On the parallel scalability and convergence of GMRES with multiplicative Schwarz preconditioner

Application to FLUOREM CFD test cases

D. Nuentsa Wakam., J. Erhel, É. Canot.

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

centre de recherche RENNES - BRETAGNE ATLANTIQUE

IRISA

Meeting of the ANR LIBRAERO project,
Lyon, May 26, 2010

Outline

GPREMS : A Parallel and distributed solver

- GPREMS : Gmres PREconditioned with Multiplicative Schwarz
- Purpose : Solve the linear system

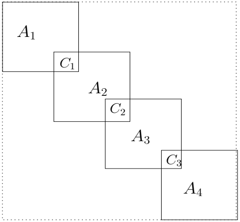
$$M^{-1}Ax = M^{-1}b$$

$A \in \mathbb{R}^{n \times n}$ nonsingular nonsymmetric, x, $b \in \mathbb{R}^n$

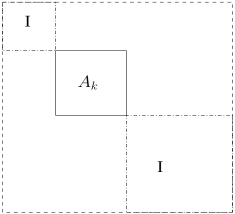
- M^{-1} : explicit formulation of the Multiplicative Schwarz preconditioner

$$M^{-1} = \bar{A}_p^{-1}\bar{C}_{p-1}\bar{A}_{p-1}^{-1}\bar{C}_{p-2}\dots\bar{A}_2^{-1}\bar{C}_1\bar{A}_1^{-1}$$

- Beforehand, the matrix A is permuted in block-diagonal form



(a) : block-diagonal form of A



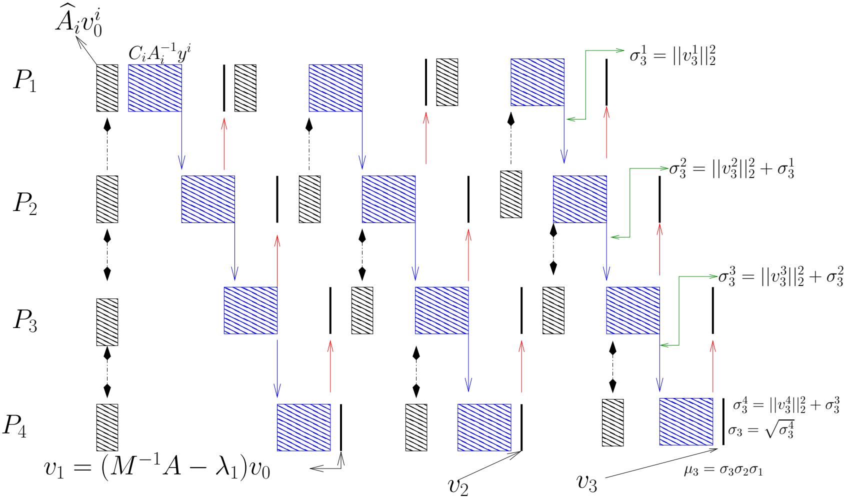
(b): Completed submatrix

Parallel GMRES implementation

- Accelerator : GMRES with Newton basis
- Initial guess : x_0, $r_0 = b - Ax_0$,
- Current approx. : $x_m \in x_0 + \mathcal{K}_m$ s.t. $b - Ax_m \perp A\mathcal{K}_m$
- $\mathcal{K}_m = span\left\{\mu_0 r_0, \mu_1(M^{-1}A - \lambda_1 I)r_0, \ldots, \mu_m \prod_{j=1}^{m}(M^{-1}A - \lambda_j I)r_0\right\}$
- A basis is built for $\mathcal{K}_m$ by :
  1. Generating a non orthonormal basis
  $$V_{m+1} = [r_0, (M^{-1}A - \lambda_1 I)r_0, \ldots, \prod_{j=1}^{m}(M^{-1}A - \lambda_j I)r_0]$$
  2. computing the scaling factors μ_j : $\sigma_{j+1} = 1/||(M^{-1}A - \lambda_j I)\tilde{v}_j||$
  $\mu_{j+1} = \sigma_{j+1}\sigma_j \ldots \sigma_0$ and $M^{-1}AV_m = V_{m+1}T_m$
  3. Orthogonalize the basis $V_{m+1} = Q_{m+1}R_{m+1}$ then $AV_m = Q_{m+1}\bar{H}_m$
- $x_m = x_0 + V_m y_m$ s.t. y_m solves $min||\beta e_1 - \bar{H}_m y_m||$, $(\beta = ||r_0||_2)$

Parallel generation of the basis V_{m+1}

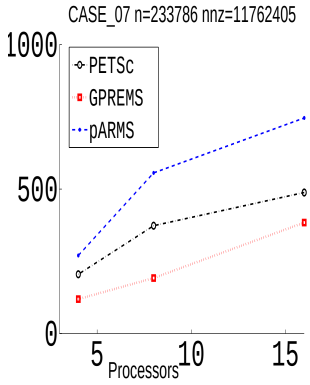
Kernel operations : $v_j = (M^{-1}A - \lambda_j I)v_{j-1}$, P_i holds A_i and $v_j^{(i)}$

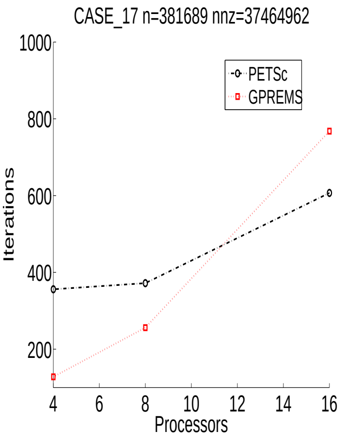


Parallel Scalability and Convergence of GMRES

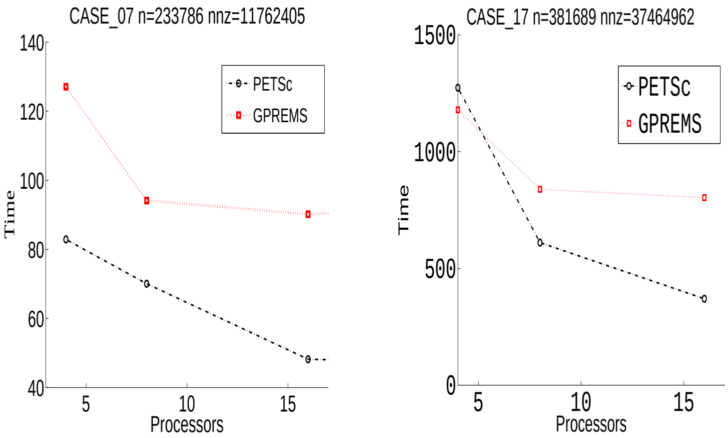
D. NUENTSA WAKAM. et al.

Initial Convergence rate





Elapsed Time



First improvement: Parallel solution of local systems

⇒ From global system :

$$M^{-1}y = \bar{A_p}^{-1}\bar{C}_{p-1}\bar{A}_{p-1}^{-1}\bar{C}_{p-2}\dots\bar{A_2}^{-1}\bar{C}_1\bar{A_1}^{-1}y = z$$

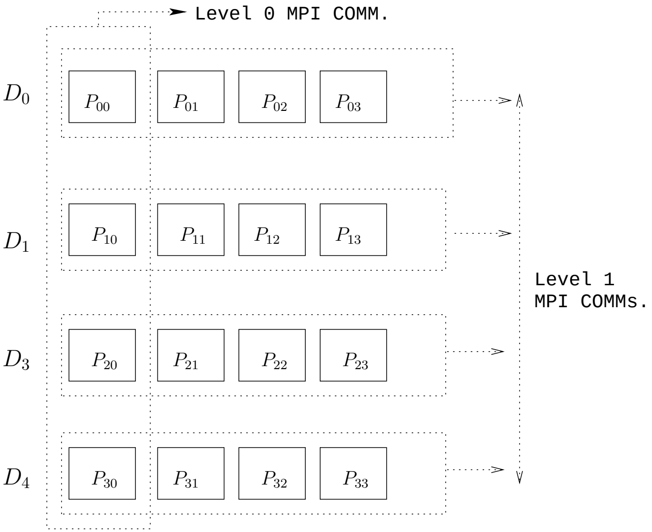
⇒ To several local subsystems :

$$A_i z_i = y_i, (i = 1\dots p)$$

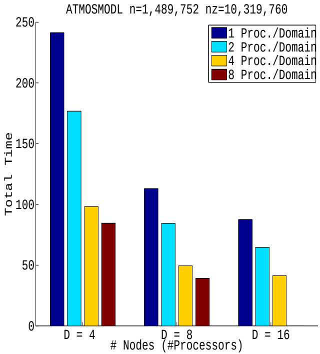
⇒ Idea : Solve the subsystems with a new level of parallelism in subdomains

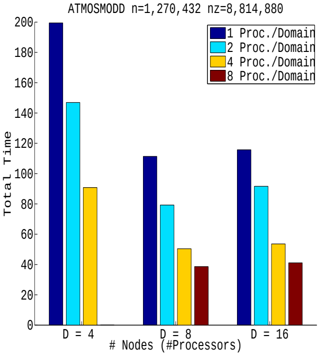
- *Exactly* : parallel direct solver(MUMPS, SuperLU_DIST, ...)
- *Approximately* : parallel ILU factorization.

Natural splitting on a Cluster of SMP Nodes

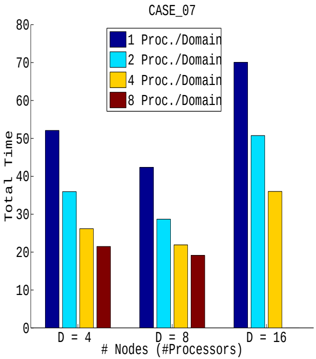


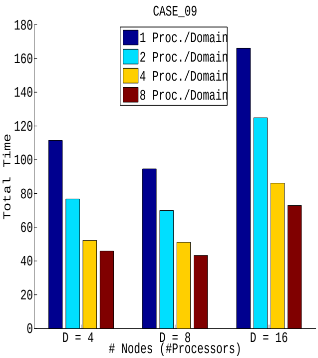
Benefits of the two levels of parallelism (1)





Benefits of the two levels of parallelism (2)





Second improvement: Deflated restarting GMRES

- Convergence of GMRES depends on the spectral distribution of $M^{-1}A$
- Removing or deflating small eigenvalues improve the convergence rate
- Deflating eigenvalues $\Rightarrow$ Add the corresponding eigenvectors in the Krylov subpace.

Eigenvectors $U = [u_1 \dots u_r]$ are deflated by

1. Augmenting the Krylov basis :

$$\mathcal{K}_m = \left\{ r_0, M^{-1}Ar_0, \dots, (M^{-1}A)^m r_0, u_1, u_2, \dots, u_r \right\}$$

2. Preconditioning : Solve $M_2^{-1}M^{-1}A = M_2^{-1}M^{-1}b$,

$$M_2^{-1} = I_n + U(|\lambda_n| T^{-1} - I_r)U^T, \quad T = U^T M^{-1} A U$$

Finding eigenvectors

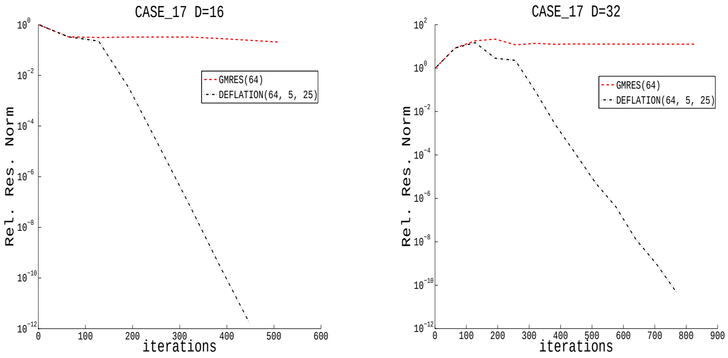
With **the Arnoldi basis** :

- $M^{-1}AV_m = V_{m+1}\bar{H}_m$
- Solve eigenvalues problem $H_m y = \lambda y$
- $V_m y$: Approximate eigenvectors of $M^{-1}A$

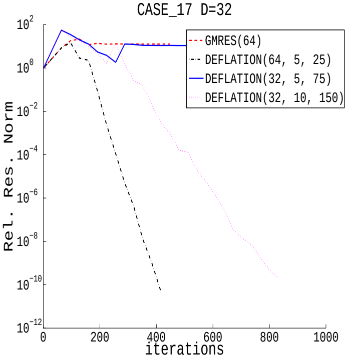
With **the Newton basis** :

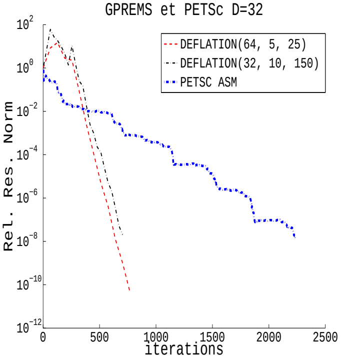
- $M^{-1}AQ_m = Q_{m+1}\underbrace{R_{m+1}\bar{T}_m R_m^{-1}}_{\bar{H}_m}$
- And $M^{-1}AV_m = Q_{m+1}\underbrace{R_{m+1}\bar{T}_m}_{\bar{C}_m}$
- Solve generalized eigenvalues problem $C_m y = \lambda R_m y$
- $Q_m y$: Approximate eigenvectors of $M^{-1}A$

Benefits of the deflation (1)

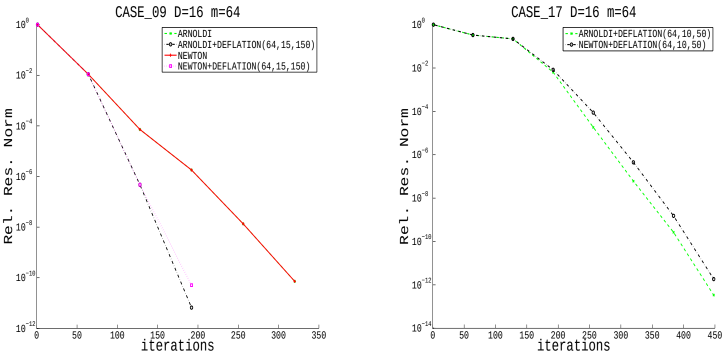


Benefits of the deflation (2)

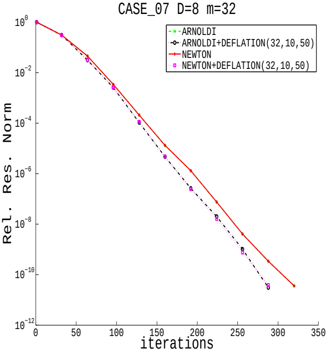


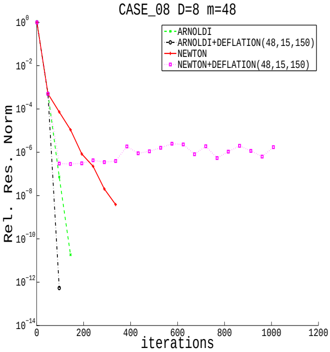


Influence of the Newton basis (1)

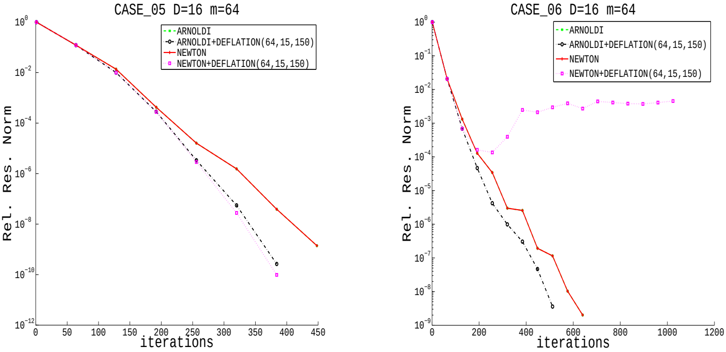


Influence of the Newton basis (2)



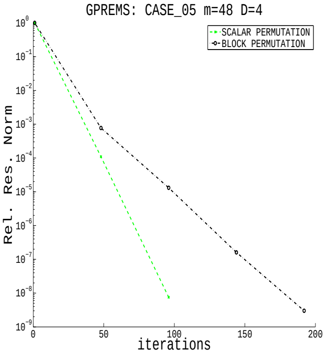


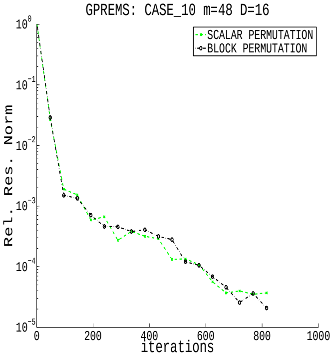
Influence of the Newton basis (3)



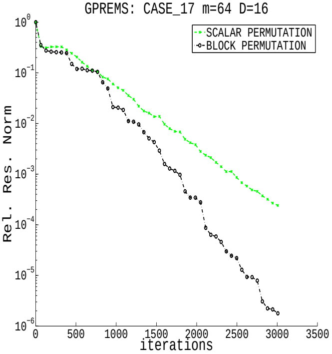
Third improvement : Exploiting the block structure

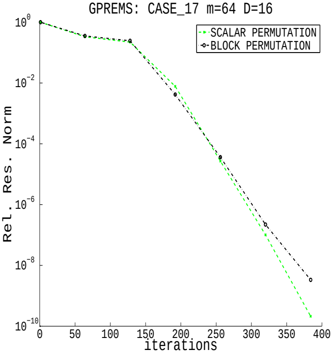
- Matrices are block-structured (5×5, 7×7)
- Perform BDO permutation only on block positions





Exploiting the block structure (2)





Present and future directions

- Introduce deflation by augmenting the Krylov basis
- Implement deflation with additive Schwarz in PETSc
- ...