Parallel sparse linear solvers and applications in CFD

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Outline

Solver interface

- Interface to direct and iterative solvers: MUMPS, SuperLU_Dist, Hypre, Petsc, pArms,etc
- SLSI [Nuentsa Wakam et al 2010] available on demand
- System solver in H2OLab platform [Erhel et al 2009]
- Application to CFD problems

GMRES(m): a Krylov method for general matrices

- combining Domain Decomposition and deflation

PCG: a Krylov method for SPD matrices

- combining Domain Decomposition and deflation

Preconditioned GMRES

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

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: generate an orthonormal basis $V_{m+1} = [v_0, \ldots, v_m]$ of $\mathcal{K}_{m+1}(B, r_0)$ such that
$$v_0 = r_0/\beta, \quad \beta = \|r_0\|_2, \quad BV_m = V_{m+1}\bar{H}_m$$
- Second step: approximate solution $x_m = x_0 + M^{-1}V_m y_m$
$$\Rightarrow r_m = r_0 - BV_m y_m = V_{m+1}(\beta e_1 - \bar{H}_m y_m)$$
$$\Rightarrow y_m = min_{y\in\mathbb{R}^m} \|\beta e_1 - \bar{H}_m y\|_2$$

GMRES ... practical issues

Arnoldi process

$v_0 = r_0 / \|r_0\|_2$
for $k = 0, \ldots$ **do**
  $p = Bv_k$
  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]

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, ...]

Complexity and stagnation 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,...]

Work in the team SAGE

Combine 'communication-avoiding' GMRES ... and Deflation ... and domain decomposition preconditioners
[Nuentsa Wakam 2011, Nuentsa Wakam+Erhel+Gropp 2013, Nuentsa Wakam+Pacull 2013, Nuentsa Wakam+Erhel 2014]

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building blocks

- Initial step: run one cycle of GMRES(m) and compute shifts for the Newton basis
- First step: build a basis $K_{m+1} = [k_0, k_1, \dots, k_m]$ 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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Communication-avoiding strategy: Newton basis

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GMRES combined with Domain Decomposition

Main steps with Domain Decomposition preconditioning

- 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 GMRES.

Deflation strategies

Restarted GMRES(m)

- $x_m = x_0 + M^{-1} V_m y_m$ where y_m minimizes $\|r_m\|_2$
- The convergence rate depends on the spectral distribution in B
- Smallest eigenvalues slow down the convergence
- Deflation occurs when the Krylov subspace is large enough
- With restarting : loss of spectral information, risk of stalling

Accelerating the restarted GMRES[Simoncini and Szyld, 2007]

- Approximate the smallest eigenvalues and the associated invariant subspace U_r
- Explicit deflation technique [Erhel et al 1996; Burrage et al 1998; Moriya et al 2000]:

$$B\bar{M}^{-1}\tilde{x} = b$$

with $\bar{M}^{-1} = (I_n + U_r(|\lambda_n| T^{-1} - I_r)U_r^T$ and $T = U_r^T B U_r$

- Augmented techniques [Morgan 2000, 2002, Giraud et al, 2010]:

$$x_m \in x_0 + span\{U_r\} + \mathcal{K}_m(B, r_0)$$

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DGMRES: GMRES with adaptive preconditioning deflation

DGMRES(m, r)

- Perform one cycle of restarted GMRES(m) and compute shifts for the Newton basis
- compute U_r, a basis of a coarse subspace
- Build $\bar{M}_r^{-1} \equiv I_n + U_r(|\lambda_n|T^{-1} - I_r)U_r^T, \quad T = U_r^T B U_r$
- Apply GMRES(m) to $B\bar{M}_r^{-1}$
- At each restart, update r and the basis U_r

Adaptive DGMRES(m,r)

- Detect a potential slow convergence [Sosonkina et al 1998]
- Switch to DGMRES(m,r) only if necessary [Nuentsa Wakam et al 2013]

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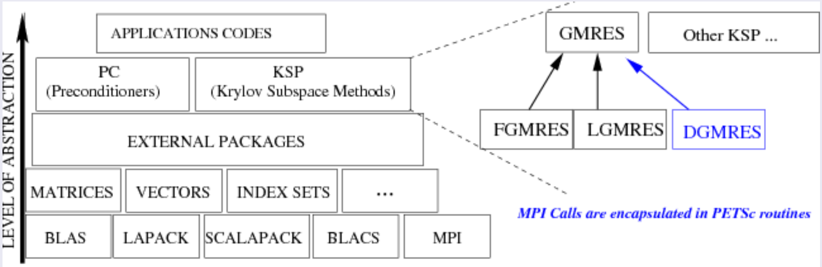
New KSP type : DGMRES



Usage in Petsc

- Available in PETSc
- Use DGMRES just as any other KSP with the following options

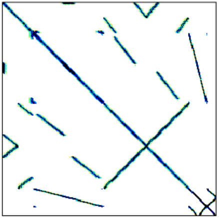
Experiments with CFD matrices

FLUOREM matrices

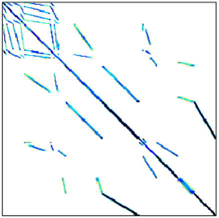
- in MatrixMarket collection
- large, sparse, nonsymmetric matrices
- linearization of Navier-Stokes: symmetric profile with structured blocks
- Schwarz preconditioning combined with GMRES or DGMRES

[Nuentsa Wakam+Erhel+Gropp 2013; Nuentsa Wakam+Pacull 2013]

RM07R n= 381,689; nnz=37,464,962

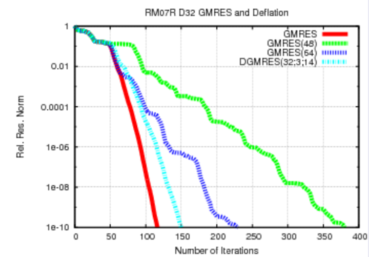


HV15R n= 2,017,169; nnz=283,073,458



Combining DGMRES with domain decomposition

RM07R



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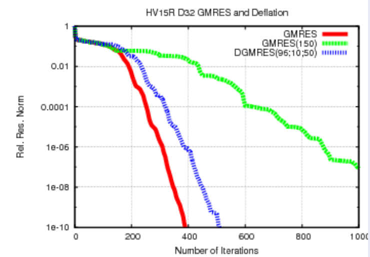

CPU time on parallel computers

RM07R, n = 381,689, nz = 37,464,962							
D	FULL-GMRES		GMRES(48)		DGMRES(32,2,15)		
	ITS	**Time (s)**	**ITS**	**Time (s)**	**ITS**	**Time (s)**	r
16	92	214	169	297	115	250	9
32	117	103	355	260	160	139	11
64	149	66	860	166	206	53	12

HV15R, n = 2,017,169, nz = 283,073,458							
D	FULL-GMRES		GMRES(150)		DGMRES(96,10,70)		
	ITS	**Time (s)**	**ITS**	**Time (s)**	**ITS**	**Time (s)**	r
32	389	1536	(8.4E-08)	3,316	510	2002	50
64	494	1024	(6.8E-01)	-	635	1500	61

AGMRES: deflation with an adaptive augmented basis

Building blocks

- Initial step: run one cycle of GMRES(m) and compute shifts for the Newton basis
  Compute $U_r = [u_0, u_1, \ldots, u_{r-1}]$ a basis of a coarse subspace
- 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

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

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

$$\left[\begin{array}{cc} K_m & U_r \end{array} \right]$$

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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AGMRES: deflation with an adaptive augmented basis

Building blocks

- Second step: Compute an orthonormal basis of $\hat{\mathcal{C}}_{s+1}$
  QR factorize the augmented basis $\begin{bmatrix} K_{m+1} & \hat{K}_r \end{bmatrix} = V_{s+1}R_{s+1}$

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

$$\Rightarrow BU_r = (V_{m+1}R_{m+1,r} + V_r R_r)D_r$$

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

$$\Rightarrow BW_s = V_{s+1}\bar{H}_s$$

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

$$\Rightarrow r_s = r_0 - BW_s y_s = V_{s+1}(\beta e_1 - \bar{H}_s y_s) \quad \text{and } \beta = \|r_0\|_2$$

$$y_s = min_{y\in\mathbb{R}^s}\|\beta e_1 - \bar{H}_s y\|_2$$

- Final step: Adaptively update r and the coarse basis U_r

AGMRES: deflation with an adaptive augmented basis

Building blocks

- Second step: Compute an orthonormal basis of $\hat{\mathcal{C}}_{s+1}$
  QR factorize the augmented basis $\begin{bmatrix} K_{m+1} & \hat{K}_r \end{bmatrix} = V_{s+1} R_{s+1}$

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

$$\Rightarrow BU_r = (V_{m+1} R_{m+1,r} + V_r R_r) D_r$$

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

$$\Rightarrow BW_s = V_{s+1} \bar{H}_s$$

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

$$\Rightarrow r_s = r_0 - BW_s y_s = V_{s+1}(\beta e_1 - \bar{H}_s y_s) \quad \text{and } \beta = \|r_0\|_2$$

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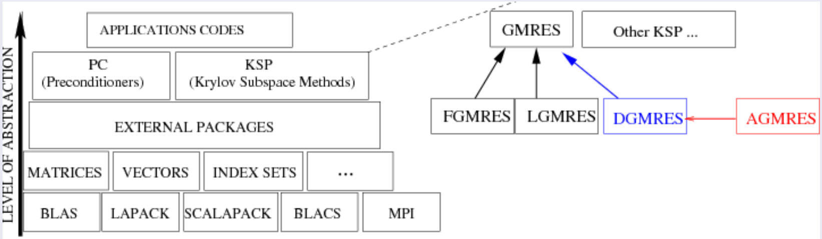
AGMRES in PETSc

New KSP type : AGMRES

figure

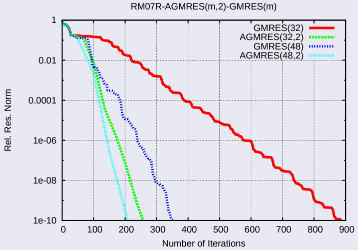


Usage in Petsc

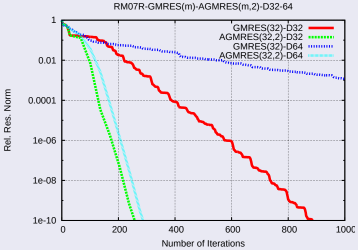
- Use AGMRES just as GMRES
- ⇒ KSPSetType(ksp, KSPAGMRES) or -ksp_type agmres, -pc_type asm, ...
- Options : -ksp_gmres_restart m, -ksp_agmres_eig r,
- -ksp_max_its maxits, -ksp_agmres_smv smv -ksp_agmres_bgv bgv, ...

Experiments with Augmented GMRES

RM07R: effect of the restarting



RM07R: effect of the number of subdomains



CPU time on parallel computers

RM07R, n = 381,689, nz = 37,464,962				
D	GMRES(32)		AGMRES(32,r)	
	ITS	**Time (s)**	**ITS**	**Time (s)**
16	254	379.3	169	224.1
32	886	573.4	212	91.41
64	-	-	287	62.39

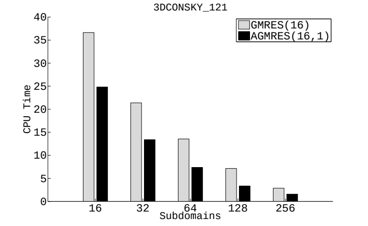
Parallel CPU Time with AGMRES

Convection-Diffusion test cases

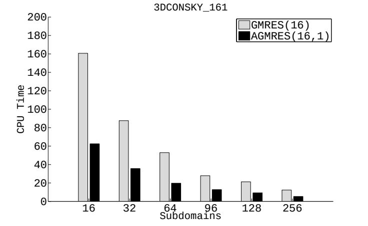
- 3DCONSKY_121 : size = 1,771,561; nonzeros = 50,178,241
- 3DCOSKY_161 : size= 4,173,281; nonzeros = 118,645,121

[Nuentsa Wakam+Erhel 2014]

3DCONSKY_121



3DCONSKY_161



Augmented Conjugate Gradient

PCG

- A Symmetric Positive Definite (SPD) matrix
- PCG is a Krylov method
- short recurrences and minimization properties
- preconditioning M^{-1}

Coarse grid and balancing

[Nicolaides 1987, Mandel 1993, DD proceedings, Giraud et al.]

- Z basis of a coarse subspace
- restriction of A: nonsingular small matrix $A_c = Z^T AZ$
- projections: $P = I - AZA_c^{-1}Z^T$ and $P^T = I - ZA_c^{-1}(AZ)^T$
- coarse grid: $ZA_c^{-1}Z^T$
- balancing: $C_b = P^T M^{-1} P + ZA_c^{-1}Z^T$

Coarse grid and augmented CG

[Erhel et al 2000, Saad et al. 2000, Tang et al. 2009, Poirriez 2011, Nataf et al]

- $x_0 = ZA_c^{-1}Z^T b$
- $C_a = P^T M^{-1}$
- C_a is equivalent to C_b (if no loss of orthogonality)

SIDNUR: AugCG and Domain Decomposition

Balancing Neumann Neumann

- PCG applied to a Schur complement
- Neumann-Neumann preconditioning M^{-1}
- Balancing with a coarse grid Z

SIDNUR

[Poirriez 2011, Pichot et al. 2014]

- domain decomposition provided by the user
- coarse grid : signature of subdomains [Frank and Vuik 2001]
- C++ library
- mutual factorization of local Schur complements and local matrices
- management of floating subdomains
- numerical experiments with 3D fracture networks

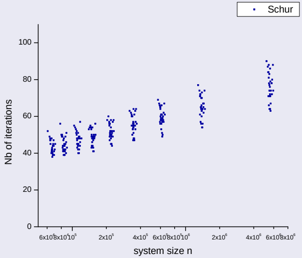
Experiments with SIDNUR

Flow computations in Discrete Fracture Networks

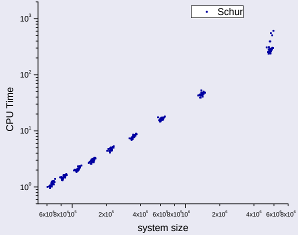
- random domain generated with MPFRAC software
- SPD sparse matrix
- solving with SIDNUR

[Poirriez 2011]

Number of iterations



CPU time

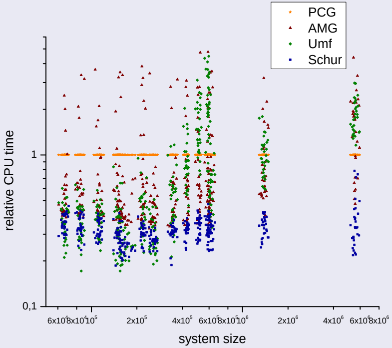


Comparing SIDNUR with other solvers

- UMFPACK: direct solver
- Boomer-AMG: algebraic multigrid
- PCG: Conjugate Gradient preconditioned by Boomer-AMG

[Poirriez 2011]

CPU time



Conclusion

GMRES

- DGMRES KSP module: deflation in GMRES(m) with or without Newton basis
- AGMRES KSP module: augmented Newton basis in GMRES(m)
- Deflation combined with Schwarz domain decomposition preconditioning
- Robustness: reduce the restarting effects and the domain decomposition effects
- Efficiency: increase granularity and scalability
- Numerical experiments with CFD problems: DGMRES and AGMRES faster than GMRES

PCG

- Deflation combined with Schur domain decomposition
- SIDNUR: Balancing Domain Decomposition
- Robustness: reduce the domain decomposition effects
- Efficiency: parallel Schur and Neumann Neumann computations
- Numerical experiments with 3D fracture networks: faster than multigrid and PCG
- Library soon available as free software