Aggregation-based algebraic multigrid

from theory to fast solvers

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Outline

ULB

1. Introduction
2. AMG preconditioning and K-cycle
3. Two-grid analysis
4. Aggregation procedure
   - Repeated pairwise aggregation
5. Multi-level analysis
6. Parallelization
7. Numerical results
8. Conclusions

1. Introduction

ULB

Ubiquitous need:

Efficient methods to solve large sparse linear systems

In many cases, the design of an appropriate iterative linear solver is much easier if one has at hand a library able to efficiently solve linear (sub)systems

$$A\,\mathbf{u} = \mathbf{b}$$

where A corresponds to the discretization of

$$-\text{div}(D\,\textbf{grad}(u)) + \mathbf{v}\,\textbf{grad}(u) + c\,u = f \qquad (+B.C.)$$

(or closely related).

Efficiently:

robustly (stable performances)

in linear time: $\frac{\text{elapsed}}{n \times \#\text{proc}}$ roughly constant

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Why algebraic multigrid (AMG)?

- Geometric multigrid: needs a predefined set of grids
- AMG attempts to obtain the same effect using only the information present in the system matrix A

  (Reminder: effect = efficient damping of “smooth” error components, that can be seen only from large scale)

1. Introduction

ULB

Two-grid Algorithm

(as in Ulrich Rüde talk)

(1) Relax several times on grid h, obtaining $\widetilde{u}^h$ with a smooth corresponding error

(2) Calculate the residual:
$r^h = f^h - L^h \widetilde{\mathbf{u}}^h$

(3) Solve approximate error-equation on the coarse grid:
$L^H v^H = f^H \equiv I_h^H r^h$

(4) Interpolate and add correction: $\widetilde{u}^h \leftarrow \widetilde{u}^h + I_H^h v^H$

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(algebraic notation for linear system $A\,\mathbf{u} = \mathbf{b}$ with smoother M ; $\mathbf{u}_k$ is the current approximation)

(1) $\widetilde{\mathbf{u}} = \mathbf{u}_k + M^{-1}(\mathbf{b} - A\,\mathbf{u}_k)$

(2) $\widetilde{\mathbf{r}} = \mathbf{b} - A\,\widetilde{\mathbf{u}}$

(3) $A_c \mathbf{v}_c = \mathbf{r}_c \equiv R\,\widetilde{\mathbf{r}}$
(R : restriction, $n_c \times n$)

(4) $\widetilde{\mathbf{u}} \leftarrow \widetilde{\mathbf{u}} + P\,\mathbf{v}_c$
(P : prolongation, $n \times n_c$)

(5) $\mathbf{u}_{k+1} = \widetilde{\mathbf{u}} + M^{-1}(\mathbf{b} - A\,\widetilde{\mathbf{u}})$

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$\rightarrow$ Try to obtain P from A

1. Intro: Why aggregation-based AMG?

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Classical AMG

- Heuristic algorithms to mimic geometric multigrid
  (Connectivity $\rightarrow$ set of coarse nodes;
  Matrix entries $\rightarrow$ interpolation rules)
- Need to be used recursively:
  $A_c = P^T A\, P \rightarrow A_{cc} = P_c^T A_c\, P_c$, etc
  Is a good algorithm for A also good for A_c ?
- Several variants and parameters;
  relevant choices depend on applications
- Main difficulty:
  Find a good tradeoff between accuracy and the mastering of “complexity” (i.e., the control of the sparsity in successive coarse grid matrices)

1. Intro: Aggregation-based AMG

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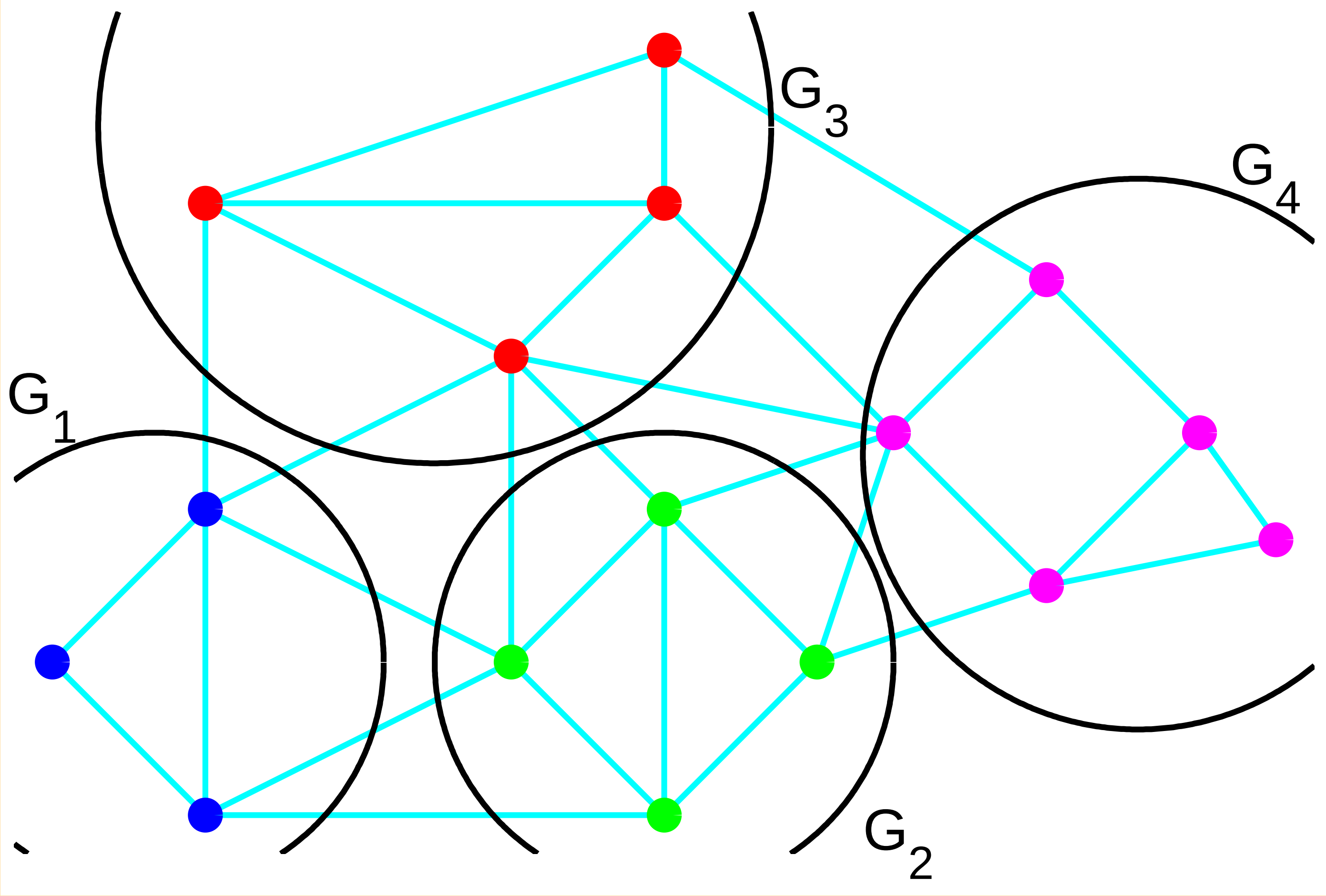
Group nodes into aggregates G_i (partitioning of $[1\,,\,n]$)

Each set corresponds to 1 coarse variable
(and vice-versa)



1. Intro: Aggregation-based AMG

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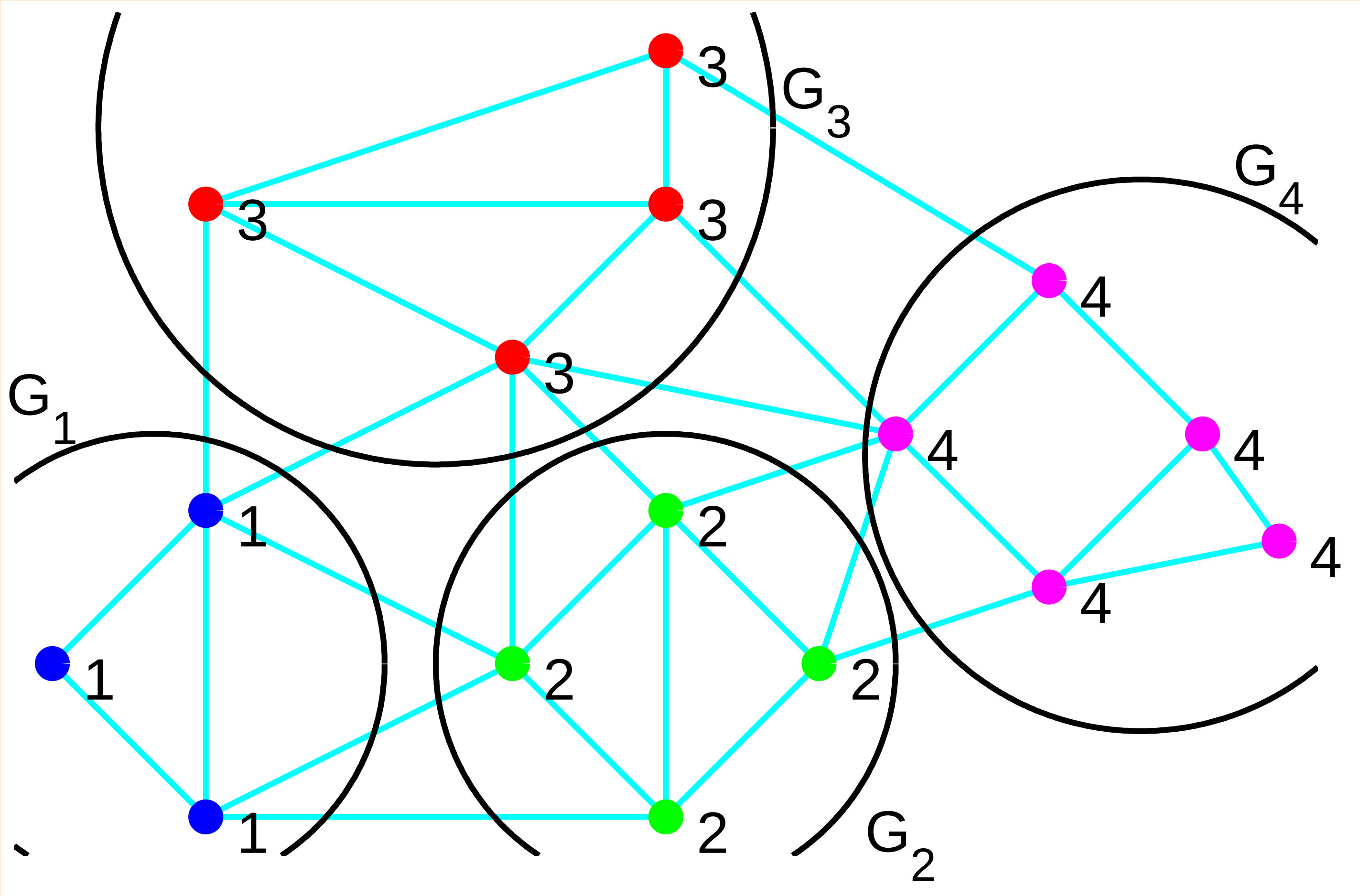
Prolongation P : $P_{ij} = \begin{cases} 1 & \text{if } i \in G_j \\ 0 & \text{otherwise} \end{cases}$

Example

$\mathbf{u}_c = \begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \end{pmatrix} \rightarrow$

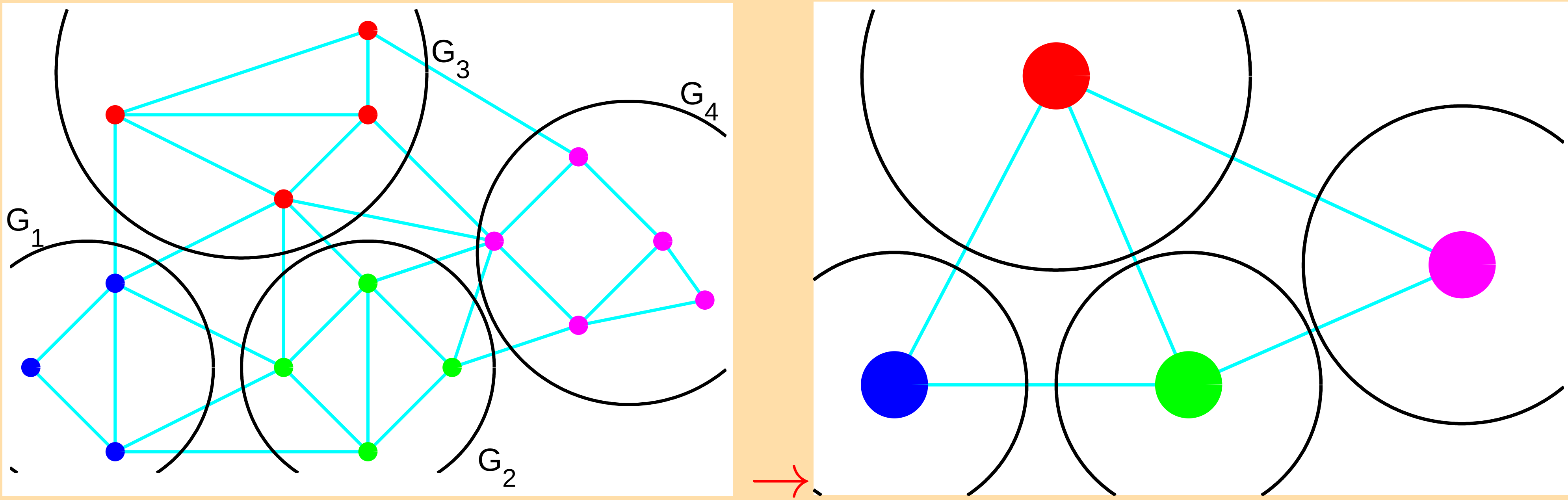


1. Intro: Aggregation-based AMG

ULB

Coarse grid matrix: $A_c = P^T A P$ given by

$$(A_c)_{ij} = \sum_{k \in G_i} \sum_{\ell \in G_j} a_{k\ell}$$



Tends to reproduce the stencil from the fine grid

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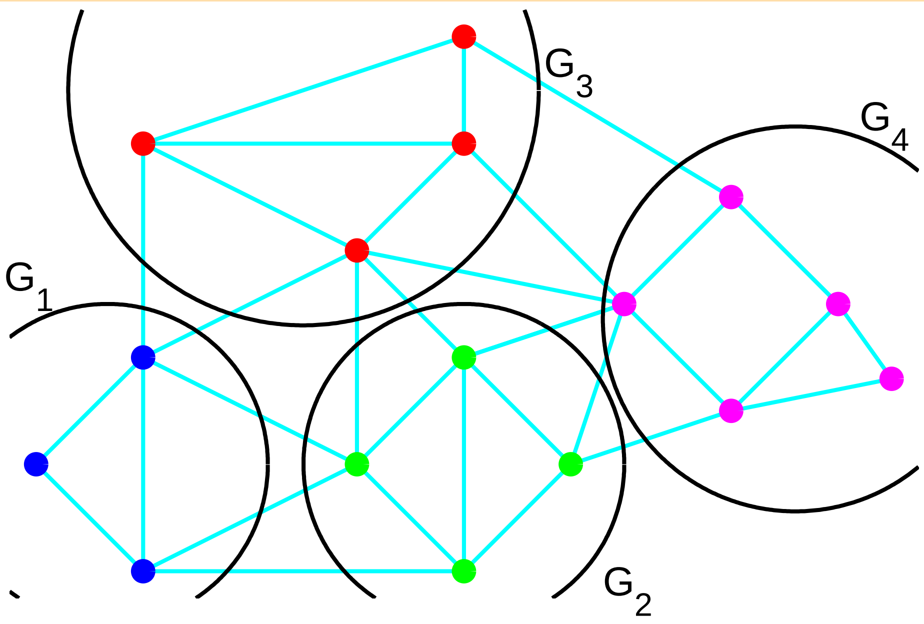

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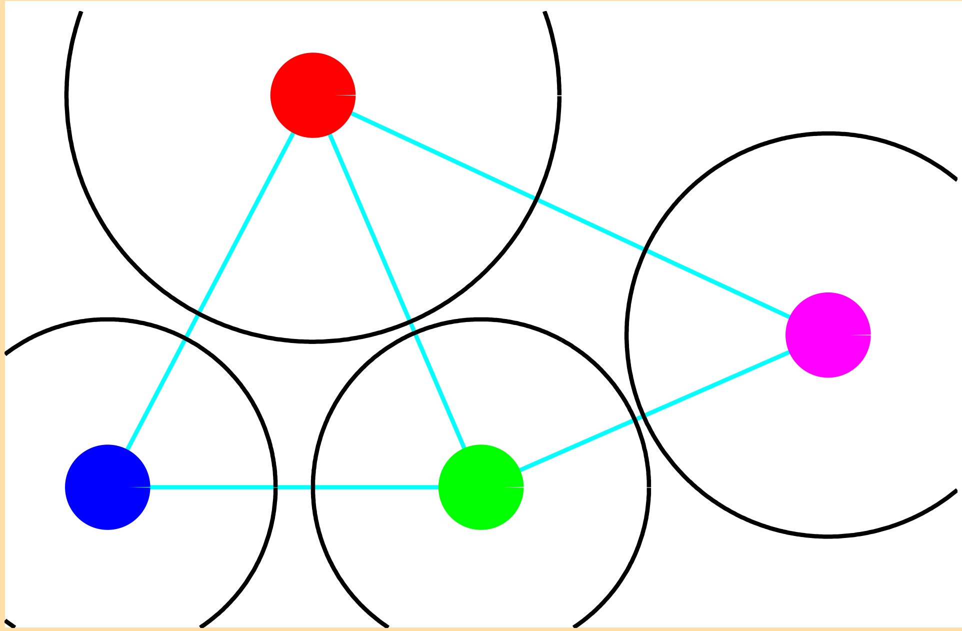

Tends to reproduce the stencil from the fine grid

Recursive use raises no difficulties

Low setup cost & memory requirements

1. Intro: Aggregation-based AMG

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- Does not mimic any classical multigrid method
- Not efficient if the piecewise constant P just substitutes the classical prolongation in a standard multigrid scheme

$\rightarrow$ has been overlooked for a long time

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Recent revival:

- Proper convergence theory (mimicry not essential for a good interplay with the smoother)
- Efficient when combined with specific components: preconditioner for a Krylov method, cheap smoother & K-cycle (Krylov for coarse problems – all levels)
- Theory and efficient solver developed hand in hand

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2. AMG preconditioning and K-cycle

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Reminder:

Stationary iteration: $\mathbf{u}_{k+1} = \mathbf{u}_k + M^{-1}(\mathbf{b} - A\,\mathbf{u}_k)$

Corresponding preconditioning step:

$$\mathbf{v}_k = M^{-1}\mathbf{r}_k \quad (\mathbf{r}_k = \mathbf{b} - A\,\mathbf{u}_k)$$

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$\rightarrow$ for multigrid, rewrite the algorithm above as

$$\mathbf{u}_{k+1} \;=\; \mathbf{u}_k + B(\mathbf{b} - A\,\mathbf{u}_k)\ ;$$

B is the inverse of the preconditioner and

$$\mathbf{v}_k \;=\; B\,\mathbf{r}_k$$

the corresponding preconditioning step

2. AMG preconditioning and K-cycle

ULB

Benefit of Krylov

- Relaxed convergence conditions
- Scaling-independent convergence, characterized by the condition number (λ_i eig of $B\,A$) :

SPD: $$\kappa = \frac{\max_i \lambda_i}{\min_i \lambda_i} = \frac{\lambda_{\max}(B\,A)}{\lambda_{\min}(B\,A)}$$

General: $$\frac{\max_i |\lambda_i|}{\min_i \Re\mathrm{e}(\lambda_i)} \quad \text{or} \quad \frac{1}{\min_i \Re\mathrm{e}(1/\lambda_i)\ \min_i \Re\mathrm{e}(\lambda_i)}$$

(All eigs with positive real part)

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Fast convergence:

if all λ_i bounded & substantially away from 0

2. AMG preconditioning and K-cycle

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K-cycle

- Reminder: recursive use of the two-grid scheme:
  - $A_c \mathbf{v}_c = \mathbf{r}_c$ not solved exactly
  - $\mathbf{v}_c \leftarrow$ approximate solution from multigrid step(s) to solve the coarse system
  - 1 step $\rightarrow$ V-cycle
    2 steps $\rightarrow$ W-cycle
- K-cycle: solve $A_c \mathbf{v}_c = \mathbf{r}_c$ with 2 steps of a Krylov method with multigrid preconditioner at coarser level

  (essentially: W-cycle with Krylov acceleration)

2. AMG preconditioning and K-cycle

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K-cycle -vs- V- & W-cycles

Number of iterations to reduce relative residual error by 10^{-12} as a function of the number of levels and of the convergence factor of the two grid method at each level

	7 levels	14 levels
$0.49 < \rho_{TG} < 0.50$ $(1.99 < \kappa_{TG} < 2.00)$		
V	188	> 999
W	37	50
K	20	20
$0.79 < \rho_{TG} < 0.80$ $(4.86 < \kappa_{TG} < 4.92)$		
V	256	> 999
W	108	315
K	42	44

2. AMG preconditioning and K-cycle

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- $\neq$ from classical multigrid theory, based on a global view of all levels (or scales)
- Classical multigrid: use “enough” smoothing steps to have spectral radius as small as desired

  Aggregation-based AMG:
  compensate for the larger condition number with Krylov, but also cheap smoothing stage (typically: one Gauss-Seidel sweep for pre- and post-smoothing)

Computational complexity

$$\text{Work} \sim C_W = \frac{\sum_{k=0}^{\ell} 2^k \, nnz(A_k)}{nnz(A)}$$

($A_0 = A$, $A_1 = A_c$, etc; $\ell =$ number of levels)

$\rightarrow$ ensure $\dfrac{nnz(A_k)}{nnz(A_{k-1})} \lesssim \dfrac{1}{4}$

(then $2^k nnz(A_k) \lesssim 2^{-k} nnz(A)$ and $C_W \lesssim 2$)

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With aggregation-based methods:

$$\frac{nnz(A_k)}{nnz(A_{k-1})} \approx \frac{1}{\text{Mean aggregates' size}}$$

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The aggregation algorithm we use is entirely based on the theory and its heuristic extensions

3. Two-grid analysis

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- Method used as a preconditioner for CG or GCR

  $\rightarrow$ Fast convergence if the eigenvalues λ_i of the preconditioned matrix are:

  - bounded
  - substantially away from 0

- Using a standard smoother (e.g., Gauss-Seidel), the eigenvalues are bounded independently of P
- If $P = 0$ the eigenvalues associated with "smooth" modes are in general very small
  - $\rightarrow$ Main difficulty: λ_i substantially away from 0
  - Role of the coarse grid correction: move the small eigenvalues enough to the right (Guideline for the choice of P)

3. Two-grid analysis: λ_i away from 0

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SPD case

Main identity [Falgout, Vassilevski & Zikatanov (2005)]:

$$\lambda_{\min} = \frac{1}{\kappa(A\,,\,P)}$$

with

$$\kappa(A,P) = \omega^{-1} \sup_{\mathbf{v}\neq 0} \frac{\mathbf{v}^T D\left(I - P(P^T D\, P)^{-1} P^T D\right)\mathbf{v}}{\mathbf{v}^T A \mathbf{v}}$$

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General case [YN (2010)]

For any λ_i :

$$\Re\mathrm{e}(\lambda_i) \geq \frac{1}{\kappa(A_S\,,\,P)}$$

with $A_S = \frac{1}{2}(A + A^T)$

The analysis of the SPD case can be sufficient

3. Two-grid analysis: λ_i away from 0

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Aggregation-based methods

$$P = \begin{pmatrix} \mathbf{1}_{n^{(1)}} & & \\ & \ddots & \\ & & \mathbf{1}_{n^{(n_c)}} \end{pmatrix} \quad , \quad D = \text{diag}(A) = \begin{pmatrix} D_1 & & \\ & \ddots & \\ & & D_{n_c} \end{pmatrix}$$

$$\rightarrow D\left(I - P(P^T D\, P)^{-1} P^T D\right)$$
$$= \text{blockdiag}\left(D_i\left(I - \mathbf{1}_{n^{(i)}}(\mathbf{1}_{n^{(i)}}^T D_i\, \mathbf{1}_{n^{(i)}})^{-1} \mathbf{1}_{n^{(i)}}^T D_i\right)\right)$$

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$\rightarrow$ find A_b, A_r nonnegative definite s.t. $A_S = A_b + A_r$ with

$$A_b = \begin{pmatrix} A_{G_1}^{(S)} & & \\ & \ddots & \\ & & A_{G_{n_c}^{(S)}} \end{pmatrix}$$

3. Two-grid analysis: λ_i away from 0

$$\kappa(A_S, P) \leq \omega^{-1} \sup_{\mathbf{v}\neq 0} \frac{\mathbf{v}^T D \left(I - P(P^T D\, P)^{-1} P^T D\right) \mathbf{v}}{\mathbf{v}^T A_b \mathbf{v}}$$

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Aggregate Quality

$$\mu_G = \omega^{-1} \sup_{\mathbf{v}\notin\mathcal{N}(A_G^{(S)})} \frac{\mathbf{v}^T D_G(I - \mathbf{1}_G(\mathbf{1}_G^T D_G \mathbf{1}_G)^{-1}\mathbf{1}_G^T D_G)\mathbf{v}}{\mathbf{v}^T A_G^{(S)} \mathbf{v}} ,$$

Then: $\kappa(A_S\,,\,P) \;\leq\; \max_i \mu_{G_i}$

Controlling μ_{G_i} ensures that eigenvalues are away from 0

3. Two-grid analysis: λ_i away from 0

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Then: $\kappa(A_S\,,\,P) \leq \max_i \mu_{G_i}$

Controlling μ_{G_i} ensures that eigenvalues are away from 0

$A_G^{(S)}$: Computed from $A_S = A_b + A_r$ with $A_r\mathbf{1} = 0$

- Rigorous for M-matrices s.t. $A_S\mathbf{1} \geq 0$
(then A_b , A_r guaranteed nonnegative definite)
- Heuristic in other cases
(A_r could have negative eigenvalue(s))

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ULB

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- For a pair $\{i,j\}$, $\mu_{\{i,j\}}$ is a simple function of the "local" entries & the row and column sum
- $\mu_G \;=\; \omega^{-1}\sup_{\mathbf{z}\notin\mathcal{N}(A_G^{(S)})} \dfrac{\mathbf{z}^T D_G(I-\mathbf{1}_G\left(\mathbf{1}_G^T D_G \mathbf{1}_G\right)^{-1}\mathbf{1}_G^T D_G)\,\mathbf{z}}{\mathbf{z}^T A_G^{(S)}\,\mathbf{z}}$

  It is always cheap to check that $\mu_G < \overline{\kappa}_{\text{TG}}$ holds:

  $$Z_G \;=\; \overline{\kappa}_{\text{TG}}\, A_G^{(S)} - \omega^{-1} D_G(I - \mathbf{1}_G\,(\mathbf{1}_G^T D_G \mathbf{1}_G)^{-1}\,\mathbf{1}_G^T D_G)$$

  is nonnegative definite if no negative pivot occurs while performing an LDL^T factorization

Pairwise aggregation

Input: threshold $\bar{\kappa}_{\text{TG}}$

Output:

n_c and aggregates G_i , $i = 1 \ldots , n_c$

Initialization: $U = [1\,,\,n] \backslash G_0$, $n_c = 0$

Algorithm: While $U \neq \emptyset$ do

1. Select $i \in U$; $n_c = n_c + 1$
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3. **If** $\mu_{\{i,j\}} < \bar{\kappa}_{\text{TG}}$ **then** $G_{n_c} = \{i, j\}$ **else** $G_{n_c} = \{i\}$
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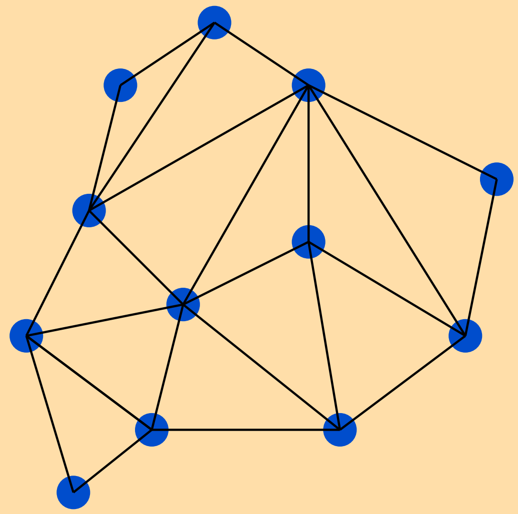

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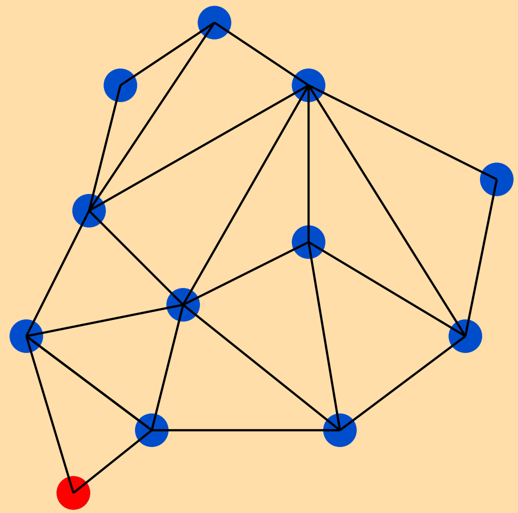

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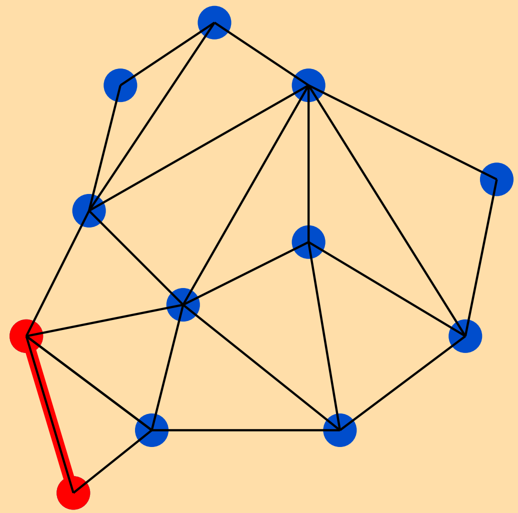

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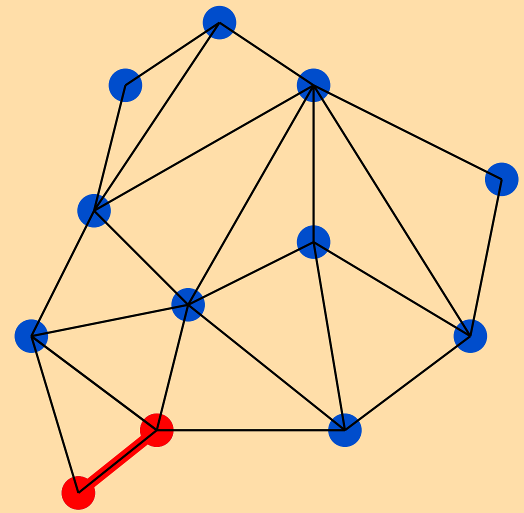

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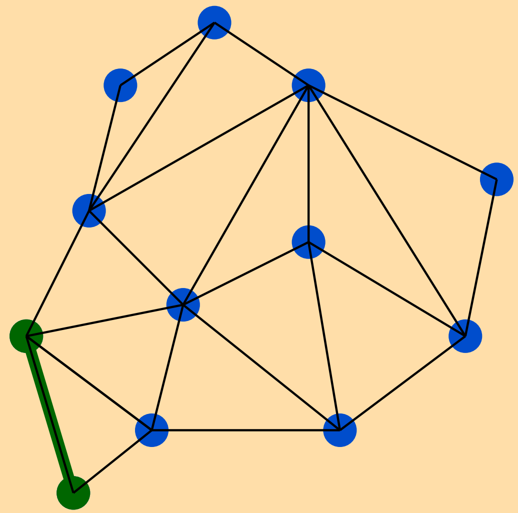

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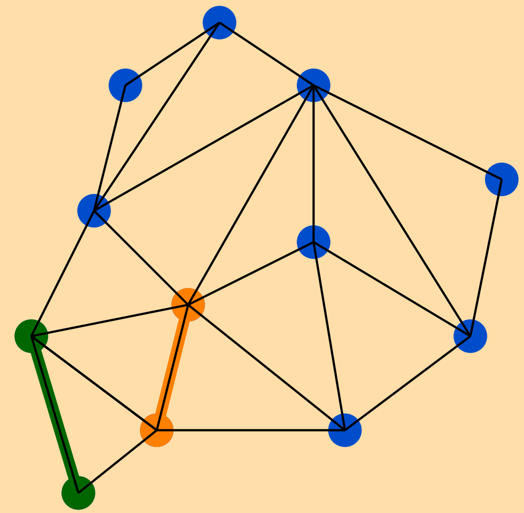

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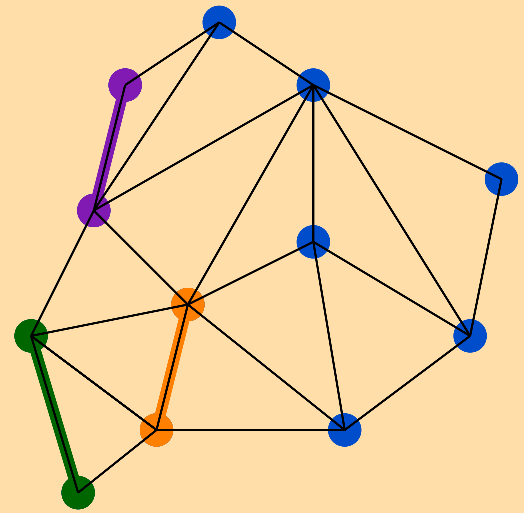


4. Repeated Pairwise aggregation

ULB

$s = 1 \; ; \; A^{(s)} = A$

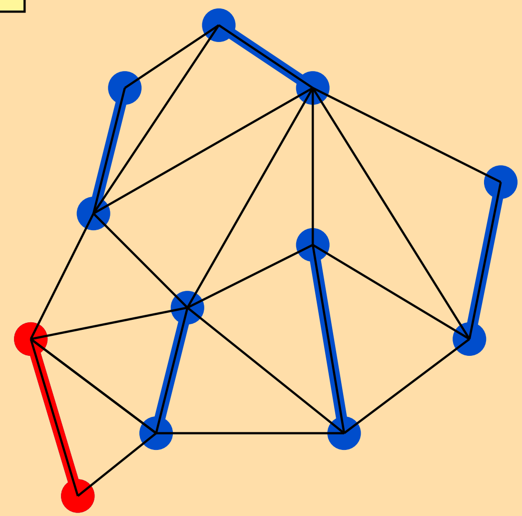
Apply pairwise aggregation to $A^{(s)}$

Form aggregated matrix $A^{(s+1)}$

$\mathit{nnz}(A^{(s+1)}) < \frac{\mathit{nnz}(A)}{\tau}$ or s==n_{pass} ?

no: $s \leftarrow s + 1$

yes: $A_c = A^{(s+1)}$



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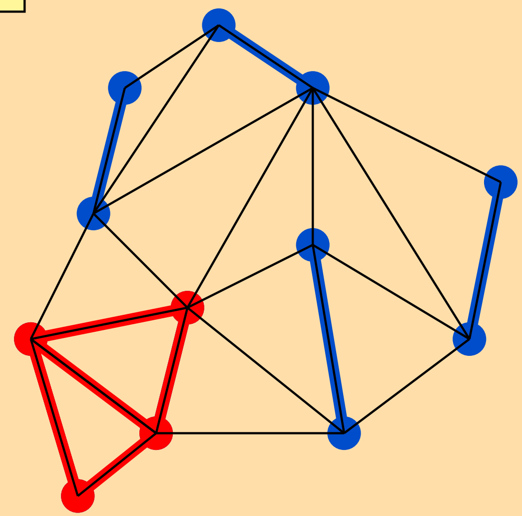

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yes ↓

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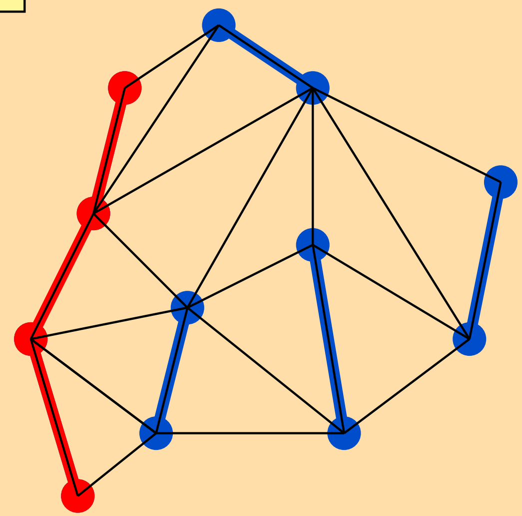

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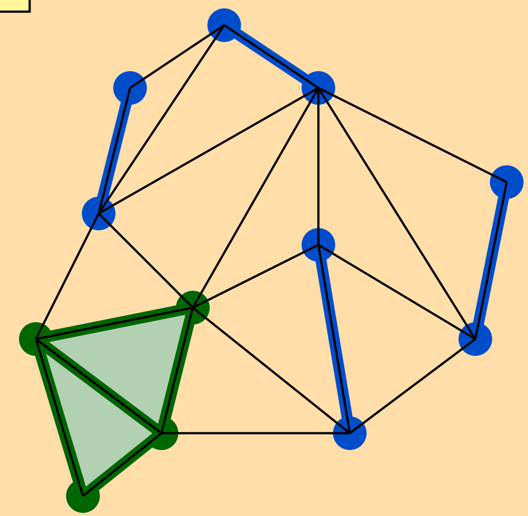

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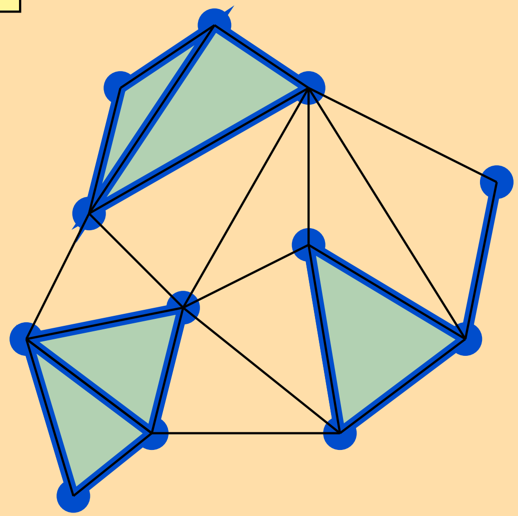
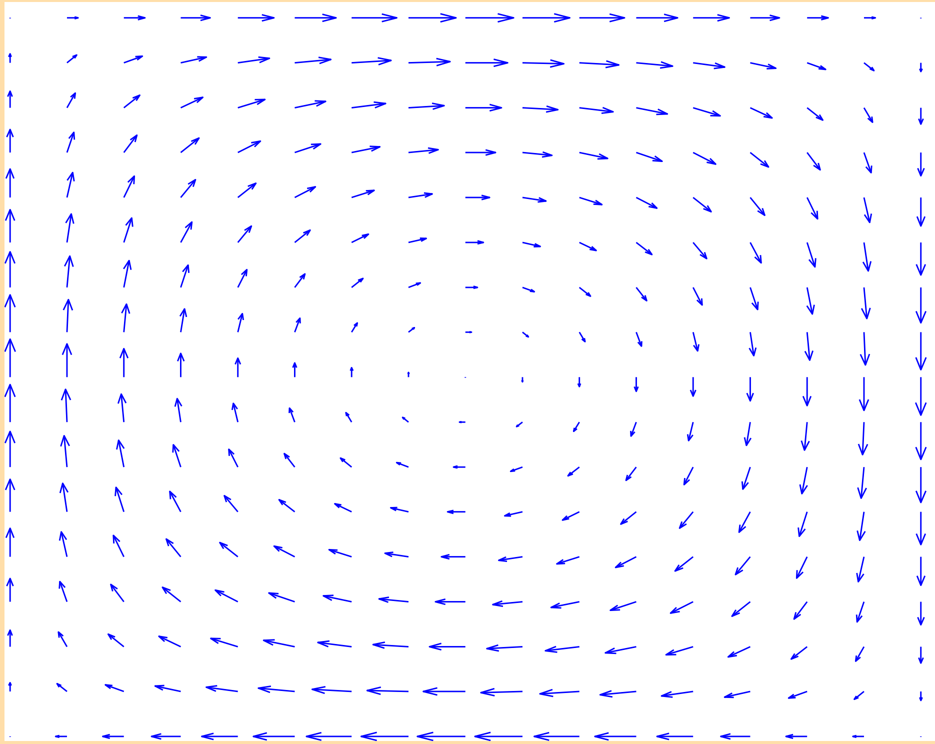


4. Aggregation procedure: Illustration

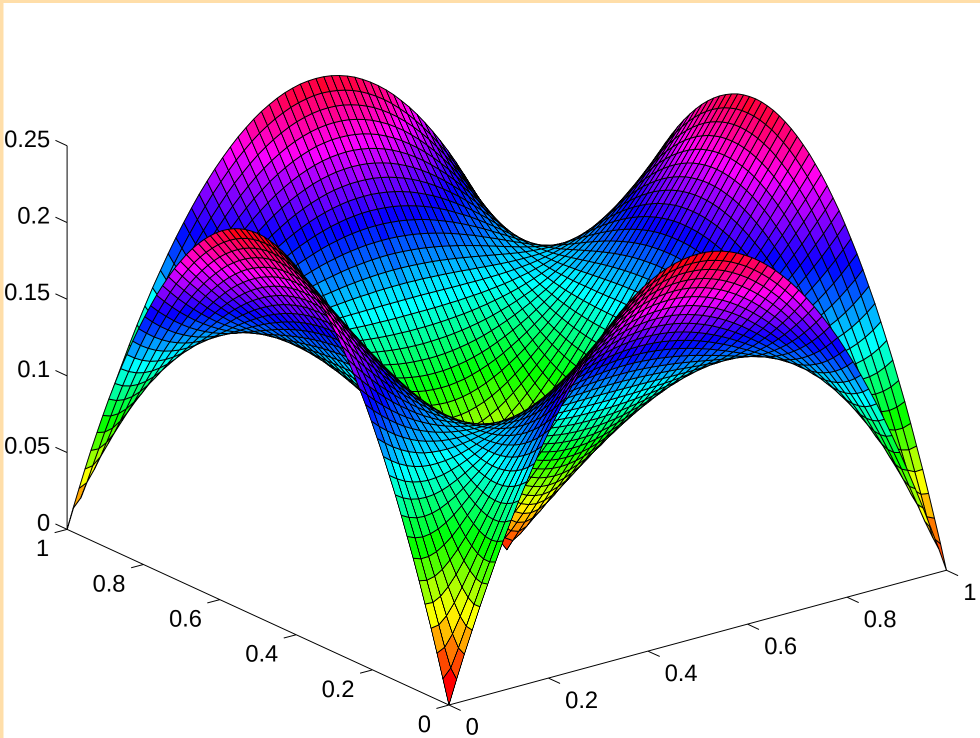
Upwind FD approximation of

$$-\nu\,\Delta\, u \;+\; \overline{v}\cdot\textbf{grad}(u) \;=\; f \quad \text{in}\;\; \Omega \;=\text{unit square}$$

with $u \;=\; g$ on $\partial\Omega$, $\overline{v}(x\,,\,y) = \begin{pmatrix} x(1-x)(2\,y-1) \\ -(2\,x-1)y(1-y) \end{pmatrix}$:



Direction of the flow

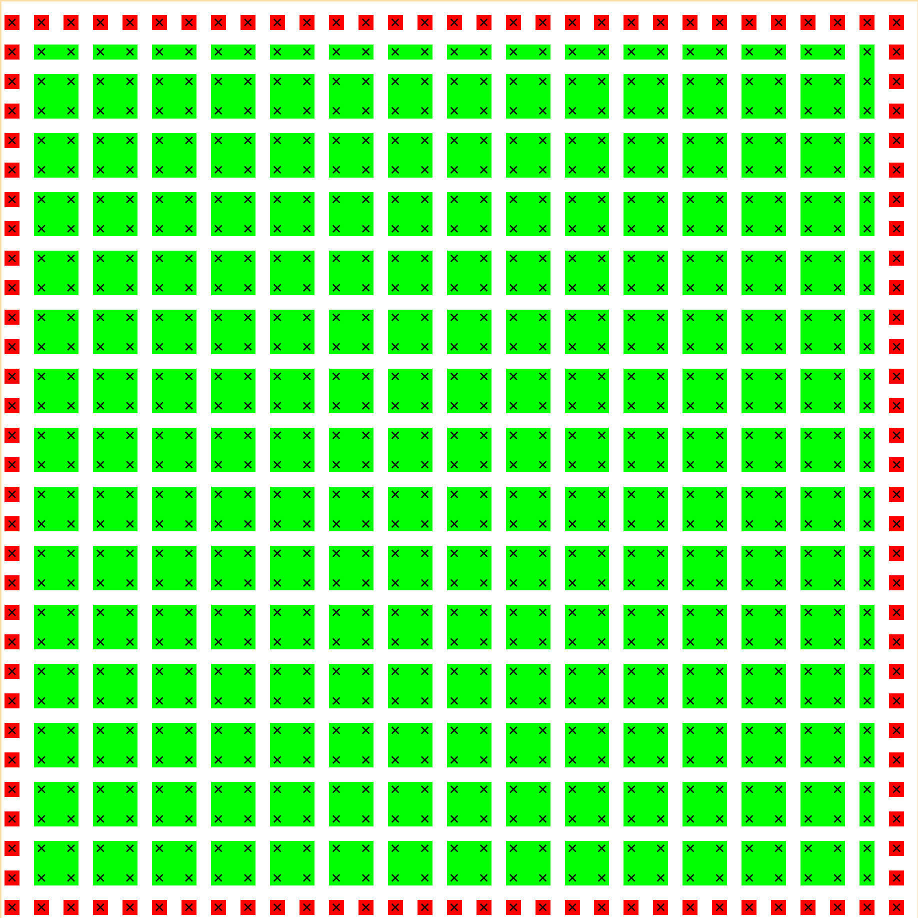


Magnitude

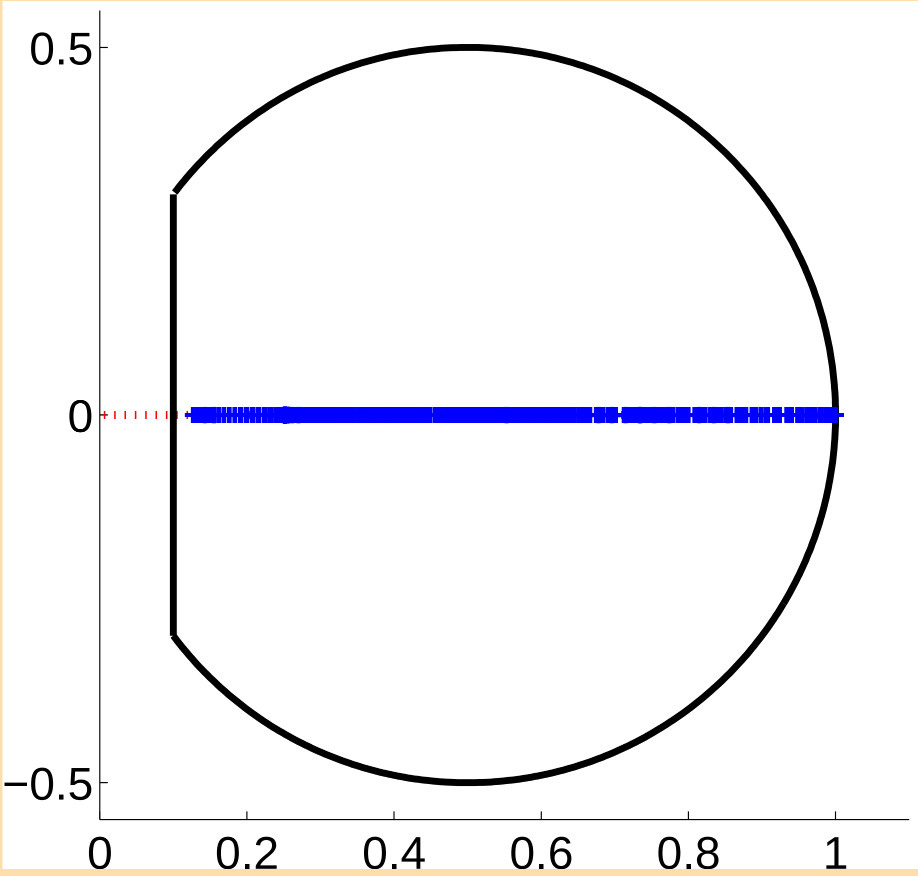
4. Aggregation procedure: Illustration

$\nu = 1$: diffusion dominating (near symmetric)

Aggregation



Spectrum



+ : $\sigma(I - T)$ — : theory

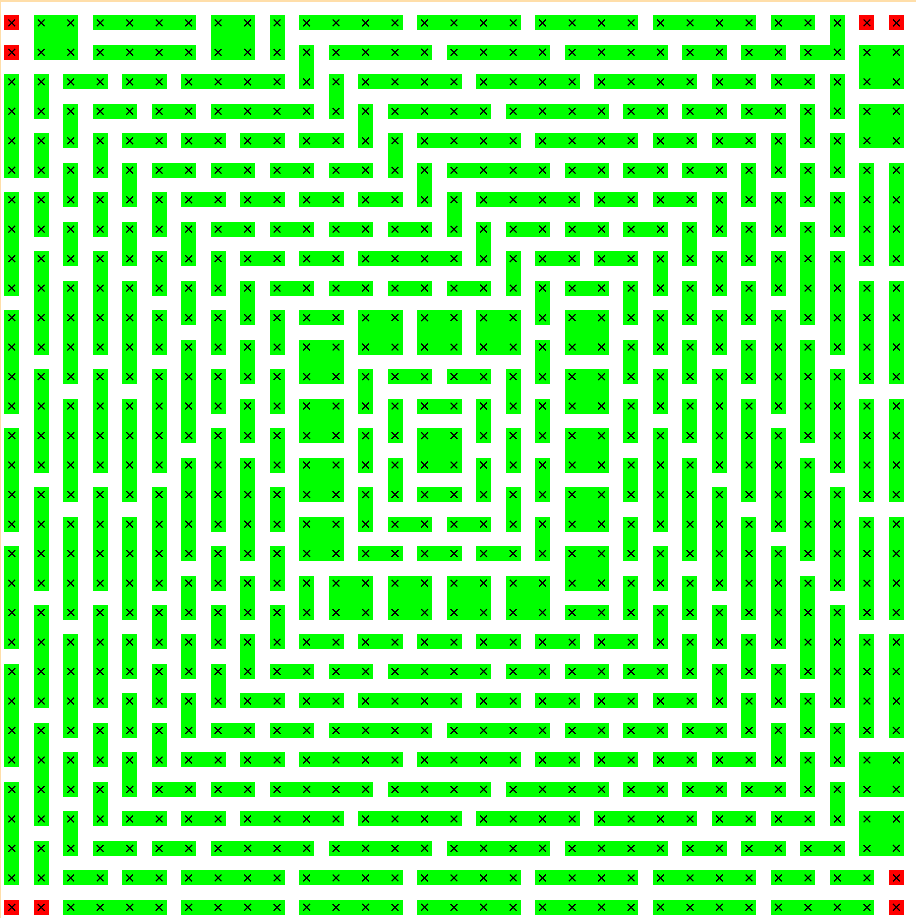
···· : $\sigma(\omega\, D^{-1} A)$ (convex hull)

4. Aggregation procedure: Illustration

ULB

$\nu = 10^{-3}$: convection dominating (strongly nonsymmetric)

Aggregation



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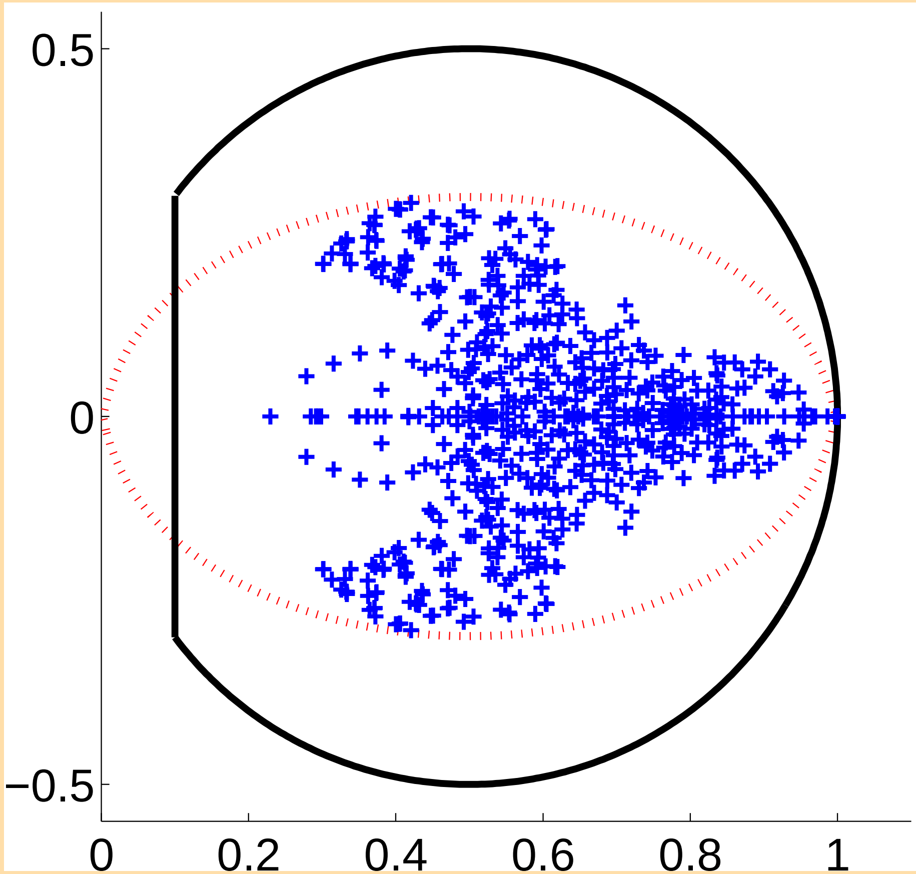

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ULB

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5. Multi-level analysis

ULB

Requires to exchange the K-cycle (Krylov acceleration) for the AMLI-cycle (polynomial acceleration; i.e., frozen coefficients)

- less flexible: requires a known bound $\overline{\rho}$ on the two-grid convergence factor
- less efficient in practice
- avoid nonlinearities $\rightarrow$ convergence proof easier
- upper bound on the convergence rate independent of the number of levels can be guaranteed with the sole assumption that $\overline{\rho}$ is below a given threshold

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Our aggregation procedure: allows to choose $\overline{\rho}$
(for symmetric M-matrices with nonnegative row sum)

5. Multi-level analysis:final result

- The method is purely algebraic and applies to any symmetric M-matrix with nonnegative row-sum

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  - independently of any regularity assumption

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Why ?

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Why ?

. . . because the upper bound is 27.056

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...because the upper bound is 27.056

Optimality requires in addition bounded complexity:

- can be proved for model problems on regular grids;
- no proof in general, but, in practice, no more complexity issues than with other AMG schemes: coarsening parameters selected for this.

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- During iterations: communications only for matvec and inner product computation

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7. Numerical results

ULB

Classical AMG talk on application

- Description of the application (beautiful pictures)
- Description of the AMG strategy and needed tuning
- Numerical results, often not fully informative:
  - no robustness study on a comprehensive test suite;
  - no comparison with state of the art competitors.

7. Numerical results

ULB

This talk

- Most applications ran by people downloading the code. Some of those I am aware of: CFD, electrocardiology (in general, I don't have the beautiful pictures at hand).

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- The code is used black box (adaptation neither sought nor needed)
- I think the most important is the robustness on a comprehensive test suite
- I like comparison with state of the art competitors

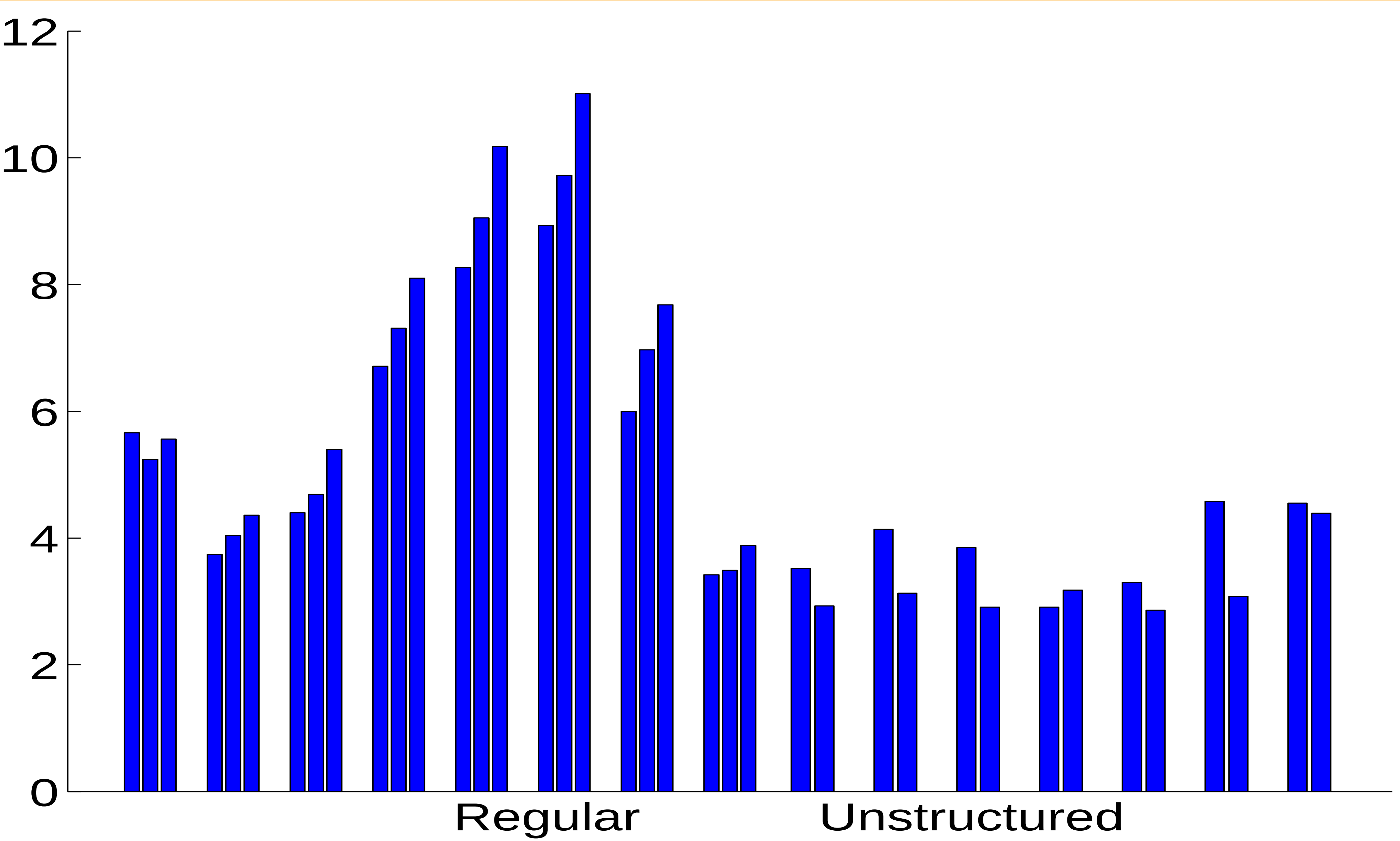
7. Numerical results

ULB

- Iterations stopped when $\frac{\|\mathbf{r}_k\|}{\|\mathbf{r}_0\|} < 10^{-6}$
- Times reported are total elapsed times in seconds (including set up) per 10^6 unknowns
- Test suite: discrete scalar elliptic PDEs
  - SPD problems with jumps and all kind of anisotropy in the coefficients (some with reentering corner)
  - convection-diffusion problems with viscosity from $1 \;\rightarrow\; 10^{-6}$ and highly varying recirculating flow
  - FD on regular grids; 3 sizes:
    2D: $h^{-1} = 600\,,\ 1600\,,\ 5000$
    3D: $h^{-1} = \ 80\,,\ \ 160\,,\ \ 320$
  - FE on (un)structured meshes (with different levels of local refinement); 2 sizes: $n = 0.15e6 \;\rightarrow\; n = 7.1e6$

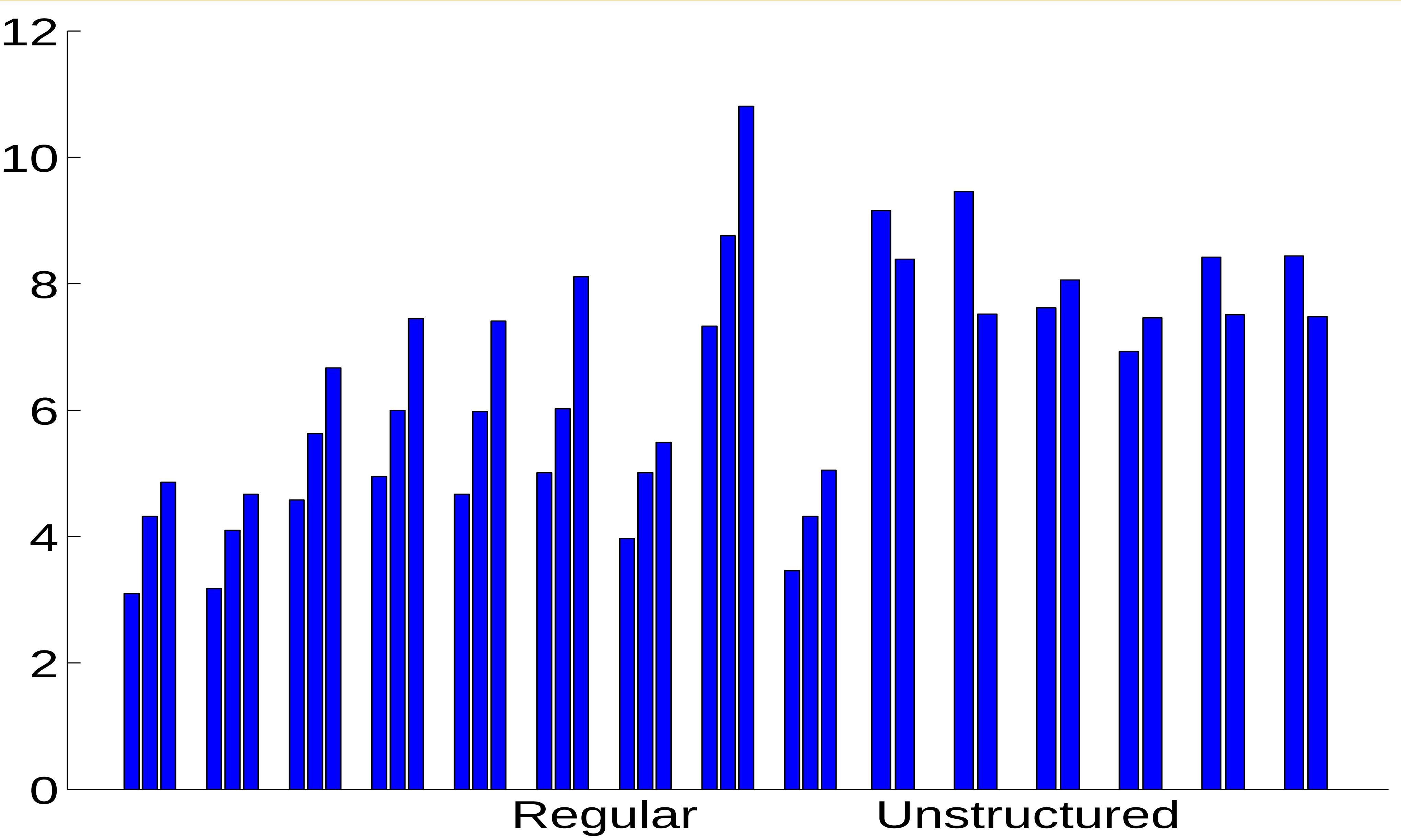
7. Numerical results

2D symmetric problems



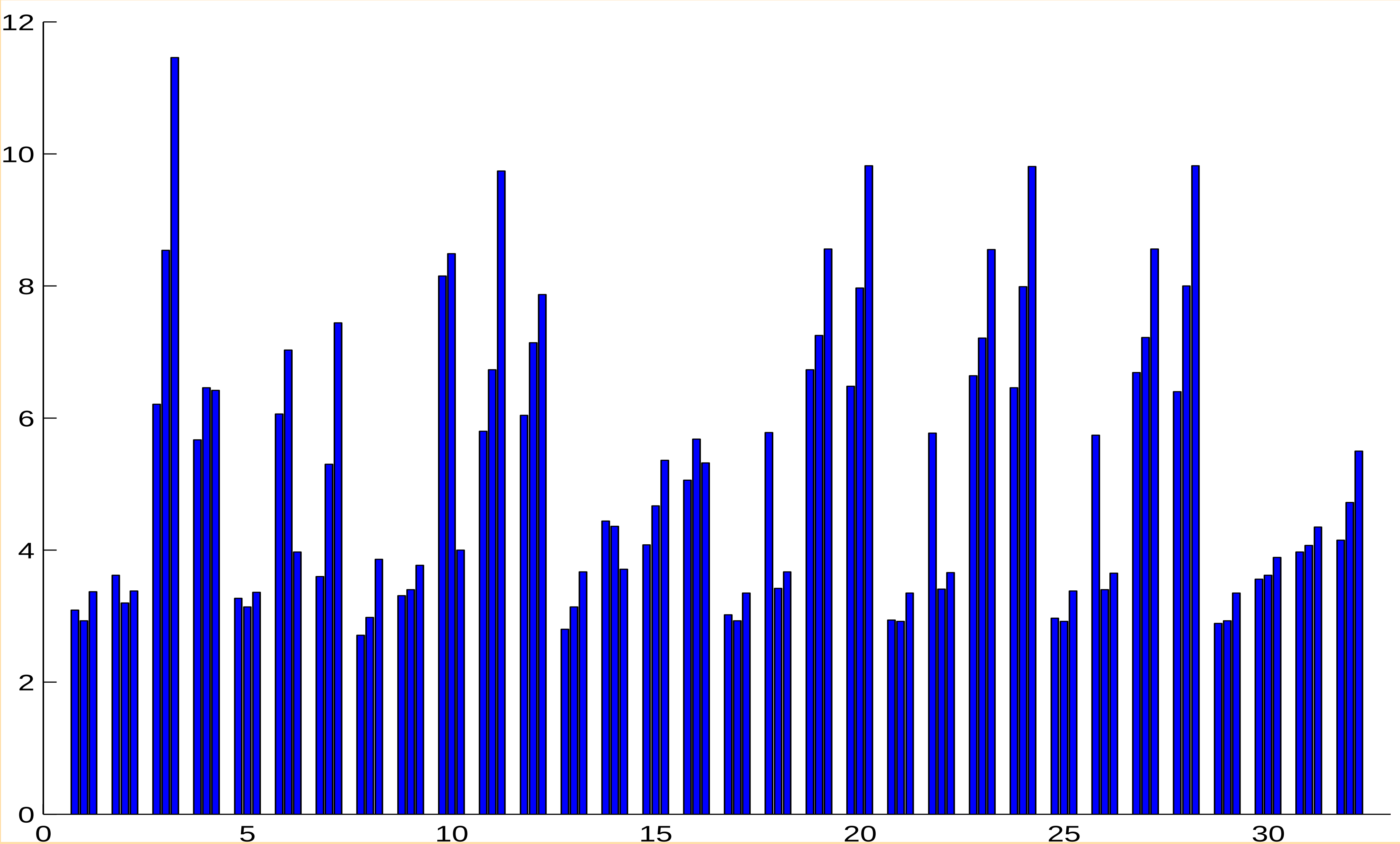
7. Numerical results

3D symmetric problems



7. Numerical results

2D nonsymmetric problems



7. Numerical results

ULB

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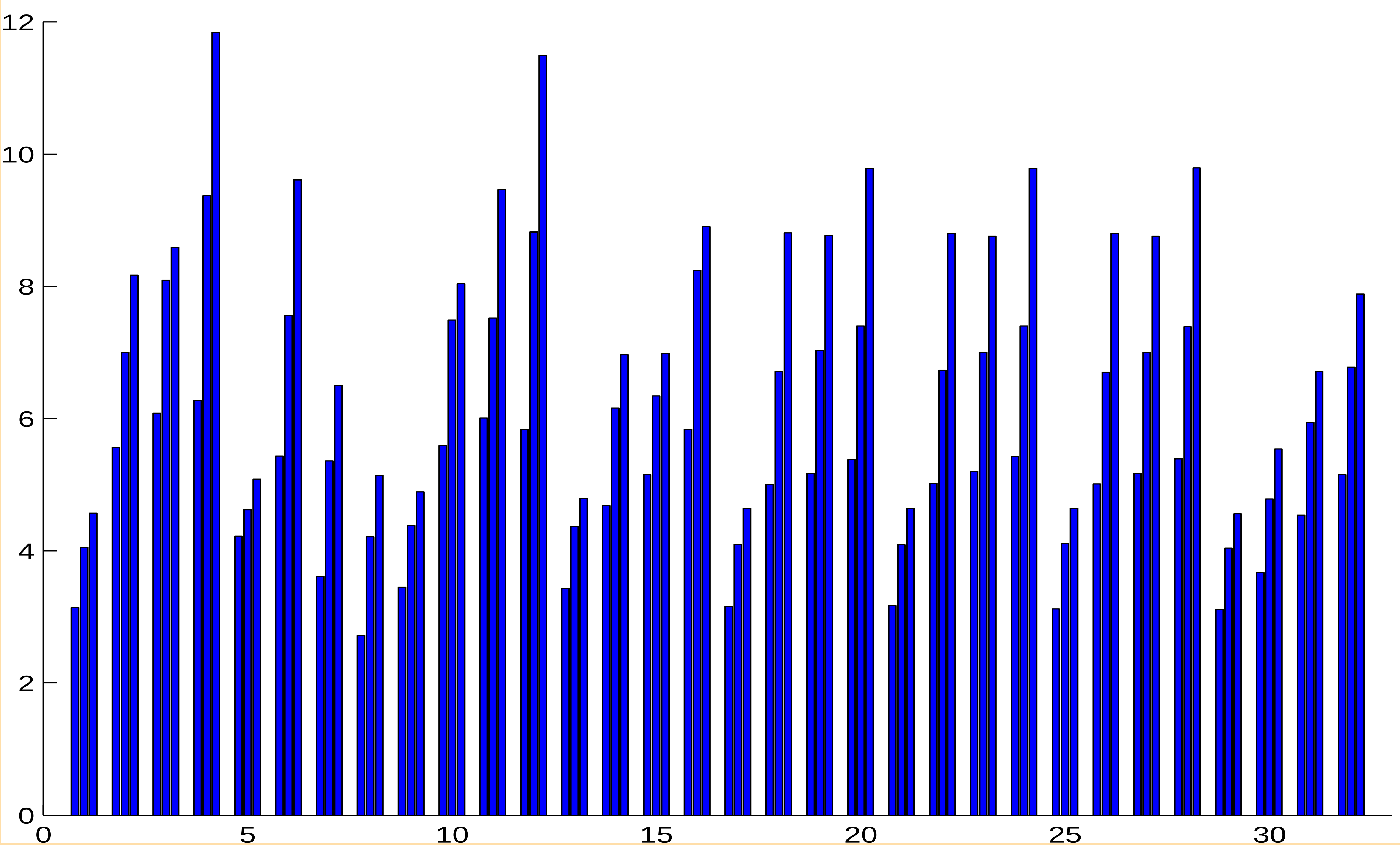


7. Numerical results

ULB

Comparison with other methods

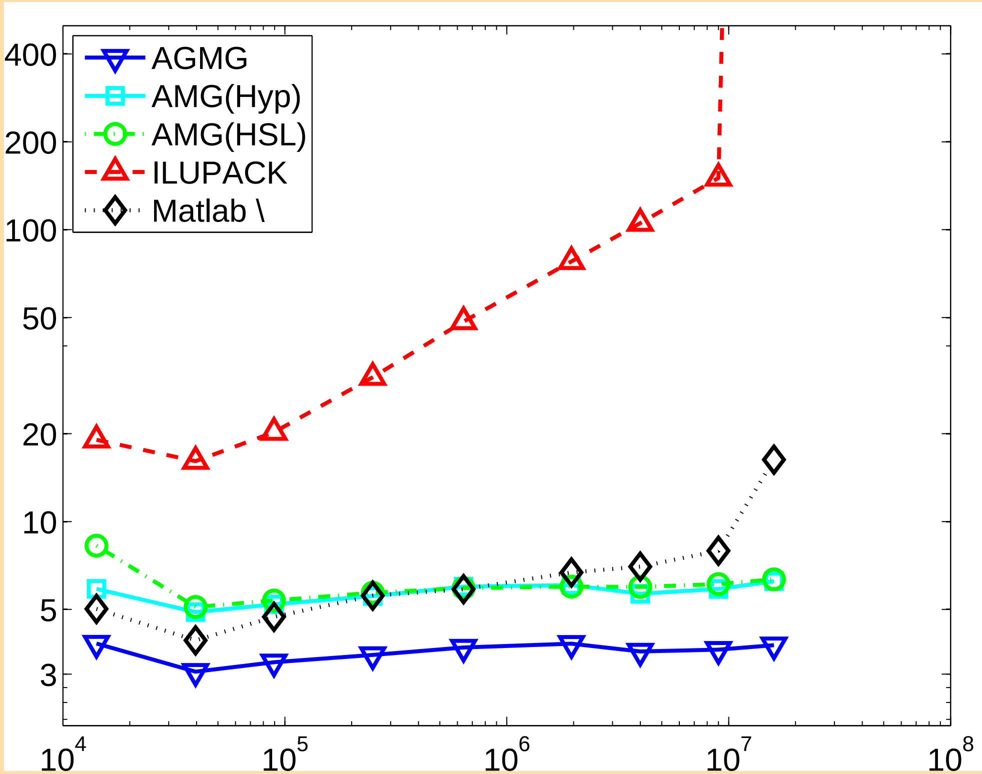
- AMG(Hyp): classical AMG method as implemented in the Hypre library (Boomer AMG)
- AMG(HSL): the classical AMG method as implemented in the HSL library
- ILUPACK: efficient threshold-based ILU preconditioner
- Matlab \: Matlab sparse direct solver (UMFPACK)

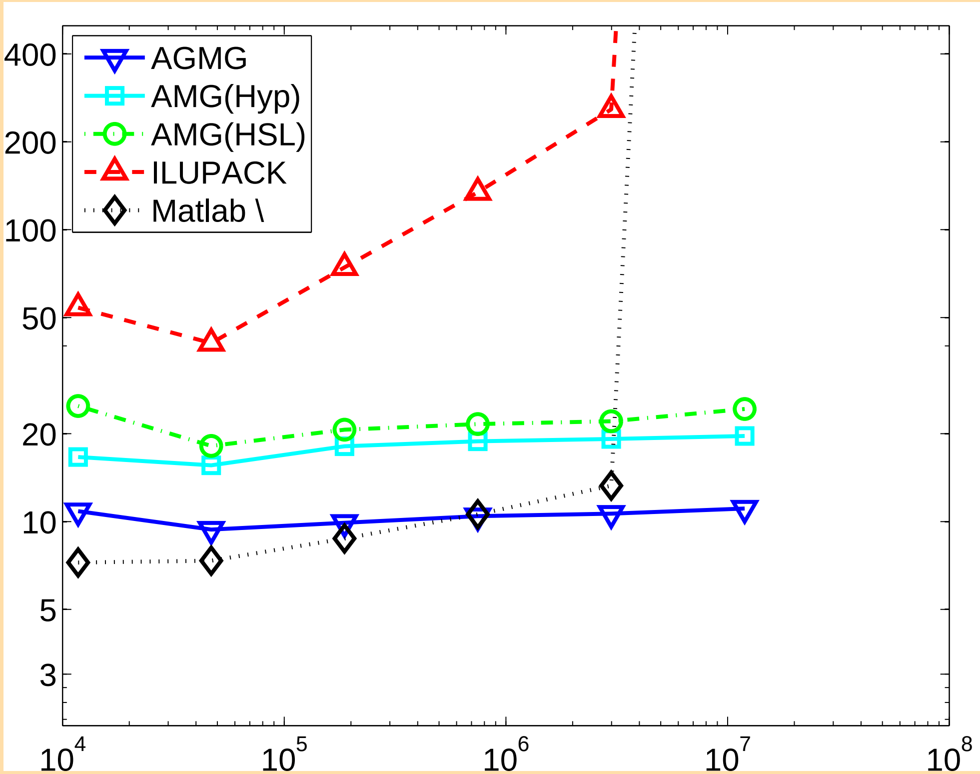
All methods but the last with Krylov subspace acceleration

7. Numerical results

ULB

Poisson 2D, FD	Laplace 2D, FE(p3)



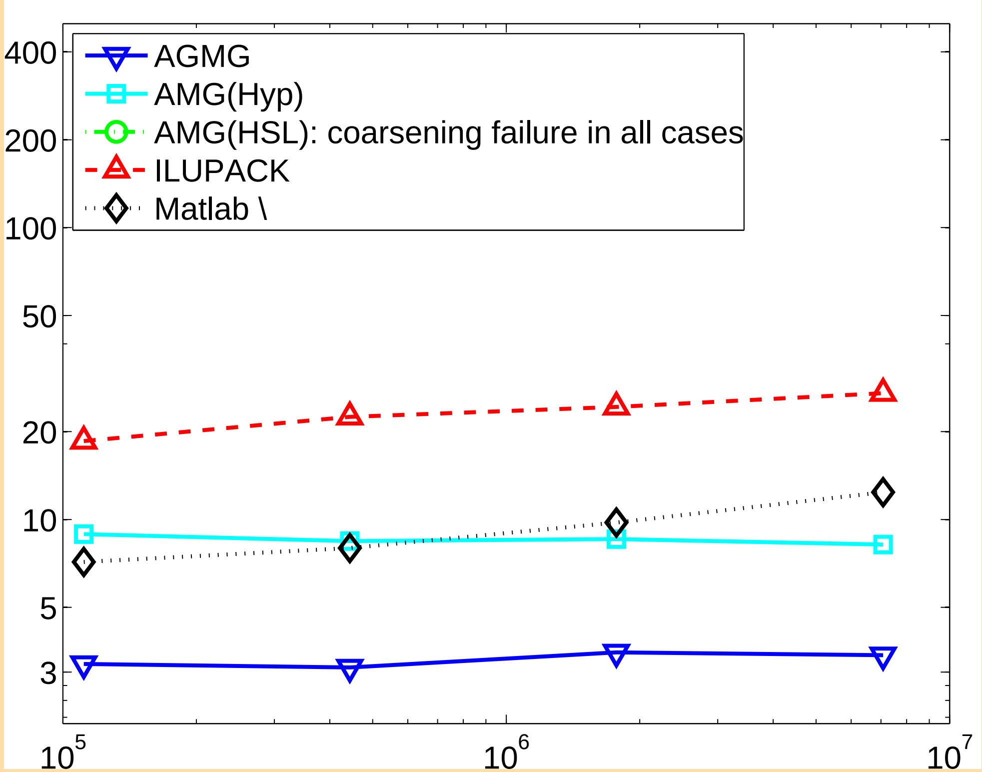


33% of nonzero offdiag > 0

7. Numerical results

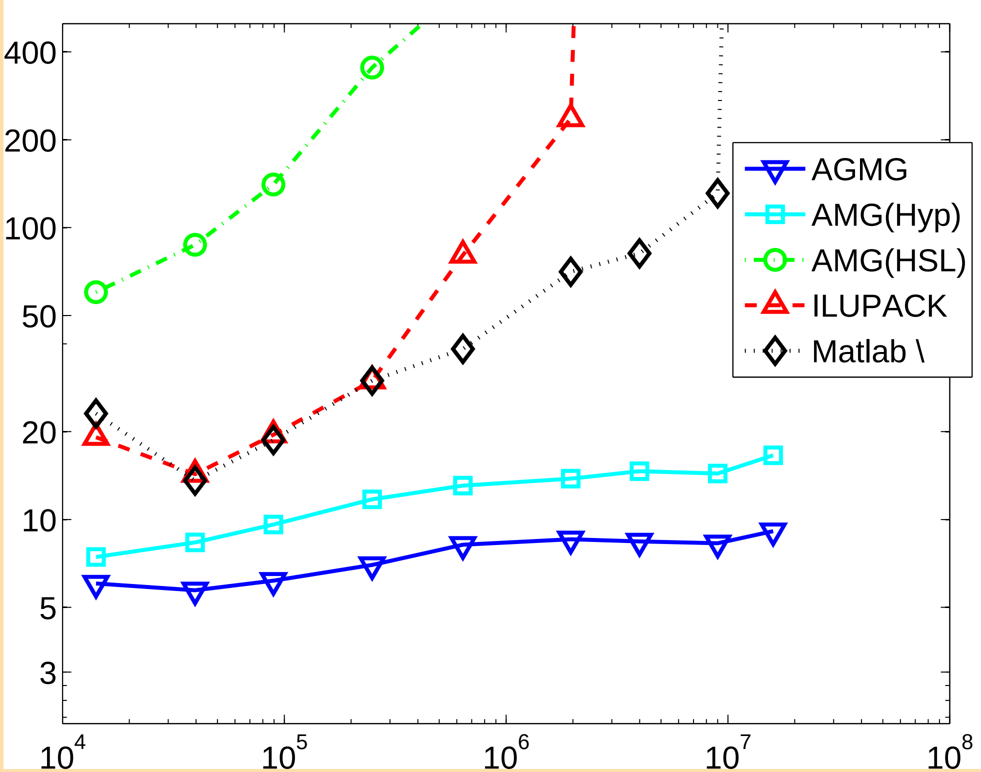
ULB

Poisson 2D, L-shaped, FE
Unstructured, Local refin.



Convection-Diffusion 2D, FD

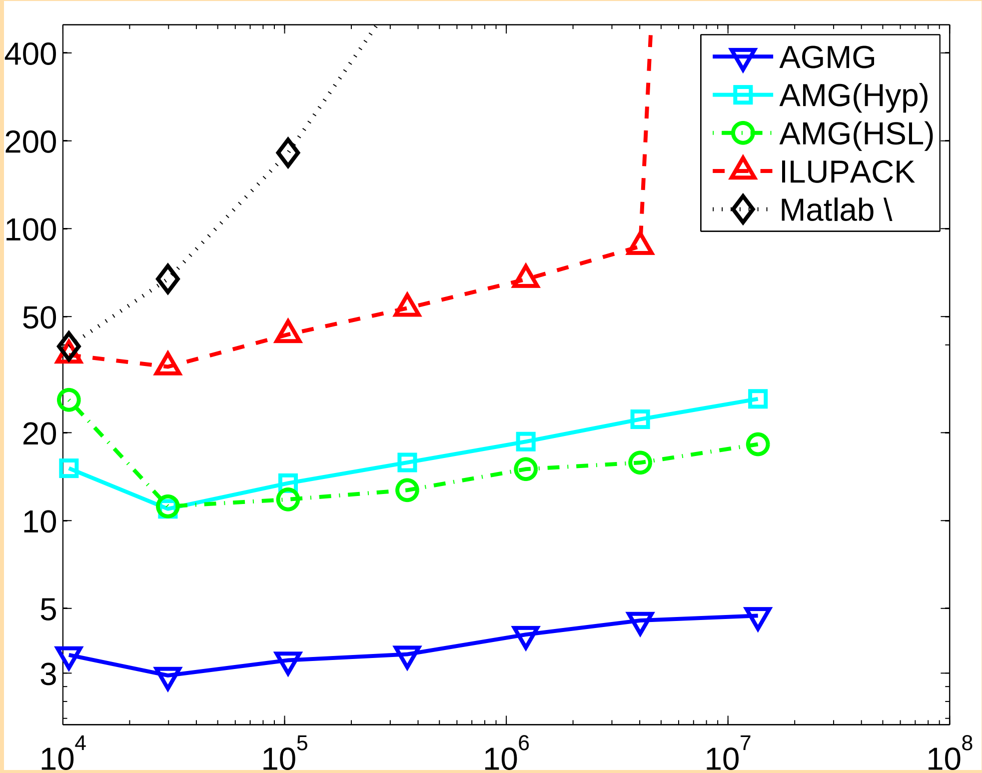
$\nu = 10^{-6}$



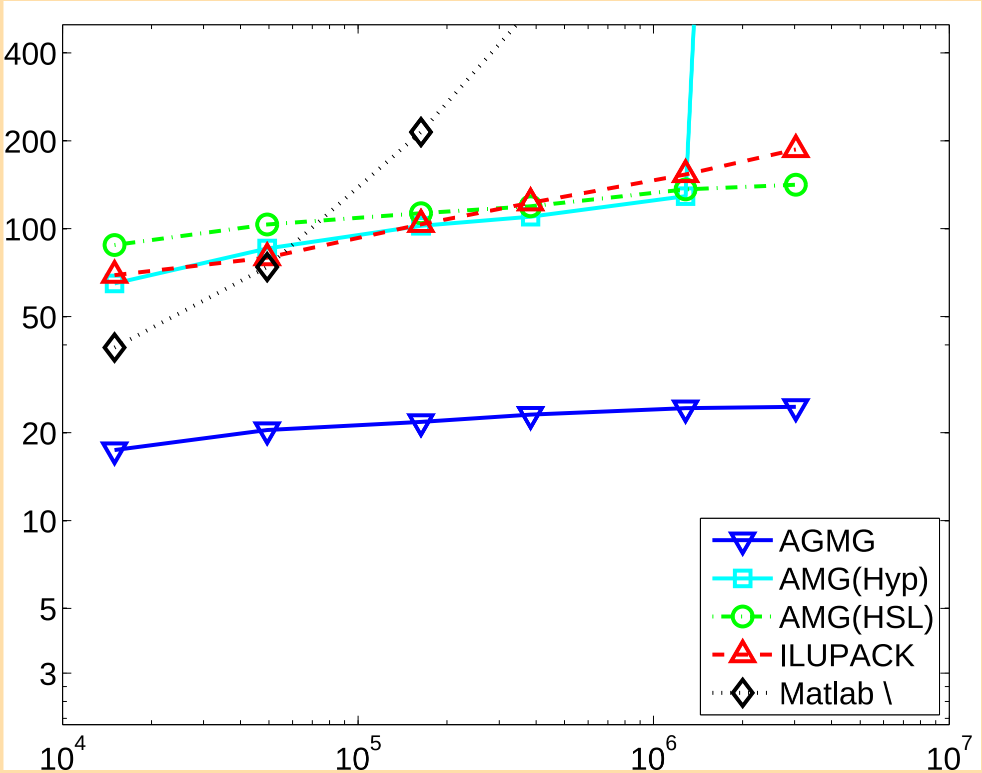
7. Numerical results

ULB

POISSON 3D, FD



LAPLACE 3D, FE(P3)

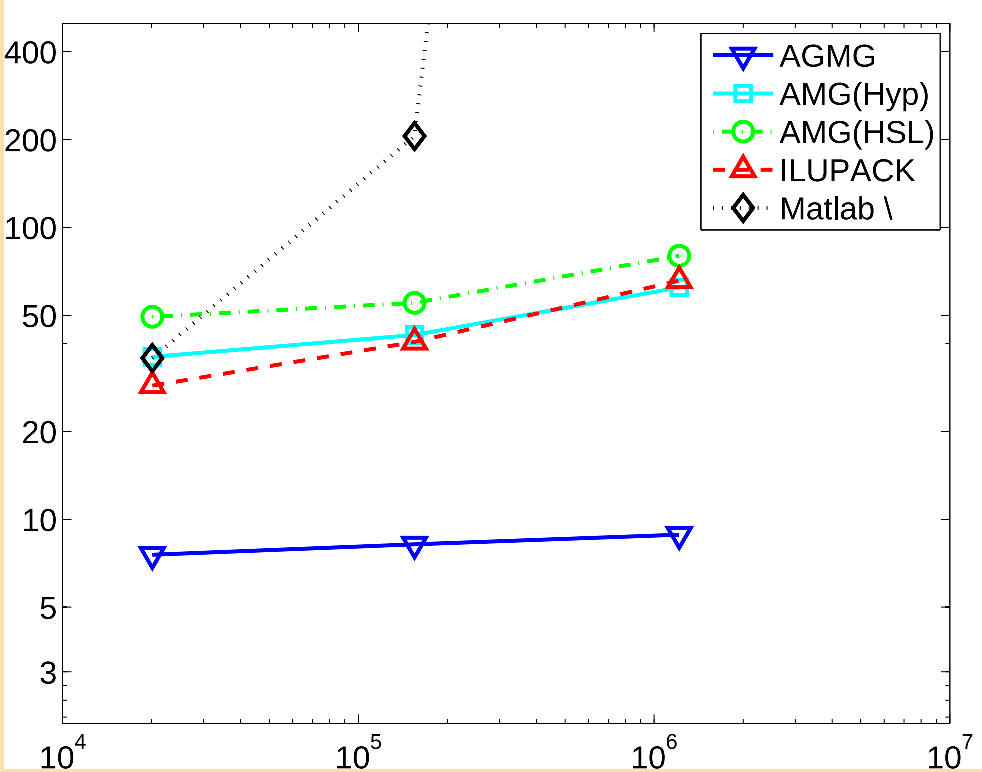


51% of nonzero offdiag > 0

7. Numerical results

Poisson 3D, FE

Unstructured, Local refin.



Convection-Diffusion 3D, FD

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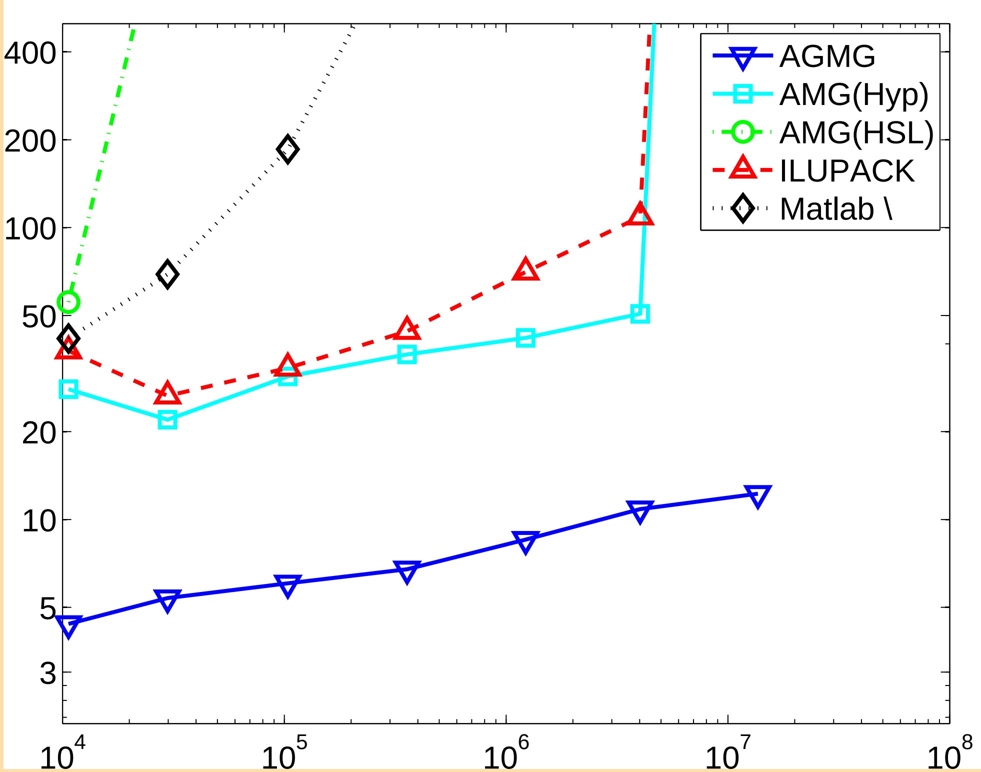

7. Numerical results

Parallel run: with direct coarsest grid solver
Cray, 32 cores/node with 1GB/node
Poisson, 3D trilinear hexahedral FE

#Nodes	#Cores	$n/10^6$	#Iter.	Setup Time	Solve Time
1	32	31	17	5.9	40.4
2	64	63	17	6.2	40.8
4	128	125	17	6.9	41.5
8	256	251	17	9.5	41.8
16	512	501	17	14.8	42.5
32	1024	1003	17	27.3	44.0
64	2048	2007	17	69.0	48.2
128	4096	4014	17	383.0	59.4

(By courtesy of Mark Walkley, Univ. of Leeds)

7. Numerical results

ULB

Parallel run: with (new) iterative coarsest grid solver
Intel(R) Xeon(R) CPU E5649 @ 2.53GHz
3D problem with jumps, FD

#Nodes	#Cores	$n/10^6$	#Iter.	Setup Time	Solve Time
1	8	64	12	14.9	89.
16	128	1026	16	17.4	191.
48	384	3065	14	18.0	165.
96	768	6155	13	17.4	170.

8. Conclusions

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- Professional code available, free academic license

References

- Analysis of aggregation–based multigrid (with A. C. Muresan), SISC (2008).
- Recursive Krylov-based multigrid cycles (with P. S. Vassilevski), NLAA (2008).
- An aggregation-based algebraic multigrid method, ETNA (2010).
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- Aggregation-based algebraic multigrid for convection-diffusion equations, SISC (2012, to appear).

AGMG software: Google AGMG
(`http://homepages.ulb.ac.be/~ynotay/AGMG`)

Thank you for your attention !