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DOMAIN DECOMPOSITION METHODS FOR CORE CALCULATIONS USING THE MINOS SOLVER

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ABSTRACT

Cell by cell homogenized transport calculations of an entire nuclear reactor core are currently too expensive for industrial applications, even if a simplified transport (SPn) approximation is used. In order to take advantage of parallel computers, we propose here two domain decomposition methods using the mixed dual finite element solver MINOS. The first one is a modal synthesis method on overlapping subdomains: several eigenmodes solutions of a local problem on each subdomain are taken as basis functions used for the resolution of the global problem on the whole domain. The second one is an iterative method based on non-overlapping domain decomposition with Robin interface conditions. At each iteration, we solve the problem on each subdomain with the interface conditions given by the solutions on the close subdomains estimated at the previous iteration. For these two methods, we give numerical results which demonstrate their accuracy and their efficiency for the diffusion model on realistic 2D and 3D cores.

Key Words: Domain decomposition, parallel calculations, eigenvalue problem.

1. INTRODUCTION

Cell by cell homogenized transport calculations of an entire nuclear reactor core are currently too expensive for industrial applications, even if a simplified transport (SP_N) approximation is used.

A way to decrease the computation time and the local memory requirement is to use a domain decomposition method. It is particularly well fitted for parallel computers: calculations are distributed on several subdomains, and as many processors as subdomains can be used. We propose here two approaches based on domain decomposition.

The first one is a modal synthesis approximation [1]: the global flux is expanded on a finite set of basis functions obtained on overlapping subdomains. The global exact cell by cell problem is solved in the finite spaces spanned by the different local functions. Two techniques are presented in order to obtain these basis functions [2].

The second approach is an iterative domain decomposition method using non overlapping subdomains and Robin interface conditions.

Even if these methods could be applied to a SP_N approximation, we demonstrate here their accuracy for the diffusion model. They are implemented in the framework of the existing MINOS solver [3], which uses a mixed dual finite element method for the resolution of diffusion and SP_N equations in 3D cartesian homogenized geometries.

We present results for these two methods on realistic 2D and 3D cores: we show the accuracy of the solutions and the efficiency of the codes on parallel computers.

2. THE MINOS SOLVER

The MINOS solver is one of the main core computational tools of the CRONOS2 system. This solver is reported in the new generation neutronic system DESCARTES and has therefore been rewritten in the C++ language [3].
MINOS solves diffusion or SP_N multigroup equations. It is based on a mixed-dual formulation of these problems, and it uses simultaneously scalar functions (even components) and vector functions (odd components). For SP_1 and diffusion equations, the even component is the scalar flux and the odd component is the current.
If *R* is a bounded domain (in fact the core) with boundary ∂R, the steady-state diffusion problem is an eigenvalue problem, and its mixed (flux φ, current $\vec{p}$) formulation reads as follows for each energy group, with zero flux boundary conditions:

$$\begin{cases} \vec{p} + D\vec{\nabla}\varphi = 0 \quad on\ R \\ \vec{\nabla}.\vec{p} + \sigma\varphi = \dfrac{1}{\lambda} S_f + S_\varphi \quad on\ R \\ \varphi = 0 \quad on\ \partial R \end{cases} \tag{1}$$

where S_f is the fission source and S_φ is the scattering source, both due to the contribution of the other groups. D is the diffusion coefficient and σ is the removal cross section.
The dual variational formulation of this problem is obtained by projecting the two equations of problem (1) on two different functional spaces, and applying the Green formula to the first equation. We obtain the variational problem for each group: find the fundamental eigenmode $\vec{p} \in H(div, R)$, $\varphi \in L^2(R)$ and λ solution of the problem

$$\begin{cases} \displaystyle\int_R -\frac{1}{D}\vec{p}.\vec{q} + \int_R \vec{\nabla}.\vec{q}\varphi = 0 \quad \forall \vec{q} \in H(div, R) \\ \displaystyle\int_R \vec{\nabla}.\vec{p}\psi + \int_R \sigma\varphi\psi = \frac{1}{\lambda}\int_R S_f\psi + \int_R S_\varphi\psi \quad \forall \psi \in L^2(R) \end{cases} \tag{2}$$

where $H(div, R) = \left\{ \vec{q} \in \left[L^2(R)\right]^S ; \vec{\nabla}.\vec{q} \in L^2(R) \right\}$ with S the space dimension.
The Raviart-Thomas-Nedelec (RT_N) elements are used to discretize the different functional spaces. To ensure consistency, the divergence of the vector space lies within the scalar space. Then it can be shown that the discrete solution converges to the exact continuous one. The use of these elements yields sparse matrices with coupling terms oriented only along each considered axis. Various boundary conditions can be taken into account in MINOS such as zero flux, reflection, void, albedo, translation and rotation. Discontinuity conditions on the scalar flux can also be taken into account.

3. THE MODAL SYNTHESIS METHOD

3.1. The Component Mode Synthesis (CMS) method

The principle of the CMS method lies in the decomposition of the global domain in subdomains, which can be overlapping or not. Here we choose overlapping subdomains, as motivated by [1]. We have adapted the CMS method to the steady state neutronic equations written in the mixed dual formulation [2]. We split the domain *R* into overlapping subdomains such that: $R = \bigcup_{k=1}^{K} R^k$.

On each R^k, we consider the first N^k eigenmodes $(\varphi_i^k, \vec{p}_i^k, \lambda_i^k)_{1\le i\le N^k}^{1\le k\le K}$ solutions of local diffusion problems using infinite medium boundary conditions on the interfaces which are not on the core boundary, and the actual core boundary conditions otherwise. In order to have functions defined on the whole domain, we extend the local solutions by 0 (denoted by a ~). Finally the global diffusion problem (2) is discretized on the finite dimension spaces spanned by all these functions:

$$\begin{aligned} W_\delta &= span\left\{ \tilde{\vec{p}}_{i,d}^{\,k} \right\}_{1\le i\le N^k,d}^{1\le k\le K} \subset H(div, R) \\ V_\delta &= span\left\{ \tilde{\varphi}_i^k \right\}_{1\le i\le N^k}^{1\le k\le K} \subset L^2(R) \end{aligned} \tag{3}$$

where the subscript d denotes a given space direction. Only the d-component of $\tilde{\vec{p}}_{i,d}^{\,k}$ is non zero:

$$\tilde{\vec{p}}_{i,x}^{\,k} = \begin{bmatrix} \tilde{p}_{i,x}^k \\ 0 \\ 0 \end{bmatrix}, \quad \tilde{\vec{p}}_{i,y}^{\,k} = \begin{bmatrix} 0 \\ \tilde{p}_{i,y}^k \\ 0 \end{bmatrix}, \quad \tilde{\vec{p}}_{i,z}^{\,k} = \begin{bmatrix} 0 \\ 0 \\ \tilde{p}_{i,z}^k \end{bmatrix}, \qquad \text{with } \tilde{p}_{i,d}^k = \tilde{\vec{p}}_i^{\,k}.\vec{d}$$

The fundamental solution $(\varphi_\delta, \vec{p}_\delta, \lambda_\delta)$ of the global diffusion problem discretized on these spaces can be written as linear combinations of the local eigenfunctions: $\vec{p}_\delta = \sum_{k=1}^{K}\sum_{i=1}^{N^k}\sum_{d} c_{i,d}^k \tilde{\vec{p}}_{i,d}^{\,k}$ for the current and $\varphi_\delta = \sum_{k=1}^{K}\sum_{i=1}^{N^k} f_i^{\,k} \tilde{\varphi}_i^k$ for the flux. A linear system of the following form (generalized eigenvalue problem) in the scalar coefficients $\left\{ \left[c_{i,d}^k\right], \left[f_i^{\,k}\right] \right\}_{i=1,N^k}^{k=1,K}$ is obtained:

$$A\begin{bmatrix} c_{i,d}^k \\ f_i^{\,k} \end{bmatrix} = \frac{1}{\lambda_\delta} T \begin{bmatrix} c_{i,d}^k \\ f_i^{\,k} \end{bmatrix} \tag{4}$$

where *A* and *T* correspond to the application of bilinear forms on the local eigenmodes used to span W_δ and V_δ. Since these forms are integrals on $R^k \overset{\circ}{\cap} R^l$ ($R^k \overset{\circ}{\cap} R^l$ is defined as the interior

of $R^k \cap R^l$), A and T are sparse: their constituting blocks vanish as soon as $R^k \overset{\circ}{\cap} R^l = \varnothing$ (see [2] for more details).

3.2. The Factorized (FCMS) method

The determination of multiple eigenfunctions on each subdomain is expensive in terms of computing time and memory storage. In the FCMS method, only the fundamental mode is performed on each subdomain, and we replace the higher order modes by suitably chosen functions. The idea, coming from homogenization results, is to factorize the higher order modes. In this view, we mention the following factorization principle for the diffusion model, proved in [4]: in a periodic core, the i-th flux eigenmode solution of the diffusion problem can be asymptotically written $\varphi_i \approx u_i \times \psi$ with ψ the fundamental periodic solution of the problem on each assembly with infinite medium boundary conditions, and u_i the i-th eigenfunction solution of a homogenized diffusion problem on the whole core.
For a non-periodic core, we adapt the above factorization principle on each subdomain of our core decomposition. Our goal is to build basis functions that take into account the heterogeneous fine structure of the core, based only on the fundamental solutions $(\vec{p}^k, \varphi^k)$ of the local problems. We define our new local flux basis functions $\tilde{\varphi}_i^k \in L^2(R)$ as follows:

$$\begin{cases} \tilde{\varphi}_1^k = \varphi^k \text{ on } R^k \\ \tilde{\varphi}_1^k = 0 \text{ on } R \setminus R^k \end{cases} \quad \text{and} \quad \begin{cases} \tilde{\varphi}_i^k = \varphi^k \times u_i^k \text{ on } R^k \\ \tilde{\varphi}_i^k = 0 \text{ on } R \setminus R^k \end{cases} \quad 1 \le k \le K,\ 2 \le i \le N^k \tag{5}$$

where u_i^k are analytical solutions (sines or cosines) of homogenized diffusion problems on R^k, with reflective boundary conditions on $\partial R^k \setminus \partial R$.
Unfortunately, we have no such factorization property for the current. We define the current basis functions in the d direction according to:

$$\begin{cases} \tilde{p}_{1,d}^k = p_d^k \text{ on } R^k \\ \tilde{p}_{1,d}^k = 0 \text{ on } R \setminus R^k \end{cases} \quad \text{and} \quad \begin{cases} \tilde{p}_{i,d}^k = \dfrac{\partial u_i^k}{\partial d} \text{ on } R^k \\ \tilde{p}_{i,d}^k = 0 \text{ on } R \setminus R^k \end{cases} \quad 2 \le i \le N^k,\ 1 \le k \le K \tag{6}$$

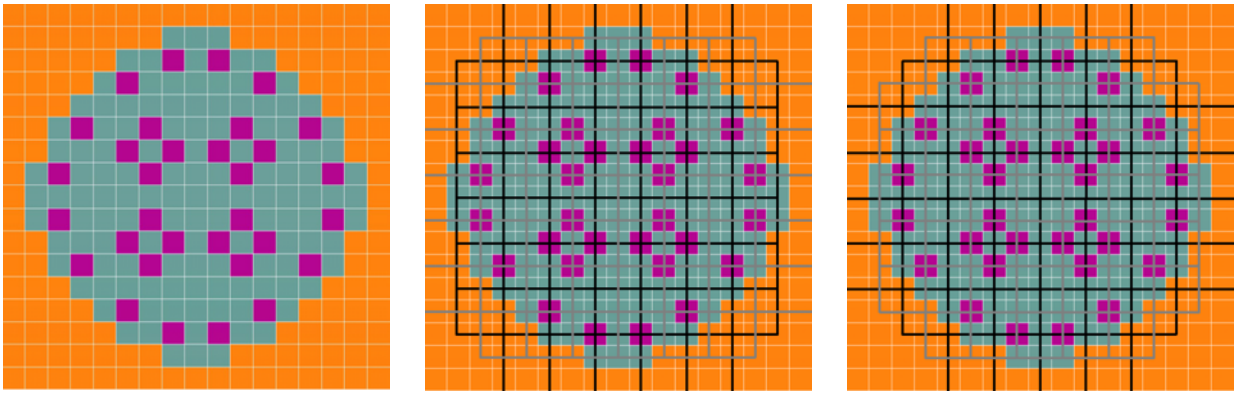
Since $\dfrac{\partial u_i^k}{\partial n} = 0$ and $\vec{p}^k.\vec{n} = 0$ on $\partial R^k \setminus \partial R$, we have $\tilde{\vec{p}}_{i,d}^k \in H(div, R)$.
The resolution of the global problem is the same as in subsection 3.1: we modify only the basis functions, replacing the higher order local eigenmodes by the functions (5) for the flux and (6) for the current.

3.3. Numerical results

In order to validate CMS and FCMS methods for neutronic core calculations, we use a realistic model of a 2D PWR 900 MWe core loaded with a set of UOX and MOX assemblies (Fig. 1a). Fig. 1b and 1c represent the proposed couple of decompositions in 201 subdomains for this core. We have chosen the internal subdomain boundaries on the middle of the assemblies, where the infinite medium boundary condition is believed to be close to the real value.We present in Table I results for CMS and FCMS methods, compared to the direct cell by cell calculation obtained by the MINOS solver. We use a 2D diffusion calculation with two energy groups.

Table I: Differences between CMS, FCMS and MINOS solutions. $k_{eff} = 1.17961$.

	CMS method 4 flux modes, 6 current modes	**FCMS method 6 flux modes, 11 current modes**
Δk_{eff} (pcm)	4.4	2.2
$\|\Delta P\|_2 / \|P\|_2$	4.3×10^{-3}	3.1×10^{-3}
$\|\Delta P\|_\infty$	5.0×10^{-2}	2.4×10^{-2}



a. PWR core b. First subdomains c. Other subdomains

Figure 1. PWR core and its domain decomposition.

3.4. Parallelization

Contrary to many domain decomposition methods, the CMS algorithm is not iterative (see Fig. 2). One can decompose it into three steps: first the local resolutions on the subdomains, second the matrix calculations and finally the global resolution on the whole domain. Each processor performs at least one subdomain calculation. No communications are requested for the local resolutions, since they are completely independent. Some exchanges of the local solutions are necessary for the matrix calculations, but only between the overlapping subdomains. Each

processor performs the submatrix calculations associated to its subdomains, and has to send them to the master processor for the sequential global resolution.
We illustrate the computing times and the efficiency of the code in parallel in Fig. 3. The 3D-core is a PWR 900-MWe split into 20 planes in the z-axis: the first and the last ones are reflectors; the other ones use the same grid as in two dimensions (see Fig. 1a). We use in these tests the FCMS method with 6 flux modes and 11 current modes. The domain is decomposed in 49 overlapping subdomains (in the X- and Y- directions). The computer used is an AMD Opteron cluster. Each node of the cluster is a 2.4 GHz quadriprocessor with 4 GB of shared memory. The nodes are connected via a high performance switch (Infiniband). We compare the computing times between the direct MINOS calculation and our FCMS method using from 1 to 25 processors.

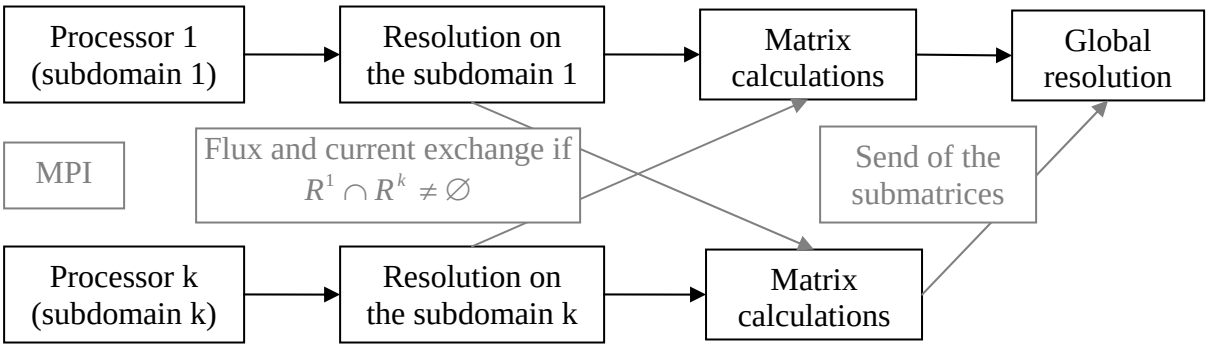


Figure 2. CMS flowchart.

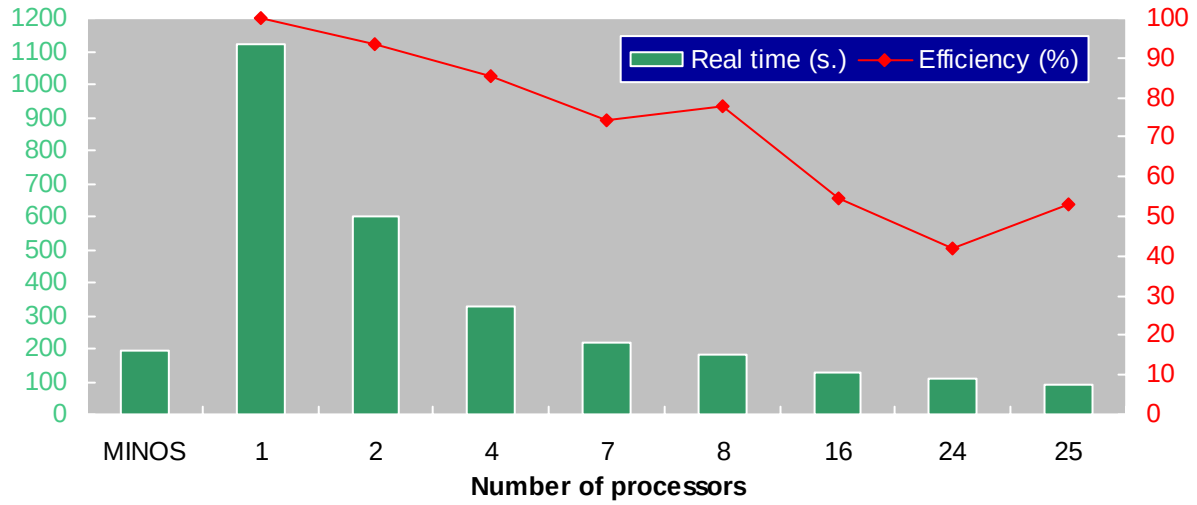


Figure 3. Real computing times and efficiency of the parallel code.

4. AN ITERATIVE DOMAIN DECOMPOSITION (IDD) METHOD

4.1. Introduction

In order to compare the previous methods with another domain decomposition technique, and to reduce the computing times and the memory requirement, we have developed an iterative scheme, proposed by P. L. Lions [5]. Let $R = \bigcup_{k=1}^{K} R^k$ a non-overlapping domain decomposition. The idea is to iterate the resolution of local problems on each subdomain, using Robin interface conditions. This condition on an internal subdomain boundary, at a given iteration, consists to impose the corresponding boundary value of the solution obtained on the close subdomain at the previous iteration. The iterative resolution of the diffusion problem (1) with the IDD method reads, on each subdomain R^k and at each outer iteration n:

$$\begin{cases} \vec{p}_n^{\,k} + D\vec{\nabla}\varphi_n^k = 0 \quad on\ R^k \\ \vec{\nabla}.\vec{p}_n^{\,k} + \sigma\varphi_n^k = \dfrac{1}{\lambda_{n-1}} S_{f,n-1}^k + S_{\varphi,n-1}^k \quad on\ R^k \\ \varphi_n^k = 0 \quad on\ \partial R^k \cap \partial R \\ -\vec{p}_n^{\,k}.\vec{n}^k + \alpha^{kl}\varphi_n^k = \vec{p}_{n-1}^{\,l}.\vec{n}^l + \alpha^{kl}\varphi_{n-1}^l \quad \text{on } \Gamma^{kl},\ \forall \Gamma^{kl} \neq \varnothing \end{cases} \tag{7}$$

where α^{kl} is a positive coefficient (α^{kl} can be different on each interface) and $\Gamma^{kl} = \partial R^k \cap \partial R^l$. $\vec{n}^k$ and $\vec{n}^l$ are the outward normals on Γ^{kl} ($\vec{n}^k = -\vec{n}^l$). The mixed dual formulation of (7) is:

$$\begin{cases} \displaystyle\int_{R^k} -\frac{1}{D}\vec{p}_n^{\,k}.\vec{q} + \int_{R^k} \vec{\nabla}.\vec{q}\,\varphi_n^k - \frac{1}{\alpha^{kl}}\int_{\Gamma^{kl}} \left(\vec{p}_n^{\,k}.\vec{n}^k\right)\left(\vec{q}.\vec{n}^k\right) = \frac{1}{\alpha^{kl}}\int_{\Gamma^{kl}} S_{n-1}^{\Gamma^{kl}}\left(\vec{q}.\vec{n}^k\right) \quad \forall \vec{q} \in H(div, R^k) \\ \displaystyle\int_{R^k} \vec{\nabla}.\vec{p}_n^{\,k}\,\psi + \int_{R^k} \sigma\varphi_n^k\,\psi = \frac{1}{\lambda_{n-1}}\int_{R^k} S_{f,n-1}^k\,\psi + \int_{R^k} S_{\varphi,n-1}^k\psi \quad \forall \psi \in L^2(R^k) \end{cases} \tag{8}$$

where $S_{n-1}^{\Gamma^{kl}} = \vec{p}_{n-1}^{\,l}.\vec{n}^l + \alpha^{kl}\varphi_{n-1}^l$. The outer iterations allow simultaneously the convergence of the eigenvalue problem and of the domain decomposition scheme.

4.2. Parallelization

We have implemented the IDD method in the DESCARTES project with the C++ language. Fig. 4 presents the flowchart of the different steps of the algorithm. One of its advantage is that it needs only minor modification of the MINOS solver. Only two data exchanges per outer iteration are necessary between the processes: one for the interface condition exchanges between the close subdomains, and one for the k_{eff} calculation. The domain decomposition is automatic, by imposing the same size for all the subdomains. It ensures a good balance of the load of the processors.

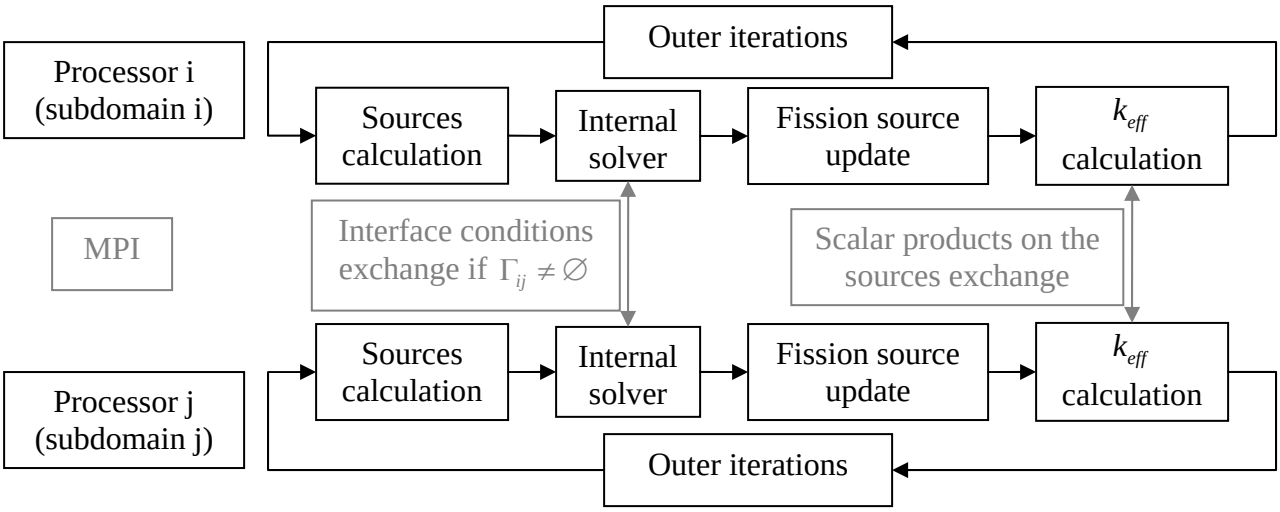


Figure 4. IDD flowchart.

4.3. Numerical results

In order to validate the IDD method for multigroup eigenvalue diffusion problems, we use two geometries: the first one is a 3D PWR 900 MWe core (the size of the mesh is $289 \times 289 \times 40$), and the second one is a 2D model of the JHR (Jules Horowitz Reactor) core [6], for which we use a very fine mesh (1000×1000) in order to have a good cartesian projection of the complex geometry. In Tables II and III we study the accuracy and the efficiency of the IDD method: we compare a reference full converged MINOS calculation to a MINOS calculation and IDD calculations converged with a criterion of 10^{-5} on the infinite norm of the fission source. Different numbers of subdomains are tested, with the same α coefficient for all the interfaces. Table II is relative to the PWR calculations with two energy groups. We use $\alpha = 1$ for the fast group and $\alpha = 5 \times 10^{-2}$ for the thermal one. Table III concerns the JHR results with 6 energy groups, and we use $\alpha = 10^{-2}$ for all the groups. The computer used is described in subsection 3.4. We obtain the same conclusions with the two geometries. In almost all the cases, the number of outer iterations is very near the MINOS one, what means that the domain decomposition does not increase it. Thus the efficiency of the IDD method is very good, especially in the JHR case. In terms of accuracy, it is very satisfactory, even with many subdomains. In the PWR case, the accuracy variations are due to the numerical discretization of the interface conditions. Thus the accuracy is better when the domain decomposition corresponds to the symmetry axes of the core. This is the case in Table II for 2, 4 and 8 subdomains. In the JHR case, the interface condition discretization is better because the mesh is finer. We plan to improve these results with optimal and automatic estimation of the values of the α coefficient in the Robin interface conditions, as motivated by [7].

Table II: Results for the 3D PWR. Comparison with a reference full converged direct MINOS calculation (10 000 outer iterations). Stop criterion: 10^{-5} **on the infinite norm of the flux. The first line corresponds to the MINOS calculation. The other ones are related to the IDD method with different domain decompositions in the three directions (** $n_x \times n_y \times n_z$ **). The number of processors is equal to the number of subdomains.** $k_{eff} = 1.05208$ **.**

	Number of iterations	Δk_{eff} (pcm)	$\|\Delta P\|_2 / \|P\|_2$ ($\times 10^{-4}$)	$\|\Delta P\|_\infty$ ($\times 10^{-3}$)	Elapsed time (s.)	Efficiency per iteration (%)
MINOS	249	12	7,7	7,8	339	100
2 (2×1×1)	247	11	7,7	7,9	214	79
4 (2×2×1)	252	11	7,8	7,6	100	86
6 (3×2×1)	278	29	21	11	95	66
8 (2×2×2)	253	11	10	10	66	65
9 (3×3×1)	280	48	25	13	61	69
12 (4×3×1)	257	63	26	15	45	65
16 (4×4×1)	251	77	28	13	34	63
18 (3×3×2)	281	48	26	18	36	59

Table III: Results for the 2D JHR (see the Table II caption). The full converged MINOS calculation uses 50 000 outer iterations. $k_{eff} = 1.30857$ **.**

	Number of iterations	Δk_{eff} (pcm)	$\|\Delta P\|_2 / \|P\|_2$ ($\times 10^{-3}$)	$\|\Delta P\|_\infty$ ($\times 10^{-2}$)	Elapsed time (s.)	Efficiency per iteration (%)
MINOS	941	78	4,2	5,1	1490	100
2 (2×1)	917	78	4,3	5,2	581	125
4 (2×2)	978	78	4,2	5,0	357	108
6 (3×2)	1068	68	4,1	5,0	344	82
8 (4×2)	950	64	4,2	5,0	165	114
9 (3×3)	1004	63	4,2	5,1	171	103
12 (4×3)	1050	53	4,1	4,8	105	132
16 (4×4)	978	55	4,1	5,0	76	127
20 (5×4)	1051	55	4,1	4,9	65	128
25 (5×5)	1129	52	4,2	4,7	55	130
30 (6×5)	1647	43	3,5	4,0	59	147
36 (6×6)	1062	58	4,2	5,0	34	138

5. CONCLUSION

The domain decomposition techniques can answer to the need of a fast 3D SP_N solver. The applications of the component mode synthesis method to cell by cell core calculations give a good accuracy for the k_{eff} as well as for the local cell power. The total independence of the local mode calculations leads to a code well-fitted for parallel computers: the computing time with enough processors is smaller than the direct calculation one. Nevertheless, this method remains expensive, thus we have developed an iterative scheme based on non-overlapping subdomains and Robin interface conditions. The results are very good: the number of outer iterations does not increase compared to the direct solver. The accuracy of the method is very satisfactory, and the efficiency on parallel computers is very high. We plan to improve it with optimal and automatic values of the α coefficient in the Robin interface conditions. We will apply this promising method on complex 3D cores (JHR, EPR…), what is currently impossible because of the computing time or the memory requirement.

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