

# DOMAIN DECOMPOSITIONS METHODS FOR REACTION-DIFFUSION SYSTEMS

by

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# ABSTRACT

Domain Decomposition (**DD**) methods have been successfully used to solve elliptic problems, as they deal with them in a more elegant and efficient way than other existing numerical methods. This is achieved through the division of the domain into subdomains, followed by the solving of smaller problems within these subdomains which leads to the solution. Furthermore **DD**-techniques can incorporate in their implementation not only the physics of the different phenomena associated with the modeling, but also the enhancement of parallel computing. They can be divided into two major categories: with and without overlapping. The most important factor in both cases is the ability to solve the interface problem referred to as the Steklov-Poincaré problem . There are two existing approaches to solving the interface problem. The first approach consists of approximating the interface problem by solving a sequence of subproblems within the subdomains, while the second approach aims to tackle the interface problem directly. The solution method presented in this thesis falls into the latter category.

This thesis presents a non-overlapping domain decomposition (**DD**) method for solving reaction-diffusion systems. This approach addresses the problem directly on the interface which allows for the presentation and analysis of a new type of interface preconditioner for the arising Schur complement problem. This thesis will demonstrate that the new interface preconditioner leads to a solution technique independent of the mesh parameter. More precisely, the technique, when used effectively, exploits the fact that the Steklov-Poincaré

operators arising from a non-overlapping **DD**-algorithm are coercive and continuous, with respect to Sobolev norms of index  $1/2$ , in order to derive a convergence analysis for a **DD**-preconditioned GMRES algorithm. This technique is the first of its kind that presents a class of substructuring methods for solving reaction diffusion systems and analyzes their behaviour using fractional Sobolev norms. All the results presented have been published in [37](linear case only), and submitted in [36](general case) for reviewing.

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# CHAPTER 1

## INTRODUCTION

Reaction-diffusion models were introduced in 1930 by Fischer [23] in the context of models for the spatial spread of an advantageous gene. Since then reaction-diffusion systems have attracted a considerable amount of scientific interest. One of the main reasons for the large amount of research dedicated to reaction-diffusion systems is their use for modeling within various fields including chemistry, biology, medicine, genetics, physics and social science [48, 57, 69, 76, 55, 15, 22, 55]. Reaction-diffusion models are generally represented as a system of nonlinear PDE:

$$\left\{ \begin{array}{l} \frac{\partial \mathbf{u}}{\partial t} = \mathbf{D}\Delta \mathbf{u} + \mathbf{f}(\mathbf{u}) \quad \text{in } \Omega, \\ \mathbf{n} \cdot (\nabla \mathbf{u}) = \mathbf{0} \quad \text{on } \partial\Omega_N, \\ \mathbf{u} = \mathbf{g} \quad \text{on } \partial\Omega_D, \\ \mathbf{u}(x, 0) = \mathbf{u}_0(x) \quad \text{for } x \in \Omega, \end{array} \right. \quad (1.1)$$

where  $\partial\Omega = \partial\Omega_D \cup \partial\Omega_N$  denotes the boundary of  $\Omega$ ,  $\mathbf{u}$  is a vector of morphogen concentrations,  $\Delta$  is the Laplace operator,  $\mathbf{f}$  is a smooth function of reaction kinetics and  $\mathbf{D}$  is a diagonal matrix with positive constant diffusion coefficients. Qualitatively speaking, the system (1.1) describes the variation of the concentration of one or more substances over time and space under the influence of two terms: a diffusion term and a nonlinear

interaction term.

One of the main features of reaction-diffusion systems is that the combination of these terms leads to the possibility of threshold phenomena, such as multiple steady states [69], spatiotemporal patterns, oscillating solutions and chaos [75, 71]. Reaction-diffusion models are generally too complex to solve analytically, therefore it becomes important to look for an efficient and accurate numerical solution. However obtaining a numerical solution for reaction-diffusion systems remains a challenging task, as they are often applied to high dimensional exotic domains [80] and require a good understanding of many areas of mathematics, such as bifurcation and stability theories, semigroup theory, singular perturbations and numerical analysis.

## 1.1 Theoretical formulation

The following reaction-diffusion system is the central problem on which this research study is based:

$$\begin{cases} -D\Delta\mathbf{u} + M\mathbf{u} = \mathbf{f} & \text{in } \Omega, \\ \mathbf{n} \cdot (\nabla\mathbf{u}) = \mathbf{0} & \text{on } \partial\Omega_N, \\ \mathbf{u} = \mathbf{g} & \text{on } \partial\Omega_D, \end{cases} \quad (1.2)$$

where:

$$\mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}, \quad M = \begin{pmatrix} \alpha_1(x, y) & \beta_1(x, y) \\ \beta_2(x, y) & \alpha_2(x, y) \end{pmatrix}, \quad \mathbf{f} = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}, \quad \text{and } D = \begin{pmatrix} d_1 & 0 \\ 0 & d_2 \end{pmatrix},$$

and  $\Omega \subset \mathbb{R}^2$  is an open simply-connected domain with boundary  $\partial\Omega$  in  $\mathbb{R}^2$ . The problem is outlined more extensively within Chapter 4. While the equation (1.2) represents the steady-state solution to the general system of (1.1), it can also represent the system

arising from the time stepping routine which results from the discretization of problem (1.1) over time. The numerical solution of reaction-diffusion problems remains a challenge as they often arise as a system containing multiple and interconnected nonlinear partial differential equations that are solved on a complex domain. Such a problem arises, for example, in mathematical models of spatial and temporal behaviour of interacting species or reactants in ecological or chemical systems [57], in the mathematical modeling of behaviour of an open system in which the transport of reactants and products relies on molecular diffusion processes [34] and for mathematical modeling of the dorsal-ventral pattern during the zebrafish embryo development [69].

Additionally, when looking for a numerical solution, one should not only take into consideration the complexity of each domain and the physics of the phenomena associated with the modeling but also exploit the emergence of parallel computing for the numerical solution as this leads to faster and more efficient algorithms. Domain decomposition (DD) methods fall into this category.

## 1.2 A domain decomposition approach

In this dissertation, the solution of problem (1.2) is obtained using a non-overlapping domain decomposition method. More precisely the domain  $\Omega$  is partitioned into  $N$  subdomains without overlap such that:

$$\bar{\Omega} = \bigcup_{i=1}^N \bar{\Omega}_i, \quad \Omega_i \cap \Omega_j = \emptyset \ (i \neq j), \quad \Gamma_i = \partial\Omega_i \setminus \partial\Omega, \quad \Gamma = \bigcup_{i=1}^N \Gamma_i.$$

It will be shown in Chapter 7 that the domain decomposition formulation of (1.2) yields a sequence of two decoupled sets of problems involving the same operator  $\mathcal{L} = -D\Delta + M$ , with essential boundary conditions on each subdomain, together with a problem set on

the interface  $\Gamma$ :

$$\left\{ \begin{array}{l} \mathcal{L}\mathbf{w}_i = \mathbf{f} \text{ in } \Omega_i, \\ \mathbf{w}_i = \mathbf{0} \text{ on } \partial\Omega_i \cap \partial\Omega_D, \\ \mathbf{n} \cdot \nabla \mathbf{w}_i = \mathbf{0} \text{ on } \partial\Omega_i \cap \partial\Omega_N, \\ \mathbf{w}_i = \mathbf{0} \text{ on } \Gamma_i, \end{array} \right. \quad (1.3a)$$

$$\left\{ \begin{array}{l} \mathcal{S}\boldsymbol{\lambda} = -\sum_{i=1}^N \mathbf{n}_i \cdot \nabla \mathbf{w}_i \text{ on } \Gamma, \end{array} \right. \quad (1.3b)$$

$$\left\{ \begin{array}{l} \mathcal{L}\mathbf{v}_i = \mathbf{0} \text{ in } \Omega_i, \\ \mathbf{v}_i = \mathbf{0} \text{ on } \partial\Omega_i \cap \partial\Omega_D, \\ \mathbf{n} \cdot \nabla \mathbf{v}_i = \mathbf{0} \text{ on } \partial\Omega_i \cap \partial\Omega_N, \\ \mathbf{v}_i = \boldsymbol{\lambda}_i \text{ on } \Gamma_i. \end{array} \right. \quad (1.3c)$$

The variational formulation of (1.3a)-(1.3c) reads as follow (See Chapter 7 for more details)

$$\left\{ \begin{array}{l} \text{Find } \mathbf{w}_i \in H_D^1(\Omega_i) \times H_D^1(\Omega_i) \text{ such that for all } \mathbf{z}_i \in H_D^1(\Omega_i) \times H_D^1(\Omega_i) \\ \quad B_i(\mathbf{w}_i, \mathbf{z}_i) = (\mathbf{f}_i, \mathbf{z}_i), \quad \forall i = 1, \dots, N. \\ \\ \text{Find } \boldsymbol{\lambda} \in \Lambda \times \Lambda \text{ such that for all } \boldsymbol{\eta} \in \Lambda \times \Lambda \\ \quad \mathcal{S}(\boldsymbol{\lambda}, \boldsymbol{\eta}) := \langle \mathcal{S}\boldsymbol{\lambda}, \boldsymbol{\eta} \rangle = \sum_{i=1}^N [(\mathbf{f}_i, F_i \boldsymbol{\eta}_i) - B_i(\mathbf{w}_i, F_i \boldsymbol{\eta}_i)]. \\ \\ \text{Find } \tilde{\mathbf{v}}_i \in H_D^1(\Omega_i) \times H_D^1(\Omega_i) \text{ such that for all } \mathbf{z}_i \in H_D^1(\Omega_i) \times H_D^1(\Omega_i) \\ \quad B_i(\tilde{\mathbf{v}}_i, \mathbf{z}_i) = B_i(\mathbf{v}_i, \mathbf{z}_i) - B_i(\mathbf{t}_i, \mathbf{z}_i) = -B_i(\mathbf{t}_i, \mathbf{z}_i), \quad \forall i = 1, \dots, N. \end{array} \right.$$

A mixed finite element method is then used to discretize the above formulations. The finite element discretization of the domain decomposition (1.3a)-(1.3c) reads:

$$\left\{ \begin{array}{l} \text{Find } \mathbf{w}_{hi} \in V_{iI}^h \times V_{iI}^h \text{ such that for all } \mathbf{z}_i \in V_{iI}^h \times V_{iI}^h \\ B_i(\mathbf{w}_{hi}, \mathbf{z}_{hi}) = (\mathbf{f}_i, \mathbf{z}_{hi}), \quad \forall i = 1, \dots, N. \end{array} \right. \quad (1.5a)$$

$$\left\{ \begin{array}{l} \text{Find } \boldsymbol{\lambda}_h \in S^h \times S^h \text{ such that for all } \boldsymbol{\eta}_h \in S^h \times S^h \\ s(\boldsymbol{\lambda}_h, \boldsymbol{\eta}_h) := \langle \mathcal{S}\boldsymbol{\lambda}_h, \boldsymbol{\eta}_h \rangle = \sum_{i=1}^N [(\mathbf{f}_i, \boldsymbol{\eta}_{hi}) - B_i(\mathbf{w}_{hi}, \boldsymbol{\eta}_{hi})]. \end{array} \right. \quad (1.5b)$$

$$\left\{ \begin{array}{l} \text{Find } \tilde{\mathbf{v}}_{hi} \in V_{iI}^h \times V_{iI}^h \text{ such that for all } \mathbf{z}_{hi} \in V_{iI}^h \times V_{iI}^h \\ B_i(\tilde{\mathbf{v}}_{hi}, \mathbf{z}_{hi}) = -B_i(\mathbf{t}_{hi}, \mathbf{z}_{hi}), \quad \forall i = 1, \dots, N. \end{array} \right. \quad (1.5c)$$

One can show that the algebraic representations of subproblems (1.5a)-(1.5c) are given by:

$$A_{II}\mathbf{w}_I = \mathbf{f}_I,$$

$$S\mathbf{u}_\Gamma = \mathbf{f}_\Gamma - A_{\Gamma I}\mathbf{w}_I,$$

$$\mathbf{v}_I = A_{II}^{-1}A_{I\Gamma}\mathbf{u}_\Gamma,$$

respectively, where  $S := A_{\Gamma\Gamma} - A_{\Gamma I}(A_{II})^{-1}A_{I\Gamma}$  and  $\mathbf{u} = (\mathbf{w}_I + \mathbf{v}_I, \mathbf{u}_\Gamma)$  is the final solution.

This corresponds to the Schur-complement algorithm for following linear system:

$$A\mathbf{u} = \begin{pmatrix} A_{II} & A_{I\Gamma} \\ A_{\Gamma I} & A_{\Gamma\Gamma} \end{pmatrix} \begin{pmatrix} \mathbf{u}_I \\ \mathbf{u}_\Gamma \end{pmatrix} = \begin{pmatrix} \mathbf{f}_I \\ \mathbf{f}_\Gamma \end{pmatrix} = \mathbf{f} \quad (1.6)$$

If the chosen discretisation is stable, as defined in Chapter 5, then (1.6) has a unique solution. However, the system matrix  $A$  may be too large to be stored in the computer memory, making a direct method too expensive to use. Therefore it becomes convenient

to use iterative methods as they approximate the solution  $\mathbf{u}$  by computing a sequence of progressively accurate iterates using simple algebraic operations (matrix vector and vector products).

### 1.3 Iterative methods and preconditioning

For a large scale problem such as (1.6), it is necessary to use an iterative method together with a suitable preconditioning technique. Among the different iterative methods, the GMRES method was selected and combined with a right preconditioner. In this research study we exploit the coercivity and continuity of the Steklov-Poincaré operators arising in a non-overlapping **DD**-algorithm with respect to the Sobolev norm of index  $1/2$ . For this reason our preconditioner incorporates two sets of solutions:

- The solution of problems posed on the interior of each domain, which can be achieved in parallel using direct methods.
- The solution of a problem involving the discrete Steklov-Poincaré operator, which is approximated iteratively.

In Chapter 9, it will be seen that the following preconditioner:

$$P_R = \begin{pmatrix} A_{II} & A_{I\Gamma} \\ 0 & \mathbf{H}_{1/2} \end{pmatrix} \text{ with;}$$

where  $\mathbf{H}_{1/2}$  is the finite element matrix representation of the norm  $\| \cdot \|_{1/2}$  can be considered as a suitable preconditioner for the arising linear system. Using the above preconditioner, the following preconditioned system has been obtained:

$$AP_R^{-1} = \begin{pmatrix} I & 0 \\ A_{\Gamma I}A_{II}^{-1} & S\mathbf{H}_{1/2}^{-1} \end{pmatrix},$$

It will also be seen that the eigenvalues of  $S\mathbf{H}_{1/2}^{-1}$  are located in a region of the complex plane that does not depend on problem size and is also located in the right half-plane.

The GMRES method is then used to solve the linear system (1.6), from an initial guess  $\mathbf{u}_0$  and an initial residual  $\mathbf{r}_0 = A\mathbf{u}_0 - \mathbf{f}$ , so that after the  $m$  iterations, the correction vector  $\mathbf{z}_m$  from the *Krylov* subspace:

$$\mathcal{K}_m = \mathcal{K}(\mathbf{r}_0, A, m) = \text{span}\{\mathbf{r}_0, A\mathbf{r}_0, \dots, A^{m-1}\mathbf{r}_0\}$$

solves the following minimization problem:

$$\min_{\mathbf{z} \in \mathcal{K}_m} \|\mathbf{f} - A(\mathbf{u}_0 + \mathbf{z})\|. \quad (1.7)$$

Due to the changing nature of our preconditioner, the flexible GMRES (FGMRES) presented in [84] described by the Algorithm 1 has been exploited in our implementation.



```

begin
  Choose  $x_0$  and  $m$ . Define a  $(m + 1) \times m$  matrix  $H_m$  with entries  $h_{i,j} = 0$ .
  Compute  $r_0 = b - Ax_0, \beta = \|r_0\|_2, v_1 = r_0/\beta$ .
  for  $j = 1, \dots, m$  do
     $z_j := M_j^{-1}v_j, w := Az_j$ 
    for  $i = 1, \dots, j$  do
       $h_{i,j} := (w, v_i), w := w - h_{i,j}v_i$ 
    end
     $h_{j+1,j} = \|w\|_2, v_{j+1} = w/h_{j+1,j}$ .
  end
  Define  $Z_m := [z_1, \dots, z_m]$ .
  Compute  $x_m = x_0 + Z_m y_m$  where  $y_m = \operatorname{argmin}_y \|\beta e_1 - H_m y\|_2$  and
   $e_1 = [1, 0, \dots, 0]^T$ .
end

```

**Algorithm 1:** FGMRES: GMRES with variable Preconditioning

For an efficient implementation of the GMRES method the reader should refer to [66, 46].

## 1.4 Thesis overview

The thesis is organized as follows. **Chapter 2** and **Chapter 3** can be considered as the building blocks of this research, as they present all the mathematical tools used in this research to tackle reaction-diffusion problems. More precisely, **Chapter 2** outlines in a simple way some definitions and fundamental results from the field of functional analysis while **Chapter 3** describes the theoretical aspects of finite element methods. **Chapter 4** presents the mathematical aspect of reaction-diffusion systems. The first section of the chapter looks at the question of how reaction-diffusion systems arise as a model. The second section presents the derivation of the basic reaction-diffusion equation using Fick's Law and the last section discusses the question of the existence and the uniqueness of its solution. **Chapter 5** demonstrates the well-posedness of the mixed variational for-

mulation of the problem (1.2) in a natural choice of norm together with all the technical details.

**Chapter 6** can be considered as a natural continuation of **Chapter 5**, as it gives a rigorous presentation of some numerical schemes available to solve the problems arising from **Chapter 5**. **Chapter 7** to **Chapter 9** contain the main theoretical contributions of the thesis. **Chapter 7** presents a rigorous formulation of non-overlapping domain decomposition methods for reaction-diffusion systems. The Steklov-Poincaré operator is derived and studied together with various technical tools from functional analysis. In **Chapter 8** and **Chapter 9** we present and analyse different types of preconditioning approaches for solving the Schur complement problem arising from non-overlapping domain decomposition methods. While the preconditioners presented in **Chapter 8** are based on the standard technique of block matrix preconditioners of the Schur-complement for solving the linear system, the preconditioners described in **Chapter 9** are motivated by the fact that the Steklov-Poincaré operators arising in a non-overlapping **DD**-algorithm are coercive and continuous with respect to Sobolev norms of index  $1/2$  [5]. Here an innovative interface preconditioner for the Steklov-Poincaré operator together with the convergence analysis for the preconditioned GMRES can be found.

In **Chapter 10**, the theoretical results obtained through different test problems are validated together with experiments outside the theoretical framework presented. Finally, **Chapter 11** outlines the conclusions of the research study and summarizes other key aspects of the thesis.

# CHAPTER 2

## MATHEMATICAL BACKGROUND

The aim of this chapter is to outline some definitions and fundamental results from the field of functional analysis given in [49, 35, 18], which are used to elaborate this research study.

### 2.1 Definitions and notation

Let  $\Omega$  be an open domain  $\in \mathbb{R}^n$ . In addition, the set of independent variables is denoted by  $\mathbf{x} = x_i, i = 1, \dots, n$ .

**Definition 2.1.1** An  $n$ -tuple of  $\alpha = (\alpha_1, \dots, \alpha_n)$ ,  $\alpha_i \in \mathbb{N}$  is called a multi-index of order  $k := |\alpha| = \alpha_1 + \dots + \alpha_n$ . Let  $\mathbf{x} \in \mathbb{R}^n$ , the product  $x_1^{\alpha_1} \dots x_n^{\alpha_n}$  is denoted by  $\mathbf{x}^\alpha$  and  $D^\alpha = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \dots \partial x_n^{\alpha_n}}$  is the partial differential operator of order  $k = |\alpha|$ .

**Definition 2.1.2** Let  $\alpha$  be a multi-index of order  $k$ . The set of continuous, real-valued functions defined on  $\Omega$ , which are  $k$  times differentiable, is denoted by  $C^k(\Omega)$ :

$$C^k(\Omega) := \{u : \Omega \rightarrow \mathbb{R} \mid D^\alpha u \text{ continuous on } \Omega, \text{ for all } \alpha \text{ with } |\alpha| \leq k\}. \quad (2.1)$$

**Definition 2.1.3** Let  $1 \leq p < \infty$ , the set of real-valued functions whose absolute value

raised to the  $p^{\text{th}}$  power is integrable is defined by  $L^p(\Omega)$ :

$$L^p(\Omega) := \left\{ u(\mathbf{x}) : \Omega \rightarrow \mathbb{R} : \int_{\Omega} |u(\mathbf{x})|^p \, d\mathbf{x} < \infty \right\}.$$

$L^p(\Omega)$  spaces are Banach spaces when endowed with the norm:

$$\|u(\mathbf{x})\|_{L^p(\Omega)} := \left( \int_{\Omega} |u(\mathbf{x})|^p \, d\mathbf{x} \right)^{1/p}$$

This study is mainly concerned with the space  $L^2(\Omega)$ , which can be seen as a Hilbert space when endowed with the inner product:

$$\langle u, v \rangle_{L^2(\Omega)} = \int_{\Omega} u(x)v(x) \, d\mathbf{x}.$$

**Definition 2.1.4** Let  $\alpha$  be a multi-index of order  $k$ . The Sobolev space of order  $k$  is denoted by:

$$W^{k,p}(\Omega) := \{u \in L^p(\Omega) \mid D^{\alpha}u \in L^p(\Omega) \text{ for all } \alpha \text{ with } |\alpha| \leq k\}.$$

$W^{k,p}(\Omega)$  are Banach spaces when equipped with the norm:

$$\|u\|_{W^{k,p}(\Omega)} := \|u\|_{k,p,\Omega} := \|u\|_{k,p} := \left( \sum_{|\alpha| \leq k} \|D^{\alpha}u\|_{L^p(\Omega)}^p \right)^{1/p}, \quad 1 \leq p < \infty.$$

Spaces  $W^{k,2}(\Omega)$ , which are denoted by  $H^k(\Omega)$  arise naturally when solving PDEs. These spaces are classed as Hilbert when equipped with the inner product:

$$\langle u, v \rangle = \sum_{|\alpha| \leq k} \langle D^{\alpha}u, D^{\alpha}v \rangle_{L^2(\Omega)}.$$

and are by Definition ref kamdef Sobolev spaces. This research study is particularly concerned with the following Sobolev spaces:

$$H^1(\Omega) = \{v \in L^2(\Omega) : \|\nabla v\|_0 < \infty\},$$

endowed with the norm:

$$\|v\|_{H^1(\Omega)}^2 = \|v\|_{1,\Omega}^2 = |v|_{0,\Omega}^2 + |v|_{1,\Omega}^2 = \|v\|_{L^2(\Omega)}^2 + \|\nabla v\|_{L^2(\Omega)}^2;$$

with:

$$|v|_{1,\Omega}^2 := \sum_{j=1}^n \left\| \frac{\partial v}{\partial x_j} \right\|_{L^2(\Omega)}^2 = |\nabla v|_{0,\Omega}^2 = \|\nabla v\|_{L^2(\Omega)}^2.$$

We also define:

$$H_D^1(\Omega) = \{v \in H^1(\Omega) : v = 0 \text{ on } \partial\Omega_D\}.$$

Another space of interest is  $H^{1/2}(U)$ , which is the interpolation space of index 1/2 between  $H^1(U)$  and  $L^2(U)$  of an open non-empty subset  $U \in \partial\Omega$  denoted by:

$$H^{1/2}(U) := [H^1(U), L^2(U)]_{1/2}$$

equipped with the norm  $\|\cdot\|_{1/2,U}$  [62]. We also define the generic space  $\Lambda$ , which is the interpolation space between the spaces  $H_*^1$  and  $L^2(U)$ :

$$\Lambda := [H_*^1, L^2(U)]_{1/2}.$$

$H_*^1$  can be one of  $H^1(U)$ ,  $H_0^1(U)$  or  $H_D^1(U)$  depending on the boundary conditions of the problem. The space  $\Lambda$  is also equipped with the same norm as  $H^{1/2}(U)$  and its dual space will be denoted throughout the thesis by  $\Lambda'$ . We will return to the illustration of this space in Chapter 9.

Finally, we introduce the following inequalities [78], [62, p. 6]:

**Lemma 2.1.5** (Poincaré-Friedrichs inequality) *Let  $\Omega \subset \mathbb{R}^n$  be a bounded open set with a sufficiently smooth boundary  $\partial\Omega$ . Then there exists a constant  $C = C(\Omega)$  so that for all  $v \in H_D^1(\Omega)$*

$$\|v\|_{L^2(\Omega)} = \|v\|_{0,\Omega} \leq C(\Omega) |v|_{1,\Omega}. \quad (2.2)$$

**Lemma 2.1.6** *The trace operator  $\gamma_0 : H^1(\Omega) \rightarrow H^{1/2}(\partial\Omega)$  is surjective and continuous i.e., there exists a constant  $C_\gamma(\partial\Omega)$  so that*

$$\|\gamma_0 v\|_{1/2,\partial\Omega} \leq C_\gamma \|v\|_{1,\Omega} \quad \forall v \in H^1(\Omega). \quad (2.3)$$

**Remark 2.1.7** *We note the following:*

1. *For the case when  $\mathbf{v} \in L^2(\Omega) \times L^2(\Omega)$  or  $\mathbf{v} \in H^1(\Omega) \times H^1(\Omega)$ , we will overload the definitions of norms  $\|\cdot\|_0$  and  $\|\cdot\|_1$  with*

$$\|\mathbf{v}\|_0^2 = \|v_1\|_{L^2(\Omega)}^2 + \|v_2\|_{L^2(\Omega)}^2, \quad \|\mathbf{v}\|_1^2 = \|v_1\|_{H^1(\Omega)}^2 + \|v_2\|_{H^1(\Omega)}^2. \quad (2.4)$$

2. *The notations  $\|\cdot\|_{1/2,\partial\Omega}$ ,  $\|\cdot\|_{1/2,\Gamma}$  will overload the notations  $\|\cdot\|_{H^{1/2}(\partial\Omega) \times H^{1/2}(\partial\Omega)}$  and  $\|\cdot\|_{H^{1/2}(\Gamma) \times H^{1/2}(\Gamma)}$  respectively.*
3. *An extension of Lemma 2.1.6 to the vector case can be easily derived.*

## 2.2 Variational formulation of PDE

We will see in Chapter 5 how to reduce a reaction-diffusion system into an integral formulation involving a bilinear form defined on some suitable space. This type of equation is known as the variational form of the PDE. All the results presented here are fully described in [49, p.116].

Let  $H$  denote a Hilbert space with the inner product  $\langle \cdot, \cdot \rangle_H$ .

**Definition 2.2.1** *A bilinear form  $a(\cdot, \cdot) : H \times H \rightarrow \mathbb{R}$  is continuous if there is a constant  $c_1 > 0$  such that:*

$$a(u, v) \leq c_1 \|u\|_H \|v\|_H \quad \forall u, v \in H.$$

**Definition 2.2.2** *A bilinear form  $a(\cdot, \cdot) : H \times H \rightarrow \mathbb{R}$  is coercive if there is a constant  $c_2 > 0$  such that:*

$$a(v, v) \geq c_2 \|v\|_H \|v\|_H \quad \forall v \in H.$$

Let  $V \subset H$  denote a closed subspace of  $H$ . Then  $V$  is also a Hilbert space when endowed with the  $H$ -inner product  $\langle \cdot, \cdot \rangle_H$ .

Let  $l$  be a linear functional on  $V$ . Furthermore, let  $a(\cdot, \cdot) : V \times V \rightarrow \mathbb{R}$  be a bilinear form on  $V$ . Consider the following abstract variational problem:

$$\begin{cases} \text{Find } u \in V \text{ such that for all } v \in V \\ a(u, v) = l(v). \end{cases} \quad (2.5)$$

The existence and uniqueness of the problem (2.5) is well-understood. We quote below the main results.

**Lemma 2.2.3** *(Lax-Milgram -see Theorem 7.2.1 in [49])*

*Let  $a(\cdot, \cdot)$  be a continuous and coercive bilinear form on  $V$  and let  $l$  denote a continuous*

linear functional on  $V$ . Then there exists a unique function  $u \in V$  such that for all  $v \in V$

$$a(u, v) = l(v).$$

**Proof:** The reader is referred to [49, p.118]. ■

In theory the variational problem posed on  $V$  is replaced by a new problem posed on a finite-dimensional subspace of  $V : V_h \subset V$ . The resulting discrete variational reads:

$$\left\{ \begin{array}{l} \text{Find } u_h \in V_h \text{ such that for all } v_h \in V_h \\ a(u_h, v_h) = l(v_h). \end{array} \right. \quad (2.6)$$

The formulation is called the Ritz-Galerkin methods, which give rise to a linear algebraic system once the basis of  $V_h$  is specified. This will be presented in the next chapter.



# CHAPTER 3

## FINITE ELEMENT METHOD

This chapter covers the main idea of finite element methods for PDE and also highlights the theoretical issues discussed in later chapters.

### 3.1 Finite element construction

As presented in the previous chapter, the first step of a finite element method is to transform the the original problem into its variational form:

$$\left\{ \begin{array}{l} \text{Find } u \in V \text{ such that for all } v \in V \\ a(u, v) = l(v). \end{array} \right. \quad (3.1)$$

Then, construct a finite-dimensional subspace of  $V : V_h \subset V$ , such that the problem (3.1) is replaced by:

$$\left\{ \begin{array}{l} \text{Find } u_h \in V_h \text{ such that for all } v_h \in V_h \\ a(u_h, v_h) = l(v_h). \end{array} \right. \quad (3.2)$$

In practice the subspace  $V_h$  subspace is formed of continuous piecewise polynomial functions of a fixed degree associated with a triangulation of the solution domain presented below.

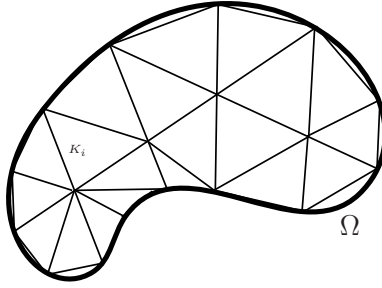


Figure 3.1: A finite element triangulation of a polygonal domain.

### 3.1.1 Domain Triangulation

The domain  $\Omega$  is divided into a set  $\mathcal{T}_h = \{K_1, \dots, K_N\}$  of non-overlapping triangles  $K_i$  as shown in Figure (3.1):

$$\bar{\Omega} = \bigcup_{K \in \mathcal{T}_h} K = K_1 \cup K_2 \dots \cup K_N.$$

Let  $h_K$  be the diameter of the circumscribed circle of  $K$ , with:

$$h = \max_{K \in \mathcal{T}_h} h_K, \quad h_{min} = \min_{K \in \mathcal{T}_h} h_K.$$

The triangulation is constructed such that no vertex of one triangle lies on the edge of another, i.e. it is a conforming subdivision of  $\Omega$  and each interior node ( $N_j$ ) is associated with a basis function  $\phi_j$ . Then, we can write:

$$\dim V_h = N(h) \quad \text{and} \quad V_h = \text{span}\{\phi_j, \dots, \phi_{N(h)}\}.$$

The basis functions  $\phi_j$  for  $j = 1, \dots, N(h)$  can be taken to be linear polynomial, in particular to satisfy:

$$\phi_j(N_i) = \delta_{ij};$$

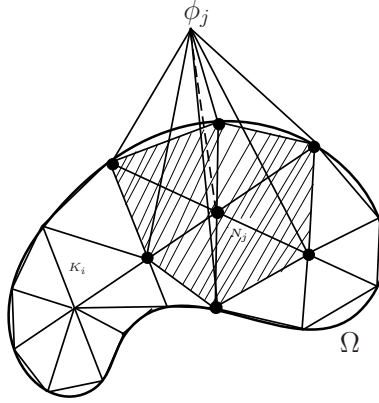


Figure 3.2: The basis function  $\phi_j$ .

We can expand  $u_h$  in terms of the basis  $\phi_j$  as:

$$u_h = \sum_{j=1}^{N(h)} u_j \phi_j(x) \quad (3.3)$$

Finally, using the discrete formulation (3.2), one should assemble and form the linear system:

$$Au = B, \quad (3.4)$$

which is equivalent to:

$$\left\{ \begin{array}{l} \text{Find } (u_1, \dots, u_{N(h)}) \in \mathbb{R}^{N(h)} \text{ such that:} \\ \sum_{i=1}^{N(h)} a(\phi_i, \phi_j) u_i = l(\phi_j), \quad j = 1, \dots, N(h). \end{array} \right. \quad (3.5)$$

Where the unknown is  $u = (u_1, \dots, u_{N(h)})$  and the matrix of the system is  $A = a(\phi_j, \phi_i)$  of size  $N(h) \times N(h)$ . Here, the matrix  $A$  is sparse as the basis functions  $\phi_i$ 's have local support. This latter property provides a great advantage from a computational point of view: They can be stored more easily and special algorithms can be employed to provide

the solution in optimal time (see Chapter 6).

## 3.2 Calculation and assembly of element matrices

In this section, we want to generalize the construction of a finite element method, when  $\Omega$  is a bounded polygonal in the plane. Consider the same triangulation as that in the previous section so that any arbitrary triangular element has its vertices indexed 1, 2, and 3. The restriction of  $u$  to the triangular element  $K \in \mathcal{T}_h$  is denoted by:

$$u^{(e)}(x_j, y_j) = c_1 + c_2x_j + c_3y_j \quad \text{for } j = 1, 2, 3. \quad (3.6)$$

Solving the linear system resulting from (3.6) we obtain:

$$c_1 = \frac{1}{2A_{123}}(\alpha_1u_1^{(e)} + \alpha_2u_2^{(e)} + \alpha_3u_3^{(e)}), \quad (3.7)$$

$$c_2 = \frac{1}{2A_{123}}(\beta_1u_1^{(e)} + \beta_2u_2^{(e)} + \beta_3u_3^{(e)}), \quad (3.8)$$

$$c_3 = \frac{1}{2A_{123}}(\theta_1u_1^{(e)} + \theta_2u_2^{(e)} + \theta_3u_3^{(e)}), \quad (3.9)$$

where:  $A_{123}$  is the area of the triangle and:

$$\alpha_i = x_jy_k - x_ky_j, \quad (3.10a)$$

$$\beta_i = y_j - y_k, \quad (3.10b)$$

$$\theta_i = -(x_j - x_k), \quad (3.10c)$$

where  $i, j, k = 1, 2, 3$ .

Substituting (3.7)-(3.9) into (3.3) we obtain:

$$u_h^{(e)}(x, y) = \sum_{i=1}^3 u_i \phi_i(x, y), \quad (3.11)$$

where

$$\phi_1 = \frac{1}{2A_{123}}(\alpha_1 + \beta_1 x + \theta_1 y), \quad (3.12a)$$

$$\phi_2 = \frac{1}{2A_{123}}(\alpha_2 + \beta_2 x + \theta_2 y), \quad (3.12b)$$

$$\phi_3 = \frac{1}{2A_{123}}(\alpha_3 + \beta_3 x + \theta_3 y). \quad (3.12c)$$

The expression (3.11) can be simplified using the so called local  $(\xi, \eta)$  coordinate system.

In the  $(\xi, \eta)$  coordinate system, each triangle  $K \in \mathcal{T}_h$  is mapped onto a unit right-angled triangle  $E$  as shown in Figure 3.3 using the following affine transformation:

$$\begin{cases} x = a\xi + b\eta + c \\ y = d\xi + e\eta + f. \end{cases} \quad (3.13)$$

Say  $E$  has vertex 1 at the origin  $(0,0)$ , vertex 2 at  $(1,0)$ , vertex 3 at  $(0,1)$  the local coordinates  $x(\xi, \eta)$  and  $y(\xi, \eta)$  have the following expression:

$$\begin{cases} x(\xi, \eta) = (x_2 - x_1)\xi + (x_3 - x_1)\eta + x_1 \\ y(\xi, \eta) = (y_2 - y_1)\xi + (y_3 - y_1)\eta + y_1 \end{cases} \quad (3.14)$$

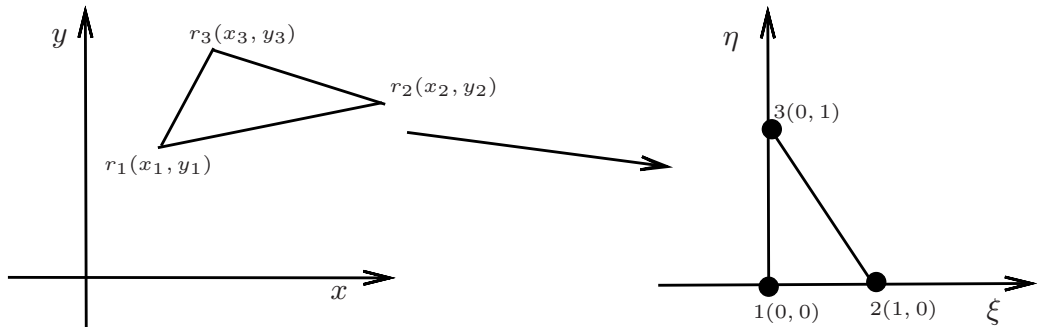


Figure 3.3: Linear transformation of a triangular element to a right-angled triangle

where  $(x_i, y_i), i = 1, 2, 3$  are the Cartesian coordinates of the vertices. The Jacobian matrix of this affine transformation is given by:

$$\mathbf{J} = \begin{pmatrix} x_2 - x_1 & x_3 - x_1 \\ y_2 - y_1 & y_3 - y_1 \end{pmatrix} \quad (3.15)$$

from which it follows that the Jacobian is given by:

$$|\mathbf{J}| = \det \begin{pmatrix} 1 & 1 & 1 \\ x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \end{pmatrix} = 2A_{123}, \quad (3.16)$$

where, as before  $A_{123}$  is the area of the triangle.

By substituting (3.10) and (3.14) into (3.12), we obtain:

$$\hat{\phi}_1(\xi, \eta) = 1 - \xi - \eta, \quad (3.17)$$

$$\hat{\phi}_2(\xi, \eta) = \xi, \quad (3.18)$$

$$\hat{\phi}_3(\xi, \eta) = \eta. \quad (3.19)$$

Therefore, from (3.11), we obtain:

$$u^{(e)}(x(\xi, \eta), y(\xi, \eta)) = \hat{u}^{(e)}(\xi, \eta) = \sum_{i=1}^3 u_i \hat{\phi}_i(\xi, \eta) \quad (3.20)$$

This new expression of  $u^{(e)}$  is then used to construct the matrix  $A$  in (3.5) by the summing of the contribution from each element over the domain  $\Omega$ . In the next section we present the derivation of some special matrices derived later in chapter 5

## 3.3 Derivation of special matrices

### 3.3.1 The mass matrix

- **The mass matrix with constant coefficient.**

The element mass matrix is given by:

$$M^{(e)} = (me)_{ij} = \int_K \phi_i(x, y) \phi_j(x, y) dx dy. \quad (3.21)$$

Mapping to the canonical element we get:

$$(me)_{ij} = \int_E \phi_i(\xi, \eta) \phi_j(\xi, \eta) |\mathbf{J}| d\xi d\eta. \quad (3.22)$$

- **The mass matrix with non constant coefficient**

$$(me)_{ij} = \int_K \tau(x, y) \phi_i(x, y) \phi_j(x, y) dx dy. \quad (3.23)$$

Mapping to the reference element, we get:

$$(me)_{ij} = \int_E \tau(x(\xi, \eta), y(\xi, \eta)) \phi_i(\xi, \eta) \phi_j(\xi, \eta) |\mathbf{J}| d\xi d\eta. \quad (3.24)$$

Where  $\tau$  is the non constant coefficient.

### 3.3.2 The stiffness matrix with constant coefficient

The element stiffness matrix is given by:

$$\begin{aligned} L^{(e)} &= (le)_{ij} = \int_K \nabla \phi_i(x, y) \nabla \phi_j(x, y) dx dy, \\ &= \int_K (\partial_x \phi_i(x, y) \partial_x \phi_j(x, y) + \partial_y \phi_i(x, y) \partial_y \phi_j(x, y)) dx dy. \end{aligned} \quad (3.25)$$

Mapping to the reference element we obtain:

$$(le)_{ij} = \int_E [(\xi_x \partial_\xi \phi_i(\xi, \eta) + \eta_x \partial_\eta \phi_i(\xi, \eta)) (\xi_x \partial_\xi \phi_j(\xi, \eta) + \eta_x \partial_\eta \phi_j(\xi, \eta)) + (\xi_y \partial_\xi \phi_i(\xi, \eta) + \eta_y \partial_\eta \phi_i(\xi, \eta)) (\xi_y \partial_\xi \phi_j(\xi, \eta) + \eta_y \partial_\eta \phi_j(\xi, \eta))] |\mathbf{J}| d\xi d\eta. \quad (3.26)$$

### 3.3.3 The right hand side approximation

Assuming that the forcing term is approximated in the FEM space by:

$$f(x, y) = \sum_i f(x_i, y_i) \phi_i(x, y).$$

The elements of the RHS are given by  $(F)^{(e)} = (fe)_j$ , where:

$$(fe)_j = \int_K \sum_i f(x_i, y_i) \phi_i(x, y) \phi_j(x, y) dx dy. \quad (3.27)$$

Mapping to the reference element we obtain:

$$(fe)_j = f(x_i, y_i) \int_E \sum_i \phi_i(\xi, \eta) \phi_j(\xi, \eta) |\mathbf{J}| d\xi d\eta = \sum_i (me)_{ji} f(x_i, y_i). \quad (3.28)$$

The integrals (3.22), (3.24), (3.26), (3.28) are evaluated using a suitable Gauss rule. All the results presented above are for the scalar case. However, when solving a system of PDEs involving more than one unknown, one should consider mixed finite element method as each unknown may require a different finite element space.

## 3.4 Mixed variational formulation

When having to deal with a system of PDEs with two or more unknowns, the continuity of the bilinear form  $a(., .)$  is never a problem, however the coercivity is not always guaranteed. The result below generalize the case of mixed finite variational formulations, i.e.



formulations which employ a bilinear form acting on mixed spaces:  $a(., .) : H_1 \times H_2 \rightarrow \mathbb{R}$ , where  $H_i, i = 1, 2$  denotes two Hilbert spaces with inner products and norms  $\langle \cdot, \cdot \rangle_{H_i}, \|\cdot\|_{H_i}, i = 1, 2$ , respectively. We state the results below [81]:

**Theorem 3.4.1** *Let  $V_1 \times V_2 \subset H_1 \times H_2$  and let  $l$  denote a continuous bilinear functional on  $V_2$ . Let  $a(., .)$  be a linear form on  $V_1 \times V_2$  which satisfies for all  $v \in V_1, w \in V_2$ :*

$$a(v, w) \leq C_1 \|v\|_{H_1} \|w\|_{H_2}, \quad (3.29a)$$

$$\sup_{u \in V_1 \setminus \{0\}} \frac{a(u, w)}{\|u\|_{H_1}} \geq C_2 \|w\|_{H_2}, \quad (3.29b)$$

$$\sup_{u \in V_1 \setminus \{0\}} \frac{a(u, w)}{\|w\|_{H_2}} \geq C_2 \|u\|_{H_1}. \quad (3.29c)$$

$$(3.29d)$$

*Then there exists a unique function  $u \in V_1$  such that for all  $v \in V_2$ :*

$$a(u, v) = l(v)$$

The conditions 3.29a-3.29c in Theorem 3.4.1 is generally referred to as the inf-sup conditions and may make the definition of the finite element spaces more complicated. However, how we show in the next chapter, our problem yields a coercive bilinear form under certain conditions and hence 3.29a-3.29c are satisfied.

# CHAPTER 4

## REACTION-DIFFUSION SYSTEMS

The aim of this chapter is to introduce the central object of the study. In doing so, the chapter will present some applications of reaction-diffusion systems. It also describes the derivation and discusses the existence and uniqueness of the solution to reaction-diffusion systems.

### 4.1 Applications

Reaction-diffusion systems may be utilized to model a vast variety of phenomena in applied mathematics. The partial list includes:

- **Biology.** There are now a large number of real life problems in biology that involve reaction-diffusion systems. Among the most notable of these are the Brusselator and the Schnakenberg model presented in [54].

The Brusselator model is represented by the following set of PDEs:

$$\left\{ \begin{array}{l} u_t = \Delta u + a - (b+1)u + u^2v \quad \text{on } \Omega; \\ v_t = d\Delta v + bu - u^2v \quad \text{on } \Omega; \\ n \cdot \nabla u = 0 \quad \text{on } \partial\Omega. \end{array} \right. \quad (4.1)$$

The Schnakenberg model is defined by the following set of PDEs:

$$\left\{ \begin{array}{l} u_t = \Delta u + \gamma(a - u + u^2v) \quad \text{on } \Omega; \\ v_t = d\Delta v + \gamma(b - u^2v) \quad \text{on } \Omega; 0 \\ n \cdot \nabla u = 0 \quad \text{on } \partial\Omega. \end{array} \right. \quad (4.2)$$

The models presented in (4.1) and (4.2) are often used to study the emergence of pattern formation. It has been shown that they describe interesting patterns such as chaos and certain structures which include self-oscillations and self-replicating spikes and stripes [56, 48].

- **Electrodynamics.** The following  $6 \times 6$  system presented in [59] represents the electro-decomposition of Nickel-Iron:

$$\left\{ \begin{array}{l} \partial_t w_i - d_i(w_i)_{xx} + b(x)(w_i)_x - [w_i \phi_x]_x = S_i(w), \\ S_1 = S_2 = 0, S_3(w) = S_4(w) = -S_5(w), \\ -[\phi]_{xx} = \sum_{i=1}^5 z_i w_i, \quad z_i \in \mathbb{R} + \text{bdy conditions}, \\ i = 1, \dots, 5. \end{array} \right. \quad (4.3)$$

The model has been studied in [4]. It is mainly used in the field of alloy deposition, namely for the recording, memory and storage devices of electronics goods.

- **Pollution effects modeling.** One of the most interesting examples of the application of reaction-diffusion systems comes from the modeling of pollutant transfers into the atmosphere. The modeling of the atmospheric dispersion of ozone and other photochemically generated pollutants can be represented by the following PDEs:

$$\frac{\partial \phi_i}{\partial t} = d_i \frac{\partial^2 \phi_i}{\partial z^2} + \nabla \cdot (\omega \phi_i) + f_i(\phi) + g_i. \quad (4.4)$$

Here  $\phi_i$  represents the molecular densities for species  $i$ , the velocity field  $\omega_i = (\omega_1, \omega_2, \omega_3)$  models the atmospheric current,  $d_i$  is the diffusion coefficient for species  $i$ ,  $f_i(\phi)$  are nonlinear reaction terms, representing the chemistry of the process, and  $g_i$  are source terms. [24] provides further details with regards to cases where  $i = 1, \dots, 20$ .

See [59, 64, 19] for further examples of applications of reaction-diffusion systems.

## 4.2 Derivation

Let  $\Omega$  be a region with boundary  $\partial\Omega$  and  $\mathbf{n}$  denotes the outer normal vector to  $\partial\Omega$ . Using Fick's law [26], we arrive at the following equation:

$$\int_{\partial\Omega} [(-\mathbf{n}) \cdot \mathbf{J}_D] \, ds = \int_{\partial\Omega} D\nabla u \cdot \mathbf{n} \, ds, \quad (4.5)$$

where  $D$  is a positive constant called the diffusivity and  $\mathbf{J}_D$  the flux density.

The rate of change of the particle mass in the domain  $\Omega$  is given by:

$$\frac{\partial}{\partial t} \int_{\Omega} u \, dx = \int_{\partial\Omega} [(-\mathbf{n}) \cdot \mathbf{J}_D] \, ds + \int_{\Omega} f(t, x, u) \, dx, \quad (4.6)$$

where  $f(t, x, u)$  is the net creation rate of the particle at  $x \in \Omega$  at time  $t$ .

Assuming that  $u$  and  $\partial\Omega$  are smooth enough, by applying the divergence theorem on the right side of (4.6) and combining with (4.5) the following equation will be obtained:

$$\int_{\Omega} \left( \frac{\partial u}{\partial t} \right) \, dx = \int_{\Omega} D\nabla^2 u \, dx + \int_{\Omega} f(t, x, u) \, dx. \quad (4.7)$$

This yields the following reaction-diffusion equation:

$$u_t = D\nabla^2 u + f(t, x, u). \quad (4.8)$$

Equation (4.8) is considered the simplest model of a reaction-diffusion system. However, the combination of a diffusion term together with a nonlinear term makes it difficult to obtain an analytical solution of the equation. It is therefore important to note that the existence and the uniqueness of the solution will depend on some conditions imposed on  $f$ .

### 4.3 Existence and uniqueness

Due to the increasing need of reaction-diffusion systems in scientific modeling, the global existence of solution to reaction-diffusion systems has received a great deal of interest.

Consider the following reaction-diffusion system:

$$\begin{cases} \partial_t u - d_1 \Delta u = f(u, v) & \text{in } \mathbb{R}^+ \times \Omega, \\ \partial_t v - d_2 \Delta v = g(u, v) & \text{in } \mathbb{R}^+ \times \Omega, \end{cases} \quad (4.9)$$

with the boundary conditions:

$$n \cdot \nabla u = 0, \quad n \cdot \nabla v = 0 \quad \text{on } \mathbb{R}^+ \times \partial\Omega \quad (4.10)$$

and initial data:

$$u(0, \cdot) = u_0, \quad v(0, \cdot) = v_0 \quad \text{in } \Omega, \quad (4.11)$$

where  $\Omega \subset \mathbb{R}^n$  is a bounded domain with smooth boundary  $\partial\Omega$ . We assume that the following basic hypotheses hold:

### Assumptions 4.3.1

- $d_1, d_2, \xi_1, \xi_2$  are constants with  $d_1, d_2, > 0$  and  $\xi_1, \xi_2 \geq 0$ ;
- $f$  and  $g$  are positive continuously differentiable functions from  $\mathbb{R}^+ \times \mathbb{R}^+$  into  $\mathbb{R}$ ;
- $u_0(\cdot)$  and  $v_0(\cdot)$  are measurable and bounded on  $\Omega$  with  $u_0(\cdot), v_0(\cdot) \geq 0$ .

Fife [22, chap. 3] has established the local existence of unique, nonnegative, classical solution of problem (4.9) on  $\Omega \times [0, T^*)$  under the conditions that assumption 4.3.1 holds. In addition to the assumptions made in 4.3.1 Haraux et al. [27], Hollis et al. [30] have obtained global existence results of problem (4.9) by imposing some additional structural conditions on  $f, g$  namely:

### Assumptions 4.3.2

$$f(r, s) + g(r, s) \leq \mathcal{C}_1(r, s)(r + s + 1) \quad \forall r, s \geq 0; \quad (4.12)$$

$$f(r, s) \leq \mathcal{C}_2(r, s)(r + s + 1) \quad \forall r, s \geq 0; \quad (4.13)$$

where  $\mathcal{C}_1, \mathcal{C}_2 : \mathbb{R}^+ \times \mathbb{R}^+ \rightarrow \mathbb{R}$  are some positive and uniformly bounded functions.

An extension to a class of reaction-diffusion problems involving more than two unknowns has been explicitly derived by Morgan [52], Hollis [31] and Martin et al. [50]. It is important to note that Assumption 4.3.2 ensures that the total mass of the components of the system (4.9) is controlled over the time, as the possibility of blow-up may occur in finite time (see for example Pierre and Schmitt [60]).

Recently, some progress has been established on the global existence results for solutions of reaction-diffusion systems: Kouachi [40, 41] and Perterson [58] have obtained global existence results for solutions of problem (4.9) by relaxing the usual monotonicity assumption on the nonlinear term  $f$ , more precisely by ignoring the condition (4.13). Chandrasekhar

et al [74] extended the work done in Morgan [52] to establish the existence and uniqueness for reaction-diffusion systems on evolving domains. A good survey on global existence in reaction-diffusion systems with the control of mass can be found in [59]. For the rest of the thesis, we assume that the assumptions 4.3.1 and 4.3.2 hold and our only focus will be the numerical approximation of problem (4.9).

# CHAPTER 5

## FINITE ELEMENT METHODS FOR REACTION-DIFFUSION SYSTEMS

In this chapter we describe the model problem and present an appropriate mixed variational finite element formulation.

### 5.1 Model problem

We consider the following problem:

$$\left\{ \begin{array}{l} -D\Delta \mathbf{u} + M(\mathbf{x})\mathbf{u} = \mathbf{f} \text{ on } \Omega, \\ \mathbf{u} = \mathbf{0} \text{ on } \partial\Omega_D, \\ \mathbf{n} \cdot \nabla \mathbf{u} = \mathbf{0} \text{ on } \partial\Omega_N, \end{array} \right. \quad (5.1)$$

where  $\Omega \subset \mathbb{R}^2$  and

$$\mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}, \quad M(\mathbf{x}) = \begin{pmatrix} \alpha_1(\mathbf{x}) & \beta_1(\mathbf{x}) \\ \beta_2(\mathbf{x}) & \alpha_2(\mathbf{x}) \end{pmatrix}, \quad \mathbf{f} = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}, \quad D = \begin{pmatrix} d_1 & 0 \\ 0 & d_2 \end{pmatrix},$$



with  $f_1, f_2 \in L^2(\Omega)$ ,  $d_1, d_2 > 0$ . We also assume that the following inequalities hold for all  $\mathbf{x} \in \Omega$ :

$$0 < \gamma_{min} < \frac{\boldsymbol{\xi}^T \mathbf{M}(\mathbf{x}) \boldsymbol{\xi}}{\boldsymbol{\xi}^T \boldsymbol{\xi}} \quad \text{for all } \boldsymbol{\xi} \in \mathbb{R}^2 \setminus \{0\}, \quad (5.2)$$

$$\|\mathbf{M}(\mathbf{x})\| < \gamma_{max}. \quad (5.3)$$

where  $\gamma_{min}, \gamma_{max}$  are positive real constants.

**Remark 5.1.1** *The following scaled version of problem (5.1) can also be considered:*

$$-\mathbf{I}_2 \Delta \mathbf{v} + \mathbf{M} \mathbf{D}^{-1} \mathbf{v} = \mathbf{f}, \quad \text{where } \mathbf{v} = \mathbf{D} \mathbf{u}. \quad (5.4)$$

As mentioned in Chapter 2, it is possible to reduce a PDE to an integral formulation involving a bilinear form defined on a suitable space. The same can be done for reaction-diffusion problems as they are simply a system of PDE.

## 5.2 Weak formulation

Choose a test function  $\mathbf{z} = (z_1, z_2) \in H_D^1(\Omega) \times H_D^1(\Omega)$ , multiply (5.1) by  $\mathbf{z}$  and integrate by parts to obtain :

$$\int_{\Omega} \mathbf{D} \nabla \mathbf{u} \cdot \nabla \mathbf{z} + (\mathbf{M} \mathbf{u}) \cdot \mathbf{z} \, d\mathbf{x} = \int_{\Omega} \mathbf{f} \cdot \mathbf{z} \, d\mathbf{x}. \quad (5.5)$$

The weak formulation of problem (5.1) can be written as:

$$\left\{ \begin{array}{l} \text{Find } \mathbf{u} \in H_D^1(\Omega) \times H_D^1(\Omega) \text{ such that for all } \mathbf{z} \in H_D^1(\Omega) \times H_D^1(\Omega) \\ B(\mathbf{u}, \mathbf{z}) = \langle \mathbf{f}, \mathbf{z} \rangle, \end{array} \right. \quad (5.6)$$

where:

$$B(\mathbf{u}, \mathbf{z}) = \int_{\Omega} \mathbf{D}\nabla\mathbf{u} : \nabla\mathbf{z} + (\mathbf{M}(\mathbf{x})\mathbf{u}) \cdot \mathbf{z} \, d\mathbf{x}, \quad \langle \mathbf{f}, \mathbf{z} \rangle = \int_{\Omega} \mathbf{f} \cdot \mathbf{z} \, d\mathbf{x}.$$

We are concerned with the existence and the uniqueness of a solution  $\mathbf{u}$  to problem (5.6).

**Theorem 5.2.1** *Consider problem (5.1) such that (5.2) and (5.3) hold. Then, problem (5.1) has a unique solution in  $H_D^1(\Omega) \times H_D^1(\Omega)$ .*

**Proof:** From (5.6) together with (5.2) and (5.3), we have:

$$\begin{aligned} B(\mathbf{u}, \mathbf{z}) &= \int_{\Omega} (\nabla\mathbf{u} : \nabla\mathbf{z} + (\mathbf{M}\mathbf{u}) \cdot \mathbf{z}) \, d\mathbf{x}, \\ &= \int_{\Omega} (\nabla\mathbf{u} : \nabla\mathbf{z} + \mathbf{u}^T \mathbf{M}\mathbf{z}) \, d\mathbf{x}, \\ &\leq \|\nabla\mathbf{u}\|_0^2 \|\nabla\mathbf{z}\|_0^2 + \gamma_{max} \|\mathbf{u}\|_0^2 \|\mathbf{z}\|_0^2, \\ &\leq \underbrace{\max\{1, \gamma_{max}\}}_{c_1} (\|\mathbf{u}\|_1^2 \|\mathbf{z}\|_1^2). \end{aligned}$$

Analogously, one can derive the following lower bound:

$$\begin{aligned} B(\mathbf{z}, \mathbf{z}) &\geq \int_{\Omega} (\nabla\mathbf{z} : \nabla\mathbf{z} + \mathbf{z}^T \mathbf{M}\mathbf{z}) \, d\mathbf{x} \\ &\geq (\|\nabla\mathbf{z}\|_0^2 + \gamma_{min} \|\mathbf{z}\|_0^2), \\ &\geq \min\{1, \gamma_{min}\} \|\mathbf{z}\|_1^2 \\ &\geq \underbrace{\min\{1, \gamma_{min}\}}_{c_2} \|\mathbf{z}\|_1^2. \end{aligned}$$

Finally it holds:

$$\begin{aligned}
l(\mathbf{z}) &:= \langle \mathbf{f}, \mathbf{z} \rangle = \int_{\Omega} \mathbf{f} \cdot \mathbf{z} \, d\mathbf{x}, \\
&\leq \|\mathbf{f}\|_0^2 \|\mathbf{z}\|_0^2, \\
&\leq C(\Omega) \|\mathbf{f}\|_1^2 \|\mathbf{z}\|_1^2.
\end{aligned}$$

Hence by Theorem (2.2.3), there exists a unique solution  $\mathbf{u} \in H_D^1(\Omega) \times H_D^1(\Omega)$  to problem (5.6). ■

### 5.3 Discrete formulation

Let  $V^h \times V^h$  be a finite dimensional subspace of  $H_D^1(\Omega) \times H_D^1(\Omega)$ . The discrete weak formulation of problem (5.1) reads:

$$\left\{ \begin{array}{l} \text{Find } \mathbf{u}_h \in V^h \times V^h \text{ such that for all } \mathbf{z}_h \in V^h \times V^h \\ B(\mathbf{u}_h, \mathbf{z}_h) = \langle \mathbf{f}_h, \mathbf{z}_h \rangle . \end{array} \right. \quad (5.7)$$

The formulation (5.7) is known as the Ritz-Galerkin method. A notable property of this formulation can be obtained by replacing  $\mathbf{z}$  by  $\mathbf{z}_h$  in (5.6) and subtracting (5.7) to get:

$$B(\mathbf{u} - \mathbf{u}_h, \mathbf{z}_h) = 0, \quad \forall \mathbf{z}_h \in V^h \times V^h. \quad (5.8)$$

This is an important result that can be used for error analysis (see Céa's Lemma- see Theorem 13.1 in [18, p.113]). The existence and uniqueness of the solution to (5.7) is also guaranteed by the Lax-Milgram Lemma, provided the continuity and coercivity conditions are satisfied.

## 5.4 Matrix formulation

Consider a triangulation of the domain as presented in Section 3.1.1 and let

$$\mathbf{u}_h = \sum_{i=1}^N \mathbf{u}_i \phi_i(\mathbf{x}), \quad \mathbf{z}_h = \sum_{i=1}^N \mathbf{z}_i \phi_i(\mathbf{x}), \quad (5.9)$$

where  $\text{span}\{\phi_i\} = V_h$ .

Inserting these approximations into the linear form of (5.7), we obtain the following system of equations:

$$\mathbf{A} \mathbf{u} = \begin{pmatrix} d_1 L + M_{\alpha_1} & M_{\beta_1} \\ M_{\beta_2} & d_2 L + M_{\alpha_2} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} M f_1 \\ M f_2 \end{pmatrix}. \quad (5.10)$$

where  $L = \int_{\Omega} \nabla \phi_i(\mathbf{x}) \nabla \phi_j(\mathbf{x}) \mathbf{d}\mathbf{x}$ ,  $M = \int_{\Omega} \phi_i(\mathbf{x}) \phi_j(\mathbf{x}) \mathbf{d}\mathbf{x}$  and  $M_{\omega} = \int_{\Omega} \omega_i \phi_i(\mathbf{x}) \phi_j(\mathbf{x}) \mathbf{d}\mathbf{x}$ ,  $\omega \in \{\alpha_1(\mathbf{x}), \alpha_2(\mathbf{x}), \beta_1(\mathbf{x}), \beta_2(\mathbf{x})\}$ . The matrices  $M$  and  $L$  are respectively the standard mass and stiffness matrix while  $M_{\alpha_1}$ ,  $M_{\alpha_2}, M_{\beta_1}, M_{\beta_2}$  represent global mass matrices resulting from the zero-order terms. They are all constructed as described in Section 3.2. It is obvious that the system (5.10) is a large sparse system. In practice iterative methods are used to solve such a system as they are more flexible and computationally cheap.

# CHAPTER 6

## SOLUTION METHODS FOR SPARSE LINEAR SYSTEMS

In practice, most PDE discretizations lead to large linear systems of the form:

$$A\mathbf{u} = \mathbf{f}, \tag{6.1}$$

where  $A$  is often a large sparse or banded matrix. To take advantage of the zero entries and to reduce the computational cost, some special iterative techniques have been developed. They are largely divided into two main classes: classical and projection iterative methods. Classical methods are easy to implement but generally too slow while projection iterative methods are robust and can be combined with other methods such as domain decomposition. This combination has been used in this research study as this leads to the derivation of efficient solvers. Additionally the resulting solvers can take advantage of the emergence of supercomputers as they can be easily implemented in parallel. In this chapter, we describe projection iterative and domain decomposition methods for large sparse linear systems. The theory and the practical aspects will be included.

## 6.1 Projection iterative methods

These are methods which compute a sequence of progressively accurate iterates  $\mathbf{u}_m$ , to approximate the solution of problem (6.1) so that the residual  $\mathbf{r}_m = \mathbf{f} - \mathbf{A}\mathbf{u}_m$  satisfies the more general *Petrov-Galerkin* condition:

$$(\mathbf{r}_m, \mathbf{y}) = 0 \quad \forall \mathbf{y} \in \mathcal{W}_m, \quad (6.2)$$

where  $\mathcal{W}_m$  is a subspace of  $\mathbb{R}^n$  of dimension  $m$ .

To obtain a matrix formulation of the problem (6.2), let  $V_m = [v_1, \dots, v_m] \in \mathbb{R}^{n \times m}$  whose column vectors form a basis of  $\mathcal{V}_m$  and  $W_m = [w_1, \dots, w_m] \in \mathbb{R}^{n \times m}$  whose column vectors form a basis of  $\mathcal{W}_m$ . The iterates  $\mathbf{u}_m$  are of the form:

$$\mathbf{u}_m = \mathbf{u}_0 + V_m \mathbf{z}_m \quad \text{with } \mathbf{z}_m \in \mathbb{R}^m, \quad (6.3)$$

from (6.2) we obtain:

$$W_m^T (\mathbf{f} - \mathbf{A}\mathbf{u}_0 - \mathbf{A}V_m \mathbf{z}_m) = 0 \Leftrightarrow W_m^T \mathbf{r}_0 = W_m^T \mathbf{A}V_m \mathbf{z}_m. \quad (6.4)$$

This leads to:

$$\mathbf{u}_m = \mathbf{u}_0 + V_m \mathbf{z}_m = \mathbf{u}_0 + V_m (W_m^T \mathbf{A}V_m)^{-1} W_m^T \mathbf{r}_0. \quad (6.5)$$

From (6.5) we can see that the existence of  $\mathbf{u}_m$  is dependent on the non-singularity of the matrix  $W_m^T \mathbf{A}V_m$ . Therefore it becomes important to carefully choose the subspaces  $\mathcal{V}_m$  and  $\mathcal{W}_m$ .

In practice, they are chosen to be *Krylov* subspaces, which are defined as:

$$\mathcal{K}_m = \mathcal{K}(\mathbf{r}_0, A, m) = \text{span}\{\mathbf{r}_0, A\mathbf{r}_0, \dots, A^{m-1}\mathbf{r}_0\}. \quad (6.6)$$

Modern iterative methods use *Krylov* subspaces divided into three main classes depending on the choice of  $\mathcal{V}_m$  and  $\mathcal{W}_m$ :

- **The Ritz-Galerkin approach** ( $\mathcal{W}_m = \mathcal{V}_m = \mathcal{K}(\mathbf{r}_0, A, m)$ ).

In this approach we seek  $\mathbf{u}_m$  so that the residual is orthogonal to the current space. If  $A$  is symmetric positive definite, then  $\|\mathbf{u}_m - \mathbf{u}\|_A$  is minimized. The conjugate gradient method falls into this category when the matrix is symmetric positive definite. Another method is the Full orthogonalization method (**FOM**).

- **The Petrov-Galerkin approach** ( $\mathcal{V}_m = \mathcal{K}(\mathbf{r}_0, A, m)$ ;  $\mathcal{W}_m = \mathcal{K}(\mathbf{r}_0, A^T, m)$ )

In the case of  $A$  symmetric, this approach is equivalent to the first one. However, this case was mainly designed for non-symmetric problems. Some illustrations of this approach are the biconjugate gradient method (BICG) and the conjugate gradient squared method (CGS).

- **The minimum residual approach** ( $\mathcal{V}_m = \mathcal{K}(\mathbf{r}_0, A, m)$ ;  $\mathcal{W}_m = A\mathcal{K}(\mathbf{r}_0, A, m)$ )

In this approach  $\mathbf{u}_m$  is obtained such that  $\|\mathbf{f} - A\mathbf{u}_m\|_2$  is minimized. Examples of these methods are the Conjugate Residual method and the very popular GMRES method.

The GMRES method is well known for being able to solve sparse linear systems with a nonsymmetric nonsingular matrix. In practice, to compute the value of  $\mathbf{x}_m$  a set of  $m$  orthogonal basis vectors has to be generated and stored and this set has to be expanded with one new basis vector in each iteration. To overcome this issue, one can restart GMRES if  $m$  exceeds a threshold. This procedure is called the restarted GMRES method (GMRES( $m$ )), where  $m$  is the maximal dimension of

the *Krylov* subspace. The price that one has to pay for restarting is that GMRES loses its optimality property, and convergence may slow down considerably [72]. An exhaustive analysis of both versions can be found in [66].

In order to predict and analyze the convergence of GMRES, several upper bounds on the residual norm have been proposed. A class of such bounds are based on the  $H$ -field of values of any matrix  $M$  defined in [65] as:

$$\mathcal{W}_H(M) = \left\{ z \in \mathbb{C} : z = \frac{x^* H M x}{x^* H x} =: \frac{\langle x, Mx \rangle_H}{\langle x, x \rangle_H}, \quad x \in \mathbb{C}^n \setminus \{0\} \right\},$$

where  $H \in \mathbb{R}^{n \times n}$  is a symmetric positive-definite matrix. This class of bounds has many advantages: they are easy to compute and play an important role in the analysis of preconditioners; more precisely, to prove that the solution technique is independent of the mesh parameters. The classical bounds of the GMRES-residual norm are based on the field of values [45, 73, 65] as:

$$\frac{\|\mathbf{r}^k\|_H}{\|\mathbf{r}^0\|_H} \leq \left( 1 - \frac{\xi_1^2}{\xi_2^2} \right)^{k/2}, \quad k = 0, 1, \dots \quad (6.7)$$

where:

$$\xi_1 = \min_{z \in \mathcal{W}_H(M)} \Re(z) = \min_{x \in \mathbb{R}^n \setminus \{0\}} \frac{\langle x, Mx \rangle_H}{\langle x, x \rangle_H}, \quad \text{and} \quad \xi_2 = \max_{z \in \mathcal{W}_H(M)} |z|.$$

More bounds can be found in [20, 73].

Many other iterative methods have been proposed in the literature. The reader may consult [9, 65, 25] for more details.



## 6.2 Domain decomposition methods (DD)

DD methods have a long history going back to the nineteenth century. They are often referred to as divide and conquer techniques as they divide the domain into subdomains and then obtain the solution by solving smaller problems on these subdomains. Such a formulation creates a very natural framework for solvers, which are easily parallelized on coarse grain parallel computers. They are commonly classified into two major categories: overlapping and non-overlapping subdomain algorithms.

### 6.2.1 Overlapping subdomains algorithms

In general, overlapping algorithms are generally referred to as Schwarz methods as they can be seen as an extension of the work done by Hermann Schwarz in 1870 [68]. In his work Hermann Schwarz [68], proposed a new approach for solving PDE on an exotic domain by dividing the domain into two simple domains, namely a disc and a rectangle. The main feature of this approach is that the original domain  $\Omega$  is subdivided into a finite number  $N$  of overlapping subdomains  $\Omega_i$  such that:

$$\Omega = \bigcup_{i=1}^N \Omega_i, \quad \text{for } i = 1, \dots, N. \quad (6.8)$$

Let  $I_i$  denote the indices of the nodes in the interior domain  $\Omega_i$ , and  $n_i$  the number of indices in  $I_i$ , we have for  $i = 1, \dots, N$

$$I = \bigcup_{i=1}^N I_i, \quad \text{and} \quad n < \sum_{i=1}^N n_i \quad (\text{due to overlap}) \quad (6.9)$$

where  $n$  is the number of unknowns in  $\Omega$ .

Let also  $R_i^T$  be the rectangular  $n \times n_i$  extension matrix of the domain  $\Omega_i$  such that:

$$(R_i^T x_i)_k = \begin{cases} (x_i)_k & \text{for } k \in I_i, \\ 0 & \text{for } k \in I - I_i \end{cases} \quad (6.10)$$

where  $x_i$  is a given subvector of length  $n_i$ . Schwarz methods can be classified into two categories:

- Additive Schwarz methods described by:

$$\mathbf{u}_{m+1} = \mathbf{u}_m + \sum_{i=1}^N R_i^T A^{-1} R_i (\mathbf{f} - A\mathbf{u}_m). \quad (6.11)$$

- Multiplicative Schwarz methods described by:

$$\mathbf{u}_{m+1} = \mathbf{u}_m + \prod_{i=1}^N R_i^T A^{-1} R_i (\mathbf{f} - A\mathbf{u}_m). \quad (6.12)$$

where  $A_i = R_i A R_i^T$  the restriction of  $A$  to  $\Omega_i$ . In practice both equations (6.12) and (6.11) are often preconditioned (See [67, 65] for more details) in a way that they can be used within an accelerator such as GMRES. One of the main drawbacks of overlapping subdomain algorithms is that they are not efficient as the overlap becomes smaller [11], and also for elliptic equations with large jump coefficients [78]. Therefore, it is better to consider non-overlapping domain decomposition algorithms. This will be covered in the next section.

## 6.2.2 Non-overlapping subdomains algorithms

In contrast to overlapping subdomains algorithms, the original domain  $\Omega$  is subdivided into a finite number  $N$  of non-overlapping subdomains  $\Omega_i$ :

$$\begin{aligned}\bar{\Omega} &= \bigcup_{i=1}^N \bar{\Omega}_i, \\ \Omega_i \cap \Omega_j &= \emptyset \quad (i \neq j).\end{aligned}\tag{6.13}$$

The main feature of any non-overlapping subdomains algorithm is that the original system (6.1) can be transformed into a reduced system on the interface  $\Gamma$ .

To understand this transformation, let us define the following sets:

$$I = \bigcup_{i=1}^N I_i, \quad \text{and} \quad \Gamma = \bigcup_{i=1}^N \Gamma_i;\tag{6.14}$$

where  $I_i$  denotes the indices of the nodes in the interior domain  $\Omega_i$ , and  $\Gamma_i$  the indices of the nodes which lie on the boundary  $\partial\Omega_i \setminus \partial\Omega$ .

Using (6.14), the original linear system (6.1) can be partitioned as:

$$\begin{pmatrix} A_{II} & A_{I\Gamma} \\ A_{\Gamma I} & A_{\Gamma\Gamma} \end{pmatrix} \begin{pmatrix} \mathbf{u}_I \\ \mathbf{u}_\Gamma \end{pmatrix} = \begin{pmatrix} \mathbf{f}_I \\ \mathbf{f}_\Gamma \end{pmatrix}.\tag{6.15}$$

where  $A_{II} = \bigoplus_{i=1}^N A_{I_i I_i}$ .

By using a block LU-factorization of  $A$ , the system (6.15) can be written as:

$$\begin{pmatrix} I & 0 \\ A_{\Gamma I}^T A_{II}^{-1} & I \end{pmatrix} \begin{pmatrix} A_{II} & A_{I\Gamma} \\ 0 & S_{\Gamma\Gamma} \end{pmatrix} \begin{pmatrix} \mathbf{u}_I \\ \mathbf{u}_\Gamma \end{pmatrix} = \begin{pmatrix} \mathbf{f}_I \\ \mathbf{f}_\Gamma \end{pmatrix}\tag{6.16}$$

where:

$$S_{\Gamma\Gamma} = A_{\Gamma\Gamma} - A_{\Gamma I}^T A_{II}^{-1} A_{I\Gamma}$$

is the Schur complement of  $A_{\Gamma\Gamma}$  in  $A$ .

By using block Gaussian elimination, the unknowns in the interior of the subdomains  $\mathbf{u}_I$  can be eliminated in (6.16), and we arrive at the following equation for  $\mathbf{u}_\Gamma$ :

$$S_{\Gamma\Gamma} \mathbf{u}_\Gamma = \mathbf{f}_\Gamma - A_{\Gamma I}^T A_{II}^{-1} \mathbf{f}_I. \quad (6.17)$$

The system (6.17) is called the Schur complement system for the interface unknowns. It presents many properties such as:

- The right hand side of the equation (6.17) can be obtained using  $N$  independent subdomain solvers,
- for second order elliptic problems the condition number of  $S_{\Gamma\Gamma}$  is  $O(h^{-1})$ , an improvement over the  $O(h^{-2})$  growth for  $A$  [9].

The main advantage of system (6.17) is that it can be solved using any type of iterative method. However, a good preconditioner is needed to improve the convergence of the system.

**Remark 6.2.1** *In practice, it is computationally cheap to perform the iteration on the larger system (6.15) with  $A_{\Gamma I} = 0$ , and construct a preconditioner from the factorization in (6.16) by replacing  $S_{\Gamma\Gamma}$  by its preconditioner  $\tilde{S}_{\Gamma\Gamma}$ . This is due to the fact that computing  $S_{\Gamma\Gamma}$  is too expensive as the matrix  $A_{II}^{-1}$  is dense.*

A good review of domain decomposition algorithms can be found in [16] and an excellent comparison between some existing non-overlapping and overlapping domain decompo-

sitions algorithms in [14, 13]. For applications and recent progress on domain decomposition the reader should refer to the the annual international conference on Domain Decomposition methods and also to the proceedings of conferences which are available electronically in [1]. The rest of the thesis will focus on designing a parallel solver using a non-overlapping domain decomposition method together with projective iterative methods. Our aim is to obtain a solver with a performance independent of the problem size and the problem parameters.

# CHAPTER 7

## NON-OVERLAPPING DOMAIN DECOMPOSITION METHODS FOR REACTION-DIFFUSION SYSTEMS

Domain Decomposition (DD) methods have been widely used to solve many different varieties of PDE. The main reason for the popularity of these methods is the straightforward applicability for parallel computing; this means domain decomposition algorithms are usually faster even when they are implemented on monoprocessor computers. Other benefits include: easy handling of global solution domains of complex and irregular domain, the possibility of using different numerical techniques in different subdomains and most importantly, they can be used as an iterative solver. A wide variety of applications and techniques of domain decomposition can be found in the proceedings of the international conference on domain decomposition [1]. It is important to observe that most of the domain decomposition algorithms used refer to a standard approach and little has been done on reaction-diffusion systems [28, 39, 47, 63, 70]. In this chapter, we present an substructuring formulation of non-overlapping domain decomposition methods for reaction-diffusion by addressing the problem directly on the interface. A similar study

for reaction diffusion equations has been carried out in [5] and for some simple model problems on uniform meshes in [3, 10, 17, 61]. The Steklov–Poincaré operator equation is derived and studied together with different technical tools from functional analysis.

## 7.1 Domain decomposition formulation

Let us recall the problem (5.1):

$$\left\{ \begin{array}{l} -D\Delta \mathbf{u} + M(\mathbf{x})\mathbf{u} = \mathbf{f} \text{ on } \Omega, \\ \mathbf{u} = \mathbf{0} \text{ on } \partial\Omega_D, \\ \mathbf{n} \cdot \nabla \mathbf{u} = \mathbf{0} \text{ on } \partial\Omega_N. \end{array} \right. \quad (7.1)$$

Consider a non-overlapping subdivision of the original domain  $\Omega \in \mathbb{R}^d$  as described in (6.13):

$$\bar{\Omega} = \bigcup_{i=1}^N \bar{\Omega}_i, \quad \Omega_i \cap \Omega_j = \emptyset \ (i \neq j), \quad \Gamma_i = \partial\Omega_i \setminus \partial\Omega, \quad \Gamma = \bigcup_{i=1}^N \Gamma_i;$$

with  $\Gamma \subset \mathbb{R}^{d-1}$ .

Let us also denote by  $\mathbf{u}_i = \mathbf{u}|_{\Omega_i}$  the solution  $\mathbf{u}$  on each subdomain  $\Omega_i$  and  $\mathbf{u}_i|_{\Gamma_i} = \boldsymbol{\lambda}_i$  the solution on each interface. The problem (7.1) can be written as:

$$\left\{ \begin{array}{l} \mathcal{L}\mathbf{u}_i + M(\mathbf{x})\mathbf{u}_i = \mathbf{f} \text{ on } \Omega_i, \\ \mathbf{u}_i = \mathbf{0} \text{ on } \partial\Omega_i \cap \partial\Omega_D, \\ \mathbf{n} \cdot \nabla \mathbf{u}_i = \mathbf{0} \text{ on } \partial\Omega_i \cap \partial\Omega_N, \\ \mathbf{u}_i = \boldsymbol{\lambda}_i \text{ on } \Gamma_i \end{array} \right. \quad (7.2)$$

where:

$$\mathcal{L} := -D\Delta + M(\mathbf{x}).$$

By setting  $\mathbf{u}_i = \mathbf{w}_i + \mathbf{v}_i$ , from (7.2) we obtain the following two sets of subproblems :

$$\left\{ \begin{array}{l} \mathcal{L}\mathbf{w}_i = \mathbf{f} \text{ in } \Omega_i, \\ \mathbf{w}_i = \mathbf{0} \text{ on } \partial\Omega_i \cap \partial\Omega_D, \\ \mathbf{n} \cdot \nabla\mathbf{w}_i = \mathbf{0} \text{ on } \partial\Omega_i \cap \partial\Omega_N, \\ \mathbf{w}_i = \mathbf{0} \text{ on } \Gamma_i \end{array} \right. \quad (7.3a)$$

$$\left\{ \begin{array}{l} \mathcal{L}\mathbf{v}_i = \mathbf{0} \text{ in } \Omega_i, \\ \mathbf{v}_i = \mathbf{0} \text{ on } \partial\Omega_i \cap \partial\Omega_D, \\ \mathbf{n} \cdot \nabla\mathbf{v}_i = \mathbf{0} \text{ on } \partial\Omega_i \cap \partial\Omega_N, \\ \mathbf{v}_i = \boldsymbol{\lambda}_i \text{ on } \Gamma_i. \end{array} \right. \quad (7.3b)$$

Here,  $\mathbf{w}_i$  is dependent only on the data  $\mathbf{f}$ , whilst  $\mathbf{v}_i$  depends solely on the value  $\boldsymbol{\lambda}_i$  on  $\Gamma_i$ . In other words,  $\mathbf{v}_i$  can be seen as the  $\mathcal{L}$ -extensions of  $\boldsymbol{\lambda}_i$  to the domain  $\Omega_i$ . Henceforth, such generalized  $\mathcal{L}$ -extensions of functions  $\boldsymbol{\lambda}$  or  $\boldsymbol{\lambda}_i$  will be denoted by  $E\boldsymbol{\lambda}$  and  $E_i\boldsymbol{\lambda}_i$  respectively. Any other extensions will be denoted by  $F\boldsymbol{\lambda}$  and  $F_i\boldsymbol{\lambda}_i$ . To find an equation for  $\boldsymbol{\lambda}_i$  we integrate the set of equations in (7.3a) and (7.3b) against  $\mathbf{z}_i \in H_D^1(\Omega_i) \times H_D^1(\Omega_i)$  on  $\Omega_i$  to obtain:

$$- \int_{\Gamma_i} \mathbf{n}_i \nabla \mathbf{w}_i \cdot \mathbf{z}_i \, ds + \int_{\Omega_i} (\nabla \mathbf{w}_i : \nabla \mathbf{z}_i + (\mathbf{M} \mathbf{w}_i) \cdot \mathbf{z}_i) \, d\Omega_i = \int_{\Omega_i} \mathbf{f} \cdot \mathbf{z}_i \, d\Omega_i; \quad (7.4)$$

and:

$$- \int_{\Gamma_i} \mathbf{n}_i \nabla \mathbf{v}_i \cdot \mathbf{z}_i \, ds + \int_{\Omega_i} (\nabla \mathbf{v}_i : \nabla \mathbf{z}_i + (\mathbf{M} \mathbf{v}_i) \cdot \mathbf{z}_i) \, d\Omega_i = \mathbf{0}. \quad (7.5)$$



Adding both (7.4) and (7.5) together and then summing over  $i$  we obtain:

$$\begin{aligned}
\sum_{i=1}^N \left( \int_{\Omega_i} \nabla(\mathbf{w}_i + \mathbf{v}_i) : \nabla \mathbf{z}_i \, d\Omega_i \right) + \sum_{i=1}^N \left( \int_{\Omega_i} (\mathbf{M}(\mathbf{w}_i + \mathbf{v}_i)) \cdot \mathbf{z}_i \, d\Omega_i \right) &= \sum_{i=1}^N \int_{\Omega_i} \mathbf{f} \cdot \mathbf{z}_i \, d\Omega_i \\
&+ \sum_{i=1}^N \int_{\Gamma_i} \mathbf{n}_i \nabla \mathbf{w}_i \cdot \mathbf{z}_i \, ds \\
&+ \sum_{i=1}^N \int_{\Gamma_i} \mathbf{n}_i \nabla \mathbf{v}_i \cdot \mathbf{z}_i \, ds.
\end{aligned} \tag{7.6}$$

Using the weak formulation of the initial problem (5.6) in (7.6), we find:

$$\sum_{i=1}^N \int_{\Gamma_i} \mathbf{n}_i \nabla E_i \lambda_i \cdot \mathbf{z}_i \, ds = - \sum_{i=1}^N \int_{\Gamma_i} \mathbf{n}_i \nabla \mathbf{w}_i \cdot \mathbf{z}_i \, ds \tag{7.7}$$

Analogously to the scalar diffusion problem, the Steklov-Poincaré matrix operator acting on  $\Lambda \times \Lambda$  can be defined as:

$$\langle \mathcal{S}\boldsymbol{\lambda}, \boldsymbol{\mu} \rangle = \sum_{i=1}^N \int_{\Gamma_i} \mathbf{n}_i \cdot \nabla(E\lambda_i) \cdot \boldsymbol{\mu}_i \, ds(\Gamma_i) := \sum_{i=1}^N \langle \mathcal{S}_i \lambda_i, \mu_i \rangle, \tag{7.8}$$

for all  $\boldsymbol{\lambda}, \boldsymbol{\mu} \in \Lambda \times \Lambda$  with  $\lambda|_{\Gamma_i} := \lambda_i$ ,  $\mu|_{\Gamma_i} := \mu_i$  and:

$$\mathcal{S} : \Lambda \times \Lambda \rightarrow \Lambda' \times \Lambda'.$$

The operator  $\mathcal{S}$  can be represented after using integration by parts as:

$$\langle \mathcal{S}\boldsymbol{\lambda}, \boldsymbol{\mu} \rangle = B(E\boldsymbol{\lambda}, F\boldsymbol{\mu}) = \sum_{i=1}^N B_i(E_i \lambda_i, F_i \mu_i), \quad \forall \boldsymbol{\lambda}, \boldsymbol{\mu} \in \Lambda \times \Lambda; \tag{7.9}$$

with the bilinear form  $B_i(\cdot, \cdot)$  defined similarly to  $B(\cdot, \cdot)$ :

$$B_i(\mathbf{u}_i, \mathbf{z}_i) = (\mathbf{D}\nabla \mathbf{u}_i, \nabla \mathbf{z}_i)_{\Omega_i} + ((\mathbf{M}(\mathbf{x})\mathbf{u}_i), \mathbf{z}_i)_{\Omega_i}. \tag{7.10}$$

The above definition of  $\mathcal{S}$  leads to a reformulation of the problem (5.1) as an ordered sequence of three decoupled sets of problems, which involve an operator  $\mathcal{L} := -D\Delta + M(\mathbf{x})$  with possibly mixed conditions on each subdomain, and a problem set on the interface  $\Gamma$ . These are given by:

$$\left\{ \begin{array}{l} \mathcal{L}\mathbf{w}_i = \mathbf{f} \text{ in } \Omega_i, \\ \mathbf{w}_i = \mathbf{0} \text{ on } \partial\Omega_i \cap \partial\Omega_D, \\ \mathbf{n} \cdot \nabla \mathbf{w}_i = \mathbf{0} \text{ on } \partial\Omega_i \cap \partial\Omega_N, \\ \mathbf{w}_i = \mathbf{0} \text{ on } \Gamma_i, \end{array} \right. \quad (7.11a)$$

$$\left\{ \begin{array}{l} \mathcal{S}\boldsymbol{\lambda} = -\sum_{i=1}^N \mathbf{n}_i \cdot \nabla \mathbf{w}_i \text{ on } \Gamma, \end{array} \right. \quad (7.11b)$$

$$\left\{ \begin{array}{l} \mathcal{L}\mathbf{v}_i = \mathbf{0} \text{ in } \Omega_i, \\ \mathbf{v}_i = \mathbf{0} \text{ on } \partial\Omega_i \cap \partial\Omega_D, \\ \mathbf{n} \cdot \nabla \mathbf{v}_i = \mathbf{0} \text{ on } \partial\Omega_i \cap \partial\Omega_N, \\ \mathbf{v}_i = \boldsymbol{\lambda}_i \text{ on } \Gamma_i. \end{array} \right. \quad (7.11c)$$

Given the representation (7.8), one can show that  $\mathcal{S}$  is a bounded positive operator on  $\Lambda \times \Lambda$ .

**Lemma 7.1.1** *Let  $\mathcal{S}$  be defined as in (7.8). Then there exist constants  $\alpha_1, \alpha_2$  such that for all  $\boldsymbol{\lambda}, \boldsymbol{\mu} \in \Lambda \times \Lambda$*

$$\alpha_1 \|\boldsymbol{\lambda}\|_{1/2, \Gamma}^2 \leq \langle \mathcal{S}\boldsymbol{\lambda}, \boldsymbol{\lambda} \rangle, \quad \langle \mathcal{S}\boldsymbol{\lambda}, \boldsymbol{\mu} \rangle \leq \alpha_2 \|\boldsymbol{\lambda}\|_{1/2, \Gamma} \|\boldsymbol{\mu}\|_{1/2, \Gamma}.$$

**Proof:** Let  $\mathbf{v}_i = E_i \boldsymbol{\lambda}_i$ ,  $\mathbf{w}_i = E_i \boldsymbol{\mu}_i$  satisfy the problem of the type (7.11c) and assume (5.2) and (5.3) hold. We have:

$$\begin{aligned} \langle \mathcal{S}_i \boldsymbol{\lambda}_i, \boldsymbol{\lambda}_i \rangle &= B_i(\mathbf{v}_i, \mathbf{v}_i) = \int_{\Omega} \nabla \mathbf{v}_i : \nabla \mathbf{v}_i + \mathbf{v}_i^T M(\mathbf{x}) \mathbf{v}_i \, d\mathbf{x}, \\ &\geq \|\nabla \mathbf{v}_i\|_0^2 + \gamma_{min} \|\mathbf{v}_i\|_0^2, \\ &\geq \min\{1, \gamma_{min}\} \|\mathbf{v}_i\|_1^2. \end{aligned}$$

$$\begin{aligned} \langle \mathcal{S}_i \boldsymbol{\lambda}_i, \boldsymbol{\mu}_i \rangle &= B_i(\mathbf{v}_i, \mathbf{w}_i) = \int_{\Omega} \nabla \mathbf{v}_i : \nabla \mathbf{w}_i + \mathbf{v}_i^T M(\mathbf{x}) \mathbf{w}_i \, d\mathbf{x}. \\ &\leq |\mathbf{v}_i|_1 |\mathbf{w}_i|_1 + \gamma_{max} \|\mathbf{v}_i\|_0 \|\mathbf{w}_i\|_0, \\ &\leq \max\{\sqrt{2}, \sqrt{2}\gamma_{max}\} \|\mathbf{v}_i\|_1 \|\mathbf{w}_i\|_1. \end{aligned}$$

Moreover, using the elliptic regularity result [2], which is known to hold for the weak solution of (7.11c), we get:

$$\|\mathbf{v}_i\|_{1, \Omega_i} = \|E_i \boldsymbol{\lambda}_i\|_{1, \Omega_i} \leq C_e \|\boldsymbol{\lambda}_i\|_{1/2, \Gamma_i}, \quad \|\mathbf{w}_i\|_{1, \Omega_i} = \|E_i \boldsymbol{\mu}_i\|_{1, \Omega_i} \leq C_e \|\boldsymbol{\mu}_i\|_{1/2, \Gamma_i}. \quad (7.12)$$

Since  $\gamma_0 \mathbf{v}_i = \boldsymbol{\lambda}_i$  and  $\gamma_0 \mathbf{w}_i = \boldsymbol{\mu}_i$ , the trace inequalities (2.3) read for all  $i = 1, \dots, N$

$$\|\boldsymbol{\lambda}_i\|_{1/2, \Gamma_i} \leq C_{\gamma}(\Omega_i) \|\mathbf{v}_i\|_1, \quad \|\boldsymbol{\mu}_i\|_{1/2, \Gamma_i} \leq C_{\gamma}(\Omega_i) \|\mathbf{w}_i\|_1$$

and the result follows from (7.12) and the definition in (7.8) of the operator  $\mathcal{S}$ . ■

## 7.2 Mixed variational formulation

The weak formulations of problems (7.11a)-(7.11c) reads:

$$\left\{ \begin{array}{l} \text{Find } \mathbf{w}_i \in H_D^1(\Omega_i) \times H_D^1(\Omega_i) \text{ such that for all } \mathbf{z}_i \in H_D^1(\Omega_i) \times H_D^1(\Omega_i) \\ B_i(\mathbf{w}_i, \mathbf{z}_i) = (\mathbf{f}_i, \mathbf{z}_i), \quad \forall i = 1, \dots, N. \end{array} \right. \quad (7.13a)$$

$$\left\{ \begin{array}{l} \text{Find } \boldsymbol{\lambda} \in \Lambda \times \Lambda \text{ such that for all } \boldsymbol{\eta} \in \Lambda \times \Lambda \\ \mathcal{S}(\boldsymbol{\lambda}, \boldsymbol{\eta}) := \langle \mathcal{S}\boldsymbol{\lambda}, \boldsymbol{\eta} \rangle = \sum_{i=1}^N [(\mathbf{f}_i, F_i \boldsymbol{\eta}_i) - B_i(\mathbf{w}_i, F_i \boldsymbol{\eta}_i)]. \end{array} \right. \quad (7.13b)$$

$$\left\{ \begin{array}{l} \text{Find } \tilde{\mathbf{v}}_i \in H_D^1(\Omega_i) \times H_D^1(\Omega_i) \text{ such that for all } \mathbf{z}_i \in H_D^1(\Omega_i) \times H_D^1(\Omega_i) \\ B_i(\tilde{\mathbf{v}}_i, \mathbf{z}_i) = B_i(\mathbf{v}_i, \mathbf{z}_i) - B_i(\mathbf{t}_i, \mathbf{z}_i) = -B_i(\mathbf{t}_i, \mathbf{z}_i), \quad \forall i = 1, \dots, N. \end{array} \right. \quad (7.13c)$$

With  $\tilde{\mathbf{v}}_i = \mathbf{v}_i - \mathbf{t}_i$ , and  $\mathbf{t}_i = F_i \boldsymbol{\lambda}_i$  any extension of  $\boldsymbol{\lambda}_i$  to  $\Omega_i$  satisfying  $\mathbf{n}_i \cdot \nabla \mathbf{t}_i = 0$  on  $\partial\Omega_i \cap \partial\Omega_N$  and  $\mathbf{t}_i = 0$  on  $\partial\Omega_i \cap \partial\Omega_D$ .

## 7.3 FEM discretization

Consider a triangulation  $\mathcal{T}_h$  of the domain  $\Omega$  by a finite union of elements  $K \in \mathcal{T}_h$  as described in subsection 5.4. Let  $P_r(\mathbf{t})$  be the space of polynomials in  $d$  variables of degree  $r$  defined on a set  $\mathbf{t} \subset \mathbb{R}^d$ . We denote by:

$$V^h = V^{h,r} := \left\{ w \in C^0(\Omega) : w|_{\mathbf{t}} \in P_r(\mathbf{t}) \quad \forall \mathbf{t} \in \mathcal{T}_h, \quad w|_{\partial\Omega_D} = 0 \right\} \subset H_D^1(\Omega)$$

a finite-dimensional space of dimension  $n$  of piecewise polynomial functions defined on a triangulation  $\mathcal{T}_h$  of  $\Omega$  into simplices  $\mathbf{t}$  of maximum diameter  $h$ . Similarly we define:

$$V_i^h = V_i^{h,r} := \left\{ w \in C^0(\Omega_i) : w|_{\mathbf{t}} \in P_r(\mathbf{t}) \quad \forall \mathbf{t} \in \mathcal{T}_h, \quad w|_{\partial\Omega_D \cap \partial\Omega_i} = 0 \right\} \subset H_D^1(\Omega_i).$$

Also let  $\phi_k^i$  denote the basis functions of  $V_i^h$  with support in  $\Omega_i$  and: write

$$V_{iI}^h = \text{span}\{\phi_k^i, k = 1 \cdots n_i^I\},$$

with:

$$n_I = \sum_i^N n_i^I, \quad \text{and} \quad n_\Gamma = n - n_I.$$

Finally, we consider:

$$S^h = \text{span}\{\psi_{k-n_I} = \gamma_0(\Gamma)\phi_k, k = n_I + 1 \cdots n_I + n_\Gamma\}.$$

Using the above definitions, the finite element discretization of problems (7.11a)-(7.11c) reads:

$$\left\{ \begin{array}{l} \text{Find } \mathbf{w}_{hi} \in V_{iI}^h \times V_{iI}^h \text{ such that for all } \mathbf{z}_i \in V_{iI}^h \times V_{iI}^h \\ B_i(\mathbf{w}_{hi}, \mathbf{z}_{hi}) = (\mathbf{f}_i, \mathbf{z}_{hi}), \quad \forall i = 1, \dots, N. \end{array} \right. \quad (7.14a)$$

$$\left\{ \begin{array}{l} \text{Find } \boldsymbol{\lambda}_h \in S^h \times S^h \text{ such that for all } \boldsymbol{\eta}_h \in S^h \times S^h \\ s(\boldsymbol{\lambda}_h, \boldsymbol{\eta}_h) := \langle \mathcal{S}\boldsymbol{\lambda}_h, \boldsymbol{\eta}_h \rangle = \sum_{i=1}^N [(\mathbf{f}_i, F_i\boldsymbol{\eta}_{hi}) - B_i(\mathbf{w}_{hi}, F_i\boldsymbol{\eta}_{hi})]. \end{array} \right. \quad (7.14b)$$

$$\left\{ \begin{array}{l} \text{Find } \tilde{\mathbf{v}}_{hi} \in V_{iI}^h \times V_{iI}^h \text{ such that for all } \mathbf{z}_{hi} \in V_{iI}^h \times V_{iI}^h \\ B_i(\tilde{\mathbf{v}}_{hi}, \mathbf{z}_{hi}) = -B_i(\mathbf{t}_{hi}, \mathbf{z}_{hi}), \quad \forall i = 1, \dots, N. \end{array} \right. \quad (7.14c)$$

Note that  $\mathbf{t}_{hi}$  is the finite element projection of  $\mathbf{t}_i = F_i\lambda_i$ .

The result of Lemma 7.1.1 also holds in the discrete case for the choice of space  $S^h \times S^h$ .

Using the above notation, we can now write the following coercivity and continuity bounds for  $s(\cdot, \cdot)$ .

**Lemma 7.3.1** *Let  $\mathcal{S}$  be defined as in (7.8). Then there exist constants  $\alpha_1, \alpha_2$  such that*

for all  $\boldsymbol{\lambda}_h, \boldsymbol{\mu}_h \in S^h \times S^h \subset \Lambda \times \Lambda$

$$\alpha_1 \|\boldsymbol{\lambda}_h\|_{1/2, \Gamma}^2 \leq s(\boldsymbol{\lambda}_h, \boldsymbol{\lambda}_h), \quad s(\boldsymbol{\lambda}_h, \boldsymbol{\mu}_h) \leq \alpha_2 \|\boldsymbol{\lambda}_h\|_{1/2, \Gamma} \|\boldsymbol{\mu}_h\|_{1/2, \Gamma}. \quad (7.15)$$

## 7.4 Matrix formulation

Let  $\{\boldsymbol{\phi}_k\}$  denote a basis of  $V^h \times V^h$ . By letting:

$$\mathbf{u}_h(\mathbf{x}) = \sum_k^{2(n_I+n_\Gamma)} \mathbf{u}_k \boldsymbol{\phi}_k(\mathbf{x}),$$

we obtain the following linear system:

$$\begin{pmatrix} A_{II}^{(1)} & A_{I\Gamma}^{(1)} & M_{II}^{(1)} & M_{I\Gamma}^{(1)} \\ A_{\Gamma I}^{(1)} & A_{\Gamma\Gamma}^{(1)} & M_{\Gamma I}^{(1)} & M_{\Gamma\Gamma}^{(1)} \\ M_{II}^{(2)} & M_{I\Gamma}^{(2)} & A_{II}^{(2)} & A_{I\Gamma}^{(2)} \\ M_{\Gamma I}^{(2)} & M_{\Gamma\Gamma}^{(2)} & A_{\Gamma I}^{(2)} & A_{\Gamma\Gamma}^{(2)} \end{pmatrix} \begin{pmatrix} u_{1I} \\ u_{1\Gamma} \\ u_{2I} \\ u_{2\Gamma} \end{pmatrix} = \begin{pmatrix} f_{1I} \\ f_{1\Gamma} \\ f_{2I} \\ f_{2\Gamma} \end{pmatrix}; \quad (7.16)$$

in which subscripts  $I$  and  $\Gamma$  refer to the interior nodes and the interface nodes respectively,  $A^{(j)} := d_j L + M(\alpha_j)$  and  $M^{(j)} := M(\beta_j)$ . The matrices  $M(\alpha_j)$  and  $M(\beta_j)$  are weighted mass matrices, whilst  $L$  represents the discrete stiffness matrix. We also denote by:

$$S_{A^{(j)}} := A_{\Gamma\Gamma}^{(j)} - A_{\Gamma I}^{(j)} (A_{II}^{(j)})^{-1} A_{I\Gamma}^{(j)}, \quad (7.17)$$

the corresponding local Schur complement associated with  $A^{(j)}$ .

Equation (8.1) can be rewritten as:

$$\mathbf{A}\mathbf{u} = \begin{pmatrix} A_{II} & A_{I\Gamma} \\ A_{\Gamma I} & A_{\Gamma\Gamma} \end{pmatrix} \begin{pmatrix} \mathbf{u}_I \\ \mathbf{u}_\Gamma \end{pmatrix} = \begin{pmatrix} \mathbf{f}_I \\ \mathbf{f}_\Gamma \end{pmatrix}, \quad (7.18)$$

where:

$$A_{\mu\nu} = \begin{pmatrix} d_1 L_{\mu\nu} + M_{\mu\nu}(\alpha_1) & M_{\mu\nu}(\beta_1) \\ M_{\mu\nu}(\beta_2) & d_2 L_{\mu\nu} + M_{\mu\nu}(\alpha_2) \end{pmatrix}, \mathbf{u}_\nu = \begin{pmatrix} u_{1\nu} \\ u_{2\nu} \end{pmatrix}, \mathbf{f}_\nu = \begin{pmatrix} f_{1\nu} \\ f_{2\nu} \end{pmatrix}, \mu, \nu \in \{I, \Gamma\}.$$

The following result is standard and follows from the equivalence between (5.7) and (7.14) [6].

**Proposition 7.4.1** *The algebraic representations of equations (7.14a), (7.14b) and (7.14c) are given by:*

$$\begin{aligned} A_{II} \mathbf{w}_I &= \mathbf{f}_I, \\ S \mathbf{u}_\Gamma &= \mathbf{f}_\Gamma - A_{\Gamma I} \mathbf{w}_I, \\ \mathbf{v}_I &= A_{II}^{-1} A_{I\Gamma} \mathbf{u}_\Gamma, \end{aligned}$$

respectively, where  $S := A_{\Gamma\Gamma} - A_{\Gamma I} (A_{II})^{-1} A_{I\Gamma}$ . The solution is then:  $\mathbf{u} = (\mathbf{w}_I + \mathbf{v}_I, \mathbf{u}_\Gamma)$

**Proof:** The proof follows that presented in [6, p. 7]. ■

**Remark 7.4.2** *Note that the following relationships hold:*

$$\mathbf{w}_I \leftrightarrow \mathbf{w}_{hi}, \quad \mathbf{v}_I \leftrightarrow \tilde{\mathbf{v}}_{hi}, \quad \mathbf{u}_\Gamma \leftrightarrow \boldsymbol{\lambda}_h$$

via the representations:

$$\mathbf{w}_{hi} = \sum_{k=1}^{2(n_I+n_\Gamma)} (\mathbf{w}_I)_k \boldsymbol{\phi}_k, \quad \tilde{\mathbf{v}}_{hi} = \sum_{k=1}^{2(n_I+n_\Gamma)} (\mathbf{v}_I)_k \boldsymbol{\phi}_k, \quad \boldsymbol{\lambda}_h = \sum_{k=1}^{2n_\Gamma} (\mathbf{u}_\Gamma)_k \boldsymbol{\psi}_k;$$

where  $\{\boldsymbol{\psi}_k\}$ ,  $\{\boldsymbol{\phi}_k\}$  are basis for the spaces  $V^h \times V^h$  and  $S^h \times S^h$  respectively. Proposition 7.4.1 indicates that we have to consider a Schur-complement problem, therefore it becomes important to look for preconditioners of the Schur complement as  $S$  is expensive to compute.

# CHAPTER 8

## INTERFACE PRECONDITIONERS

Consider problem (5.1) with  $M \in \mathbb{R}^{2 \times 2}$  the matrix formulation of the finite element approximation presented in Chapter 5 is given by:

$$\begin{pmatrix} d_1 L + \alpha_1 M & \beta_1 M \\ \beta_2 M & d_2 L + \alpha_2 M \end{pmatrix} = \begin{pmatrix} M f_1 \\ M f_2 \end{pmatrix}. \quad (8.1)$$

It is easy to see that equation (8.1) will have the following form:

$$A \mathbf{u} = \begin{pmatrix} A_{II} & A_{I\Gamma} \\ A_{\Gamma I} & A_{\Gamma\Gamma} \end{pmatrix} \begin{pmatrix} \mathbf{u}_I \\ \mathbf{u}_\Gamma \end{pmatrix} = \begin{pmatrix} \mathbf{f}_I \\ \mathbf{f}_\Gamma \end{pmatrix}, \quad (8.2)$$

where:

$$A_{\mu\nu} = \begin{pmatrix} d_1 L_{\mu\nu} + M_{\mu\nu}(\alpha_1) & M_{\mu\nu}(\beta_1) \\ M_{\mu\nu}(\beta_2) & d_2 L_{\mu\nu} + M_{\mu\nu}(\alpha_2) \end{pmatrix}, \mathbf{u}_\nu = \begin{pmatrix} u_{1\nu} \\ u_{2\nu} \end{pmatrix}, \mathbf{f}_\nu = \begin{pmatrix} f_{1\nu} \\ f_{2\nu} \end{pmatrix}, \mu, \nu \in \{I, \Gamma\}.$$



We can see that the Schur complement  $S$  arising from the linear system (8.2) is of the form:

$$S = \begin{pmatrix} S_1 & S_2 \\ S_3 & S_4 \end{pmatrix}$$

where  $S_i$  for  $i = 1, 2, 3, 4$  are to be determined. This is a very difficult and expensive task, therefore it becomes important to look for a good preconditioner of the Schur-complement. In this chapter we present and analyze different block preconditioners of the Schur-complement for solving the linear system arising from a non-overlapping domain decomposition formulation.

## 8.1 Case of two subdomains

The domain  $\Omega$  is partitioned into two non-overlapping equal domains  $\Omega_i = (-1, 1) \times (-a, a)$  for  $i = 1, 2$ ,  $a > 0$  and uniformly subdivided into equal triangles. We denote by  $I_k$  the identity matrix of order  $k$ , where  $k$  is a positive integer. The global stiffness matrix  $L$  and the global mass matrix  $M$  can be written as:

$$L = T_n \otimes I_n + I_n \otimes T_n \quad \text{and} \quad M = \widetilde{M}_n \otimes I_n + I_n \otimes \widetilde{M}_n;$$

where:

$$T_k := \text{tridiag}[-1, 2, -1] \in \mathbb{R}^{k \times k} \quad \text{and} \quad \widetilde{M}_k := \text{tridiag} \frac{1}{6}[1, 4, 1] \in \mathbb{R}^{k \times k} \quad (8.3)$$

are respectively the element stiffness matrix and element mass matrix on a mesh with  $k$  interior points.

### 8.1.1 Eigenvalue analysis

Let us recall the system (7.18) in Chapter 7:

$$\begin{pmatrix} A_{II} & A_{IR} \\ A_{RI} & A_{RR} \end{pmatrix} \begin{pmatrix} \mathbf{u}_I \\ \mathbf{u}_R \end{pmatrix} = \begin{pmatrix} \mathbf{f}_I \\ \mathbf{f}_R \end{pmatrix}. \quad (8.4)$$

Using the notation presented in the section above the original matrices presented in (8.1) as  $L_{m,n}$  and  $M_{m,n}$ , which are respectively the corresponding stiffness and mass matrix with  $m$  interior nodes in the x-direction and  $n$  interior nodes in the y-direction. We have:

$$L_{n,n} = \begin{pmatrix} L_{m,n} & & -e_m \otimes I_n \\ & L_{m,n} & -e_1 \otimes I_n \\ -e_m^T \otimes I_n & -e_1^T \otimes I_n & T \end{pmatrix}, \quad M_{n,n} = \begin{pmatrix} M_{m,n} & & -e_m \otimes I_n \\ & M_{m,n} & -e_1 \otimes I_n \\ -e_m^T \otimes I_n & -e_1^T \otimes I_n & \bar{M} \end{pmatrix}; \quad (8.5)$$

where:

$$L_{m,n} = T_m \otimes I_n + I_m \otimes T_n, \quad M_{m,n} = N_m \otimes I_n + I_m \otimes N_n,$$

$$T = 2I_n + T_n, \quad \bar{M} = \frac{4}{6}I_n + \tilde{M}_n, \quad N = \frac{4}{6}\tilde{M},$$

and  $e_i$  denotes the  $i$ th column of  $I_m$ .

The block matrices of the system (8.1) are:

$$\begin{aligned}
A_{II} &= \begin{pmatrix} d_1 L_{m,n} + \alpha_1 M_{m,n} & \beta_1 M_{m,n} & & \\ \beta_2 M_{m,n} & d_2 L_{m,n} + \alpha_2 M_{m,n} & & \\ & & d_1 L_{m,n} + \alpha_1 M_{m,n} & \beta_1 M_{m,n} \\ & & \beta_2 M_{m,n} & d_2 L_{m,n} + \alpha_2 M_{m,n} \end{pmatrix}; \\
A_{GI} &= \begin{pmatrix} (d_1 + \alpha_1)(-e_m \otimes I_n) & \beta_1(-e_m \otimes I_n) & (d_1 + \alpha_1)(-e_1 \otimes I_n) & \beta_1(-e_1 \otimes I_n) \\ \beta_2(-e_m \otimes I_n) & (d_2 + \alpha_2)(-e_m \otimes I_n) & \beta_2(-e_1 \otimes I_n) & (d_2 + \alpha_2)(-e_1 \otimes I_n) \end{pmatrix}; \\
&= [\mathcal{C} \otimes (-e_m \otimes I_n) \quad \mathcal{C} \otimes (-e_1 \otimes I_n)] \quad \text{with} \quad \mathcal{C} = \begin{pmatrix} d_1 + \alpha_1 & \beta_1 \\ \beta_2 & d_2 + \alpha_2 \end{pmatrix}; \\
&= A_{GI}^T; \\
A_{GR} &= \begin{pmatrix} d_1 T + \alpha_1 \bar{M} & \beta_1 \bar{M} \\ \beta_2 \bar{M} & d_2 T + \alpha_2 \bar{M} \end{pmatrix}.
\end{aligned}$$

From the eigenvalues decomposition of  $T_m, N_m$  [79]:

$$T_m = V_m D_m V_m^T, \quad \text{and} \quad N_m = V_m B_m V_m^T; \quad (8.6)$$

with:

$$(D_m)_{ii} = 2 \left( 1 - \cos \frac{i\pi}{k+1} \right) =: \mu_i^{(k)} \quad (B_m)_{ii} = \frac{1}{6} \left( 4 - 2 \cos \frac{i\pi}{k+1} \right) =: \vartheta_i^{(k)} \quad (8.7)$$

and:

$$V_m = [v_1, \dots, v_m], \quad (v_j)_i = \sqrt{\frac{2}{k+1}} \sin \frac{ij\pi}{k+1}, \quad i, j = 1, \dots, k. \quad (8.8)$$

It follows:

$$L_{n,n} = (V_m \otimes V_n)D_{m,n}(V_m \otimes V_n)^T, \quad M_{n,n} = (V_m \otimes V_n)B_{m,n}(V_m \otimes V_n)^T; \quad (8.9)$$

where:

$$D_{m,n} = I_m \otimes D_n + D_m \otimes I_n \quad B_{m,n} = I_m \otimes B_n + B_m \otimes I_n.$$

Similarly,

$$d_i L_{n,n} + \alpha_i M_{n,n} = (V_m \otimes V_n)C_{m,n}^{(i)}(V_m \otimes V_n)^T \quad (8.10)$$

with:

$$C_{m,n}^{(i)} = d_i D_{m,n} + \alpha_i B_{m,n}.$$

and:

$$T = 2I_n + T_n = V_n (2I_n + D_n) V_n^T \quad \bar{M} = V_n \left( \frac{4}{6}I_n + \frac{6}{4}B_n \right) V_n^T. \quad (8.11)$$

The Schur complement of the system (8.4) is given by:

$$\begin{aligned}
S &= A_{\Gamma\Gamma} - A_{\Gamma I} A_{II}^{-1} A_{I\Gamma} = A_{\Gamma\Gamma} - \sum_{i \in \{1, m\}} C \otimes (e_i \otimes I_n) \mathcal{B}^{-1} C^T \otimes (e_i \otimes I_n)^T; \quad \text{with } \mathcal{B} = \begin{pmatrix} d_1 L_{m,n} + \alpha_1 M_{m,n} & \beta_1 M_{m,n} \\ \beta_2 M_{m,n} & d_2 L_{m,n} + \alpha_2 M_{m,n} \end{pmatrix}; \\
&= A_{\Gamma\Gamma} - 2C \otimes \underbrace{(e_m \otimes I_n) \mathcal{B}^{-1} C^T \otimes (e_m \otimes I_n)^T}_{\mathfrak{F}} \quad (8.12)
\end{aligned}$$

We have:

$$A_{\Gamma\Gamma} = \begin{pmatrix} V_n \\ V_n \end{pmatrix} \begin{pmatrix} d_1(2I_n + D_n) + \alpha_1 \left(\frac{4}{6}I_n + \frac{6}{4}B_n\right) & \beta_1 \left(\frac{4}{6}I_n + \frac{6}{4}B_n\right) \\ \beta_2 \left(\frac{4}{6}I_n + \frac{6}{4}B_n\right) & d_2(2I_n + D_n) + \alpha_2 \left(\frac{4}{6}I_n + \frac{6}{4}B_n\right) \end{pmatrix} \begin{pmatrix} V_n \\ V_n \end{pmatrix}^T. \quad (8.13)$$

Using the inverse of a partitioned matrix described by Prasolov 1991 in [51], we can write:

$$\begin{aligned}
\mathcal{B}^{-1} &= \begin{pmatrix} V_m \otimes V_n & \\ & V_m \otimes V_n \end{pmatrix} \begin{pmatrix} C_{m,n}^1 & \beta_1 B_{m,n} \\ \beta_2 B_{m,n} & C_{m,n}^2 \end{pmatrix}^{-1} \begin{pmatrix} V_m \otimes V_n & \\ & V_m \otimes V_n \end{pmatrix}^T \\
&= \begin{pmatrix} V_m \otimes V_n & \\ & V_m \otimes V_n \end{pmatrix} \begin{pmatrix} \underbrace{\left( C_{m,n}^1 - \beta_1 B_{m,n} (C_{m,n}^2)^{-1} \beta_2 B_{m,n} \right)^{-1}}_{\mathfrak{E}^1} & \\ \underbrace{\left( \beta_1 B_{m,n} - C_{m,n}^1 (\beta_2 B_{m,n})^{-1} C_{m,n}^2 \right)^{-1}}_{\mathfrak{E}^3} & \underbrace{\left( \beta_2 B_{m,n} - C_{m,n}^2 (\beta_1 B_{m,n})^{-1} C_{m,n}^1 \right)^{-1}}_{\mathfrak{E}^2} \end{pmatrix} \begin{pmatrix} V_m \otimes V_n & \\ & V_m \otimes V_n \end{pmatrix}^T
\end{aligned}$$

We also have:

$$\mathcal{C} \otimes (e_m \otimes I_n) = \begin{pmatrix} (d_1 + \alpha_1)(e_m \otimes I_n) & \beta_1(e_m \otimes I_n) \\ \beta_2(e_m \otimes I_n) & (d_2 + \alpha_2)(e_m \otimes I_n) \end{pmatrix}$$

This leads to:

$$\begin{aligned} \mathcal{C} \otimes (e_m \otimes I_n) & \begin{pmatrix} V_m \otimes V_n \\ V_m \otimes V_n \end{pmatrix} = \begin{pmatrix} (d_1 + \alpha_1)(e_m \otimes I_n) & \beta_1(e_m \otimes I_n) \\ \beta_2(e_m \otimes I_n) & (d_2 + \alpha_2)(e_m \otimes I_n) \end{pmatrix} \begin{pmatrix} V_m \otimes V_n \\ V_m \otimes V_n \end{pmatrix}; \\ & = \begin{pmatrix} (d_1 + \alpha_1)(v_m \otimes V_n) & \beta_1(v_m \otimes V_n) \\ \beta_2(v_m \otimes V_n) & (d_2 + \alpha_2)(v_m \otimes V_n) \end{pmatrix}; \end{aligned}$$

and:

$$\begin{aligned} \mathfrak{F} & = \begin{pmatrix} (d_1 + \alpha_1)(v_m \otimes V_n) & \beta_1(v_m \otimes V_n) \\ \beta_2(v_m \otimes V_n) & (d_2 + \alpha_2)(v_m \otimes V_n) \end{pmatrix} \begin{pmatrix} \mathfrak{E}^1 & \mathfrak{E}^2 \\ \mathfrak{E}^3 & \mathfrak{E}^4 \end{pmatrix} \begin{pmatrix} (d_1 + \alpha_1)(v_m \otimes V_n) & \beta_1(v_m \otimes V_n) \\ \beta_2(v_m \otimes V_n) & (d_2 + \alpha_2)(v_m \otimes V_n) \end{pmatrix}^T; \\ & = \begin{pmatrix} \mathfrak{H}^1 & \mathfrak{H}^2 \\ \mathfrak{H}^3 & \mathfrak{H}^4 \end{pmatrix}. \end{aligned}$$

Where:

$$\left\{ \begin{array}{l} \mathfrak{Y}^1 = (v_m \otimes V_n) \left( (d_1 + \alpha_1) \left( (d_1 + \alpha_1) \mathfrak{E}^1 + \beta_1 \mathfrak{E}^3 \right) + \beta_2 \left( (d_1 + \alpha_1) \mathfrak{E}^2 + \beta_1 \mathfrak{E}^4 \right) \right) (v_m \otimes V_n)^T; \\ \mathfrak{Y}^2 = (v_m \otimes V_n) \left( \beta_1 \left( (d_1 + \alpha_1) \mathfrak{E}^1 + \beta_1 \mathfrak{E}^3 \right) + (d_2 + \alpha_2) \left( (d_1 + \alpha_1) \mathfrak{E}^2 + \beta_1 \mathfrak{E}^4 \right) \right) (v_m \otimes V_n)^T; \\ \mathfrak{Y}^3 = (v_m \otimes V_n) \left( (d_1 + \alpha_1) \left( \beta_2 \mathfrak{E}^1 + (d_2 + \alpha_2) \mathfrak{E}^3 \right) + \beta_2 \left( \beta_2 \mathfrak{E}^2 + (d_2 + \alpha_2) \mathfrak{E}^4 \right) \right) (v_m \otimes V_n)^T; \\ \mathfrak{Y}^4 = (v_m \otimes V_n) \left( \beta_1 \left( \beta_2 \mathfrak{E}^1 + (d_2 + \alpha_2) \mathfrak{E}^3 \right) + (d_2 + \alpha_2) \left( \beta_2 \mathfrak{E}^2 + (d_2 + \alpha_2) \mathfrak{E}^4 \right) \right) (v_m \otimes V_n)^T. \end{array} \right. \quad (8.14)$$

(8.14) can be written as:

$$\left\{ \begin{array}{l} \mathfrak{Y}^1 = \sum_{i=1}^m (v_m)_i^2 V_n \left( (d_1 + \alpha_1) \left( (d_1 + \alpha_1) \mathfrak{E}^1 + \beta_1 \mathfrak{E}^3 \right) + \beta_2 \left( (d_1 + \alpha_1) \mathfrak{E}^2 + \beta_1 \mathfrak{E}^4 \right) \right) V_n^T; \\ \mathfrak{Y}^2 = \sum_{i=1}^m (v_m)_i^2 V_n \left( \beta_1 \left( (d_1 + \alpha_1) \mathfrak{E}^1 + \beta_1 \mathfrak{E}^3 \right) + (d_2 + \alpha_2) \left( (d_1 + \alpha_1) \mathfrak{E}^2 + \beta_1 \mathfrak{E}^4 \right) \right) V_n^T; \\ \mathfrak{Y}^3 = \sum_{i=1}^m (v_m)_i^2 V_n \left( (d_1 + \alpha_1) \left( \beta_2 \mathfrak{E}^1 + (d_2 + \alpha_2) \mathfrak{E}^3 \right) + \beta_2 \left( \beta_2 \mathfrak{E}^2 + (d_2 + \alpha_2) \mathfrak{E}^4 \right) \right) V_n^T; \\ \mathfrak{Y}^4 = \sum_{i=1}^m (v_m)_i^2 V_n \left( \beta_1 \left( \beta_2 \mathfrak{E}^1 + (d_2 + \alpha_2) \mathfrak{E}^3 \right) + (d_2 + \alpha_2) \left( \beta_2 \mathfrak{E}^2 + (d_2 + \alpha_2) \mathfrak{E}^4 \right) \right) V_n^T. \end{array} \right. \quad (8.15)$$

Using (8.13) and (8.15) in (8.12), then:

$$S = \begin{pmatrix} V_n & & \\ & V_n & \\ & & V_n \end{pmatrix} \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} V_n \\ V_n \\ V_n \end{pmatrix}^T; \quad (8.16)$$

where:

$$\begin{cases} S_{11} = d_1(2I_n + D_n) + \alpha_1\left(\frac{4}{6}I_n + \frac{6}{4}B_n\right) - 2\sum_{i=1}^m (v_m)_i^2 \left( (d_1 + \alpha_1)\mathfrak{E}^1 + \beta_1\mathfrak{E}^3 \right) + \beta_2 \left( (d_1 + \alpha_1)\mathfrak{E}^2 + \beta_1\mathfrak{E}^4 \right); \\ S_{12} = \beta_1\left(\frac{4}{6}I_n + \frac{6}{4}B_n\right) - 2\sum_{i=1}^m (v_m)_i^2 \left( \beta_1 \left( (d_1 + \alpha_1)\mathfrak{E}^1 + \beta_1\mathfrak{E}^3 \right) + (d_2 + \alpha_2) \left( (d_1 + \alpha_1)\mathfrak{E}^2 + \beta_1\mathfrak{E}^4 \right) \right); \\ S_{21} = \beta_2\left(\frac{4}{6}I_n + \frac{6}{4}B_n\right) - 2\sum_{i=1}^m (v_m)_i^2 \left( (d_1 + \alpha_1)(\beta_2\mathfrak{E}^1 + (d_2 + \alpha_2)\mathfrak{E}^3) + \beta_2 \left( \beta_2\mathfrak{E}^2 + (d_2 + \alpha_2)\mathfrak{E}^4 \right) \right); \\ S_{22} = d_2(2I_n + D_n) + \alpha_2\left(\frac{4}{6}I_n + \frac{6}{4}B_n\right) - 2\sum_{i=1}^m (v_m)_i^2 \left( \beta_1 \left( \beta_2\mathfrak{E}^1 + (d_2 + \alpha_2)\mathfrak{E}^3 \right) + (d_2 + \alpha_2) \left( \beta_2\mathfrak{E}^2 + (d_2 + \alpha_2)\mathfrak{E}^4 \right) \right). \end{cases} \quad (8.17)$$

Thus, the eigenvalue  $\lambda_{S_{i,j}}$  of  $S_{i,j}$  for  $i, j = 1, 2$  are:

$$\begin{cases} \lambda_j(S_{11}) = d_1(2 + \lambda_{D_n}) + \alpha_1\left(\frac{4}{6} + \frac{6}{4}\lambda_{B_n}\right) - 2\sum_{i=1}^m (v_m)_i^2 \left( (d_1 + \alpha_1)\lambda_{\mathfrak{E}^1} + \beta_1\lambda_{\mathfrak{E}^3} \right) + \beta_2 \left( (d_1 + \alpha_1)\lambda_{\mathfrak{E}^2} + \beta_1\lambda_{\mathfrak{E}^4} \right); \\ \lambda_j(S_{12}) = \beta_1\left(\frac{4}{6} + \frac{6}{4}\lambda_{B_n}\right) - 2\sum_{i=1}^m (v_m)_i^2 \left( \beta_1 \left( (d_1 + \alpha_1)\lambda_{\mathfrak{E}^1} + \beta_1\lambda_{\mathfrak{E}^3} \right) + (d_2 + \alpha_2) \left( (d_1 + \alpha_1)\lambda_{\mathfrak{E}^2} + \beta_1\lambda_{\mathfrak{E}^4} \right) \right); \\ \lambda_j(S_{21}) = \beta_2\left(\frac{4}{6} + \frac{6}{4}\lambda_{B_n}\right) - 2\sum_{i=1}^m (v_m)_i^2 \left( (d_1 + \alpha_1)(\beta_2\lambda_{\mathfrak{E}^1} + (d_2 + \alpha_2)\lambda_{\mathfrak{E}^3}) + \beta_2 \left( \beta_2\lambda_{\mathfrak{E}^2} + (d_2 + \alpha_2)\lambda_{\mathfrak{E}^4} \right) \right); \\ \lambda_j(S_{22}) = d_2(2 + \lambda_{D_n}) + \alpha_2\left(\frac{4}{6} + \frac{6}{4}\lambda_{B_n}\right) - 2\sum_{i=1}^m (v_m)_i^2 \left( \beta_1 \left( \beta_2\lambda_{\mathfrak{E}^1} + (d_2 + \alpha_2)\lambda_{\mathfrak{E}^3} \right) + (d_2 + \alpha_2) \left( \beta_2\lambda_{\mathfrak{E}^2} + (d_2 + \alpha_2)\lambda_{\mathfrak{E}^4} \right) \right); \end{cases} \quad (8.18)$$



where:

$$\begin{cases} \lambda_j(\mathfrak{S}^1) = \frac{\lambda C_{m,n}^2}{\lambda C_{m,n}^1 - \lambda C_{m,n}^2 - \beta_1 \beta_2 \lambda_{B_{m,n}}^2}; \\ \lambda_j(\mathfrak{S}^2) = \frac{\beta_1 \beta_2 \lambda_{B_{m,n}}^2}{\beta_1 \lambda_{B_{m,n}}} = -\frac{\beta_1 \lambda_{B_{m,n}} \lambda(\mathfrak{S}^4)}{\lambda C_{m,n}^2}; \\ \lambda_j(\mathfrak{S}^3) = \frac{\beta_2 \lambda_{B_{m,n}}}{\beta_1 \beta_2 \lambda_{B_{m,n}} - \lambda C_{m,n}^1} = -\frac{\beta_2 \lambda_{B_{m,n}} \lambda(\mathfrak{S}^4)}{\lambda C_{m,n}^2}; \\ \lambda_j(\mathfrak{S}^4) = \frac{\lambda C_{m,n}^1}{\lambda C_{m,n}^1 - \lambda C_{m,n}^2 - \beta_1 \beta_2 \lambda_{B_{m,n}}^2} = \frac{\lambda C_{m,n}^1 \lambda(\mathfrak{S}^1)}{\lambda C_{m,n}^2}. \end{cases} \quad (8.19)$$

If we consider only the diagonal entries of the matrix  $S$ , using (8.19) we obtain:

$$\begin{aligned} \lambda_j(S_{11}) &= d_1(2 + \lambda_{D_n}) + \alpha_1 \left( \frac{4}{6} + \frac{6}{4} \lambda_{B_n} \right) - 2 \sum_{i=1}^m (v_m)_i^2 \left( (d_1 + \alpha_1) \lambda_{\mathfrak{S}^1} + \beta_1 \lambda_{\mathfrak{S}^3} + \beta_2 ((d_1 + \alpha_1) \lambda_{\mathfrak{S}^2} + \beta_1 \lambda_{\mathfrak{S}^4}) \right)_i; \\ &= d_1(2 + \lambda_{D_n}) + \alpha_1 \left( \frac{4}{6} + \frac{6}{4} \lambda_{B_n} \right) - 2 \sum_{i=1}^m (v_m)_i^2 \left( (d_1 + \alpha_1)^2 - \frac{\beta_1 \beta_2 (d_1 + \alpha_1) \lambda_{B_{m,n}}}{\lambda C_{m,n}^2} - \frac{\beta_1 \beta_2 (d_1 + \alpha_1) \lambda_{B_{m,n}}}{\lambda C_{m,n}^1} + \frac{\beta_1 \beta_2 \lambda C_{m,n}^2}{\lambda C_{m,n}^1} \right)_i \left[ \frac{1}{\lambda C_{m,n}^1 - \frac{\beta_1 \beta_2 \lambda_{B_{m,n}}^2}{\lambda C_{m,n}^2}} \right]_i; \\ &= d_1(2 + \lambda_{D_n}) + \alpha_1 \left( \frac{4}{6} + \frac{6}{4} \lambda_{B_n} \right) - 2 \sum_{i=1}^m (v_m)_i^2 \left( (d_1 + \alpha_1)^2 - 2 \frac{\beta_1 \beta_2 (d_1 + \alpha_1) \lambda_{B_{m,n}}}{\lambda C_{m,n}^2} + \frac{\beta_1 \beta_2 \lambda C_{m,n}^2}{\lambda C_{m,n}^1} \right)_i \left[ \frac{1}{\lambda C_{m,n}^1 - \frac{\beta_1 \beta_2 \lambda_{B_{m,n}}^2}{\lambda C_{m,n}^2}} \right]_i. \end{aligned} \quad (8.20)$$

Similarly:

$$\begin{aligned} \lambda_j(S_{22}) &= d_2(2 + \lambda_{D_n}) + \alpha_2 \left( \frac{4}{6} + \frac{6}{4} \lambda_{B_n} \right) - 2 \sum_{i=1}^m (v_m)_i^2 \left( \beta_1 (\beta_2 \lambda_{\mathfrak{S}^1} + (d_2 + \alpha_2) \lambda_{\mathfrak{S}^3}) + (d_2 + \alpha_2) (\beta_2 \lambda_{\mathfrak{S}^2} + (d_2 + \alpha_2) \lambda_{\mathfrak{S}^4}) \right)_i; \\ &= d_1(2 + \lambda_{D_n}) + \alpha_1 \left( \frac{4}{6} + \frac{6}{4} \lambda_{B_n} \right) - 2 \sum_{i=1}^m (v_m)_i^2 \left( (d_2 + \alpha_2)^2 - 2 \frac{\beta_1 \beta_2 (d_2 + \alpha_2) \lambda_{B_{m,n}}}{\lambda C_{m,n}^1} + \frac{\beta_1 \beta_2 \lambda C_{m,n}^1}{\lambda C_{m,n}^2} \right)_i \left[ \frac{1}{\lambda C_{m,n}^2 - \frac{\beta_1 \beta_2 \lambda_{B_{m,n}}^2}{\lambda C_{m,n}^1}} \right]_i. \end{aligned} \quad (8.21)$$

In order to derive the approximations for  $\lambda_j(S_{22})$  and  $\lambda_j(S_{11})$ , lets recall the Schur-complement for a reaction diffusion

equation:

$$s_i = d_i(2I_n + D_n) + \alpha_i \left( \frac{4}{6} I_n + \frac{6}{4} B_n \right) - 2 \sum_{i=1}^m (v_m)_i^2 \frac{(d_i + \alpha_i)^2}{C_{m,n}^i}; \quad (8.22)$$

which eigenvalues are given by:

$$\lambda(s_i) = d_i(2 + \lambda_{D_n}) + \alpha_i \left( \frac{4}{6} + \frac{6}{4} \lambda_{B_n} \right) - 2 \sum_{i=1}^m (v_m)_i^2 \frac{(d_i + \alpha_i)^2}{\lambda_{C_{m,n}^i}}. \quad (8.23)$$

If we use the argument that  $\alpha_i \gg \beta_i$  for  $i = 1, 2$ , we can have the following approximations for eigenvalues of  $\lambda_j(S_{22})$  and

$\lambda_j(S_{11})$ :

$$\begin{aligned} \lambda_j(S_{11}) &= d_1(2 + \lambda_{D_n}) + \alpha_1 \left( \frac{4}{6} + \frac{6}{4} \lambda_{B_n} \right) - 2 \sum_{i=1}^m (v_m)_i^2; \left( \left[ (d_1 + \alpha_1)^2 - 2 \frac{\beta_1 \beta_2 (d_1 + \alpha_1) \lambda_{B_{m,n}}}{\lambda_{C_{m,n}^2}} + \frac{\beta_1 \beta_2 \lambda_{C_{m,n}^2}}{\lambda_{C_{m,n}^1}} \right] \left[ \frac{1}{\lambda_{C_{m,n}^1} - \frac{\beta_1 \beta_2 \lambda_{B_{m,n}}^2}{\lambda_{C_{m,n}^2}}} \right] \right)_i \\ &\approx \lambda(s_1); \end{aligned} \quad (8.24)$$

and:

$$\begin{aligned} \lambda_j(S_{22}) &= d_1(2 + \lambda_{D_n}) + \alpha_1 \left( \frac{4}{6} + \frac{6}{4} \lambda_{B_n} \right) - 2 \sum_{i=1}^m (v_m)_i^2; \left( \left[ (d_2 + \alpha_2)^2 - 2 \frac{\beta_1 \beta_2 (d_2 + \alpha_2) \lambda_{B_{m,n}}}{\lambda_{C_{m,n}^1}} + \frac{\beta_1 \beta_2 \lambda_{C_{m,n}^1}}{\lambda_{C_{m,n}^2}} \right] \left[ \frac{1}{\lambda_{C_{m,n}^2} - \frac{\beta_1 \beta_2 \lambda_{B_{m,n}}^2}{\lambda_{C_{m,n}^1}}} \right] \right)_i \\ &\approx \lambda(s_2); \end{aligned} \quad (8.25)$$

The equations (8.25), (8.25) give us a good idea of what one should consider when looking for a block preconditioner of the Schur complement of a reaction-diffusion system. The same idea is also obtained when having to deal with more than two subdomains. This is discussed in the next section.

## 8.2 Case of many subdomains

Consider a non-overlapping subdivision of the original domain  $\Omega \in \mathbb{R}^d$  such that:

$$\bar{\Omega} = \bigcup_{i=1}^N \bar{\Omega}_i, \quad \Omega_i \cap \Omega_j = \emptyset \ (i \neq j), \quad \Gamma_i = \partial\Omega_i \setminus \partial\Omega, \quad \Gamma = \bigcup_{i=1}^N \Gamma_i;$$

with  $\Gamma \subset \mathbb{R}^{d-1}$ . The same system (8.4) is obtained with:

$$A_{II} = \begin{pmatrix} d_1 L_{II} + \alpha_1 M_{II} & \beta_1 M_{II} \\ \beta_2 M_{II} & d_2 L_{II} + \alpha_2 M_{II} \end{pmatrix};$$

$$A_{I\Gamma} = \begin{pmatrix} d_1 L_{I\Gamma} + \alpha_1 M_{I\Gamma} & \beta_1 M_{I\Gamma} \\ \beta_2 M_{I\Gamma} & d_2 L_{I\Gamma} + \alpha_2 M_{I\Gamma} \end{pmatrix};$$

$$A_{\Gamma I} = \begin{pmatrix} d_1 L_{\Gamma I} + \alpha_1 M_{\Gamma I} & \beta_1 M_{\Gamma I} \\ \beta_2 M_{\Gamma I} & d_2 L_{\Gamma I} + \alpha_2 M_{\Gamma I} \end{pmatrix};$$

$$A_{\Gamma\Gamma} = \begin{pmatrix} d_1 L_{\Gamma\Gamma} + \alpha_1 M_{\Gamma\Gamma} & \beta_1 M_{\Gamma\Gamma} \\ \beta_2 M_{\Gamma\Gamma} & d_2 L_{\Gamma\Gamma} + \alpha_2 M_{\Gamma\Gamma} \end{pmatrix}.$$

Since the matrices  $L, M$  are symmetric and positive-definite, there exists a matrix  $Q$  such that [Section 7.6][32]:

$$Q^T L Q = D \quad \text{and} \quad Q^T M Q = I; \quad (8.26)$$

where  $(D)_{ii} = \lambda_i(M^{-1}L)$ , denotes the  $i$ th eigenvalue of the matrix  $M^{-1}L$ .

The system (8.4) can be re-written as:

$$\tilde{A}\tilde{\mathbf{u}} = \begin{pmatrix} \tilde{A}_{II} & 0 \\ 0 & \tilde{A}_{\Gamma\Gamma} \end{pmatrix} \begin{pmatrix} \tilde{\mathbf{u}}_I \\ \tilde{\mathbf{u}}_\Gamma \end{pmatrix} = \begin{pmatrix} \tilde{\mathbf{f}}_I \\ \tilde{\mathbf{f}}_\Gamma \end{pmatrix}, \quad (8.27)$$

where:

$$\tilde{A}_{II} = \begin{pmatrix} d_1 D_{II} + \alpha_1 I_{II} & \beta_1 I_{II} \\ \beta_2 I_{II} & d_2 D_{II} + \alpha_2 I_{II} \end{pmatrix};$$

$$\tilde{A}_{\Gamma\Gamma} = \begin{pmatrix} d_1 D_{\Gamma\Gamma} + \alpha_1 I_{\Gamma\Gamma} & \beta_1 I_{\Gamma\Gamma} \\ \beta_2 I_{\Gamma\Gamma} & d_2 D_{\Gamma\Gamma} + \alpha_2 I_{\Gamma\Gamma} \end{pmatrix}.$$

The Schur complement of the system (8.27) is given by:

$$\tilde{S}_{\Gamma\Gamma} = \tilde{A}_{\Gamma\Gamma}. \quad (8.28)$$

The expression of the Schur-complement  $\tilde{S}_{\Gamma\Gamma}$  in (8.28) confirms that a good preconditioner requires an efficient approximation of the Steklov-Poincaré operator on the interface. It is well known that the inverse of the Steklov-Poincaré operator can be expressed explicitly using the Green's function restricted to the interface [77], however computing the Green's function remains a difficult task.

Following the discussions in [53, 33, 17], it is feasible to consider the following precondi-

tioner for  $\tilde{S}_{\Gamma\Gamma}$ :

$$\tilde{P}_{\tilde{S}_{\Gamma\Gamma}} = \begin{pmatrix} d_1 D_{\Gamma\Gamma} + \alpha_1 I_{\Gamma\Gamma} & 0 \\ 0 & d_2 D_{\Gamma\Gamma} + \alpha_2 I_{\Gamma\Gamma} \end{pmatrix}. \quad (8.29)$$

### 8.2.1 Eigenvalue analysis

Consider a triangulation of the solution domain  $\Omega$  as described in section 5.4:  $\Omega$  into a set  $\mathcal{T}_h = \{K_1, \dots, K_N\}$  of non-overlapping triangles  $K_i$  such that:

$$\bar{\Omega} = \bigcup_{K \in \mathcal{T}_h} K = K_1 \cup K_2 \dots \cup K_N; \quad (8.30)$$

where  $h_K$  be the diameter of the circumscribed circle of  $K$ , with:

$$h = \max_{K \in \mathcal{T}_h} h_K, \quad h_{min} = \min_{K \in \mathcal{T}_h} h_K. \quad (8.31)$$

We will make use of the eigenvalue bounds for the Galerkin Mass matrix and Stiffness Matrix presented in [21, p. 57-60] for the two dimensional case:

**Lemma 8.2.1** *Given a finite element approximation such that (8.30) and (8.31) hold. A realistic bounds for eigenvalues of the Mass matrix and the Stiffness matrix are given by:*

$$\kappa_2 h^2 < \lambda_i(M) \leq \kappa_1 h^2 \quad \text{and} \quad \tilde{\kappa}_2 h^2 < \lambda_i(L) \leq \tilde{\kappa}_1; \quad \kappa_2, \kappa_1, \tilde{\kappa}_1, \tilde{\kappa}_2 \in \mathbb{R}. \quad (8.32)$$

The above Lemma allows us to derive the following theorem: Then, it holds:

**Theorem 8.2.2** *Given a finite element approximation such that (8.30) and (8.31) hold, the eigenvalues of the matrix  $M^{-1}L$  are bound below and above by:*

$$\gamma < \lambda_i(LM^{-1}) \leq \zeta h^{-2}; \quad \gamma, \zeta \in \mathbb{R}. \quad (8.33)$$

**Proof:**

$$\begin{aligned}\lambda_i(M^{-1}L) &= \lambda_i(M^{-1})\lambda_i(L); \\ &= \frac{1}{\lambda_i(M)}\lambda_i(L);\end{aligned}$$

The result follows from the Lemma 8.2.1. ■

**Theorem 8.2.3** *The eigenvalues of  $\tilde{P}_{\tilde{S}_{\Gamma\Gamma}}^{-1}\tilde{S}_{\Gamma\Gamma}$  satisfy*

$$\lambda_i(\tilde{P}_{\tilde{S}_{\Gamma\Gamma}}^{-1}\tilde{S}_{\Gamma\Gamma}) \in \left[ 1 - \sqrt{\frac{\beta_1\beta_2}{(d_1\gamma + \alpha_1)(d_2\gamma + \alpha_2)}}, \quad 1 + \sqrt{\frac{\beta_1\beta_2}{(d_1\gamma + \alpha_1)(d_2\gamma + \alpha_2)}} \right]. \quad (8.34)$$

**Proof:** The eigenvalues of  $\tilde{P}_{\tilde{S}_{\Gamma\Gamma}}^{-1}\tilde{S}_{\Gamma\Gamma}$  satisfy:

$$\begin{pmatrix} d_1D + \alpha_1I & 0 \\ 0 & d_2D + \alpha_2I \end{pmatrix}^{-1} \begin{pmatrix} d_1D + \alpha_1I & \beta_1I \\ \beta_2I & d_2D + \alpha_2I \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \lambda \begin{pmatrix} x \\ y \end{pmatrix}. \quad (8.35)$$

From (8.35), we obtain the following system of equations:

$$\begin{cases} Ix + \mathcal{B}y = \lambda Ix \\ \mathcal{F}x + Iy = \lambda Iy \end{cases} \implies \begin{cases} \mathcal{B}y = xI(\lambda - 1) \\ \mathcal{F}x = yI(\lambda - 1) \end{cases} \quad (8.36)$$

where:

$$\mathcal{B} = (d_1D + \alpha_1I)^{-1}\beta_1I \quad \text{and} \quad \mathcal{F} = (d_2D + \alpha_2I)^{-1}\beta_2I.$$

The matrices  $\mathcal{B}$  and  $\mathcal{F}$  are diagonal matrices with entries:

$$(\mathcal{B}_n)_{ii} = b_i = \frac{\beta_1}{d_1\lambda_i(M^{-1}L) + \alpha_1}, \quad \text{and} \quad (\mathcal{F}_n)_{ii} = f_i = \frac{\beta_2}{d_2\lambda_i(M^{-1}L) + \alpha_2} \quad (8.37)$$

From (8.36) we obtain the following:

$$\mathcal{F}x = x\mathcal{B}^{-1}(\lambda - 1)(\lambda - 1) \implies x(I(\lambda - 1)(\lambda - 1) - \mathcal{B}\mathcal{F}) = 0.$$

The value of  $\lambda_i$  is obtained by solving the following quadratic equation:

$$\lambda_i^2 - 2\lambda_i + 1 - b_i f_i = 0.$$

This yields:

$$\lambda_i = 1 \pm \sqrt{b_i f_i} \implies \lambda_i = 1 \pm \sqrt{\frac{\beta_1 \beta_2}{(d_1 \lambda_i (M^{-1}L) + \alpha_1)(d_2 \lambda_i (M^{-1}L) + \alpha_2)}} \quad (\text{using (8.37)}).$$

From inequality (8.33), we obtain:

$$\lambda_i \in \left[ 1 - \sqrt{\frac{\beta_1 \beta_2}{(d_1 \gamma + \alpha_1)(d_2 \gamma + \alpha_2)}}, \quad 1 + \sqrt{\frac{\beta_1 \beta_2}{(d_1 \gamma + \alpha_1)(d_2 \gamma + \alpha_2)}} \right].$$

■

We can also consider the preconditioner for  $\tilde{S}_{\Gamma\Gamma}$  to be:

$$\tilde{P}_{\tilde{S}_{\Gamma\Gamma}} = \begin{pmatrix} d_1 D_{\Gamma\Gamma} + \alpha_1 I_{\Gamma\Gamma} & \beta_1 I_{\Gamma\Gamma} \\ 0 & D_{\Gamma\Gamma} + \alpha_2 I_{\Gamma\Gamma} \end{pmatrix}. \quad (8.38)$$

**Theorem 8.2.4** *The eigenvalues of  $\tilde{P}_{\tilde{S}_{\Gamma\Gamma}}^{-1} \tilde{S}_{\Gamma\Gamma}$  satisfy:*

$$\lambda_i(\tilde{P}_{\tilde{S}_{\Gamma\Gamma}}^{-1} \tilde{S}_{\Gamma\Gamma}) \in \left[ 1 - \frac{\beta_1 \beta_2}{(d_1 \gamma + \alpha_1)(d_2 \gamma + \alpha_2)}, \quad 1 \right]. \quad (8.39)$$

**Proof:** The eigenvalues of  $\tilde{P}_{\tilde{S}_{rr}}^{-1} \tilde{S}_{rr}$  satisfy:

$$\begin{pmatrix} d_1 D + \alpha_1 I & \beta_1 I \\ 0 & d_2 D + \alpha_2 I \end{pmatrix}^{-1} \begin{pmatrix} d_1 D + \alpha_1 I & \beta_1 I \\ \beta_2 I & d_2 D + \alpha_2 I \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \lambda \begin{pmatrix} x \\ y \end{pmatrix}. \quad (8.40)$$

using the fact that:

$$\begin{pmatrix} d_1 D + \alpha_1 I & \beta_1 I \\ 0 & d_2 D + \alpha_2 I \end{pmatrix}^{-1} = \begin{pmatrix} (d_1 D + \alpha_1 I)^{-1} & -(d_1 D + \alpha_1 I)^{-1} \beta_1 I (d_2 D + \alpha_2 I)^{-1} \\ 0 & (d_2 D + \alpha_2 I)^{-1} \end{pmatrix};$$

we obtain:

$$\begin{cases} \mathcal{A}x = \lambda Ix \\ \mathcal{C}x + Iy = \lambda Iy \end{cases} \quad (8.41)$$

where:

$$\mathcal{A} = I - (d_1 D + \alpha_1 I)^{-1} \beta_1 I (d_2 D + \alpha_2 I)^{-1} \beta_2 I$$

and:

$$\mathcal{C} = (d_1 D + \alpha_1 I)^{-1} \beta_2 I.$$

$\mathcal{A}$  and  $\mathcal{C}$  are diagonal matrices with the following entries:

$$\begin{aligned} (\mathcal{A}_n)_{ii} = a_i &= 1 - \frac{\beta_1 \beta_2}{(d_1 \lambda_i (M^{-1} L) + \alpha_1)(d_2 \lambda_i (M^{-1} L) + \alpha_2)} \\ (\mathcal{C}_n)_{ii} = c_i &= \frac{\beta_2}{d_1 \lambda_i (M^{-1} L) + \alpha_1}. \end{aligned} \quad (8.42)$$

From (8.41) the following cases are obtained:

**if**  $x = 0 \Rightarrow \lambda = 1$ .

This means that we have at least  $n$  eigenvalues equal to 1. We just have to look at



the  $n$  other eigenvalues.

if  $\mathcal{A} = \lambda I$ .

We obtain from (8.42):

$$\lambda_i = a_i = 1 - \frac{\beta_1 \beta_2}{(d_1 \lambda_i(M^{-1}L) + \alpha_1)(d_2 \lambda_i(M^{-1}L) + \alpha_2)}. \quad (8.43)$$

Therefore using the inequality (8.33), we can write:

$$\lambda_i \in \left[ 1 - \frac{\beta_1 \beta_2}{(d_1 \gamma + \alpha_1)(d_2 \gamma + \alpha_2)}, \quad 1 \right].$$

■

We observe from (8.39) and (8.34) that both intervals are closer to 1 and independent of the mesh-size  $h$ . However, one of the main drawbacks associated with these approaches is that they are not convenient if the grid on the interface is non-uniform or does not have a natural multigrid structure [77].

All of the preconditioners presented in this chapter are related to the block structure of the Schur-complement. Therefore it would be interesting to look into the Schur-complement operator itself. In other words, to exploit the fact the Steklov-Poincaré operators arising in a non-overlapping **DD**-algorithm are coercive and continuous with respect to Sobolev norms of index  $1/2$  as in [5, 7, 8]. This will be considered in the next chapter.

# CHAPTER 9

## INTERFACE PRECONDITIONERS ASSOCIATED WITH FRACTIONAL SOBOLEV NORMS

In a recent paper, Caetano et al. [12] introduced a non-overlapping domain decomposition algorithm of Schwarz waveform relaxation type for semilinear reaction-diffusion equations. For solving the interface problem they proposed a new type of nonlinear transmission: using Robin or Ventcell transmission conditions, which leads to a solution technique independent of the mesh parameter. However, this has not been extended to reaction-diffusion systems. In this chapter we present an alternative approach to approximate the Steklov-Poincaré operators arising from a non-overlapping **DD**-algorithm for reaction diffusion systems. Our approach is related to that in [6]. The coercivity and the continuity of the Steklov-Poincaré operators arising in a non-overlapping domain decomposition algorithm for scalar elliptic problems with respect to Sobolev norms of index  $1/2$  allow us to construct a new interface preconditioner, which leads to solution techniques independent of the mesh size  $h$ .

## 9.1 Interpolation space

We briefly review the interpolation theory for Hilbert spaces presented in Lions and Magenes 1968 [43, chapter 1, section 2]. Let  $X, Y$  be two Hilbert spaces with scalar products  $(\cdot, \cdot)_X, (\cdot, \cdot)_Y$  and norms  $\| \cdot \|_X, \| \cdot \|_Y$  respectively. We assume that:

$$X \subset Y, \quad X \text{ dense in } Y \quad \text{with continuous injection.} \quad (9.1)$$

Then there exists a positive self-adjoint operator:  $\mathcal{L} : X \rightarrow Y$  (see Riesz Sz-Nagy, 1956), such that:

$$(u, v)_X = (u, \mathcal{L}v)_Y, \quad \forall u, v \in X \quad (9.2)$$

The spectral properties of  $\mathcal{L}$  allow us to define a new operator  $\zeta = \mathcal{L}^{1/2}$  which is also positive definite and self-adjoint in  $Y$  with domain  $X$  denoted  $D(\zeta)$ . Furthermore, the norm of  $X$  is equivalent to the graph norm:  $\| \cdot \|_\zeta$ :

$$\|u\|_X \sim \|u\|_\zeta := \left( \|u\|_Y^2 + \|\zeta u\|_Y^2 \right)^{1/2}. \quad (9.3)$$

It is also possible to define any real power of  $\zeta$  by using the spectral decomposition of  $\zeta$ .

**Definition 9.1.1** *Let  $0 < \theta < 1$ . We denote by:*

1.  $[X, Y]_\theta := D(\zeta^{1-\theta})$  *the interpolation space of index  $\theta$  for the pair  $[X, Y]$ .*
2.  $\|u\|_\theta := \left( \|u\|_Y^2 + \|\zeta^{1-\theta}u\|_Y^2 \right)^{1/2}$  *the norm on  $[X, Y]_\theta$ .*

**Remark 9.1.2** 1.  $D(\zeta^{1-\theta})$  *is endowed with the inner product  $(u, v)_\theta = (u, v)_Y + (u, \zeta^{1-\theta}v)_Y$ ;*

2.  $[X, Y]_0 = X$  and  $[X, Y]_1 = Y$ .

3. For any  $\theta_1, \theta_2$  such that  $0 < \theta_1 < \theta_2 < 1$ , we have

$$X \subset [X, Y]_{\theta_1} \subset [X, Y]_{\theta_2} \subset Y.$$

Finally, it is important to note the main interpolation theorem presented in Lions and Magenes 1968 [43, chapter 1, section 5].

**Theorem 9.1.3** *Let  $\mathfrak{X}, \mathfrak{Y}$  be two Hilbert spaces with the same properties as  $X$  and  $Y$  respectively. Let  $\pi$  be a continuous linear operator from  $X$  into  $\mathfrak{X}$ , and from  $Y$  into  $\mathfrak{Y}$  i.e.*

$$\pi \in \mathcal{L}(X, \mathfrak{X}) \cap \mathcal{L}(Y, \mathfrak{Y}),$$

then for all  $\theta \in (0, 1)$

$$\pi \in \mathcal{L}([X, Y]_{\theta}; [\mathfrak{X}, \mathfrak{Y}]_{\theta}).$$

## 9.2 Finite dimensional spaces

In the following section we consider the case when  $X = \mathcal{X} \times \mathcal{X}, Y = \mathcal{Y} \times \mathcal{Y}, X_h = \mathcal{X}_h \times \mathcal{X}_h, Y_h = \mathcal{Y}_h \times \mathcal{Y}_h$ , with  $\mathcal{X}_h \subset \mathcal{X}, \mathcal{Y}_h \subset \mathcal{Y}$  two finite-dimensional subspaces with dimension  $n$ . They are Hilbert spaces when endowed with the inner-products  $\langle \cdot, \cdot \rangle_X, \langle \cdot, \cdot \rangle_Y$ . As in the previous subsection we define the corresponding positive, self-adjoint operator

$\zeta_h = \mathcal{L}_h^{1/2}, \mathcal{L}_h : \mathcal{X}_h \times \mathcal{X}_h \rightarrow \mathcal{Y}_h \times \mathcal{Y}_h$  such that:

$$(u_h, v_h)_X = (u_h, \mathcal{L}_h v_h)_Y, \quad u_h, v_h \in X_h \times X_h. \quad (9.4)$$

Similarly, we denote the domain of  $\zeta_h$  by  $D(\zeta_h)$ , which in turn is  $X_h \times X_h$ , and the scale of discrete norms as:

$$\|u_h\|_{1/2,h} := \left( \|u_h\|_Y^2 + \|\zeta_h u_h\|_Y^2 \right)^{1/2}, \quad \forall u_h \in X_h \times X_h. \quad (9.5)$$

Furthermore using the definition (9.1.1), we can define:

$$[X_h, Y_h]_\theta := D(\zeta_h^{1-\theta});$$

and the scale of discrete norms as:

$$\|u_h\|_{\theta,h} := \left( \|u_h\|_Y^2 + \|\zeta_h^{1-\theta} u_h\|_Y^2 \right)^{1/2}, \quad \forall u_h \in X_h \times X_h. \quad (9.6)$$

Let  $\mathbf{H}_X$  and  $\mathbf{H}_Y$  be the Grammian matrices corresponding to the inner products  $(\cdot, \cdot)_X$ ,  $(\cdot, \cdot)_Y$  respectively and  $\{\psi_i\}_{1 \leq i \leq n}$  denotes a basis of  $\mathcal{X}_h$ .

Let also  $\mathcal{Q}$  be the basis of  $\mathcal{X}_h \times \mathcal{X}_h$  such that:

$$\mathcal{Q} = \left\{ \begin{pmatrix} \psi_j \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \psi_j \end{pmatrix}, j = 1, \dots, n \right\}. \quad (9.7)$$

Then  $\mathbf{H}_X, \mathbf{H}_Y$  can be written as:

$$\mathbf{H}_X = G_X \oplus G_X, \quad \mathbf{H}_Y = G_Y \oplus G_Y, \quad (9.8)$$

where:

$$(G_X)_{ij} = \langle \psi_i, \psi_j \rangle_X; \quad (G_Y)_{ij} = \langle \psi_i, \psi_j \rangle_Y \quad 1 \leq i, j \leq n.$$

And the corresponding norms  $\| \cdot \|_X, \| \cdot \|_Y$  as:

$$\|u_h\|_X = \|\mathbf{u}\|_{\mathbf{H}_X} = \left(\mathbf{u}^T \mathbf{H}_X \mathbf{u}\right)^{1/2}, \quad \|u_h\|_Y = \|\mathbf{u}\|_{\mathbf{H}_Y} = \left(\mathbf{u}^T \mathbf{H}_Y \mathbf{u}\right)^{1/2},$$

with  $\mathbf{u}$  the vector of coefficients of  $u_h$  in the basis  $\mathcal{Q}$ .

Furthermore, equality (9.4) can be written in the discrete case as:

$$\mathbf{u}^T \mathbf{H}_X \mathbf{u} = \mathbf{u}^T \mathbf{H}_Y \mathbf{J} \mathbf{u}; \tag{9.9}$$

where  $\mathbf{J} = \mathbf{H}_Y^{-1} \mathbf{H}_X$  is a positive-definite matrix. Since  $\mathbf{J}$  is the matrix representation of the corresponding positive self-adjoint operator.

Finally, lets us recall definition of the  $\theta$  power of a matrix studied in [42, section 5.4] and [29, Chap. 6-7]:

**Definition 9.2.1** *Let  $M \in \mathbb{R}^n \times \mathbb{R}^n$  be a positive diagonalizable matrix with a real positive definite spectrum, which eigenvalue decomposition is denoted by  $M = Q^{-1} D_M Q$ . The matrix  $D_M$  is a diagonal matrix with positives entries labeled in increasing order as:*

$$0 < \lambda_1 < \dots < \lambda_n.$$

Let  $\theta \in \mathbb{R}$ . The  $\theta$  power of  $M = Q^{-1} D_M Q$  is given by:

$$M^\theta = Q^{-1} D_M^\theta Q.$$

Using the above definition together with the expression of  $H_X$  and  $H_Y$ , it holds:

**Proposition 9.2.2** *The matrix representation of the norm  $\| \cdot \|_{\theta,h} : [X_h, Y_h]_\theta \rightarrow \mathbb{R}_+$  is*

$$\mathbf{H}_{\theta,h} = \mathbf{H}_Y + \mathbf{H}_Y (\mathbf{H}_Y^{-1} \mathbf{H}_X)^{1-\theta}; \tag{9.10}$$

and the reduced form of  $\mathbf{H}_{\theta,h}$  is given by:

$$\mathbf{H}_\theta = \mathbf{H}_Y(\mathbf{H}_Y^{-1}\mathbf{H}_X)^{1-\theta}. \quad (9.11)$$

**Proof:** The proof follows that in [8, p. 1-5] ■

**Remark 9.2.3** Using the fact that the matrices  $\mathbf{H}_Y$  and  $\mathbf{H}_X$  are symmetric and positive definite, one can find a matrix  $Q$  such that: [32, Section 7.6]:

$$\mathbf{H}_X = Q^T D Q, \quad \mathbf{H}_Y = Q^T Q,$$

where  $D$  is a diagonal matrix with positives entries.

Using definition 9.2.1, the matrices  $\mathbf{H}_{\theta,h}$  and  $\mathbf{H}_\theta$  can be written as:

$$\mathbf{H}_{\theta,h} = Q^T(I + D^{1-\theta})Q, \quad \mathbf{H}_\theta = Q^T(D^{1-\theta})Q, \quad (9.12)$$

### 9.3 Discrete interpolation norms

Our aim in this section is to describe an optimal preconditioner for the Schur complement  $S$  acting on the space  $\Lambda \times \Lambda$  (see (7.9)). In the following we will make use of the basis  $\mathcal{Q}$  given in (9.7) to denote a basis of  $S^h \times S^h$ . Let it be defined by:

$$\nabla_\Gamma \psi(x) := \nabla \psi(x) - \mathbf{n}(\mathbf{n} \cdot \nabla \psi(x))$$

the projection of the gradient of  $\psi(x)$  onto the plane tangent to  $\Gamma$ . Additionally, we also defined the following Sobolev space:

$$H_D^1(\Gamma) = \left\{ v \in L^2(\Gamma) : \int_\Gamma |\nabla_\Gamma v|^2 ds(\Gamma) < \infty; v|_{\Gamma \cap \partial\Omega} = 0 \right\}, \quad (9.13)$$

where  $\Gamma = \bigcup_{i=1}^N \Gamma_i$ .

By considering the space  $\Lambda$  to be the interpolation space between  $\mathcal{X} = H_D^1(\Gamma)$  and  $\mathcal{Y} = L^2(\Gamma)$ , which is equipped with norm  $\|\cdot\|_\Lambda$ , we can choose:

$$X_h = (S^h \times S^h, \|\cdot\|_{H^1(\Gamma) \times H^1(\Gamma)}) \subset X, \text{ and } Y_h = (S^h \times S^h, \|\cdot\|_{L^2(\Gamma) \times L^2(\Gamma)}) \subset Y.$$

Similar to the work done in [6], we derive the following finite element matrix representation of the norm  $\mathbf{H}_{1/2}$

$$\mathbf{H}_{1/2} := \begin{pmatrix} H_{1/2} & 0 \\ 0 & H_{1/2} \end{pmatrix} \text{ with } H_{1/2} = M_\Gamma (M_\Gamma^{-1} L_\Gamma)^{1/2}, \quad (9.14)$$

where  $M_\Gamma$  and  $L_\Gamma$  represent respectively the mass matrix and the Laplace-Beltrami operator assembled on  $\Gamma$  [6]:

$$(M_\Gamma)_{ij} = (\psi_i, \psi_j)_{L^2(\Gamma)}, \quad (L_\Gamma)_{ij} = (\nabla_\Gamma \psi_i, \nabla_\Gamma \psi_j)_{H^1(\Gamma)};$$

where  $\psi_i \in S^h$  for  $i = 1, \dots, n_\Gamma$ .

Finally, let  $\pi_h \in \mathcal{L}(X, X_h) \cap \mathcal{L}(Y, Y_h)$  from Theorem 9.1.3 we can derive an equivalence between the continuous and the discrete interpolation norms of index 1/2 as in [5, p.8] namely: for all  $\boldsymbol{\lambda}_h \in S^h \times S^h$  there exist constants  $\kappa_1, \kappa_2$  such that:

$$\kappa_1 \|\mathbf{u}_\Gamma\|_{1/2, \Gamma} \leq \|\boldsymbol{\lambda}_h\|_{\mathbf{H}_{1/2}} \leq \kappa_2 \|\mathbf{u}_\Gamma\|_{1/2, \Gamma}. \quad (9.15)$$

Let us consider some examples to illustrate the above derivation.

**Example** Consider  $X = H_0^1(\Omega), Y = L^2(\Omega)$ . We want to derive the matrix representation



of a norm defined on a discrete subspace of the following interspace:

$$H_{00}^{1/2} = [H_0^1(\Omega), L^2(\Omega)]_{1/2}.$$

Let  $X_h \subset X$  being the finite element space spanned by a basis  $\{\phi\}_{1 \leq i \leq n}$  of piecewise polynomials defined on subdivision of  $\Omega$ . Use the same procedure as presented above we described the following Grammian matrices with respect of the set  $\{\phi\}_i$  corresponding to the following inner product:

$$(L)_{i,j} = (\nabla \phi_i, \nabla \phi_j)_{L^2(\Omega)}, \quad (M)_{i,j} = (\phi_i, \phi_j)_{L^2(\Omega)}.$$

The matrices  $L, M$  represent the discrete Dirichlet Laplacian and mass matrix respectively. Therefore a norm for the interpolation space  $[X_h, Y_h]_\theta$  is given by

$$H_\theta = M(M^{-1}L)^{1-\theta}.$$

Assuming that we have a uniform subdivision of the domain  $\Omega$ , then  $L, M$  are simultaneous diagonalisable and  $H_\theta$  becomes

$$H_\theta = M^{\theta/2}(M^{1-\theta}L)^{\theta/2}.$$

For the case where  $\theta = 1/2$ , we obtain

$$H_{1/2} = M^{1/4}(M^{1/2}L)^{1/4}.$$

The above example show us that the computation of  $H_{1/2}$  is done in two steps: The first step consists of assembly the matrices  $L, M$  on the interfaces, which consist of a segment in a triangular mesh. The second step is just simple matrix algebra(matrix multiplication

and inversion).

Finally, If we consider the coercivity and continuity bounds for  $s(\cdot, \cdot)$  given in (7.15) together with the above result, we get for all  $\boldsymbol{\mu}_h, \boldsymbol{\lambda}_h \in S^h \times S^h$ :

$$\frac{\alpha_1}{\kappa_2^2} \|\mathbf{u}_\Gamma\|_{\mathbf{H}_{1/2}}^2 \leq s(\mathbf{u}_\Gamma, \mathbf{u}_\Gamma), \quad s(\mathbf{u}_\Gamma, \mathbf{v}_\Gamma) \leq \frac{\alpha_2}{\kappa_1^2} \|\mathbf{u}_\Gamma\|_{\mathbf{H}_{1/2}} \|\mathbf{v}_\Gamma\|_{\mathbf{H}_{1/2}}. \quad (9.16)$$

The above inequalities indicate that  $\mathbf{H}_{1/2}$  and the Schur complement  $S$  have the same spectral properties. This will be described and used in the construction of a new type of interface preconditioners presented in the next section.

## 9.4 Analysis

Preconditioned GMRES is often used to solve the linear system (7.18) due to the size and the sparsity of the matrix  $A$ . In our case a suitable strategy would be to use a GMRES solver combined with a right preconditioner, which requires the solution of a large subsystem posed on the interior of each subdomain and a small subsystem involving the discrete Steklov-Poincaré operator. The speed of convergence of the preconditioned system will depend on the ability of the preconditioner  $P_S$  to approximate the Schur complement  $S$ . To see this, consider the following eigenvalue problem:

$$\begin{pmatrix} A_{II} & A_{I\Gamma} \\ A_{\Gamma I} & A_{\Gamma\Gamma} \end{pmatrix} \begin{pmatrix} \mathbf{u}_I \\ \mathbf{u}_\Gamma \end{pmatrix} = \mu \begin{pmatrix} A_{II} & A_{I\Gamma} \\ 0 & P_S \end{pmatrix} \begin{pmatrix} \mathbf{u}_I \\ \mathbf{u}_\Gamma \end{pmatrix}. \quad (9.17)$$

One can prove that  $\mu = 1$  or  $\mu$  satisfies:

$$S\mathbf{u}_\Gamma = \mu P_S \mathbf{u}_\Gamma. \quad (9.18)$$

Therefore if the eigenvalues of the problem (9.18) are clustered, we expect fast convergence.

Given the inequalities in (9.16), a natural choice of  $P_S$  is:

$$\widehat{S}_1 = \begin{pmatrix} S_{A^{(1)}} & 0 \\ 0 & S_{A^{(2)}} \end{pmatrix}; \quad (9.19)$$

where  $S_{A^{(i)}} = A_{\Gamma\Gamma}^{(i)} - A_{\Gamma\Gamma}^{(i)}(A_{II}^{(i)})^{-1}A_{\Gamma\Gamma}^{(i)}$ , with  $A^{(i)} := d_i L + \alpha_i M$  for  $i = 1, 2$ .

**Proposition 9.4.1** *Let  $S_{A^{(j)}}$  be defined as in (7.17). Then there exist two constants  $\sigma_j, \delta_j$  such that for  $j = 1, 2$ :*

$$\sigma_i \|\tilde{v}\|_{H_{1/2}^{(i)}}^2 \leq \langle S_{A^{(i)}} \tilde{v}, \tilde{v} \rangle, \quad \langle S_{A^{(i)}} \tilde{v}, \tilde{\mu} \rangle \leq \delta_i \|\tilde{v}\|_{H_{1/2}^{(i)}} \|\tilde{\mu}\|_{H_{1/2}^{(i)}}; \quad i = 1, 2. \quad (9.20)$$

**Proof:** Let  $\mathbf{v}_i = E_i \boldsymbol{\lambda}_i, \mathbf{w}_i = E_i \boldsymbol{\mu}_i$  satisfy (7.11c) with  $\mathcal{L} := -\Delta + \alpha_j(\mathbf{x})$ , and  $\mathcal{S}_{A^{(j)}}$  the corresponding Steklov-Poincaré operator. Define  $\alpha_{j_{max}} = \max_{\mathbf{x} \in \Omega} \alpha_j(\mathbf{x})$ , and  $\alpha_{j_{min}} = \min_{\mathbf{x} \in \Omega} \alpha_j(\mathbf{x})$ . Then, we have:

$$\begin{aligned} \langle \mathcal{S}_{A^{(j)}} \boldsymbol{\lambda}_i, \boldsymbol{\lambda}_i \rangle &= B_i(\mathbf{v}_i, \mathbf{v}_i) = \int_{\Omega} \nabla \mathbf{v}_i : \nabla \mathbf{v}_i + \alpha_j(\mathbf{x}) \mathbf{v}_i^T \mathbf{v}_i \, \mathbf{d}\mathbf{x}, \\ &\geq \|\nabla \mathbf{v}_i\|_0^2 + \alpha_{j_{min}} \|\mathbf{v}_i\|_0^2, \quad (\text{as (5.2) holds}) \\ &\geq \min\{1, \alpha_{j_{min}}\} \|\mathbf{v}_i\|_1^2. \\ \langle \mathcal{S}_{A^{(j)}} \boldsymbol{\lambda}_i, \boldsymbol{\mu}_i \rangle &= B_i(\mathbf{v}_i, \mathbf{w}_i) = \int_{\Omega} \nabla \mathbf{v}_i : \nabla \mathbf{w}_i + \alpha_j(\mathbf{x}) \mathbf{v}_i^T \mathbf{w}_i \, \mathbf{d}\mathbf{x}, \\ &\leq \|\nabla \mathbf{v}_i\|_0 \|\nabla \mathbf{w}_i\|_0 + \alpha_{j_{max}} \|\mathbf{v}_i\|_0 \|\mathbf{w}_i\|_0, \quad (\text{as (5.2) holds}) \\ &\leq \max\{\sqrt{2}, \sqrt{2}\alpha_{j_{max}}\} \|\mathbf{v}_i\|_1 \|\mathbf{w}_i\|_1. \end{aligned}$$

Since  $\gamma_0 \mathbf{v}_i = \boldsymbol{\lambda}_i$  and  $\gamma_0 \mathbf{w}_i = \boldsymbol{\mu}_i$ , the trace inequalities (2.3) read for all  $i = 1, \dots, N$

$$\|\boldsymbol{\lambda}_i\|_{1/2, \Gamma_i} \leq C_\gamma(\Omega_i) \|\mathbf{v}_i\|_1, \quad \|\boldsymbol{\mu}_i\|_{1/2, \Gamma_i} \leq C_\gamma(\Omega_i) \|\mathbf{w}_i\|_1.$$

The inequality (9.20) follows from (7.12) and the definition of the operator  $\mathcal{S}$  given in (7.8). ■

Proposition 9.4.1 suggests the following more practical choice of  $P_S$ ,

$$\widehat{S}_2 := \begin{pmatrix} H_{1/2}^{(1)} & 0 \\ 0 & H_{1/2}^{(2)} \end{pmatrix};$$

where  $H_{1/2}^{(i)} = M_{\Gamma\Gamma} \left( M_{\Gamma\Gamma}^{-1} (d_i L_{\Gamma\Gamma} + \alpha_i M_{\Gamma\Gamma}) \right)^{1/2}$  for  $i = 1, 2$ .

The preconditioner  $\widehat{S}_2$  can be implemented using sparse linear algebra techniques. In particular the action of the inverse of  $H_{1/2}^{(i)}$  on a given vector  $\mathbf{z} \in \mathbb{R}^n$  can be approximated via generalised Lanczos algorithms. In that case mesh independence can only be obtained when the number of lanczos vectors  $k = n_{\Gamma}$ . However, the number of iterations required to compute  $H_{1/2}^{-(i)} \mathbf{z}$  is of the order  $\mathcal{O}(kn_{\Gamma})$ , which is still very low. A intensive study of the numerical approximation for  $H^{1/2}$ -norm using Lanczos algorithms can be found in [8, 6].

**Proposition 9.4.2** *There exist two constants  $\tilde{\varepsilon}_1, \tilde{\varepsilon}_2$  such that  $\forall \boldsymbol{\beta}, \boldsymbol{\mu} \in S^h \times S^h$*

$$\tilde{\varepsilon}_1 \|\boldsymbol{\beta}\|_{\widehat{S}_2}^2 \leq \boldsymbol{\beta}^T S \boldsymbol{\beta}, \quad \boldsymbol{\mu}^T S \boldsymbol{\beta} \leq \tilde{\varepsilon}_2 \|\boldsymbol{\beta}\|_{\widehat{S}_2} \|\boldsymbol{\mu}\|_{\widehat{S}_2}. \quad (9.21)$$

**Proof:** Using the Poincaré-Friedrichs inequality (see Lemma 2.1.5), we obtain

$$\mathbf{v}^T M_{\Gamma} \mathbf{v} \leq C^2(\Gamma) \mathbf{v}^T L_{\Gamma} \mathbf{v}.$$

This gives:

$$d_i \mathbf{v}^T L_{\Gamma} \mathbf{v} \leq \mathbf{v}^T (d_i L_{\Gamma} + M_{\Gamma}(\alpha_i)) \mathbf{v} \leq (d_i + C^2(\Gamma)) \mathbf{v}^T L_{\Gamma} \mathbf{v},$$

which means  $A_\Gamma^{(j)} = d_j L_\Gamma + M_\Gamma(\alpha_j)$  is spectrally equivalent to  $L_\Gamma$  and  $H_{1/2}^{(j)}$  is spectrally equivalent to  $H_{1/2}$  for  $j = 1, 2$ . Therefore the matrix  $\widehat{S}_2$  is spectrally equivalent to  $\mathbf{H}_{1/2}$  defined in (9.14).  $\blacksquare$

The inequalities (9.20), (9.21) indicate that the eigenvalues of  $S\widehat{S}_k^{-1}$  for  $k = 1, 2$  can be bounded independently of the meshsize  $h$ , which means the preconditioners  $\widehat{S}_k$  (for  $k = 1, 2$ ) are optimal in some sense to be described below.

## 9.5 GMRES convergence

To establish the mesh independence of GMRES convergence, one can study the bounds of the field of values of the preconditioned matrix  $S\widehat{S}_2^{-1}$ . We will make use of the  $H$ -field of values of any matrix  $M$  presented in subsection 6.1.

**Proposition 9.5.1** *Let  $P_S$  be a symmetric and positive definite matrix such that  $\forall \boldsymbol{\beta}, \boldsymbol{\mu} \in S^h \times S^h$ , there exist two constants  $\tilde{\alpha}_1, \tilde{\alpha}_2$  with:*

$$\tilde{\alpha}_1 \|\boldsymbol{\beta}\|_{P_S}^2 \leq \boldsymbol{\beta}^T S \boldsymbol{\beta}, \quad \boldsymbol{\mu}^T S \boldsymbol{\beta} \leq \tilde{\alpha}_2 \|\boldsymbol{\beta}\|_{P_S} \|\boldsymbol{\mu}\|_{P_S}.$$

*Then the  $P_S^{-1}$ -field of values of  $SP_S^{-1}$  lies in the right half-plane and is bounded independently of the meshsize  $h$ .*

**Proof:** We have for all  $\mathbf{z} \in \mathcal{W}_{P_S^{-1}}(SP_S^{-1})$ ,

$$\min_{\mathbf{z}} |\mathbf{z}| = \min_{\boldsymbol{\beta} \in \mathbb{R}^{n_\Gamma} \setminus \{\mathbf{0}\}} \frac{\langle \boldsymbol{\beta}, SP_S^{-1} \boldsymbol{\beta} \rangle_{P_S^{-1}}}{\langle \boldsymbol{\beta}, \boldsymbol{\beta} \rangle_{P_S^{-1}}} = \min_{\tilde{\boldsymbol{\beta}} \in \mathbb{R}^{n_\Gamma} \setminus \{\mathbf{0}\}} \frac{\tilde{\boldsymbol{\beta}}^T S \tilde{\boldsymbol{\beta}}}{\tilde{\boldsymbol{\beta}}^T P_S \tilde{\boldsymbol{\beta}}} \geq \tilde{\alpha}_1 > 0;$$

and

$$|\mathbf{z}| \leq \max_{\boldsymbol{\beta} \in \mathbb{R}^{n_\Gamma} \setminus \{\mathbf{0}\}} \frac{\|S\boldsymbol{\beta}\|_{P_S^{-1}}}{\|\boldsymbol{\beta}\|_{P_S}} = \max_{\boldsymbol{\beta} \in \mathbb{R}^{n_\Gamma} \setminus \{\mathbf{0}\}} \max_{\boldsymbol{\mu} \in \mathbb{R}^{n_\Gamma} \setminus \{\mathbf{0}\}} \frac{\boldsymbol{\beta} \boldsymbol{\mu}^T \boldsymbol{\beta}}{\|\boldsymbol{\beta}\|_{P_S} \|\boldsymbol{\mu}\|_{P_S}} \leq \tilde{\alpha}_2.$$

Therefore the  $P_S^{-1}$ -field of values of  $SP_S^{-1}$  is contained in the intersection of the regions:

$$\mathcal{R}_1 = \{z \in \mathbb{C} : \operatorname{Re} z \geq \tilde{\alpha}_1\} \quad \text{and} \quad \mathcal{R}_2 = \{z \in \mathbb{C} : \operatorname{Re} z \geq \tilde{\alpha}_2\};$$

which lies in the right half-plane. Furthermore:

$$\frac{\|\mathbf{r}^k\|_{P_S}}{\|\mathbf{r}^0\|_{P_S}} \leq \left(1 - \frac{\tilde{\alpha}_1^2}{\tilde{\alpha}_2^2}\right)^{k/2}.$$

■

All the preconditioners presented in this chapter are proved to be independent of the problem size and the problem parameters, however it is necessary to validate the obtained results on numerical experiments. This is done in the next chapter.

# CHAPTER 10

## NUMERICAL RESULTS

In this chapter we validate the theoretical results obtained in various numerical experiments. The numerical experiments are obtained by solving reaction-diffusion problems in two dimensions. The problems are solved either on a square domain or on the unit disc.

- **Square Domain**

On the square domain, we used two types of partition: A uniform partition, where  $\Omega$  is divided into  $N = N_x \times N_y$  subdomains of size  $2/N_x \times 2/N_y$  each, with  $N_x = N_y \in \{2, 4, 8\}$  (see Figure 10.3), and an automatical partition using METIS [38], which is a graph-partitioning tool publicly available.

- **Unit Disc**

As it is not possible to have a uniform partition in that case, only the automatical partition provided by METIS [38] is considered (see Figure 10.2).

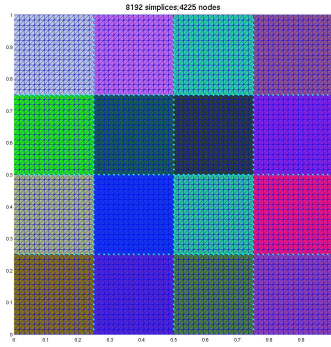


Figure 10.1: Unit square

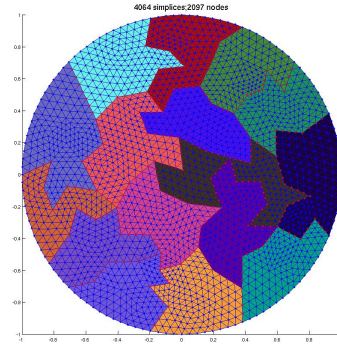


Figure 10.2: Unit circle

The iterative method employed in all cases is the GMRES method with a right preconditioner  $P_S$  as indicated. Additionally, GMRES is stopped when the relative residual norm  $\frac{\|\mathbf{r}^k\|_2}{\|\mathbf{r}^0\|_2}$  is brought below  $10^{-6}$ .

## 10.1 Test problem 1

### 10.1.1 Manual partitioning

Consider now the problem (5.1)

$$\begin{cases} -D\Delta\mathbf{u} + M(\mathbf{x})\mathbf{u} = \mathbf{f} & \text{on } \Omega, \\ \mathbf{u} = \mathbf{0} & \text{on } \partial\Omega_D, \\ \mathbf{n} \cdot \nabla\mathbf{u} = \mathbf{0} & \text{on } \partial\Omega_N, \end{cases} \quad (10.1)$$

with the following parameters:

- $\mathbf{u} = \mathbf{0}$  on  $\partial\Omega$  with  $\Omega = [0, 1]^2$ .

- Matrices

$$M = \begin{pmatrix} \alpha_1 & \beta_1 \\ \beta_2 & \alpha_2 \end{pmatrix}; \quad D = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \quad \mathbf{f} = \begin{pmatrix} 1 + x + y \\ 1 - x - y \end{pmatrix}$$



The following interface preconditioner is used:

$$P_{S_j} = \begin{pmatrix} A_{II} & A_{IG} \\ 0 & \widehat{S}_j \end{pmatrix} \quad (j = 1, 2); \quad (10.2)$$

where:

$$\widehat{S}_1 = \begin{pmatrix} S_{A^{(1)}} & 0 \\ 0 & S_{A^{(2)}} \end{pmatrix}, \quad S_{A^{(i)}} = A_{IG}^{(i)} - A_{IG}^{(i)}(A_{II}^{(i)})^{-1}A_{IG}^{(i)}, \quad \text{with } A^{(i)} := d_i L + \alpha_i M;$$

$$\widehat{S}_2 = \begin{pmatrix} H_{1/2, \alpha_1} & 0 \\ 0 & H_{1/2, \alpha_2} \end{pmatrix}; \quad \text{with } H_{1/2, \alpha_i} = M_{GG} \left( M_{GG}^{-1} (d_i L_{GG} + \alpha_i M_{GG}) \right)^{1/2}.$$

The results represented in Table 10.1 and 10.2 show us that  $P_{S_1}$  is an optimal preconditioner for problem (5.1), as the number of iterations is independent of the problem size and the number of subdomains. However, it remains computationally expensive. A more practical option is  $P_{S_2}$ . We indeed find that working with  $P_{S_2}$  still gives us virtually no dependence on the size of the problem, but a dependence on the number of subdomains (see Table 10.3). However, this dependence disappears with increasing  $\alpha_i$ . This latter property is due to the fact that the problem becomes ‘*easier*’ to solve iteratively as the mass matrix becomes more and more dominant (see Table 10.1).

Preconditioner=	$P_{S_1}$						$P_{S_2}$											
$k_1$ =	1		2		3		1		2		3							
domains =	4	16	64	4	16	64	4	16	64	4	16	64	4	16	64			
size = 8,450	4	4	4	4	4	4	3	3	3	10	14	18	10	12	13	11	11	11
33,282	4	4	4	4	4	4	3	3	3	10	14	18	10	12	14	10	11	11
132,098	4	4	4	4	4	4	3	3	3	10	14	19	10	12	14	10	10	11

Table 10.1: GMRES iterations for Problem 1 with  $\alpha_1 = \alpha_2 = 10^{k_1}$ ,  $\beta_1 = \beta_2 = 1$ .

Preconditioner=	$P_{S_1}$									$P_{S_2}$								
$k_1$ =	1			2			3			1			2			3		
domains =	4	16	64	4	16	64	4	16	64	4	16	64	4	16	64	4	16	64
size = 8,450	0.3	0.3	0.3	0.2	0.1	0.18	0.25	0.05	0.17	0.5	1	4	0.5	0.6	2	1	1	9
33,282	2	2	2	1.5	1	1	1	1	0.9	3	4	18	3	4	14	3	5	10
132,098	8	8	8	5	6	6	4	4	6	13	23	261	13	20	205	15	23	170

Table 10.2: CPU time in Seconds

Preconditioner=	$P_{S_2}$								
$k_2$	0			1			2		
doms =	4	16	64	4	16	64	4	16	64
size = 8,450	10	15	18	12	16	20	15	26	49
33,282	10	15	19	11	16	20	15	28	55
132,098	10	15	19	12	16	20	15	28	56

Table 10.3: GMRES iterations for Problem 1 with  $\alpha_1 = \alpha_2 = 1, \beta_1 = \beta_2 = 10^{k_2}$ .

### 10.1.1.1 Computational results beyond the theory

As described in chapter 9 the optimal matrix exponent required for our preconditioner is  $1/2$ . However, we found when using the preconditioner  $P_{S_2}$  with:

$$H_{\varsigma, \alpha_i} = M_{\Gamma\Gamma} \left( M_{\Gamma\Gamma}^{-1} (d_i L_{\Gamma\Gamma} + \alpha_i M_{\Gamma\Gamma}) \right)^\varsigma; \quad (10.3)$$

where  $\varsigma = 0.6, 0.7$  for  $doms = 16, 64$  respectively. The number of iterations is independent of the problem size and the number of subdomains (see Table 10.4-10.5). However, we do not have any theoretical results to indicate the independence on the number of subdomains.

### 10.1.2 Automatic partitioning

The results from Table 10.6 shows us that, when using automatic partitioning of the domain, our precondition maintains the  $h$ -independence with a much reduced dependence on the number of subdomains. However, the independence on the number of subdomains

Preconditioner=	$P_{S_2, \varsigma}$								
$k_1$	1			2			3		
$\varsigma =$	0.5	0.6	0.7	0.5	0.6	0.7	0.6	0.6	0.7
doms =	4	16	64	4	16	64	4	16	64
size = 8,450	10	11	12	10	9	9	11	9	8
33,282	10	11	13	10	9	10	10	8	7
132,098	10	12	14	10	10	12	10	8	8

Table 10.4: GMRES iterations for Problem 1 with  $\alpha_1 = \alpha_2 = 10^{k_1}, \beta_1 = \beta_2 = 1$ .

Preconditioner=	$P_{S_2, \varsigma}$								
$k_2$	0			1			2		
$\varsigma =$	0.5	0.6	0.7	0.5	0.6	0.7	0.6	0.6	0.7
doms =	4	16	64	4	16	64	4	16	64
size = 8,450	10	11	12	12	13	14	15	28	50
33,282	10	11	13	11	14	16	15	30	52
132,098	10	12	15	12	14	17	15	31	55

Table 10.5: GMRES iterations for Problem 1 with  $\alpha_1 = \alpha_2 = 1, \beta_1 = \beta_2 = 10^{k_2}$ .

can be achieved by modifying the exponent as shown in Table 10.7.

Preconditioner=	$P_{S_2}$								
$k_1$	0			1			2		
doms =	4	16	64	4	16	64	4	16	64
size = 8,450	14	19	26	14	19	26	13	15	22
33,282	14	19	27	14	19	27	13	16	23
132,098	15	20	28	15	19	28	14	16	23

Table 10.6: GMRES iterations for Problem 1 with  $\alpha_1 = \alpha_2 = 10^{k_1}, \beta_1 = \beta_2 = 1$ .

### 10.1.3 Other type of preconditioners

In this section, we consider a uniform partition of the domain  $\Omega$  and present some different preconditioning approaches.

Preconditioner=	$P_{S_2, \varsigma}$								
$k_1$	0			1			2		
$\varsigma$ =	0.5	0.6	0.7	0.5	0.6	0.7	0.6	0.6	0.7
doms =	4	16	64	4	16	64	4	16	64
size = 8,450	14	18	22	14	17	21	13	13	18
33,282	14	18	23	14	18	23	13	14	20
132,098	15	19	24	15	18	26	14	14	22

Table 10.7: GMRES iterations for Problem 1 with  $\alpha_1 = \alpha_2 = 10^{k_1}, \beta_1 = \beta_2 = 1$ .

First, we consider the following preconditioner:

$$\hat{P}_{S_2} = \begin{pmatrix} A_{II} & A_{IG} \\ 0 & \hat{S}_2 \end{pmatrix};$$

where:

$$\hat{S}_2 = \begin{pmatrix} H_{1/2, \alpha_1} & 0 \\ 0 & H_{1/2, \alpha_2} \end{pmatrix}; \quad (10.4)$$

with:

$$H_{1/2, \alpha_i} = M_{GG} \left( M_{GG}^{-1} (d_i L_{GG} + (\alpha_i - \beta_1 \beta_2) M_{GG}) \right)^{1/2}. \quad (10.5)$$

This is mainly inspired by the work presented in section 8.1 and the results obtained in Tables 10.5 and 10.3, which illustrated a poor performance of our preconditioner for  $\beta_i \gg \alpha_i$  for  $i = 1, 2$ . We found that the number of iterations remains independent of the problem size but increases at worst logarithmic with the number of subdomains (see Table 10.8, 10.9). However, the performance of the preconditioner deteriorates badly with increasing  $\beta_i$  compared to the initial preconditioner  $P_{S_2}$  but is very similar when  $\alpha_i \gg \beta_i$  for  $i = 1, 2$ .

Preconditioner=	$\widehat{P}_{S_2}$								
$k_1$	1			2			3		
doms =	4	16	64	4	16	64	4	16	64
size = 8,450	14	14	18	10	12	13	11	11	11
33,282	10	14	18	10	12	14	10	11	11
132,098	10	14	18	10	12	14	10	10	11

Table 10.8: GMRES iterations for Problem 1 with  $\alpha_1 = \alpha_2 = 10^{k_1}, \beta_1 = \beta_2 = 1$ .

Preconditioner=	$\widehat{P}_{S_2}$								
$k_2$	0			1			2		
$\varsigma$ =	0.5	0.6	0.7	0.5	0.6	0.7	0.6	0.6	0.7
doms =	4	16	64	4	16	64	4	16	64
size = 8,450	10	14	18	39	88	141	286	790	1714
33,282	10	14	18	40	91	145	297	866	2010
132,098	10	15	19	40	93	146	312	870	N/A

Table 10.9: GMRES iterations for Problem 1 with  $\alpha_1 = \alpha_2 = 1, \beta_1 = \beta_2 = 10^{k_2}$ .

Finally, consider the following preconditioner:

$$P_S = \begin{pmatrix} P_{S_{\alpha_1}} & \beta_2 M \\ 0 & P_{S_{\alpha_2}} \end{pmatrix};$$

where:

$$P_{S_{\alpha_i}} = \begin{pmatrix} (d_i L + \alpha_i M)_{II} & (d_i L + \alpha_i M)_{I\Gamma} \\ 0 & H_{1/2, \alpha_i} \end{pmatrix} \quad (i = 1, 2). \quad (10.6)$$

This preconditioner is inspired by the work carried out in [44], where the block matrix  $A$  in (5.10), is the preconditioner by an upper triangular matrix. Here instead we approximated the diagonal entries using a **DD**-preconditioner. We found that the number of iterations is dependent on the problem size and the number of subdomains and decreases for increasing  $\alpha_i$ . This poor performance is due to the fact that we are preconditioning a coupled problem using a decoupled approach. One should mention that the preconditioner (10.1.3) will

require twice as many processors as our original preconditioner if implemented in parallel.

Preconditioner=	$P_S$								
$k_1$	0			1			2		
doms =	4	16	64	4	16	64	4	16	64
size = 8,450	63	86	104	31	36	40	17	18	18
33,282	102	184	250	56	67	75	22	24	25
132,098	161	302	384	102	125	320	39	44	44

Table 10.10: GMRES iterations for Problem 1 with  $\alpha_1 = \alpha_2 = 10^{k_1}$ ,  $\beta_1 = \beta_2 = 1$ .

As a result of our investigations, we will consider only the preconditioner  $P_{S_2}$  for the remaining test problems.

## 10.2 Test problem 2

We consider now the problem (5.1), with the following parameters:

$$d_1 = 1, d_2 = 0.1, \alpha_1 = \alpha_2 = 10^{k_1}, \beta_1 = \beta_2 = 1;$$

with  $\mathbf{f}$  such that  $\mathbf{u}^T = \left( (x - \frac{1}{3}x^3)(y - \frac{1}{3}y^3), (x - \frac{1}{3}x^3)(y - \frac{1}{3}y^3) + 2 \right)$ . Since  $d_1 \neq d_2$  two set of results have been obtained (see Table 10.13). The first set of results is obtained by applying the preconditioner directly to the problem (5.1). The second set of results is obtained by applying the preconditioner to a scaled version of problem (5.1), namely:

$$-I_2 \Delta \mathbf{v} + \mathbf{M} \mathbf{D}^{-1} \mathbf{v} = \mathbf{f}, \quad \text{where } \mathbf{v} = \mathbf{D} \mathbf{u}. \quad (10.7)$$

In both cases, we find indeed that the number of iterations is independent of the problem size but exhibits at worst logarithmic dependence on the number of subdomains. However, the number of iterations remains higher than in the Test problem 1. This is due to the fact that the preconditioned matrices are no longer symmetric.

	Without Scaling						With Scaling											
$k_1 =$	1			2			3			1			2			3		
domains =	4	16	64	4	16	64	4	16	64	4	16	64	4	16	64	4	16	64
size = 8,450	20	24	26	17	19	19	16	17	16	13	14	17	12	12	13	9	11	10
33,282	20	24	27	17	20	21	15	19	19	13	14	18	12	13	13	10	12	11
132,098	20	24	28	18	21	22	15	19	19	14	14	18	12	13	13	10	12	12

Table 10.11: GMRES iterations for Problem 2 .

**Remark 10.2.1** *The similarity between the second part of the results in Table cdttable:a@ tells us that the performance of our preconditioner will not be affected if  $d_1 \ll d_2$ . In that case the scaled version (10.7) of the problem is used.*

### 10.3 Test problem 3

Finally we consider problem (5.1) with  $d_1 = 1; d_2 = 0.1; \mathbf{f} = (1, 1)^T$  and

$\mathbf{u} = \mathbf{0}$  on  $\partial\Omega$  together with the following jump coefficients such that assumptions (4.3.2) are satisfied:

$$\alpha_1 = \begin{cases} 1 & \text{if } x^2 + y^2 < 1/4; \\ 100 & \text{otherwise.} \end{cases} ; \quad \alpha_2 = \begin{cases} 100 & \text{if } x^2 + y^2 < 1/4; \\ 1 & \text{otherwise.} \end{cases}$$

$$\beta_1 = \begin{cases} 0.1 & \text{if } x^2 + y^2 < 1/4; \\ 1 & \text{otherwise.} \end{cases} \quad \beta_2 = \begin{cases} 1 & \text{if } x^2 + y^2 < 1/4; \\ 0.1 & \text{otherwise.} \end{cases}$$

An illustration of the final solution  $\mathbf{u}$  is provided in Figure 10.3, while the iteration count is presented in Table 10.12. We observe a similar convergence behaviour: independence of the problem size and logarithmic dependence on the number of subdomains.

domains =	$h$	4	16	64
size = 8,450	0.0313	19	24	28
33,282	0.0156	18	25	28
132,098	0.0078	18	26	28

Table 10.12: GMRES iterations for Problem 3.

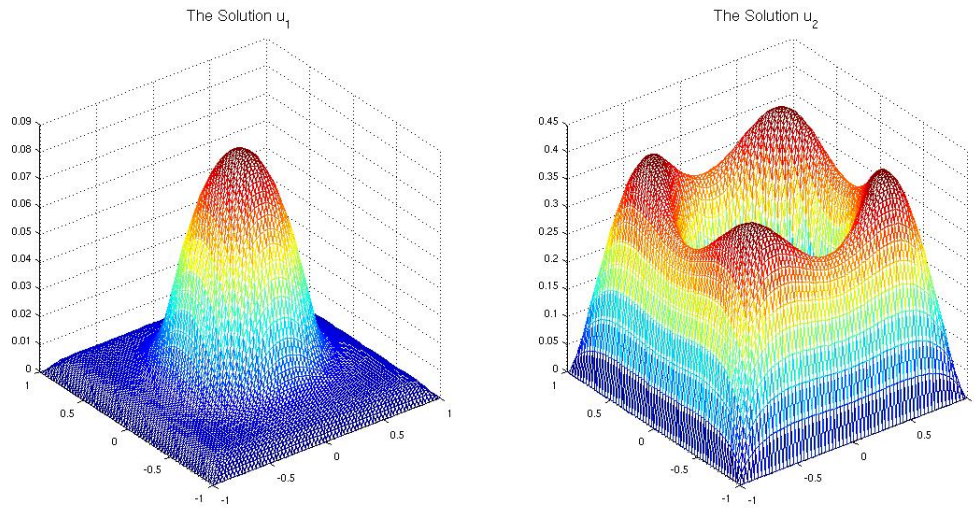


Figure 10.3: Solution for Problem 3.

## 10.4 Test problem 4

The problem (5.1) is solved on domain  $\Omega = (-1, 1)^2$  with  $\partial\Omega_N = \emptyset$ . The rest of the parameters are:  $\mathbf{f} = (1, 1)^T$ ,  $\mathbf{u} = 0$  on  $\partial\Omega_D$  and

$$M(\mathbf{x}) = \begin{pmatrix} 1 + x^2 + y^2 & x^2 + y^2 \\ x^2 - y^2 & x^2 + y^2 \end{pmatrix}.$$



As we are dealing with non constant coefficients the matrix  $\widehat{S}_2$  is adapted as:

$$\widehat{S}_2 = \begin{pmatrix} H_{1/2}^{\alpha_1} & 0 \\ 0 & H_{1/2}^{\alpha_2} \end{pmatrix}; \quad (10.8)$$

with:

$$H_{1/2}^{\alpha_i} := [d_i L + M_{\omega_i}, M]_{1/2} \quad \text{and} \quad M_{\omega_i} = \int_{\Gamma} \omega \phi_i \phi_j \, d\Gamma.$$

The other parameters together with the number of iterations are given in Table 10.13 and Table 10.14. We indeed find that the number of iterations is independent of the size of the problem but increases with the number of subdomains.

$d_1 = d_2 = 1$			
doms =	4	16	64
size = 8,450	14	15	19
33,282	15	16	20
132,098	16	17	20

Table 10.13: GMRES iterations for Problem 4.

$d_1 = 0.1, d_2 = 1$			
doms =	4	16	64
size = 8,450	21	25	29
33,282	22	26	31
132,098	24	27	31

Table 10.14: GMRES iterations for Problem 4.

## 10.5 Test problem 5

In this section we present the numerical experiments obtained by solving the Schnakenberg system: Schnakenberg model is defined by the following set of PDEs:

$$\begin{cases} u_t = \Delta u + \gamma(a - u + u^2v) & \text{on } \Omega; \\ v_t = d\Delta v + \gamma(b - u^2v) & \text{on } \Omega; 0 \\ n \cdot \nabla u = 0 & \text{on } \partial\Omega. \end{cases} \quad (10.9)$$

This model is widely used in biology to model the emergence of patterns (see [48, 76, 54]) and can be written as:

$$\begin{cases} \frac{\partial \mathbf{u}}{\partial t} = D\Delta \mathbf{u} + \mathbf{f}(\mathbf{u}) & \text{in } \Omega, \\ \mathbf{n} \cdot (\nabla \mathbf{u}) = \mathbf{0} & \text{on } \partial\Omega_N, \\ \mathbf{u} = \mathbf{g} & \text{on } \partial\Omega_D, \\ \mathbf{u}(x, 0) = \mathbf{u}_0(x) & \text{for } x \in \Omega, \end{cases} \quad (10.10)$$

with  $\partial\Omega_D = \emptyset$ , where:

$$\mathbf{f}(\mathbf{u}) = \begin{pmatrix} \gamma(a - u_1 + u_1^2 u_2) \\ \gamma(b - u_1^2 u_2) \end{pmatrix}, \quad D = \begin{pmatrix} 1 & 0 \\ 0 & d \end{pmatrix}, \quad a, b, \gamma, d > 0. \quad (10.11)$$

If we denote by

$$f(u_1, u_2) = \gamma(a - u_1 + u_1^2 u_2), \quad g(u_1, u_2) = \gamma(b - u_1^2 u_2),$$

then for all  $u, v \geq 0$ ,

$$f(0, u_2) = \gamma a > 0, \quad g(u_1, 0) = \gamma b > 0, \quad f(u_1, u_2) + g(u_1, u_2) \leq \gamma(a + b),$$

so that (4.3.2) holds.

The steady state for the problem (10.10) is given by the solution of the system:

$$\begin{cases} -\frac{1}{\gamma}D\Delta\mathbf{u} + M_{\theta_1,\theta_2}(\mathbf{u})\mathbf{u} = \mathbf{f} & \text{on } \Omega, \\ \mathbf{n} \cdot \nabla\mathbf{u} = 0 & \text{on } \partial\Omega, \end{cases}$$

where  $\theta_1 = 1 - \theta_2$ ,  $\theta_2 \in \mathbb{R}$  and:

$$M_{\theta_1,\theta_2}(\mathbf{u}) = \begin{pmatrix} 1 - (1 - \theta_1)u_1u_2 & -\theta_1u_1^2 \\ \theta_2u_1u_2 & (1 - \theta_2)u_1^2 \end{pmatrix}, \quad \mathbf{f} = \begin{pmatrix} a \\ b \end{pmatrix}.$$

Again the determinant of  $M_{\theta_1,\theta_2}(\mathbf{u})$  is denoted by

$$\begin{aligned} \det_{M_{\theta_1,\theta_2}(\mathbf{u})} &= (1 - \theta_2u_1u_2)\theta_1u_1^2 + \theta_1\theta_2u_1^3u_2 \\ &= \theta_1u_1^2 > 0. \end{aligned}$$

so that (5.2) holds. We solve this nonlinear problem using the following Picard iteration with  $k \in \mathbb{N}_0$ :

$$\begin{cases} -\frac{1}{\gamma}D\Delta\mathbf{u}^{k+1} + M_{\theta_1,\theta_2}(\mathbf{u}^k)\mathbf{u}^{k+1} = \mathbf{f} & \text{on } \Omega, \\ \mathbf{n} \cdot \nabla\mathbf{u}^{k+1} = 0 & \text{on } \partial\Omega, \\ \mathbf{u}^{k+1}(0, \cdot) = \mathbf{u}^0. \end{cases} \quad (10.12)$$

together with the following adaptive stopping criterion:

$$\frac{\|\mathbf{r}^\omega\|}{\|\mathcal{F}(\mathbf{u}^k)\|^q} \leq \text{tol}, \quad q > 0; \quad (10.13)$$

where  $\mathbf{r}^\omega$  denotes the GMRES residual and  $\mathcal{F}(\mathbf{u}^k) := -\frac{1}{\gamma}D\Delta\mathbf{u}^{k+1} + M_{\theta_1,\theta_2}(\mathbf{u}^k)\mathbf{u}^{k+1} - \mathbf{f}$ .

Note that for the small value of  $q$  we relax the stopping criterion for GMRES.

The starting value is obtained after using an explicit time stepping integration. More precisely, a Crank-Nicolson scheme is applied on the reaction diffusion system (10.9) with final time  $t_F = 110$  and time-step  $\delta t = 5 \times 10^{-2}$  following the setup in (10.11). The parameters values are the same as used in [80], namely:

$$\gamma = 100, a = 0.1305, b = 0.7695, d_1 = 0.05, d_2 = 1$$

$$\text{and } \mathbf{u}^0(\mathbf{x}) = \left( a + b + 10^{-3} \exp \left( -100 \left( x - \frac{1}{3} \right)^2 - 100 \left( y - \frac{1}{2} \right)^2 \right), \frac{b}{(a+b)^2} \right)^T.$$

The preconditioner used here is the same as in the previous case and is also adapted as in (10.8). Before solving problem (10.12), it is important to run some selective tests in order to find the best value for  $\theta_1$  and  $\theta_2$  as they have an impact on the preconditioner as shown in the Table 10.15. We solve the system (10.12) on the unit square domain (see

$\theta_1 = 1 - \theta_2$	0.3	0.35	0.4	0.45
	2178	819	698	738
	8450	657	561	593
			625	

Table 10.15: Total number of nonlinear iterations

Figure 10.3). An illustration of the solution to the steady state is shown in Figure 10.4 and iteration counts in Table 10.16 for  $\theta_2 = 0.35$ . We find indeed that the number of iterations is independent of the problem size but exhibits at worst logarithmic dependence on the number of subdomains.

$q = 10^{-2}$	$\text{tol} = 10^{-1}$		
doms =	4	16	64
size = 2, 178	3, 152	9, 180	8, 082
8, 450	2, 540	4, 015	4, 956
33, 282	3, 324	4, 949	3, 525

Table 10.16: Total number of GMRES iterations for Problem 5.

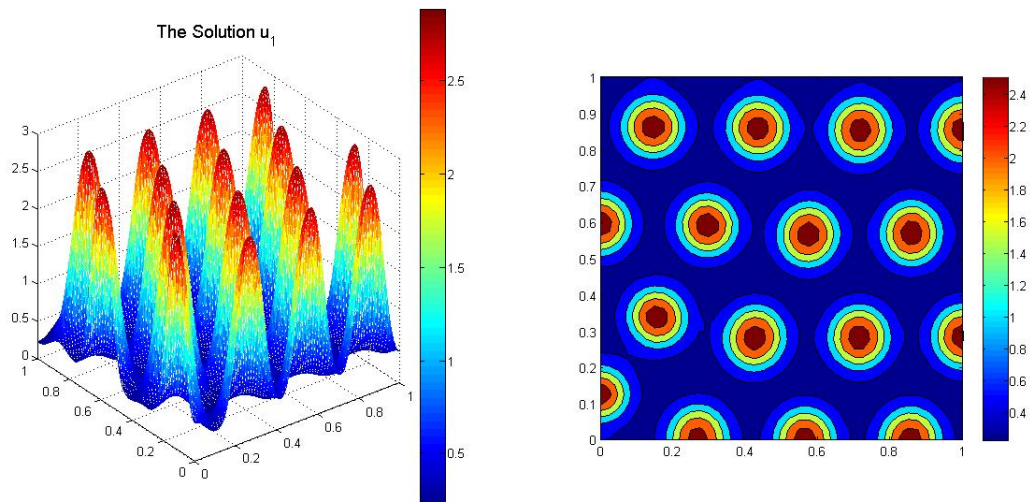


Figure 10.4: One steady state of the Schnakenberg model.

Next we change the shape and the size of the domain, using a METIS [38] partitioning of the domain (see Figure 10.2), but keep all other parameters unchanged. An illustration of the solutions of the steady state is shown in Figure 10.5 and iteration counts in Table 10.17. As in the previous case, the number of iterations is independent of the size of the problem, but exhibits a logarithmic dependence on the number of subdomains.

$q = 10^{-2}$	$\text{tol} = 10^{-1}$		
doms =	4	16	64
size = 4, 258	10, 045	14, 210	16, 248
16, 770	7, 620	11, 457	11, 430
66, 562	6, 762	10, 593	11, 556

Table 10.17: Total number of GMRES iterations for Problem 5.

**Remark 10.5.1** *The results obtained in Table 10.17 and 10.16 show that the approach presented in this thesis is an important contribution for finding the steady state of reaction-diffusions systems. Our approach produces the results in more efficient and faster way than any other approaches existing in the literature (See for example [48, 76, 80]).*

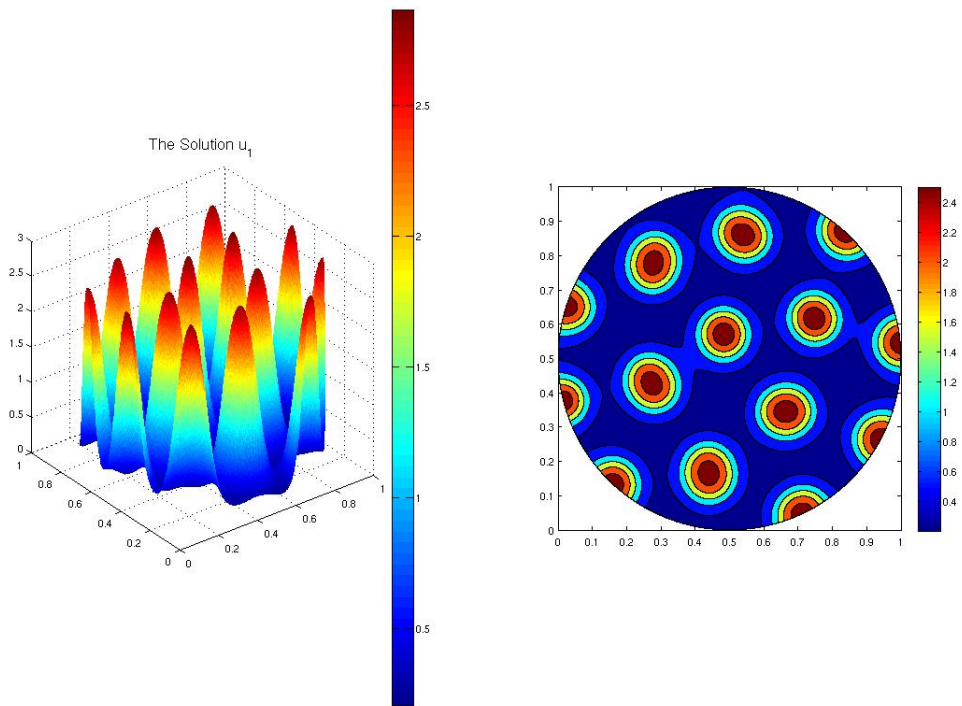


Figure 10.5: One steady state of the Schnakenberg model.

# CHAPTER 11

## CONCLUSION

### 11.1 Summary

We presented a general non-overlapping domain decomposition method for solving reaction-diffusion systems. We derived the corresponding Steklov-Poincaré operator together with the associated linear algebra problem. In addition, by exploiting the fact that the Steklov-Poincaré operators arising in a non-overlapping **DD**-algorithm are coercive and continuous with respect to Sobolev norms of index  $1/2$ , an interface preconditioner for the Schur complement problem was constructed. This was shown to be strongly related to the finite element representation of the norm  $\| \cdot \|_{1/2, \Gamma}$ . Its implementation can be achieved via sparse Lanczos procedures, which do not add to the complexity of the problem. We used various numerical examples to validate our theoretical results. We found that the performance of our preconditioner is independent of the mesh parameters when having a uniform or a METIS [38] partitioning of the domain but exhibits at worst logarithmic dependence on the number of subdomains. However, the subdomain independence can be achieved when using a fractional power greater than  $1/2$ . Although we do not have any theory to back up this affirmation, it has been validated in various numerical experiments.

## 11.2 Further directions

The results obtained in this thesis are very satisfactory and its extension to larger reaction-diffusions systems would be straightforward and would exhibit similar properties. However, some issues concerning the performance and the robustness need to be addressed as there is still room for improvement.

- **Block diagonal preconditioning of the Schur-complement**

In this thesis we have considered a block diagonal precondition for the Schur complement of reaction-diffusion systems. However, we found that when  $\beta_i \gg \alpha_i$  for  $i = 1, 2$ , our preconditioner deteriorates (See Test problem 1). Another approach will be to consider a new type of preconditioner, the structure of which would take into consideration the parameters  $\beta_i$  for  $i = 1, 2$  as shown by the equations (8.25), (8.25) while remaining extendable to large systems and easily implementable.

- **The linearization problem**

For our non-overlapping algorithm to remain valid for any non-linear reaction diffusion systems, it is necessary to transform the given non-linear reaction diffusion systems into linear reaction diffusion systems. However, the linearization techniques can have an impact on the performance of the solver (see Table 10.15). Therefore it becomes important to run some selective tests.

- **Subdomains dependence**

We found that the subdomain dependence can be eliminated by using a fractional power greater than  $1/2$ . However this can not be proved theoretically. That is why we believe it would be interesting to explore the idea of envisaging a coarse grid correction, if the performance of our preconditioner deteriorates badly with the number of subdomains. Another option would be to try to devise an algorithm,



which would allow us to find the optimal number of subdomains in order for our preconditioner to remain subdomain independent.

- **Lanczos algorithm**

In this thesis all the results have been obtained without using a Lanczos algorithm as our aim was to study the performance of the exact preconditioner. However, this has been suggested in chapter 9 and done in [8, 6] for reaction diffusion equations but the demonstration of the effect of the lanczos space dimension of reaction-diffusion systems still remains an open problem.

- **Multigrid methods (MG)** In this thesis we have presented only Krylov subspace method. It would be interesting have look into MG, as they belong to the category of iterative solver, which solve the problem by taking into account the underlying PDE systems together with a hierarchy of discretization of the problem. More precisely, they consist of combining computed results obtained on different scales, using results from one scale to reduce certain error components of the approximation of the solution on another scale. Some applications can be found in [82, 83].

- **Parallel performance**

It is well known that the main purpose of using domain decomposition is to devise parallel algorithms that can exploit the emergence of multiprocessor computers. However, the results presented in this thesis have been obtained from a single processor computer. It would be quite tempting to investigate the degree of parallelism that can be achieved by the approach presented in this session. This would open the road to test the approach presented in this paper on more complicated reaction-diffusion systems, such as problems (4.4).

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*"In God, we trust".*