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

M. Arioli, I. S. Duff, S. Gratton, and S. Pralet

Outline

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

Linear system

We wish to solve large sparse systems

$$\mathbf{A}\mathbf{x} = \mathbf{b} \qquad \text{where } \mathbf{A} \in \mathbf{R}^{n\times n}$$

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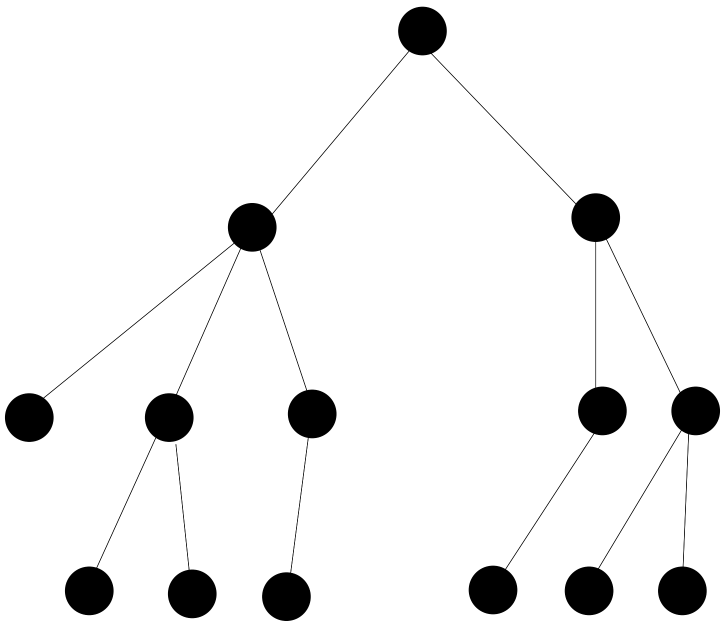
$$\mathbf{A}\mathbf{x} = \mathbf{b} \qquad \text{where } \mathbf{A} \in \mathbf{R}^{n\times n}$$

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

Multifrontal method

ASSEMBLY TREE



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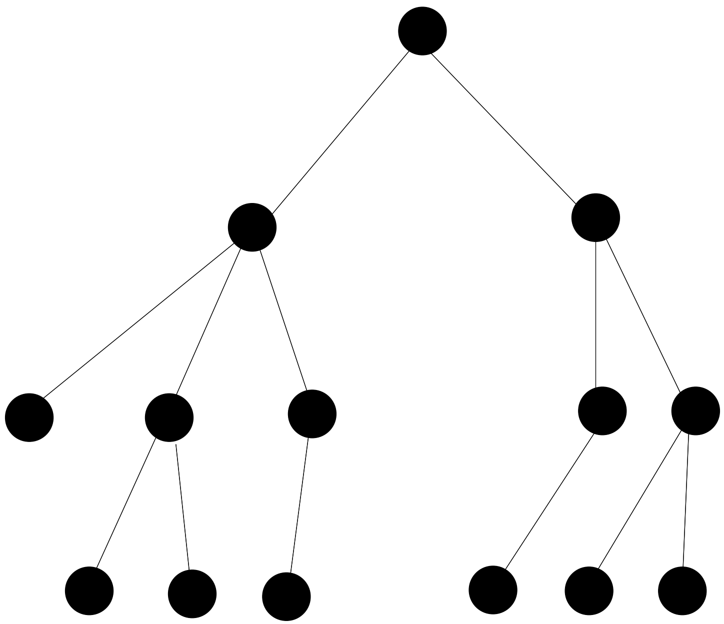
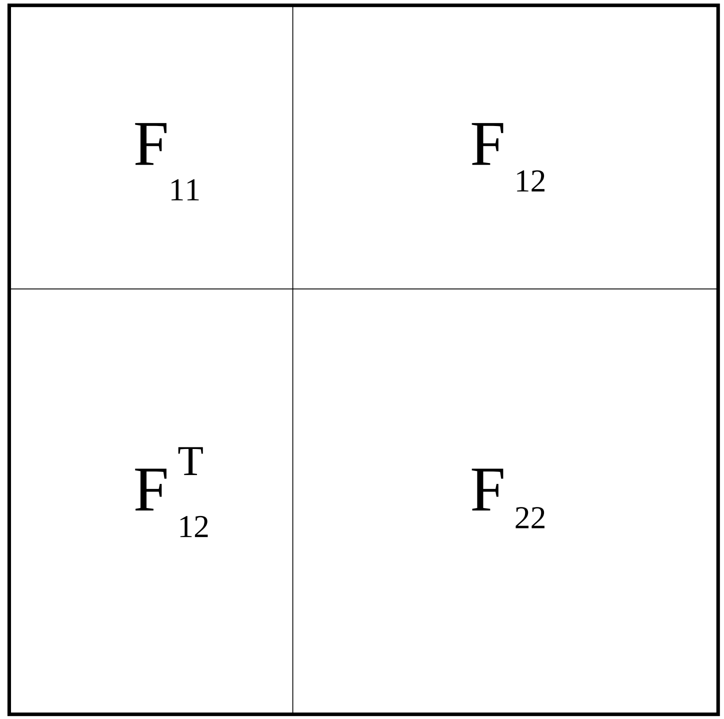


AT EACH NODE



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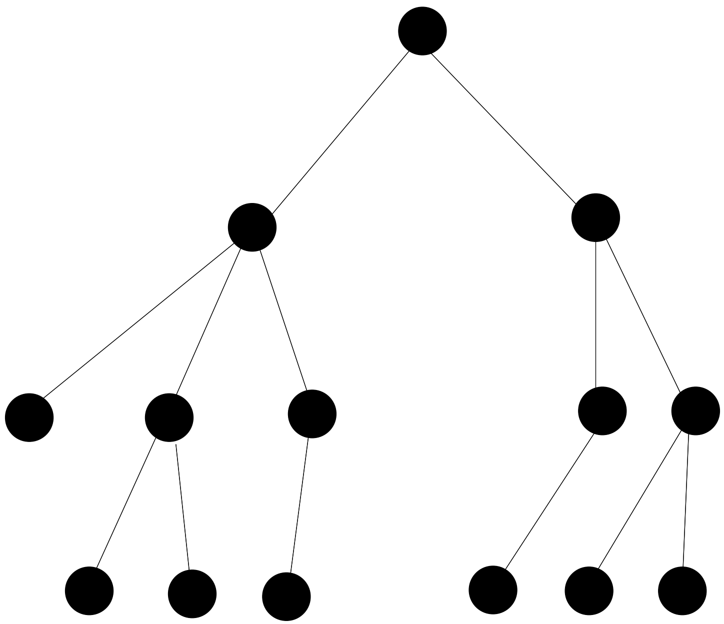

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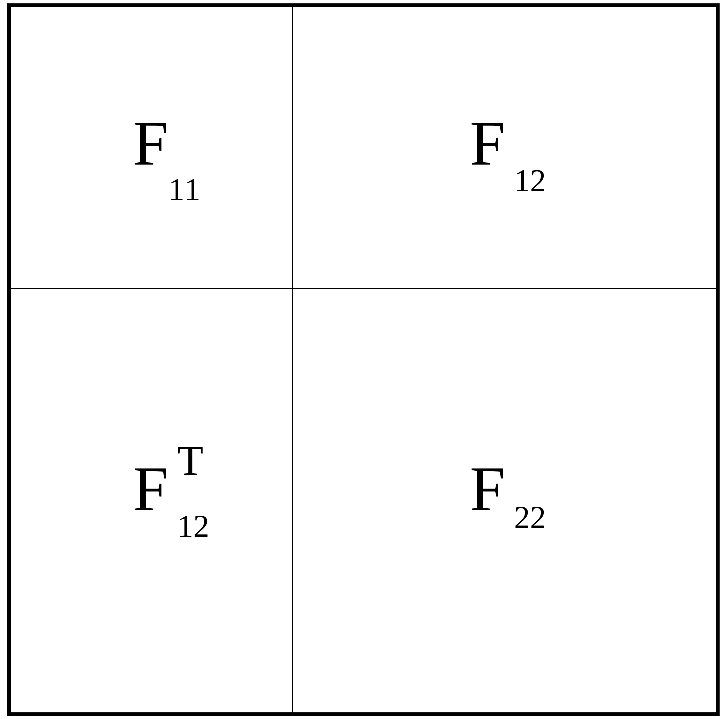
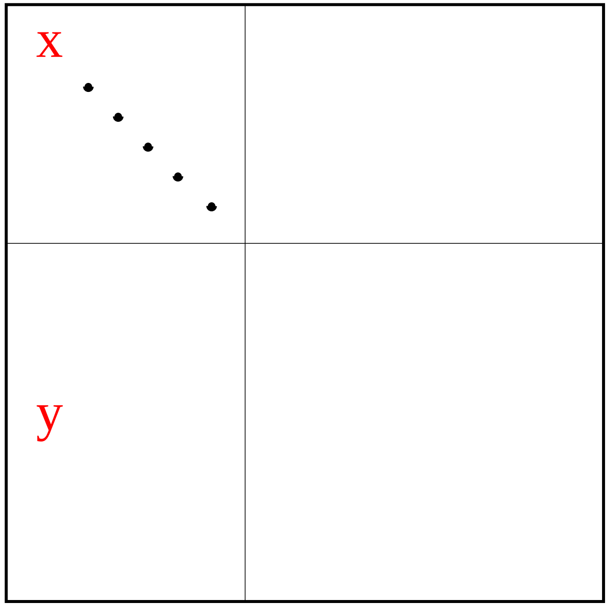


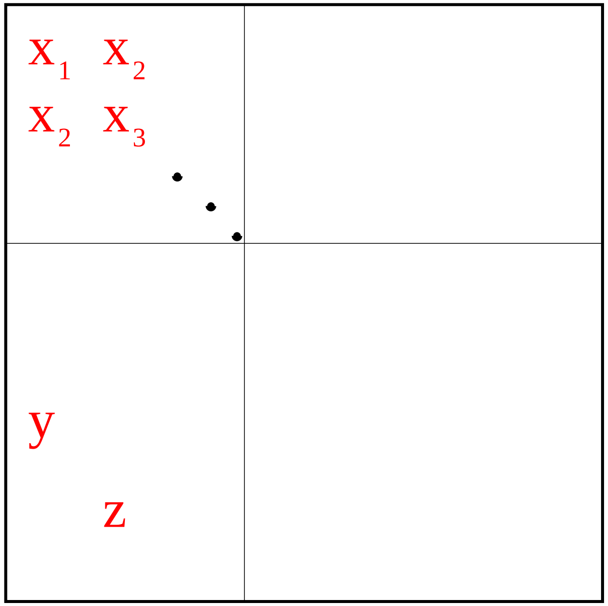
$$F_{22} \leftarrow F_{22} \; - \; F_{12}^T F_{11}^{-1} F_{12}$$

Pivoting (1×1)



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

Pivoting (2×2)

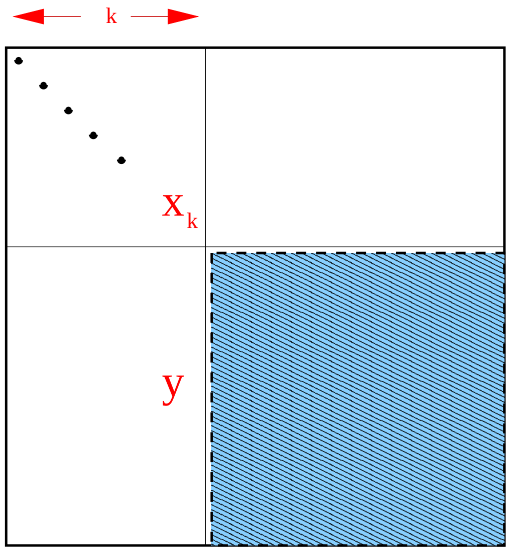


For the indefinite case, we can choose 2×2 **pivot** where we require

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

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

Pivoting



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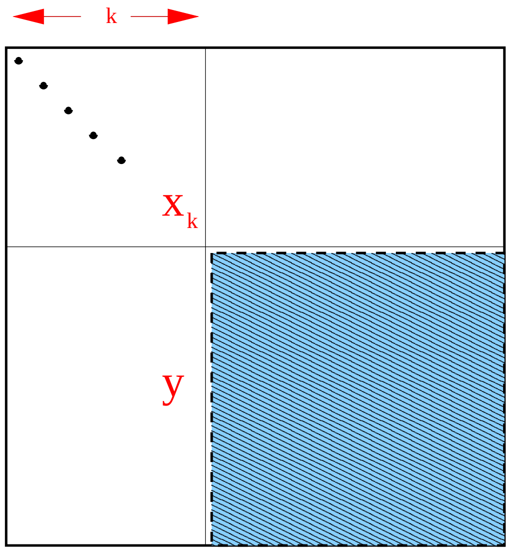

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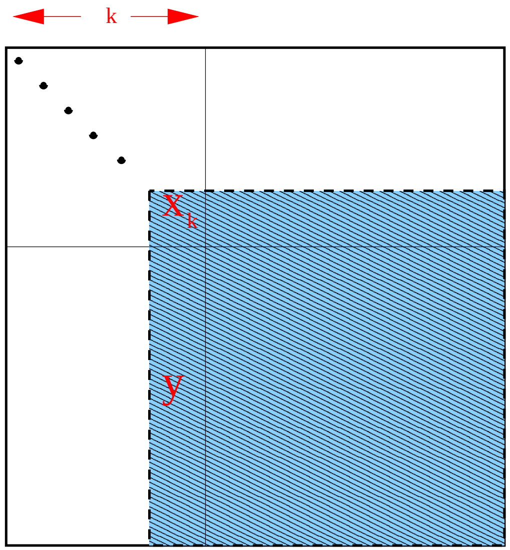

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- **DELAY** the pivot and then send to the parent a larger Schur complement.

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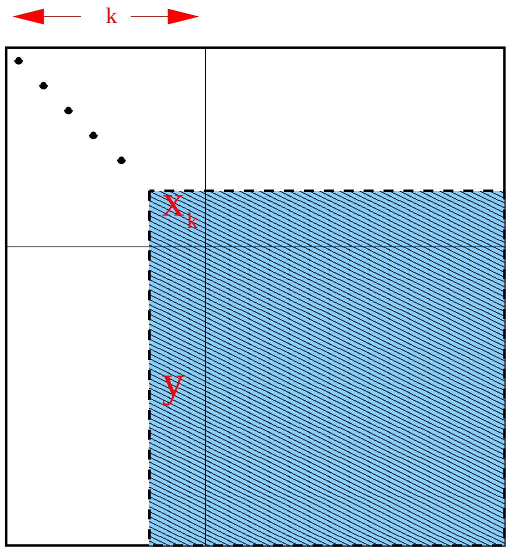

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This can cause more work and storage

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and CONTINUE.

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

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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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and CONTINUE.
We thus have factorized

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

where $|E| \leq \tau I$

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

Roundoff error 1

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

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

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

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

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Right preconditioned GMRES and Flexible GMRES

procedure [x] = right_Prec_GMRES(A,M,b)
$x_0 = M^{-1}b, r_0 = b - Ax_0$ and $\beta = ||r_0||$
$v_1 = r_0/\beta$; k = 0;
while $||r_k|| > \mu(||b|| + ||A||\ ||x_k||)$
$k = k + 1$;
$z_k = M^{-1}v_k; w = Az_k$;
for $i = 1, \ldots, k$ do
$h_{i,k} = v_i^T w$;
$w = w - h_{i,k}v_i$;
end for;
$h_{k+1,k} = ||w||$;
$v_{k+1} = w/h_{k+1,k}$;
$V_k = [v_1, \ldots, v_k]$;
$H_k = \{h_{i,j}\}_{1 \le i \le j+1; 1 \le j \le k}$;
$y_k = \arg\min_y ||\beta e_1 - H_k y||$;
$x_k = x_0 + M^{-1}V_k y_k$ and $r_k = b - Ax_k$;
end while ;
end procedure.

procedure [x] =FGMRES(A,M_i,b)
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$h_{k+1,k} = ||w||$;
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$Z_k = [z_1, \ldots, z_k]$; $V_k = [v_1, \ldots, v_k]$;
$H_k = \{h_{i,j}\}_{1 \le i \le j+1; 1 \le j \le k}$;
$y_k = \arg\min_y ||\beta e_1 - H_k y||$;
$x_k = x_0 + Z_k y_k$ and $r_k = b - Ax_k$;
end while ;
end procedure.

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

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

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

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:

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

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

Giraud and Langou, Björck and Paige, and generalise Paige, Rozložník, and Strakoš

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

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*

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

MA57 tests

	n	nnz	nnz(L)+nnz(D)	Fact. time
CONT_201	80595	239596	9106766	9.0 sec
CONT_300	180895	562496	22535492	28.8 sec

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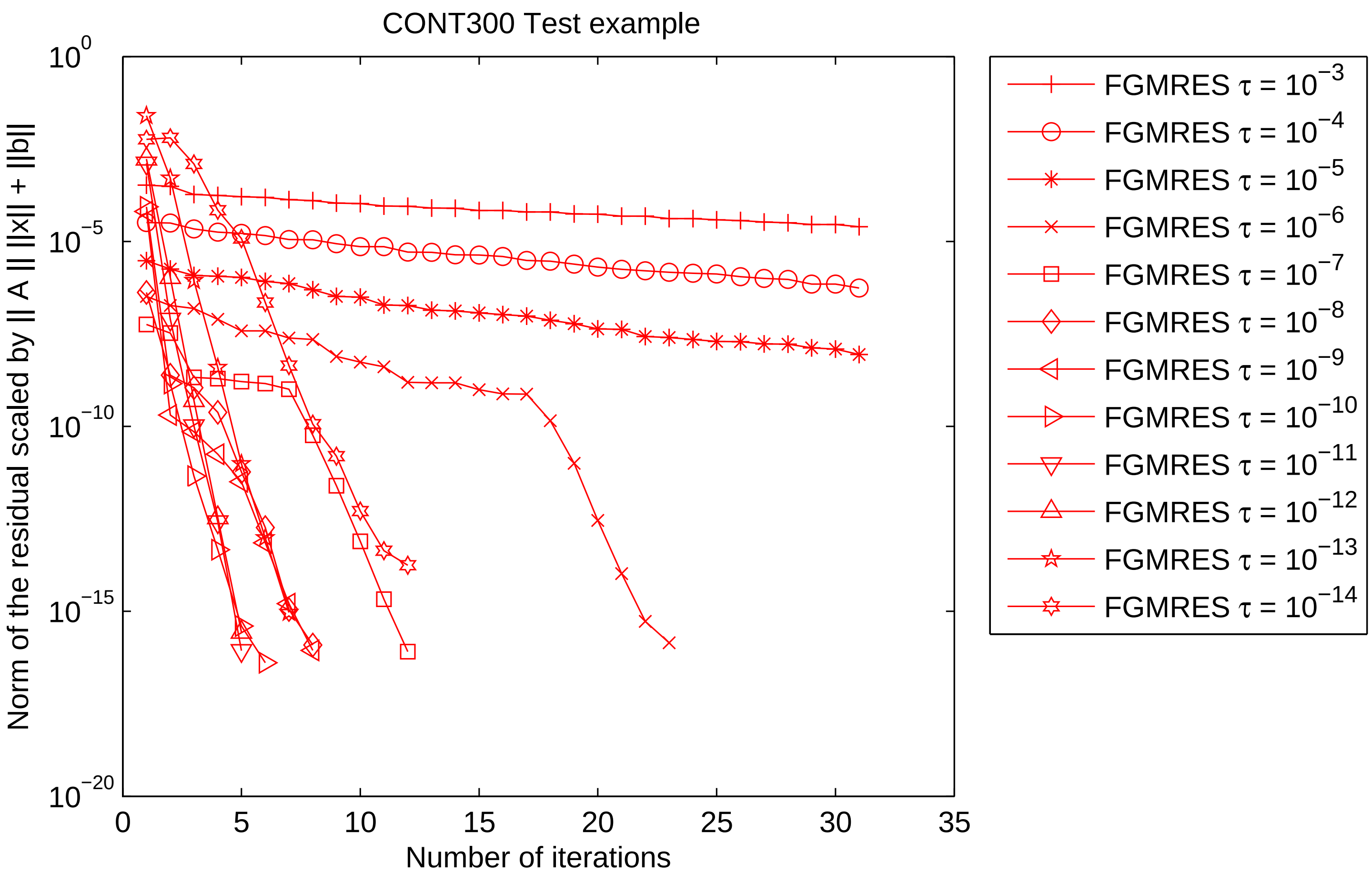
IR does not converge!

Numerical experiments



FGMRES on CONT-300 test example

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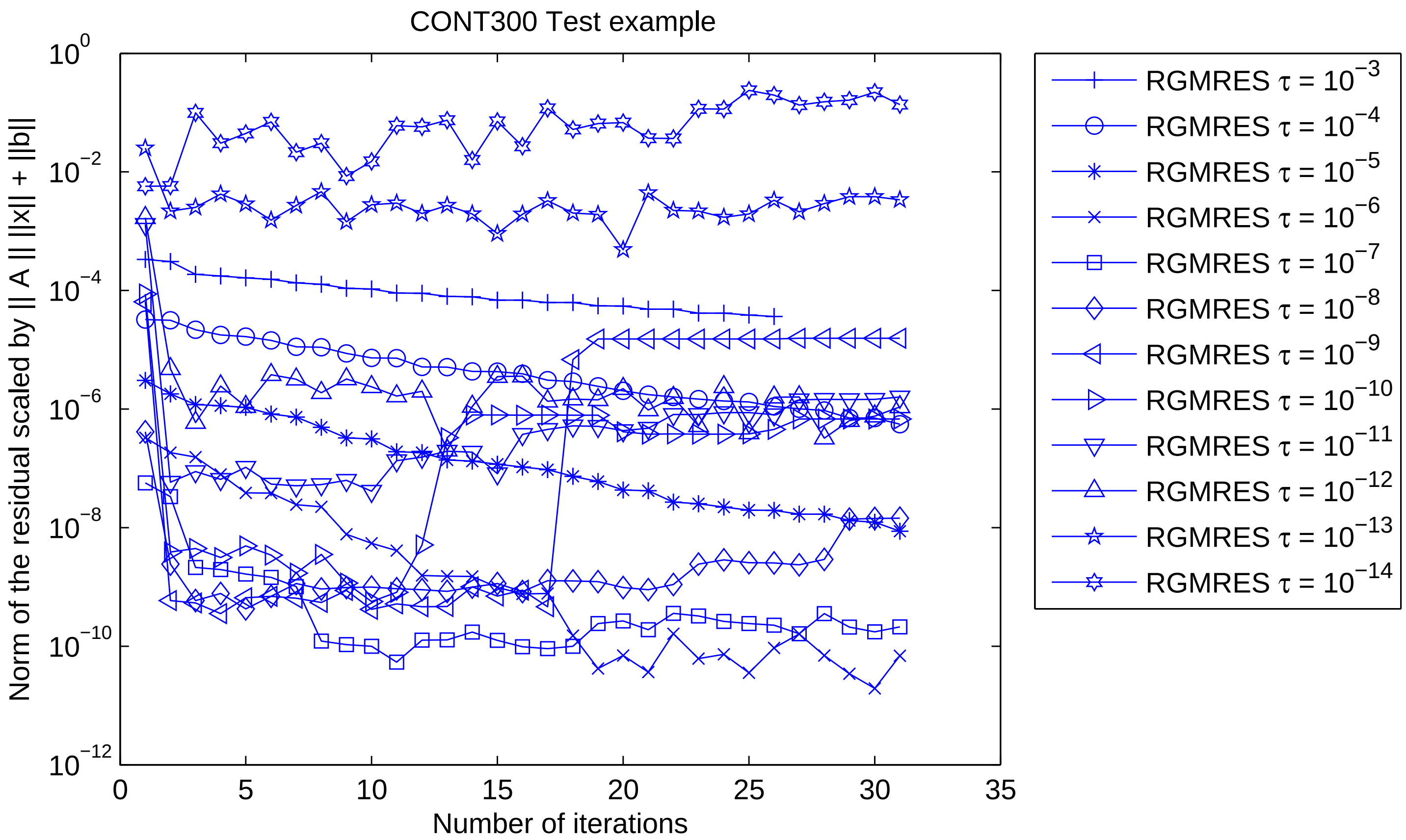

GMRES on CONT-300 test example

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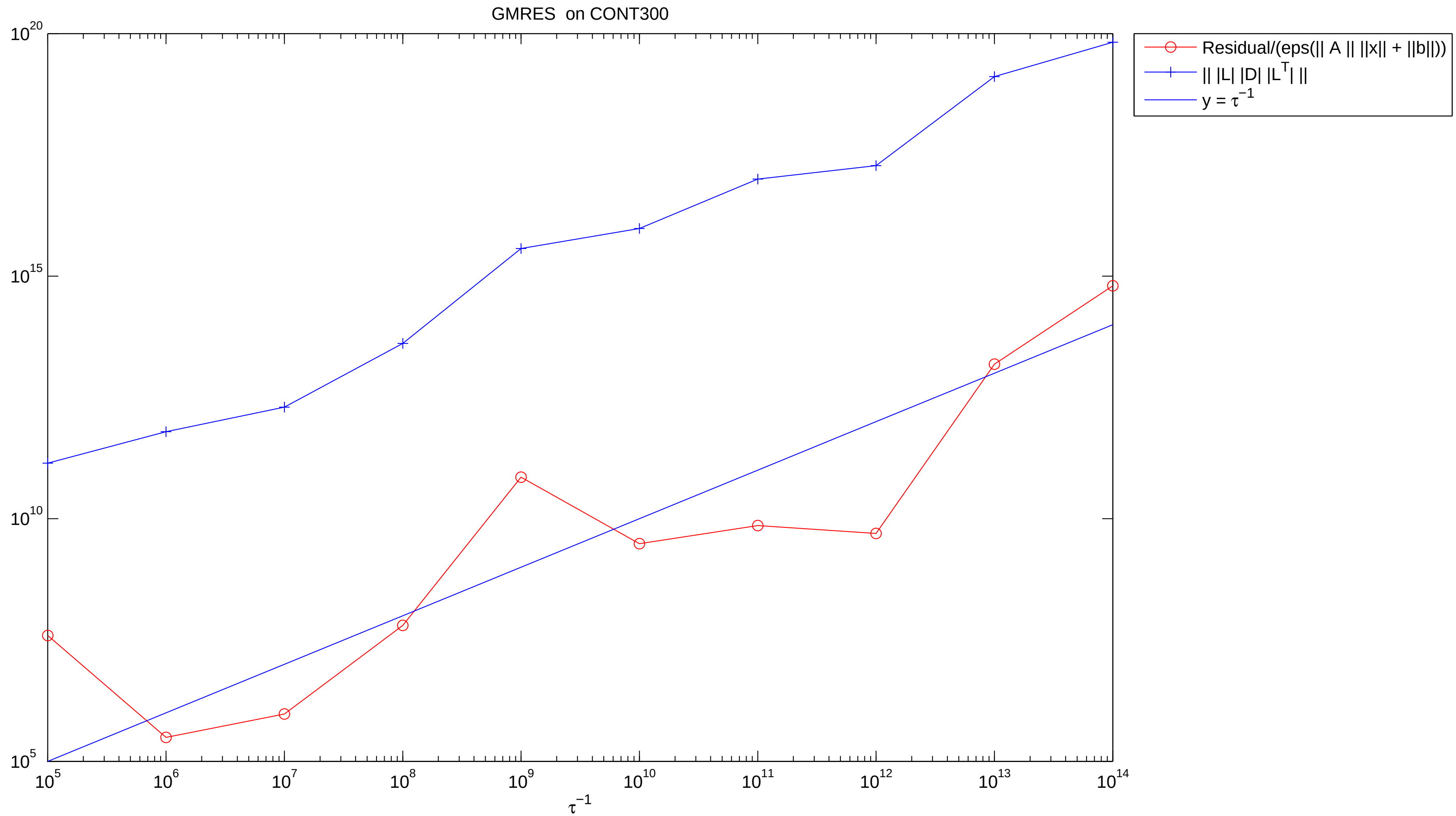

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- IR with static pivoting is very sensitive to τ and not robust

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- GMRES is also sensitive and not robust
- FGMRES is robust and less sensitive (see roundoff analysis)
- Gains from restarting. Makes GMRES more robust, saves storage in FGMRES (but not really needed)