The Augmented Block-Cimmino Distributed Method

Improvements to the Conjugate Gradient accelerated Block Cimmino Method

Mohamed Zenadi[1], Ronan Guivarch[1] Iain S. Duff[2] Daniel Ruiz[1],

IRIT - ENSEEIHT[1], CERFACS and Rutherford Appleton Laboratory[2]

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Block Cimmino : The basic facts

- Block row projection method [Elfving (Numer. Math. 1980)]

Partitioning the system $Ax = b$

$$\begin{pmatrix} A_1 \\ A_2 \\ \vdots \\ A_p \end{pmatrix} x = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_p \end{pmatrix}$$

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The Block Cimmino Iteration

$$\begin{aligned} \delta_i^{(k)} &= A_i^+ b_i - P_{\mathcal{R}(A_i^T)} x^{(k)} \\ x^{(k+1)} &= x^{(k)} + \nu \sum_{i=1}^{p} \delta_i^{(k)} \end{aligned}$$

where: $A_i^+ = A_i^T \left(A_i A_i^T\right)^{-1}$ and $P_{\mathcal{R}(A_i^T)} = A_i^+ A_i$

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- Block row projection method [Elfving (Numer. Math. 1980)]
- CG acceleration: iteration matrix is $\sum_{i=1}^{p} A_i^+ A_i = \sum_{i=1}^{p} P_{\mathcal{R}(A_i^T)}$

Acceleration

Apply CG to solve the SPD system

$$\sum_{i=1}^{p} A_i^+ A_i \; x = \sum_{i=1}^{p} A_i^+ b_i$$

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- Offers a natural parallelism

Acceleration

Solve independently using MUMPS the systems for each partition

$$\begin{bmatrix} I & A_i^T \\ A_i & 0 \end{bmatrix} \begin{bmatrix} u_i \\ v_i \end{bmatrix} = \begin{bmatrix} 0 \\ b_i - A_i x \end{bmatrix}$$

$$\begin{aligned} \text{where : } u_i &= A_i^+ (b_i - A_i x) \\ &= \delta_i \end{aligned}$$

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- Offers a natural parallelism
- Can also exploit 2nd and 3rd levels of parallelism (sparsity structure, BLAS3 Kernels)

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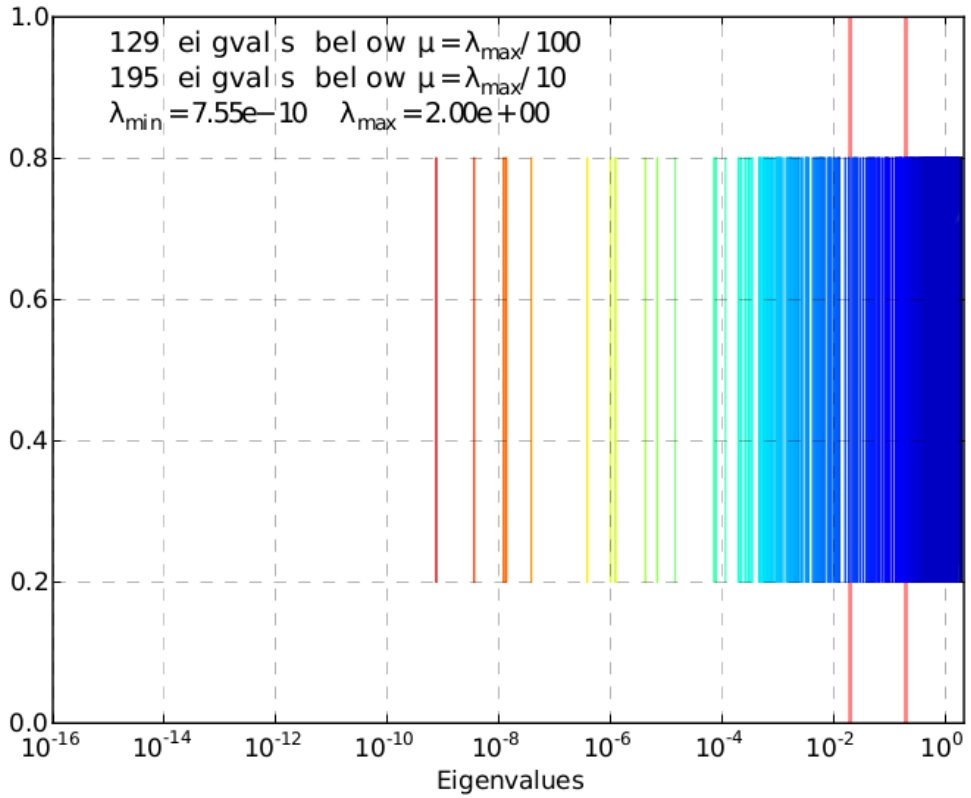
Block Cimmino : Numerical considerations

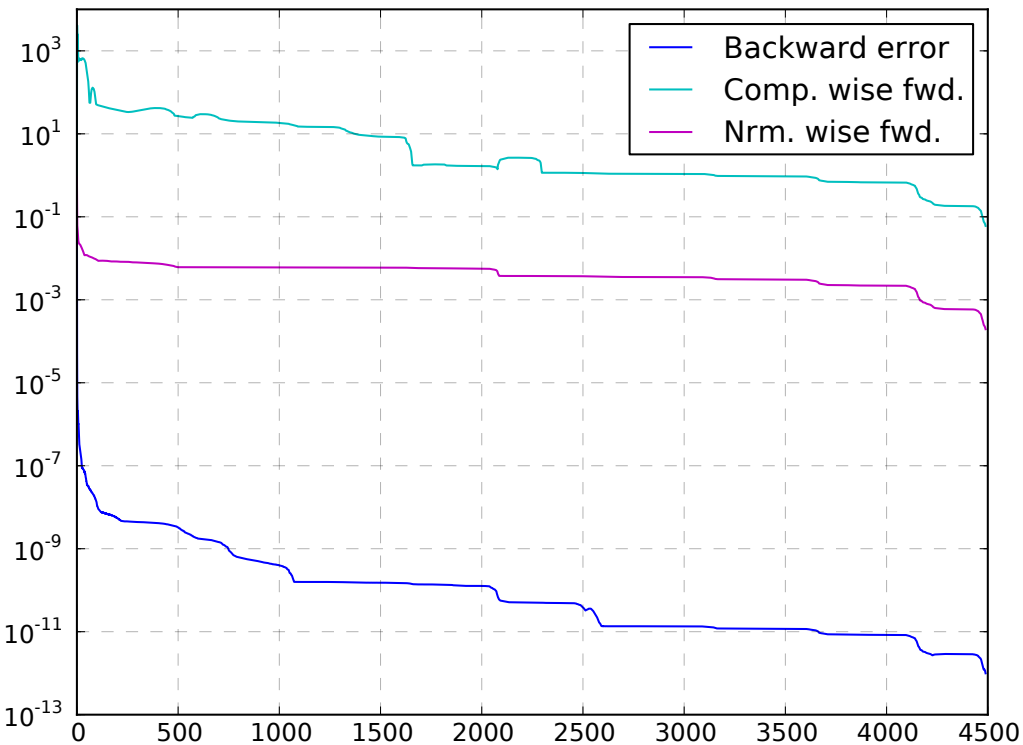
- Block Cimmino iteration matrix exhibits in general good eigenvalue clustering around 1



[bayer01 - 57k - 16 parts] Smallest eigenvalues values of the iteration matrix

Block Cimmino : Numerical considerations

- Block Cimmino iteration matrix exhibits in general good eigenvalue clustering around 1
- However, combination of ill-conditioning with clusters of few eigenvalues at the extremes implies CG convergence with plateaus



`[bayer01 - 57k - 16 parts]` Backward error iteration profile $\omega_k = \|r_k\| / (\|A\| \, \|x_k\| + \|b\|)$

Block Cimmino : Numerical considerations

To improve the convergence one can:

- Preprocess the matrix (scaling, permutation, partitioning strategy) to improve the orthogonality between the partitions [Drummond, Duff, Guivarch, Ruiz, and Zenadi (Precond'11)]
- Use Stabilized Block CG to reduce the length of the plateaus [Arioli, Duff, Ruiz, and Sadkane (SIMAX 1995)]

For successive solves with he same matrix :

- Combine Chebyshev filters (as preconditioners) with conjugate gradient [Golub, Ruiz, Touhami (SIMAX 2007)]

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However,

- Effectiveness is problem dependent
- For very large problems, difficult to control explicitly the spread of the intermediate eigenvalues in the iteration matrix (length of plateaus in convergence, memory issues for Krylov basis extraction)

A path to orthogonality

Objectives

- Control explicitly the behavior of the method
- A better and explicit control of the memory needed
- Maintain the efficiency in the case of multiple solves

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- Extract a condensed smaller subsystem (similar to Schur complement techniques) that can be reused for efficient further solves

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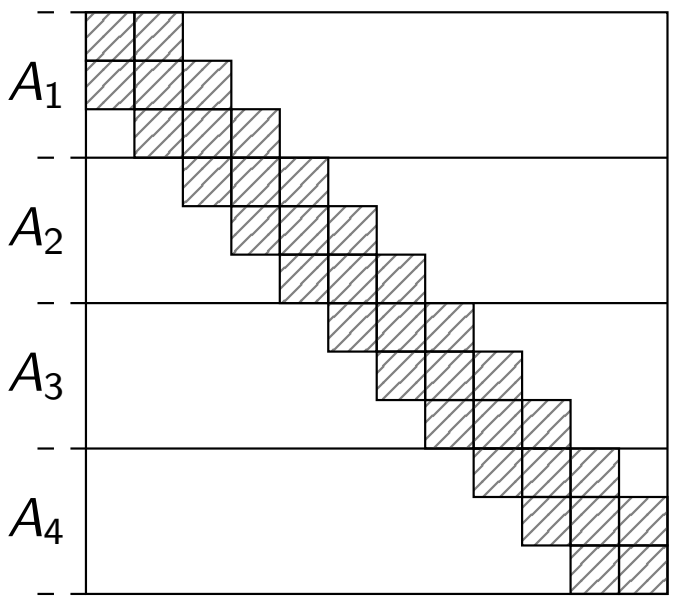
$\Rightarrow$ **A**ugmented **B**lock **C**immino **D**istributed solver (`ABCD solver`)

The augmentation process

- Partition the matrix with respect to its structure (not necessarily in block-tridiagonal form)



`Illustrative example`

The augmentation process

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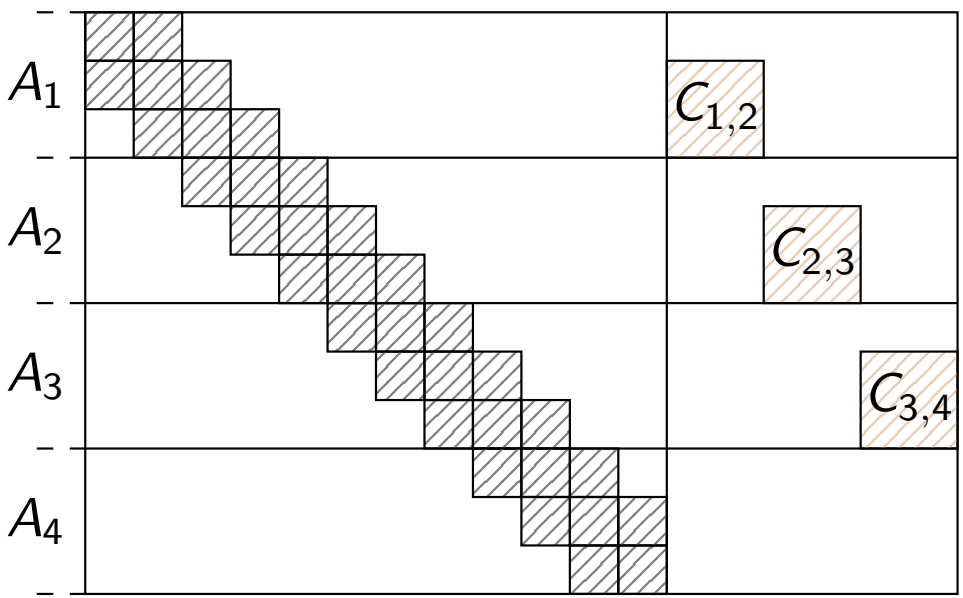
- For each pair of partitions ($j > i$), expand with $C_{i,j} = A_i A_j^T$,



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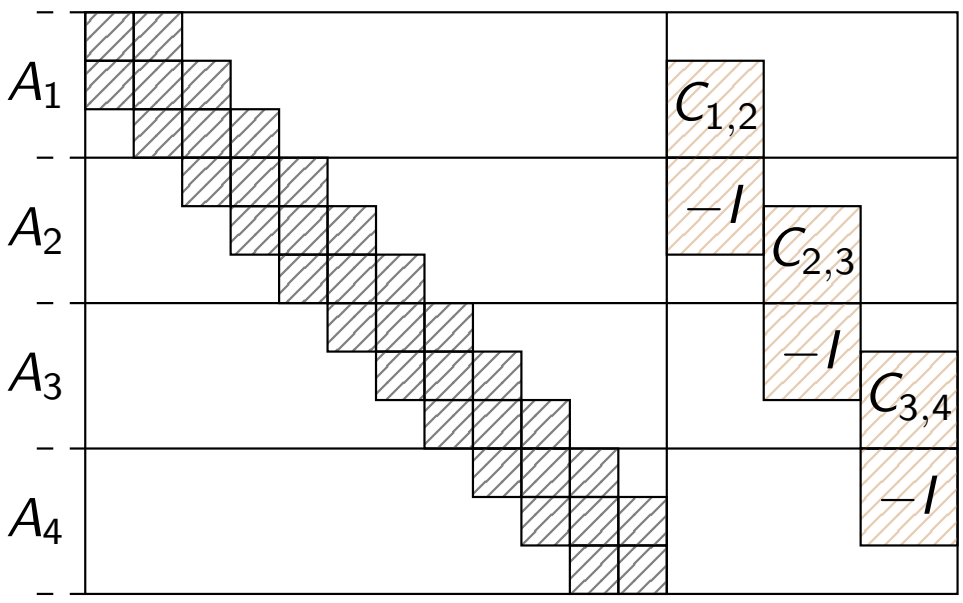

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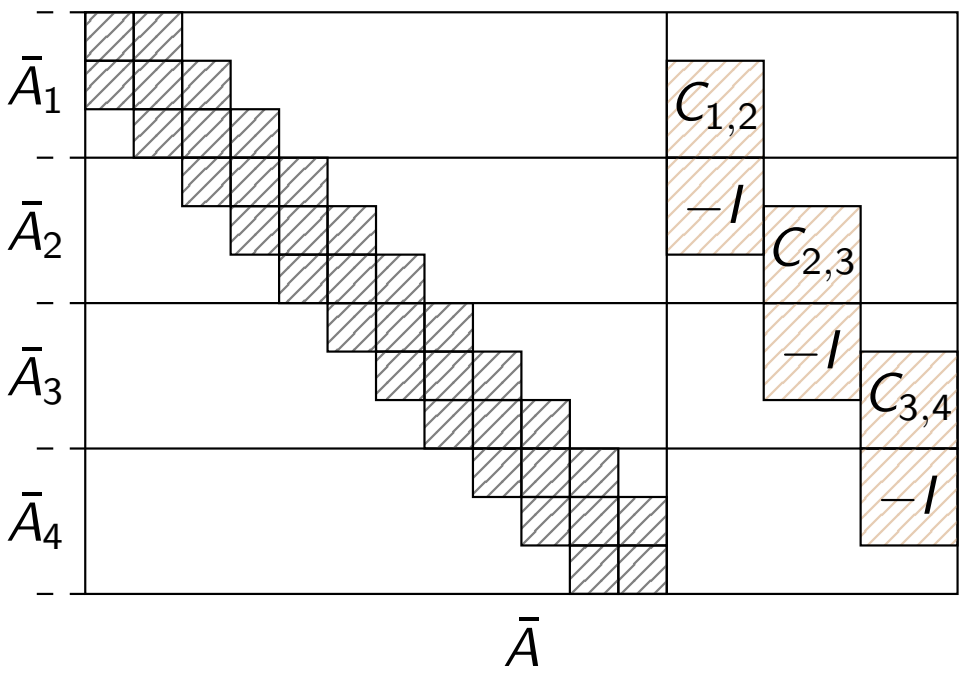

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- Add extra constraints to build an equivalent linear system :

$$\begin{bmatrix} A & C \\ 0 & I \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix},$$

where $y = 0$ ensures the same solution x.

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Problem

the extra partition $Y = \begin{bmatrix} 0 & I \end{bmatrix}$, linked to the constraints equations, is not orthogonal to the previous partitions in $\bar{A} = \begin{bmatrix} A & C \end{bmatrix}$.

The augmentation process

To enforce this orthogonality, we project the column vectors Y^T onto the null space of $\bar{A} = \begin{bmatrix} A & C \end{bmatrix}$ (orthogonal complement of $\mathcal{R}\left(\bar{A}^T\right)$) :

$$W^T = (I - P)\, Y^T,$$

where (as a result of the enforced orthogonality) :

$$P = P_{\mathcal{R}(\bar{A}^T)} = P_{\bigoplus_{i=1}^{p} \mathcal{R}(\bar{A}_i^T)} = \sum_{i=1}^{p} P_{\mathcal{R}(\bar{A}_i^T)}$$

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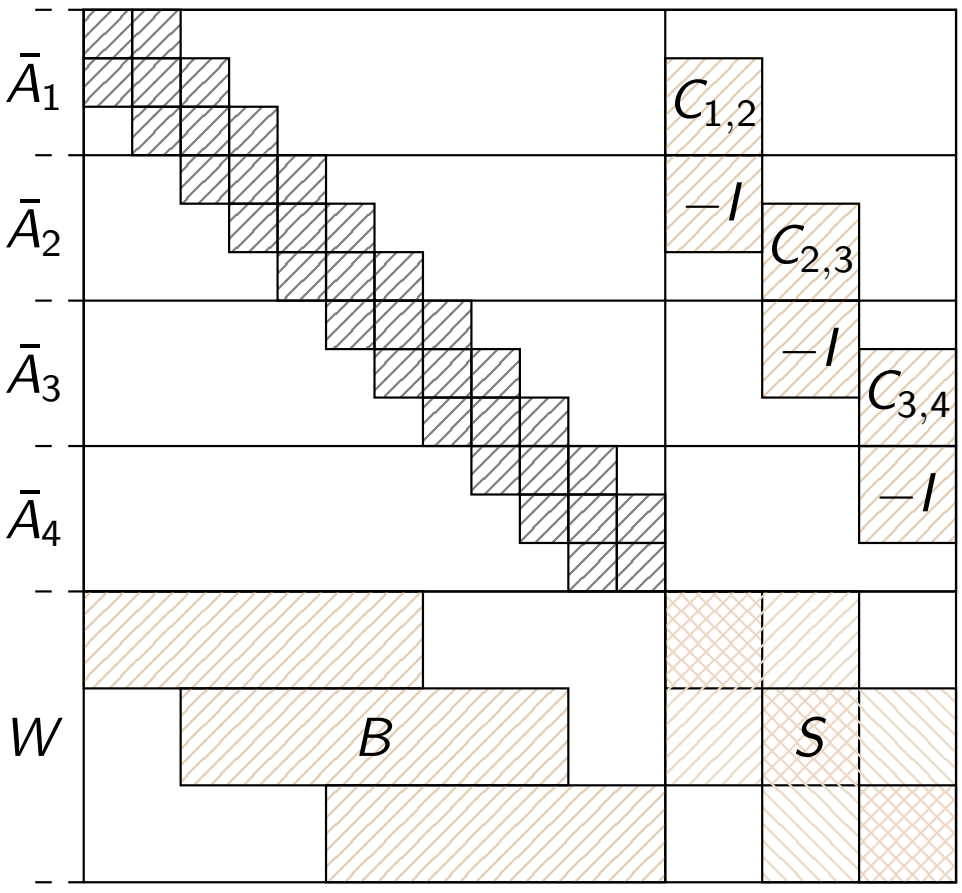
We finally obtain $\begin{bmatrix} A & C \\ B & S \end{bmatrix}$, where $\begin{bmatrix} B & S \end{bmatrix} = W$, an augmented matrix with mutually numerically orthogonal partitions

The augmentation process



Illustrative example

The augmentation process

To keep the consistency within the solution of the new system :

$$\begin{bmatrix} A & C \\ B & S \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} b \\ f \end{bmatrix}$$

we compute the right hand side f as :

$$f \quad = \quad \begin{bmatrix} B & S \end{bmatrix} \begin{bmatrix} x \\ 0 \end{bmatrix} \quad = \quad Y\,(I - P) \begin{bmatrix} x \\ 0 \end{bmatrix}$$

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$$\begin{aligned} f &= \begin{bmatrix} B & S \end{bmatrix} \begin{bmatrix} x \\ 0 \end{bmatrix} &&= Y(I-P) \begin{bmatrix} x \\ 0 \end{bmatrix} \\ &&&= -YP \begin{bmatrix} x \\ 0 \end{bmatrix} \qquad (\text{since } Y = \begin{bmatrix} 0 & I \end{bmatrix}) \\ &&&= -Y\bar{A}^{+}\bar{A} \begin{bmatrix} x \\ 0 \end{bmatrix} \\ f &= -Y\bar{A}^{+}b \end{aligned}$$

Since all the partitions in the new equivalent linear system

$$\begin{bmatrix} A & C \\ B & S \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} b \\ f \end{bmatrix}$$

are mutually numerically orthogonal, the Cimmino iteration matrix becomes the `Identity` matrix,

Implicit Direct Solver

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$$\begin{aligned} \begin{bmatrix} x \\ y \end{bmatrix} &= \bar{A}^{+} b + W^{+} f \\ &= \bar{A}^{+} b - W^{+} Y \bar{A}^{+} b \\ &= \sum_{i=1}^{p} \bar{A}_i^{+} b_i - W^{+} Y \sum_{i=1}^{p} \bar{A}_i^{+} b_i \end{aligned}$$

Computational Ingredients

Knowing that $W = \begin{bmatrix} B & S \end{bmatrix} = Y\,(I - P)$, with $Y = \begin{bmatrix} 0 & I \end{bmatrix}$, we have :

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and the pseudo inverse $W^+ = W^T(WW^T)^{-1}$ is given by

$$\begin{aligned} W^+ &= W^T S^{-1} \\ W^+ &= (I-P)\,Y^T S^{-1} \end{aligned}$$

The solution is thus given by :

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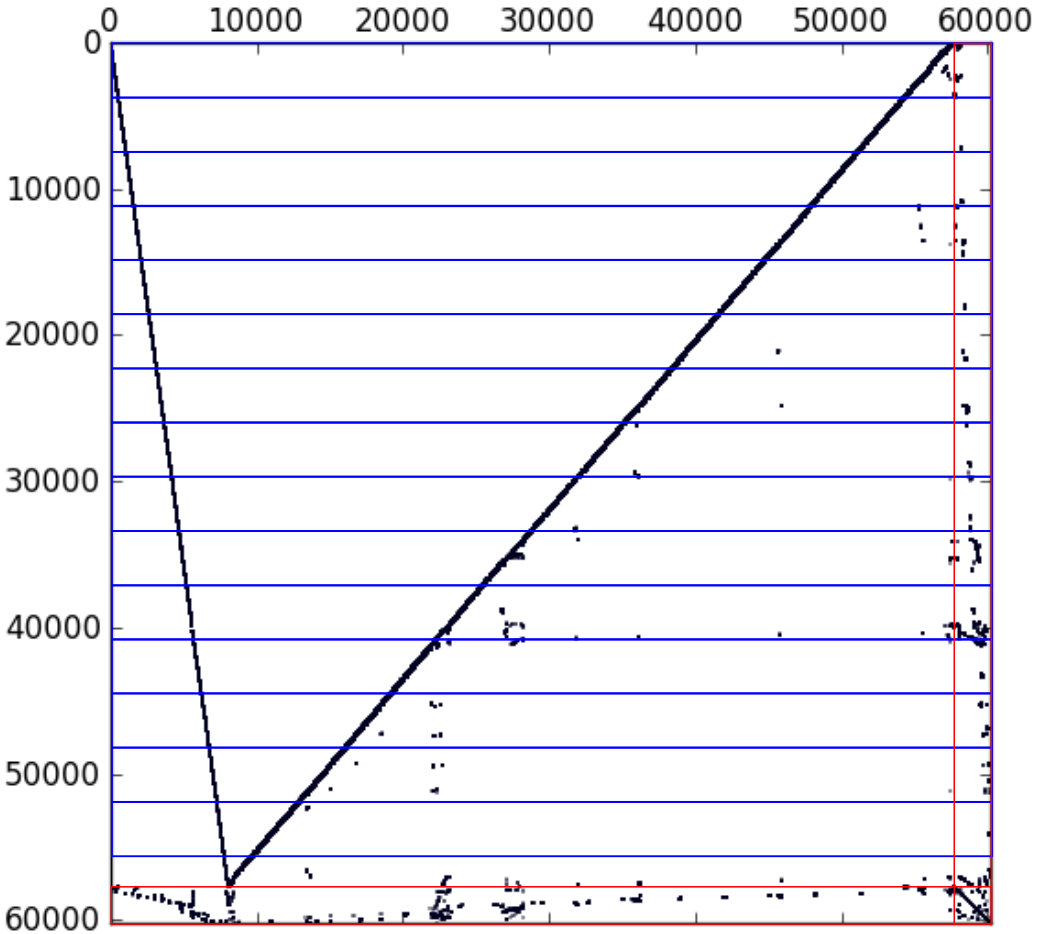
Note that we don't need to build B, only S is used

Example : bayer01 (57k) - 16 partitions



Solution Quality	
$\frac{\|x^*-x\|}{\|x^*\|}$	$3.05e-09$
$\frac{\|r\|}{\|b\|}$	$5.23e-14$

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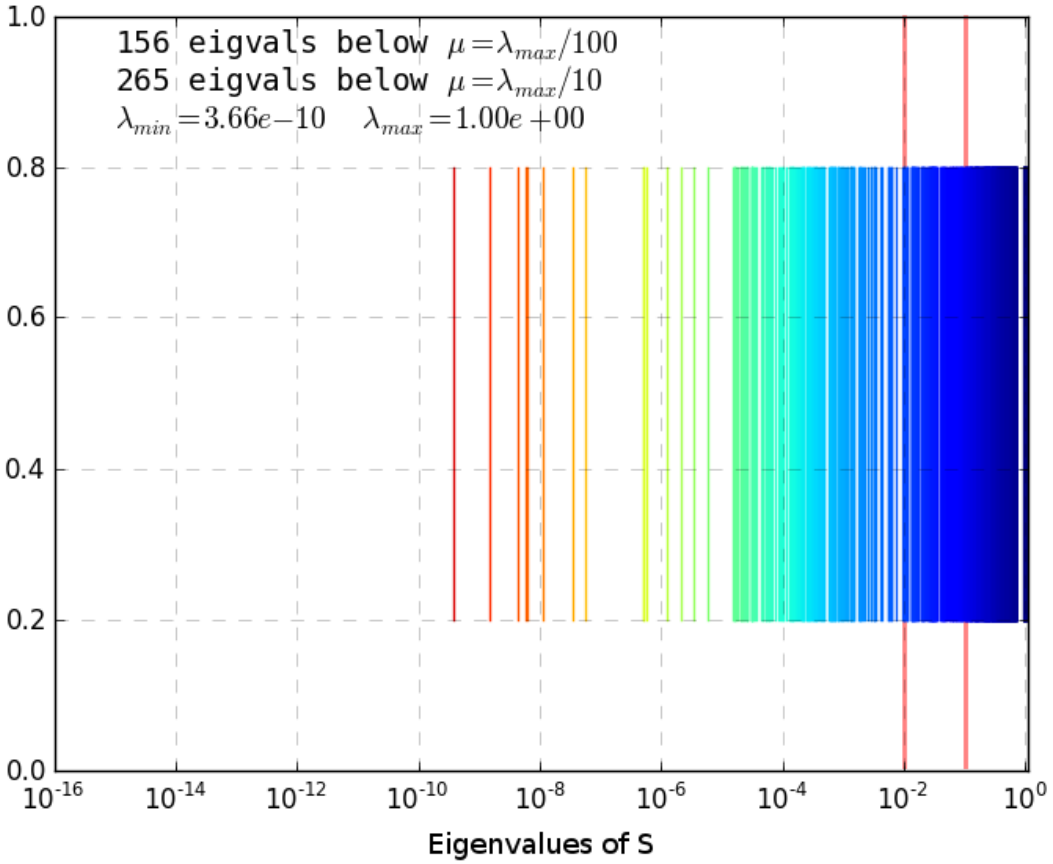

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Several Issues

- The size of S is problem dependent :
  - sparsity structure (preprocessing, permutations...)
  - number and size of partitions
  - interconnections between partitions

Matrix	**Size**	**#Part.**	**Size of S**
`gre_1107`	1107	5	1227
`bayer01`	57735	16	2951
`lhr34c`	35152	8	10108

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- The size of S can be reduced with the alternative use of the transpose of the augmentation process
- The ill-conditioning of S can be as close as that of the original iteration matrix, but the density of eigenvalues will be less
- Open choice : build S and factorize it, or use S implicitly (MV products) in an iterative process (CG, S is SPD)

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Relaxation of the augmentation process

To better control the size of S, we propose to drop entries in the contributing blocks $C_{i,j}$ to reduce the number of added columns.
Target:

- A reduced size of S with respect to the size of A : better control of memory requirements
- Build and factorize S : takes care of the ill-conditioning in S, factors can be reused for efficient further solves

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Issues:

- The augmented partitions $\bar{A}_i$ lose *"partly"* their mutual numerical orthogonality
- $(I - P)$ is no longer explicitly available, and must be recovered via an iterative process
- The iteration matrix in this process is $\sum_{i=1}^{p} P_{\mathcal{R}(\bar{A}_i^T)}$

Inner iterations for $(I - P)$

- To recover the effect of $(I - P)$ onto any vector z, we use CG to solve the symmetric semi-positive definite linear system

$$\sum_{i=1}^{p} \bar{A}_i^+ \bar{A}_i \; x = \sum_{i=1}^{p} \bar{A}_i^+ \bar{A}_i z$$

- $\sum_{i=1}^{p} \bar{A}_i^+ \bar{A}_i$ corresponds to the Block Cimmino iteration matrix on the first set of augmented partitions, and has the same kernel as that of $\bar{A}$
- CG on consistent symmetric semi-positive definite linear systems computes the minimum norm solution : $x = Pz$

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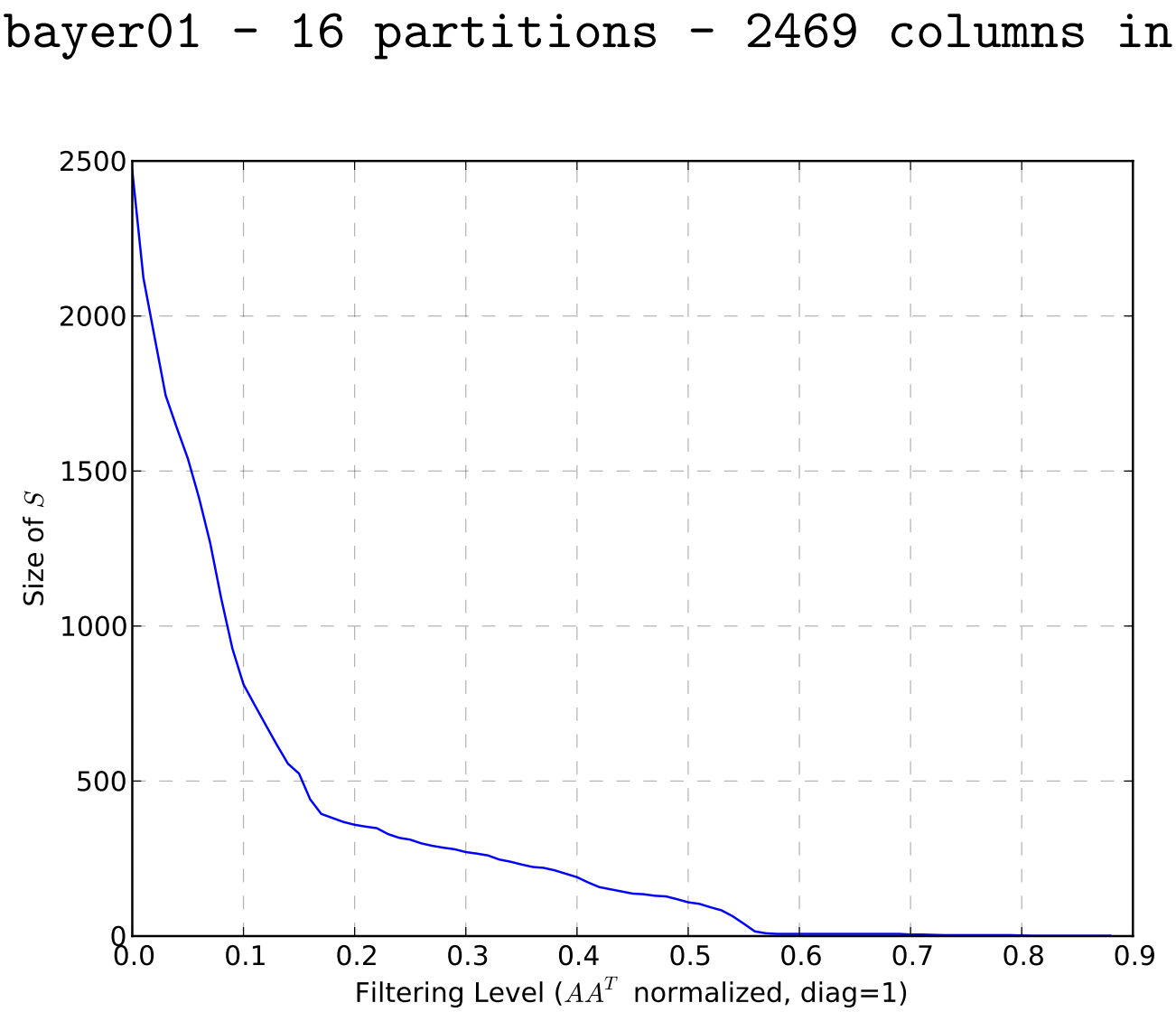
- CG on consistent symmetric semi-positive definite linear systems computes the minimum norm solution : $x = Pz$
- Possible numerical stability issues : investigate alternative techniques such as MINRES-QLP `[Choi, Paige, and Saunders (SISC 2011)]`

Example of C filtering



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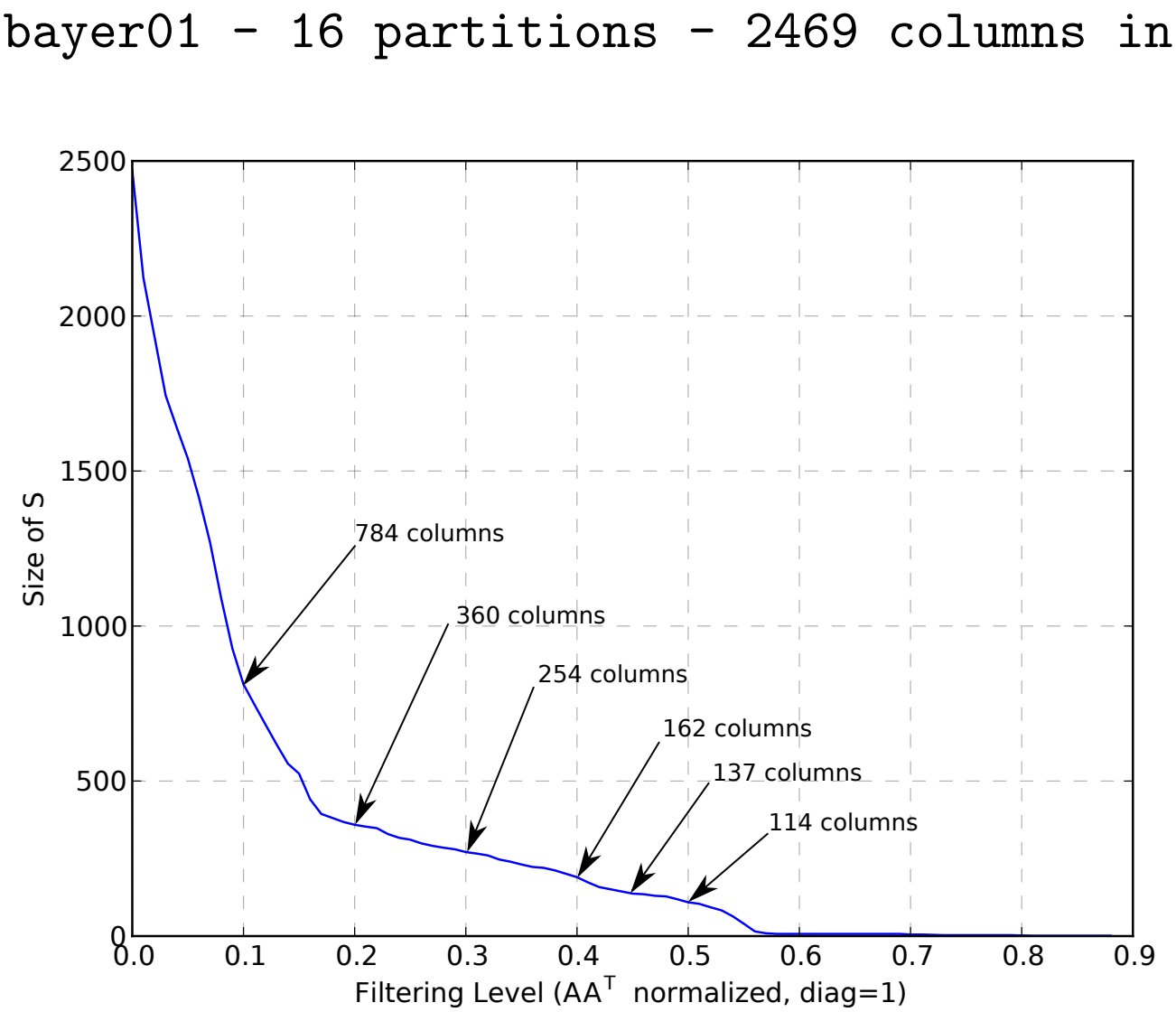
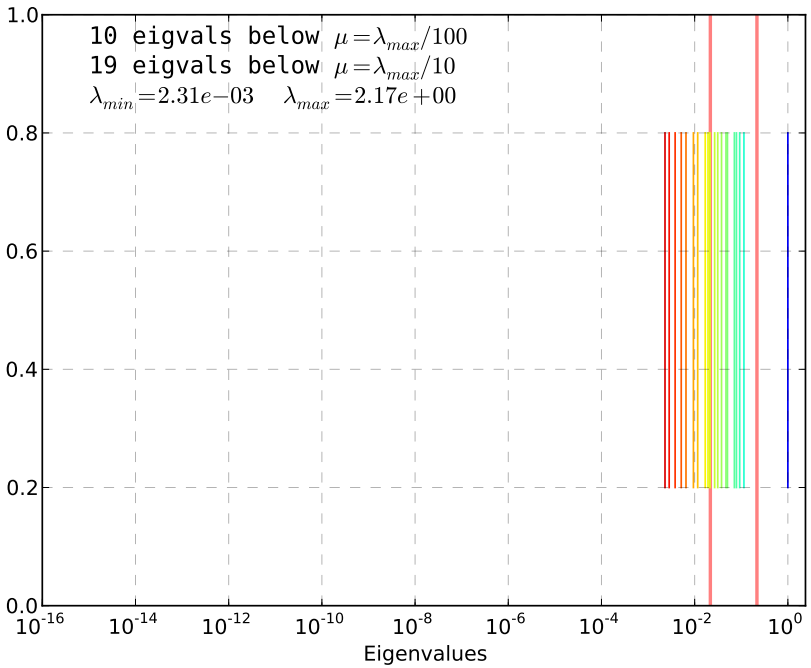


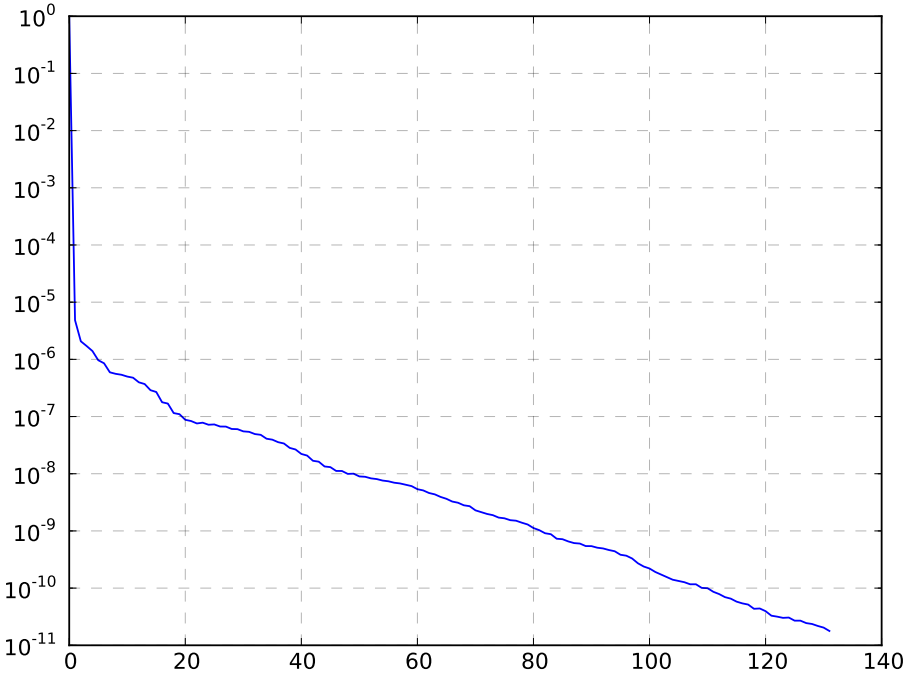
Example of C filtering

bayer01 | 16 partitions | Filter C at 0.10 | 784 cols

Ritz values of the iteration matrix



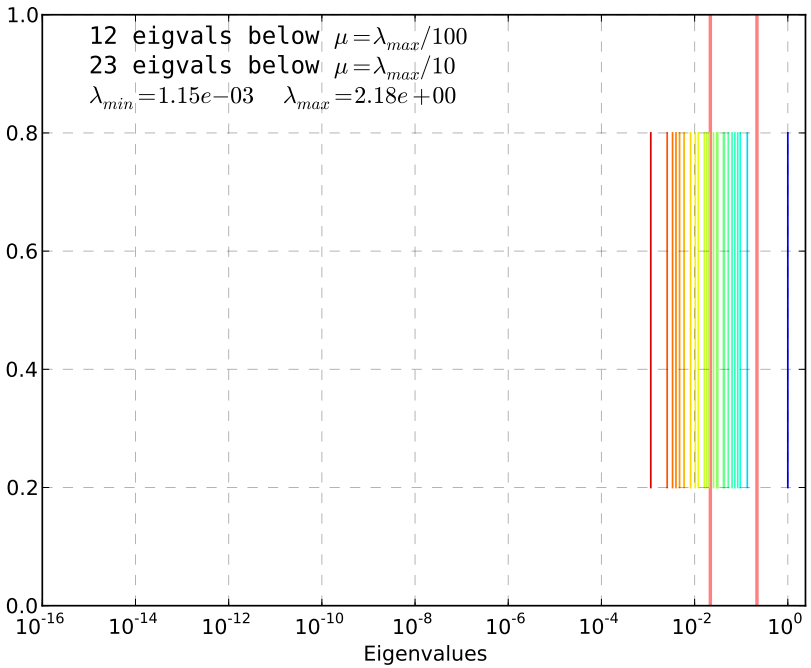
Backward error iteration profile of $w = \bar{A}^{+} b$



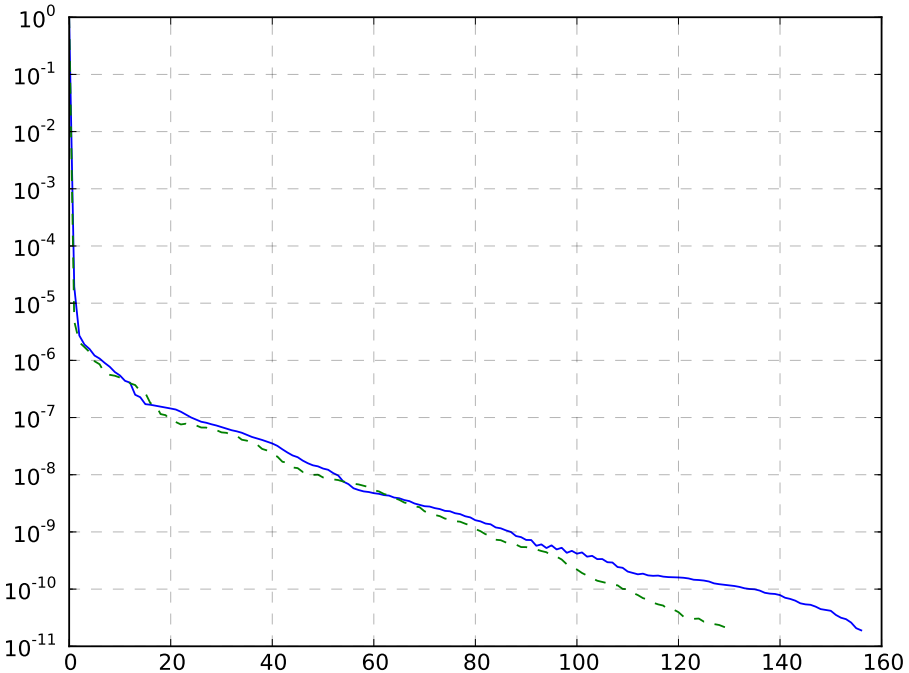
Example of C filtering

bayer01 | 16 partitions | Filter C at 0.20 | 360 cols

Ritz values of the iteration matrix



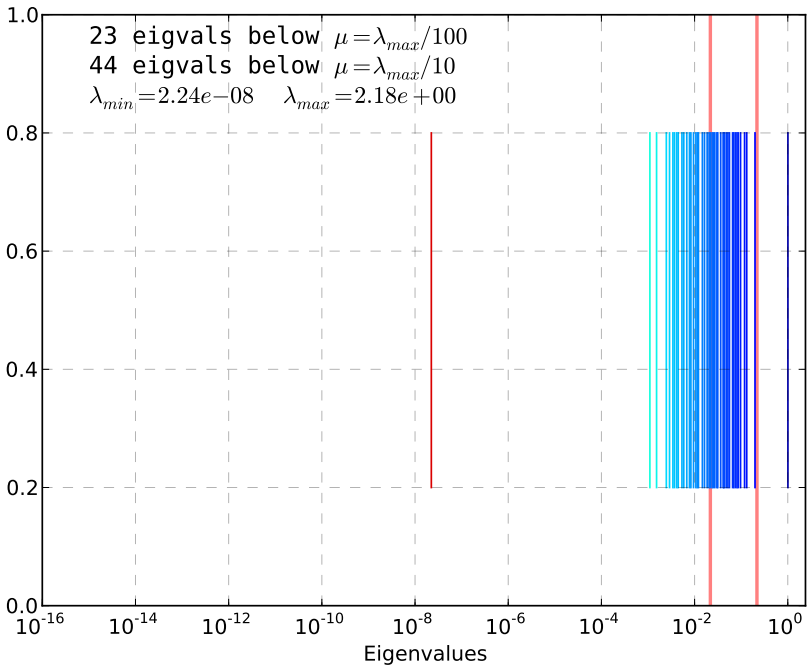
Backward error iteration profile of $w = \bar{A}^{+} b$



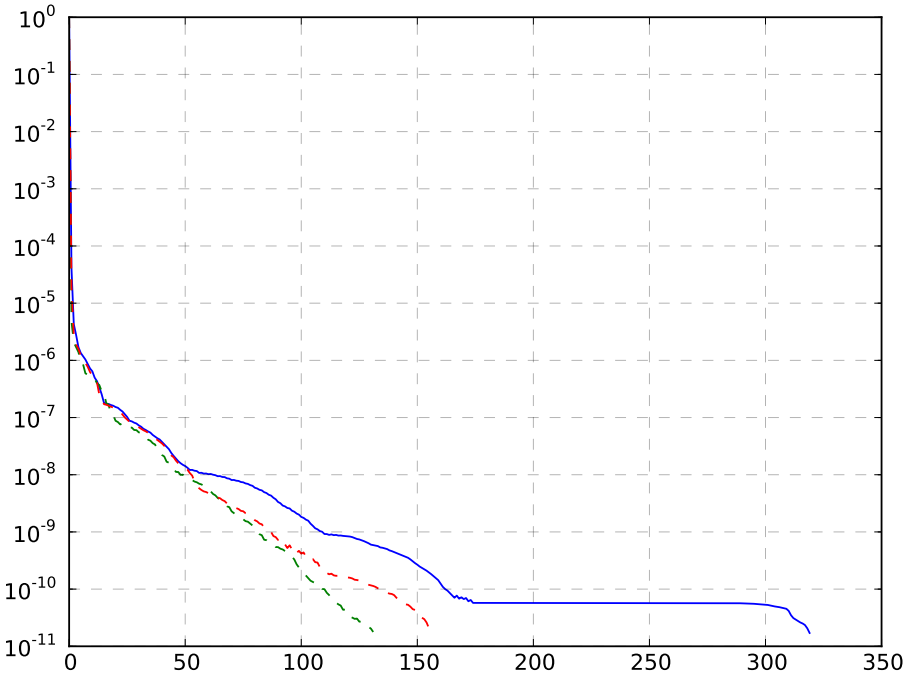
Example of C filtering

bayer01 | 16 partitions | Filter C at 0.30 | 254 cols

Ritz values of the iteration matrix



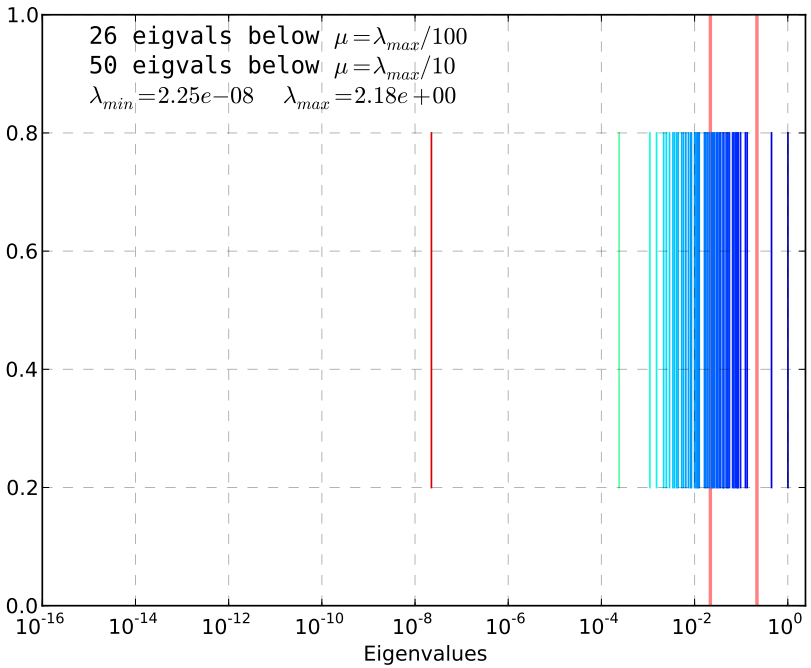
Backward error iteration profile of $w = \bar{A}^{+} b$



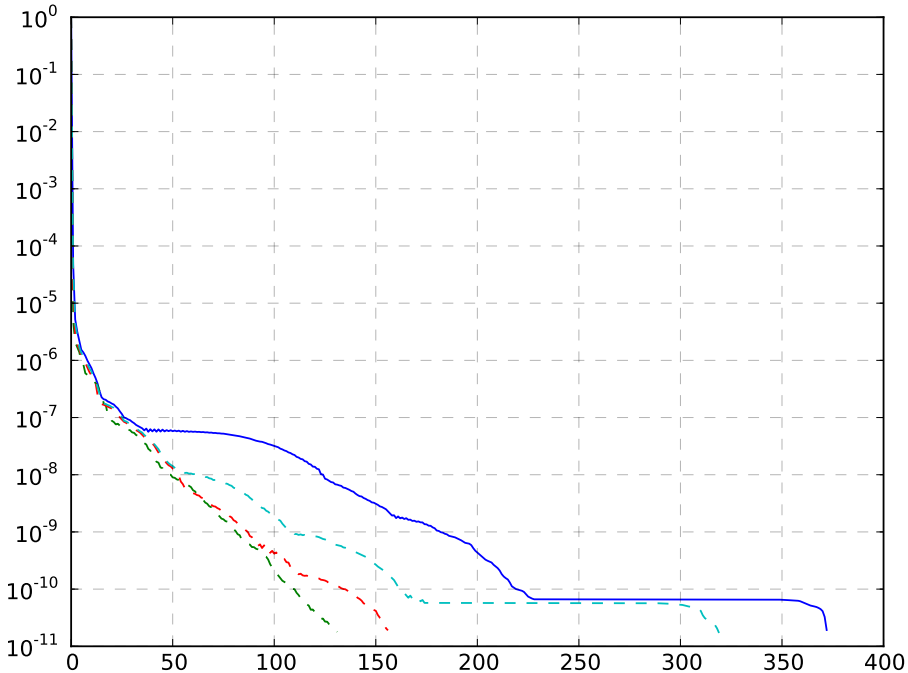
Example of C filtering

bayer01 | 16 partitions | Filter C at 0.35 | 201 cols

Ritz values of the iteration matrix



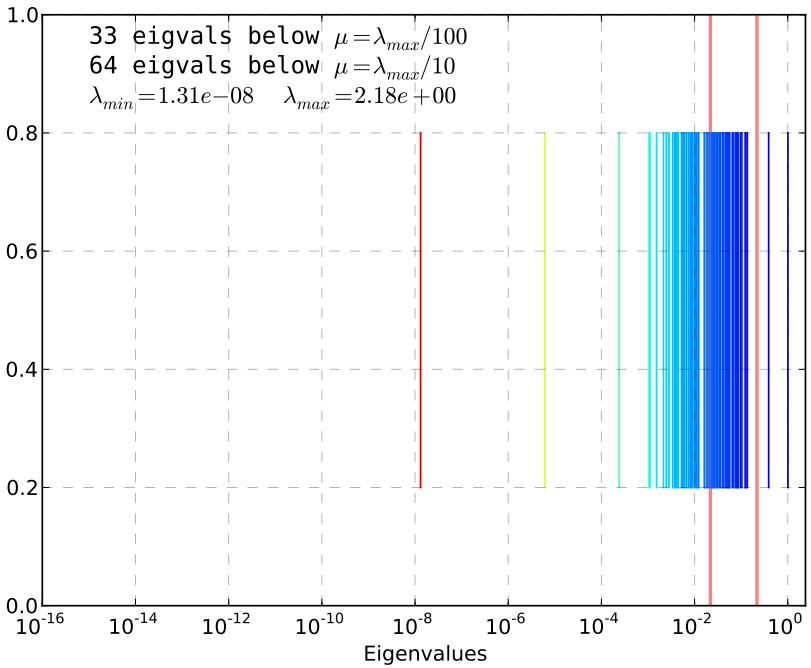
Backward error iteration profile of $w = \bar{A}^{+} b$



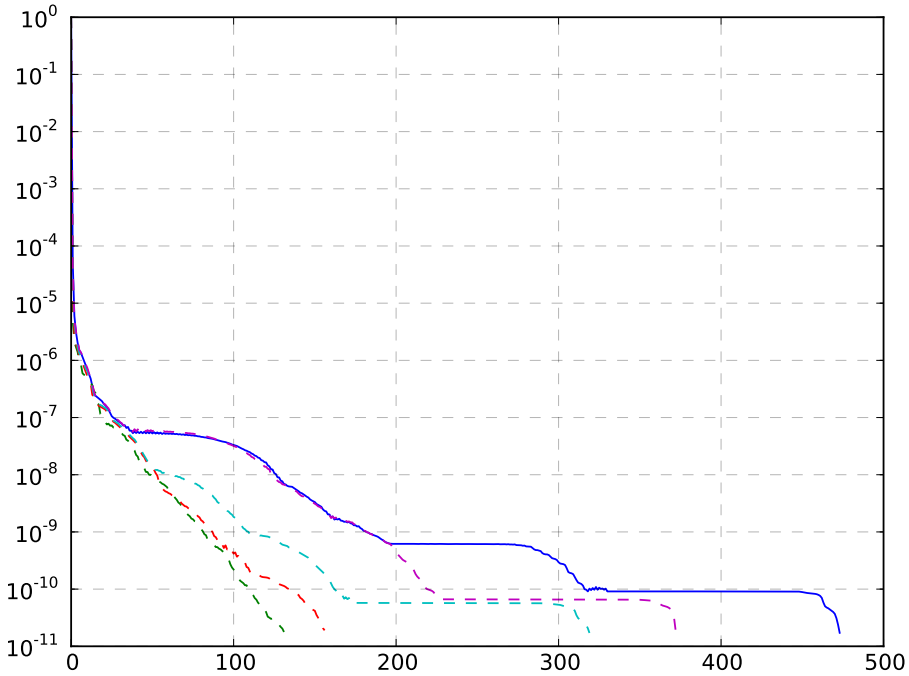
Example of C filtering

bayer01 | 16 partitions | Filter C at 0.4 | 162 cols

Ritz values of the iteration matrix



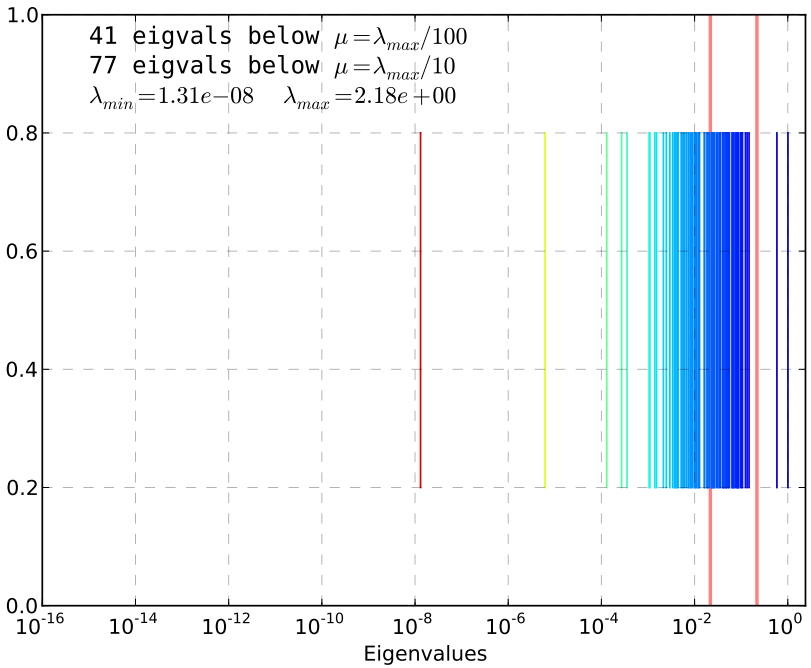
Backward error iteration profile of $w = \bar{A}^{+} b$



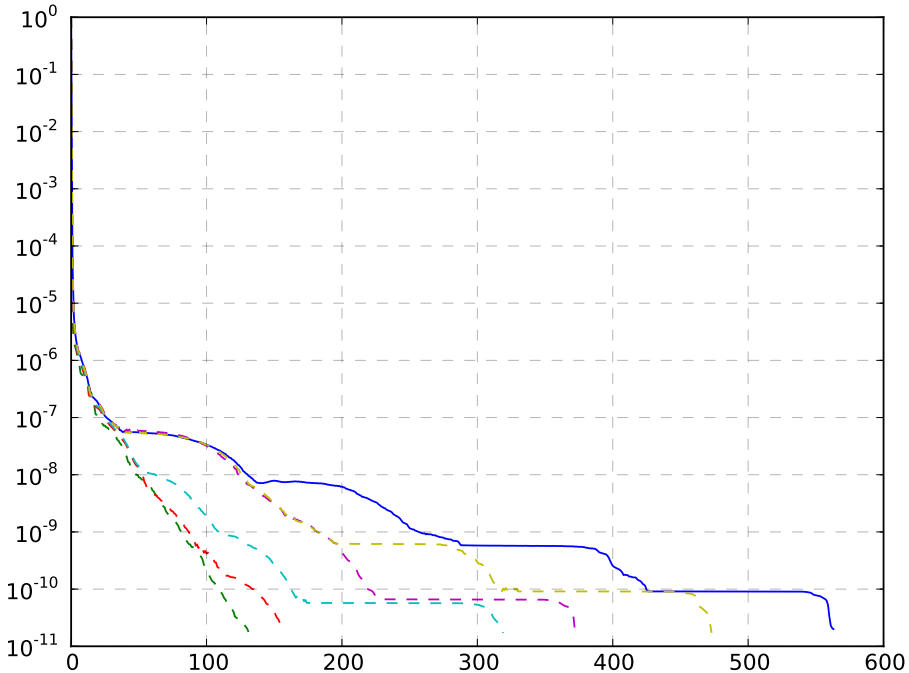
Example of C filtering

bayer01 | 16 partitions | Filter C at 0.45 | 137 cols

Ritz values of the iteration matrix



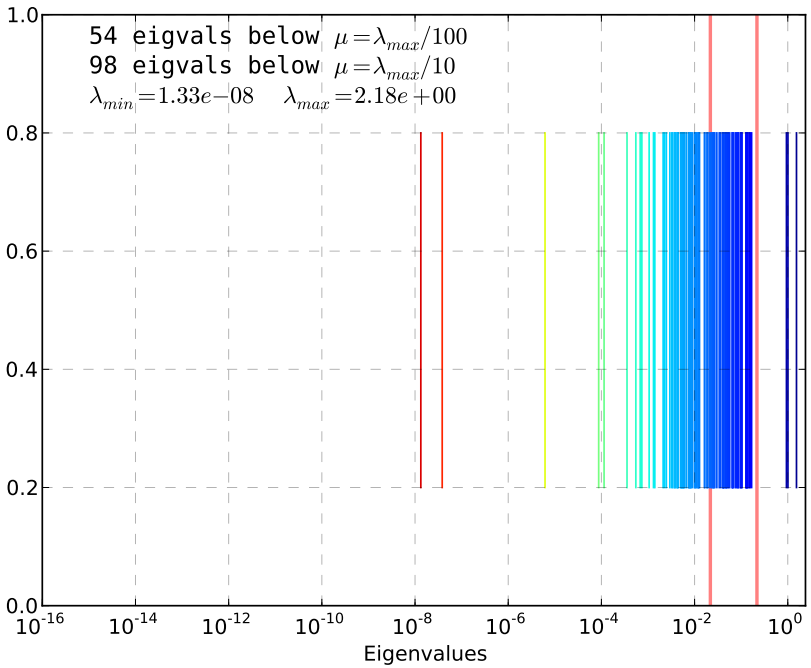
Backward error iteration profile of $w = \bar{A}^{+} b$



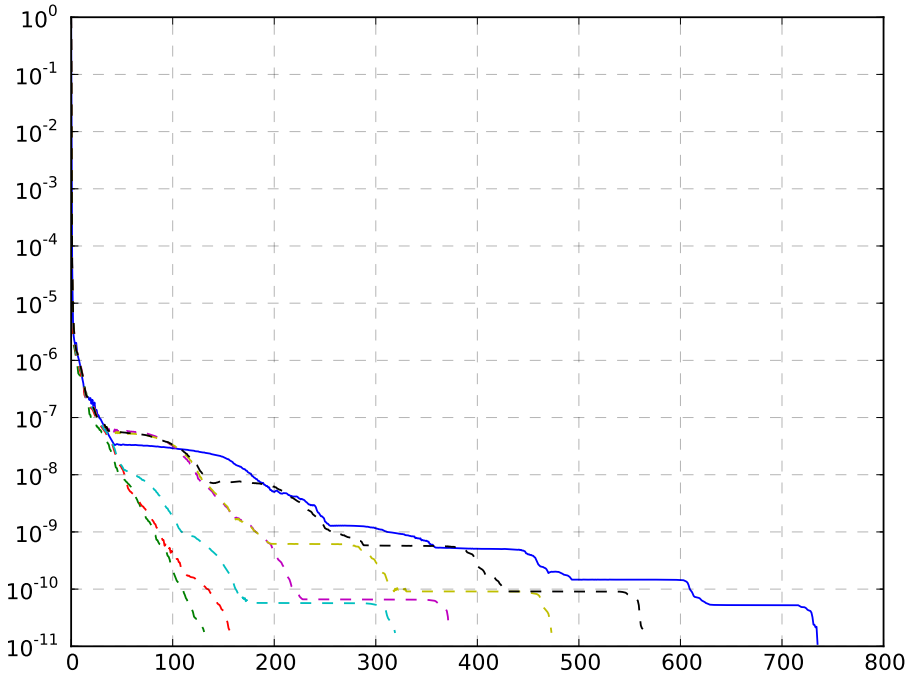
Example of C filtering

bayer01 | 16 partitions | Filter C at 0.5 | 114 cols

Ritz values of the iteration matrix

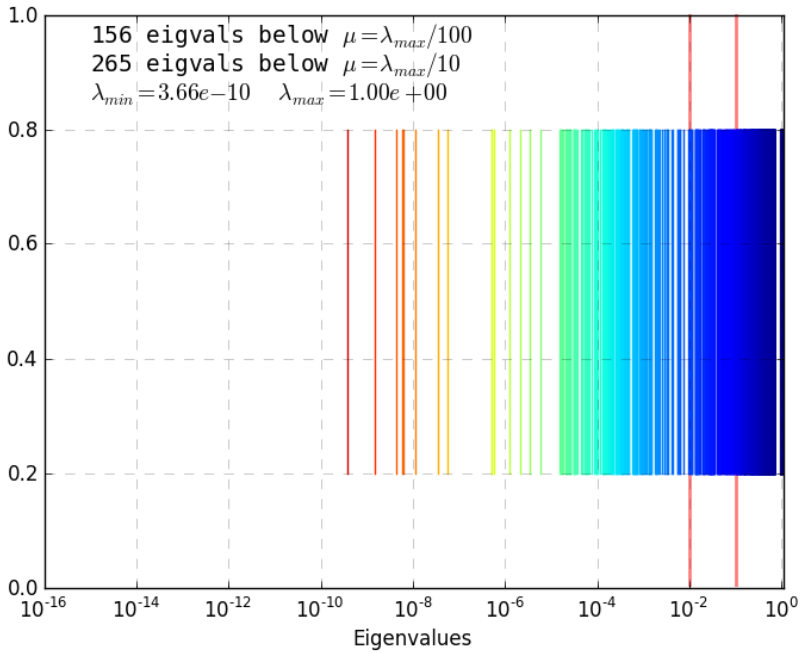


Backward error iteration profile of $w = \bar{A}^{+} b$

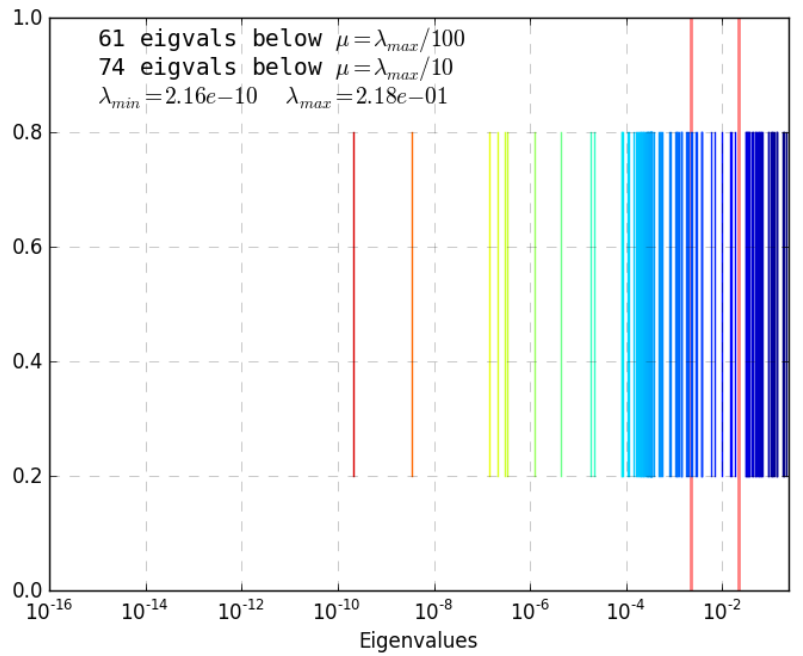


Example of C filtering

Eigenvalues of S without filtering of C (2469 cols)



Eigenvalues of S with filtering of C at 0.5 (114 cols)



Example of C filtering : summary

bayer01 - 16 partitions

	0	0.1	0.3	0.4	0.45
Size of S	2469	784	254	162	137
Nb. Iter. $w = \bar{A}^{+}b$	1	155	334	491	577
Med./Max Iter. S	1	24/43	33/64	51/121	59/160
$\|r\|/\|b\|$	$5e-14$	$3e-9$	$1e-7$	$1e-9$	$2e-9$
$\|x^* - x\|_\infty/\|x^*\|_\infty$	$3e-9$	$4e-6$	$4e-5$	$9e-6$	$7e-5$

lhr34c - 8 partitions

0	0.1	0.3
1803	1299	465
1	44	192
1	24/43	166/496
$2e-7$	$9e-3$	$7e-2$
$2e-2$	$1e-1$	$3e-1$

gre_1107 - 5 partitions

0	0.1	0.45
1138	904	86
1	9	122
1	9/10	127/133
$1e-10$	$9e-8$	$1e-7$
$9e-5$	$2e-2$	$4e-2$

Open Issues / Future Work

- Build simultaneously, and in parallel, multiple columns of S
- Investigate iteration solution without building S
- Sparse approximation of S as a preconditioner
- Investigate numerically stable alternatives to CG for semi-positive definite systems
- Analyze the benefit in the case of multiple (successive) RHS
- Investigate memory requirements and trade-offs with respect to computational work
- Chebyshev filters to precondition Pz computation
- Extensive analysis of the parallel implementation of the method

Thank you for your attention!

email:
mohamed.zenadi@enseeiht.fr