Component mode synthesis methods applied to 3D heterogeneous core calculations, using the mixed dual finite element solver MINOS

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Abstract

This paper describes a new technique for determining the pin power in heterogeneous core calculations. It is based on a domain decomposition with overlapping subdomains and a component mode synthesis technique for the global flux determination. Local basis functions are used to span a discrete space that allows fundamental global mode approximation through a Galerkin technique. Two approaches are given to obtain these local basis functions: in the first one (Component Mode Synthesis method), the first few spatial eigenfunctions are computed on each subdomain, using periodic boundary conditions. In the second one (Factorized Component Mode Synthesis method), only the fundamental mode is computed, and we use a factorization principle for the flux in order to replace the higher order eigenmodes. These different local spatial functions are extended to the global domain by defining them as zero outside the subdomain. These methods are well-fitted for heterogeneous core calculations because the spatial interface modes are taken into account in the domain decomposition. Although these methods could be applied to higher order angular approximations - particularly easily to a SP_N approximation - the numerical results we provide are obtained using a diffusion model. We show the methods' accuracy for reactor cores loaded with UOX and MOX assemblies, for which standard reconstruction techniques are known to perform poorly. Furthermore, we show that our methods are highly and easily parallelizable.

KEYWORDS: Domain decomposition, Eigenvalue problem, Parallelization, Steady state neutronic equations

1. Introduction

Cell by cell homogenized transport calculations of the entire core are currently too expensive for industrial applications, even if a simplified transport (SP_N) approximation is used. The standard reconstruction technique to obtain the local pin power consists in superposing a large scale diffusion calculation with a fine mesh pre-calculated function coming from a local transport calculation. Unfortunately this method does not work well for MOX reloaded cores due to the interface modes between UOX and MOX assemblies.

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We propose here a new approach based on modal synthesis approximation. 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 space spanned by the different local functions. We propose two methods to obtain these basis functions :

- The first one is adapted from the component mode synthesis (CMS) method [1]: the basis functions are several eigenfunctions (modes), solutions of a local problem on each subdomain.
- The second one computes only the fundamental mode on each subdomain, which leads to an important reduction of calculation time and memory storage. We then enlarge the basis using a homogenization theorem on a periodic core (factorization of the flux eigenfunctions, [2]).

We implement here our methods in the framework of the existing MINOS solver [3]. The mixed dual finite element method is used in this solver for the resolution of the SP_N equations in 3D cartesian homogenized geometries. Even if these methods could be applied to any angular approximation – particularly easily to a SP_N approximation, we here demonstrate their accuracy for the diffusion model. In this view, we give results obtained on a realistic PWR core, compared to a direct cell by cell calculation obtained by MINOS. We also study the parallelization efficiency of our code.

2. The MINOS solver

The MINOS solver is one of the main core computational tools of the CRONOS2 system ([3], [4]). This solver is reported in the new generation neutronic system DESCARTES and has therefore been rewritten in the C++ language ([5], [6]).

MINOS solves the diffusion or SP_N multigroup equations. It is based on a mixed-dual formulation of these problems. This formulation uses simultaneously scalar functions (φ_e, the even components) and vector functions ($\vec{\varphi}_o$, the odd components). The first even component corresponds to the scalar flux.

If R is a bounded domain with boundary ∂R, the SP_N transport equations written in the mixed (odd-even) form read as follows for each energy group of the multigroup equations:

$$\begin{cases} H\,\vec{\nabla}\varphi_e + T_o\vec{\varphi}_o = \vec{S}_o \quad \text{on } R \\ H^T\,\vec{\nabla}.\vec{\varphi}_o + T_e\varphi_e = S_e \quad \text{on } R \\ H^T\left(\vec{\varphi}_o.\vec{n}\right) = \Lambda\varphi_e \quad \text{on } \Gamma_1 \\ \vec{\varphi}_o.\vec{n} = 0 \quad \text{on } \Gamma_2 \end{cases}, \tag{1}$$

where $\varphi_e = [\varphi_0, \varphi_2, \varphi_4, ...]^T$, $\vec{\varphi}_o = [\vec{\varphi}_1, \vec{\varphi}_3, \vec{\varphi}_5, ...]^T$,

$\Gamma_1 \cup \Gamma_2 = \partial R$,

Λ is a full matrix associated to vacuum conditions,

T_e and T_o are respectively the even and odd removal diagonal matrices:

$T_e = diag(\sigma_0, \sigma_2, \sigma_4..)$, $T_o = diag(\sigma_1, \sigma_3, \sigma_5..)$ with σ_l the removal cross-sections,

H is a bidiagonal matrix with spatially constant coefficients coupling the odd and even harmonics: $H = \begin{bmatrix} 1 & 2 & \\ & 3 & 4 \\ & & . \end{bmatrix}$.

The dual variational formulation of the SP_N equations is obtained by projecting the odd and even equations on two different functional spaces, and applying the Green formula to the odd equation. We obtain the variational problem for each energy group:

find $\vec{\varphi}_o \in \left[H_{0,\Gamma_2}(div,R)\right]^{N_h}$ and $\varphi_e \in [L^2(R)]^{N_h}$ such that

$$\begin{cases} \int_R H\varphi_e\left(\vec{\nabla}.\vec{\psi}_o\right) - \int_R T_o\vec{\varphi}_o.\vec{\psi}_o - \int_{\partial R}\left(H\Lambda^{-1}H^T\right)\left(\vec{\varphi}_o.\vec{n}\right)\left(\vec{\psi}_o.\vec{n}\right) = -\int_R \vec{S}_o.\vec{\psi}_o \quad \forall \vec{\psi}_o \in \left[H_{0,\Gamma_2}(div,R)\right]^{N_h} \\ \int_R H^T\left(\vec{\nabla}.\vec{\varphi}_o\right)\psi_e + \int_R T_e\varphi_e\psi_e = \int_R S_e\psi_e \quad \forall \psi_e \in [L^2(R)]^{N_h}, \end{cases} \tag{2}$$

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,

$H_{0,\Gamma_2}(div,R) = \left\{\vec{q} \in H(div,R), \vec{q}.\vec{n} = 0 \text{ on } \Gamma_2\right\}$,

N_h is the number of odd and even harmonics.

More details on variational formulations and functional spaces are given in [7].

The Raviart-Thomas-Nedelec (RTN) elements [8] 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 component mode synthesis method

The CMS method for the computation of partial differential equations' eigenmodes has been used for a long time in structural analysis as well as in the asymptotic analysis of time dependent problems. This method provides a powerful tool for computing the eigenmodes of large domains thanks to its high accuracy and its high degree of parallelization. The main idea of this method lies in the decomposition of the global structure in subdomains: a finite number of local eigenmodes of the same operator over each subdomain are chosen, and constitutes a finite basis of functions for approximating the global problem with a Galerkin method. The subdomains can be overlapping or not. Here, we choose overlapping subdomains, as motivated by [1]. Note that CMS with non-overlapping subdomains has already been briefly considered in [9] for the diffusion equation.

To explain the CMS method, we consider a general variational formulation of the steady state neutronic equations: find $u_0 \in V$ and $\lambda_0 \in \mathbb{R}$ such that

$$a(u_0,v) = \frac{1}{\lambda_0} b(u_0,v) \quad \forall v \in V, \tag{3}$$

where a and b are bilinear forms describing the problem. For the sake of simplicity we specify neither these forms nor the V space. To determine the first global eigenpair (u_0,λ_0), we construct an overlapping subdomain decomposition of R such that: $R = \bigcup_{k=1}^{K} R^k$.

On each R^k, we consider the first N^k eigenpairs $(u_i^k,\lambda_i^k)_{1\le i\le N^k}^{1\le k\le K}$ which are solutions of the local problems: find $u_i^k \in V^k$ and $\lambda_i^k \in \mathbb{R}$ such that

$$a^k\left(u_i^k,v\right) = \frac{1}{\lambda_i^k} b^k\left(u_i^k,v\right) \quad \forall v \in V^k, \tag{4}$$

where a^k, b^k and V^k are restrictions to R^k of a, b and V respectively, with reflective boundary conditions on interfaces $\partial R^k \setminus \partial R$, and the actual boundary conditions on ∂R. Now, in order to work with functions defined on the whole domain, we extend the local solutions by zero and denote by $\tilde{u}_i^k$ these extended functions (we explain in the next section why this extension yields conformal basis functions in our case). Then, we look for an approximate solution of problem (3) in the space spanned by all the $\tilde{u}_i^k$ functions: find $\tilde{u}_0 = \sum_{k=1}^{K} \sum_{i=1}^{N^k} \alpha_i^k \tilde{u}_i^k$ and $\tilde{\lambda}_0 \in \mathbb{R}$ such that

$$a(\tilde{u}_0, \tilde{u}_j^l) = \frac{1}{\tilde{\lambda}_0} b(\tilde{u}_0, \tilde{u}_j^l) \quad \forall 1 \le l \le K, 1 \le j \le N^l . \tag{5}$$

4. Extension of the CMS method to the mixed dual formulation

We now extend the CMS method to mixed-dual variational approximations [10]. In this case, the prolongation by zero of the local functions is consistent with the different functional spaces. Indeed, the even space $[L^2(R)]^{N_h}$ allows for discontinuous functions, thus their prolongation by zero is permissible. As for the odd space $\left[H_{0,\Gamma_2}(div, R)\right]^{N_h}$, conformity requires the normal trace of the odd fluxes to be continuous, and the natural way to proceed is to build local functions with reflection conditions on any subdomain boundary (except on the boundary ∂R, where the prescribed boundary conditions are always applied), and to extend them by zero outside the subdomain.

Thus our local basis functions are several eigenmodes which are solution of a problem similar to (2), but defined locally on each subdomain, with the above mentioned boundary conditions. These local eigenmodes on each R^k extended on R by zero give global functions on R (denoted by ~) in the appropriate spaces, thanks to the infinite medium boundary conditions. We define the discretized spaces W_δ for the odd components and V_δ for the even ones:

$$\begin{aligned} W_\delta &= span\left\{ \tilde{\vec{\varphi}}_{o,i,d}^k \right\}_{1 \le i \le N^k, d}^{1 \le k \le K} \subset H(div, R) \\ V_\delta &= span\left\{ \tilde{\varphi}_{e,i}^k \right\}_{1 \le i \le N^k}^{1 \le k \le K} \subset L^2(R) \end{aligned} \tag{6}$$

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

If we look for an approximate global solution of problem (2) in these spaces, the unknowns can be written: $\vec{\varphi}_{o,\delta} = \sum_{k=1}^{K} \sum_{i=1}^{N^k} \sum_{d} c_{i,d}^k \tilde{\vec{\varphi}}_{o,i,d}^k$ for the odd components and $\varphi_{e,\delta} = \sum_{k=1}^{K} \sum_{i=1}^{N^k} f_i^k \tilde{\varphi}_{e,i}^k$ for the even ones. 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:

$$A \begin{bmatrix} c_{i,d}^k \\ f_i^k \end{bmatrix} = \frac{1}{\lambda_\delta} T \begin{bmatrix} c_{i,d}^k \\ f_i^k \end{bmatrix}, \tag{7}$$

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 $R^k \overset{\circ}{\cap} R^l = \varnothing$.

5. The factorized CMS (FCMS) method for the diffusion (SP_1) model

The determination of multiple eigenfunctions on each subdomain is expensive in terms of computing time and memory storage. Our goal in this section is to perform only the fundamental mode calculation on each subdomain, and to replace the higher order modes by suitably chosen functions. The idea, coming from homogenization results, is to factorize the higher order modes ([2], [11], [12]). In this view, we mention the following factorization principle for the diffusion model, proved in [2]: in a periodic core, the i-th (even) flux eigenmode solution of the diffusion problem can be asymptotically written $\varphi_i \approx u_i \times \psi$ with ψ the fundamental rapidly varying solution of the problem on each assembly with infinite medium boundary conditions, and u_i the i-th smooth shape 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 obtain our new local (even) flux basis functions $\tilde{\varphi}_i^k \in L^2(R)$:

$$\begin{cases} \tilde{\varphi}_1^k = \varphi^k \text{ on } R^k \\ \tilde{\varphi}_1^k = 0 \text{ on } R \setminus R^k \end{cases} \quad \textit{and} \quad \begin{cases} \tilde{\varphi}_i^k = \varphi^k \times u_i^k \text{ on } R^k \\ \tilde{\varphi}_i^k = 0 \text{ on } R \setminus R^k \end{cases} \quad 1 \le k \le K,\ 2 \le i \le N^k . \tag{8}$$

where u_i^k are analytical solutions (sines or cosines) of local 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 (odd flux). At this time we define the current basis functions in the d direction according to:

$$\begin{cases} \tilde{p}_{1,d}^k = p_d^k \text{ on } E^k \\ \tilde{p}_{1,d}^k = 0 \text{ on } E \setminus E^k \end{cases} \quad \textit{and} \quad \begin{cases} \tilde{p}_{i,d}^k = \dfrac{\partial u_i^k}{\partial d} \text{ on } E^k \quad (\textit{if } \dfrac{\partial u_i^k}{\partial d} \neq 0) \\ \tilde{p}_{i,d}^k = 0 \text{ on } E \setminus E^k \end{cases} \quad 2 \le i \le N^k,\ 1 \le k \le K . \tag{9}$$

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 $\vec{\tilde{p}}_{i,d}^{\,k} \in H(div, R)$.

The resolution of the global problem is the same as in Section 4: we modify only the basis functions, replacing the higher order local eigenmodes by the functions (8) for the flux and (9) for the current.

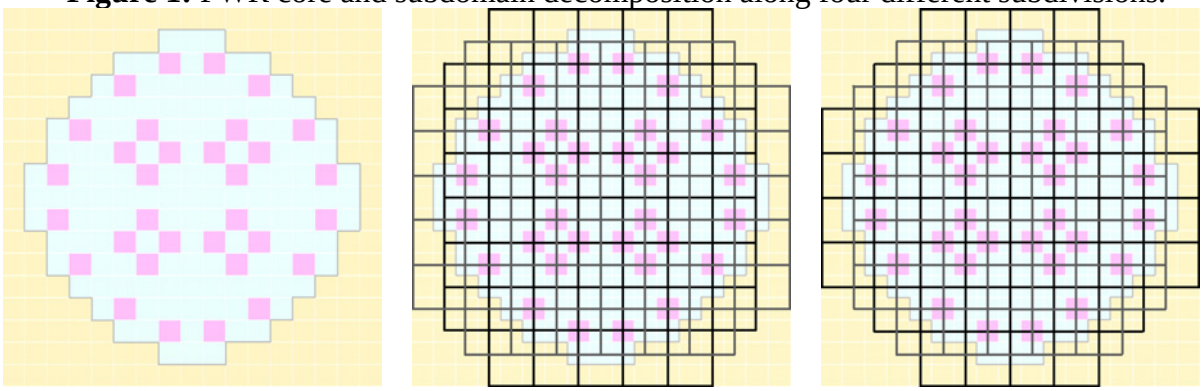
6. Accuracy of our methods: numerical results in 2D

In order to validate the methods for neutronic core calculations, we use a realistic model of a PWR 900 MWe core loaded with a set of UOX and MOX assemblies (Fig. 1a). Each assembly contains 289 cells (17 in each radial direction). Fig. 1b and 1c represent the proposed decomposition of the core along four different subdivisions, yielding a total of 201 overlapping subdomains. As shown in these figures, we have chosen the internal subdomains boundaries $\partial R^k \setminus \partial R$ on the middle of the assemblies, where the infinite medium boundary condition is believed to be close to the real value. Furthermore, with this decomposition we

avoid the interface problem between UOX and MOX assemblies, because such interfaces lie within a subdomain, not on its boundary.

The implementation of CMS and FCMS methods for core calculations is based on the existing SP_N MINOS solver. We present here 2D diffusion results with two energy groups and zero-flux boundary conditions. We always take the number of current modes larger than the number of flux modes in order to avoid a numerical locking phenomenon (see [13] for more explanations).

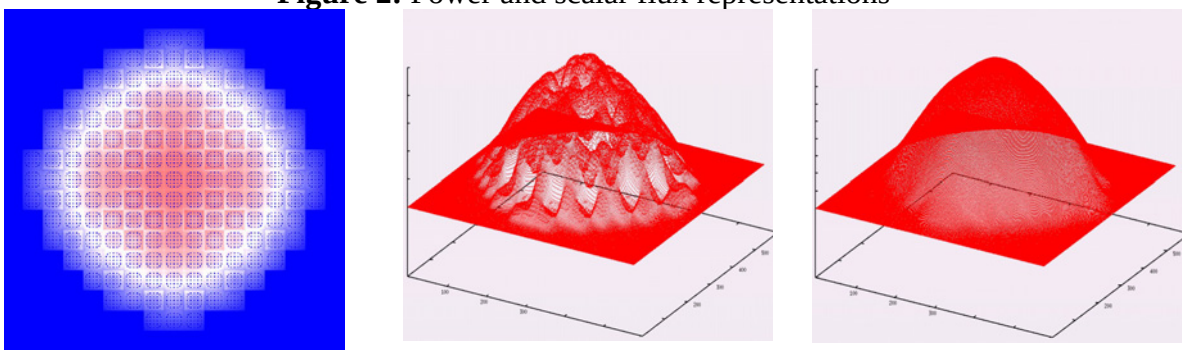
Figure 1: PWR core and subdomain decomposition along four different subdivisions.



a. PWR core b. First two subdivisions c. Other two subdivisions

The core grid used for direct (done by MINOS), CMS and FCMS calculations is made out of 17×17 assemblies subdivided into 17×17 cells. Each cell (where cross-sections are constant) is itself subdivided into 4 sub-cells. We use a RT_0 approximation. This amounts to 334,084 flux unknowns. Fig. 2 gives graphical representations of the power on the whole core (2a), and of the scalar flux for thermal (2b) and fast energy groups (2c).

Figure 2: Power and scalar flux representations



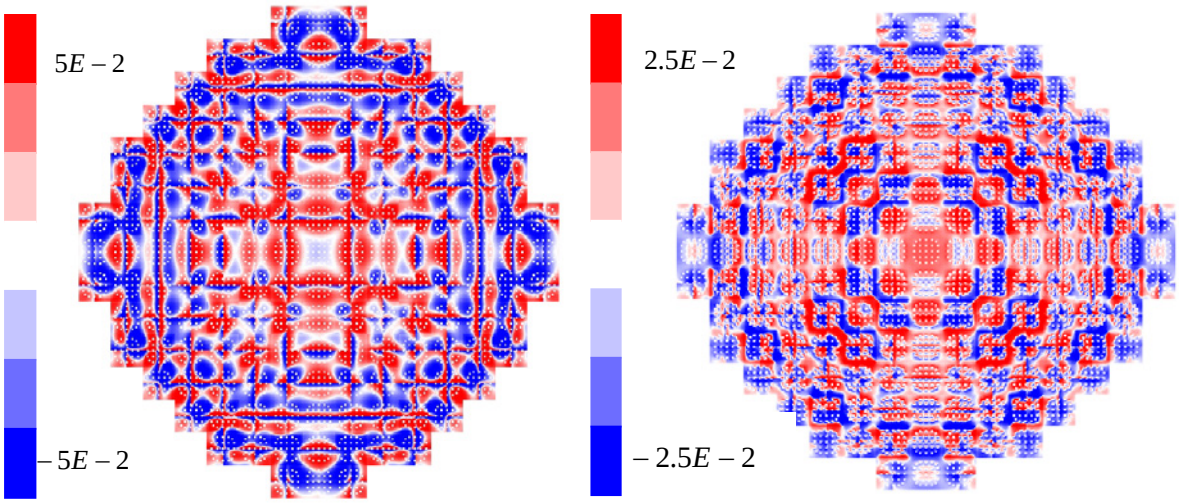
a. Power on the core b. Thermal flux c. Fast flux

We compare two results: 4 flux and 6 current modes on each subdomain for the CMS method, 6 flux and 11 current modes for the FCMS method. Fig. 3, 4 and Table 1 present numerical differences between the direct MINOS calculation and our methods with the domain decomposition presented on Fig. 1b and 1c. As shown in Table 1, we obtain good converged and accurate calculations even with only a few modes: the L^2- Norm and the L^∞-Norm of the power difference between our methods and MINOS are small, and the Keff differences are smaller than 5 pcm for the two methods. Fig. 3 presents the maps of the power

difference between the direct MINOS calculation and our methods: we can see lines parallel to the X- and Y-axis, corresponding to the jump of the flux at the interface between two subdomains. However the accuracy of the local cell power is good (Fig. 4): for more than 95% of the cells, the power gaps between our methods and the direct MINOS calculation are less than 1%.

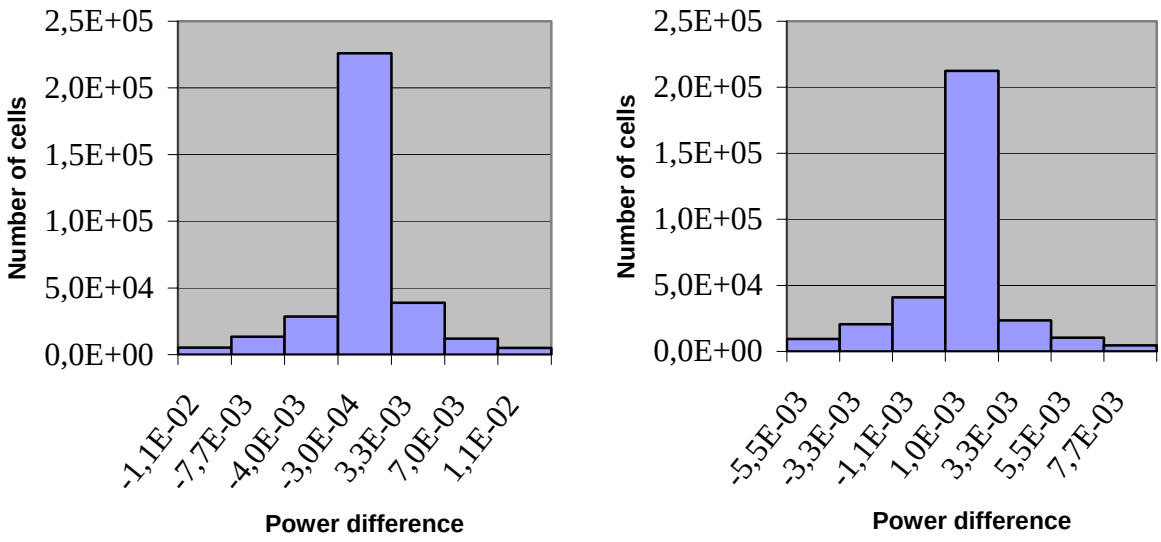
For the same accuracy, the FCMS method based only on the fundamental mode is more efficient in terms of calculation time and memory storage than the CMS method which spends most of the computing time in determining several eigenfunctions on each subdomain.

Fig. 3. Graphical representations of the power gap between our methods and direct MINOS solution in 2D.



CMS FCMS

Fig. 4. Histograms of the power cell difference between our methods and direct MINOS solution in 2D.



CMS FCMS

Table 1. Keff difference, L^2 and L^∞ Norm of the power difference between our methods and direct MINOS solution in 2D. $Keff \approx 1.180$.

	CMS	FCMS
Δ Keff (pcm)	4.4	2.2
$\|\Delta P\|_2$	3.8×10^{-3}	2.8×10^{-3}
$\|\Delta P\|_\infty$	5.0×10^{-2}	2.4×10^{-2}

7. Parallelization in 3D

CMS and FCMS methods are easily parallelizable: each local calculation on a subdomain can be performed independently by a process without communication. The matrix calculations need exchanges of messages, but it can also be parallelized. At this time, we parallelize it on energy groups and space directions. For example, in a 2-energy group case, if a given process does the calculation of the matrix *A* for the fast group in the Z-direction, this process needs to get from all the other processes the local eigenmodes for the fast group in the Z-direction, for all the subdomains. This kind of parallelization is not very satisfactory: a lot of communications are necessary. A better way to proceed is to use the fact that the matrices are sparse: as explain in Section 4, the non-null terms correspond only to the close subdomains. Thus the process which performs the local calculation on the subdomain R^k can compute the k-th line of all the matrices. In this case this process only needs to get the local basis functions from the processes which perform the local calculations on R^l, with $R^k \overset{\circ}{\cap} R^l \neq \varnothing$.

We illustrate the computing times in Fig. 5. We use in these tests the FCMS method with 6 flux modes and 11 current modes. The 3D-core is split into 20 planes in the Z-axis: the first and the last one are reflectors, the other ones use the same grid as in 2D (see Fig. 1a). Now we have 6,681,680 flux unknowns. We use the same domain decomposition as in 2D (Fig. 1b and 1c): we do not make a decomposition of the core in the Z-axis (the Z-size of the subdomains is equal to the one of the core). The computer used is an AMD Opteron cluster. Each node of the cluster is a 4 AMD Opteron 1.8 GHz processor server with 4 GB of shared memory. The nodes are connected via a high performance switch (Infiniband). We compare the computing time between the direct MINOS calculation and our method from 1 to 32 processors. As shown in Fig. 6, the efficiency of the parallel code is good (up to 70% on 26 processors). Most of the time is spent in local solves and matrix calculations. The FCMS global solve is not parallelized, but the corresponding time is very small. The computing time with our method is comparable with the direct MINOS calculation if 8 processors are used, and becomes smaller with more processors. We can observe in Fig. 6 that the optimal splitting is achieved for 26 processors. This equilibrium may change depending on the algorithm improvement. In terms of memory storage, the direct MINOS calculation requires about 1.7 GB for this calculation, whereas our method only needs 1.1GB. We plan to improve the parallelization efficiency by decreasing communication and matrix calculations times with the mentioned above technique. Moreover, the code is not optimized yet. We will give results in the oral talk on calculation servers with more processors and different core configurations.

Fig. 5. Computing time of the FCMS method from 1 to 32 processors. Reference: direct MINOS calculation.

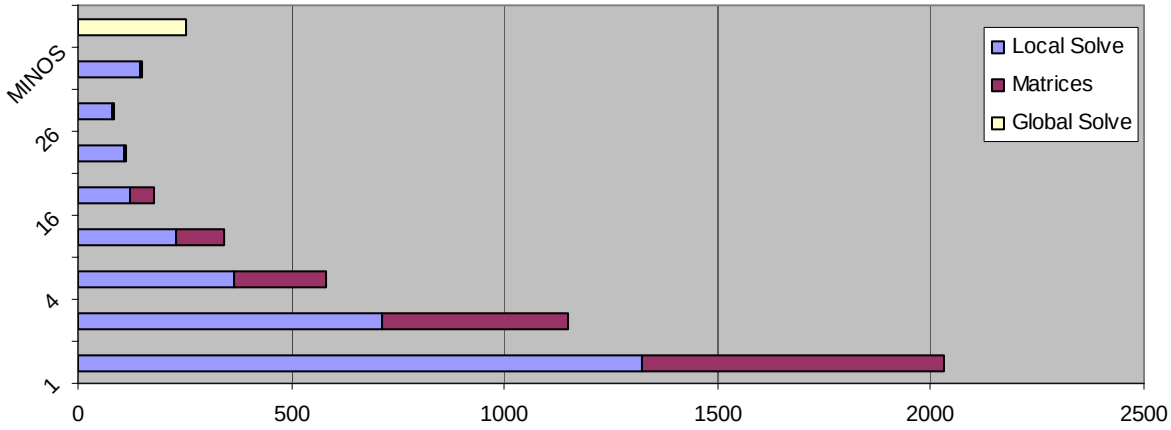
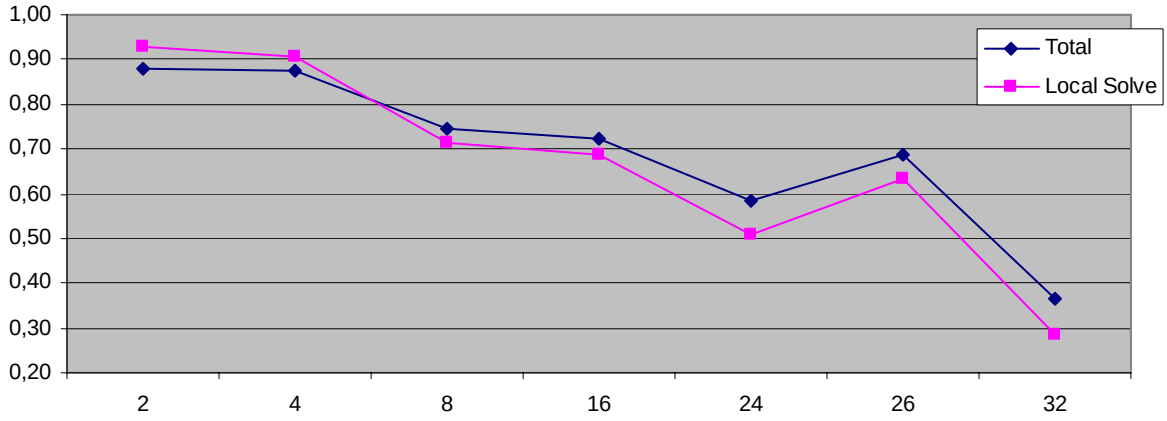


Fig. 6. Local solve and FCMS solver (Total) efficiencies.



8. Conclusion

The numerical results show that the applications of the component mode synthesis method to cell-by-cell core calculations give a good accuracy for the Keff as well as for the local cell power. The total independence of the local mode calculations gives methods very well-fitted for parallel computers.

Presently the tests have been done only in the diffusion approximation. The next step will be to perform 3D SP_N calculations. The size of the mesh is not limited to the cell, and we can refine it for pin-by-pin calculations. Our methods could have a great interest for the calculations of future generation reactors with complex geometries, for which the mesh must be very fine (EPR, HTR, VHTR…). Another interesting application is the time dependent problems: we can keep the same basis functions for several time steps, and do only a few "updates" of the local fine functions in order to decrease the calculation time. Furthermore our methods are not related to the SP_N or diffusion models, and we intend to apply them to some transport models (the factorization principle used in the FCMS method holds true also

in the transport case, see [14]). Also we can consider coupling a transport or a SP_N model for local calculations, and a diffusion model for the global resolution.

In conclusion these methods offer interesting prospects for large 3D calculations with an important potential gain on parallel computers.

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