A Parallel Augmented GMRES algorithm

Application to design optimization in CFD

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Preconditioned GMRES

$Ax = b, \quad A \in \mathbb{R}^{n \times n} \quad x, b \in \mathbb{R}^n \quad B \equiv AM^{-1}$

GMRES(m): a Krylov subspace method

- [Saad and Schultz 1986, Meurant's book 1999, Saad's book 2003, Simoncini and Szyld 2007, Erhel 2011, ...]
- Fix x_0, then $r_0 = b - Ax_0$
- $\mathcal{K}_m(B, r_0) = span\{r_0, Br_0, \ldots B^{m-1} r_0\}$
- Find $x_m \in x_0 + \mathcal{K}_m(B, r_0)$ such that $\|r_m\|_2 = \|b - Bx_m\|_2 = \min_{u \in x_0 + \mathcal{K}_m(B, r_0)} \|b - Bu\|_2$

Building blocks of GMRES

- Initial step: choose x_0, compute r_0
- First step: generation of an orthonormal basis $V_{m+1} = [v_0, \ldots, v_m]$ of $\mathcal{K}_{m+1}(B, r_0)$ such that

$$v_0 = r_0/\beta, \quad \beta = \|r_0\|, \quad BV_m = V_{m+1}\bar{H}_m$$

- Second step: approximate solution $x_m = x_0 + M^{-1} V_m y_m$

$$\Rightarrow r_m = r_0 - BV_m y_m = V_{m+1}(\beta e_1 - \bar{H}_m y_m) \quad \text{with } \beta = \|r_0\|_2$$

$$\Rightarrow y_m = min_{y \in \mathbb{R}^m} \|\beta e_1 - \bar{H}_m y\|_2$$

GMRES ... practical issues

Arnoldi process

```
v_0 = r_0/||r_0||_2
for k = 0, ... do
    p = B v_k
    for i = 1 : k do
        h_ik = v_i^T p
        p = p - h_ik v_i
    end for
    h_{k+1,k} = ||p||_2
    v_{k+1} = p/h_{k+1,k}
end for
```

$\Downarrow$

$$BV_m = V_{m+1}\bar{H}_m$$

Granularity issues in parallel algorithms

$\Rightarrow$ Communication-avoiding strategies

- Generate the basis vectors [Reichel 1990, Bai et al 1994]
- Orthogonalize the basis [De Sturler 1994, Erhel 1995, Sidje 1997]
- Improve the strategy [Hoemmen 2010, Demmel et al 2011]

Complexity issues with restarted GMRES(m)

$\Rightarrow$ Use deflation to recover possible loss of information

- Deflation by preconditioning [Erhel et al 1996, Burrage et al 1998, Baglama et al 1998, ...]
- Deflation by augmented basis [Morgan 1995, Morgan 2002,...]

Preconditioning issues

$\Rightarrow$ use multilevel methods to deal with large systems

- Schwarz preconditioning [Atenekeng Kahou et al 2007, Dufaud+Tromeur-Dervout 2010, Giraud+Haidar 2009, Smith et al's book 1996,...]
- Filtering and Schur complement [Li et al 2003, Grigori et al 2011]
- Multilevel parallelism [Nuentsa Wakam et al 2011, Giraud et al 2010, ...]

Proposal of this work

Combine 'communication-avoiding' GMRES ... and Deflation ... and domain decomposition preconditioners

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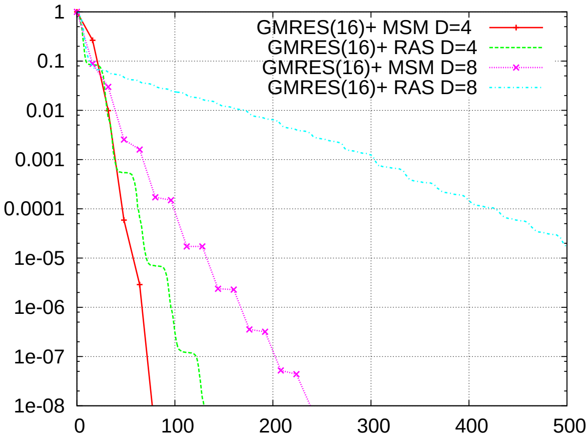
Illustration : Domain decomposition and Restarting

- 2D Helmholtz problem on a 164×164 grid
- GMRES(16) + RAS or MSM (4 or 8 domains), LU as subdomain solver



Outline

1. Newton basis
2. Adaptive deflation
3. Numerical experiments
   - Software package
   - CFD application
   - Numerical convergence
   - CPU Time

building blocks

- Initial step: run one cycle of GMRES(m) and compute shifts for the Newton basis
- First step: build a basis $K_{m+1} = [k_0, k_1, \ldots, k_m]$ of the Krylov subspace $\mathcal{K}_{m+1}(B, r_0)$ such that

$$BK_m = K_{m+1}\bar{T}_m$$

- Second step: compute an orthonormal basis of $\mathcal{K}_{m+1}(B, r_0)$
  Compute the QR factorization $K_{m+1} = V_{m+1}R_{m+1}$
  RODDEC [Sidje 1997, Erhel 1995] or TSQR [Demmel et al 2011]

$$\Rightarrow BK_m = V_{m+1}R_{m+1}\bar{T}_m \Rightarrow BV_m = V_{m+1}\underbrace{R_{m+1}\bar{T}_m R_m^{-1}}_{\bar{H}_m}$$

- Third step: approximate solution $x_m = x_0 + M^{-1}V_m y_m$

$$\Rightarrow r_m = r_0 - BK_m y_m = V_{m+1}(\beta e_1 - \bar{H}_m y_m) \quad \text{with } \beta = \|r_0\|_2$$

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GMRES with a Newton basis

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Computation of the Newton basis

Shifts and matrix-vector products

- Initial step: Compute m Ritz values $\lambda_j \quad j = 0, \ldots m-1$ and get their Leja ordering
  Alternative [Philippe+Reichel, 2011]
- At each cycle:

  $tmp = r_0$
  $\sigma_0 = \|tmp\|_2$
  $k_0 = tmp/\sigma_0$
  $j = 0$
  while $j \leq m-1$ **do**
      if $Im(\lambda_{j+1}) = 0$ **then**
          $tmp = (B - \lambda_{j+1} I)k_j$
          $\sigma_{j+1} = \|tmp\|_2$
          $k_{j+1} = tmp/\sigma_{j+1}$
          $j = j+1$
      else if $Im(\lambda_{j+1} > 0)$ **then**
          $tmp = (B - Re(\lambda_{j+1})I)k_j$
          $\sigma_{j+1} = \|tmp\|_2$
          $k_{j+1} = tmp/\sigma_{j+1}$
          $tmp = (B - Re(\lambda_{j+1})I)tmp + Im(\lambda_{j+1})^2 k_j$
          $\sigma_{j+2} = \|tmp\|_2$
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  end while

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Building blocks

- Initial step: run one cycle of GMRES(m) and compute shifts for the Newton basis
  Compute $U_r = [u_0, u_1, \dots, u_{r-1}]$ a basis of a coarse subspace
- First step: build a basis $K_{m+1} = [k_0, k_1, \dots, k_m]$ of the Krylov subspace $\mathcal{K}_{m+1}(B, r_0)$ such that

$$BK_m = K_{m+1}\bar{T}_m$$

  Define the augmented subspace $\mathcal{C}_s = \mathcal{K}_m(B, r_0) + span\{U_r\}$ with $s = m + r$ with the basis

$$\begin{bmatrix} K_m & U_r \end{bmatrix}$$

- compute

$$BU_r = \hat{K}_r D_r$$

  Define the augmented subspace $\hat{\mathcal{C}}_{s+1} = \mathcal{K}_{m+1}(B, r_0) + span\{BU_r\}$ with the basis

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GMRES with an adaptive augmented Newton basis

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  Define the basis $W_s = \begin{bmatrix} V_m & U_r \end{bmatrix}$

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- Third step: $x_s = x_0 + M^{-1} W_s y_s$

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Adaptive strategy

Update r and U_r using convergence estimation

- At each restart, estimate *Iter*, the remaining number of steps [Sosonkina et al, 1998]

$$Iter = s * log(\frac{\epsilon}{||r_s||})/log(\frac{||r_s||}{||r_0||});$$

- If ($Iter \leq smv * itmax$): fast convergence $\Rightarrow$ keep U_r
- If ($smv * itmax < Iter \leq bgv * itmax$): slow convergence $\Rightarrow$ update U_r
- If ($Iter > bgv * itmax$): possible stagnation $\Rightarrow$ Increase r by l until r_{max} and update U_r

Coarse subspace

Approximate invariant subspace

- Initial step: Compute m Ritz values $\lambda_j \quad j = 0, \ldots m-1$ and get their Leja ordering extract r Ritz vectors $u_j, \quad j = 0, \ldots r-1$ with $u_j = V_m g_j$ in the subspace $\mathcal{K}_m$ using the Galerkin condition $V_m^T(B - \lambda_j I)V_m g_j = 0$

$$\Rightarrow H_m g_j = \lambda_j g_j$$

- At each cycle: update U_r with $u_j = W_s g_j$ in the augmented subspace $\mathcal{C}_s$ using the Galerkin condition $(BW_s)^T(B - \lambda_j I)W_s g_j = 0$

$$\Rightarrow \bar{H}_s^T \bar{H}_s g_j = \lambda_j \bar{H}_s^T V_{s+1}^T W_s g_j$$

with

$$V_{s+1}^T W_s = \begin{bmatrix} V_{s+1}^T V_m & V_{s+1}^T U_r \end{bmatrix}$$

$$V_{s+1}^T V_m = \begin{bmatrix} I_m \\ 0 \end{bmatrix}$$

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AGMRES algorithm

AGMRES(m,itmax, r, l, rmax)

B, $r_0 = b/\|b\|_2$
Compute one cycle of Arnoldi-GMRES
Generate m shifts λ_j
Compute r vectors U_r
while no convergence **do**
    Compute K_{m+1} such that $BK_m = K_{m+1}\bar{T}_m$
    Compute $BU_r = \hat{K}_r D_r$
    Orthogonolize $\begin{bmatrix} K_{m+1} & \hat{K}_r \end{bmatrix} = V_{s+1}R_{s+1}$
    Define $W_s = \begin{bmatrix} V_m & U_r \end{bmatrix}$
    Get $BW_s = V_{s+1}\bar{H}_s$
    solve $y_s = \min_y J(y)$ with $J(y) = ||\beta e_1 - \bar{H}_s y||_2$
    Compute $x_s = x_0 + W_s y_s$
    Test of convergence
    Adaptively udpate r and U_r
end while

Complexity issues: comparison with GMRES(m)

- memory additional requirements: $2r$ vectors U_r and $[v_{m+1} \dots v_{m+r}]$
- CPU additional requirements in GMRES process: BU_r and $[v_{m+1} \dots v_{m+r}]$
- CPU overhead in adaptive strategy: $V_{s+1}^T U_r$

AGMRES algorithm

AGMRES(m,itmax, r, l, rmax)

```
B, r_0 = b/||b||_2
Compute one cycle of Arnoldi-GMRES
Generate m shifts λ_j
Compute r vectors U_r
while no convergence do
    Compute K_{m+1} such that B K_m = K_{m+1} T̄_m
    Compute B U_r = K̂_r D_r
    Orthogonolize [ K_{m+1}  K̂_r ] = V_{s+1} R_{s+1}
    Define W_s = [ V_m  U_r ]
    Get B W_s = V_{s+1} H̄_s
    solve y_s = min_y J(y) with J(y) = ||β e_1 − H̄_s y||_2
    Compute x_s = x_0 + W_s y_s
    Test of convergence
    Adaptively udpate r and U_r
end while
```

Complexity issues: comparison with GMRES(m)

- memory additional requirements: $2r$ vectors U_r and $[v_{m+1} \dots v_{m+r}]$
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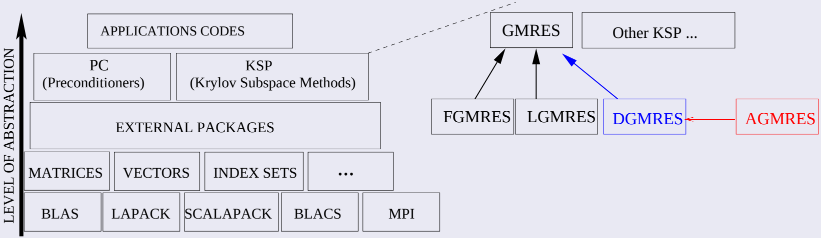
Implementation using PETSc

New KSP type : AGMRES



Usage in Petsc

- Use AGMRES just as GMRES
- ⇒ KSPSetType(ksp, KSPAGMRES) or -ksp_type agmres, -pc_type asm, ...
- Options : -ksp_gmres_restart m, -ksp_agmres_eig r,
- -ksp_max_its maxits, -ksp_agmres_smv smv -ksp_agmres_bgv bgv, ...

Using AGMRES with Schwarz preconditioning

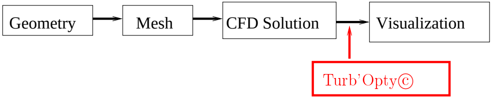
Main steps when using AGMRES

- Partition the weighted graph of the matrix in parallel with PARMETIS.
- Redistribute the matrix and right-hand-side according to the PARMETIS partitioning.
- Perform a parallel iterative row and column scaling on the matrix and the right-hand side vector [Amestoy et al, 2008].
- Define the overlap between the submatrices for the additive Schwarz preconditioner.

$$M_{RAS}^{-1} = \sum_{k=1}^{D} (R_k^0)^T (A_k^\delta)^{-1} R_k^\delta$$

- Setup the submatrices (ILU or LU factorization).
- Solve iteratively the preconditioned system using either AGMRES or GMRES.

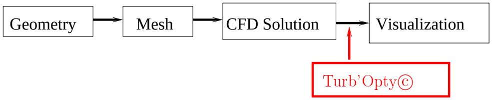
A CFD application



- At steady state, the solution of the stationary Navier-Stokes writes $F(q_{ref}, p_{ref}) = 0$
- $q = \{\rho, \rho U, \rho V, \rho W, \rho E, \rho k, \rho\omega\}$ flow variables (mass, momentum, energy, turbulence)
- $p =$ physical and geometrical flow parameters (pressure, temperature, shape, distance, ...)
- Turb'Opty©, FLUOREM : Find new solutions q with respect to the parameters p

About Turb'Opty [S. Aubert et al 2001]
About using AGMRES for Turb'Opty matrices [Nuentsa Wakam + Pacull, Computer & Fluids 2012]

A CFD application



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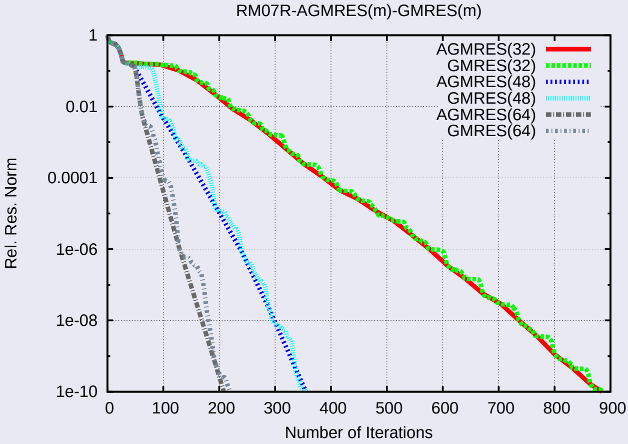
About using AGMRES for Turb'Opty matrices [Nuentsa Wakam + Pacull, Computer & Fluids 2012]

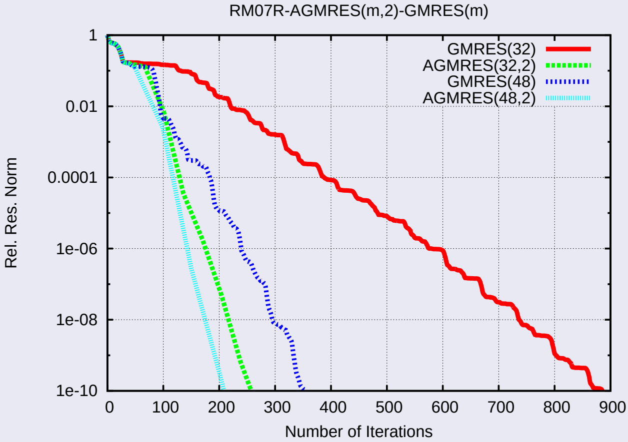
RM07R size = 381,689 nonzeros = 37,464,962

Experimental stability of AGMRES (without deflation)



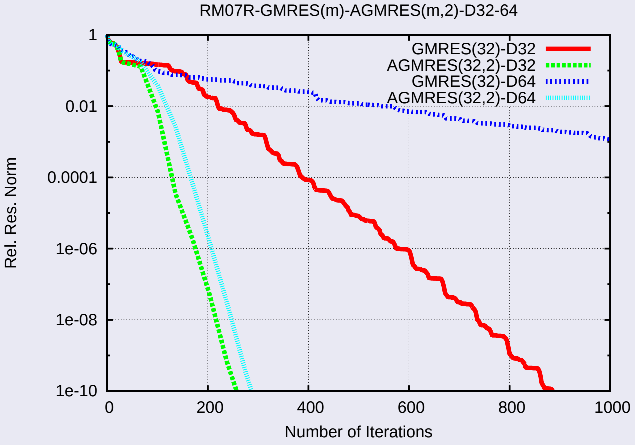
RM07R size = 381,689 nonzeros = 37,464,962

Influence of the augmented basis (no adaptive strategy)



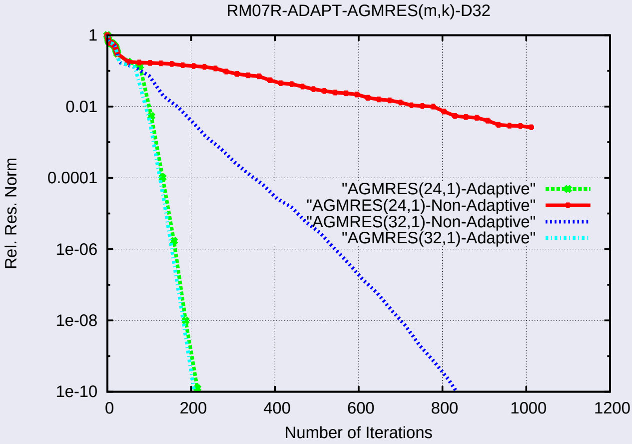
RM07R size $= 381{,}689$ nonzeros $= 37{,}464{,}962$

Influence of the number of subdomains (no adaptive strategy)



RM07R size = 381,689 nonzeros = 37,464,962

Influence of the adaptive strategy ($l = 2$ and $r_{max} = 5$)



IM07R and VV11R: CPU Time and communications

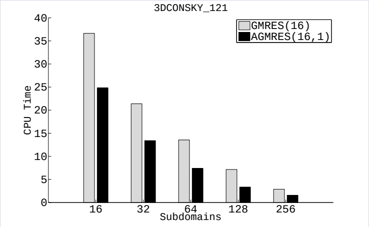
- IM07R Size = 261,465 entries : 26,872,530
- VV11R Size = 277,095 entries : 30,000,952
- $r = 2$, $l = 2$, $r_{max} = 6$

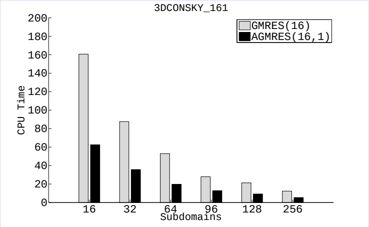
D \ m	24		32		48		
	Iter. Time	MSG	Iter. Time	MSG	Iter. Time	MSG	
GMRES(m)							VV11R
8	92.84	2.05	68.95	1.69	77.7	1.47	
16	101.1	12.27	89.37	11.47	63.2	7.66	
32	-	-	31.2	22.5	29.7	18.54	
AGMRES(m, r)							
8	52.8	1.28	38.5	1.02	40.5	1.05	
16	51.8	7.4	34.5	4.91	28.08	3.87	
32	38.3	25.6	31.2	22.5	29.7	18.5	
GMRES(m)							IM07R
8	76.219	2.6	73.3	2.63	63.669	2.31	
16	111.74	20.06	96.246	18.25	83.583	15.76	
32	-	-	-	-	77.066	59.87	
AGMRES(m, r)							
8	45.781	1.65	40.905	5.48	40.85	1.52	
16	36.492	21.65	34.803	24.12	33.65	23.64	
32	33.262	94.54	27.837	93.27	27.109	105.35	

3D Convection-Diffusion problems

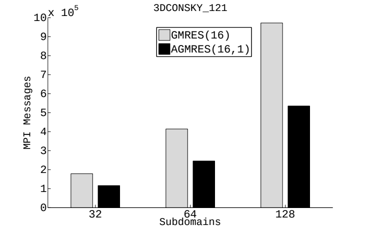
- 3DCONSKY_121 : size = 1,771,561; nonzeros = 50,178,241
- 3DCOSKY_161 : size= 4,173,281; nonzeros = 118,645,121

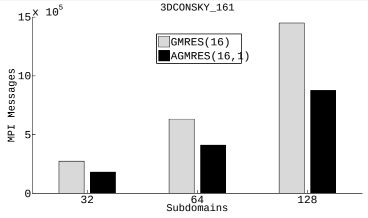
CPU Time





Number of MPI messages





Conclusion

- AGMRES: augmented Newton basis in GMRES(m)
- AGMRES + Schwarz: domain decomposition preconditioning
- Robustness: reduce the restarting effects and the domain decomposition effects
- Efficiency: increase granularity and scalability
- Numerical experiments with CFD problems: AGMRES faster than GMRES

AGMRES module

- Will be made available in PETSc in 2012

Paper in revision for publication in ETNA
preprint at http://www.irisa.fr/sage/desire