Algebraic multigrid and multilevel methods

A general introduction

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May 20, 2005, Leuven

* Supported by the "Fonds National de la Recherche Scientifique", Maître de recherches

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Introduction

Large sparse discrete PDE systems

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

- Iterative methods accelerated by preconditioning: easily invertible B such that $B \approx A$.
- Multigrid & multilevel methods: often very efficient.
- Basic principle (two-grid): obtain fast the convergence by solving a smaller problem, on a coarser grid.
- Recursive use: the coarse grid problem is solved using the same two-grid preconditioner.
- This seminar: emphasis on *algebraic* methods (that work using only the information in A).

Algebraic methods: field of application

- Robust for scalar elliptic PDEs with standard discretization.
- Emphasis on (theory for) symmetric problems (self-adjoint PDEs), but work in unsymmetric cases as well (e.g. convection diffusion problems).
- Ongoing research for systems of PDEs (efficient preconditioning of each diagonal block).
- Does not work well for indefinite problems (some eigenvalues with negative real part); e.g.: Helmholtz.

Remark: AMG is the generic name of a family of methods, but also the specific name of Ruge & Stüben method.

Outline

1. An introductory example.
2. Needed ingredients: algebraic coarsening and algebraic interpolation.
3. The different schemes and their algebraic properties.
4. Algebraic interpolation.
5. Algebraic coarsening: standard from AMG and aggregation.
6. Checking & correcting the coarsening.
7. From two- to multi-level: cycling strategies.
8. Some numerical illustrations

An example

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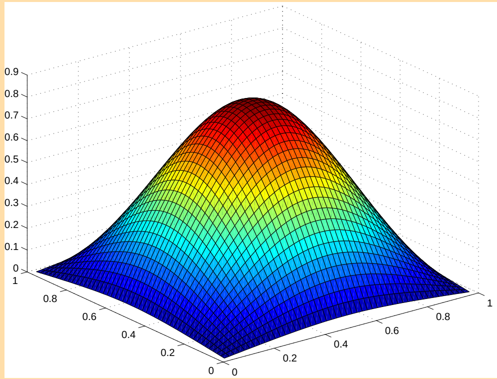
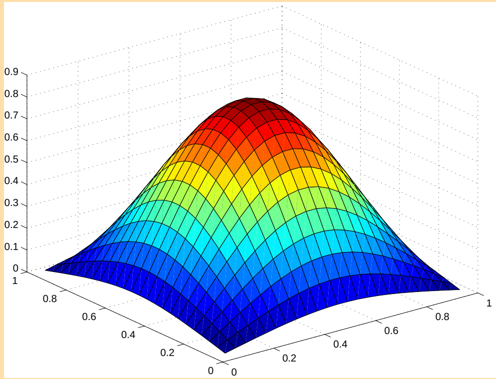
PDE: $-\Delta\, u \;=\; 20\, e^{-10\,((x-0.5)^2+(y-0.5)^2)}$ in $\Omega = (0,1)\times(0,1)$

$u \;=\; 0$ on $\partial\Omega$

Uniform grid with mesh size h , five-point finite difference.



Solution with $h^{-1} = 50$



Solution with $h^{-1} = 25$

An idea

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Fine grid (system to solve):

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

Coarse grid (auxiliary system):

$$A_C\,\mathbf{u}_C \;=\; \mathbf{b}_C\;.$$

$\mathbf{u}_C$ may be computed and prolongated (by interpolation) on the fine grid:

$$\mathbf{u}^{(1)} = p\,\mathbf{u}_C$$

$\mathbf{u}^{(1)}$ may serve as initial approximation, i.e., one solves

$$A\,(\mathbf{u}^{(1)}+\mathbf{x}) \;=\; \mathbf{b} \qquad \text{or} \qquad A\,\mathbf{x} \;=\; \mathbf{b} - A\,p\,A_C^{-1}\,\mathbf{b}_C\;.$$

How it works

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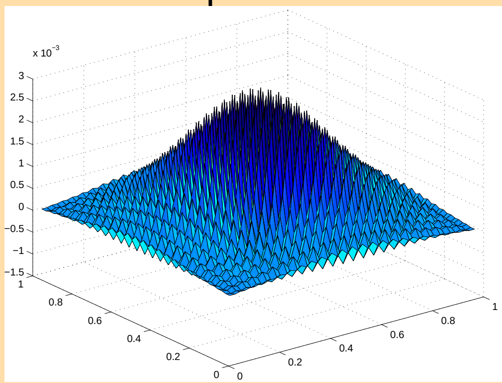
Error on the fine grid after interpolation



$$\frac{\|\mathbf{u}-\mathbf{u}^{(1)}\|}{\|\mathbf{u}\|} = 0.0019$$

Let us repeat

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$$A\,(\mathbf{u}^{(1)}+\mathbf{x}) \;=\; \mathbf{b} \qquad \text{or} \qquad A\,\mathbf{x} \;=\; \mathbf{b} - A\,p\,A_C^{-1}\mathbf{b}_C \;=\; \mathbf{r}^{(1)}\;.$$

(1) Restrict on the coarse grid:

$$\mathbf{r}_C \;=\; r\,\mathbf{r}(1)\;.$$

(2) Solve on the coarse grid:

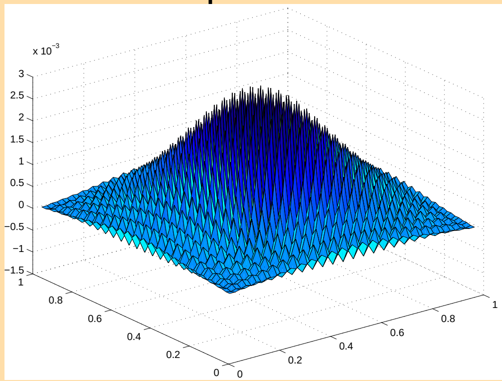
$$\mathbf{x}_C^{(2)} \;=\; A_C^{-1}\,\mathbf{r}_C\;.$$

(3) Prolongate:

$$\mathbf{x}^{(2)} \;=\; p\,\mathbf{x}_C^{(2)}\;,$$
$$\mathbf{u}^{(2)} \;=\; \mathbf{u}^{(1)} + \mathbf{x}^{(2)}\;.$$

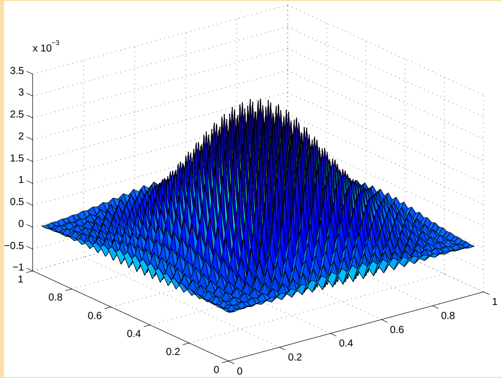
Still working ?

Error on the fine grid after interpolation



$$\frac{\|\mathbf{u}-\mathbf{u}^{(1)}\|}{\|\mathbf{u}\|} = 0.0019$$

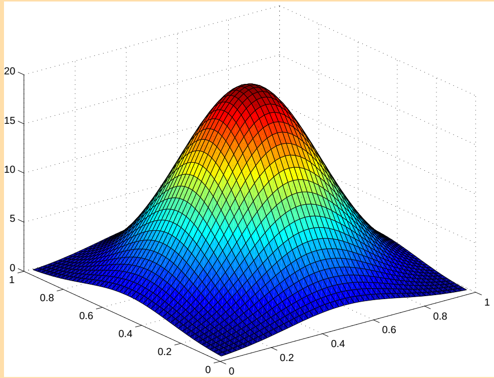
Repeating the process . . .



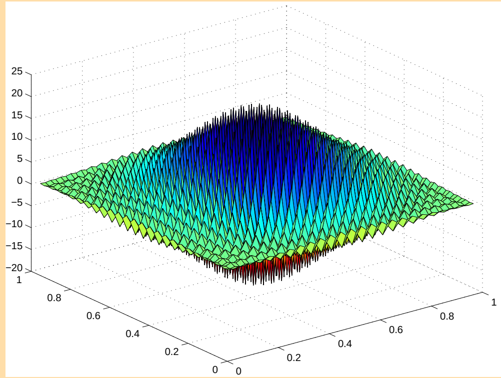
$$\frac{\|\mathbf{u}-\mathbf{u}^{(2)}\|}{\|\mathbf{u}\|} = 0.0018$$

Error controlled through residual

Initial residual (r.h.s.)



After coarse grid correction



$$\frac{\|\mathbf{b}-A\,p\,A_C^{-1}\mathbf{b}_C\|}{\|\mathbf{b}\|} = 0.7142$$

Explanation

Assume (for simplicity) that $\mathbf{b}_C = r\,\mathbf{b}$.

One has

$$\begin{aligned}\mathbf{u}-\mathbf{u}^{(1)} &= \mathbf{u}-p\,A_C^{-1}\,r\,\mathbf{b}\\ &= \left(I-p\,A_C^{-1}\,r\,A\right)\,\mathbf{u}\,,\\ \mathbf{u}-\mathbf{u}^{(2)} &= \left(I-p\,A_C^{-1}\,r\,A\right)^2\,\mathbf{u}\,,\end{aligned}$$

etc. Similarly

$$\begin{aligned}\mathbf{r}^{(1)} &= \mathbf{b}-A\,p\,A_C^{-1}\,r\,\mathbf{b}\\ &= \left(I-A\,p\,A_C^{-1}\,r\right)\,\mathbf{r}^{(0)}\,.\end{aligned}$$

$p\,A_C^{-1}\,r$ has rank n_C $\rightarrow$

$$\rho\left(I-A\,p\,A_C^{-1}\,r\right) = \rho\left(I-p\,A_C^{-1}\,r\,A\right) \geq 1\,.$$

Smoother enters the scene

$\mathbf{u}-\mathbf{u}^{(1)}$ and $\mathbf{r}^{(1)}$ very oscillatory

$\rightarrow$ improve $\mathbf{u}^{(1)}$ with a simple iterative method, efficient in smoothing the error & residual.

Example: symmetric Gauss-Seidel (SGS)

$$\begin{aligned}L\,\mathbf{u}^{(1+1/2)} &= \mathbf{b}-(A-L)\,\mathbf{u}^{(1)}\,, \qquad (L=\mathrm{low}(A))\\ U\,\mathbf{u}^{(2)} &= \mathbf{b}-(A-U)\,\mathbf{u}^{(1+1/2)}\,. \qquad (U=\mathrm{upp}(A))\end{aligned}$$

Same as

$$\mathbf{u}^{(2)} = \mathbf{u}^{(1)}+M^{-1}\mathbf{r}^{(1)}\,, \qquad M=L\,D^{-1}\,U \quad (D=\mathrm{diag}(A))$$

Thus:

$$\begin{aligned}\mathbf{u}-\mathbf{u}^{(2)} &= \left(I-M^{-1}A\right)\left(\mathbf{u}-\mathbf{u}^{(1)}\right)\\ \mathbf{r}^{(2)} &= \left(I-A\,M^{-1}\right)\mathbf{r}^{(1)}\end{aligned}$$

One may repeat: $\mathbf{r}^{(m+1)} = \left(I-A\,M^{-1}\right)^m\,\mathbf{r}^{(1)}$.

Smoothing effect

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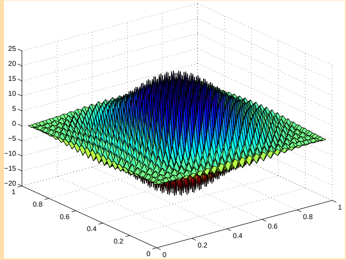
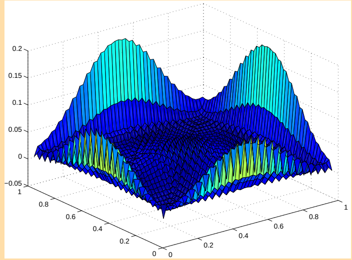
Residual after CG correction



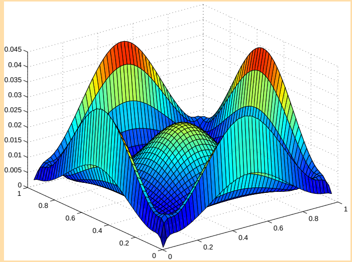
$\frac{\|\mathbf{r}\|}{\|\mathbf{b}\|} = 0.7142$

Adding 1 SGS step



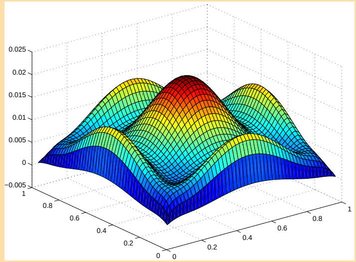
$\frac{\|\mathbf{r}\|}{\|\mathbf{b}\|} = 0.0039$

Adding 3 SGS steps



$\frac{\|\mathbf{r}\|}{\|\mathbf{b}\|} = 0.0018$

Adding 8 SGS steps



$\frac{\|\mathbf{r}\|}{\|\mathbf{b}\|} = 0.0012$

Smoothing + coarse grid correction

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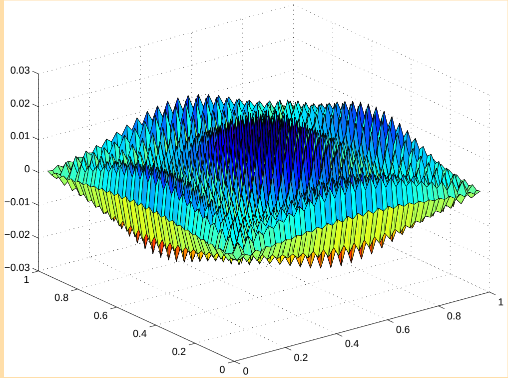
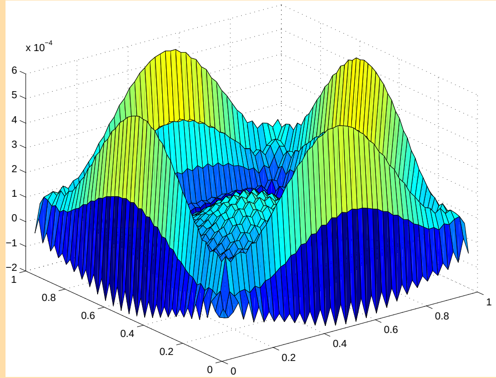
Adding now a CG correction



$$\frac{\|\mathbf{r}\|}{\|\mathbf{r}_{\text{previous}}\|} = 0.746$$

. . . and again 1 SGS step



$$\frac{\|\mathbf{r}\|}{\|\mathbf{r}_{\text{previous}}\|} = 0.0155$$

What we learned

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For each coarse grid correction:

$$\mathbf{u} - \mathbf{u}^{(m+1)} \;=\; \left(I - p\,A_C^{-1}\,r\,A\right)\left(\mathbf{u} - \mathbf{u}^{(m)}\right).$$

Cannot work alone because $\rho\left(I - p\,A_C^{-1}\,r\,A\right) \;\geq\; 1\,.$

For each smoothing step

$$\mathbf{u} - \mathbf{u}^{(m+1)} \;=\; \left(I - M^{-1}\,A\right)\left(\mathbf{u} - \mathbf{u}^{(m)}\right).$$

Not efficient alone because $\rho\left(I - M^{-1}\,A\right) \;\approx\; 1\,.$

However

$$\rho\Big(\left(I - M^{-1}\,A\right)\left(I - p\,A_C^{-1}\,r\,A\right)\left(I - M^{-1}\,A\right)\Big) \;\ll\; 1$$

Rmk: if $A = A^T$, we assume $M = M^T$.

How it works

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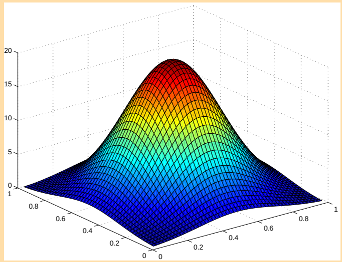
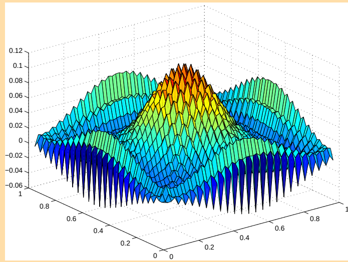
Initial residual

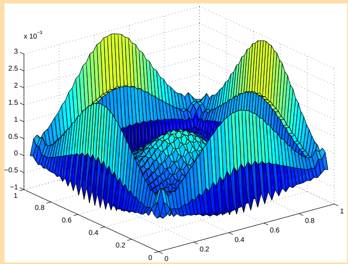


1 multigrid step



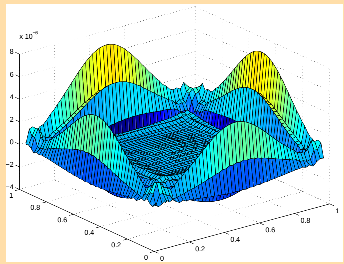
$\frac{\|\mathbf{r}\|}{\|\mathbf{b}\|} = 3.9\,10^{-3}$

2 multigrid steps



$\frac{\|\mathbf{r}\|}{\|\mathbf{b}\|} = 7.7\,10^{-5}$

4 multigrid steps



$\frac{\|\mathbf{r}\|}{\|\mathbf{b}\|} = 1.7\,10^{-7}$

Some remarks

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Geometric multigrid

- Simple in its principles.
- Complicate to analyze.
- Not robust: simple ideas not always lead to efficient schemes.
- There is a lot of research works on multigrid applications.

Algebraic multigrid

- More user friendly ("black box").
- More robust.
- ...sacrificing somewhat on efficiency.

Algebraic multigrid: ingredients

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- Coarsening: F/C partitioning of the unknowns.
- Interpolation J_{FC} and prolongation $p = \begin{pmatrix} J_{FC} \\ I \end{pmatrix}$ satisfying $p\,\mathbf{e}_C = \mathbf{e}$.
- For the restriction, one often takes $r = \beta \begin{pmatrix} J_{FC}^T & I \end{pmatrix} = \beta\, p^T$ with β such that $r\,\mathbf{e} = \mathbf{e}_C$.
- For A_C one may rely on the Galerkin approximation:

$$A_C = r\,A\,p \qquad \text{or} \qquad \widehat{A}_C = p^T A\,p$$

with coarse grid correction given by $p\,\widehat{A}_C^{-1}\,p^T$.

- $I - p\,\widehat{A}_C^{-1}\,p^T A = \left(I - p\,\widehat{A}_C^{-1}\,p^T A\right)^2$ (projector)

Two-grid AMG as a preconditioner

ULB

AMG as preconditioner

$\mathbf{v} = B_{\text{AMG}}^{-1}\,\mathbf{r}$ computed as

1. $\mathbf{t} = M^{-1}\mathbf{r}$; $\mathbf{w} = \mathbf{r} - A\,\mathbf{t}$
2. $\mathbf{y}_C = \mathbf{w}_C + J_{FC}^T\,\mathbf{w}_F$
3. Solve $\widehat{A}_C\,\mathbf{z}_C = \mathbf{y}_C$
4. $\mathbf{z}_F = J_{FC}\,\mathbf{z}_C$
5. $\mathbf{v} = \mathbf{t} + \mathbf{z} + M^{-1}(\mathbf{w} - A\,\mathbf{z})$

$$I - B_{\text{AMG}}^{-1}\,A = (I - M^{-1}A)(I - p\,\widehat{A}_C^{-1}\,p^T A)(I - M^{-1}A)\,.$$

Multilevel is not multigrid !

ULB

Coarse grid correction:

$$p\,\widehat{A}_C^{-1}\,p^T \qquad \text{with} \qquad p = \begin{pmatrix} J_{FC} \\ I \end{pmatrix}\,.$$

Let's try an additive complement

$$q\,Q_{FF}^{-1}\,q^T \qquad \text{with} \qquad q = \begin{pmatrix} I \\ 0 \end{pmatrix}\,.$$

($Q_{FF} \approx q^T A\,q = A_{FF}$)
Corresponding preconditioner:

$$B_{\text{HBBD}}^{-1} = \begin{pmatrix} I & J_{FC} \\ & I \end{pmatrix} \begin{pmatrix} Q_{FF}^{-1} & \\ & \widehat{A}_C^{-1} \end{pmatrix} \begin{pmatrix} I & \\ J_{FC}^T & I \end{pmatrix}\,.$$

Hierarchical finite element bases

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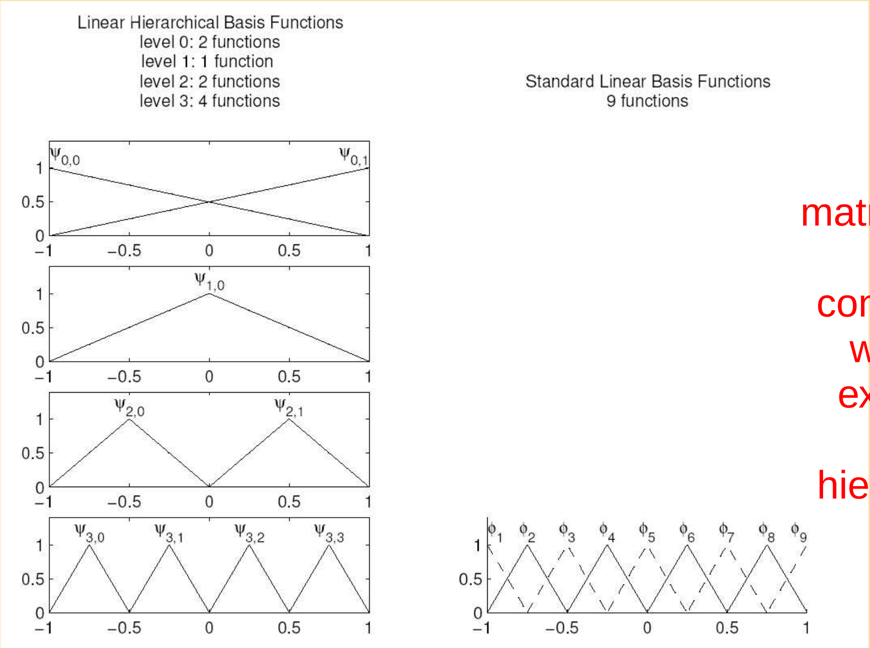

Finite element matrices are better conditioned whenever expressed in the hierarchical basis

(Generalized) hierarchical basis

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In finite element applications with regular refinement,

$$J = \begin{pmatrix} I & J_{FC} \\ & I \end{pmatrix}$$

performs the basis transformation *(hb_tl)*$\to$*(nb)*
(*(hb_tl)*: coarse nodal basis ($2\,h$) + compl. functions (h)).

Matrix in this basis:

$$\widehat{A} = J^T A\, J = \begin{pmatrix} I & \\ J_{FC}^T & I \end{pmatrix} \begin{pmatrix} A_{FF} & A_{FC} \\ A_{CF} & A_{CC} \end{pmatrix} \begin{pmatrix} I & J_{FC} \\ & I \end{pmatrix}$$

$$= \begin{pmatrix} A_{FF} & A_{FC}+A_{FF}\,J_{FC} \\ A_{CF}+J_{FC}^T A_{FF} & \widehat{A}_C \end{pmatrix} .$$

Additive two-level

ULB

Matrix in *(hb_tl)*: $\widehat{A} = J^T A\, J$.

Two-grid with additive complement:

$$B_{\text{HBBD}}^{-1} = \begin{pmatrix} I & J_{FC} \\ & I \end{pmatrix} \begin{pmatrix} Q_{FF}^{-1} & \\ & \widehat{A}_C^{-1} \end{pmatrix} \begin{pmatrix} I & \\ J_{FC}^T & I \end{pmatrix} = J\, \widehat{B}_{\text{HBBD}}^{-1}\, J^T ,$$

where

$$\widehat{B}_{\text{HBBD}} = \begin{pmatrix} Q_{FF} & \\ & \widehat{A}_C \end{pmatrix} \approx \begin{pmatrix} A_{FF} & \\ & \widehat{A}_C \end{pmatrix} ,$$

which is the block diagonal part of $\widehat{A}$. Further,

$$B_{\text{HBBD}}^{-1} A = \left(J\, \widehat{B}_{\text{HBBD}}^{-1}\, J^T\right)\left(J^{-T}\, \widehat{A}\, J^{-1}\right) = J\, \widehat{B}_{\text{HBBD}}^{-1} \widehat{A}\, J^{-1} .$$

The strengthened C.B.S. constant

ULB

We assume A symmetric and positive definite

Definition

$$\widehat{\gamma} = \max_{\mathbf{v}=\begin{pmatrix}\mathbf{v}_F \\ 0\end{pmatrix}\neq 0\ ,\ \mathbf{w}=\begin{pmatrix}0 \\ \mathbf{w}_C\end{pmatrix}\neq 0} \frac{|\,\mathbf{v}^T\,\widehat{A}\,\mathbf{w}\,|}{\left(\mathbf{v}^T\,\widehat{A}\,\mathbf{v}\right)^{1/2}\left(\mathbf{w}\,\widehat{A}\,\mathbf{w}\right)^{1/2}} .$$

Property. If $\widehat{A} = \sum_\ell \widehat{A}_\ell$ and if, $\forall \ell$, $\widehat{\gamma}_\ell$ is such that,
for all $\mathbf{v} = \begin{pmatrix}\mathbf{v}_F \\ 0\end{pmatrix}$, $\mathbf{w} = \begin{pmatrix}0 \\ \mathbf{w}_C\end{pmatrix}$

$$|\,\mathbf{v}^T\,\widehat{A}_\ell\,\mathbf{w}\,| \le \widehat{\gamma}_\ell\,\left(\mathbf{v}^T\,\widehat{A}_\ell\,\mathbf{v}\right)^{1/2}\left(\mathbf{w}\,\widehat{A}_\ell\,\mathbf{w}\right)^{1/2} ,$$

then: $\widehat{\gamma} \le \max_\ell \widehat{\gamma}_\ell$

$\to$ $\widehat{\gamma}$ may often be bounded away from 1.

The strengthened C.B.S. constant (cont.) ULB

Let

$$\widehat{A} = \begin{pmatrix} A_{FF} & \widehat{A}_{FC} \\ \widehat{A}_{CF} & \widehat{A}_C \end{pmatrix} \quad , \quad \widehat{D} = \begin{pmatrix} A_{FF} & \\ & \widehat{A}_C \end{pmatrix} \quad ,$$

One has

$$\kappa\left(\widehat{D}^{-1}\widehat{A}\right) = \frac{\lambda_{\max}\left(\widehat{D}^{-1}\widehat{A}\right)}{\lambda_{\min}\left(\widehat{D}^{-1}\widehat{A}\right)} = \frac{1+\widehat{\gamma}}{1-\widehat{\gamma}} \,.$$

Let $S_A = A_{CC} - A_{CF}\,A_{FF}^{-1}\,A_{FC} = \widehat{A}_C - \widehat{A}_{CF}\,A_{FF}^{-1}\,\widehat{A}_{FC}\,.$

One has

$$\lambda_{\min}\left(\widehat{A}_C^{-1} S_A\right) = 1 - \widehat{\gamma}^2 \,,$$

$$\lambda_{\max}\left(\widehat{A}_C^{-1} S_A\right) \le 1 \,.$$

Two-grid HBBD preconditioning ULB

Preconditioning by HBBD

$\mathbf{v} = B_{\text{HBBD}}^{-1}\,\mathbf{r}$ computed as

1. $\mathbf{y}_F = Q_{FF}^{-1}\,\mathbf{r}_F$
2. $\mathbf{y}_C = \mathbf{r}_C + J_{FC}^T\,\mathbf{r}_F$
3. Solve $\widehat{A}_C\,\mathbf{v}_C = \mathbf{y}_C$
4. $\mathbf{z}_F = J_{FC}\,\mathbf{v}_C$
5. $\mathbf{v}_F = \mathbf{z}_F + \mathbf{y}_F$

$$\kappa \approx \frac{1+\widehat{\gamma}}{1-\widehat{\gamma}}$$

$$B_{\text{HBBD}}^{-1} = \begin{pmatrix} I & J_{FC} \\ & I \end{pmatrix} \begin{pmatrix} Q_{FF}^{-1} & \\ & \widehat{A}_C^{-1} \end{pmatrix} \begin{pmatrix} I & \\ J_{FC}^T & I \end{pmatrix}$$

$$= q\,Q_{FF}^{-1}\,q^T + p\,\widehat{A}_C^{-1}\,p^T \,.$$

Two-level block factorization ULB

$$\begin{aligned}
\widehat{A} &= \begin{pmatrix} A_{FF} & \widehat{A}_{FC} \\ \widehat{A}_{CF} & \widehat{A}_C \end{pmatrix} \\
&= \begin{pmatrix} I & \\ \widehat{A}_{CF}\,A_{FF}^{-1} & I \end{pmatrix} \begin{pmatrix} A_{FF} & \\ & S_A \end{pmatrix} \begin{pmatrix} I & A_{FF}^{-1}\widehat{A}_{FC} \\ & I \end{pmatrix} \\
&\approx \begin{pmatrix} I & \\ \widehat{A}_{CF}\,Q_{FF}^{-1} & I \end{pmatrix} \begin{pmatrix} Q_{FF} & \\ & \widehat{A}_C \end{pmatrix} \begin{pmatrix} I & Q_{FF}^{-1}\,\widehat{A}_{FC} \\ & I \end{pmatrix} \,. \\
&= \widehat{B}_{\text{HBBF}}
\end{aligned}$$

$$B_{\text{HBBF}}^{-1} = J\,\widehat{B}_{\text{HBBF}}^{-1}\,J^T$$

Two-level block factorization (cont.) ULB

Preconditioning by HBBF

$\mathbf{v} = B_{\text{HBBF}}^{-1}\,\mathbf{r}$ computed as

1. $\mathbf{y}_F = Q_{FF}^{-1}\,\mathbf{r}_F$
2. $\mathbf{y}_C = \mathbf{r}_C - A_{CF}\,\mathbf{y}_F + J_{FC}^T(\mathbf{r}_F - A_{FF}\,\mathbf{y}_F)$
3. Solve $\widehat{A}_C\,\mathbf{v}_C = \mathbf{y}_C$
4. $\mathbf{z}_F = J_{FC}\,\mathbf{v}_C$
5. $\mathbf{v}_F = \mathbf{z}_F + Q_{FF}^{-1}\,(\mathbf{r}_F - A_{FC}\,\mathbf{v}_C - A_{FF}\,\mathbf{z}_F)$

$$\kappa \approx \frac{1}{1-\widehat{\gamma}^2}$$

$$B_{\text{HBBF}}^{-1} = J \begin{pmatrix} I & -Q_{FF}^{-1}\,\widehat{A}_{FC} \\ & I \end{pmatrix} \begin{pmatrix} Q_{FF}^{-1} & \\ & \widehat{A}_C^{-1} \end{pmatrix} \begin{pmatrix} I & -Q_{FF}^{-1}\,\widehat{A}_{FC} \\ & I \end{pmatrix} J^T$$

Two-level hierarchical basis multigrid

Preconditioning by HBMG

$\mathbf{v} = B_{\text{HBMG}}^{-1}\,\mathbf{r}$ computed as

1. $\mathbf{y}_F = Q_{FF}^{-1}\,\mathbf{r}_F$
2. $\mathbf{y}_C = \mathbf{r}_C - A_{CF}\,\mathbf{y}_F + J_{FC}^T(\mathbf{r}_F - A_{FF}\,\mathbf{y}_F)$
3. Solve $\widehat{A}_C\,\mathbf{v}_C = \mathbf{y}_C$
4. $\mathbf{z}_F = J_{FC}\,\mathbf{v}_C + \mathbf{y}_F$
5. $\mathbf{v}_F = \mathbf{z}_F + Q_{FF}^{-1}\,(\mathbf{r}_F - A_{FC}\,\mathbf{v}_C - A_{FF}\,\mathbf{z}_F)$

$$\kappa \approx \frac{1}{1-\widehat{\gamma}^2}$$

$$B_{\text{HBMG}}^{-1} = J\begin{pmatrix} I & -Q_{FF}^{-1}\widehat{A}_{FC} \\ & I \end{pmatrix}\begin{pmatrix} 2\,Q_{FF}^{-1} - Q_{FF}^{-1}\,A_{FF}\,Q_{FF}^{-1} & \\ & \widehat{A}_C^{-1} \end{pmatrix}\cdots$$

Hierarchical basis & multigrid

Elementary algebra yields

$$I - B_{\text{HBMG}}^{-1}\,A = (I - R\,A)(I - p\,\widehat{A}_C^{-1}\,p^T\,A)(I - R\,A)$$

with

$$R = \begin{pmatrix} Q_{FF}^{-1} & 0 \\ 0 & 0 \end{pmatrix}.$$

Reminder:

$$I - B_{\text{AMG}}^{-1}\,A = (I - M^{-1}\,A)(I - p\,\widehat{A}_C^{-1}\,p^T\,A)(I - M^{-1}\,A).$$

Block factorization without h.b.

$$\begin{aligned}
A &= \begin{pmatrix} A_{FF} & A_{FC} \\ A_{CF} & A_{CC} \end{pmatrix} \\
&= \begin{pmatrix} I & \\ A_{CF}\,A_{FF}^{-1} & I \end{pmatrix}\begin{pmatrix} A_{FF} & \\ & S_A \end{pmatrix}\begin{pmatrix} I & A_{FF}^{-1}A_{FC} \\ & I \end{pmatrix} \\
&\approx \begin{pmatrix} I & \\ A_{CF}\,P_{FF}^{-1} & I \end{pmatrix}\begin{pmatrix} P_{FF} & \\ & \widehat{A}_C \end{pmatrix}\begin{pmatrix} I & P_{FF}^{-1}\,A_{FC} \\ & I \end{pmatrix}. \\
&= B_{\text{MBF}}
\end{aligned}$$

Block factorization without h.b. (cont.)

Preconditioning by MBF

$\mathbf{v} = B_{\text{MBF}}^{-1}\,\mathbf{r}$ computed as

1. $\mathbf{y}_F = P_{FF}^{-1}\,\mathbf{r}_F$
2. $\mathbf{y}_C = \mathbf{r}_C - A_{CF}\,\mathbf{y}_F$
3. Solve $\widehat{A}_C\,\mathbf{v}_C = \mathbf{y}_C$
4. $\mathbf{v}_F = P_{FF}^{-1}\,(\mathbf{r}_F - A_{FC}\,\mathbf{v}_C)$

$$\kappa \approx \frac{1}{1-\widehat{\gamma}^2}$$

Possibly unstable !

$$B_{\text{MBF}}^{-1} = \begin{pmatrix} I & -P_{FF}^{-1}A_{FC} \\ & I \end{pmatrix}\begin{pmatrix} P_{FF}^{-1} & \\ & \widehat{A}_C^{-1} \end{pmatrix}\begin{pmatrix} I & \\ -A_{CF}\,P_{FF}^{-1} & I \end{pmatrix}$$

Block factorization without h.b. (cont.)

$$B_{\text{HBBD}}^{-1} = q\,Q_{FF}^{-1}\,q^T + p\,\widehat{A}_C^{-1}\,p^T \;.$$

$$B_{\text{HBBF}}^{-1} = q\,Q_{FF}\,q^T + \widetilde{p}\,\widehat{A}_C^{-1}\,\widetilde{p}^T \;,$$

$$B_{\text{HBMG}}^{-1} = q\,\left(Q_{FF}^{-1} + Q_{FF}^{-T} - Q_{FF}^{-1}\,A_{FF}\,Q_{FF}^{-T}\right)\,q^T + \widetilde{p}\,\widehat{A}_C^{-1}\,\widetilde{p}^T \;,$$

$$\widetilde{p} = \begin{pmatrix} -Q_{FF}^{-1}A_{FC} + (I - Q_{FF}^{-1}A_{FF})J_{FC} \\ I \end{pmatrix} \;.$$

$$B_{\text{MBF}}^{-1} = q\,P_{FF}^{-1}\,q^T + \overline{p}\,\widehat{A}_C^{-1}\,\overline{p}^T \;,$$

$$\overline{p} = \begin{pmatrix} -P_{FF}^{-1}A_{FC} \\ I \end{pmatrix} \;.$$

$\overline{p}$ has to define a “correct” interpolation.

Block factorization without h.b. (cont.)

h^{-1}	$P_{FF}^{-1}A_{FF}$ λ_{min}	$\lambda_{\max}$	κ	$B_{\text{MBF}}^{-1}A$ λ_{min}	$\lambda_{\max}$	κ
MILU preconditioning of A_{FF}						
16	1.00	1.20	1.20	0.51	1.25	2.45
32	1.00	1.21	1.21	0.50	1.27	2.54
64	1.00	1.21	1.21	0.50	1.29	2.58
128	1.00	1.21	1.21	0.50	1.29	2.58
ILU preconditioning of A_{FF}						
16	0.88	1.09	1.24	0.510	1.42	2.78
32	0.88	1.09	1.24	0.380	2.28	6.00
64	0.87	1.09	1.25	0.176	4.97	28.30
128	0.87	1.09	1.25	0.058	15.00	258.00

Correct interpolation

- Essential requirement:

$$\overline{p} = \begin{pmatrix} -P_{FF}^{-1}A_{FC} \\ I \end{pmatrix}$$ good for low energy modes,

  i.e. vectors $\mathbf{v}$ such that $A\mathbf{v} \approx 0$.

- Scalar elliptic PDEs: one such vector:

$$\mathbf{e} = \begin{pmatrix} 1 & \dots & 1 \end{pmatrix}^T .$$

- If one satisfies the row-sum criterion

$$P_{FF}\,\mathbf{e}_F = A_{FF}\,\mathbf{e}_F \;,$$

  then

$$A_{FF}\,\mathbf{e}_F + A_{FC}\,\mathbf{e}_C \approx 0 \quad \Rightarrow \quad P_{FF}^{-1}A_{FC}\,\mathbf{e}_C \approx \mathbf{e}_F \;.$$

Correct interpolation (cont.)

If A is a symmetric M-matrix with nonnegative row-sum (SPD with nonpositive offdiagonal entries), several results available.

For instance:

$$\overline{A} = \overline{J}^T\,A\,\overline{J}$$

with

$$\overline{J} = \begin{pmatrix} I & -P_{FF}^{-1}A_{FC} \\ & I \end{pmatrix}$$

satisfies

$$\overline{\gamma} \le \sqrt{1 - \frac{1}{\kappa(P_{FF}^{-1}A_{FF})}} \;.$$

Algebraic analysis of AMG

ULB

HBBF, HBMG: $\kappa \approx \dfrac{1}{1-\widehat{\gamma}^2}$; MBF: $\kappa \approx \dfrac{1}{1-\widehat{\gamma}^2}$ (!).

AMG

Assumption: $2\,M - A$ SPD or, equivalently, $\rho\left(I - M^{-1}\,A\right) < 1$. One has

$$\kappa\left(B_{\text{AMG}}^{-1}\,A\right) \le \mu$$

where

$$\mu = \max_{\mathbf{z}\neq 0} \frac{(\mathbf{z}_F - J_{FC}\,\mathbf{z}_C)^T\,X_{FF}\,(\mathbf{z}_F - J_{FC}\,\mathbf{z}_C)}{\mathbf{z}^T\,A\,\mathbf{z}}\,,$$

with X_{FF} being the top left block of

$$X = M\,(2\,M - A)^{-1}\,M\,.$$

Algebraic analysis of AMG (cont.)

ULB

Further,

$$\frac{1}{1-\widehat{\gamma}^2} \le \mu \le \frac{1}{\lambda_{\min}(X_{FF}^{-1}A_{FF})}\,\frac{1}{1-\widehat{\gamma}^2} \le \frac{1}{\lambda_{\min}(M_{FF}^{-1}A_{FF})\,(2-\lambda_{\max}(M^{-1}A))}\,\frac{1}{1-\widehat{\gamma}^2}\,.$$

Example: SGS smoothing: $\lambda_{\max}(M^{-1}A) = 1$.

$$\frac{1}{1-\widehat{\gamma}^2} \le \mu \le \frac{1}{\lambda_{\min}(M_{FF}^{-1}A_{FF})}\,\frac{1}{1-\widehat{\gamma}^2}\,.$$

Algebraic analysis of AMG (cont.)

ULB

Quality of the interpolation measured with

$$\tau = \max_{\mathbf{z}\neq 0} \frac{(\mathbf{z}_F - J_{FC}\,\mathbf{z}_C)^T\,D_{FF}\,(\mathbf{z}_F - J_{FC}\,\mathbf{z}_C)}{\mathbf{z}^T\,A\,\mathbf{z}}$$

($D_{FF} = \text{diag}(A_{FF})$).

There holds

$$\tau \le \frac{1}{\lambda_{\min}(D_{FF}^{-1}A_{FF})}\,\frac{1}{1-\widehat{\gamma}^2}$$

$$\tau \ge \max\left(\frac{1}{\lambda_{\max}(D_{FF}^{-1}A_{FF})}\,\frac{1}{1-\widehat{\gamma}^2}\,,\;\frac{1}{\lambda_{\min}(D_{FF}^{-1}A_{FF})}\right)\,.$$

What we learned

ULB

- All methods work or fail together.
- They are relatively equivalent with respect to algebraic analysis (except “additive” HBBD).
- However they mimic “geometric” methods that behave differently in a multigrid or multilevel context.
- The F/C partitioning has to be such that A_{FF} is well conditioned.
- The interpolation J_{FC} has to be such that $\widehat{\gamma}$ is away from 1.
- MBF needs special care; it does not require explicitly J_{FC} , but $\widehat{A}_C$ needs to be provided.

Algebraic interpolation

Consider

$$\begin{pmatrix} I & \\ -A_{CF}A_{FF}^{-1} & I \end{pmatrix} \begin{pmatrix} A_{FF} & A_{FC} \\ A_{CF} & A_{CC} \end{pmatrix} \begin{pmatrix} I & -A_{FF}^{-1}A_{FC} \\ & I \end{pmatrix}$$
$$= \begin{pmatrix} A_{FF} & \\ & S_A \end{pmatrix} .$$

Block diagonal $\rightarrow \gamma = 0$.

$\rightarrow$ $-A_{FF}^{-1}A_{FC}$ is the ideal algebraic interpolation.

However: $\widehat{A}_C = \begin{pmatrix} J_{FC}^T & I \end{pmatrix} A \begin{pmatrix} J_{FC} \\ I \end{pmatrix}$

$\rightarrow$ J_{FC} has to remain sparse.

Algebraic interpolation (cont.)

Direct interpolation in AMG for M-matrices with nonnegative row-sum:

$$(J_{FC})_{ij} = \begin{cases} \dfrac{-\sum_{j\neq i}|(A)_{ij}|}{(A_{FF})_{ii}} \dfrac{(A_{FC})_{ij}}{\sum_{\substack{j\in C \\ a_{ij} \text{ "strong"}}} |(A_{FC})_{ij}|} & \text{if } a_{ij} \text{ "strong"} \\ 0 & \text{if } a_{ij} \text{ "weak"} . \end{cases}$$

Property:

$$\tau \leq \max_{i\in F} \frac{\sum_{j\neq i}|(A)_{ij}|}{\sum_{\substack{j\in C \\ a_{ij} \text{ "strong"}}} |(A_{FC})_{ij}|}$$

(Reminder: $\tau \approx \frac{1}{1-\widehat{\gamma}^2}$).

Algebraic interpolation (cont.)

- Possible improvement: take also into account “indirect” couplings (J_{FC} less sparse).
- Essentially positive-type matrices with nonnegative row-sum: split $A = A_M + A_P$ where
  $\text{offdiag}(A_P) = \max(O, \text{offdiag}(A))$ and $A_P\, e = 0$;
  apply previous scheme to A_M ;
  the bound on τ depends now on $\kappa(A_M^{-1}A)$.
- General case: no obvious solution so far if A is not (weakly) diagonally dominant.

Algebraic coarsening

Standard coarsening in AMG

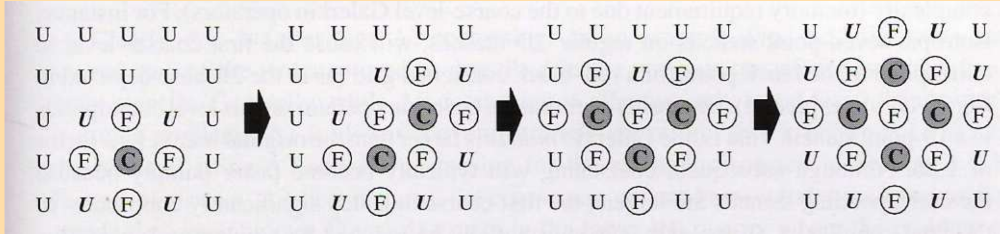
First classify the negative couplings in strong and weak, according some given threshold.

Next, repeat, till all nodes are marked either coarse or fine :

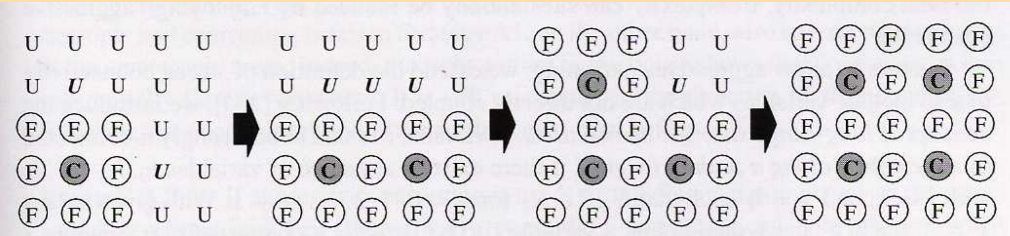
1. select an unmarked node as next coarse grid node, according to some priority rule
   (designed so as to favor a regular covering of the matrix graph);
2. select as fine grid nodes all nodes strongly negative coupled to this new coarse grid node.

AMG coarsening: how it works

Five-point stencil



Nine-point stencil



AMG coarsening: pros and cons

- Each F node is strongly negative coupled to at least 1 C node
  $\rightarrow$ standard interpolation works.
- Slow coarsening in case of low connectivity, anisotropy or strong asymmetry. (Too fast coarsening in case of high connectivity).
- May be cured with aggressive coarsening. Requires specialized interpolation.
- The number of nonzero entries per row tends to grow from level to level.
- May be sensitive to the Strong/Weak coupling threshold.
- All in all, works reasonably in many cases.

Aggregation

- Group nodes into aggregates G_i (partitioning of $[1\,,\,n]$).
- (Possible) prolongation p:

$$(p)_{ij} = \begin{cases} 1 & \text{if } i \in G_j \\ 0 & \text{otherwise}. \end{cases}$$

- Coarse grid matrix: $\widehat{A}_C = p^T A\, p$ given by

$$\left(\widehat{A}_C\right)_{ij} = \sum_{k\in G_i} \sum_{\ell \in G_j} a_{k\ell}\,.$$

- Optionally select a C node in each aggregates; other nodes are then F nodes. Associated interpolation:

$$\forall\, i \in F\,,\, j \in C\ :\ (J_{FC})_{ij} = \begin{cases} 1 & \text{if } i \in G_j \\ 0 & \text{otherwise}. \end{cases}$$

Example: pairwise aggregation

Definition: $S_i = \{\, j \neq i \mid a_{ij} < -\beta \max_{a_{ik}<0} |a_{ik}| \,\}$

Initialization: $F = \emptyset$; $C = \emptyset$; $U = [1\,,\,n]$;
For all i : $m_i = |\{\, j \in U \mid i \in S_j \,\}|$.

Algorithm: While $U \neq \emptyset$ do

1. select $i \in U$ with minimal m_i
2. select $j \in U$ such that $a_{ij} = \min_{k \in U} a_{ik}$
3. if $j \in S_i$:

3a. $C = C \cup \{j\}$, $F = F \cup \{i\}$, $G_j = \{i, j\}$, $U = U \backslash \{i, j\}$
3b. update: $m_k = m_k - 1$ for $k \in S_i$ and $k \in S_j$

otherwise:

3a'. $C = C \cup \{i\}$, $G_i = \{i\}$, $U = U \backslash \{i\}$
3b'. update: $m_k = m_k - 1$ for $k \in S_i$

Double pairwise aggregation

Algorithm:

1. Apply simple pairwise aggregation to A.
   Output: $(F_1\,,\,C_1)$, and $G_i^{(1)}$, $i\in C_1$.
2. Compute the auxiliary matrix $A_1=\left(a_{ij}^{(1)}\right)$, $i,j\in C_1$
   with
   $$a_{ij}^{(1)} = \sum_{k\in G_i^{(1)}}\sum_{\ell\in G_j^{(1)}} a_{k\ell}\ .$$
3. Apply simple pairwise aggregation to A_1.
   Output: $(F_2\,,\,C_2)$, and $G_i^{(2)}$, $i\in C_2$.
4. $C=C_2$, $F=F_1\cup F_2$, $G_i=\cup_{j\in G_i^{(2)}}G_j^{(1)}$, $i\in C$.

Example

2D problem with anisotropy & discontinuity
Five-point finite difference approx. (uniform mesh) of

$$-a_x\frac{\partial^2 u}{\partial x^2}-a_y\frac{\partial^2 u}{\partial y^2} = f \qquad \text{in} \quad \Omega=(0,1)\times(0,1)$$

$$\begin{cases} u = 0 & \text{on } y=1\,,\ 0\le x\le 1 \\ \frac{\partial u}{\partial n} = 0 & \text{elsewhere on } \partial\Omega \end{cases}$$

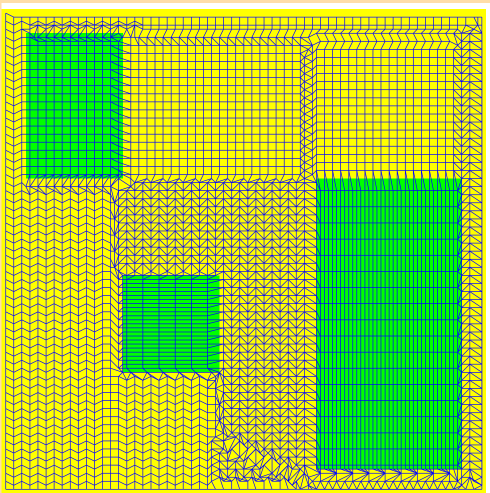
$$\begin{cases} a_x=d\ ,\ a_y=1\ ,\ f=0 & \text{in } (0.65\,,\,0.95)\times(0.05\,,\,0.65) \\ a_x=1\ ,\ a_y=d\ ,\ f=0 & \text{in } (0.25\,,\,0.45)\times(0.25\,,\,0.45) \\ a_x=d\ ,\ a_y=d\ ,\ f=1 & \text{in } (0.05\,,\,0.25)\times(0.65\,,\,0.95) \\ a_x=1\ ,\ a_y=1\ ,\ f=0 & \text{elsewhere}\ , \end{cases}$$

where d is a parameter.

Example ($d=100$)

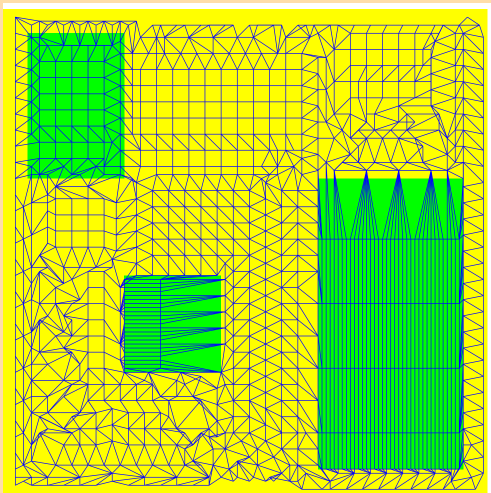
Double pairwise aggregation

First coarse grid



$n_c=3794$, $\frac{n}{n_c}=3.83$, $\frac{nz}{n_c}=5.46$

Second coarse grid



$n_c=1025$, $\frac{n}{n_c}=14.2$, $\frac{nz}{n_c}=6.02$

Some remarks

Geometric multigrid does not benefit from semi-coarsening
→ A_{FF} may be badly conditioned
→ has to be compensated by specialized smoothers.

Geometric schemes fix the coarsening and the interpolation; the smoother (the approximation to A_{FF}) is adapted to the problem.

Algebraic schemes fix the smoother (the approximation to A_{FF}); the coarsening is adapted to the problem.

With algebraic schemes, the adaptation is automatic.

Aggregation: pros and cons

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- Control of the coarsening speed.
- Insensitive to the Strong/Weak coupling threshold.
- Maintain the sparsity in coarse grid matrices, that are nevertheless “reasonable”, up to some scaling factor.
- The interpolation that is naturally associated with aggregation is bad (not an issue for MBF-based methods).
- Smoothed aggregation: optionally sparsify A into $\widetilde{A}$, in such a way that $A\mathbf{e} = \widetilde{A}\mathbf{e}$; then:

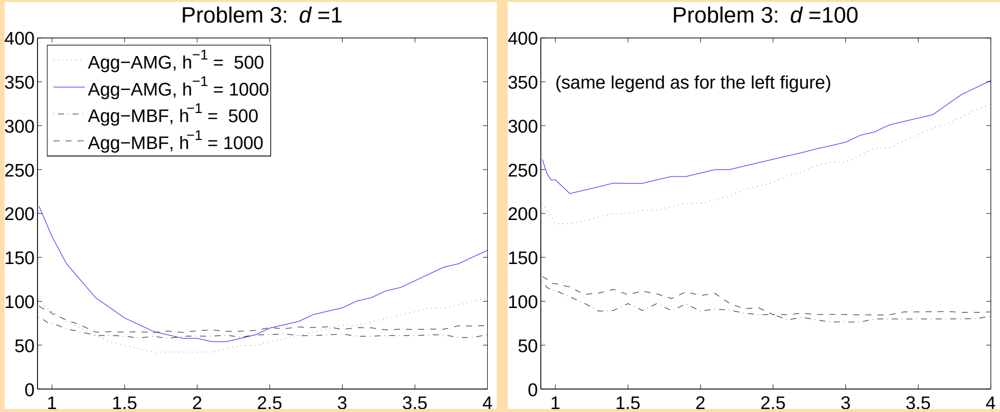
$$p_{\text{sm agg}} = \left(I - \omega\, \widetilde{D}^{-1}\widetilde{A}\right) p_{\text{agg}}$$

where $\widetilde{D} = \text{diag}(\widetilde{A})$.

Illustration

ULB

Performance of AMG and MBF with aggregation



Relative solution cost – vs – scaling of the coarse grids

Checking the F/C partitioning

ULB

A_{FF} has to be well conditioned.
This may be a posteriori checked.

Compatible relaxation (AMG)

Perform smoothing on a random r.h.s while frozing the values at C variables. If the error at F variables does not decay quickly, adapt the partioning by moving to C some of the slowly convergent F variables.

Remark
Amounts to check the conditioning of $M_{FF}^{-1}A_{FF}$.
Remember that
$\kappa_{\text{AMG}} \sim \left(\lambda_{\min}(M_{FF}^{-1}A_{FF})\left(2 - \lambda_{\max}(M^{-1}A)\right)\right)^{-1}$.

Checking the F/C partitioning (cont.)

ULB

Dynamic MILU

The size of the pivots in a modified ILU ($P_{FF}\mathbf{e}_F = A_{FF}\mathbf{e}_F$) factorization is a good indication of the conditioning.

For instance, in some cases, letting $P_{FF} = L_{FF}\, Q_{FF}^{-1} U_{FF}$ with $\text{diag}(L_{FF}) = \text{diag}(U_{FF}) = Q_{FF}$,
if $Q_{FF} \geq \xi \text{diag}(A_{FF})$ for some $\xi > \frac{1}{2}$, then

$$\kappa(P_{FF}^{-1}A_{FF}) \leq \frac{1}{2-\xi^{-1}} .$$

Dynamic MILU: algorithm

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1. *Repeat*=*False* .
2. (re)initialize:
   $Q_{FF} = \text{diag}(A_{FF})$, $L_{FF} = \text{lower}(A_{FF})$,
   $U_{FF} = \text{upper}(A_{FF})$.
3. for $k = 1, \ldots, n$, $k \in F$:
   if $q_{kk} \geq \gamma\, a_{kk}$:
   eliminate row & column k in A_{FF} according to the MILU algorithm
   otherwise: $F = F\backslash\{k\}$, $C = C \cup \{k\}$;
   Repeat=*True* .
4. If (*Repeat*), GoTo 1, possibly decreasing the value of γ .

Dynamic MILU: example

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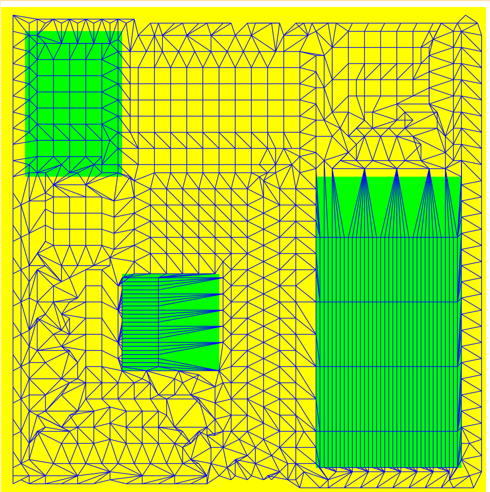
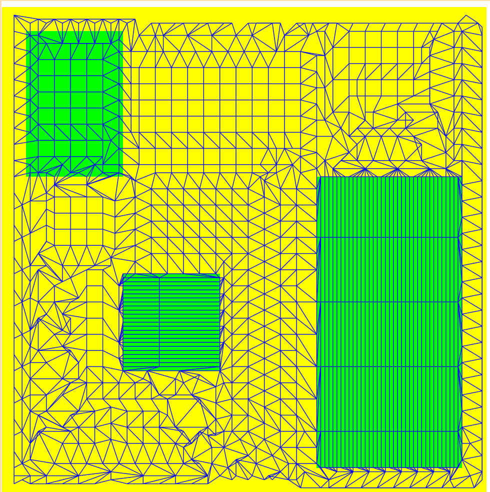
Double pairwise aggregation, second coarse grid

Without dynamic MILU



$n_c = 1025$, $\frac{n}{n_c} = 14.2$, $\frac{nz}{n_c} = 6.02$

With dyanmic MILU



$n_c = 1124$, $\frac{n}{n_c} = 12.9$, $\frac{nz}{n_c} = 5.94$

From two- to multi-level

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- Exploit recursively the same ideas.
- Succession of grids (levels), each with its own F/C partitioning and interpolation J_{FC} , and also with its “ideal” preconditioner in which the matrix at the coarser level is inverted exactly.
- At some point the coarse grid matrix in indeed small enough to be factorized exactly.
- At every other level, the “ideal” preconditioner is adapted, exchanging the exact solution to $\widehat{A}_C \mathbf{v}_C = \mathbf{y}_C$ for an approximate solution.
- Approximate $\widehat{A}_C \mathbf{v}_C = \mathbf{y}_C$ with
  1 application of the preconditioner: V cycle.
  inner iterations: W cycle.

From two- to multi-level (cont.)

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W cycles may be based on fixed point iterations, but Krylov (CG, GMRES) is more robust. Then:

- Except at the coarsest level, the so defined preconditioner is slightly variable from step to step $\rightarrow$
  Flexible Krylov subspace methods (FCG, FGMRES).
- Inner iterations are exited when the relative residual error is less than 0.35 , or when the number of iterations reaches *int*$[nz(A)/nz(\widehat{A}_C)]$.

From two- to multi-level (cont.)

ULB

AMG: often efficient with V cycle
$\longrightarrow$ simplicity, consistency with slow coarsening.

The use of V cycle is based on experiment and mimicry of geometric schemes
$\longrightarrow$ it may be not robust to rely on V cycle.

Block factorization methods: require W cycle (geometric schemes do require it too)

$\longrightarrow$ need coarsening fast enough.

Numerical results (previous problem)

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MBF with aggregation & dynamic MILU

$$\text{"sol"} = \frac{\text{Cost of resolution}}{\text{Cost of 1 unprec. CG iter.}} \approx 28 \text{ for geom. multigrid (on model problems).}$$

	$h^{-1}=600$				$h^{-1}=1200$			
d	$\frac{n}{n_c}$	inner	iter.	sol.	$\frac{n}{n_c}$	inner	iter.	sol.
1	3.99	1.76	21	67.1	4.00	1.76	21	68.8
2	3.97	2.00	20	69.8	3.99	2.00	23	82.9
4	3.96	2.04	24	84.1	3.98	2.00	25	90.3
10	3.95	2.04	24	84.2	3.98	2.04	26	94.0
10^2	3.95	2.04	24	82.5	3.98	2.00	26	90.6
10^4	3.95	1.96	26	88.0	3.98	2.04	27	95.6
10^6	3.95	2.15	26	92.2	3.98	2.00	31	107.9

A non self-adjoint 3D problem

ULB

Seven-point FD approx. (upwind scheme) of

$$-\nu\,\Delta u + \overline{v}\,\overline{\nabla} u = 0 \quad \text{in } \Omega = (0,1)\times(0,1)\times(0,1)$$

$$\begin{cases} u = 1 & \text{on } z = 1,\ 0 \le x,\ y \le 1 \\ u = 0 & \text{elsewhere on } \partial\Omega \end{cases}$$

$$\overline{v}(x,y,z) = \begin{pmatrix} 2x(1-x)(2y-1)z \\ -(2x-1)y(1-y) \\ -(2x-1)(2y-1)z(1-z) \end{pmatrix};$$

$\nu = \infty$ corresponds to the Laplace equation.

Uniform mesh with constant mesh size h.

Stretched mesh: refined in such a way that the ratio of maximum mesh size to minimum mesh size is equal to 200, the ratio of subsequent mesh sizes being constant.

3D problem: numerical results

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	$101\times101\times101$ grid				$201\times201\times201$ grid			
ν	$\frac{n}{n_c}$	inner	iter.	sol.	$\frac{n}{n_c}$	inner	iter.	sol.
Uniform mesh								
∞	4.00	2.00	15	79.6	4.00	2.00	15	82.0
1	3.76	2.00	17	109.7	3.81	2.00	17	108.3
10^{-2}	3.75	2.00	18	119.7	3.84	1.94	18	111.7
10^{-4}	3.93	2.00	21	136.9	3.93	2.00	21	136.8
10^{-6}	3.93	2.00	26	167.2	3.96	2.00	30	203.0
Stretched mesh								
∞	3.91	1.94	16	79.3	3.94	1.88	17	85.8
1	3.91	1.94	16	80.0	3.94	1.88	17	85.8
10^{-2}	3.92	1.65	20	95.5	3.95	1.94	17	85.3
10^{-4}	3.46	1.81	21	117.1	3.64	1.87	23	125.8
10^{-6}	3.64	2.00	27	171.0	3.28	2.00	27	186.3

Some references

ULB

Many textbooks on multigrid, but few address algebraic schemes.

- U. Trottenberg, C.W. Oosterlee, and A. Schüller. Multigrid. Academic Press, London, 2001.

is recommended for a general introduction to multigrid; it contains in appendix the best available review on AMG:

- K. Stüben. An Introduction to Algebraic Multigrid. In Trottenberg et al., 2001. Appendix A.

Other results in research papers. Let mention mine !

- Algebraic multigrid and algebraic multilevel methods: a theoretical comparison
- Aggregation-based algebraic multilevel preconditioning

(see homepage for details and download)

ULB

PhD Fellowship

Area: numerical nuclear reactor simulation

Collaboration between ULB and Framatome ANP

Location: Framatome ANP GmbH in Erlangen, Germany (main European research center of the group) with periodical stays in Brussels.

Task: adaptation of advanced preconditioned iterative techniques to nuclear reactor simulation.

Please contact me for further information.

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