Parallel sparse linear solvers in the team SAGE

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Joint work with Désiré Nuentsa Wakam (GMRES)
and Baptiste Poirriez (PCG)

SAGE team, Inria Rennes, France

Workshop on linear solvers, organized by C2S@EXA, 23rd September 2013

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

- 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

⇒ 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)

⇒ 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

⇒ 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, ...]

Work in the team SAGE

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

[Nuentsa Wakam et al 2013 and to appear]

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Communication-avoiding strategy: Newton basis

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]

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

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

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

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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 a coarse subspace of basis U_r
- Build $\bar{M}^{-1} \equiv I_n + U_r(|\lambda_n| T^{-1} - I_r)U_r^T, \quad T = U_r^T B U_r$
- At each restart, update r and the basis U_r

Adaptive DGMRES(m,r)

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

Module DGMRES

- KSP module in Petsc library
- Distributed with Petsc
- Application to CFD problems [Nuentsa Wakam Pacull 2013]

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DGMRES combined with Domain Decomposition

Implementation in PETSc

Options for DGMRES accelerator

-ksp_type <dgmres>, -ksp_dgmres_eigen <1>, -ksp_dgmres_smv <0.5>, -ksp_gmres_restart <48, 64>, -ksp_maxit <1000>

ASM Preconditioner

ParMETIS partitioning, RAS preconditioner ($D = 16, 32, 64, 128$), overlap $= 1$, Sequential MUMPS in subdomains.

Cluster Parapide @ GRID'5000; 25 nodes (2 CPUs Intel@2.93GHz, 4 cores/CPU, 24GB RAM), Infiniband network

RM07R : $n = 381{,}689$; $nz = 37{,}464{,}962$

D	GMRES(48)		DGMRES(47,1)		GMRES(64)		DGMRES(63,1)		Memory (MB)
	Matvecs	Time	Matvecs	Time	Matvecs	Time	Matvecs	Time	
16	551	230	212	173.4	355	193.8	208	168.9	1,070
32	-	-	533	109.2	2217	244.6	455	94.6	513
64	-	-	410	56.8	-	-	453	50.8	299
128	-	-	791	51.5	-	-	638	44.3	225

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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

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

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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

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

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

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

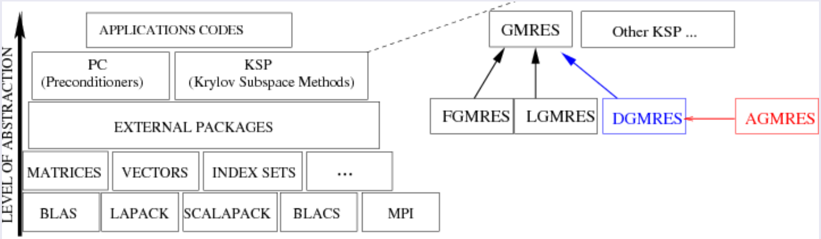
$$y_s = min_{y \in \mathbb{R}^s} \|\beta e_1 - \bar{H}_s y\|_2$$

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

AGMRES in PETSc

New KSP type : AGMRES

figure



LEVEL OF ABSTRACTION

APPLICATIONS CODES

PC (Preconditioners)

KSP (Krylov Subspace Methods)

EXTERNAL PACKAGES

MATRICES | VECTORS | INDEX SETS | ...

BLAS | LAPACK | SCALAPACK | BLACS | MPI

GMRES | Other KSP ...

FGMRES | LGMRES | DGMRES | AGMRES

Usage in Petsc

- Use AGMRES just as GMRES
- $\Rightarrow$ 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, ...

AGMRES combined with Domain Decomposition

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.

Augmented Conjugate Gradient

PCG

- A Symmetric Positive Definite (SPD) matrix
- 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
- $A_c = Z^T AZ$ restriction of A nonsingular small matrix
- $P = I - AZA_c^{-1}Z^T$ and $P^T = I - ZA_c^{-1}(AZ)^T$
- $C_b = P^T M^{-1} P + ZA_c^{-1} Z^T$

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

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. DD21 proceedings to appear]

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

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