

Schur Complement Technique for Advection-Diffusion Equation using Matching Structured Finite Volumes

Samir Khallouq and Hassan Belhadj

University of Abdelmalek Essaadi
Faculty of Sciences and Techniques of Tangier
Department of Mathematics
BP. 416, 90000 Tangier, Morocco
samir.khallouq@gmail.com
hassan.belhadj@gmail.com

Abstract

The Schur complement technique is often used in finite elements context. In this paper we are interested in a coupling implicit finite volumes scheme and a Schur complement method applied to an advection-diffusion equation on a 2D structured and matching mesh. The domain of calculation is decomposed into $q \geq 2$ nonoverlapping sub-domains and the proposed approach is applied to solve the local boundary sub-problems. The numerical experiments show the advantages of the method compared to global calculation. The proposed algorithm is both stable and efficient. It can be applied to more general PDEs.

AMS Subject Classifications: 65C20, 65M08, 65M55.

Keywords: PDEs, advection-diffusion equation, domain decomposition method, implicit finite volumes, matching structured mesh, nonoverlapping sub-domains, Schur complement.

1 Introduction

Domain decomposition methods (DDM) have enjoyed an increasing popularity among the scientific community, because they define a good framework to derive efficient solvers for the resulting systems using the mathematical properties of PDEs. DDM has been developed for structural mechanics problems (elliptic PDEs) and for computational fluid dynamics problems (hyperbolic and mixed hyperbolic-parabolic PDEs). DDM are generally classified according to two criteria:

- Overlapping or nonoverlapping method according to the spatial decomposition of the the global domain.
- Multiplicative or additive method according to the independence of the local solution at each iteration.

As nonoverlapping DDM, we can use Schwarz or Schur Complement (SC) method, the latest being related to block Gaussian elimination techniques (each block corresponding to a different sub-domain). At the continuous level, one has to deal with an operator acting on interface variables whose discretization is the Schur complement of the global operator [2–4].

Our objective is to propose a new coupled implicit finite volumes (FV) and SC (FV–SC) algorithm, and apply it to the following advection-diffusion problem:

$$\begin{cases} \partial_t c + \operatorname{div}(Uc - D\nabla c) = f & \text{on } \Omega \times (0, T) \\ c(x, t) = c_D(x, t) & \text{on } \partial\Omega \times (0, T) \\ c(x, 0) = c_0(x) & \text{on } \Omega, \end{cases} \quad (1.1)$$

where $\Omega \subset \mathbb{R}^2$ is an open connected and bounded domain supposed to be polygonal, c is the concentration, $D = \begin{pmatrix} \delta & 0 \\ 0 & \delta \end{pmatrix}$ is the diffusion coefficient where δ is a nonnegative constant real number, $U = \begin{pmatrix} u & v \end{pmatrix}$ is the velocity field and $f \in L^2(\Omega \times (0, T))$ is a given source term. The function c_0 and c_D denote the initial value and the Dirichlet boundary value, respectively.

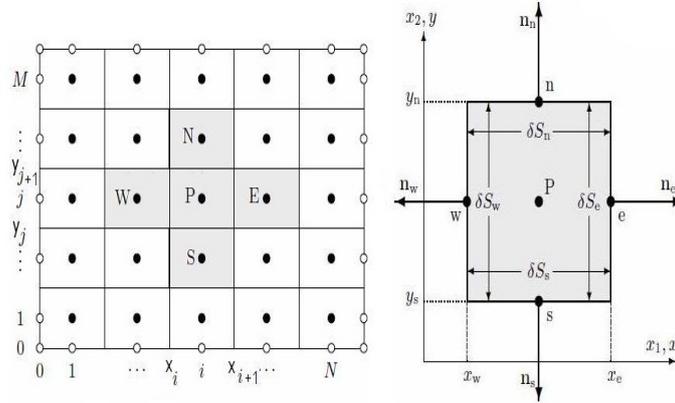
The paper is organized as follows. In the next section, we present the implicit finite volumes (FV) scheme [1]. In Section 3, we describe the Schur complement and the proposed new algorithm. Finally, in Section 4 we discuss the obtained results and we finish by some concluding remarks and perspectives.

2 Finite Volumes Approach

The finite volumes approach consists of dividing the domain of calculation Ω into a finite number of control volumes (CVs) V_i ($i = 1, \dots, N \times M$) with $\Omega = \cup_{i=1}^{N \times M} V_i$. For a general CV, we use the notation of the distinguished points (midpoint, midpoints of faces) and the unit normal vectors according to the notation as indicated in Figure 2.1 (right). The midpoints of neighboring CVs we denote with capital letters W, S , etc. (see Figure 2.1 left). By integrating the equation (1.1) over an arbitrary CV V_P and applying the Green formula, one obtains

$$\mu(V_P) \frac{\partial c}{\partial t} + \sum_a \int_{S_a} (Uc - D\nabla c) n_a dS_a = \int_{V_P} f(x, t) dV_P, \quad (2.1)$$

where S_a ($a = e, n, w, s$) are the four faces of volume V_P (Figure 2.1), n_a is the unit normal vectors to the face S_a and $\mu(V_P)$ is the volume of cell V_P . Approximating the

Figure 2.1: FV structured mesh of domain Ω .

time derivative at time t_{n+1} by the implicit Euler method,

$$\frac{c_P^{n+1} - c_P^n}{\Delta t} + \frac{1}{\mu(V_P)} \sum_{S_a} F_P^{n+1} = f_P^{n+1}, \quad (2.2)$$

where $F_P^{n+1} = \int_{S_a} (U c^{n+1} - D \nabla c^{n+1}) n_a dS_a$ denote the advection and diffusion fluxes through the CV V_P faces,

$$f_P^{n+1} = \frac{1}{\mu(V_P)} \int_{V_P} f(x, t_{n+1}) dV_P,$$

and $c_P^0 = \frac{1}{\mu(V_P)} \int_{V_P} c_0(x) dV_P.$

- The discretization of advection term is done through the flow coming on a cell V_P using the upwind scheme.
- For discretization of diffusion term, we have considered a centred difference scheme.
- For approximation of the volume and surface integrals, we have employed the midpoint rule.

Let us denote by c_I^n the concentration on the volume V_I ($I=P, E, W, N$ or S) at time t_n . The concentration variables c_I^{n+1} and c_I^n ($I=P, E, W, N$ or S) in equation (2.2) can be arranged as follows:

$$a_P c_P^{n+1} + a_E c_E^{n+1} + a_W c_W^{n+1} + a_N c_N^{n+1} + a_S c_S^{n+1} = c_P^n + \zeta_P, \quad (2.3)$$

where ζ_P is a constant depending on the boundary, initial conditions and f_P^{n+1} . In the case $u \geq 0$ and $v \geq 0$, the coefficients a_I ($I=P, E, W, N$ or S) are defined as follows:

- $a_P = 1 + \frac{\Delta t}{\Delta x \Delta y} \left(u_P \Delta y + v_P \Delta x + 2\delta \left(\frac{\Delta y}{\Delta x} + \frac{\Delta x}{\Delta y} \right) \right)$;
- $a_W = -\frac{\Delta t}{\Delta x} \left(u_W + \frac{\delta}{\Delta x} \right)$;
- $a_E = -\delta \frac{\Delta t}{(\Delta x)^2}$;
- $a_S = -\frac{\Delta t}{\Delta y} \left(v_S + \frac{\delta}{\Delta y} \right)$;
- $a_N = -\delta \frac{\Delta t}{(\Delta y)^2}$.

The numerical scheme is then expressed as the linear system

$$AC_P^{n+1} = C_P^n + \zeta_P,$$

where A is a $(N \times M, N \times M)$ type matrix of coefficients a_I ($I=P, E, W, N$ or S).

3 Schur Complement Method

Before describing the Schur complement and the proposed new algorithm, we detail the decomposition of Ω .

3.1 Domain Decomposition

The domain Ω is decomposed into a multi-domain nonoverlapping strip decomposition $\Omega_1, \dots, \Omega_q$, where $\bar{\Omega} = \cup_{i=1}^q \bar{\Omega}_i$ and $\Omega_i \cap \Omega_j = \emptyset$ when $i \neq j$ (Figure 3.1). Let Γ_{ij} denote the interface between Ω_i and Ω_j and $\Gamma = \cup_{ij} \Gamma_{ij}$, and by n^i the normal direction (oriented outward) on Γ_{ij} for $i = 1, \dots, q-1$ and $j = i+1$. For simplicity of notation, we also set $n = n^i$. Considering a rectangular mesh of Ω , each sub-domain Ω_i is partitioned into n_i ($i = 1, \dots, q$) cells in X direction and m cells in Y direction (Figure 3.2). The problem (1.1) can then be expressed as

$$\left\{ \begin{array}{ll} \frac{\partial c_i}{\partial t} + \text{div}(Uc_i - D\nabla c_i) = f & \text{on } \Omega_i \times (0, T), i = 1, \dots, q \\ c_i(x, t) = c_D(x, t) & \text{on } (\partial\Omega_i - \Gamma) \times (0, T) \\ c_i(x, 0) = c_0(x) & \text{on } \Omega_i \\ c_i = c_j & \text{on } \Gamma_{ij}, i, j = 1, \dots, q \\ \frac{\partial c_i}{\partial n} = \frac{\partial c_j}{\partial n} & \text{on } \Gamma_{ij}. \end{array} \right. \quad (3.1)$$

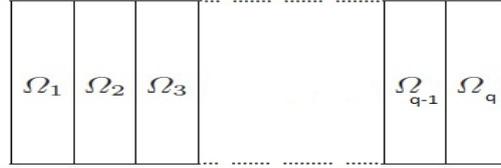
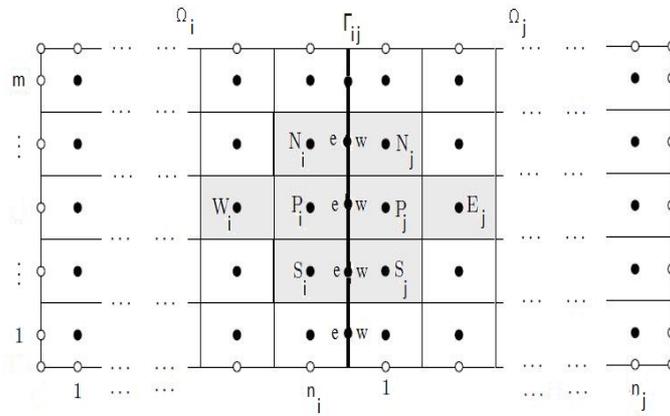


Figure 3.1: Nonoverlapping strip decomposition.

Figure 3.2: Domain decomposition and matching structured mesh of domain Ω .

The last two interface conditions are known as transmission conditions on Γ_{ij} . The decomposed problem (3.1) is discretized on each sub-domain Ω_i , $i = 1, \dots, q$ using the implicit finite volume scheme described in Section 2. For the interface conditions we have used the centred differences scheme. We obtain the following system, $i = 1, \dots, q - 1$, $j = i + 1$:

$$\left\{ \begin{array}{l} a_{P_i} c_{P_i}^{n+1} + a_{W_i} c_{W_i}^{n+1} + a_{N_i} c_{N_i}^{n+1} \\ + a_{S_i} c_{S_i}^{n+1} + a_{\sigma_i} c_{\sigma_i}^{n+1} = c_{P_i}^n + \zeta_{P_i} \quad \text{on } \Omega_i \quad \text{(a)} \\ \\ a_{P_j} c_{P_j}^{n+1} + a_{E_j} c_{E_j}^{n+1} + a_{N_j} c_{N_j}^{n+1} \\ + a_{S_j} c_{S_j}^{n+1} + a_{\sigma_j} c_{\sigma_j}^{n+1} = c_{P_j}^n + \zeta_{P_j} \quad \text{on } \Omega_j \quad \text{(b)} \\ \\ c_{ei}^{n+1} = c_{wj}^{n+1} \quad \text{on } \Gamma_{ij} \quad \text{(c)} \\ \\ c_{ei}^{n+1} + c_{wj}^{n+1} - c_{P_i}^{n+1} - c_{P_j}^{n+1} = 0 \quad \text{on } \Gamma_{ij} \quad \text{(d)} \end{array} \right. \quad (3.2)$$

where

$$\begin{cases} \sigma_i = e_i \text{ and } \sigma_j = w_j, & \text{if } V_{P_i} \cap \Gamma_{ij} \neq \emptyset \text{ (} i = 1, \dots, q-1 \text{ and } j = i+1 \text{)} \\ \sigma_i = E_i \text{ and } \sigma_j = W_j, & \text{otherwise,} \end{cases}$$

and ζ_{P_i} are constants depending on initial, boundary conditions, and $f_{P_i}^{n+1}$ on Ω_i , $i = 1, \dots, q$.

3.2 Schur Complement

The methods based on Schur complement exist in two versions. The first one uses the Steklov Poincaré operator and the second one is an algebraic version. In [2–4], one finds presentations of these methods used in the context of a finite elements method. In this work, we have used an algebraic version of Schur complement method. Let c_i^{n+1} and c_Γ^{n+1} denote the vector of the unknowns of Ω_i ($i = 1, \dots, q$) and Γ at time t_{n+1} (respectively), so the decomposed problem (3.2) can be written in the matrix form

$$\begin{pmatrix} A_1 & 0 & \cdot & \cdot & \cdot & 0 & A_{1\Gamma} \\ 0 & A_2 & 0 & \cdot & \cdot & 0 & A_{2\Gamma} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & 0 & A_q & A_{q\Gamma} \\ A_{\Gamma 1} & A_{\Gamma 2} & \cdot & \cdot & \cdot & A_{\Gamma q} & A_{\Gamma\Gamma} \end{pmatrix} \cdot \begin{pmatrix} c_1^{n+1} \\ c_2^{n+1} \\ \cdot \\ \cdot \\ \cdot \\ c_q^{n+1} \\ c_\Gamma^{n+1} \end{pmatrix} = \begin{pmatrix} c_1^n + \zeta_1 \\ c_2^n + \zeta_2 \\ \cdot \\ \cdot \\ \cdot \\ c_q^n + \zeta_q \\ 0 \end{pmatrix}, \quad (3.3)$$

where A_i , $A_{i\Gamma}$ describe respectively (a) and (b) of system (3.2), and $A_{\Gamma i}$, $A_{\Gamma\Gamma}$ ($i = 1, \dots, q$) describe respectively (c) and (d) of system (3.2). The matrix A_i presents the coupling of the unknowns in Ω_i , $A_{\Gamma\Gamma}$ is related to the unknowns on the interface, $A_{\Gamma i}$ and $A_{i\Gamma}$ representing the coupling of the unknowns of each sub-domain Ω_i with those of the interface Γ_{ii+1} for ($i = 1, \dots, q-1$). The system (3.3) can be solved formally by block Gaussian elimination. Eliminating c_i^{n+1} ($i = 1, \dots, q$) in the system (3.3) yields the following reduced linear system for c_Γ^{n+1} :

$$S c_\Gamma^{n+1} = \chi_\Gamma, \quad (3.4)$$

where

$$\chi_\Gamma = - \sum_{i=1, \dots, q} A_{\Gamma i} A_i^{-1} (c_i^n + \zeta_i),$$

$$S = A_{\Gamma\Gamma} - \sum_{i=1, \dots, q} A_{\Gamma i} A_i^{-1} A_{i\Gamma},$$

and S is the Schur complement matrix. After calculating c_Γ^{n+1} , c_i^{n+1} can be obtained immediately and independently (in parallel) by solving $A_i c_i^{n+1} = (c_i^n + \zeta_i) - A_{i\Gamma} c_\Gamma^{n+1}$ ($i = 1, \dots, q$).

4 Numerical Simulations

In this section, we consider a bidimensional advection-diffusion problem with analytical solution. Let us consider a linear model problem of the type (1.1) with constant coefficients given by

$$f = 0, \quad D = \delta \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad U = \begin{pmatrix} u & v \end{pmatrix}.$$

The initial and boundary conditions are given by the exact solution [5]

$$c(x, y, t) = \frac{1}{200\delta t + 1} e^{-50 \frac{(x-x_0-ut)^2 + (y-y_0-vt)^2}{200\delta t + 1}}$$

representing a Gaussian peak starting at the point (x_0, y_0) , being transported by advection and diffusion. Let us in particular consider:

$$\Omega = (0, 3) \times (0, 3), \quad T = 2, \quad u = 0.8, \quad v = 0.4, \quad x_0 = 0.5, \quad y_0 = 1.35.$$

We consider the discretization of the domain Ω into N^2 squares (with $N = 12, 36, 108$, and 324), and the time interval $(0, T)$ into 200 time steps and we give two values to the parameter δ : for $\delta = 0.1$, the problem is diffusion-dominated, and for $\delta = 0.001$, the problem is convection-dominated. In order to validate the FV and the proposed FV-SC algorithms, we have plotted on the exact and the numerical solutions (FV and FV-SC for 2 sub-domains) and for all test cases, we have computed the analytical solution and numerical ones at the stopped time $t = 2$ and considered three values of y ($y = 0.375, 1.625$ and 2.875).

- For $\delta = 0.1$ (diffusion-dominated), we have plotted Figures 4.1, 4.2 and 4.3 (left) for FV algorithm and Figures 4.1, 4.2 and 4.3 (right) for 2 sub-domains FV-SC algorithm.
- For $\delta = 0.001$ (convection-dominated), we have plotted Figures 4.4, 4.5 and 4.6 (left) for FV algorithm, Figures 4.4, 4.5 and 4.6 (right) for 2 sub-domains FV-SC algorithm, in this case we have used the logarithmic scale for a better visualization.

All figures show the convergence of the proposed algorithm to the exact solution with the increasing of the unknown numbers and also its stability.

We also have computed the discrete $L^2(\Omega)$ errors at time $t = 2$ for different values of N ($N^2=144, 1296, 11664$, and 104976), for $\delta = 0.1$ (see Table 1), and for $\delta = 0.001$ (see Table 2). The estimate errors in Tables 1 and 2 show at the same time the convergence of FV-SC algorithm and a good accuracy of calculation with the increasing of the sub-domain numbers compared to FV method.

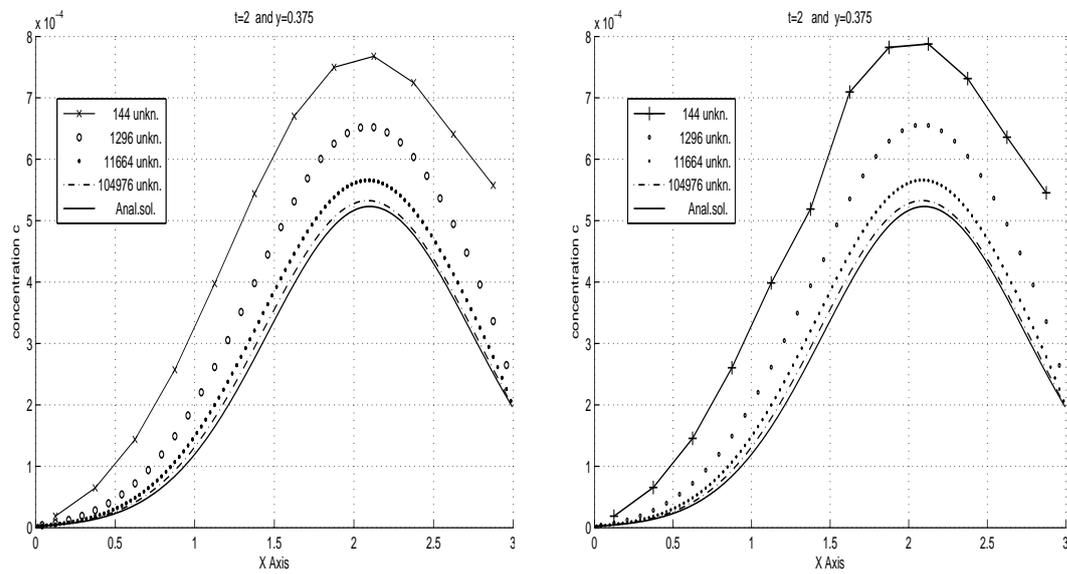


Figure 4.1: Exact solution with FV (left) and FV-SC (right) for different values of N^2 at $t = 2$, $y = 0.375$ and $\delta = 0.1$.

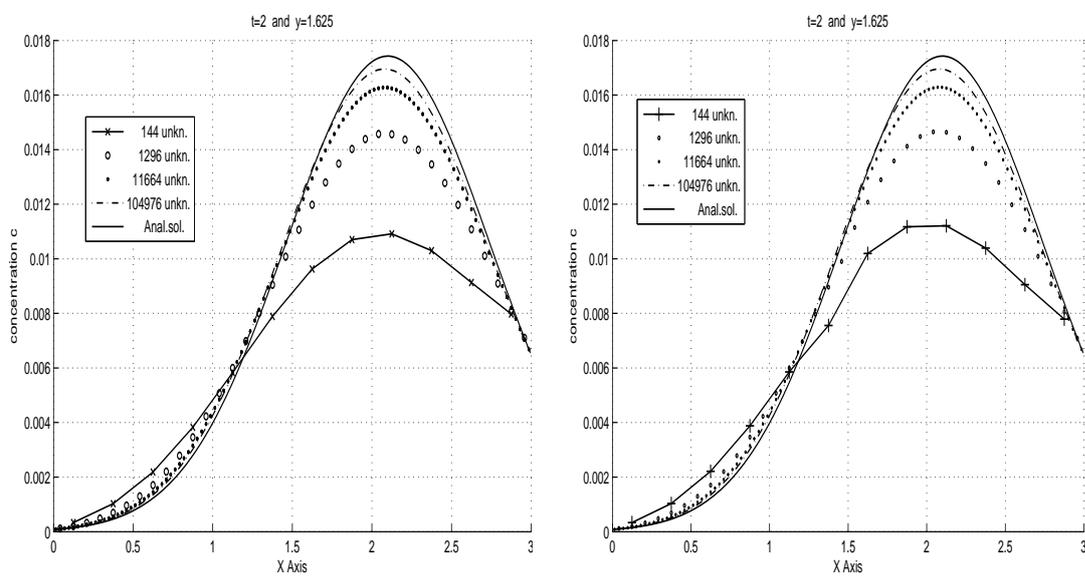


Figure 4.2: Exact solution with FV (left) and FV-SC (right) for different values of N^2 (numbers of unknowns) at $t = 2$, $y = 1.625$ and $\delta = 0.1$.

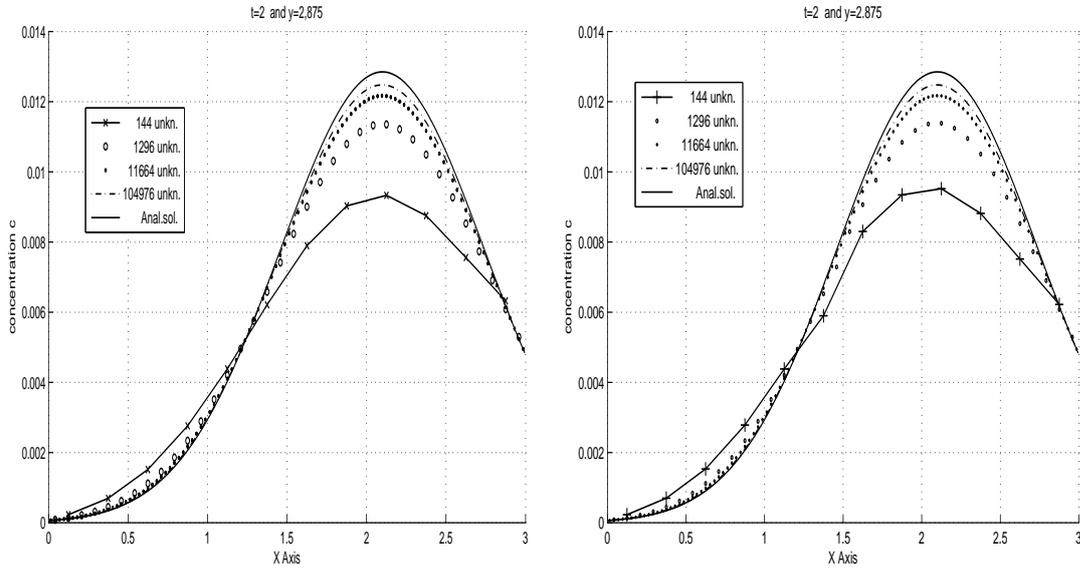


Figure 4.3: Exact solution with FV (left) and FV-SC (right) for different values of N^2 (numbers of unknowns) at $t = 2$, $y = 2.875$ and $\delta = 0.1$.

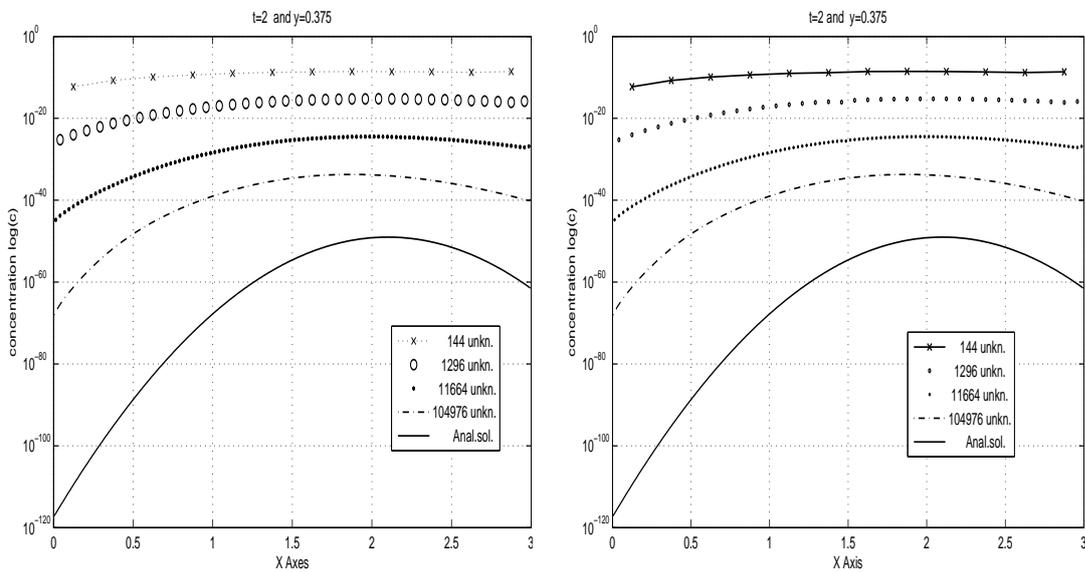


Figure 4.4: Exact solution with FV (left) and FV-SC (right) for different values of N^2 (numbers of unknowns) at $t = 2$, $y = 0.375$ and $\delta = 0.001$.

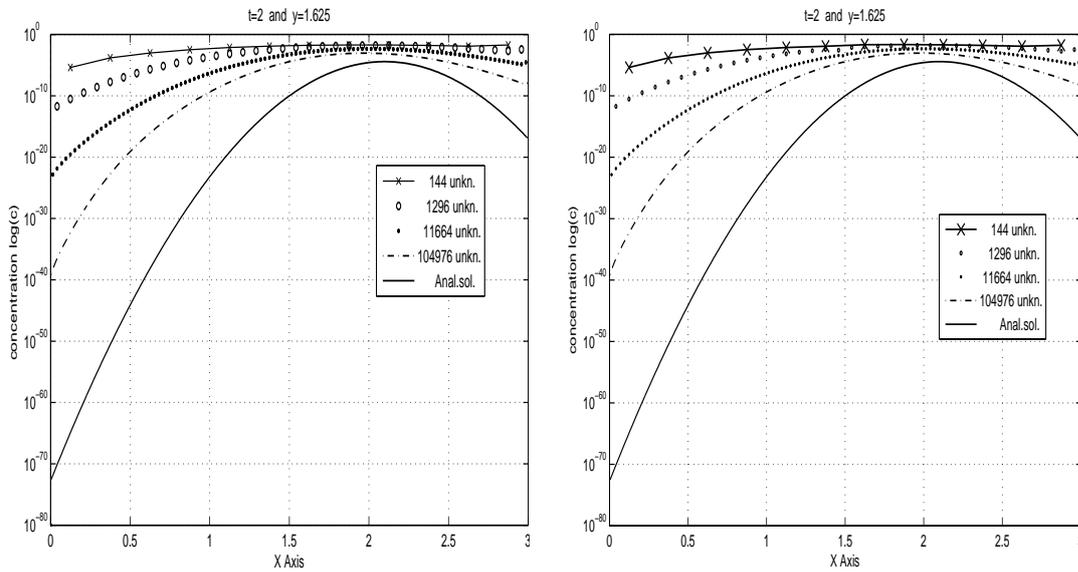


Figure 4.5: Exact solution with FV (left) and FV-SC (right) for different values of N^2 (numbers of unknowns) at $t = 2$, $y = 1.625$ and $\delta = 0.001$.

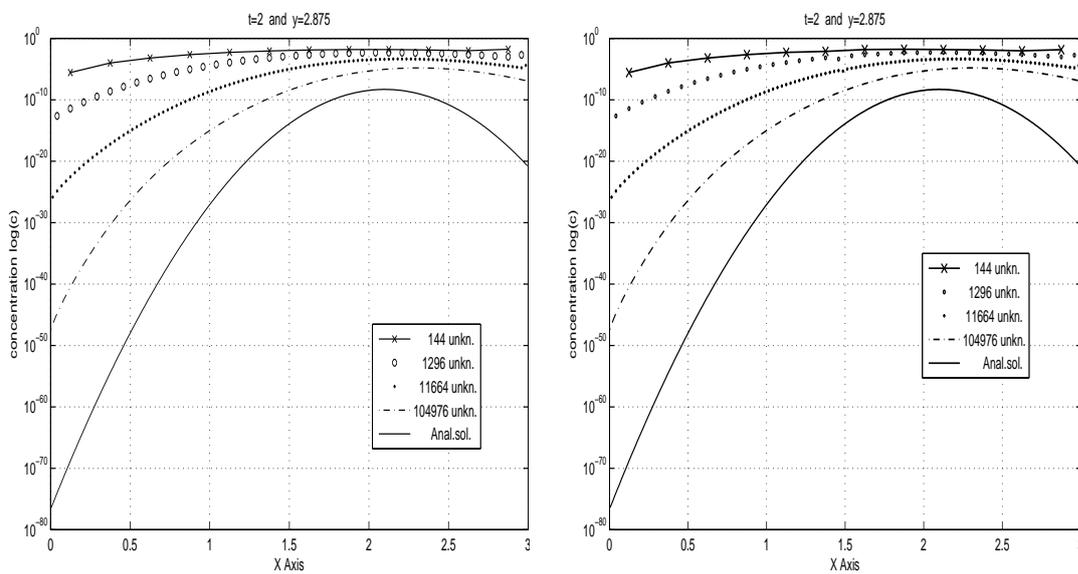


Figure 4.6: Exact solution with FV (left) and FV-SC (right) for different values of N^2 (numbers of unknowns) at $t = 2$, $y = 2.875$ and $\delta = 0.001$.

N	Unkns	error-1D	error-2DD	error-3DD	error-4DD
12	144	0.0095	0.0092	0.0088	0.0084
36	1296	0.0042	0.0042	0.0041	0.0040
108	11664	0.0018	0.0018	0.0018	0.0018
324	104976	0.00087447	0.00087336	0.00087254	0.00087138

Table 1: N , number of unknowns, and discrete $L^2(\Omega)$ errors for $\delta = 0.1$ at $t = 2$ for FV approach and 2, 3, 4 strip sub-domains FV-SC approach (respectively).

N	Unkns	error-1D	error-2DD	error-3DD	error-4DD
12	144	0.1684	0.1680	0.1680	0.1661
36	1296	0.1248	0.1240	0.1232	0.1226
108	11664	0.0985	0.0981	0.0977	0.0974
324	104976	0.0712	0.0711	0.0710	0.0709

Table 2: N , number of unknowns, and discrete $L^2(\Omega)$ errors for $\delta = 0.001$ at $t = 2$ for FV approach and 2, 3, 4 strip sub-domains FV-SC approach (respectively).

5 Conclusion

A new approach coupling implicit FV and Schur complement methods applied to the equation of advection-diffusion, on 2D structured and matching mesh, is presented. The algorithm applied to nonoverlapping multi-domains decomposition has the proprieties of stability and convergence. On the other hand, it reduces the error of calculation compared to global calculation by FV method. As future perspectives, we plan to: generalize the algorithm to the convection-diffusion-reaction problem; apply the FV-SC method to the nonlinear advection-diffusion problem; use an unstructured and matching/nonmatching mesh for complex applications.

References

- [1] H.-J. Bungartz and M. Schäfer, *Fluid-structure interaction*, Lecture Notes in Computational Science and Engineering, 53, Springer, Berlin, 2006.
- [2] T. P. A. Mathew, *Domain decomposition methods for the numerical solution of partial differential equations*, Lecture Notes in Computational Science and Engineering, 61, Springer, Berlin, 2008.
- [3] A. Quarteroni and A. Valli, Theory and application of Steklov-Poincaré operators for boundary-value problems, in *Applied and industrial mathematics (Venice, 1989)*, 179–203, Math. Appl., 56 Kluwer Acad. Publ., Dordrecht, 1991.

- [4] A. Quarteroni and A. Valli, *Domain decomposition methods for partial differential equations*, Numerical Mathematics and Scientific Computation, Oxford Univ. Press, New York, 1999.
- [5] M. Vohralík, Numerical methods for nonlinear elliptic and parabolic equation — Application to flow problems in porous and fractured media, PhD thesis, University of Paris XI and Technical University of Prague, 2004.