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Solving large sparse linear systems with a variable s-step GMRES preconditioned by DD

David Imberti and Jocelyne Erhel
Joint work with Désiré Nuentza Wakam (first part)

FLUMINANCE team, Inria Rennes, France

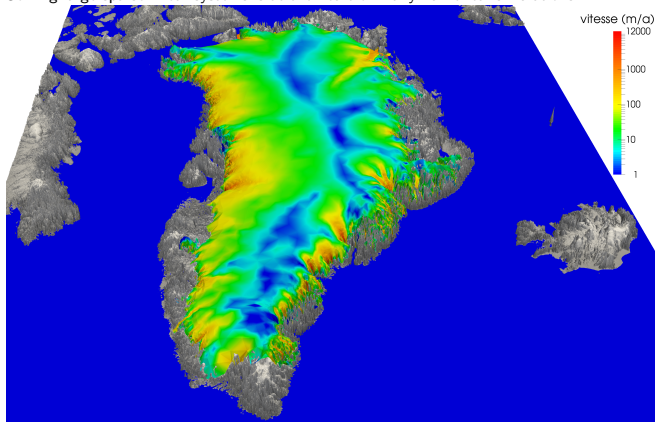


DD24

Longyearbyen - Svalbard, Norway, February 2017

Numerical simulations

Solving large sparse linear systems is at the heart of many numerical simulations



Simulation of the velocity field on the Greenland inlandsis, with Elmer/Ice model

Image : Fabien Gillet-Chaulet, CNRS and LGGE, Grenoble.

More information on the website [Interstices](#) for the general public

[["modéliser-et-simuler-la-fonte-des-calottes-polaires"](#), Nodet and JE, 2015]

FibGMRES

DI & JE
&DNW

GMRES

DGMRES
and
AGMRES

VGMRES

- 1 Krylov subspace algorithm GMRES
- 2 m -step preconditioned and deflated GMRES
- 3 Variable s -step algorithm VGMRES(m,s)

$$Ax = b, \quad A \in \mathbb{R}^{n \times n} \quad x, b \in \mathbb{R}^n \quad B = AM^{-1} \quad x_0 \in \mathbb{R}^n \quad r_0 = b - Ax_0$$

GMRES(m): a Krylov subspace method

- [Saad and Schultz 1986, Meurant's book 1999, Saad's book 2003, Simoncini and Szyld 2007, JE 2011, ...]
- $\mathcal{K}_m(B, r_0) = \text{span}\{r_0, Br_0, \dots, B^{m-1}r_0\}$
- Find $x_m \in x_0 + M^{-1}\mathcal{K}_m(B, r_0)$ such that $\|r_m\|_2 = \|b - Bx_m\|_2 = \min_{x \in x_0 + M^{-1}\mathcal{K}_m(B, r_0)} \|b - Bx\|_2$

Building blocks of GMRES(m)

- Build an orthonormal basis V_{k+1} of the Krylov subspace \mathcal{K}_{k+1}
get the Arnoldi-like relation $BV_k = V_{k+1}H_k$ for $k = 1, \dots, m$
- Minimize the residual in the Krylov subspace
 $x = x_0 + M^{-1}V_k y$ implies $r = r_0 - BV_k y = V_{k+1}(\beta e_1 - H_k y)$
Solve the least-squares problem: $\min_{y \in \mathbb{R}^k} \|\beta e_1 - H_k y\|$
- Restart if not converged

$$x_0 = x_0 + M^{-1}V_m y_m$$

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Arnoldi process

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1:  $v_1 = r_0 / \|r_0\|_2$ 
2: for  $k = 1, m$  do
3:    $p = Bv_k$ 
4:   for  $i = 1 : k$  do
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$$BV_m = V_{m+1}H_m$$

Granularity issues in parallel algorithms

⇒ Communication-avoiding strategies

- Generate the basis vectors [Reichel 1990, Bai et al 1994]
- Orthogonalize the basis [JE 1995, Sidje 1997, Demmel et al 2011]
- Compute the basis block by block [De Sturler 1994, Hoemmen 2010]

Preconditioning issues

⇒ multilevel methods to deal with large systems

- Schwarz preconditioning [Atenekeng Kahou et al 2007, Dufaud+Tromeur-Dervout 2010, Giraud+Haidar 2009,...]
- 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)

⇒ deflation to recover possible loss of information

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

Strategy

Combine 'communication-avoiding' GMRES ... and Deflation ... and Domain Decomposition preconditioners [Nuentsa Wakam et al 2013, Nuentsa Wakam and Pacull 2013, Nuentsa Wakam and JE 2013]

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- Minimize the residual in the Krylov subspace
 $x = x_0 + M^{-1}V_my$ implies $r = r_0 - BV_my = V_{m+1}(\beta e_1 - H_mR_m^{-1}y)$
Solve the least-squares problem:

$$\min_{y \in \mathbb{R}^m} \|\beta e_1 - H_m R_m^{-1} y\|$$

- Alternative to minimize the residual in the Krylov subspace
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Computation of vectors w_k

- Monomial basis: $w_{k+1} = Bw_k$
- Newton basis: $\sigma_{k+1}w_{k+1} = (B - \alpha_{k+1}I)w_k$
where the shifts α_k are computed during a preliminary cycle of GMRES(m)
and scaling is done with σ_k
[Reichel 1990, Bai et al 1994, JE 1995, Nuentza Wakam and JE 2013]
- Chebyshev basis [Joubert+Carey 1992, Philippe+Reichel 2012]

Stability and parallelism issues

- the condition number of W_m increases with m
- Parallel performances increases with m

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 [Cai and Sarkis 1999, Efstathiou and Gander 2003]

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

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

Restarted GMRES(m)

- 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
[JE et al 1996; Burrage et al 1998; Moriya et al 2000, Nuentza Wakam et al 2013]:

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

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
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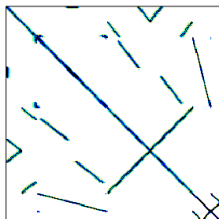
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FLUOREM matrices

- in MatrixMarket collection
- large, sparse, nonsymmetric matrices
- linearization of Navier-Stokes: symmetric profile with structured blocks

[Nuentsa Wakam+Pacull 2013]

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



Software

Krylov solvers integrated in Petsc
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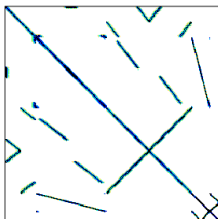
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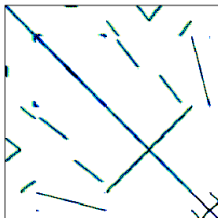
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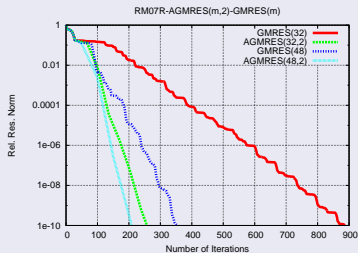
Krylov solvers integrated in Petsc

[Nuentsa Wakam 2011]

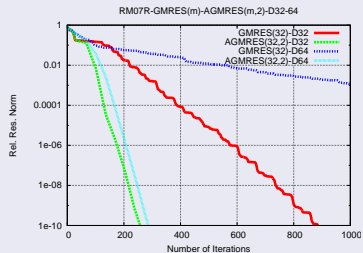
- Schwarz preconditioning combined with GMRES, Newton basis and deflation
- DGMRES: preconditioning deflation
- AGMRES: augmented subspace

Convergence with Augmented GMRES (AGMRES)

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

FibGMRES

DI & JE
&DNW

GMRES

DGMRES
and
AGMRES

VGMRES

Parallel CPU Time with AGMRES

FibGMRES

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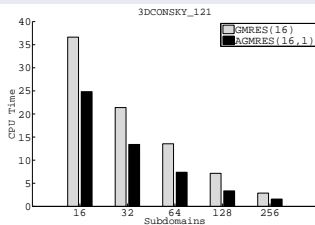
VGMRES

Convection-Diffusion test cases

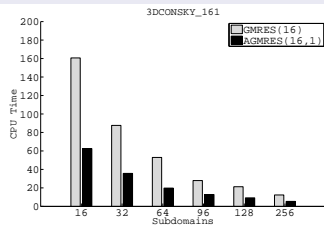
- 3DCONSKY_121 : size = 1,771,561; nonzeros = 50,178,241
- 3DCOSKY_161 : size= 4,173,281; nonzeros = 118,645,121

[Nuentsa Wakam and JE 2013]

3DCONSKY_121



3DCONSKY_161



- 1 Krylov subspace algorithm GMRES
- 2 m -step preconditioned and deflated GMRES
- 3 Variable s -step algorithm VGMRES(m,s)

Variable s step GMRES: VGMRES(m,s)

Variable block size s_j and Krylov size $l_1 = s_1, l_j = l_{j-1} + s_j, j \geq 2$

[Imberti and JE 2016]

- Build a basis W_j of the Krylov subspace \mathcal{K}_j for $1 \leq j \leq J$
- Build an orthonormal basis V_{j+1} of the Krylov subspace \mathcal{K}_{l_j+1}
get the Arnoldi-like relation $BW_j = V_{j+1}H_j$
- Minimize the residual in the Krylov subspace
 $x = x_0 + M^{-1}W_j y$ implies $r = r_0 - BW_j y = V_{j+1}(\beta e_1 - H_j y)$
Solve the least-squares problem:

$$\min_{y \in \mathbb{R}^j} \|\beta e_1 - H_j y\|$$

Test convergence at each step j

- Restart if not converged at step J with $l_j = m$

$$x_0 = x_0 + M^{-1}W_m y_m$$

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$$x_0 = x_0 + M^{-1}W_m y_m$$

Step j of VGMRES(m,s)

Initialization: $r_0 = b - Ax_0$, $\beta = \|r_0\|$, $v_1 = r_0/\beta$, $W_0 = \emptyset$, $V_1 = [v_1]$

Block j of size s_j , with $1 \leq j \leq J$

with an adaptive choice of s_j such that $s_j \leq s$

- First step: s_j matrix vector products
Compute the block C_j as a basis of $\mathcal{K}_{s_j}(B, u)$ with $u = v_{j-1+1}$
Compute the block BC_j
Parallel preconditioning $t = M^{-1}u$ then parallel matrix-vector product At
Define the Krylov basis by

$$W_j = [W_{j-1}, C_j]$$

- Second step: orthogonalization

$$BC_j = V_{j+1}S_j$$

RODDEC [Sidje 1997, JE 1995] or TSQR [Demmel et al 2011]

By induction, get the Arnoldi-like relation

$$[v_1, BW_j] = V_{j+1}R_{j+1}, BW_j = V_{j+1}H_j$$

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Condition number of BC_j and BW_j

- block basis

$$W_j = [C_1, C_2, \dots, C_j]$$

$$\kappa(BW_j) \geq \max_{1 \leq k \leq j} \kappa(BC_k)$$

- symmetric case: exponential growth of the condition number of a Krylov basis [Beckermann 2000]
- nonsymmetric case with $|\lambda_1| > |\lambda_2|$
monomial basis $C_j = \{u, Bu, \dots, B^{s_j-1}u\}$
[Imberti and JE 2016]

$$\kappa(BC_j) \geq \text{cste} |\lambda_1/\lambda_2|^{s_j-1}$$

Choice of the block size s_j

Objective: small condition numbers of the first blocks

- fixed sequence $s_j = s$: SGMRES(m,s)
[Hoemmen 2010, ...]
- adaptive increasing sequence s_j with $s_j \leq s$: VGMRES(m,s)
[Imberti and JE 2016]

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The number of messages is related to the number of steps J

Objective: reduce the number of steps

Number of steps

- SGMRES(m,s): $J = m/s$ steps
- VGMRES(m,s): J steps with $l_J = m$ and $J = J_1 + J_2$
- FibGMRES(m,s): Fibonacci sequence capped at s

$$J_2 = O(m/s), J_1 = O(\log_{\phi}(s))$$

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$$J_2 = O(m/s), J_1 = O(\log_\phi(s))$$

Sequences with $m = 48$ and $s = 16$

j	1	2	3	4	5	6	7
s_j	1	2	3	5	8	13	16
l_j	1	3	6	11	19	32	48

Variable increasing block size for $m = 48$ and $s = 16$.

j	1	2	3	4	5	6	7
s_j	16	13	8	5	3	2	1
l_j	16	29	37	42	45	47	48

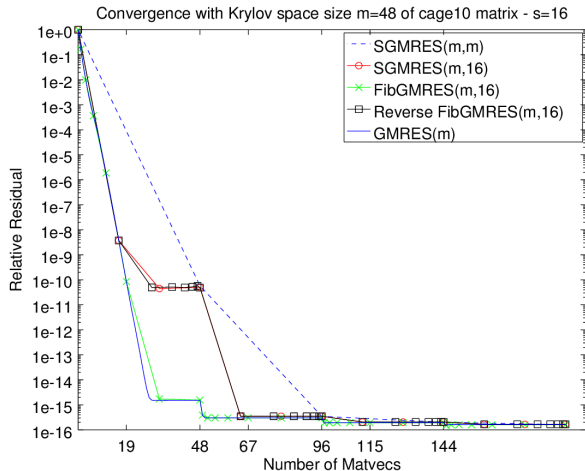
Variable decreasing block size for $m = 48$ and $s = 16$.

Numerical experiments done with a monomial basis

Numerical experiment with a small nonsymmetric matrix

Nonsymmetric matrix CAGE10 of size $n = 11397$ and nonzeros $nz = 150645$

Convergence curves with $m = 48$ and $s = 16$



FibGMRES

DI & JE
&DNW

GMRES

DGMRES
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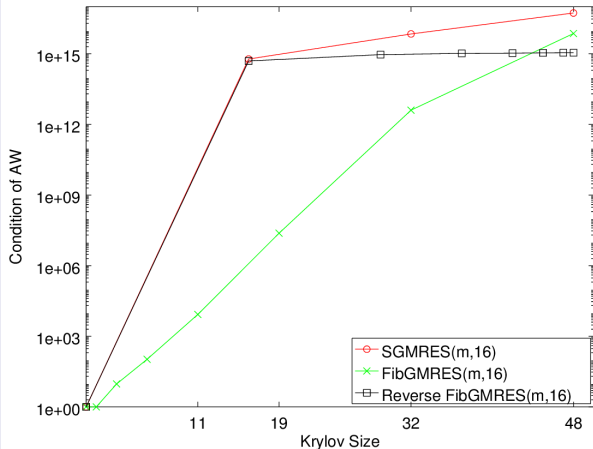
VGMRES

Numerical experiment with a small nonsymmetric matrix

Nonsymmetric matrix CAGE10 of size $n = 11397$ and nonzeros $nz = 150645$

Condition numbers of AW with $m = 48$ and $s = 16$

Condition for size $m=48$ of cage10 matrix - $s=16$



FibGMRES

DI & JE
&DNW

GMRES

DGMRES
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VGMRES

Sequences of FibGMRES(m,s) with $m = 96$

j	1	2	3	4	5	6	7	8	9	10
s_j	1	2	3	5	8	13	16	16	16	16
l_j	1	3	6	11	19	32	48	64	80	96

Variable increasing block size for $m = 96$ and $s = 16$

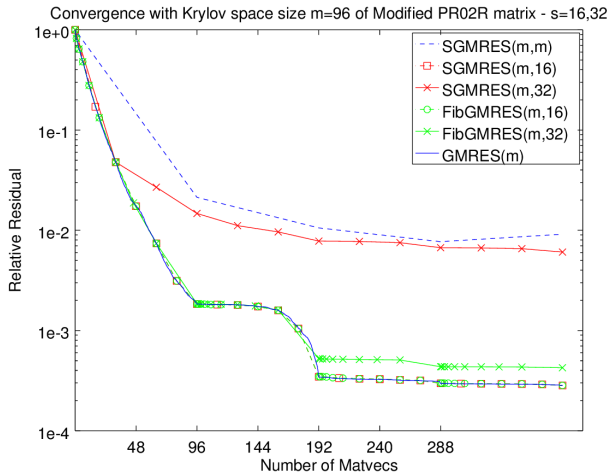
j	1	2	3	4	5	6	7	8	9
s_j	1	2	3	5	8	13	14	18	32
l_j	1	3	6	11	19	32	46	64	96

Variable increasing block size for $m = 96$ and $s = 32$

Numerical experiment with a large nonsymmetric matrix

Nonsymmetric matrix (PR02R + 1000 I) with $n = 161070$ and $nz = 8185136$

Convergence curves with $m = 96$ and $s = 16$ or $s = 32$



FibGMRES

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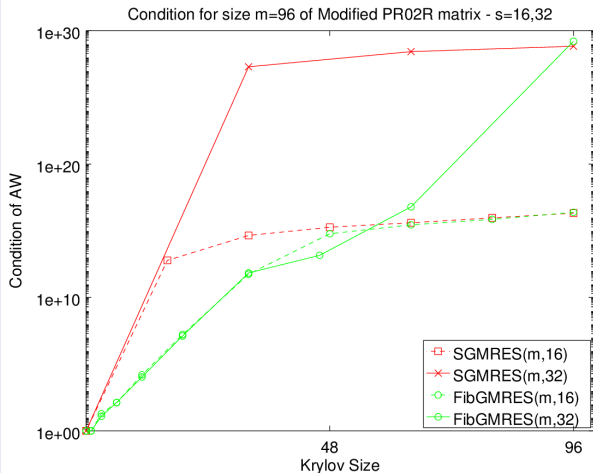
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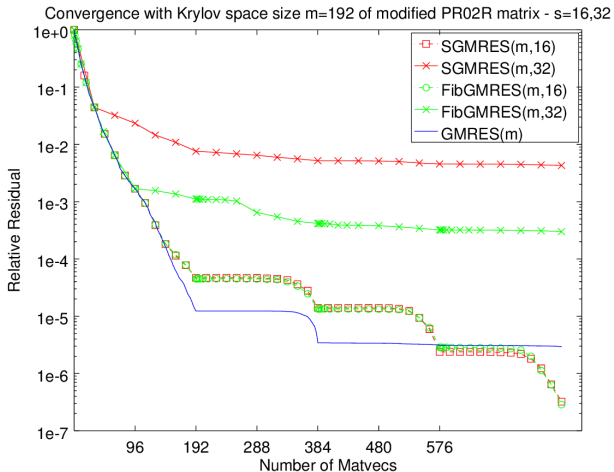
DGMRES
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Numerical experiment with a large restarting parameter

Nonsymmetric matrix (PR02R + 1000 I) with $n = 161070$ and $nz = 8185136$

Convergence curves with $m = 192$ and $s = 16$ or $s = 32$



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DI & JE
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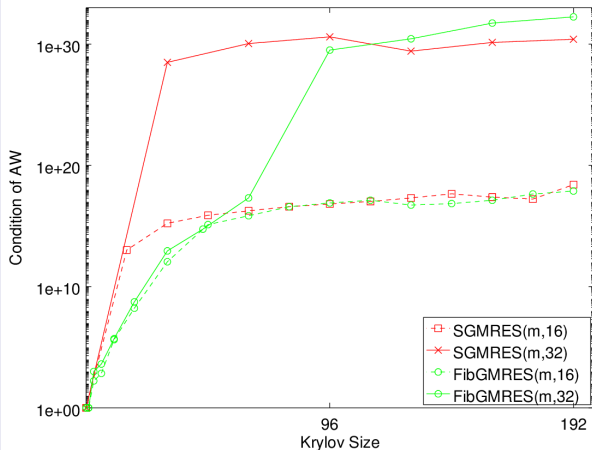
VGMRES

Numerical experiment with a large restarting parameter

Nonsymmetric matrix (PR02R + 1000 I) with $n = 161070$ and $nz = 8185136$

Condition numbers of AW with $m = 192$ and $s = 16$ or $s = 32$

Condition for size $m=192$ of modified PR02R matrix - $s=16,32$



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DGMRES(m,r) and AGMRES(m,r)

- Combined DD preconditioning with m -step GMRES and deflation
- Parallel efficiency and fast convergence with a large number of subdomains
- Difficult choice of the restarting parameter m

VGMRES(m,s) and FibGMRES(m,s)

- s -step algorithm combined with a variable block size s_j
- Relationship between convergence rate and condition numbers of the blocks
- Numerical experiments with a Fibonacci sequence

Future work

- Adaptive variation of s
- Blocks computed via a Newton basis
- Schwarz preconditioning with deflation
- Parallel computations

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