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GMRES preconditioned by a perturbed LDL^T decomposition with static pivoting

M. Arioli, I. S. Duff, S. Gratton, and S. Pralet
http://www.numerical.rl.ac.uk/people/marioli/marioli.html

Outline

- Multifrontal
- Static pivoting
- GMRES and Flexible GMRES
- Flexible GMRES: a roundoff error analysis
- GMRES right preconditioned: a roundoff error analysis
- Test problems
- Numerical experiments

Linear system

We wish to solve large sparse systems

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

where $\mathbf{A} \in \mathbf{R}^{\mathrm{N}\times\mathrm{N}}$ is symmetric indefinite

Linear system

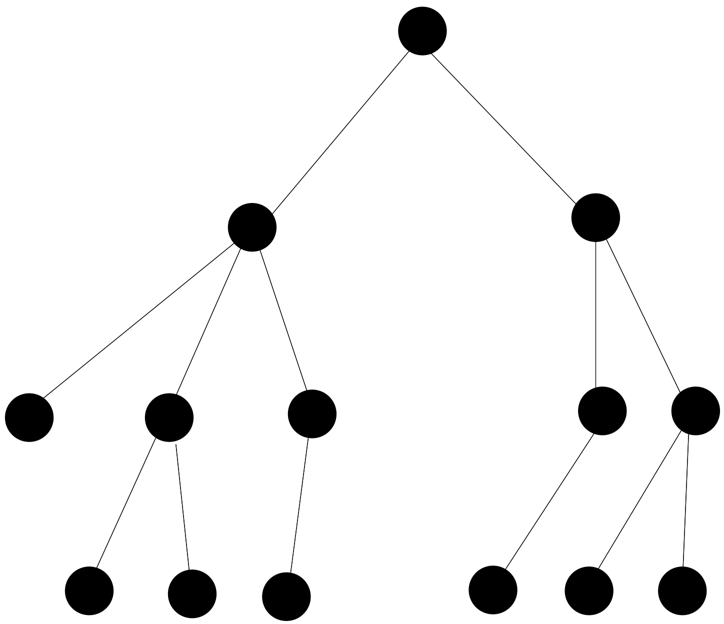
A particular and important case arises in saddle-point problems where the coefficient matrix is of the form

$$\begin{bmatrix} H & A \\ A^T & 0 \end{bmatrix}$$

Since we want accurate solutions, we would prefer to use a direct method of solution and our method of choice uses a multifrontal approach.

Multifrontal method

ASSEMBLY TREE



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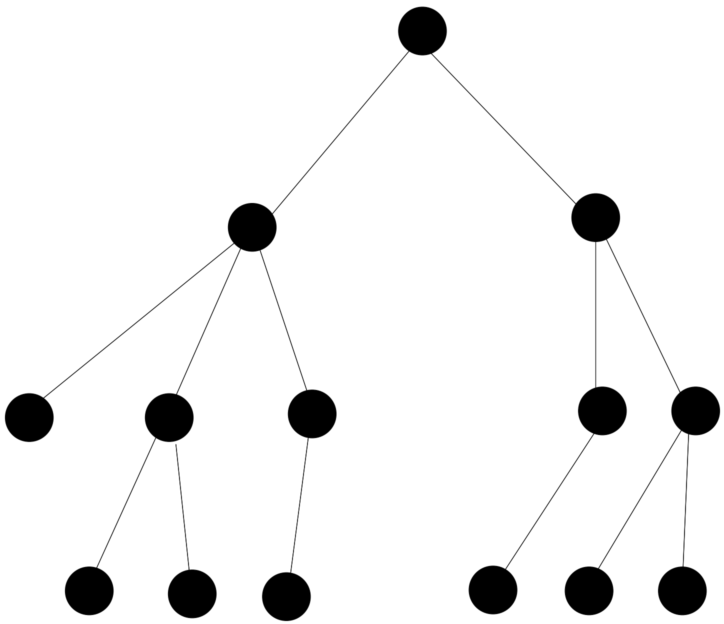
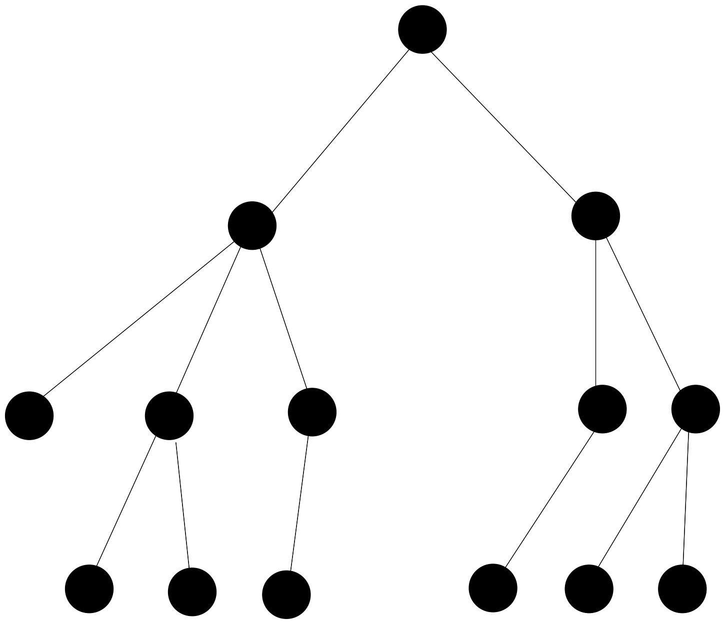


AT EACH NODE

$$\begin{array}{|c|c|} \hline F_{11} & F_{12} \\ \hline F_{12}^{T} & F_{22} \\ \hline \end{array}$$

Multifrontal method

ASSEMBLY TREE



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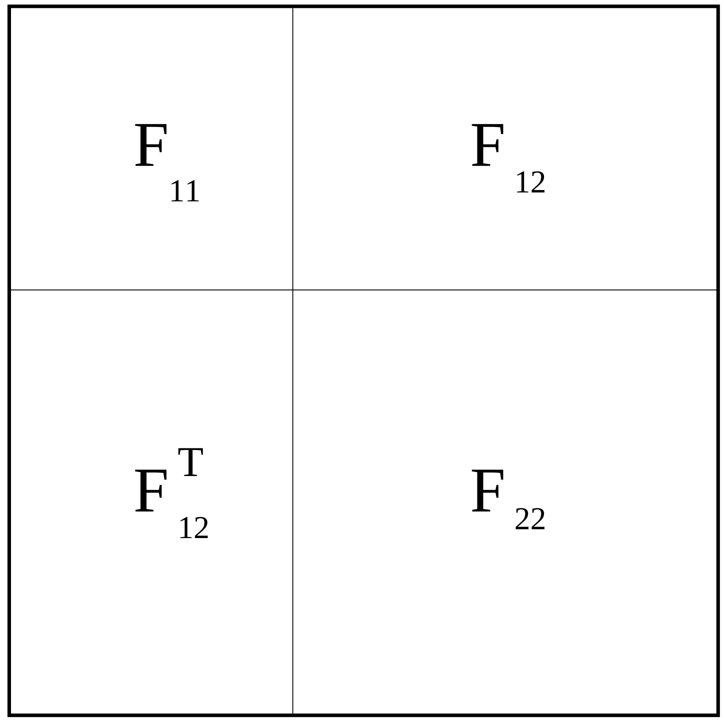
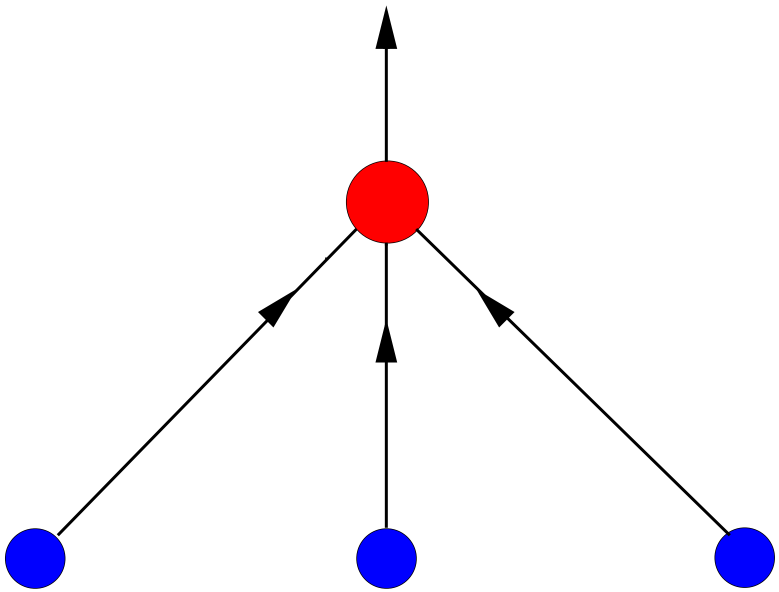


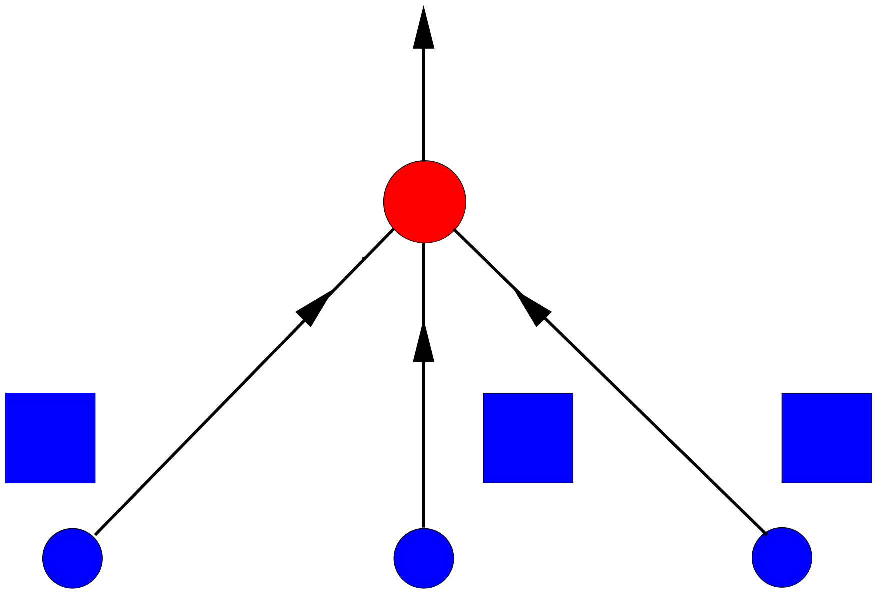
$$F_{22} \leftarrow F_{22} \; - \; F_{12}^{T} F_{11}^{-1} F_{12}$$

Multifrontal method



- From children to parent

Multifrontal method



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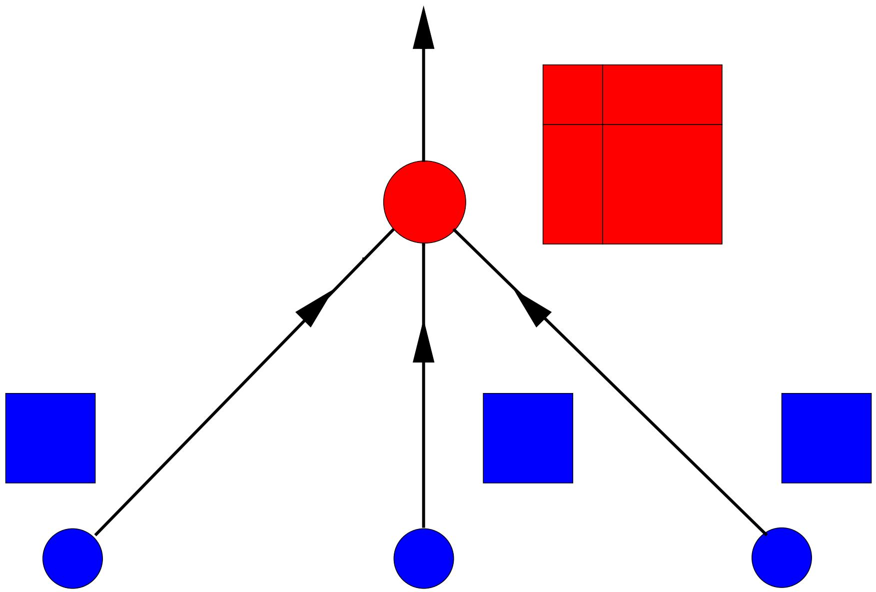
- **ASSEMBLY** Gather/Scatter operations (indirect addressing)

Multifrontal method



- From children to parent
- **ASSEMBLY** Gather/Scatter operations (indirect addressing)
- **ELIMINATION** Full Gaussian elimination, Level 3 BLAS (TRSM, GEMM)

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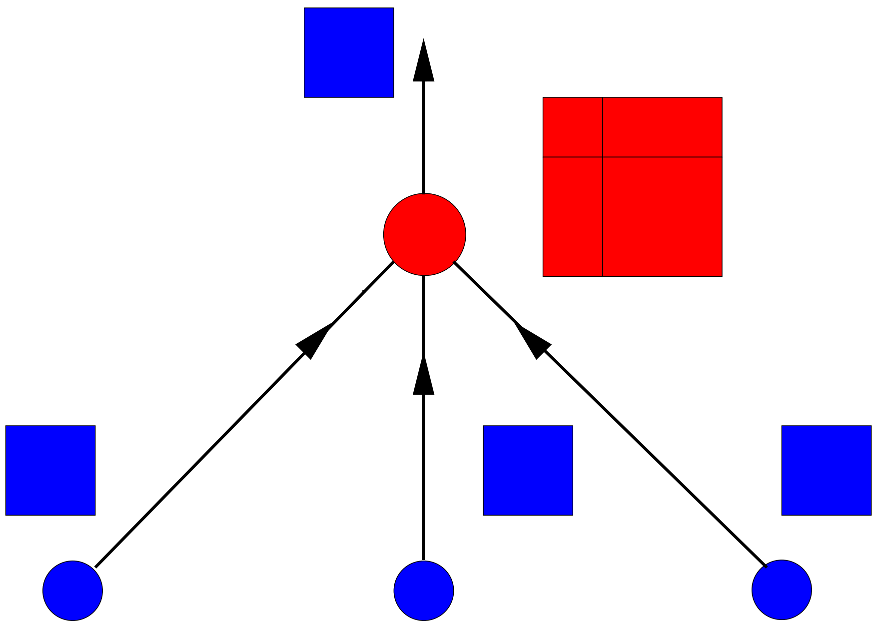

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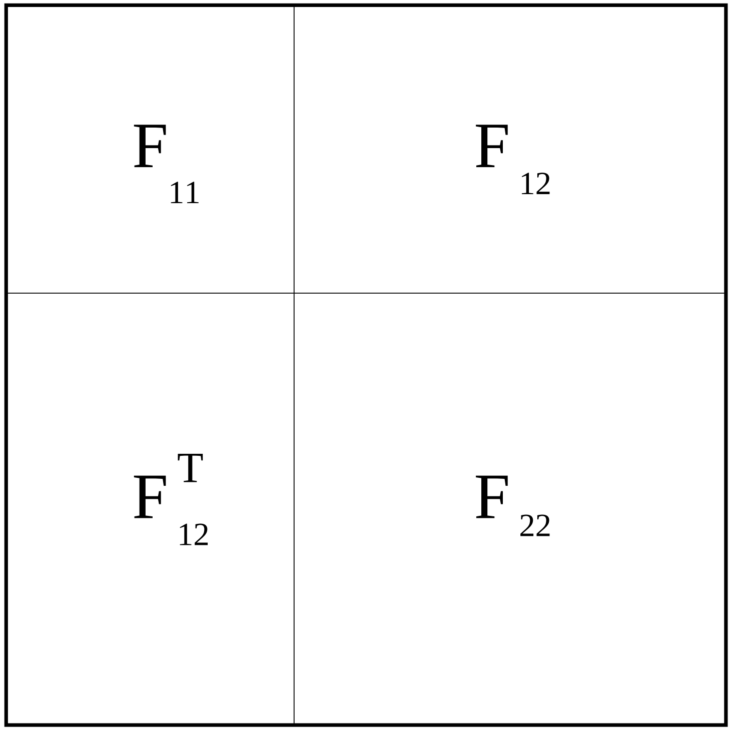
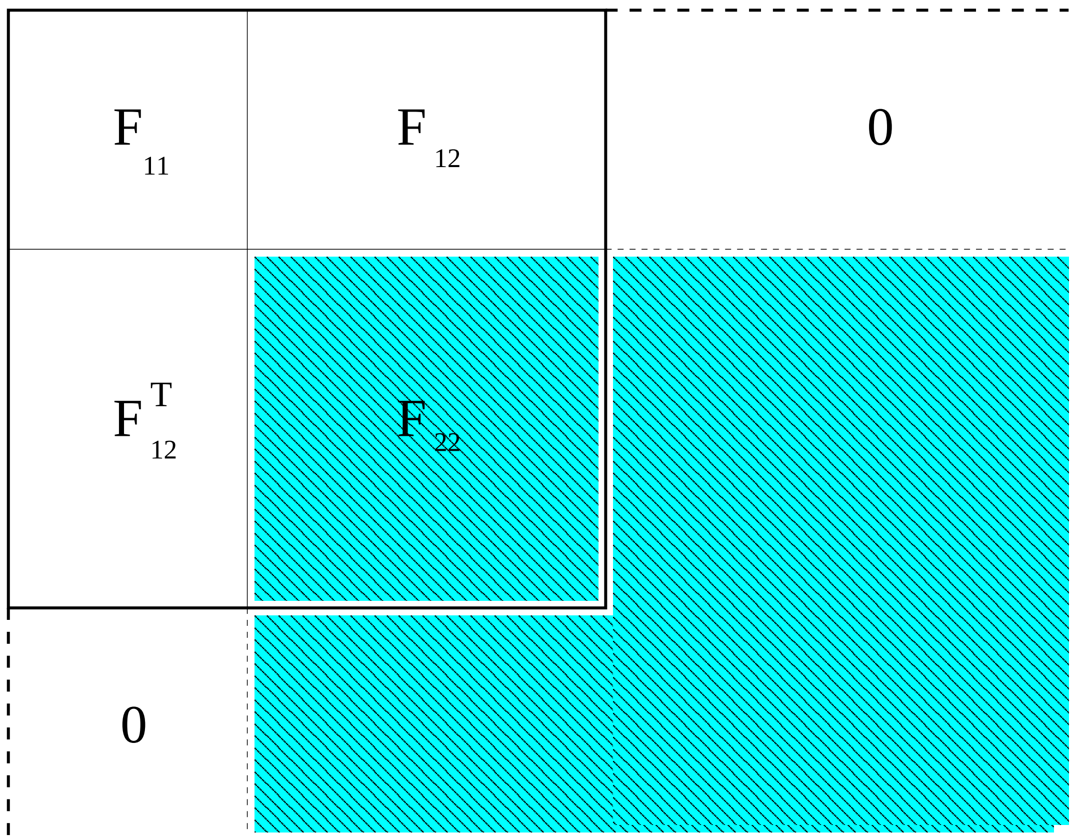


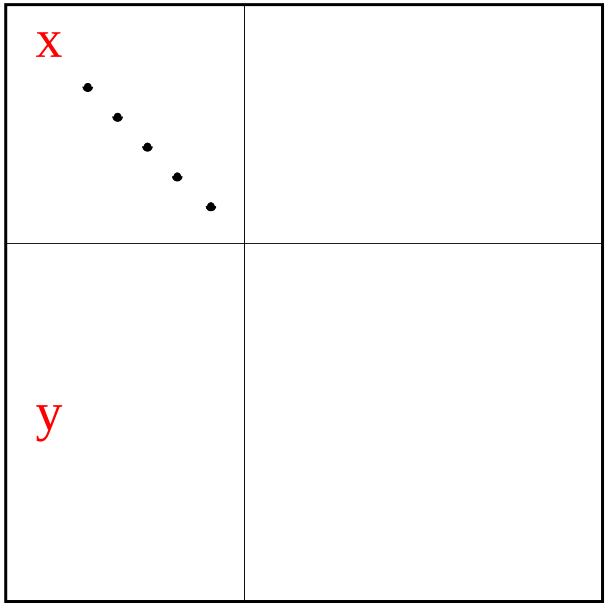
Pivot can only be chosen from F_{11} block since F_{22} is **NOT** fully summed.

Multifrontal method



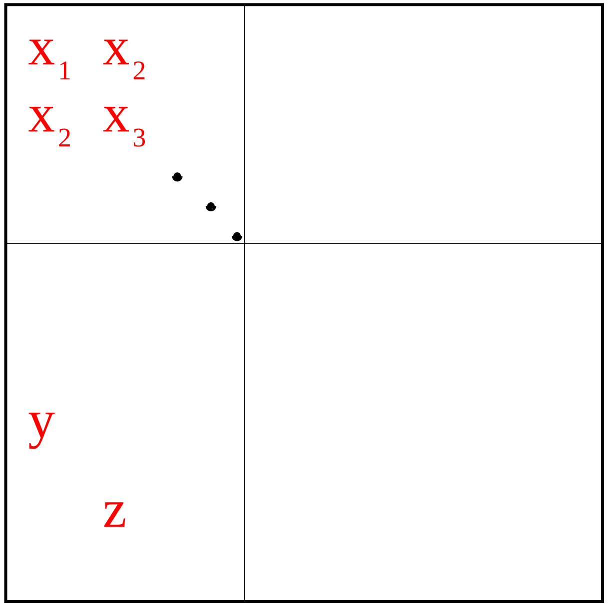
Situation wrt rest of matrix

Pivoting (1×1)



Choose x as 1×1 **pivot** if $|x| > u|y|$
where $|y|$ is the largest in column.

Pivoting (2×2)

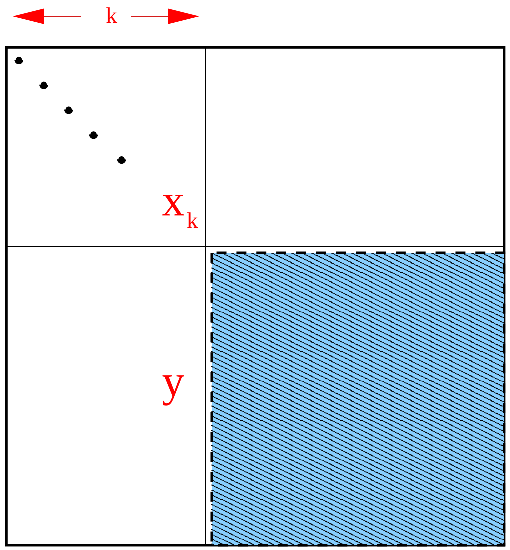


For the indefinite case, we can choose 2×2 **pivot** where we require

$$\left| \begin{bmatrix} x_1 & x_2 \\ x_2 & x_3 \end{bmatrix}^{-1} \right| \begin{bmatrix} |y| \\ |z| \end{bmatrix} \leq \begin{bmatrix} \frac{1}{u} \\ \frac{1}{u} \end{bmatrix}$$

where again $|y|$ and $|z|$ are the largest in their columns.

Pivoting



If we assume that $k-1$ pivots are chosen but $|x_k| < u|y|$:

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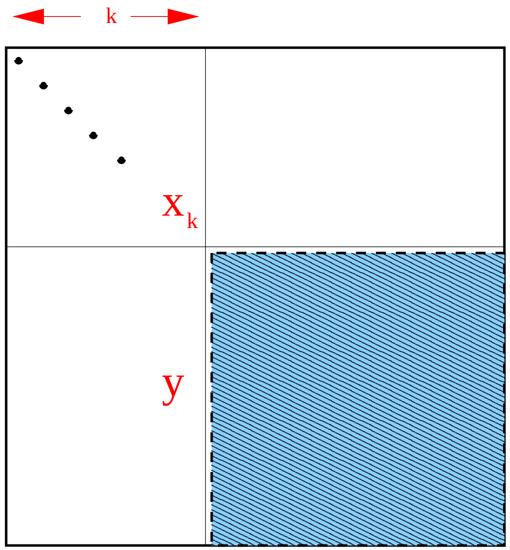

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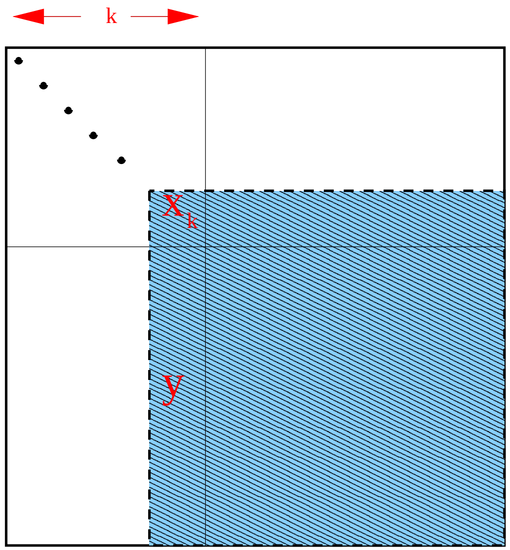

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- **DELAY** the pivot and then send to the parent a larger Schur complement.

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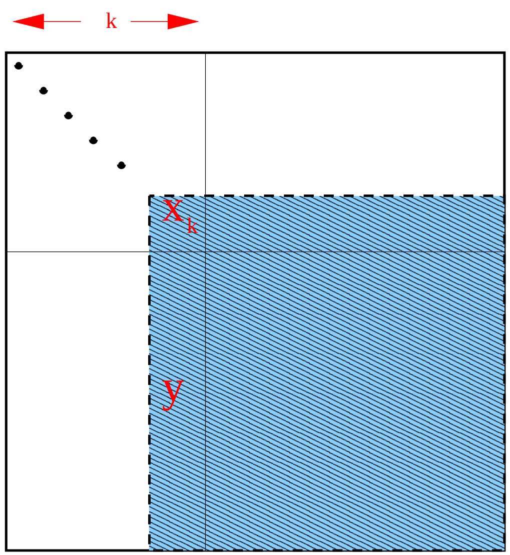

If we assume that $k-1$ pivots are chosen but $|x_k| < u|y|$:

- we can either take the **RISK** and use it or
- **DELAY** the pivot and then send to the parent a larger Schur complement.

This can cause more work and storage

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An **ALTERNATIVE** is to use **Static Pivoting**, by replacing x_k by

$$x_k + \tau$$

and CONTINUE.

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This is even more important in the case of parallel implementation where static data structures are often preferred

Static Pivoting

Several codes use (or have an option for) this device:

- SuperLU (Demmel and Li)
- PARDISO (Gärtner and Schenk)
- MA57 (Duff and Pralet)

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We thus have factorized

$$A + E = LDL^T = M$$

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The three codes then have an **Iterative Refinement** option.
IR will converge if $\rho(M^{-1}E) < 1$

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- $\approx \varepsilon \Longrightarrow$ big growth in preconditioning matrix M
- $\approx 1 \Longrightarrow$ huge error $||E||$.

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In real life $\rho(M^{-1}E) > 1$

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If $\rho(M^{-1}E) > 1$ then

PLAN A (Iterative Refinement Algortithm) fails!!!

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We have Plan B

GMRES and Flexible GMRES

Right preconditioned GMRES and Flexible GMRES

```
procedure [x] = right_Prec_GMRES(A,M,b)
    x_0 = M^{-1} b, r_0 = b − A x_0 and β = ||r_0||
    v_1 = r_0/β; k = 0;
    while ||r_k|| > μ(||b|| + ||A|| ||x_k||)
        k = k + 1;
        z_k = M^{-1} v_k; w = A z_k;
        for i = 1, . . . , k do
            h_{i,k} = v_i^T w ;
            w = w − h_{i,k} v_i;
        end for;
        h_{k+1,k} = ||w||;
        v_{k+1} = w/h_{k+1,k};
        V_k = [v_1, . . . , v_k];
        H_k = {h_{i,j}}_{1≤i≤j+1; 1≤j≤k};
        y_k = arg min_y ||β e_1 − H_k y||;
        x_k = x_0 + M^{-1} V_k y_k and r_k = b − A x_k;
    end while ;
end procedure.
```

```
procedure [x] =FGMRES(A,M_i,b)
    x_0 = M_0^{-1} b, r_0 = b − A x_0 and β = ||r_0||
    v_1 = r_0/β; k = 0;
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        end for;
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end procedure.
```

Roundoff error 1

The computed $\hat{L}$ and $\hat{D}$ in floating-point arithmetic satisfy

$$\begin{cases} A + \delta A + \tau E = M \\ ||\delta A|| \leq c(n)\varepsilon || \, |\hat{L}| \, |\hat{D}| \, |\hat{L}^T| \, || \\ ||E|| \leq 1. \end{cases}$$

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$\| \, |\hat{L}| \, |\hat{D}| \, |\hat{L}^T| \, \| \approx \frac{n}{\tau} \Longrightarrow \varepsilon \leq \frac{\tau^2}{n^2}$

Moreover, we assume that $\boxed{\max\{\|M^{-1}\|, \|\bar{Z}_k\|\} \leq \frac{\tilde{c}}{\tau}}$.

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   MGS applied to

$$C = (z_1, Az_1, Az_2, \dots)$$

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The first two stages of the roundoff error analysis are the same for both FGMRES and GMRES. the last two stages are specific to each one of the two algorithms.

Roundoff error FGMRES

Theorem 1.

$$\sigma_{\mathit{min}}(\bar{H}_k) > c_7(k,1)\varepsilon||\bar{H}_k|| + \mathcal{O}(\varepsilon^2) \quad \forall k,$$

$$|\bar{s}_k| < 1 - \varepsilon, \ \forall k,$$

(where $\bar{s}_k$ are the sines computed during the Givens algorithm)

and

$$2.12(n+1)\varepsilon < 0.01 \text{ and } 18.53\varepsilon n^{\frac{3}{2}}\kappa(C^{(k)}) < 0.1 \ \forall k$$

$$\exists \hat{k}, \qquad \hat{k} \leq n$$

such that, $\forall k \geq \hat{k}$*, we have*

$$||b - A\bar{x}_k|| \leq c_1(n,k)\varepsilon\Big(||b|| + ||A||\,||\bar{x}_0|| + ||A||\,||\bar{Z}_k||\,||\bar{y}_k||\Big) + \mathcal{O}(\varepsilon^2).$$

Roundoff error FGMRES

Moreover, if $M_i = M, \forall i$,

$$\rho = 1.3\, ||\hat{W}_k|| + c_2(k,1)\varepsilon ||M||\, ||\bar{Z}_k|| < 1 \quad \forall k < \hat{k},$$

where

$$\hat{W}_k = [M\bar{z}_1 - \bar{v}_1, \ldots, M\bar{z}_k - \bar{v}_k]\,,$$

we have:

$$||b - A\bar{x}_k|| \leq c(n,k)\gamma\varepsilon(||b|| + ||A||\, ||\bar{x}_0|| + ||A||\, ||\bar{Z}_k||\, ||M(\bar{x}_k - \bar{x}_0)||) + \mathcal{O}(\varepsilon^2)$$

$$\gamma = \frac{1.3}{1-\rho}.$$

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Roundoff error FGMRES

Theorem 2

Under the Hypotheses of Theorem 1, and

$$\boxed{\mathbf{c}(n)\varepsilon|| \, |\hat{L}| \, |\hat{D}| \, |\hat{L}^T| \, || < \tau}$$

$$\boxed{c(n,k)\gamma\varepsilon||A|| \, ||\bar{Z}_k|| < 1 \quad \forall k < \hat{k}}$$

$$\boxed{\max\{||M^{-1}||, ||\bar{Z}_k||\} \leq \frac{\tilde{c}}{\tau}}$$

we have

Roundoff error FGMRES

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$$\boxed{\max\{||M^{-1}||, ||\bar{Z}_k||\} \leq \frac{\tilde{c}}{\tau}}$$

we have

$$||b - A\bar{x}_k|| \leq 2\mu\varepsilon(||b|| + ||A||\,(||\bar{x}_0|| + ||\bar{x}_k||)) + \mathcal{O}(\varepsilon^2).$$

$$\mu = \frac{c(n,k)}{1 - c(n,k)\varepsilon||A||\,||\bar{Z}_k||}$$

Roundoff error right preconditioned GMRES

Theorem 3

We assume of applying Iterative Refinement for solving $M(\bar{x}_k - \bar{x}_0) = \bar{V}_k \bar{y}_k$ *at last step.*

Under the Hypotheses of Theorem 1 and $\boxed{c(n)\varepsilon\,\kappa(M) < 1}$

$$\exists \hat{k}, \qquad \hat{k} \leq n$$

such that, $\forall k \geq \hat{k}$*, we have*

$$\begin{aligned} ||b - A\bar{x}_k|| \leq \; & c_1(n,k)\varepsilon \Big\{ ||b|| + ||A||\,||\bar{x}_0|| + ||A||\,||\bar{Z}_k||\,||M(\bar{x}_k - \bar{x}_0)|| + \\ & ||AM^{-1}||\,||M||\,||\bar{x}_k - \bar{x}_0|| + \\ & ||AM^{-1}||\,||\,|\hat{L}|\,|\hat{D}|\,|\hat{L}^T|\,||\,||M(\bar{x}_k - \bar{x}_0)|| \Big\} + \mathcal{O}(\varepsilon^2). \end{aligned}$$

Roundoff error right preconditioned GMRES

As we did for FGMRES, if

$$\boxed{\mathbf{c}(n)\varepsilon \| \, |\hat{L}| \, |\hat{D}| \, |\hat{L}^T| \, \| < \tau}$$

Roundoff error right preconditioned GMRES

As we did for FGMRES, if

$$\mathbf{c}(n)\varepsilon || \, |\hat{L}| \, |\hat{D}| \, |\hat{L}^T| \, || < \tau$$

we can prove that $\exists k^*$ s.t $\forall k \geq k^*$ the right preconditioned GMRES computes a $\bar{x}_k$ s.t.

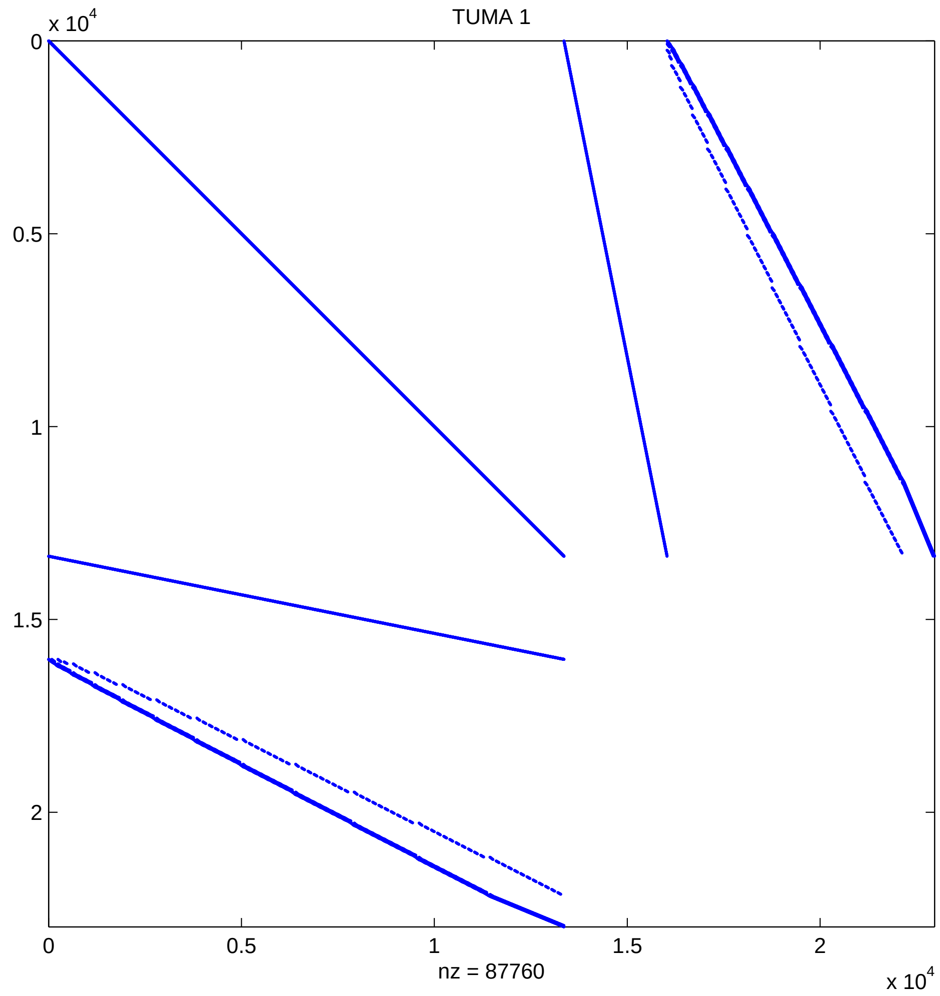
$$||b - A\bar{x}_k|| \leq \quad c(n,k)\,\varepsilon \Big[\, ||b|| + ||A|| \, ||\bar{x}_0|| + ||A|| \, ||\bar{Z}_k|| \, || \, M\,(\bar{x}_k - \bar{x}_0)|| + \\ || \, |\hat{L}| \, |\hat{D}| \, |\hat{L}^T| \, || \, ||M\,(\bar{x}_k - \bar{x}_0)|| \, \Big] + \mathcal{O}(\varepsilon^2).$$

Test Problems

	n	nnz	Description
CONT_201	80595	239596	KKT matrix Convex QP (M2)
CONT_300	180895	562496	KKT matrix Convex QP (M2)
TUMA_1	22967	76199	Mixed-Hybrid finite-element

Test problems

Test Problems: TUMA 1



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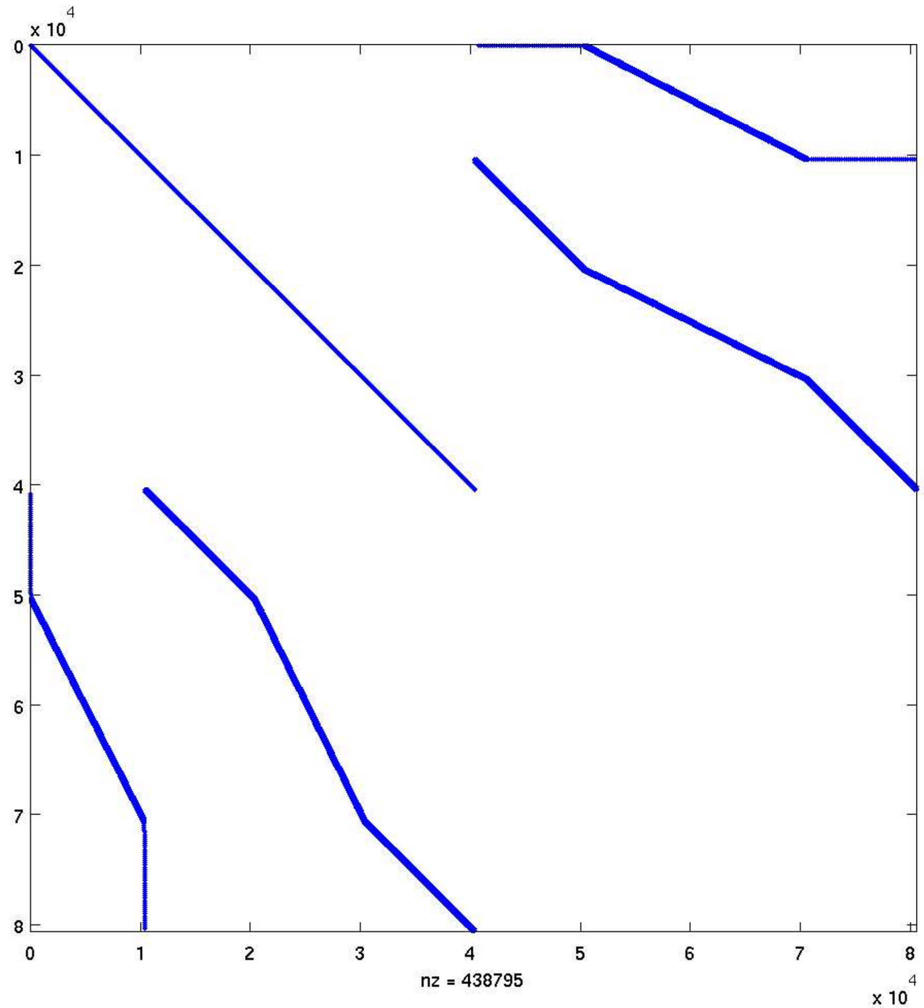
Test Problems: CONT-201



MA57 tests

	n	nnz(L)+nnz(D)	Factorization time
CONT_201	80595	9106766	9.0 sec
CONT_300	180895	22535492	28.8 sec

MA57 without static pivot

MA57 tests

	n	nnz(L)+nnz(D)	Factorization time
CONT_201	80595	9106766	9.0 sec
CONT_300	180895	22535492	28.8 sec

MA57 without static pivot

	nnz(L)+nnz(D)+ FGMRES (#it)	Factorization time	# static pivots
CONT_201	5563735 (6)	3.1 sec	27867
CONT_300	12752337 (8)	8.9 sec	60585

MA57 with static pivot $\tau = 10^{-8}$

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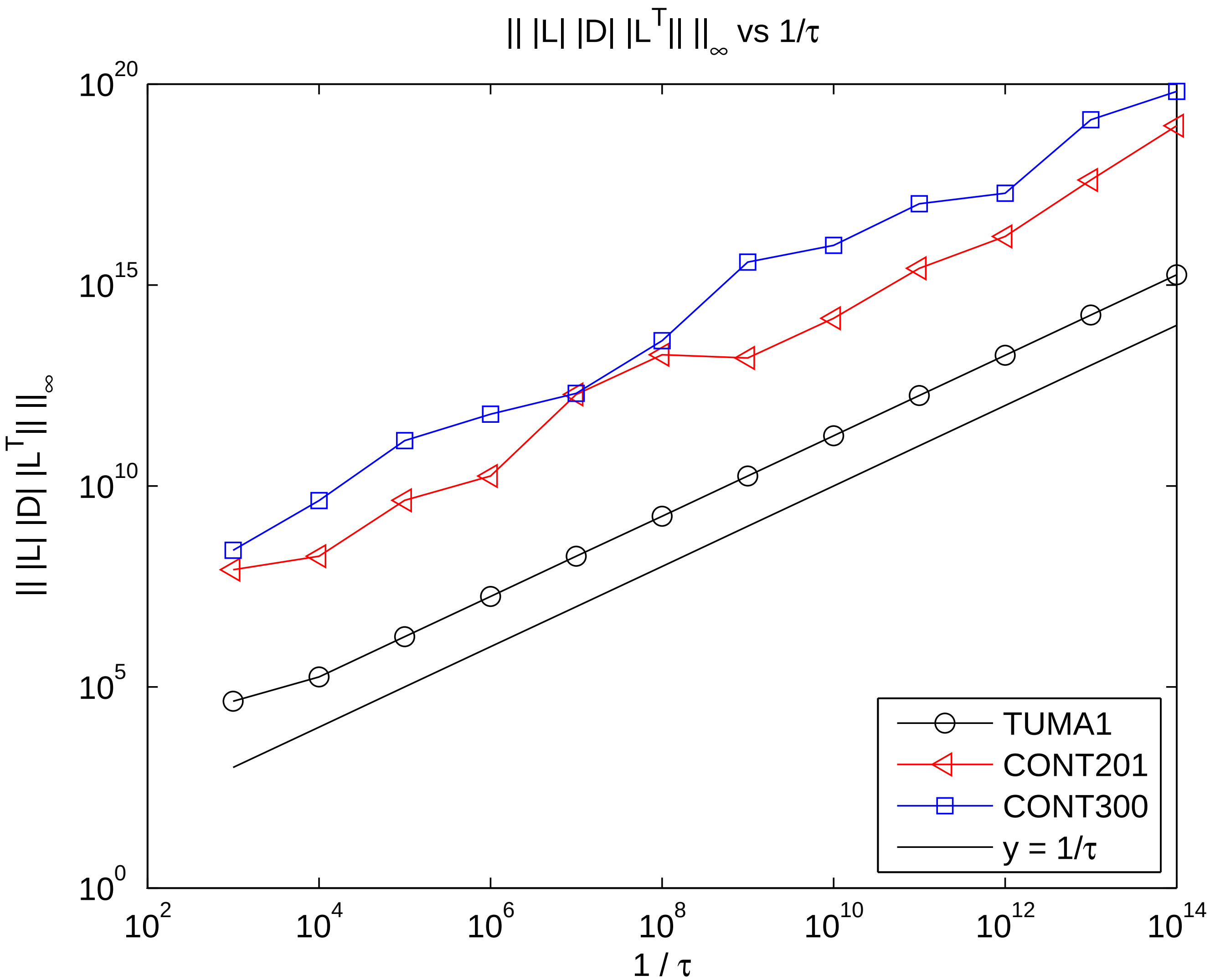
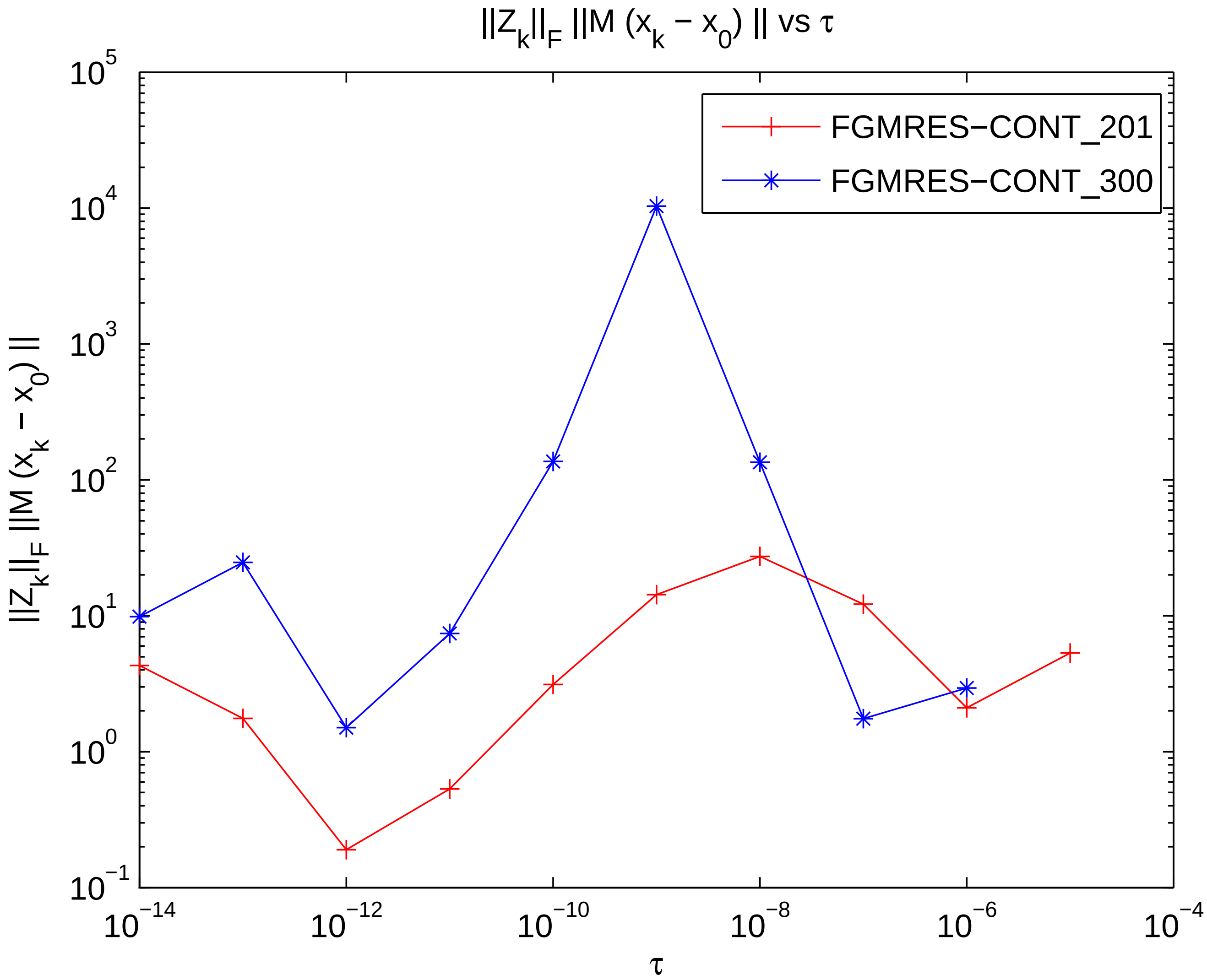
$\| \, |\hat{L}| \, |\hat{D}| \, |\hat{L}^T| \, \|$ vs $1/\tau$



$\|\bar{Z}_k\|_F \, \|M(x_k - x_0)\|$ vs τ



Numerical experiments: TUMA 1

	$\frac{\|\|b - A\bar{x}_k\|\|}{\|\|b\|\| + \|\|A\|\|\|\|\bar{x}_k\|\|}$				$\|\|M(\bar{x}_k - \bar{x}_0)\|\|$		
τ	IR	GMRES	FGMRES	$\|\|Z_k\|\|$	GMRES	FGMRES	$\|\|\,\|L\|\,\|D\|\,\|L^T\|\,\|\|$
1.0e-03	3.0e-03	1.0e-14	7.2e-17	1.2e+02	3.5e-03	3.5e-03	4.4e+04
1.0e-04	5.3e-17	1.8e-16	3.1e-17	4.7e+01	4.4e-04	4.4e-04	1.8e+05
1.0e-05	5.1e-17	1.3e-16	1.9e-17	4.4e+01	4.5e-05	4.5e-05	1.8e+06
1.0e-06	1.5e-16	1.3e-16	1.9e-17	4.4e+01	4.5e-06	4.5e-06	1.8e+07
1.0e-07	1.8e-17	1.2e-16	2.0e-17	4.3e+01	4.5e-07	4.5e-07	1.8e+08
1.0e-08	1.7e-17	1.3e-16	1.8e-17	4.3e+01	4.5e-08	4.5e-08	1.8e+09
1.0e-09	1.8e-17	2.8e-15	1.8e-17	2.6e+01	4.0e-08	4.0e-08	1.8e+10
1.0e-10	1.7e-17	4.2e-13	1.8e-17	8.8e+00	4.0e-07	4.0e-07	1.8e+11
1.0e-11	6.7e-17	1.0e-10	6.2e-17	6.8e+00	4.0e-06	4.0e-06	1.8e+12
1.0e-12	2.1e-17	1.0e-08	2.2e-17	3.2e+01	4.3e-05	4.3e-05	1.8e+13
1.0e-13	2.0e-17	2.4e-07	1.9e-17	1.3e+02	3.9e-04	3.9e-04	1.8e+14
1.0e-14	8.6e-17	8.6e-06	2.1e-17	1.8e+02	4.3e-03	4.3e-03	1.8e+15

TUMA 1 results

Numerical experiments: CONT_201

	$\frac{\|\|b - A\bar{x}_k\|\|}{\|\|b\|\| + \|\|A\|\|\|\|\bar{x}_k\|\|}$				$\|\|M(\bar{x}_k - \bar{x}_0)\|\|$		
τ	IR	GMRES	FGMRES	$\|\|Z_k\|\|$	GMRES	FGMRES	$\|\| \|L\| \|D\| \|L^T\| \|\|$
1.0e-03	4.0e-04	1.8e-05	9.8e-06	*	7.1e-04	1.5e-04	8.3e+07
1.0e-04	4.0e-05	2.0e-07	2.0e-07	*	1.5e-05	1.9e-05	1.8e+08
1.0e-05	3.5e-06	1.8e-12	1.1e-16	4.1e+05	5.9e-06	1.3e-05	4.4e+09
1.0e-06	3.5e-07	1.1e-11	2.1e-16	2.7e+06	7.8e-07	7.8e-07	1.8e+10
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1.0e-10	7.7e-17	3.2e-09	7.2e-17	3.4e+05	9.2e-06	9.2e-06	1.5e+14
1.0e-11	4.6e-17	2.1e-09	4.5e-17	1.9e+03	2.8e-04	2.8e-04	2.6e+15
1.0e-12	5.2e-17	4.5e-07	3.8e-17	2.0e+02	9.5e-04	9.5e-04	1.6e+16
1.0e-13	1.3e-16	1.3e-04	2.6e-16	1.6e+02	1.1e-02	1.1e-02	4.1e+17
1.0e-14	1.2e-03	2.3e-01	2.5e-14	4.3e+02	1.9e-02	1.0e-02	9.2e+18

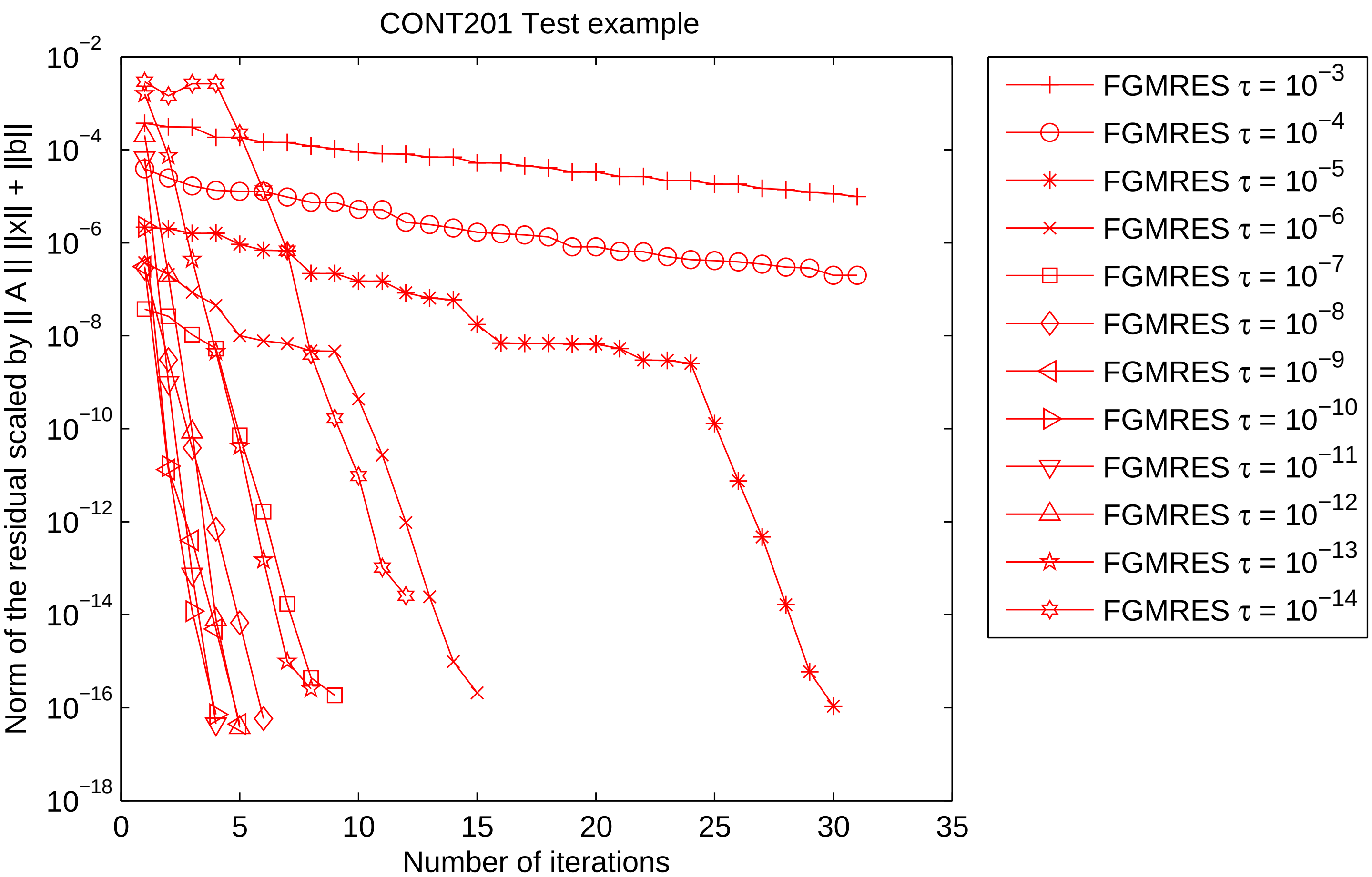
CONT_201 results

Numerical experiments: CONT_300

	$\frac{\|\|b - A\bar{x}_k\|\|}{\|\|b\|\| + \|\|A\|\|\|\|\bar{x}_k\|\|}$				$\|\|M(\bar{x}_k - \bar{x}_0)\|\|$		
τ	IR	GMRES	FGMRES	$\|\|Z_k\|\|$	GMRES	FGMRES	$\|\|\,\|L\|\,\|D\|\,\|L^T\|\,\|\|$
1.0e-03	3.8e-04	3.6e-05	2.5e-05	*	8.7e-04	1.3e-04	2.5e+08
1.0e-04	3.6e-05	5.5e-07	5.5e-07	*	6.5e-05	2.8e-05	4.3e+09
1.0e-05	4.3e-06	8.7e-09	8.7e-09	*	3.7e-06	6.1e-06	1.4e+11
1.0e-06	3.7e-07	6.9e-11	1.4e-16	3.0e+06	5.7e-07	9.8e-07	6.2e+11
1.0e-07	6.8e-08	2.1e-10	8.2e-17	7.6e+06	2.3e-07	2.3e-07	2.0e+12
1.0e-08	2.1e-09	1.4e-08	1.2e-16	7.5e+07	1.8e-06	1.8e-06	4.1e+13
1.0e-09	1.1e-16	1.6e-05	8.8e-17	3.7e+07	2.8e-04	2.8e-04	3.7e+15
1.0e-10	3.9e-17	6.8e-07	4.1e-17	3.8e+05	3.6e-04	3.6e-04	9.6e+15
1.0e-11	4.0e-17	1.6e-06	8.7e-17	1.4e+03	5.3e-03	5.3e-03	1.0e+17
1.0e-12	7.3e-17	1.1e-06	2.7e-16	1.5e+02	1.0e-02	1.0e-02	1.9e+17
1.0e-13	1.8e-16	3.4e-03	9.2e-16	1.3e+02	1.9e-01	1.9e-01	1.3e+19
1.0e-14	1.1e-15	1.4e-01	1.8e-14	2.1e+02	4.7e-02	4.7e-02	6.6e+19

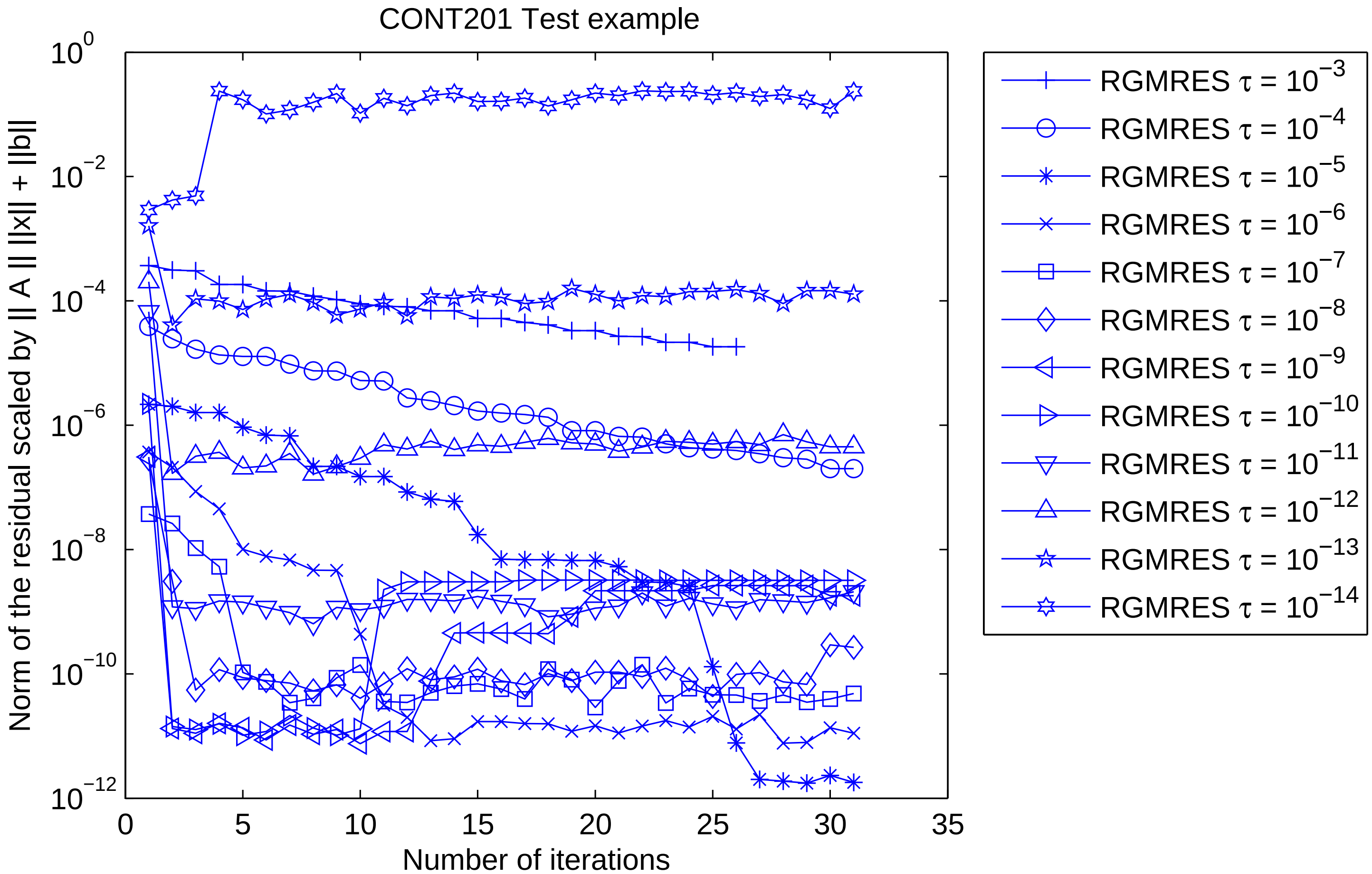
CONT_300 results

Numerical experiments



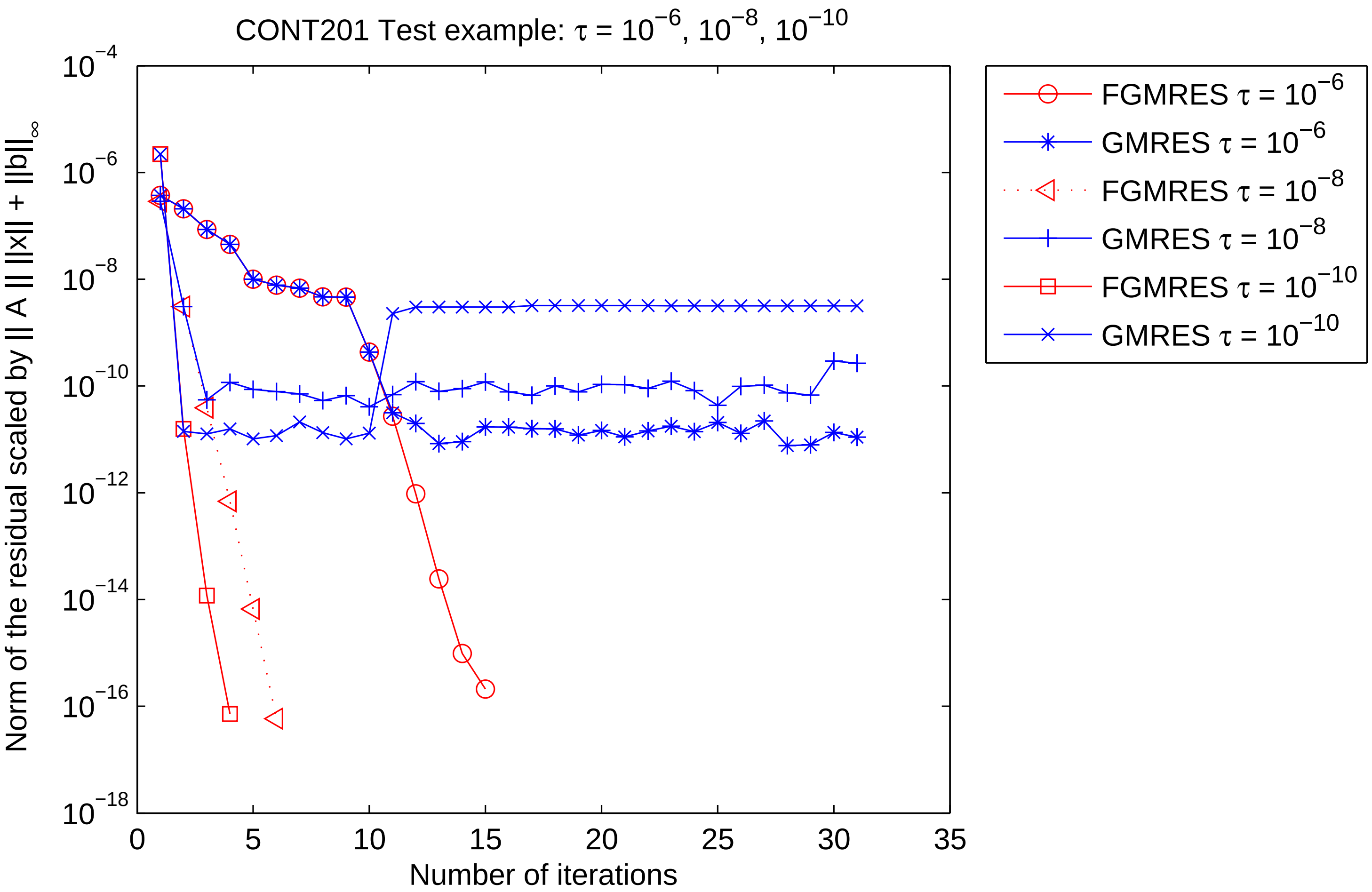
FGMRES on CONT-201 test example

Numerical experiments



GMRES on CONT-201 test example

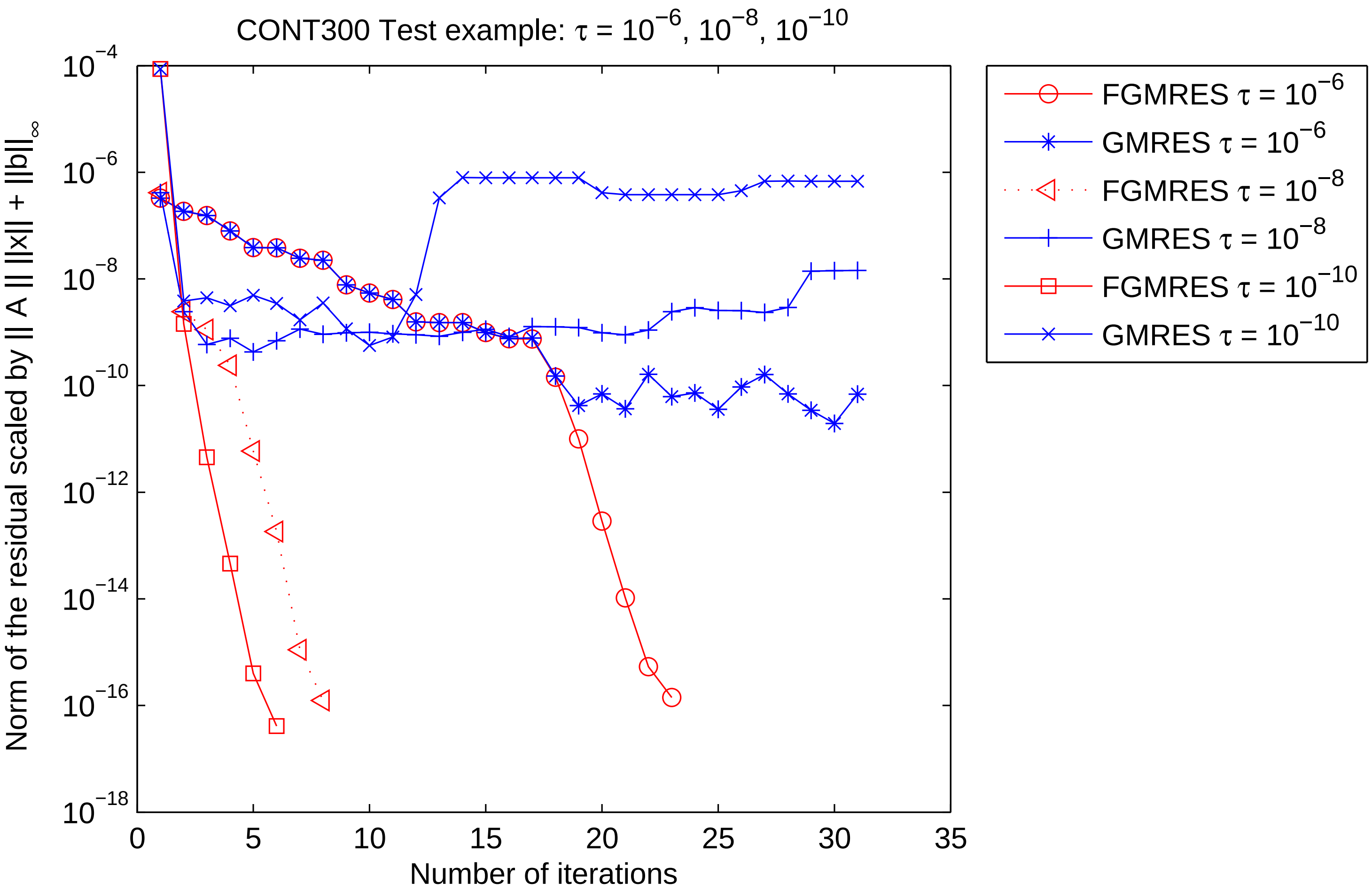
Numerical experiments



GMRES vs. FGMRES on CONT-201 test example:

$$\tau = 10^{-6}, 10^{-8}, 10^{-10}$$

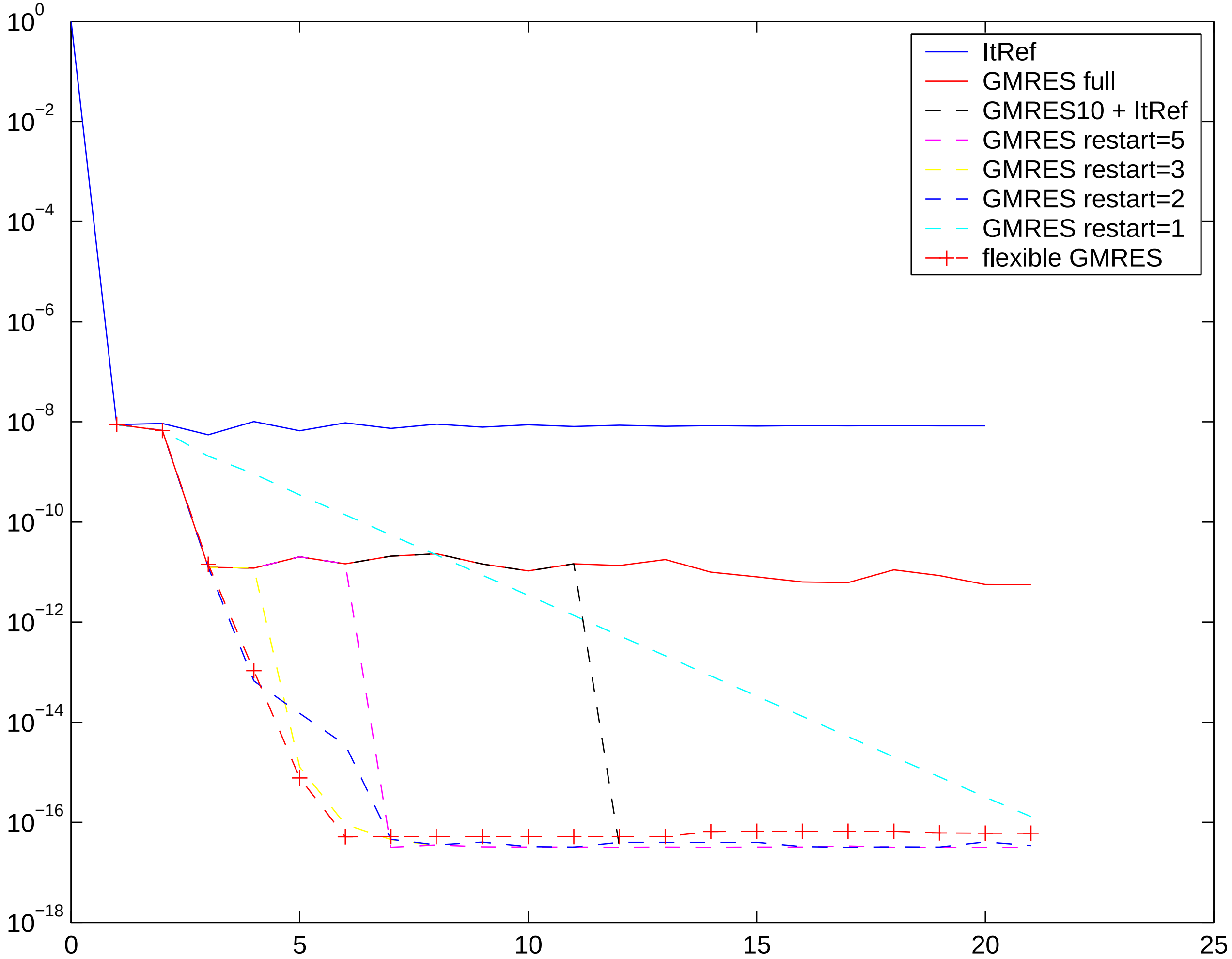
Numerical experiments



GMRES vs. FGMRES on CONT-300 test example:

$$\tau = 10^{-6}, 10^{-8}, 10^{-10}$$

Numerical experiments



Restarted GMRES vs. FGMRES on CONT-201 test example: $\tau = 10^{-8}$

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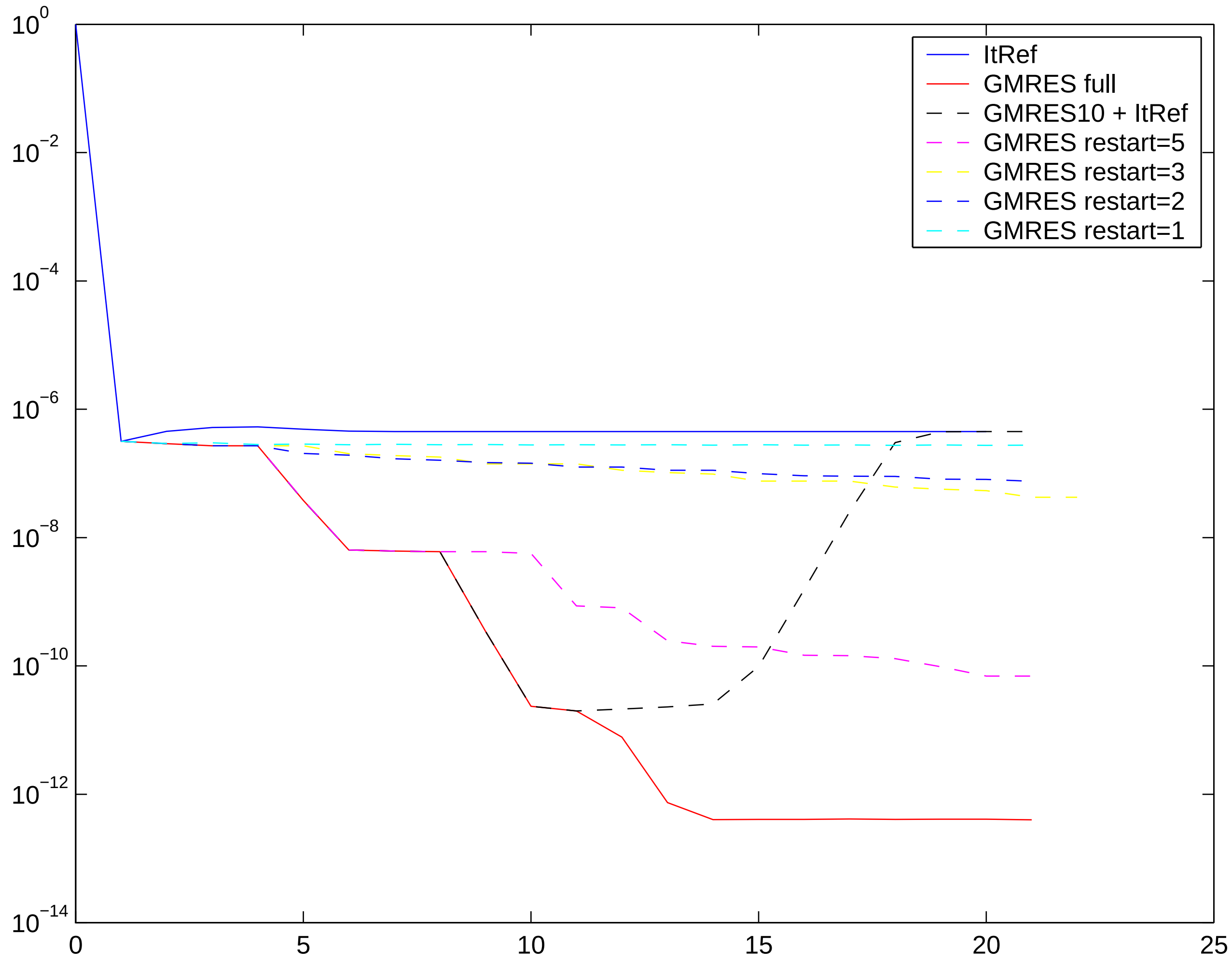
Numerical experiments



Restarted GMRES on CONT-201 test example: $\tau = 10^{-6}$

Summary

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- PLAN B is working