



# Domain decomposition multigrid methods for nonlinear reaction–diffusion problems



A. Arrarás<sup>a</sup>, F.J. Gaspar<sup>b</sup>, L. Portero<sup>a,\*</sup>, C. Rodrigo<sup>b</sup>

<sup>a</sup>Departamento de Ingeniería Matemática e Informática, Universidad Pública de Navarra, Edificio de Las Encinas, Campus de Arrosadía, 31006 Pamplona, Spain  
<sup>b</sup>IUMA, Departamento de Matemática Aplicada, Universidad de Zaragoza, Pedro Cerbuna 12, 50009 Zaragoza, Spain

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## ABSTRACT

In this work, we propose efficient discretizations for nonlinear evolutionary reaction–diffusion problems on general two-dimensional domains. The spatial domain is discretized through an unstructured coarse triangulation, which is subsequently refined via regular triangular grids. Following the method of lines approach, we first consider a finite element spatial discretization, and then use a linearly implicit splitting time integrator related to a suitable decomposition of the triangulation nodes. Such a procedure provides a linear system per internal stage. The equations corresponding to those nodes lying strictly inside the elements of the coarse triangulation can be decoupled and solved in parallel using geometric multigrid techniques. The method is unconditionally stable and computationally efficient, since it avoids the need for Schwarz-type iteration procedures. In addition, it is formulated for triangular elements, thus yielding much flexibility in the discretization of complex geometries. To illustrate its practical utility, the algorithm is shown to reproduce the pattern-forming dynamics of the Schnakenberg model.

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## 1. Introduction

Let us consider the nonlinear evolutionary reaction–diffusion equation

$$u_t = \nabla \cdot (D\nabla u) + r(u) + f, \quad \text{in } \Omega \times (0, T], \quad (1)$$

where  $\Omega \subset \mathbb{R}^2$  is a bounded, open, polygonal domain with boundary  $\Gamma$ . Here, we seek for  $u(\mathbf{x}, t)$ , provided that a symmetric and positive definite diffusion tensor  $D(\mathbf{x})$ , a nonlinear reaction term  $r(u)$ , and a source/sink term  $f(\mathbf{x}, t)$  are given. The equation is supplemented with the initial condition

$$u = u_0, \quad \text{in } \Omega \times \{0\} \quad (2)$$

and the boundary conditions

$$u = g_1, \quad \text{on } \Gamma_D \times (0, T], \quad (3a)$$

$$\nabla u \cdot \mathbf{n} = g_2, \quad \text{on } \Gamma_N \times (0, T], \quad (3b)$$

where  $\mathbf{n}$  is the outward unit normal vector to  $\Gamma$ . The Dirichlet and Neumann boundaries are denoted by  $\Gamma_D$  and  $\Gamma_N$ , respectively, and satisfy  $\Gamma = \overline{\Gamma_D} \cup \overline{\Gamma_N}$  and  $\Gamma_D \cap \Gamma_N = \emptyset$ .

\* Corresponding author.

E-mail addresses: [andres.arraras@unavarra.es](mailto:andres.arraras@unavarra.es) (A. Arrarás), [fjgaspar@unizar.es](mailto:fjgaspar@unizar.es) (F.J. Gaspar), [laura.portero@unavarra.es](mailto:laura.portero@unavarra.es) (L. Portero), [carmenr@unizar.es](mailto:carmenr@unizar.es) (C. Rodrigo).

Reaction–diffusion problems of the form (1)–(3) are typically related to dissipative dynamical systems modeling physical, chemical and biological phenomena. In particular, they have been used along the years to model chemical systems or population dynamics (see, e.g., [29,30,47]). A classical example is given by the Fisher equation, for which  $r(u) = \beta u(1 - u)$  and  $f \equiv 0$ , with  $\beta > 0$ , first proposed as a one-dimensional model for the propagation of a mutant gene (cf. [13]). The extension to systems of partial differential equations (PDEs) involving  $m$  equations of the form (1) in the unknown  $u_i$ , for  $i = 1, 2, \dots, m$ , is studied in [1,18,28,37,39], among others. If each of these unknowns represents the concentration of a chemical species, and the equations are coupled in the nonlinear reaction terms, then spatial patterns of chemical concentrations may develop under certain conditions. Such pattern-forming dynamics provides a possible explanation for the evolution of pattern and form in developmental biology (cf. [30,43,48]). In the sequel, for the sake of clarity in the exposition, we shall be concerned with the scalar Eq. (1). The behaviour of systems of PDEs will be illustrated by the simulation of the Schnakenberg model (cf. [39]) at the end of the paper.

In the present work, we propose efficient discretizations for the problem (1)–(3) that suitably combine non-iterative domain decomposition techniques and geometric multigrid methods. To this end, using the method of lines approach, we first formulate a finite element spatial discretization of the given problem on so-called block-structured triangular grids. This type of grids is generated by first considering an unstructured coarse triangulation  $\mathcal{T}_0$  of  $\Omega$ , and then refining its elements via regular triangular meshes to obtain a fine triangulation  $\mathcal{T}_h$ . The use of block-structured grids permits to consider complex geometries and to deal with problems that contain abrupt variations in the material properties (i.e., jump discontinuities in the diffusion coefficients).

The continuous-in-time semidiscrete scheme is a nonlinear system of stiff ordinary differential equations (ODEs) of the form

$$U'_h = A_h U_h + R_h(U_h) + F_h, \quad (4)$$

where  $A_h U_h$  and  $R_h(U_h)$  represent the semidiscrete diffusion and reaction terms, respectively,  $F_h$  is a suitable approximation to  $f$ , and the initial datum  $U_h(0) \approx u_0(\mathbf{x})$  is given. Note that the stiffness of the system (4) is mainly due to the presence of the diffusion operator  $A_h$ . As a result, an efficient integration of such a system may be achieved by using a so-called linearly implicit method, which considers an implicit contribution of the linear diffusion term, while explicitly treating the nonlinear reaction term. Although (4) is nonlinear, this strategy yields a linear system to be solved at each internal stage. Previous works on linearly implicit time integrators can be found in [2,7,8]. Note that this class of methods is closely related to the so-called implicit–explicit (IMEX) schemes, which have also been studied in the framework of convection–diffusion (cf. [3,4]) and reaction–diffusion (cf. [37]) problems.

In this work, we take a step forward and further consider a suitable splitting of the implicit part and the source/sink term, thus obtaining a so-called linearly implicit splitting scheme (cf. [12]). More precisely, we split both  $A_h$  and  $F_h$  into two sub-terms, which are related to a decomposition of the fine triangulation  $\mathcal{T}_h$  into two sets of nodes: (a) those lying strictly inside the elements of  $\mathcal{T}_0$ ; and (b) those lying on the edges of  $\mathcal{T}_0$ . Since the equations corresponding to the first set of nodes decouple across the elements of  $\mathcal{T}_0$ , they can be solved in parallel using geometric multigrid techniques.

Multigrid methods are well known to be among the fastest numerical algorithms for solving the algebraic equations arising from the discretization of PDEs. They are mainly based on the acceleration of convergence of common iterative methods by using solutions obtained on coarser levels as corrections. There are two basic approaches to multigrid solvers, namely, algebraic multigrid (cf. [36]) and geometric multigrid (cf. [42]). In the former, no information is used concerning the grid on which the governing PDE is discretized; in the latter, a hierarchy of grids must be used. Algebraic multigrid is capable of handling large problems with irregular structure, but geometric multigrid always has a lower cost per iteration, because of its ability to take advantage of the geometry within the used data structures. The performance of these methods strongly depends on the choice of their components. For each particular problem, they have to be carefully chosen by taking into account the main features of the equations under consideration. Consequently, when dealing with new applications, it is always a challenge to find the most suitable ones. In this context, the local Fourier analysis (LFA) has been shown to be a helpful technique to facilitate this demanding task (cf. [15,16]). In this work, we shall introduce a specific geometric multigrid method that is designed to take advantage of the block structure of the triangulation  $\mathcal{T}_h$  (cf. [34]). To this end, suitable components will be chosen on each structured patch of the grid with the help of the LFA.

The proposed domain decomposition multigrid algorithm belongs to the class of non-iterative domain decomposition methods, which have been previously studied by several authors in the context of parabolic problems (see, e.g., [27,31,38,44,45] in the overlapping case, and [10,11,14,21,22,40,49–51] in the non-overlapping case). To be precise, we formulate a non-overlapping domain decomposition scheme that extends the ideas discussed in [46] for linear diffusion equations on rectangular meshes to the case of nonlinear reaction–diffusion problems on triangular grids. Unlike classical domain decomposition schemes (cf. [33]), this technique does not involve any Schwarz iteration procedure, thus reducing the computational cost of the overall solution process.

The rest of the paper is organized as follows. In Section 2, we describe the construction of a block-structured triangular grid and formulate the finite element spatial discretization of the given problem. The time integration is addressed in Section 3, where we introduce a domain decomposition operator splitting for both  $A_h$  and  $F_h$ , and consider a two-component linearly implicit splitting formula. Section 4 is devoted to the solution of the linear systems arising in the fully discrete scheme via a suitable geometric multigrid approach. This technique considers different components depending on the

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