Domain Decompostion and Associate Block-Jacobi Method for the Diffusion Equation

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ABSTRACT Among the classical methods used for solving the neutron diffusion equation, we are interested in methods based on a classical finite element discretization and well suited for use on parallel computers. Domain decomposition methods seem to answer this preoccupation. This study deals with the convergence of the block-Jacobi method associated with a decomposition of the domain. A theoretical study is carried for Lagrange finite elements and some examples are given ; in the case of mixed dual finite elements, the study is based on examples.

INTRODUCTION The neutron multigroup diffusion equation is usually solved by an iterative power method combined with a finite element method (Lagrange elements, mixed elements). For the numerical studies we plan to use a multiprocessor computer ; that is why, for solving the diffusion equation, we are interested in methods based on a classical discretization of finite elements type and well suited for use on multiprocessor computers. Domain decomposition methods seem to answer this preoccupation, each subdomain being assigned to a processor. For solving the linear system associated with a decomposition, we have chosen to use the block-Jacobi method because it is always parallelizable.

At first, I will briefly recall the diffusion equation and its primal and mixed dual variational formulations ; their approximation by a finite element method will also be given. The second and third parts will be devoted to the study of the convergence of the block-Jacobi method associated with a decomposition of the domain ; the case of the Lagrange elements and the case of mixed finite elements are both considered ; convergence conditions are established for the block-Jacobi method. For the Lagrange elements, a theoretical study is led, and examples are given ; in the mixed dual case, the study is essentially based on examples.

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1. The diffusion equation and its variationnal formulations . The transport equation describes the evolution of a population of neutrons in a medium. Various hypotheses and approximations lead to the multigroup diffusion equation, which is considered under its stationnary eigenvalue problem formulation [1, 2] :

$$(1) \quad \begin{cases} - \operatorname{div} (D_g(r) \nabla\phi_g(r)) + \sum_g^t(r) \, \phi_g(r) - \sum\limits_{g'=1}^{G} \sum_{g',g}^t(r) \, \phi_{g'}(r) \\ \qquad = \frac{\chi_g}{\lambda} \sum\limits_{g'=1}^{G} \nu_g(r) \sum_{g'}^f(r) \, \phi_{g'}(r) \\ \text{for } g = 1, \ldots, G \end{cases}$$

with : ϕ_g = neutron flux in group g.

D_g = diffusion coefficient in group g.

$\sum_g^t$ = total removal cross section in group g.

$\sum_g^f$ = macroscopic fission cross section for group g.

$\sum_{g,g'}^t$ = macroscopic scattering cross section from group g to group g'.

χ_g = fission spectrum for prompt neutrons.

ν_g = average number of neutrons produced per fission.

λ = effective multiplication factor.

G = total number of energy groups.

r = spacial dependence.

The boundary conditions are of Dirichlet-Neumann type.

The multigroup diffusion equation (1) is generally solved by the iterative power method [1, 2] ; at each iteration, we have to solve problems of the following form :

$$(2) \quad \begin{cases} - \operatorname{div} (D \vec{\nabla} u) + \sum u = S & \text{in } \Omega, \\ u = 0 & \text{on } \Gamma_o, \\ D \frac{\partial u}{\partial n} = 0 & \text{on } \Gamma_1, \end{cases}$$

Ω being a bounded domain of $R^n (n \le 3)$ and $\partial\Omega = \Gamma_o \cup \Gamma_1$, $\Gamma_o \cap \Gamma_1 = \emptyset$, meas $(\Gamma_o) > 0$. The present study treats of this equation, which is here refered as the diffusion equation. Functions D and $\sum$ statisfy the following inequalities :

$$(3) \quad \begin{cases} 0 < \nu \le D(x) \le D_\infty < + \infty \\ 0 \le \sum(x) \le \sum_\infty < + \infty \end{cases} \quad \text{in } \Omega \; ;$$

they make certain the existence and unicity of the solution of the undermentioned variational problems.

The diffusion equation can be written under different variational formulations, the most used being [3, 4].

$$X = \begin{pmatrix} X_1 \\ \vdots \\ X_n \\ X_{n+1} \end{pmatrix} \quad X' = \begin{pmatrix} X_1 \\ \vdots \\ X_n \\ -X_{n+1} \end{pmatrix}, \text{ in the } 3^{rd} \text{ case.}$$

We have : ${}^tX\, M'\, X = {}^tX'\, M\, X'$; so : ${}^tX\, M'\, X \geq 0$, and :

$${}^tX\, M'\, X = 0 \iff X' = 0 \iff X = 0.$$

And consequently M' is positive definite.

2.2. General theoretical study

2.2.a. Notations

K : any element of the triangulation T_n

A_K : contribution of K to matrix A (*)

$\hat{A}_K$: square matrix extracted from A_K corresponding to the nodes of K. it is of order N^2, if N is the number of unknowns by rectangle (or parallelepiped rectangle).

A'_K : contribution of K to matrix A'.

We have : $A'_K = 2 \text{ diag } (A_K) - A_K$, so there is no ambiguity in the notations.

$\hat{A}'_K$: square matrix extracted from A'_K corresponding to the nodes of K

We have : $\hat{A}'_K = 2 \text{ diag } (\hat{A}_K) - \hat{A}_K$; so the notation is not ambigous.

Let i be a positive integer.

$T_i = \{K \in T_h \ / \ K \text{ is splitted into i subdomains}\}$, the decomposition being considered in the sense of nodes.

An example is represented on figure 1 : the finite element is the Lagrange element, the decomposition corresponds to a splitting along the dotted lines ; we have indicated to which set T_i belongs each rectangle of the triangulation.

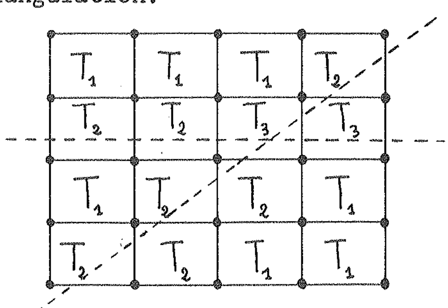


FIGURE 1

Example of sets T_i

(*) $A_{ij} = \int_\Omega D\, \vec{\nabla}\phi_i \cdot \vec{\nabla}\phi_j + \Sigma\, \phi_i\, \phi_j$

$(A_K)_{ij} = \int_K D\, \vec{\nabla}\phi_i \cdot \vec{\nabla}\phi_j + \Sigma\, \phi_i\, \phi_j$

- The primal formulation :

(4) $$\begin{cases} \text{Find } u \in H^1_{o,\Gamma_o}(\Omega) \text{ so that :} \\ \int_\Omega D\, \vec{\nabla}u.\vec{\nabla}v + \sum uv = \int_\Omega Sv \qquad \forall v \in H^1_{o,\Gamma_o}(\Omega) \end{cases}$$

- The mixed dual formulation :

(5) $$\begin{cases} \text{Find } (\vec{p},u) \in H_{o,\Gamma_1}(\text{div}, \Omega) \times L^2(\Omega) \text{ so that :} \\ \int_\Omega \frac{1}{D}\, \vec{p}.\vec{q} + \text{div}\, \vec{q}\, u = 0 \qquad \forall \vec{q} \in H_{o,\Gamma_1}(\text{div}\, \Omega) \\ \int_\Omega -\text{div}\, \vec{p}\, v + \sum uv = \int_\Omega Sv \qquad \forall v \in L^2(\Omega) \end{cases}$$

where $$\begin{cases} H^1_{o,\Gamma_o}(\Omega) = \{ v \in H^1(\Omega) \;/\; \gamma_o(v) = 0 \quad \text{on } \Gamma_o \} \\ \gamma_o(v) = \text{trace of } v \\ H_{o,\Gamma_1}(\text{div},\Omega) = \{\vec{q} \in H(\text{div},\Omega) \;/\; \langle \gamma_1(\vec{q}), v \rangle = 0 \\ \qquad\qquad\qquad \forall v \in H^1_{o,\Gamma_o}(\Omega)\} \\ \gamma_1(\vec{q}) = \text{normal derivative of } \vec{q}. \end{cases}$$

In the mixed formulation, in addition to the flux u, a second unknown $\vec{p}$ occurs as an independant variable ; $\vec{p}$ is equal to $D\,\vec{\nabla}\,u$ and is called the current.

Equations (4) and (5) are discretized by finite element technics ; we mainly use :

- The Lagrange elements in the primal case :

  (*) $P_K = P_{k,k}$ for each rectangular element of the triangulation.

- The elements of Raviart and Thomas in the mixed dual case :

  (*) $$\begin{cases} P_K = P_{k,k} & \text{for each rectangular element of the triangulation.} \\ Q_K = P_{k+1,k} \times P_{k,k+1} \end{cases}$$

In all what follows, every triangulation of the domain will be constituted by rectangles or parallelepiped rectangles ($\bar{\Omega} = \cup K_i$, K_i = "rectangle").

(*) $P_{k,\ell} = \{P \in R[X,Y] \;/\; \text{Deg}_x P \leq k \quad \text{deg}_y P \leq \ell\}$

2. Study of the convergence of the block-Jacobi method associated with a decomposition of the domain, in the case of Lagrange elements [5].

This paragraph is devoted to the study of the convergence of the block-Jacobi method associated with a decomposition of the domain, in the case of Lagrange elements.

A triangulation of the domain: T_h, a Lagrange element and a decomposition of the domain are given. The matrix of the linear system is called A ; it has a block-structure according to the decomposition.

Notation : For every square matrix M, with a block-structure, Diag(M) represents the matrix constituted of the diagonal blocks of M, and M' = 2diag(M) - M.

Matrix A is a positive definite matrix, so we examine whether A' is positive definite or not.

2.1. General examples Some decompositions yield a block-Jacobi method which is convergent without any assumption ; here are some examples.

The basic result is the following :

Proposition : let M be a symmetric positive definite matrix with a block-structure.

If M has a 2 block-structure
or
If M is block-tridiagonal
or
If M is of the following form : M =

$$M = \begin{pmatrix} M_{11} & & & M_{1,n+1} \\ & M_{22} & & \vdots \\ & & \ddots\ M_{n,n} & M_{n,n+1} \\ {}^tM_{1,n+1} & \cdots & {}^tM_{n,n+1} & M_{n+1,n+1} \end{pmatrix}$$

then M' is positive definite.

Demonstration : Let X be a vector. It has a block-structure corresponding to the one of M. We define a vector M' as follows :

$$X = \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \qquad X' = \begin{pmatrix} X_1 \\ -X_2 \end{pmatrix}, \text{ in the } 1^{st} \text{ case.}$$

$$X = \begin{pmatrix} X_1 \\ \vdots \\ X_n \end{pmatrix} \qquad X' = \begin{pmatrix} X_1 \\ -X_2 \\ X_3 \\ -X_4 \\ \vdots \end{pmatrix}, \text{ in the } 2^{nd} \text{ case.}$$

There is only a finite number of integers i so that $T_i \neq \emptyset$, and of course, they are the only ones that are considered.

A_i : contribution of the elements K of T_i to matrix A.

A'_i : contribution of the elements K of T_i to matrix A' ; we have $A'_i = 2\,\mathrm{diag}\,(A_i) - A_i$

$\hat{A}'_i$: square matrix extracted from A'_i corresponding to the nodes belonging to elements K of T_i ; we have : $\hat{A}'_i = 2\,\mathrm{diag}\,(\hat{A}_i) - \hat{A}_i$

The following relations hold :

$$(6) \qquad \begin{cases} A' = \sum_i A'_i \\ \forall i,\ A'_i = \sum_{K \in T_i} A'_K \end{cases}$$

2.2.b. Convergence result - According to relation (6), for A' to be positive definite it is enough that matrices A'_i or A'_K are positive semi definite and A' is invertible (**).

Generally $T_1 \neq \emptyset$; and then, $A'_1 = A_1$ is positive semi definite.

In practise, $T_2 \neq \emptyset$. Then, for each element K of T_2, the block-structure of the positive semi definite matrix $\hat{A}_K$ is a 2 block-structure ; therefore $\hat{A}'_K$ is positive semi definite and so is A'_K.

Let us suppose that for each $i \geq 3$ and each $K \in T_i$, $\hat{A}'_K$ is positive semi definite ; then the corresponding matrices A'_K are positive semi definite ; therefore for each $i \geq 3$, A'_i is positive semi definite. Consequently, A' is positive semi definite. If one of the matrices A'_i is invertible, then A' is positive definite, being the sum of a positive definitive matrix and positive semi definite matrices. But, for a matrix A'_i to be invertible it is necessary that each node of the triangulation belongs to an element K of T_i, otherwise, except for a permutation of the nodes, $A'_i = \begin{pmatrix} \hat{A}'_i & 0 \\ 0 & 0 \end{pmatrix}$ and A'_i is not inversible ; this is not the general case.

The convergence result is the following :

Theorem : if for each K belonging to $\bigcup_{i \geq 3} T_i$, matrix $\hat{A}'_K$ is positive definite and if $\hat{A}_1$ and $\hat{A}'_2$ are invertible, then A' is positive definite and the block-Jacobi method associated with the decomposition is convergent.

Remarks : If $T_1 = \emptyset$ (resp. $T_2 = \emptyset$), the hypothesis concerning $\hat{A}_1$

(**) It is recalled that for a positive semi definite symmetric matrix M : M is positive definite $\Longleftrightarrow$ M is invertible.

(resp. $\hat{A}'_2$) is to omit in the text of the theorem.

If for $i \geq 3$ $T_i = \emptyset$, the hypothesis relative to matrices A'_K for $K \in T_i$ is to omit in the theorem.

Demonstration of the theorem : It has already been shown that A' is positive semi definite assuming weaker hypotheses than the ones of the theorem.

For every vector X, the following notations will be used :

- For each element K of the triangulation, X_K is the vector constituted of the components of X relative to the nodes of K.

- For each integer i, X_i is the vector constituted of the components of X relative to the nodes of elements K of T_i.

Let X be any vector so that ${}^tX\, A'\, X = 0$.

${}^tX\, A'\, X = \sum_i {}^tX\, A'_i\, X = \sum_i \left(\sum_{K \in T_i} {}^tX\, A'_K\, X\right)$. Then, matrices A'_i and A'_K being positive semi definite :

$$\begin{cases} \forall i \quad {}^tX\, A'_i\, X = 0 \\ \forall K \quad {}^tX\, A'_K\, X = 0 \end{cases}$$

Now, $\begin{cases} \forall i \quad {}^tX\, A'_i\, X = {}^tX_i\, \hat{A}'_i\, X_i \\ \forall K \quad {}^tX\, A'_K\, X = {}^tX_K\, \hat{A}'_K\, X_K \end{cases}$, therefore $\begin{cases} X_1 = 0 \\ X_2 = 0 \\ \forall i \geq 3, \; \forall K \in T_i, \; X_K = 0 \end{cases}$

according to the hypotheses of the theorem. Consequently, X = 0.

Therefore A' is positive definite and the block-Jacobi method associated to the decomposition of the domain is convergent.

Remark : Hypothesis : "A'_2 is invertible", can be replaced by a stronger hypothesis : "$\forall K \in T_2$, $\hat{A}'_K$ is positive definite". However, for $K \in T_2$:

$$\hat{A}'_K \text{ is positive definite} \iff \hat{A}_K \text{ is positive definite,}$$

and $\hat{A}_K$ is not positive definite if $\sum = 0$ in K and if K is an inner element.

In practise, sets T_i that are susceptible of being not empty are : $\begin{cases} T_1,\ T_2,\ T_4 \\ \text{and possibly } T_8 \text{ in the three dimensional case.} \end{cases}$

Then it is advisable to study the conditions for $\hat{A}'_K$ to be positive definite for an element K of T_4.

2.2.c. - Conditions for $\hat{A}'_K$ to be positive definite, $K \in T_4$: particular case of the linear Lagrange element.

For the sake of simplicity, we restrict ourselves to the 2D case.

Let K be a rectangle of the triangulation belonging to T_4 ; the lengths of its sides are called hx and hy. Functions D ans Σ are supposed to be constant on K.

Except for a permutation of the nodes, the elementary matrix $\hat{A}_K$ is equal to :

$$\begin{pmatrix} a & b & c & d \\ b & a & d & c \\ c & d & a & b \\ d & c & b & a \end{pmatrix}$$

with :

$$\begin{cases} a = \frac{D}{3}\left(\frac{hy}{hx} + \frac{hx}{hy}\right) + \frac{\Sigma\, hx\, hy}{9} \\ b = \frac{D}{6}\left(-2\frac{hy}{hx} + \frac{hx}{hy}\right) + \frac{\Sigma\, hx\, hy}{18} \\ c = \frac{D}{6}\left(\frac{hy}{hx} - 2\frac{hx}{hy}\right) + \frac{\Sigma\, hx\, hy}{18} \\ d = -\frac{D}{6}\left(\frac{hy}{hx} + \frac{hx}{hy}\right) + \frac{\Sigma\, hx\, hy}{36} \end{cases}$$

Then : $\hat{A}'_K = \begin{pmatrix} a & -b & -c & -d \\ -b & a & -d & -c \\ -c & -d & a & -b \\ -d & -c & -b & a \end{pmatrix}$, and its eigenvalues are : $\begin{cases} a-b-c-d \\ a+b-c+d \\ a-b+c+d \\ a+b+c-d \end{cases}$

A necessary and sufficient condition for $\hat{A}'_K$ to be positive definite is that its four eigenvalues are positive. The calculation of the four eigenvalues as functions of D, Σ, hx, hy and the study of their sign, permits to show that $\hat{A}'_K$ is positive definite if and only if one of the following cases occurs :

1) $\frac{1}{hx^2} - \frac{2}{hy^2} > 0$ and $m(hx,hy)\,\Sigma < D < M(hx,hy)\,\Sigma$

2) $\frac{1}{hy^2} - \frac{2}{hx^2} > 0$ and $m(hy,hx)\,\Sigma < D < M(hy,hx)\,\Sigma$

3) $\frac{1}{hx^2} - \frac{2}{hy^2} < 0$, $\frac{1}{hy^2} - \frac{2}{hx^2} < 0$ and $m(hx,hy)\,\Sigma < D$

4) $\left(\frac{1}{hx^2} = \frac{2}{hy^2}\right.$ or $\left.\frac{1}{hy^2} = \frac{2}{hx^2}\right)$ and $m(hx,hy)\,\Sigma < D$ and $0 < \Sigma$

with : $m(hx,hy) = \frac{1}{24}\left(\frac{1}{hx^2} + \frac{1}{hy^2}\right)^{-1}$, $M(hx,hy) = \frac{5}{12}\left(\frac{1}{hx^2} - \frac{2}{hy^2}\right)^{-1}$

It is to notice that, if hx = hy, by refining the mesh, it will possible to satisfy the condition. On the other hand, if $\frac{hx}{hy}$ is constant and $\frac{hx}{hy} > \sqrt{2}$, when hx and hy tend to 0, then $M(hy,hx) \sum$ also tends to 0 and consequently the condition is no more satisfied ; but it does not mean that A' is not positive definite.

2.2.d. - So, the theoretical study gives sufficient conditions for the convergence of the block-Jacobi method. Some simple examples have been analyzed, for which a necessary and sufficient condition have been found.

2.3. - Examples

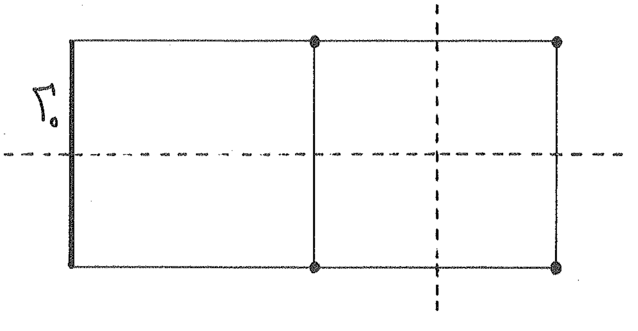
2.3.1. - <u>First example</u> - The framework of this example is the following :

- Ω is a rectangle : $\Omega =]A,B[\times]C,D[$, and $B-A=2(D-C)=2h$
- the boundary conditions are : $\begin{cases} u = 0 & \text{on } \Gamma_o , \\ D \frac{\partial u}{\partial n} = 0 & \text{on } \Gamma_1 \end{cases}$

with : $\begin{cases} \Gamma_o = \{A\} \times [C,D] \\ \Gamma_1 = ([A,B] \times \{C\}) \cup (\{B\} \times [C,D]) \cup ([A,B] \times \{D\}). \end{cases}$

- the triangulation is defined by : $\bar{\Omega} = K_1 \cup K_2$, $K_1 = [A,M] \times [C,D]$, $K_2 = [M,B] \times [C,D]$ and $M = \frac{A+B}{2}$
- D and $\sum$ are constant on Ω.
- the finite element is the linear Lagrange element

The domain Ω, is splitted into four parts along the lines : $X \equiv \frac{M+B}{2}$ and $Y \equiv \frac{C+D}{2}$. The nodes and the decomposition are represented on figure 2.



<u>FIGURE 2</u>

Linear Lagrange element - First example

Here : $T_2 = \{K_1\}$, $T_4 = \{K_2\}$, $T_i = \emptyset \quad \forall i \notin \{2,4\}$.

According to the previous study, $A'_4 = \hat{A}'_{K_2}$ is positive definite if and only if $\frac{\sum h^2}{48} < D$. At that time, the theoretical study permits to conclude that if $\frac{\sum h^2}{48} < D$, then A' is positive definite and the block-Jacobi method is convergent.

On the other hand, a direct study looking for the sign of the eigenvalues of A' shows that :

A' is positive definite $\Longleftrightarrow$ $r \sum h^2 < D$, where $r = \frac{-174 + \sqrt{31752}}{1476}$.

We note that : $r \approx 0{,}003$ and $\frac{1}{48} \approx 0{,}021$.

2.3.2. - Second example - The framework of this example is the following :

- Ω is a rectangle : $\Omega =]A,B[\times]C,D[$, and $B-A = 3(D-C) = 3h$
- The boundary conditions are : $\begin{cases} u = 0 & \text{on } \Gamma_o \\ D \frac{\partial u}{\partial n} = 0 & \text{on } \Gamma_1 \end{cases}$

with = $\Gamma_o = (\{A\} \times [C,D]) \cup (\{B\} \times [C,D])$, $\Gamma_1 = ([A,B] \times \{C\}) \cup ([A,B] \times \{D\})$

- The triangulation is defined by : $\bar{\Omega} = K_1 \cup K_2 \cup K_3$,

  $K_1 = [A,M] \times [C,D]$, $K_2 = [M,N] \times [C,D]$, $K_3 = [N,B] \times [C,D]$,

  $M = A + \frac{B-A}{3}$, $N = A + 2\,\frac{B-A}{3}$

- Functions D and $\sum$ are constant on Ω.
- The finite element is the linear Lagrange element.

The domain, Ω, is splitted into four parts along the lines : $X \equiv \frac{A+B}{2}$ and $Y \equiv \frac{C+D}{2}$. The nodes and the decomposition are represented on figure 3.

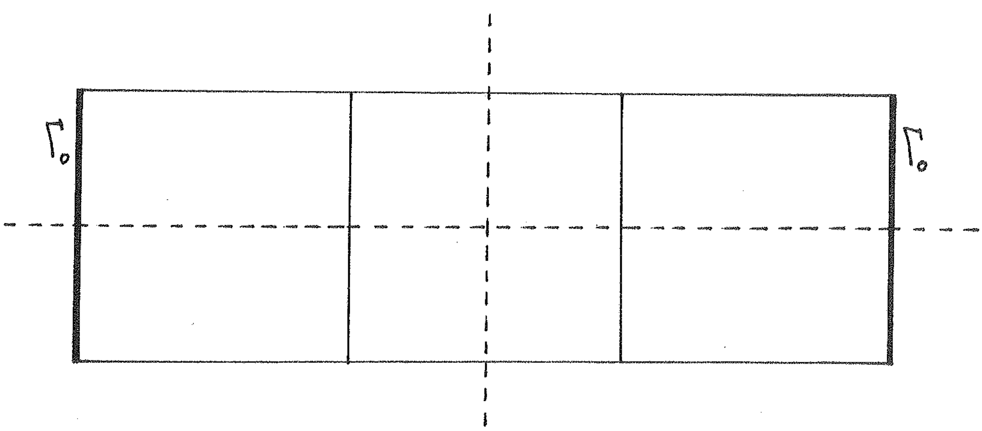


FIGURE 3

Linear Lagrange element - Second example

Here : $T_2 = \{K_1, K_3\}$ $T_4 = \{K_2\}$, $T_i = \emptyset$ $\forall i \notin \{2,4\}$.

According to the study led previously, $A'_4 = \hat{A}'_{K_2}$ is positive definite if and only if $\frac{\sum h^2}{48} < D$. The theoretical study permits to conclude that if $\frac{\sum h^2}{48} < D$, then A' is positive definite and the block-Jacobi method is convergent.

The direct study, consisting of calculations of the four eigenvalues of A', shows that they are positive, and consequently A' is positive definite ; therefore, the block-Jacobi method is convergent.

2.4. - Conclusion A direct study yield a necessary and sufficient convergence condition of the form : $D > C \sum h^2$, where C is a constant belonging to $[0, +\infty[$ and depending on the geometry of the domain, the boundary conditions, the finite element and the decomposition, and also on the geometry of the triangulations. However, a direct study, as the one performed on the above examples, is quite often impossible in concrete cases. The theoretical study, though giving less precise results, as seen on the examples, has the advantage of being always applicable and of giving a convergence condition depending only on the finite element and the decomposition.

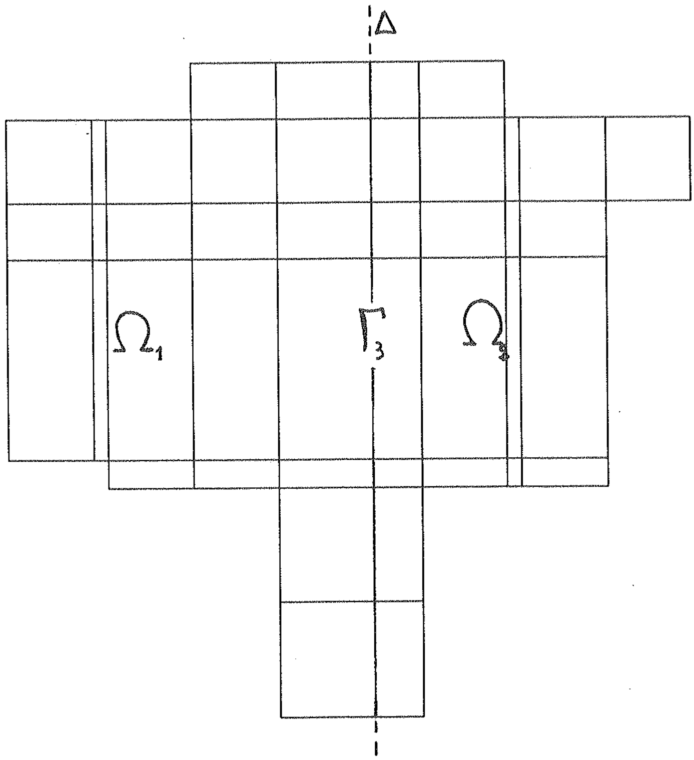
3. - Study of the convergence of the block-Jacobi method associated with a decomposition of the domain, in the case of mixed dual elements of Raviart and Thomas [5].

In this paragraph, we study the convergence of the block-Jacobi method associated with a decomposition of the domain, in the case of a discretization by mixed dual elements of Raviart and Thomas. With the aim of having simple notations, the study takes place in the two dimensional case.

A triangulation of the domain, T_h, an element of Raviart and Thomas, and a decomposition of the domain are given.

The matrix of the linear system is not positive definite, so it is not sure that the Block-Jacobi method can be defined. It is the first problem to look at.

3.1. Definition of the block-Jacobi method Suppose that an axis Δ cuts Ω along sides of rectangles of the triangulation ; Ω is decomposed into two subdomains along Δ ; we have the possibility of considering the interface Γ_3 as a third subdomain (dissection decomposition) or integrating it to one of the subdomains (decomposition with an integrated interface) (see figure 4).



. Dissection decomposition :

$\begin{cases} \text{domain 1 : nodes of } \Omega_1 \\ \text{domain 2 : nodes of } \Omega_2 \\ \text{domain 3 : nodes of } \Omega_3 \end{cases}$

. Decomposition with an integrated interface :

$\begin{cases} \text{domain 1 : nodes of } \Omega_1 \text{ and nodes of } \Gamma_3 \\ \text{domain 2 : nodes of } \Omega_2 \end{cases}$

or $\begin{cases} \text{domain 1 : nodes of } \Omega_1 \\ \text{domain 2 : nodes of } \Omega_2 \text{ and nodes of } \Gamma_3 \end{cases}$

FIGURE 4

Dissection decomposition and decomposition with an integrated interface

The matrix of the linear system can be written under the following form :

$$A = \begin{pmatrix} A_{11} & 0 & A_{13} \\ 0 & A_{22} & A_{23} \\ {}^tA_{13} & {}^tA_{23} & A_{33} \end{pmatrix}$$

A_{33} is symmetric and positive definite, because the nodes situated on the interface are current nodes. For i = 1 and i = 2, A_{ii} is the matrix of the approximate problem corresponding to the equation :

$$\begin{cases} -\operatorname{div}(D\,\vec{\nabla}u) + \sum u = S & \text{in } \Omega_i \\ u = 0 & \text{on } \Gamma_o \cap \partial\Omega_i \\ D\,\frac{\partial u}{\partial n} = 0 & \text{on } (\Gamma_1 \cap \partial\Omega_i) \cup \Gamma_3 \end{cases}$$

and so is invertible if : ($\exists\, \sum_o > 0$ so that : $\sum(x) \geq \sum_o > 0$ in Ω_i or meas $(\Gamma_o \cap \partial\,\Omega_i) > 0$) ; the second condition is satisfied if Ω and the boundary conditions (that is to say : Γ_o and Γ_1) are symmetric with respect to Δ. The block-Jacobi method associated with the dissection decomposition is defined, if one of the above hypotheses is verified ; it is now supposed that we are in that case.

Now, let us examine if matrix $\bar{A}_{ii} = \begin{pmatrix} A_{ii} & A_{i3} \\ {}^tA_{i3} & A_{33} \end{pmatrix}$ for i = 1 or 2 is invertible. Let $A_{33}^{(i)}$ be the contribution of Ω_i to matrix A_{33}(*). Then, $\tilde{A}_{ii} = \begin{pmatrix} A_{ii} & A_{i3} \\ {}^tA_{i3} & A_{33}^{(i)} \end{pmatrix}$ is the matrix of the problem on Ω_i :

$$\begin{cases} -\operatorname{div}(D\,\nabla u) + \sum u = S & \text{in } \Omega_i \\ u = 0 & \text{on } (\Gamma_o \cap \partial\,\Omega_i) \cup \Gamma_3 \\ D\,\frac{\partial u}{\partial n} = 0 & \text{on } \Gamma_1 \cap \partial\,\Omega_i \end{cases}$$

and so is invertible because meas $((\Gamma_o \cap \partial\Omega_i) \cup \Gamma_3) \geq$ meas $(\Gamma_3) > 0$.

The following general result holds :

<u>Theorem</u> : let $M = \begin{pmatrix} A & B & D \\ {}^tB & C & E \\ {}^tD & {}^tE & F \end{pmatrix}$ be a symmetric and invertible matrix. If $\begin{pmatrix} A & B \\ {}^tB & C \end{pmatrix}$ is positive definite, F semi negative definite and $\begin{pmatrix} C & E \\ {}^tE & F \end{pmatrix}$ invertible, then $A - (B\text{–}D) \begin{pmatrix} C & E \\ {}^tE & F \end{pmatrix}^{-1} \begin{pmatrix} {}^tB \\ {}^tD \end{pmatrix}$ is symmetric positive definite.

We apply this theorem with $M = \begin{pmatrix} A_{33}^{(i)} & {}^tA_{i3} \\ A_{i3} & A_{ii} \end{pmatrix}$, $A = A_{33}^{(i)}$,

(*) If $(A_{33})_{k,\ell} = \int_\Omega \frac{1}{D} \vec{P}_k \cdot \vec{P}_\ell$, then $(A_{33}^{(i)})_{k,\ell} = \int_{\Omega_i} \frac{1}{D} \vec{P}_k \cdot \vec{P}_\ell$

$\begin{pmatrix} C & E \\ {}^tE & F \end{pmatrix} = A_{ii}$, and we conclude that $A_{33}^{(i)} - {}^tA_{i3}\, A_{ii}^{-1}\, A_{i3}$ is symmetric positive definite. But, $A_{33}^{(1)}$ and $A_{33}^{(2)}$ are symmetric positive definite, and this implies that the two matrices :

$$\begin{cases} A_{33} - {}^tA_{13}\, A_{11}^{-1}\, A_{13} = (A_{33}^{(1)} - {}^tA_{13}\, A_{11}^{-1}\, A_{13}) + A_{33}^{(2)} \\ A_{33} - {}^tA_{23}\, A_{22}^{-1}\, A_{23} = (A_{33}^{(2)} - {}^tA_{23}\, A_{22}^{-1}\, A_{23}) + A_{33}^{(1)} \end{cases} \quad \text{are positive}$$

definite, and in particular they are invertible. Consequently, $\bar{A}_{11}$ and $\bar{A}_{22}$ are invertible, and the block-Jacobi method associated with the two decompositions with an integrated interface can be defined.

The results are similar to the previous ones for a decomposition into four parts along two perpendicular axes.

All this can be generalized to the three dimensional case for decompositions along planes of symmetry.

Demonstration of the theorem :

Let us define the following notations :

$$\mathcal{A} = A - (B\text{-}D)\begin{pmatrix} C & E \\ {}^tE & F \end{pmatrix}^{-1} \begin{pmatrix} {}^tB \\ {}^tD \end{pmatrix}, \quad \mathcal{M} = \begin{pmatrix} C & E \\ {}^tE & F \end{pmatrix}, \quad \mathcal{A}_o = A - BC^{-1}\,{}^tB$$

$\begin{pmatrix} A & B \\ {}^tB & C \end{pmatrix}$ is symmetric positive definite, and so is $\mathcal{A}_o$; we note :

$$\mathcal{A}_1 = \mathcal{A} - \mathcal{A}_o$$

$$\mathcal{A}_1 = B\,C^{-1}\,{}^tB - (B\ D)\,\mathcal{M}^{-1}\begin{pmatrix} {}^tB \\ {}^tD \end{pmatrix} = (B\ D)\left[\begin{pmatrix} C^{-1} & 0 \\ 0 & 0 \end{pmatrix} - \mathcal{M}^{-1}\right]\begin{pmatrix} {}^tB \\ {}^tD \end{pmatrix}$$

$$\mathcal{A}_1 = {}^tH\left[\mathcal{M}\begin{pmatrix} C^{-1} & 0 \\ 0 & 0 \end{pmatrix}\mathcal{M} - \mathcal{M}\right] H, \quad \text{with } H = \mathcal{M}^{-1}\begin{pmatrix} {}^tB \\ {}^tD \end{pmatrix}.$$

$$\mathcal{A}_1 = {}^tH\begin{pmatrix} 0 & 0 \\ 0 & {}^tE\,C^{-1}\,E - F \end{pmatrix} H.$$

$\begin{pmatrix} C & E \\ {}^tE & F \end{pmatrix}$ is invertible, C is positive definite and F is negative semi definite, therefore ${}^tE\,C^{-1}\,E - F$ is positive semi definite. Consequently $\mathcal{A}_1$ is positive semi-definite.

Then $\mathcal{A} = \mathcal{A}_o + \mathcal{A}_1$ is positive definite.

3.2. Numerical tests

Numerical tests have been carried out. The first ones, led in 3D, are relative to the dissection decomposition associated with the splitting of a cube into eight equal parts, the finite element being the element of Raviart and Thomas of order 1 [5].

For :
- numbers of points in the 3 directions equal to 3.
- $\sum = 1$, $S = 10^{-3}$, length of the side of a cube of the triangulation : $h = 1$.
- X^o = initial vector for the Jacobi iterations so that : $X^o(i) = 1 \ \forall i$.

the numerical results are indicated on table 5.

D	Number of iterations	Precision
100	50 100	151,89 297 912 288
30	100	539,23
20	100 200 300	0,74 5815,59 45591 728
15	19	convergence
10	15	convergence
1	21	convergence

. precision=pr(n) = $\frac{\| X^n - X \|}{\| X \|}$

X = exact solution

. In the last 3 cases we have indicated the number of iterations that are necessary for the convergence.

TABLE 5

Numerical results about a dissection decomposition

The results of theses tests are not enough to conclude but they allow to think that for $\frac{D}{\sum h^2}$ greater than a constant, the block-Jacobi methodes diverges.

Other tests, led on 2 examples of reactors, have also suggested that the dissection algorithm could diverge and that decompositions with an integrated interface are more stable [5, 6].

An analytical study has been led on examples.

3.3. Examples

3.3.1. First example - The framework of this example is the following :

- Ω is a square : $\Omega =]A,B[\times]C,D[$, and $D-C = B-A = 2\ h$
- the boundary conditions are : $u = 0$ on $\partial\Omega$
- the triangulation of Ω is defined by : $\bar{\Omega} = K_1 \cup K_2 \cup K_3 \cup K_4$,

  $K_1 = [A,M] \times [C,N]$, $K_2 = [M,B] \times [C,N]$, $K_3 = [A,M] \times [N,D]$,

  $K_4 = [M,B] \times [N,D]$, $M = \frac{A+B}{2}$, $N = \frac{C+D}{2}$.
- D and $\sum$ are constant on Ω.
- the finite element is the element of Raviart and Thomas of order 1.

The domain is splitted into four parts along the lines : $X \equiv M$ and $Y \equiv N$, and we consider the dissection decomposition. The nodes and the decomposition are represented on figure 6.

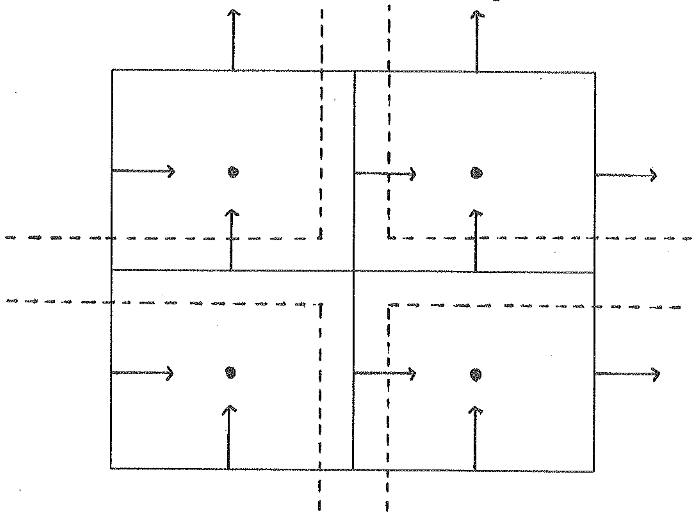


FIGURE 6

Element of Raviart and Thomas - First example

By calculating the iteration matrix and studying its eigenvalues [5], it is shown that :

The block-Jacobi method is convergent if and only if : $D < \frac{5}{24} \sum h^2$.

3.3.2. Second example - The framework of this example is the following :

- Ω is a rectangle : $\Omega =]A,B[\times]C,D[$ and $B,A=2(D-C) = 2h$
- the boundary conditions are : $\begin{cases} u = 0 & \text{on } \Gamma_o \\ D \frac{\partial u}{\partial n} = 0 & \text{on } \Gamma_1 \end{cases}$

with : $\Gamma_o = \{A\} \times [C,D]$, $\Gamma_1 = ([A,B]x\{C\}) \cup (\{B\}x[C,D]) \cup ([A,B]x\{D\})$

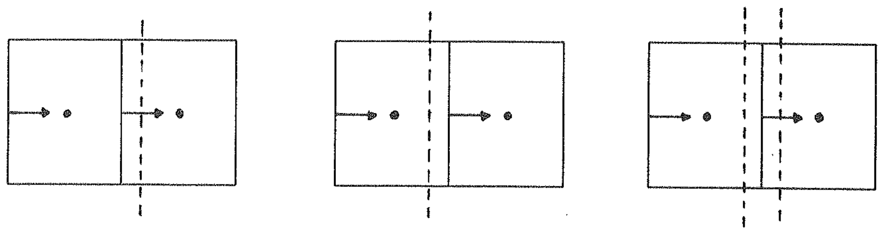
- the triangulation of Ω is defined by : $\bar{\Omega} = K_1 \cup K_2$,

  $K_1 = [A,M]x[C,D]$, $K_2 = [M,B]x[C,D]$ and $M = \frac{A+B}{2}$

- D and $\sum$ are constant on Ω

- the finite element is the element of Raviart and Thomas of order 1

Ω is splitted into two parts by the line : $X \equiv M$, and three decompositions are considered, whether the interface is or is not integrated to one of the two subdomains ; they are represented on figure 7.



decomposition 1 decomposition 2 decomposition 3

FIGURE 7

Element of Raviart and Thomas - Second example

By calculating the 3 iteration matrices and their eigenvalues, we have found a necessary and sufficient condition for the convergence of the block-Jacobi method associated to each decomposition [5] ; these results are indicated in table 8. We notice the block-Jacobi method associated to the dissection decomposition is the one that converges the least.

	decomposition 1 (interface integ. to domain 1)	decomposition 2 (interface integ. to domain 2)	decomposition 3 (dissection decomposition)
convergence condition	$\frac{D}{\sum h^2} < \frac{7}{6}$	any $\frac{D}{\sum h^2}$	$\frac{D}{\sum h^2} < \frac{\sqrt{10} - 1}{6}$

$\frac{7}{6} \approx 1{,}167$ $\frac{\sqrt{10} - 1}{6} \approx 0{,}360$

TABLE 8

Convergence condition for each decomposition

3.4. Conclusion On examples it has been established that the convergence criterion of the block-Jacobi method is of the form : $\sum \frac{D}{h^2} < C$, where C is a constant belonging to]0, +∞], and depending on the geometry of the domain, the boundary conditions, the finite element, the decomposition and also on the geometry of the triangulation.

We may note that here the inequality is the opposite of the one we have in the case of Lagrange elements.

REFERENCES

/1/ J.J. DUDERSTADT, L.J. HAMILTON
"Nuclear Reactor Analysis", John Wiley & Sons, inc., 1976.

/2/ R. DAUTRAY, J.L. LIONS
"Analyse mathématique et calcul numérique pour les sciences et les techniques", Collection du Commissariat à l'Energie Atomique, Masson, 1984 (in French).

/3/ P.G. CIARLET
"The Finite Element Method for Elliptic Problems" - North Holland, 1978.

/4/ P.A. RAVIART, J.M. THOMAS
"A Mixed Finite Element Method for 2nd Order Elliptic Problems" Lecture Notes in Mathematics 606, Springer Verlag, 1977.

/5/ F. COULOMB
"Algorithmes parallèles pour la résolution de l'équation de diffusion par les méthodes éléments finis et par les méthodes nodales", Thèse de l'Université Pierre et Marie Curie, PARIS, March 1989 (in french).

/6/ F. COULOMB
"Domain Decomposition and Mixed Finite Elements for the Neutron Diffusion Equation", Proceedings of the Second International Symposium on Domain Decomposition methods, LOS ANGELES, 14-16 january 1988, SIAM.