}_n$ in $L_p(D)$ one has to utilize the inequality $\|u(n)\|_p \leq h^{d/p} \|\mathbf{u}_n\|_p$. A similar proof can be carried out for $U_i \mathbf{u}_n$. Thus the existence of a weak limit $u = \lim_{J(p)} u(n)$ in $\dot{W}_p^1(D)$ for some $J(p) \subset \mathbb{N}$ is proved. Let \mathbf{f}_n be the discretizations of a function $f \in \dot{C}^{(1)}(\bar{D})$. Then

$$h^d \langle \mathbf{f}_n | A_n \mathbf{u}_n \rangle + h^d \langle \mathbf{f}_n | L_n(\mathbf{u}_n) \rangle = h^d \langle \mathbf{f}_n | \boldsymbol{\mu}_n \rangle.$$

The weak consistency [8], Section 6., implies $\lim_{J(p)} h^d \langle \mathbf{f}_n | A_n \mathbf{u}_n \rangle = a(f, u)$. The remaining two terms converge obviously to $\langle f | L(u) \rangle$ and $\langle f | \mu \rangle$, respectively. Hence, u is a solution to (4). **QED**

For nonlinear IVP which are defined by (5) results on the existence of solution are given in Theorem 3.2. Various numerical methods are described in [9], Chapter 4. One of such methods, a discretization of (5) by a system of nonlinear ODE, is utilized in the next section.

6 EXAMPLES

To test the method numerically we need examples in which we know solutions in closed forms. However, it is not easy to construct a single example demonstrating all of the important properties of this numerical method. We thus give two examples in \mathbb{R}^2 , in the first one we consider a boundary value problem for a diffusion-reaction operator with nonlinearity in the reaction term, and in the second one an IVP with a measure on the right hand side. The differential operators are the same in both examples, as well as the diffusion tensor $a(\mathbf{x}) = \begin{pmatrix} 10 & 2 \\ 2 & 1 \end{pmatrix}$. Because $a_{22} < a_{12} < a_{11}$ a monotone scheme can be obtained by applying methods of Section 4 with a non-trivial choice of parameters $\mathbf{r}(\mathbf{x})$. Examples are constructed by supposing solutions, applying the operators to supposed solutions and calculating the right hand sides. The calculated right hand sides are Radon measures, unfortunately, having both signs. They have the structure as demanded by Theorem 3.2. For examples with a diffusion with jumps, for the linear problem, see [6–8].

Next we compare numerical solutions to the solutions in the closed form in terms of $l_1(G_n(D))$ and $l_\infty(G_n(D))$ -norms, denoted by $\|\cdot\|_1, \|\cdot\|_\infty$, respectively. The values of solutions at grid-knots $u^*(\mathbf{x}_i), \mathbf{x}_i \in G_n(D)$ determine the grid-solutions \mathbf{u}^* with components $u^*(\mathbf{x}_i)$. In both examples numerical grid-solutions \mathbf{u} are compared with \mathbf{u}^* by measuring the relative error:

$$\varepsilon_1 = \frac{\|\mathbf{u} - \mathbf{u}^*\|_1}{\|\mathbf{u}^*\|_1}, \quad \varepsilon_\infty = \|\mathbf{u} - \mathbf{u}^*\|_\infty. \quad (12)$$

Table 1
Numerical results for the examples

	h	ε_1	ε_∞	K	t
BVP	5×10^{-3}	0.04	0.009	1.2×10^4	
BVP	2.5×10^{-3}	0.005	0.002	9.1×10^4	
IVP	5×10^{-3}	0.004	0.003	5.9×10^4	0.15
IVP	2.5×10^{-3}	0.003	0.002	1.9×10^5	0.11

EXAMPLE 6.1 (Nonlinear elliptic problem) The boundary value problem is defined on the domain $D = (-1/2, 1/2) \times (-1/2, 1/2)$, and the differential operator is defined by $u(\mathbf{x}) \mapsto A(u(\mathbf{x}))u(\mathbf{x}) = -2 \sum_{i,j} \partial_i a_{ij} u(\mathbf{x}) \partial_j u(\mathbf{x}) + cu(\mathbf{x})$, where c is a positive constant. The problem $A(u(\mathbf{x}))u(\mathbf{x}) = \mu(\mathbf{x})$ with the homogeneous Dirichlet boundary condition on ∂D can be transformed to an equivalent nonlinear problem:

$$- \sum_{i,j=1}^2 \partial_i a_{ij} \partial_j u(\mathbf{x}) + c \sqrt{u(\mathbf{x})} = \mu(\mathbf{x}), \quad \mathbf{x} \in D, \quad (13)$$

where μ , c and boundary conditions are as before.

Let $z \mapsto \phi(z)$ be the hat function at zero with the unit support and $u(x_1, x_2) = \phi(x_1)\phi(x_2)$. For the differential operator $A(\mathbf{x}) = -\sum_{i,j} \partial_i a_{ij} \partial_j + c\sqrt{u(\mathbf{x})}$ we have $A(\mathbf{x})u(\mathbf{x}) = \mu(\mathbf{x})$ where the measure μ is defined in terms of δ -functions: $\mu(\mathbf{x}) = 20 \delta(x_1) \phi(x_2) + 2 \delta(x_2) \phi(x_1) - 4 \text{sign}(x_1)\text{sign}(x_2) + c \phi(x_1)^{1/2} \phi(x_2)^{1/2}$. Obviously, μ is a Radon measure and u is a solution to (13). Since the operator $u \mapsto A(u)u$ is monotone for non-negative functions, the solution u is unique.

Now we apply the developed monotone scheme of Section 5 to Problem (13) where the parameters of the scheme are $r_1 = 3, r_2 = 1$. The discretized problems with the compartmental matrix $\mathbf{u} \mapsto A_n(\mathbf{u})$ are solved by iterations. We write $A_n(\mathbf{u})\mathbf{u} = D_n\mathbf{u} - B_n\mathbf{u} + c\sqrt{\mathbf{u}}$ where D_n and B_n are described in Section 4, and $\sqrt{\mathbf{u}}$ is the grid-function with components $\sqrt{(\mathbf{u})_i}, i \in J_n(D)$. The entries of D_n are denoted by d_{ii} . The iterations are defined by

$$\mathbf{u}(k+1) = F_n(\mathbf{u}(k)) (B_n\mathbf{u}(k) + \boldsymbol{\mu}_n),$$

where $\mathbf{v} \mapsto F_n(\mathbf{v})$ is a diagonal matrix with the entries $\sqrt{v_i}/(c + \sqrt{v_i}d_{ii})$. The scheme is monotone and produces $\mathbf{u}(k) \geq \mathbf{0}$ for $\boldsymbol{\mu}_n \geq \mathbf{0}$. In our case $\boldsymbol{\mu}_n$ has components with both signs, but nevertheless $\mathbf{u}(k) \geq \mathbf{0}$.

We specify $c = 5$ in (13) and discretize the domain D by choosing the spatial step sizes $h = 1/200$ and $h = 1/400$. The comparison with exact solution in

terms of relative errors (12) is given in Table 1. The number of iterations K is also given in Table 1.

EXAMPLE 6.2 (Nonlinear parabolic problem) Here we consider an IVP of the form (5) with the differential operator as in Example 6.1. For a non-negative initial condition and μ as in Example 6.1, we get asymptotically $u(t) \rightarrow u_\infty$, where $u_\infty(\mathbf{x}) = \phi(x_1)^{1/2}\phi(x_2)^{1/2}$. A numerical test of this fact is carried out by using the same discretizations of D, μ and $A(\mathbf{x})$ as in the previous example. The time discretization is carried out by using Forward Euler method with a temporal grid size of the same order as the CFL-condition. The scheme is:

$$\mathbf{u}(k+1) = F_n(\mathbf{u}_+(k)) \mathbf{u}(k) + \tau B_n \mathbf{u}(k)^2 + \tau \boldsymbol{\mu}_n,$$

where $u_+ = \max\{u, 0\}$, and $\mathbf{v} \mapsto F_n(\mathbf{v})$ is the diagonal matrix with entries $1 - \tau d_{ii} v_i - \tau c$ and the temporal step size is generally variable. Thus for $h = 1/400$ and larger values of k we have $\tau = 10^{-6}$. Since the scheme is monotone, grid-solutions are non-negative for $\boldsymbol{\mu}_n \geq \mathbf{0}$. In our case the grid-functions $\boldsymbol{\mu}_n$ have components with both signs. Still, grid-solutions are positive asymptotically on $G_n(D)$, *i.e.* for larger value of k we have $\mathbf{u}(k) > \mathbf{0}$ on $G_n(D)$.

Some results are given in Table 1 for times t which are written in the last column of table. After the specified time t further iterations do not change the numerical solution $u(n, t_k, \cdot) = \Phi_n \mathbf{u}(k)$, $t_k = \sum_{j \leq k} \tau_j$, *i.e.* the numerical asymptotic value is reached for the given times t .

In the above two examples nonlinear algebraic systems (NLS) and ODE which result in the process of discretizations of respective BVPs and IVPs have system matrices A_n of the order $N_{sys} = h^{-2}$ where h is the spatial step size. The matrices A_n are band matrices with bandwidth $\approx 1/h$. For $h = 1/400$ we get $N_{sys} > 1.5 \times 10^5$ with bandwidth > 400 . This fact forced us to use iterative methods in solving NLS and explicit methods in solving ODE. An implicit method or a mixed method based on the band structure of A_n is difficult to apply to ODE with system matrices of such huge order, unless there is enough information on the sparsity structure of the system matrix. However, the sparsity is influenced by the diffusion tensor, thus performing fast LU-decomposition does not seem to be easy. At the present level of our knowledge we do not know how to implement an efficient implicit method on a single processor machine to problems involving non-homogeneous diffusion on arbitrary domains. On parallel architectures the possibility of constructing such methods should be a matter of further research.

7 DISCUSSION

Monotone schemes in Section 4 are constructed in terms of system matrices A_n . For bounded domains these matrices are simultaneously M-matrices and compartmental matrices. We give the construction for linearized problems, in such a way that they can be applied in computation of solutions to nonlinear PDE by iterations. In the case of dimension $d = 2$, we can apply the proposed monotone schemes to problems with a general diffusion coefficients $a_{ij}(\mathbf{x})$, whereas for $d \geq 3$ this can be done only if an additional condition holds, as formulated in the Assumption 4.1. If this condition breaks down, we can still make use of the schemes after the rotation of coordinates, but this possibility was not analyzed here. Although we analyze schemes for PDE with nonlinear diffusion, we can also apply them to PDE with linear diffusion and nonlinear lower order differential operators. In this case, we must discretize the lower order operators by upwinding.

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