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INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

*Sparse approximations of the Schur complement for  
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## Sparse approximations of the Schur complement for parallel algebraic hybrid linear solvers in 3D

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**Abstract:** In this report we study the computational performance of variants of an algebraic additive Schwarz preconditioner for the Schur complement for the solution of large sparse linear systems. In earlier works, the local Schur complements were computed exactly using a sparse direct solver. The robustness of the preconditioner comes at the price of this memory and time intensive computation that is the main bottleneck of the approach for tackling huge problems. In this work we investigate the use of sparse approximation of the dense local Schur complements. These approximations are computed using a partial incomplete  $LU$  factorization. Such a numerical calculation is the core of the multi-level incomplete factorization such as the one implemented in pARMS. The numerical and computing performance of the new numerical scheme is illustrated on a set of large 3D convection-diffusion problems; preliminary experiments on linear systems arising from structural mechanics are also reported.

**Key-words:** Hybrid direct/iterative solver, parallel scientific computing, scalable preconditioner, incomplete/partial factorization, large 3D problems, high performance computing.

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## Approximation creuse du complément de Schur pour des solveurs linéaires hybrides pour des problèmes 3D

**Résumé :** Dans ce rapport nous étudions les performances de variantes d'un préconditionneur de type Schwarz additif pour le complément de Schur pour la résolution de systèmes linéaires creux de grande taille. Dans des travaux précédents, les compléments de Schur pour ce préconditionneur étaient calculés explicitement en utilisant un solveur direct creux. La robustesse de ce préconditionneur avait un coût calculatoire et mémoire important qui constituait le principal frein pour la résolution de problèmes de très grande dimension. Dans ce travail, nous étudions l'utilisation d'approximation creuse de ces compléments de Schur denses. Ces approximations sont calculées via une factorisation  $LU$  incomplète partielle telle que celle utilisée dans pARMS. Les performances numériques et calculatoires de ce nouveau schéma sont illustrées sur un ensemble de problèmes de convection-diffusion en 3D; des résultats préliminaires sur des systèmes issus de mécanique des structures sont également présentés.

**Mots-clés :** Solveurs linéaires hybrides directs/itératifs, calcul parallèle scientifique, préconditionneurs scalables, factorisation incomplète/partielle, problèmes 3D de grandes tailles, calcul haute performance.

## 1 Introduction

The solution of partial differential equations (PDE) problems on large three dimensional (3D) meshes often leads to the solution of large sparse possibly unstructured linear systems. In this work, we mainly consider unsymmetric matrices resulting from the discretization of convection-diffusion type of problems. For their solution, we consider a parallel hybrid iterative-direct numerical technique. It is based on an algebraic preconditioner for the Schur complement system that classically appears in non-overlapping domain decomposition method. In earlier papers [3, 4], we studied the numerical and parallel scalability of this algebraic additive Schwarz preconditioners [2, 5, 6] where the preconditioner is built using exact local Schur complement matrices. This exact calculation is performed thanks to sparse direct solvers such as [1]. This calculation becomes prohibitive for large 3D problems both from a memory and computing time perspectives. To alleviate these costs while preserving its numerical robustness, we consider in this report an approximation of the local Schur complement computed using a partial incomplete factorization following the approach implemented in the multi-level incomplete factorization schemes such as pARMS [7].

In Section 2, we describe the main components of the preconditioner that are the algebraic additive Schwarz approach and the variant of the dual thresholding  $ILLU(t, p)$  [10] enabling us to build the approximation of the local Schur complement. The memory and CPU-time benefits as well as the numerical and parallel behaviours are discussed in Section 4 through an extensive scalability study on large numbers of processors for model problems. More precisely, we mainly consider the 3D convection-diffusion problems defined by Equation (1)

$$\begin{cases} -\epsilon \operatorname{div}(K \cdot \nabla u) + v \cdot \nabla u = f & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega, \end{cases} \quad (1)$$

where  $\epsilon$  is a scalar,  $K$  a positive definite bounded tensor and  $v$  a velocity field defined on the computational domain  $\Omega$ . Some preliminary experiments on linear systems arising from industrial structural mechanics computational are also reported.

## 2 The main components of the parallel preconditioner

Motivated by parallel distributed computing and the potential for coarse grain parallelism, considerable research activity developed around iterative domain decomposition schemes [8, 9, 13, 14]. The governing idea behind sub-structuring or Schur complement methods is to split the unknowns in two subsets. This induces the following block reordered linear system associated with the discretization of Equation (1):

$$\begin{pmatrix} A_{II} & A_{I\Gamma} \\ A_{\Gamma I} & A_{\Gamma\Gamma} \end{pmatrix} \begin{pmatrix} x_I \\ x_\Gamma \end{pmatrix} = \begin{pmatrix} b_I \\ b_\Gamma \end{pmatrix}, \quad (2)$$

where  $x_\Gamma$  contains all unknowns associated with sub-domain interfaces and  $x_I$  contains the remaining unknowns associated with sub-domain interiors. The matrix  $A_{II}$  is block diagonal where each block corresponds to a sub-domain interior. Eliminating  $x_I$  from the second block row of Equation (2) leads to the reduced system

$$Sx_\Gamma = b_\Gamma - A_{\Gamma I}A_{II}^{-1}b_I, \text{ where } S = A_{\Gamma\Gamma} - A_{\Gamma I}A_{II}^{-1}A_{I\Gamma} \quad (3)$$

and  $S$  is referred to as the *Schur complement matrix*. This reformulation leads to a general strategy for solving (2). Specifically, an iterative method can be applied to (3). Once  $x_\Gamma$  is determined,  $x_I$  can be computed with one additional solve on the sub-domain interiors.

For the sake of simplicity, we describe the basis of our algebraic preconditioner in two dimensions as its generalization to three dimensions is straightforward. In Figure 1, we depict an internal sub-domain  $\Omega_i$  with its edge interfaces  $E_m, E_g, E_k,$  and  $E_\ell$  that define  $\Gamma_i = \partial\Omega_i \setminus \partial\Omega$ . Let  $R_{\Gamma_i} : \Gamma \rightarrow \Gamma_i$

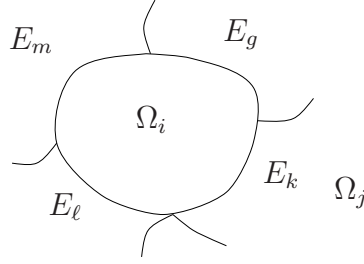


Figure 1: An internal sub-domain.

be the canonical pointwise restriction that maps full vectors defined on  $\Gamma$  into vectors defined on  $\Gamma_i$ , and let  $R_{\Gamma_i}^T : \Gamma_i \rightarrow \Gamma$  be its transpose. For a matrix  $A$  arising from a finite element discretization, the Schur complement matrix (2) can also be written

$$S = \sum_{i=1}^N R_{\Gamma_i}^T S^{(i)} R_{\Gamma_i},$$

where

$$S^{(i)} = A_{\Gamma\Gamma}^{(i)} - A_{\Gamma_i i} A_{ii}^{-1} A_{i\Gamma_i}$$

is referred to as the local Schur complement associated with the sub-domain  $\Omega_i$ . The matrix  $S^{(i)}$  involves submatrices from the local stiffness matrix  $A^{(i)}$ , defined by

$$A^{(i)} = \begin{pmatrix} A_{ii} & A_{i\Gamma_i} \\ A_{\Gamma_i i} & A_{\Gamma_i \Gamma_i} \end{pmatrix}. \quad (4)$$

The matrix  $A^{(i)}$  corresponds to the discretization of Equation (1) on the sub-domain  $\Omega_i$  with Neumann boundary condition on  $\Gamma_i$  and  $A_{ii}$  corresponds to the discretization of Equation (1) on the sub-domain  $\Omega_i$  with homogeneous Dirichlet boundary conditions on  $\Gamma_i$ .

For convection diffusion problems the discretization matrix  $A$  is unsymmetric. Hence, systems with the matrix  $S$  can be solved using a unsymmetric Krylov subspace method such as GMRES [12] without forming the Schur complement matrix explicitly. While the Schur complement system is often much more amenable to solution using a Krylov subspace method than the original system, it is important to consider further preconditioning.

We now describe in Section 2.1 the algebraic Schwarz preconditioner that, in its original form, relies on the knowledge of some block entries of the Schur complement matrix  $S$  that have to be computed explicitly using some entries of the matrices  $S^{(i)}$ . This explicit calculation of these matrix entries can become prohibitive for large 3D problems. To overcome this penalty we introduce in Section 2.2 an approximation of the local Schur complement matrices  $S^{(i)}$  that is computed by a partial incomplete dual thresholding LU factorisation [10].

## 2.1 The algebraic additive Schwarz preconditioner

The local Schur complement matrix, associated with the sub-domain  $\Omega_i$  depicted in Figure 1, is dense and has the following  $4 \times 4$  block structure:

$$S^{(i)} = \begin{pmatrix} S_{mm}^{(i)} & S_{mg} & S_{mk} & S_{ml} \\ S_{gm} & S_{gg}^{(i)} & S_{gk} & S_{gl} \\ S_{km} & S_{kg} & S_{kk}^{(i)} & S_{kl} \\ S_{lm} & S_{lg} & S_{lk} & S_{ll}^{(i)} \end{pmatrix},$$

where each block accounts for the interactions between the degrees of freedom of the four edges of the interface  $\Gamma_i$ .

To describe the preconditioner we define the local assembled Schur complement,  $\bar{S}^{(i)} = R_{\Gamma_i} S R_{\Gamma_i}^T$ , that corresponds to the restriction of the Schur complement to the interface  $\Gamma_i$ . This local assembled preconditioner can be built from the local Schur complements  $S^{(i)}$  by assembling their diagonal blocks thanks to a few neighbour to neighbour communications in a parallel distributed computing environment. For instance, the diagonal blocks of the complete matrix  $S$  associated with the edge interface  $E_k$ , depicted in Figure 1, is  $S_{kk} = S_{kk}^{(i)} + S_{kk}^{(j)}$ . That is, it results from the contribution of domain  $\Omega_i$  and  $\Omega_j$  that share the edge interface  $E_k$ . Assembling each diagonal block of the local Schur complement matrices, we obtain the local assembled Schur complement, that is:

$$\bar{S}^{(i)} = \begin{pmatrix} S_{mm} & S_{mg} & S_{mk} & S_{m\ell} \\ S_{gm} & S_{gg} & S_{gk} & S_{g\ell} \\ S_{km} & S_{kg} & S_{kk} & S_{k\ell} \\ S_{\ell m} & S_{\ell g} & S_{\ell k} & S_{\ell\ell} \end{pmatrix}.$$

With these notations the preconditioner reads

$$M_d = \sum_{i=1}^N R_{\Gamma_i}^T \left( \bar{S}^{(i)} \right)^{-1} R_{\Gamma_i}. \quad (5)$$

In a matrix form this preconditioner can be viewed as a block diagonal preconditioner with overlap among the blocks. Consequently, it is referred to as algebraic additive Schwarz preconditioner for the Schur complement.

In three dimensional problems the size of the dense local Schur matrices can be large, consequently it might be computationally expensive to factorize and perform forward/backward substitutions with these factors. One possible alternative to get a cheaper preconditioner is to consider a sparse approximation for  $\bar{S}^{(i)}$  in (5), which may result in a saving of memory to store the preconditioner and saving of computation time to factorize and apply it. This approximation  $\hat{S}^{(i)}$  can be constructed by dropping the elements of  $\bar{S}^{(i)}$  that are smaller than a given threshold. More precisely, the following dropping policy can be applied:

$$\hat{s}_{\ell j} = \begin{cases} 0, & \text{if } |\bar{s}_{\ell j}| \leq \xi(|\bar{s}_{\ell\ell}| + |\bar{s}_{jj}|), \\ \bar{s}_{\ell j}, & \text{otherwise.} \end{cases}$$

The resulting preconditioner reads

$$M_{sp} = \sum_{i=1}^N R_{\Gamma_i}^T \left( \hat{S}^{(i)} \right)^{-1} R_{\Gamma_i}. \quad (6)$$

While this strategy enables us to reduce the memory storage and computational complexity to apply the preconditioner, it does require a memory peak while the local Schur complement are assembled (before to be sparsified). In the next section we describe a solution to avoid this expensive calculation.

## 2.2 Sparse approximation based on partial $ILU(t, p)$

One can design a computationally and memory cheaper alternative to approximate the local Schur complements  $S^{(i)}$ . Among the possibilities, we consider in this report a variant based on the  $ILU(t, p)$  [10] that is also implemented in pARMS [7].

The approach consists in applying a partial incomplete factorisation to the matrix  $A^{(i)}$ . The incomplete factorisation is only run on  $A_{ii}$  and it computes its ILU factors  $\tilde{L}_i$  and  $\tilde{U}_i$  using to the dropping parameter threshold  $t_{factor}$ .

$$pILU(A^{(i)}) \equiv pILU \begin{pmatrix} A_{ii} & A_{i\Gamma_i} \\ A_{\Gamma_i i} & A_{\Gamma_i \Gamma_i}^{(i)} \end{pmatrix} \equiv \begin{pmatrix} \tilde{L}_i & 0 \\ A_{\Gamma_i} \tilde{U}_i^{-1} & I \end{pmatrix} \begin{pmatrix} \tilde{U}_i & \tilde{L}_i^{-1} A_{i\Gamma} \\ 0 & \tilde{S}^{(i)} \end{pmatrix}$$



where

$$\tilde{S}^{(i)} = A_{\Gamma_i \Gamma_i}^{(i)} - A_{\Gamma_i i} \tilde{U}_i^{-1} \tilde{L}_i^{-1} A_{i \Gamma_i}$$

The incomplete factors are then used to compute an approximation of the local Schur complement. Because our main objective is to get an approximation of the local Schur complement we switch to another less stringent threshold parameter  $t_{Schur}$  to compute the sparse approximation of the local Schur complement.

Such a calculation can be performed using a IKJ-variant of the Gaussian elimination [11], where the  $\tilde{L}$  factor is computed but not stored as we are only interested in an approximation of  $\tilde{S}_i$ . This further alleviate the memory cost.

The local approximations of the Schur complement are then assembled thanks to a few neighbour to neighbour communications to form  $\tilde{\underline{S}}^{(i)}$ . These matrices are used to build a preconditioner similar to (6) that reads

$$M_{app} = \sum_{i=1}^N R_{\Gamma_i}^T \left( \tilde{\underline{S}}^{(i)} \right)^{-1} R_{\Gamma_i}. \quad (7)$$

### 3 Exact vs. approximated Schur algorithm

In a parallel distributed memory environment, the domain decomposition strategy is followed to assign each local PDE problem (sub-domain) to one processor that works independently of other processors and exchange data using message passing. In that computational framework, the implementation of the algorithms based on preconditioners built from the exact or approximated local Schur complement only differ in the preliminary phases. The parallel SPMD algorithm is as follow:

1. Initialization phase:
  - Exact Schur : using the sparse direct solver [1] we compute at once the  $LU$  factorization of  $A_{ii}$  and the local Schur complement  $S^{(i)}$ ;
  - Approximated Schur : using the sparse direct solver we only compute the  $LU$  factorization of  $A_{ii}$ , then we compute the approximation of the local Schur complement  $\tilde{S}^{(i)}$  by performing a partial  $ILU$  factorization of  $A^{(i)}$ .
2. Set-up of the preconditioner:
  - Exact Schur : we first assemble the diagonal problem thanks to few neighbour to neighbour communications (computation of  $\tilde{S}^{(i)}$ ), we sparsify the assembled local Schur (i.e.,  $\hat{S}^{(i)}$ ) that is then factorized.
  - Approximated Schur : we assemble the sparse approximation also thanks to few neighbour to neighbour communications and we factorize the resulting sparse approximation of the assembled local Schur.
3. Krylov subspace iteration: the same numerical kernels are used. The only difference is the sparse factors that are considered in the preconditioning step dependent on the selected strategy (exact v.s. approximated).

From a high performance computing point of view, the main difference relies in the computation of the local Schur complement. In the exact situation, this calculation is performed using sparse direct techniques which make intensive use of BLAS-3 technology as most of the data structure and computation schedule are performed in a symbolic analysis phase when fill-in is analyzed. For partial incomplete factorization, because fill-in entries might be dropped depending on their numerical values, no prescription of the structure of the pattern of the factors can be symbolically computed. Consequently this calculation is mainly based on sparse BLAS-1 operations that are

much less favorable to an efficient use of the memory hierarchy and therefore less effective in terms of their floating point operation rate. In short, the second case leads to fewer operations but at a lower computing rate, which might result in higher overall elapsed time in some situations. Nevertheless, in all cases the approximated Schur approach consumes much less memory as illustrated later on in this report.

## 4 Numerical experiments

We first describe in Section 4.1 the computational framework considered for our parallel numerical experiments then we illustrate in Section 4.2 the benefits from a computational resources viewpoint of the approximated approach. We investigate in Section 4.3 the numerical behaviours of the sparsified approximated variants and compare them with the classical sparse preconditioner based on an exact computation of the Schur complement. In Section 4.4 we briefly study the numerical scalability of the preconditioners by conducting weak scalability experiments where the global problem size is increased linearly with the number of processors.

### 4.1 Computational framework

We investigate the numerical behaviour and the parallel scalability of the hybrid solver on parallel computing facilities. These computers are: the IBM JS21 that is a 4-way SMP of PowerPC 970MP processors running at 2.5 GHz and equipped with 8 GBytes of main memory per node. The IBM Blue Gene/L that consists of 1024 chips, where each chip has two modified PowerPC 440s running at 700 MHz and 512 MBytes of memory per CPU.

We consider various 3D model problems defined by Equation (1) with different diffusion and convection terms. A scalar term is used in front of the diffusion term that enables us to vary the Péclet number so that the robustness with respect to this parameter can be investigated. These various choices of 3D model problems are thought to be difficult enough and representative for a large class of applications. We consider for the diffusion coefficient the matrix  $K$  in Equation (1) as diagonal with piecewise constant function entries defined in the unit cube as depicted in Figure 2. The diagonal entries  $a(x, y, z)$ ,  $b(x, y, z)$ ,  $c(x, y, z)$  of  $K$  are bounded positive functions on  $\Omega$  enabling us to define heterogeneous and/or anisotropic problems.

To vary the difficulties we consider both discontinuous and anisotropic diffusion coefficients defined along vertical beams according to the pattern displayed in Figure 2.

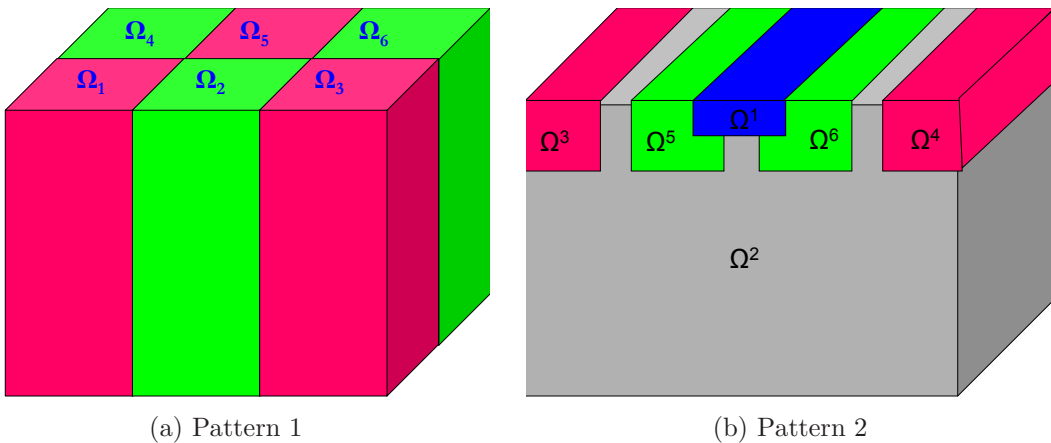


Figure 2: variable diffusion coefficient domains.

More precisely we define the following set of diffusion coefficients to define  $K$ .

Problem 1: heterogeneous diffusion problem defined on Pattern 1

$$a(\cdot) = b(\cdot) = c(\cdot) = \begin{cases} 1 & \text{in } \Omega^1 \cup \Omega^3 \cup \Omega^5, \\ 10^3 & \text{in } \Omega^2 \cup \Omega^4 \cup \Omega^6. \end{cases}$$

Problem 2: heterogeneous and anisotropic diffusion problem defined on Pattern 1

$$a(\cdot) = 1 \text{ and } b(\cdot) = c(\cdot) = \begin{cases} 1 & \text{in } \Omega^1 \cup \Omega^3 \cup \Omega^5, \\ 10^3 & \text{in } \Omega^2 \cup \Omega^4 \cup \Omega^6. \end{cases}$$

Problem 3: heterogeneous and anisotropic diffusion problem defined on Pattern 2

$$a(\cdot) = 1 \text{ and } b(\cdot) = c(\cdot) = \begin{cases} 1 & \text{in } \Omega^1, \\ 10^3 & \text{in } \Omega^2, \\ 10^{-3} & \text{in } \Omega^3 \cup \Omega^4 \cup \Omega^5 \cup \Omega^6. \end{cases}$$

For each of the diffusion problems described above we define a 3D convection-diffusion problem by considering a convection term with a circular flow in the  $xy$  direction and a sinusoidal flow in the  $z$  direction; that is:

$$\begin{cases} v_x(\cdot) &= (x - x^2)(2y - 1), \\ v_y(\cdot) &= (y - y^2)(2x - 1), \\ v_z(\cdot) &= \sin(\pi z). \end{cases}$$

We depict in Figure 3 the streamlines of the convection field.

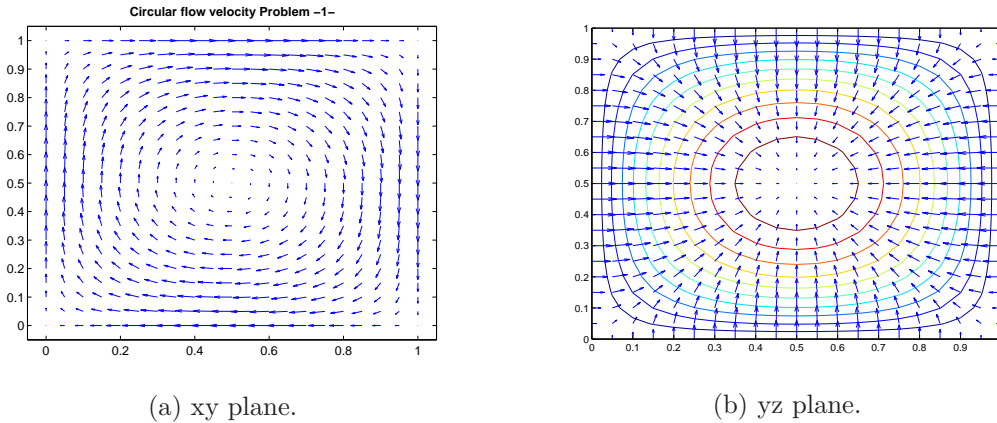


Figure 3: circular convection flow.

Each problem is discretized on the unit cube using standard second order finite difference discretization with a seven point stencil; a centered finite difference scheme is considered for the first order term.

## 4.2 Comparison between exact and approximated Schur method

In this section we illustrate the difference of computing resource consumption of the two approaches. We first illustrate the requirement of each approach in term of memory. We depict in Table 1 the memory required for each sub-problem to compute the exact Schur complement or to calculate the approximated sparse Schur complement. In the row of Table 1 we report the amount of memory (expressed in MBytes) when the size of the local sub-problem is varied. These results were observed for a given setup of the parameters governing the model problem but there are representative of a general trend seen with many experiments we have run.

It can be seen that the exact Schur computation requires a large amount of memory especially for large sub-problem ( $55^3$  local mesh, that is about 166 000 unknowns). The memory is mainly used to store the  $L$  and  $U$  parts associated with the interface unknowns as well as the local dense exact Schur complement. A feature of the approximated sparse variant is that it reduces dramatically this memory requirement. For all the problem sizes, the approximated Schur approach reduces the memory requirement by a factor of 5. This feature enables us to perform much larger computation using the same computing resources as most of the memory was used to exactly compute the local Schur complement in our earlier work [4, 3]. For example, on the IBM-JS21 supercomputer with  $2GB/proc$ , the maximal sub-domain size allowed to perform a simulation using the exact Schur method is  $35^3$  (i.e., 43 000 unknowns per sub-problem), whereas it can be bigger than  $50^3$  (i.e., 125 000 unknowns) using the approximated Schur method. In other words, on 1728 processors, we can solve a problem with more than 216 million degrees of freedom using the approximated Schur method instead of a problem with 74 million degrees of freedom using the exact Schur method.

We now examine the approximated Schur method from a computing time view point, and compare it with the exact Schur method. Those tests were performed on the IBM-JS21 supercomputer because of the memory requirement on the large sub-problems. We report in Table 2 the elapsed time required to compute the exact or the approximated local Schur complement for different sub-problem sizes (i.e., sub-domain size). For the approximated Schur method this elapsed time corresponds to the exact local sparse factorisation of  $A_{ii}$  (that is the (1,1) block of  $A^{(i)}$  in Equation (4)) and the partial incomplete factorisation of the complete matrix  $A^{(i)}$  to compute the approximated Schur complement  $\tilde{S}^{(i)}$ . We display the percentage of retained entries in the  $U$  factor for two values of the dropping parameter for each sub-problem size. It can be seen that on the small problems, higher computing speed of the BLAS-3 computation compensates the extra computation performed by the exact approach. This is no longer true for large problem sizes where the amount of fill-in increases significantly. In this latter situation, the reduction of the amount of computation introduced by the dropping strategy is large enough to compensate for its slower computational speed due to its sparse BLAS-1 nature. In Table 2, we can observe that for a value of 10% in the  $U$  factor (that leads to a sparse Schur with only 4% of entries compared to the exact

memory/sub-domain $MB$		sub-domain mesh size						
		$25^3$ 15 Kdof	$30^3$ 27 Kdof	$35^3$ 43 Kdof	$40^3$ 64 Kdof	$45^3$ 91 Kdof	$50^3$ 125 Kdof	$55^3$ 166 Kdof
$\tilde{S}^{(i)}$	100% in $U$ , 4% in $S$	254	551	1058	1861	3091	4760	7108
$\tilde{\tilde{S}}^{(i)}$	21% in $U$ , 4% in $S$	55	114	216	383	654	998	1506

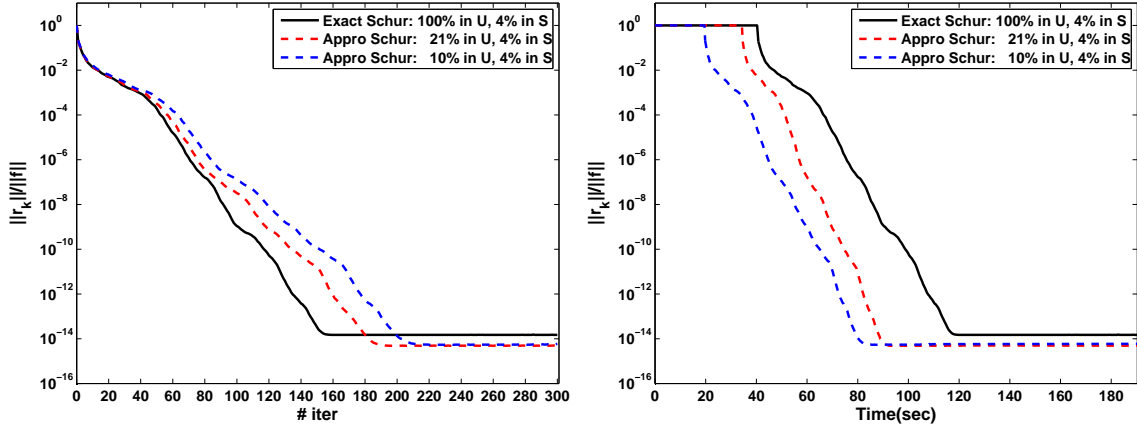
Table 1: Memory comparison between an exact and an approximated computation of the local Schur complement  $S^{(i)}$  using sparse direct factorisation for exact approach and partial incomplete factorisation for the approximated approach.

Time $sec$		kept entries in factor		sub-domain grid size						
				$25^3$ 15 Kdof	$30^3$ 27 Kdof	$35^3$ 43 Kdof	$40^3$ 64 Kdof	$45^3$ 91 Kdof	$50^3$ 125 Kdof	$55^3$ 166 Kdof
$\tilde{S}^{(i)}$	100% in $U$ , 4% in $S$	4.1	12.1	35.4	67.6	137	245	581		
$\tilde{\tilde{S}}^{(i)}$	21% in $U$ , 4% in $S$	6.1	15.1	31.2	60.8	128	208	351		
$\tilde{\tilde{\tilde{S}}}^{(i)}$	10% in $U$ , 4% in $S$	2.9	7.5	16.5	29.8	64	100	169		

Table 2: Elapsed time comparison between an exact and an approximated computation of the local Schur complement  $S^{(i)}$  using sparse direct factorisation for exact approach and partial incomplete factorisation for the approximated approach.

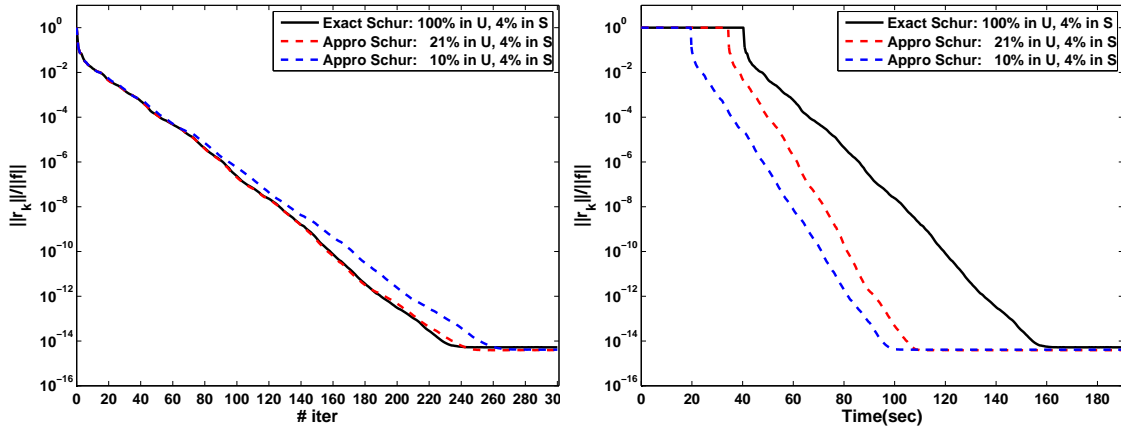
full), the approximated Schur method performs more than twice faster than the exact one for all decompositions.

### 4.3 Influence of the sparsification threshold



(a) Heterogeneous diffusion  
Problem 1 with Convection 1  
(history v.s. iterations).

(b) Heterogeneous diffusion  
Problem 1 with Convection 1  
(history v.s. time).



(c) Heterogeneous and anisotropic diffusion  
Problem 2 with Convection 1  
(history v.s. iterations).

(d) Heterogeneous and anisotropic diffusion  
Problem 2 with Convection 1  
(history v.s. time).

Figure 4: Convergence history for a  $420 \times 420 \times 420$  mesh mapped onto 1728 processors for various sparsification dropping thresholds (Left: scaled residual versus iterations, Right: scaled residual versus time). ( $\epsilon = 10^{-3}$ ) in Equation (1).

The attractive feature of  $M_{\text{app}}$  compared to  $M_{\text{sp}}$  is that it enables us not only to reduce the memory requirement to store and factorize the preconditioner but also to reduce the computational cost to construct it (exact versus approximated sparse factorization) especially for large problems size. However, the counterpart of this computing resource saving could be a deterioration of the preconditioner quality that would slow down the convergence of GMRES. We study the effect of the sparse approximation on a set of model problems. For these experiments, we consider a

420 × 420 × 420 mesh mapped onto 1728 processors of the IBM-JS21 supercomputer. That is, each sub-domain has a size of about 43 000 unknowns and the overall problem is about 74 millions unknowns. We note that this is the largest example that we can conduct on this platform using the exact computation, whereas we can perform a problem with 216 millions unknowns using the approximated computation.

We briefly compare and show the effect of the ILU dropping parameter for the different problems mentioned above. For those problems, it has been observed [4, 3] that an amount of 2-4% of kept entries in the Schur complement are suitable values to provide a good trade-off between convergence speed and computational cost per iteration for  $M_{sp}$ . We display in Figure 4 the convergence history for various choices of the ILU dropping parameters  $t_{factor}$  and  $t_{Schur}$  involved in the definition of  $M_{app}$  in (7). For those experiments  $t_{factor}$  is defined so that 21% and 10% of the entries are kept in the incomplete  $U$  compared to its exact counterpart computed by the sparse direct factorization. The parameter  $t_{Schur}$  is chosen so that only 4% of entries are eventually kept (compared to its dense counterpart). We also plot the convergence history of the exact sparsified  $M_{sp}$  preconditioner, where the sparsification parameter is also chosen to keep only 4% of the entries. The left graphs in Figure 4 show the convergence history as a function of the iterations, whereas the right graphs give the convergence as a function of the computing time. The black curve corresponds to the sparse preconditioner based on an exact Schur computation sparsified by keeping around 4% of the Schur entries. The red curve illustrates the sparse preconditioner based on an approximated Schur computation, where we keep around 21% of the factor  $U$  entries during the ILU factorization and around 4% of the resulting approximated Schur complement entries. Whereas the blue curve corresponds to the sparse preconditioner based on an approximated Schur computation, where we kept around 10% of the incomplete factor  $U$  and around 4% of the resulting approximated Schur complement entries.

We should mention that the initial plateaus in the right graphs correspond to the setup time that is the sum of the initialization time and the time to setup the preconditioner (assembling and factorization).

It can be observed that, as  $t_{factor}$  is increased the amount of entries kept in factor  $U$  is decreased, the setup time (initial plateaus of the graphs) decreases but the convergence deteriorates slightly (blue dashed curve). For a small dropping parameter for ILU (red dashed curve), the numerical performance of the approximated sparse preconditioner is closer to the exact sparse one and the convergence behaviours are similar. It can be observed that, even though the approximated sparse variants require more iterations, with respect to time they converge faster as the setup is cheaper and the time per iteration is comparable.

#### 4.4 Parallel performance

In this section we first study the weak numerical scalability of the preconditioner. We perform weak scalability experiments where the global problem size is varied linearly with the number of processors. Such experiments illustrate the ability of parallel computation to perform large simulations (fully exploiting the local memory of the distributed platforms) in ideally a constant elapsed time. We mention that these experiments have been conducted on the Blue Gene supercomputer. In the numerical experiments below, the iterative method used to solve these problems is the right preconditioned GMRES algorithm. We choose the ICGS (Iterative Classical Gram-Schmidt orthogonalization) strategy which is suitable for parallel implementation. The initial guess is the zero vector and the iterations are stopped when the normwise backward error on the right-hand side, that is defined by  $\frac{\|r_k\|}{\|f\|}$ , becomes smaller than  $10^{-8}$  or when more than 500 iterations are performed. In that expression  $f$  denotes the right-hand side of the Schur complement system to be solved and  $r_k$  the true residual at the  $k^{th}$  iteration (i.e.,  $r_k = f - Sx_{\Gamma}^{(k)}$ ).

#### 4.4.1 Numerical scalability on massively parallel platforms

In this section we describe, evaluate and analyze how the preconditioners ( $M_{\text{app}}$ ) affect the convergence rate of the iterative hybrid solver and what numerical performance is achieved on various model problems when the convection term is varied. Various results are presented in Tables 3 and 4. In these tables, we report the number of iterations when the local problem size is varied when we increase the number of sub-domains from 27 up-to 1728; in Table 4 we vary the Péclet number. For the sake of readability, the size of the sub-domain is fixed to  $35 \times 35 \times 35$ , that is approximately 43 000 dof. We also indicate the percentage of the kept entries in both the approximated factor U and the approximated computed Schur complement. We divide the discussion into three parts:

- the numerical scalability according to the local problem size (column reading in Table 3),
- the numerical scalability of the Krylov solver when the number of sub-domains increases (weak scalability),
- the numerical efficiency of the preconditioner when the Péclet number is varied.

In Table 3, we can observe that for all the problems, the dependency of the convergence rate on the mesh size is rather low. When we go from sub-domains with about 15 625 dof to sub-domains with about 43 000 dof, the gap in the number of iterations is between 3-10 iterations (10%-18%). Notice that with such an increase in the sub-domain size, the overall system size is multiplied by a factor of 3; on 1728 processors the global system size varies from 27 million dof up-to about 74 million dof.

We now comment on the numerical scalability of the approximated Schur method when the number of sub-domains is varied while the Péclet number is constant. This behaviour can be observed in Tables 3 and 4 by reading these tables by row. It can be seen that the increase in the number of iterations is moderate when the sub-domain number varies from 27 up-to 1728. When we multiply the number of sub-domains by 64, the number of iterations increases between 3 to 4 times. Such a numerical behaviour can be considered as satisfactory on this type of difficult problems. For the characteristics of the problems and the associated difficulties, we can consider that the preconditioner performs reasonably well. The behaviour is similar for the different dropping thresholds. We mention that the approximated sparse preconditioner convergence is similar to the one observed using the exact dense/sparse preconditioner [3].

Moreover, we study the effect of varying the dropping thresholds for the incomplete factorisation ( $t_{\text{factor}}$ ) and for the approximated Schur complement ( $t_{\text{Schur}}$ ). As explained in Section 4.3, as these thresholds increase, the sparsity of  $\tilde{S}^{(i)}$  and the U factor increases; the preconditioner behaves poorly. For example in Table 4, we observe that the gap between  $M_{\text{app}}$  with 21% of kept entries in the factor U and  $M_{\text{app}}$  with 10% of kept entries in the factor U is significant; between 3 to 20 iterations (5%-15%). Furthermore, we see that, when we increase the number of sub-domains, the sparser the preconditioner, the larger the number of iterations is. The gap is larger when the Péclet number is increased.

Regarding the behaviour of the preconditioners for convection dominated problems, although those problems are more difficult to solve, the preconditioners are still effective. We recall that the preconditioners do not exploit any specific information about the problem (e.g., direction of flow). From a numerical point of view, if we read Table 4 by column, we can observe the effect of the Péclet number increase on number of GMRES iterations to converge. With respect to this parameter the preconditioners perform reasonably well. This robustness is illustrated by the fact that the solution is tractable even for large Péclet numbers.



#### 4.4.2 Parallel weak scalability on massively parallel platforms

This section is devoted to the presentation and analysis of the parallel performance of the approximated sparse preconditioners  $M_{\text{app}}$ . It is believed that parallel performance is the most important means of improving/reducing turn around time and computational cost of applications. In this context, we consider scaled experiments where we increase the number of processors while the size of the sub-domain (i.e., sub-domain size) is kept constant. Such weak scalability experiments mainly emphasize the interest of parallel computation in keeping constant the elapsed time to solve a problem for which the overall size and the number of processors increase proportionally.

In Table 5 are reported the elapsed time to exactly factorize the local internal problem of the matrix associated with each sub-domain  $A_{ii}^{(i)}$ , using [1] (LU[ $A_{ii}$ ]), to perform the partial incomplete LU factorization on  $A^{(i)}$  to construct  $\tilde{S}^{(i)}$ . Different problem sizes are considered for these experiments. The initialization times, displayed in Table 5, are independent of the number of sub-domains and only depend on their size. It can be seen that the BLAS-3 implementation of the sparse direct solver outperforms the sparse BLAS-1 like computation of the partial incomplete factorization.

We report in Table 6 the setup time for the two values of the dropping threshold of the preconditioner and for different sizes of the sub-domains. As mentioned above the setup time to build the preconditioner depends on the size of the local Schur complement and especially on the amount of the kept entries on the local Schur complements. This cost includes the time to assemble the local approximated Schur complement, and to factorize it using a sparse direct solver. We should mention that the assembly time does not depend much on the number of processors; the key is that to assemble the preconditioner, a few neighbour to neighbour communications are performed to exchange informations with processors owning neighbouring regions. In our 3D case the maximum communication is performed among 27 neighbours for the internal sub-domains. As already observed in earlier work, the time per iteration does not depend much on the number of processors. For example increasing the number of processors from 125 to 1728, the time goes from 0.32 seconds up to 0.39 seconds. This illustrates the parallel efficiency of the implementation of the iterative

sub-domain grid size		# sub-domains $\equiv$ # processors									
		27	64	125	216	343	512	729	1000	1331	1728
Heterogeneous diffusion term defined by Problem 1											
25 <sup>3</sup>	21% in U, 5% in S	29	39	44	56	60	73	81	86	91	108
	10% in U, 5% in S	32	45	48	63	67	81	90	97	101	119
30 <sup>3</sup>	21% in U, 4% in S	32	43	47	60	62	80	86	92	96	114
	10% in U, 4% in S	36	49	52	68	73	90	101	107	107	130
35 <sup>3</sup>	21% in U, 4% in S	34	46	50	65	70	77	94	98	97	123
	10% in U, 4% in S	38	50	55	73	79	92	105	114	111	136
Heterogeneous and anisotropic diffusion term defined by Problem 2											
25 <sup>3</sup>	21% in U, 5% in S	33	47	54	73	73	83	92	100	101	127
	10% in U, 5% in S	35	51	59	78	79	91	100	108	110	133
30 <sup>3</sup>	21% in U, 4% in S	33	49	56	75	75	86	100	102	107	131
	10% in U, 4% in S	37	54	63	82	83	97	105	114	117	139
35 <sup>3</sup>	21% in U, 4% in S	35	51	58	78	77	89	97	105	110	134
	10% in U, 4% in S	43	57	65	85	84	101	110	120	121	144

Table 3: Number of preconditioned GMRES iterations for various diffusion terms combined when the number of sub-domains are varied (horizontal view) and when the sub-domain mesh size is varied (vertical view).



		# sub-domains $\equiv$ # processors									
		27	64	125	216	343	512	729	1000	1331	1728
Heterogeneous diffusion term defined by Problem 1 with Convection 1											
$\epsilon = 1$	21% in U, 4% in S	34	46	50	65	70	77	94	98	97	123
	21% in U, 2% in S	35	45	50	66	68	78	93	104	100	126
	10% in U, 4% in S	38	50	55	73	79	92	105	114	111	136
	10% in U, 2% in S	38	52	56	73	80	88	107	113	113	137
$\epsilon = 10^{-3}$	21% in U, 4% in S	34	48	53	67	77	89	100	112	118	135
	21% in U, 2% in S	35	46	55	68	77	91	101	112	124	139
	10% in U, 4% in S	38	54	60	76	90	102	114	129	136	154
	10% in U, 2% in S	40	54	61	76	89	102	116	126	140	157
$\epsilon = 10^{-4}$	21% in U, 4% in S	36	52	62	72	85	96	105	116	128	138
	21% in U, 2% in S	37	52	64	74	86	98	111	118	132	143
	10% in U, 4% in S	41	59	69	81	96	108	119	131	144	155
	10% in U, 2% in S	43	58	71	82	95	108	122	131	147	159
$\epsilon = 10^{-5}$	21% in U, 4% in S	126	170	163	169	201	217	231	259	276	290
	10% in U, 4% in S	128	179	183	197	232	253	269	296	321	338
Heterogeneous and anisotropic diffusion term defined by Problem 2 with Convection 1											
$\epsilon = 1$	21% in U, 4% in S	35	51	58	78	77	89	97	105	110	134
	21% in U, 2% in S	36	52	59	79	78	91	99	109	113	136
	10% in U, 4% in S	43	57	65	85	84	101	110	120	121	144
	10% in U, 2% in S	43	57	65	85	84	101	111	120	123	146
$\epsilon = 10^{-3}$	21% in U, 4% in S	41	53	64	84	87	102	118	122	129	150
	21% in U, 2% in S	38	55	66	86	89	105	120	126	133	153
	10% in U, 4% in S	47	60	74	91	100	116	129	141	148	167
	10% in U, 2% in S	47	61	74	91	101	116	129	142	151	170
$\epsilon = 10^{-4}$	21% in U, 4% in S	48	65	82	103	117	143	168	189	210	248
	21% in U, 2% in S	49	67	86	109	124	151	178	201	223	263
	10% in U, 4% in S	62	86	107	136	156	189	222	250	273	299
	10% in U, 2% in S	62	87	108	137	157	190	225	252	279	302
Heterogeneous and anisotropic diffusion term defined by Problem 3 with Convection 1											
$\epsilon = 1$	21% in U, 4% in S	44	61	72	91	109	122	132	143	151	161
	21% in U, 2% in S	44	61	73	92	111	122	134	145	153	163
	10% in U, 4% in S	51	64	80	98	115	128	138	155	166	179
	10% in U, 2% in S	50	64	80	99	115	128	138	156	166	180
$\epsilon = 10^{-3}$	21% in U, 4% in S	49	61	73	94	118	134	157	166	186	200
	21% in U, 2% in S	50	62	75	95	121	136	160	169	189	202
	10% in U, 4% in S	52	67	82	103	126	144	171	187	208	225
	10% in U, 2% in S	52	67	84	103	126	145	171	188	209	226
$\epsilon = 10^{-4}$	21% in U, 4% in S	62	67	85	109	146	170	213	215	227	260
	10% in U, 4% in S	62	70	89	111	151	177	221	228	238	272

Table 4: Number of preconditioned GMRES iterations for various diffusion terms when the number of sub-domains and the Péclet number are varied. For sake of readability, the size of the sub-domain is fixed into  $35 \times 35 \times 35$ ; that is, the size of each sub-domains is 43 000 dof.

solver. This nice scalability is mainly due to the network available on the BlueGene computer dedicated to the reductions.

Finally, we consider the overall computing time with the aim of showing the parallel scalability of the complete algorithms. We display in the left graphs of Figure 5 the number of iterations required to solve the linear systems whereas the right graphs summarize the corresponding elapsed time for the complete solution. For each of these tests, we recall that the sub-domains are  $35 \times 35 \times 35$  grid mesh with 43 000 dof. The growth in the number of iterations as the number of sub-domains increases is rather pronounced, whereas it is rather moderate for the global solution time as the initialization step represents a significant part of the overall calculation.

#### 4.4.3 Preliminary investigations on real life structural mechanics problems

To further assess the robustness of the proposed numerical scheme, we have investigated the numerical behaviour of our approximated preconditioner for the solution of linear systems arising in three dimensional structural mechanics problems representative of difficulties encountered in this application area. Our purpose is to evaluate the robustness and the performance of our preconditioner on the solution of the challenging linear systems that are often solved using direct solvers. In this respect we consider a section of fuselage depicted in Figure 6. It is composed of its skin, stringers (longitudinal) and frames (circumferential, in light blue on Figure 6. This problem is related to the solution of the linear elasticity equations with constraints such as rigid bodies and cyclic conditions. These constraints are handled using Lagrange multipliers, that give rise to symmetric indefinite augmented systems.

The Fuselage problem is a relatively difficult problem with high heterogeneity. In Table 7, we display the number of iterations obtained for this unstructured mesh with 0.6 million dof. The

elapsed time <i>sec</i>	kept entries in factor	sub-domain grid size			
		$25^3$ 15 Kdof	$30^3$ 27 Kdof	$35^3$ 43 Kdof	$40^3$ 64 Kdof
LU( $A_{ii}^{(i)}$ )		2.1	5.3	12.2	23.6
ILU( $A^{(i)}$ )+ $\tilde{S}^{(i)}$	21% in U	24.1	56.6	120.1	230.2
ILU( $A^{(i)}$ )+ $\tilde{S}^{(i)}$	10% in U	12.2	27.2	55.5	115.8
Init time	21% in U	26.2	61.9	132.3	253.8
Init time	10% in U	14.3	32.5	67.7	139.4

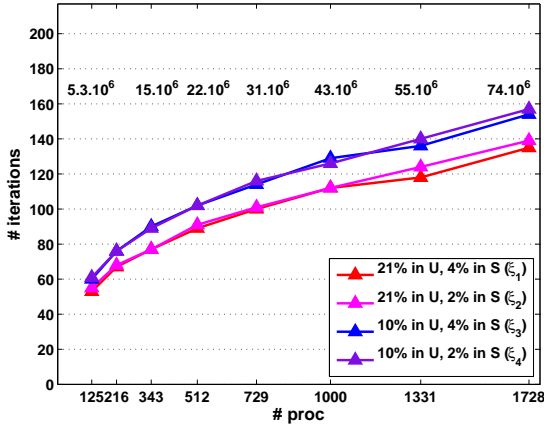
Table 5: Initialization time on a BlueGene supercomputer.

Sub-domain grid size		$25^3$	$30^3$	$35^3$	$40^3$
Time	4% in $S$	2.8	6.1	10.1	14.4
	2% in $S$	1.7	2.9	5.2	7.5

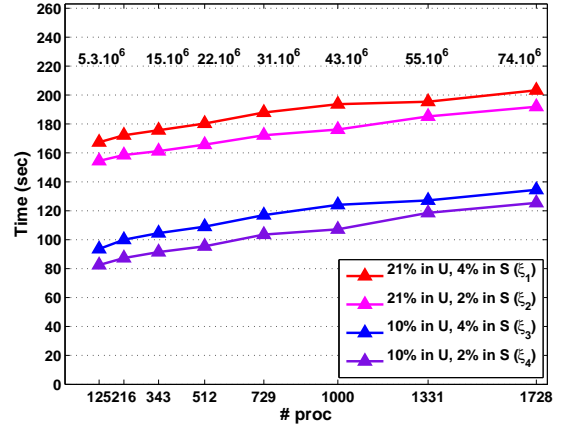
Table 6: Preconditioner setup time (sec) on the Blue Gene supercomputer.

# iterations	exact variant	approximated variant			
	100% in U	65% in U	50% in U	45% in U	25% in U
	100% in $S$	30% in $S$	30% in $S$	30% in $S$	30% in $S$
	64	66	74	106	-

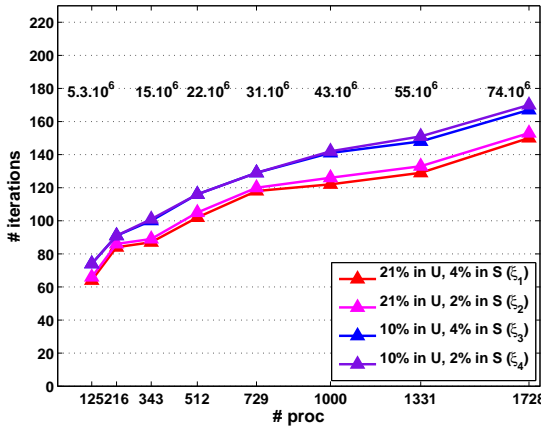
Table 7: Number of preconditioned GMRES iterations when varying the percentage of the kept entries in the approximated factor U for the structural mechanics fuselage problem with 0.6 M dof. For the sake of completeness we give a comparison of the number of iterations between the exact and the approximated variants. “-” means no convergence.



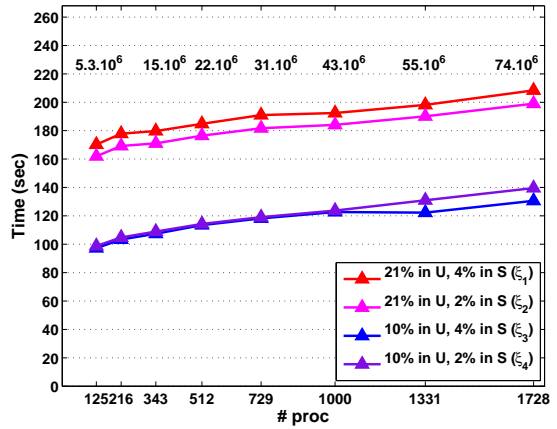
(a) Heterogeneous diffusion Problem 1 with convection 1.



(b) Heterogeneous diffusion Problem 1 with convection 1.

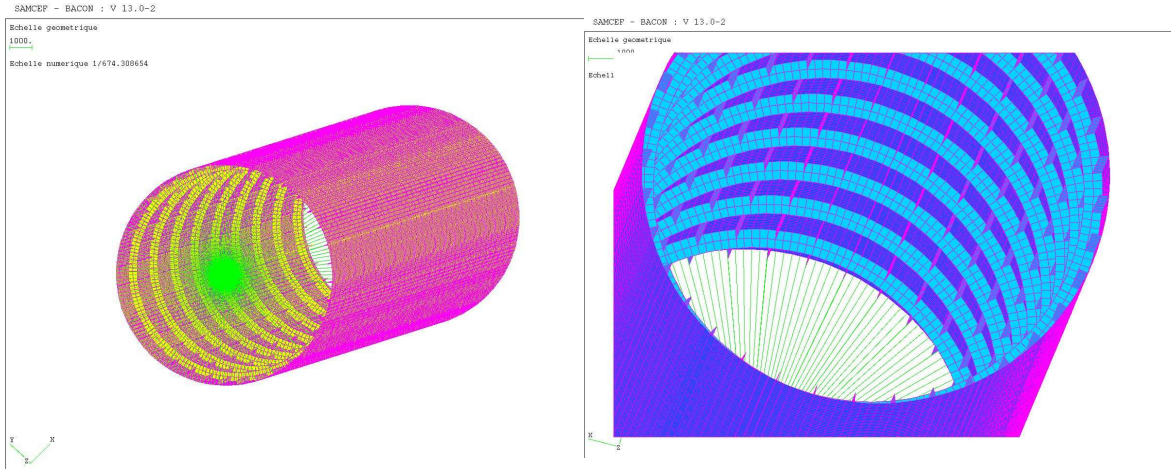


(c) Heterogeneous anisotropic diffusion Problem 2 with convection 1.



(d) Heterogeneous anisotropic diffusion Problem 2 with convection 1.

Figure 5: Parallel weak scalability of a fixed sub-domain size ( $35^3$ ), when varying the number of processors from 125 up to 1728. The convection term is defined by the circular convection and  $\epsilon = 10^{-3}$ . (Left: number of iterations, Right: overall computing time for the solution).



Part of a Fuselage.

Figure 6: structural mechanics meshes.

problem is split into 8 sub-domains. We test the quality of the approximated sparse preconditioner generated by varying the percentage of the kept entries in the incomplete factor  $U$  and in the approximated local Schur complement  $\tilde{S}^{(i)}$ . We compare the results to the exact variant where we keep 100% of the factor entries and also 100% of the local Schur entries.

The results show that, for these real engineering problems, the sparse preconditioner has to retain more information about the Schur complement than for the model convection diffusion test cases. For these problems, in order to preserve the numerical quality similar to the exact dense variant, the approximated variant needs to keep more than 45% of the entries of the factor  $U$  whereas 10% in the convection diffusion test cases were enough. This result is not surprising, however the gain in memory is significant (around 50%).

## 5 Concluding remarks

In this report, we propose an alternative to build an additive Schwarz preconditioner for the Schur complement for designing a parallel hybrid linear solver. In earlier works [4, 3], the main bottleneck of this robust preconditioner was the explicit computation of the local Schur complements. The robustness of the preconditioner comes at the price of this memory and time intensive computation which constitute the main bottleneck of the approach when dealing with very large problems. We have investigated in this report the use of sparse approximation of the dense local Schur complements. These approximations are computed using a partial incomplete  $LU$  factorization. Such a numerical calculation is the core of the multi-level incomplete factorization such as the one implemented in pARMS. The numerical and computing performance of the new numerical scheme have been illustrated on a set of large 3D convection-diffusion problems. The results indicated that most of the numerical features of the initial preconditioner are preserved while both the memory and computing time requirements have been relaxed.

In order to further assess the relevance of the new approach, preliminary experiments on symmetric indefinite linear systems have been conducted. The results show that, for these very difficult engineering problems, to keep a convergence similar to the exact variant, the approximated variant should keep more than 45% of the entries of the factor  $U$ . A possible source of gain for the approximated variant would be a more sophisticated dropping strategy. More work on this aspect would deserve to be undertaken to also investigate strategies for the automatic tuning of the threshold parameter.

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