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## About Parallel Variants of GMRES Algorithm

Jocelyne Erhel

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## About Parallel Variants of GMRES Algorithm

Jocelyne Erhel

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

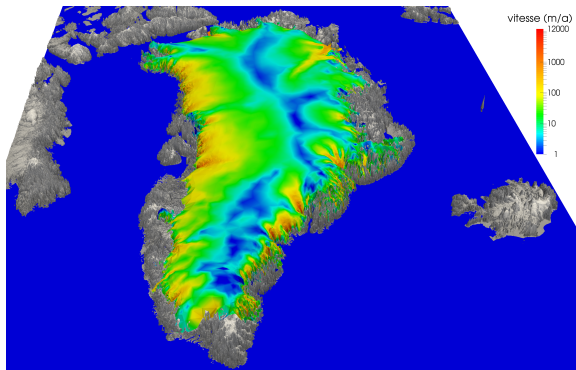
FLUMINANCE team, Inria Rennes, France



SIAM on Parallel Processing  
Tokyo, Japan, February 2018

# 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.  
website [Interstices](#) for the general public*

["Simulating the melting of ice caps", Nodet and JE,  
First prize of the second Mathematics of Planet Earth competition, 2017]

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 [Nuentsia 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 [Nuentsia Wakam et al 2013, Nuentsia Wakam and Pacull 2013, Nuentsia Wakam and JE 2013]

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- Build a basis  $W_{m+1}$  of the Krylov subspace  $\mathcal{K}_{m+1}$  such that  $BW_m = W_{m+1}T_{m+1}$
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[Nuentza Wakam and JE 2013, Hoemmen 2010]

- 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:

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

- 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  $\alpha_k$  are computed during a preliminary cycle of GMRES( $m$ )  
and scaling is done with  $\sigma_k$   
[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  
[Morgan 2000, 2002, Giraud et al 2010, Nuentza Wakam and JE 2013]

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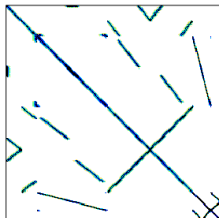
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## FLUOREM matrices

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

[Nuentsa Wakam and Pacull 2013]

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



## Software

Krylov solvers integrated in Petsc  
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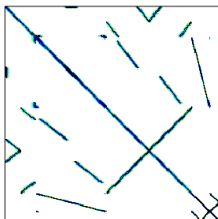
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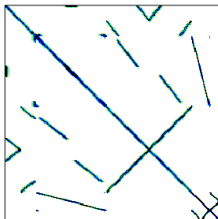


## FLUOREM matrices

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

[Nuentsa Wakam and Pacull 2013]

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



## Software

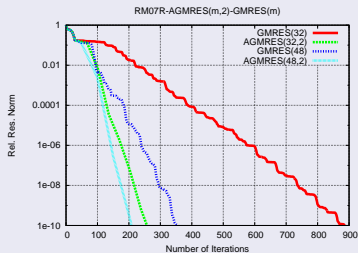
Krylov solvers integrated in Petsc

[Nuentsa Wakam 2011]

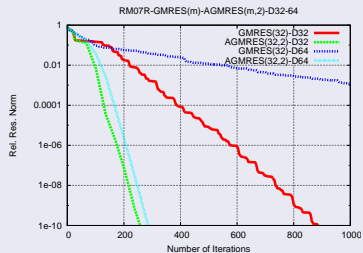
- Schwarz preconditioning combined with GMRES, Newton basis and deflation
- DGMRES: preconditioning deflation
- AGMRES: augmented subspace

# 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

DI & JE  
&DNW

GMRES

DGMRES  
and  
AGMRES

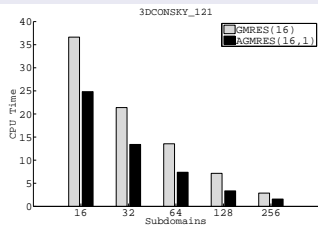
VGMRES

## Convection-Diffusion test cases

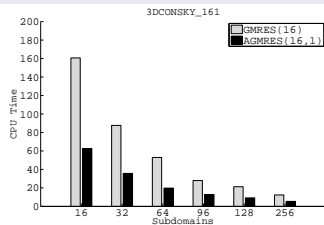
- 3DCONSKY\_121 : size = 1,771,561; nonzeros = 50,178,241
- 3DCOSKY\_161 : size= 4,173,281; nonzeros = 118,645,121

[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 2017]

- 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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FibGMRES

DI & JE  
&DNW

GMRES

DGMRES  
and  
AGMRES

VGMRES

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## 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 2017]

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

## 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 2017]

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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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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

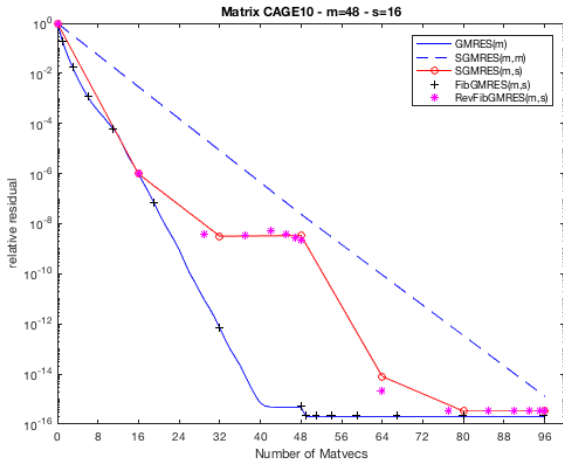
**Variable decreasing block size for  $m = 48$  and  $s = 16$ .**

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

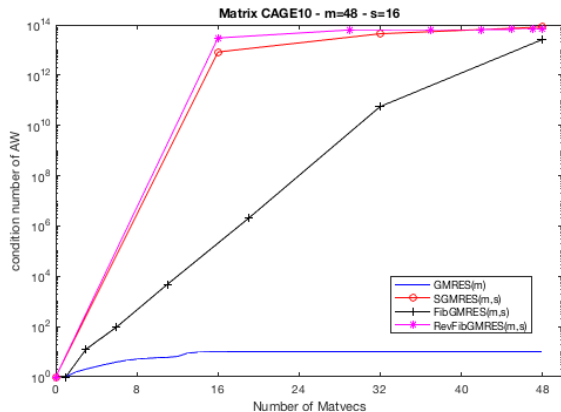
DGMRES  
and  
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DI & JE  
&DNW

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DGMRES  
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AGMRES

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  $s = 16$**

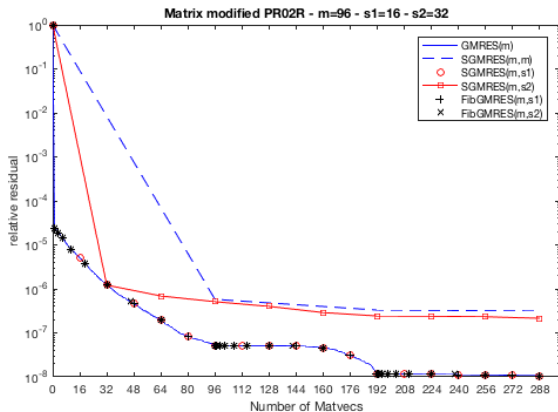
$j$	1	2	3	4	5	6	7	8	9
$s_j$	1	2	3	5	8	13	14	18	32
$l_j$	1	3	6	11	19	32	46	64	96

**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

DI & JE  
&DNW

GMRES

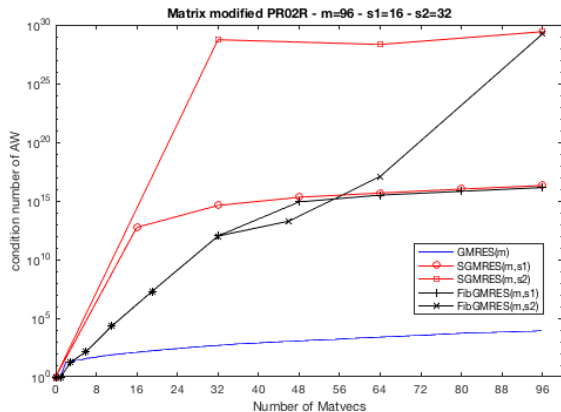
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FibGMRES

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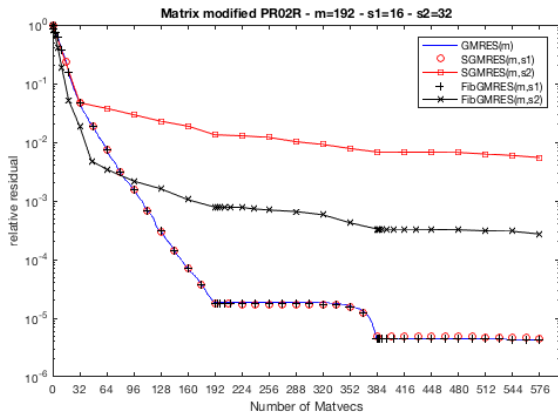
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Nonsymmetric matrix (PR02R + 1000 I) with  $n = 161070$  and  $nz = 8185136$

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

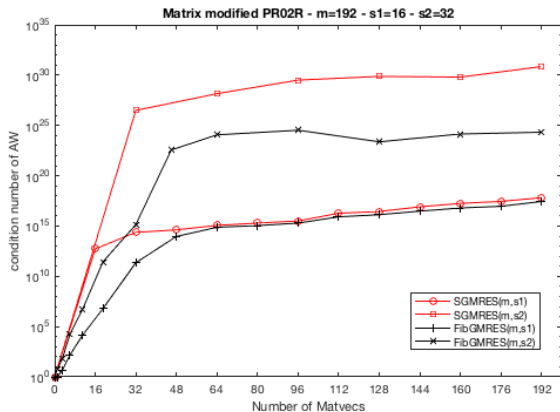




# Numerical experiment with a large restarting parameter

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



FibGMRES

DI & JE  
&DNW

GMRES

DGMRES  
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AGMRES

VGMRES

### 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 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
- Combined DD preconditioning with variable  $s$ -step GMRES and deflation
- Parallel computations

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