# Multigrid-based augmented block-Cimmino method

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Sparse Days

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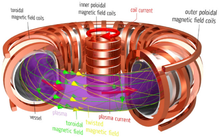
CERFACS - Toulouse[1] IRIT - Université de Toulouse[2]

Erlangen-Nuremberg Univ.[3]

# General Problem: From physics to Linear Algebra




$$
\begin{cases}
\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0 \\
\rho \partial_t \mathbf{v} + \rho \mathbf{v} \cdot \nabla \mathbf{v} + \nabla(p) = \mathbf{J} \times \mathbf{B} + \nu \triangle \mathbf{v} \\
\partial_t p + \mathbf{v} \cdot \nabla p + \gamma p \nabla \cdot \mathbf{v} = 0 \\
\partial_t \mathbf{B} = -\nabla \times \mathbf{E} = \nabla \times (\mathbf{v} \times \mathbf{B} - \eta \mathbf{J}) \\
\nabla \times \mathbf{B} = \mathbf{J} \\
\nabla \cdot \mathbf{B} = 0
\end{cases}
$$

$\mathbf{Ax} = \mathbf{b}$

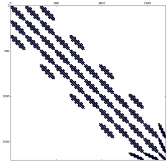
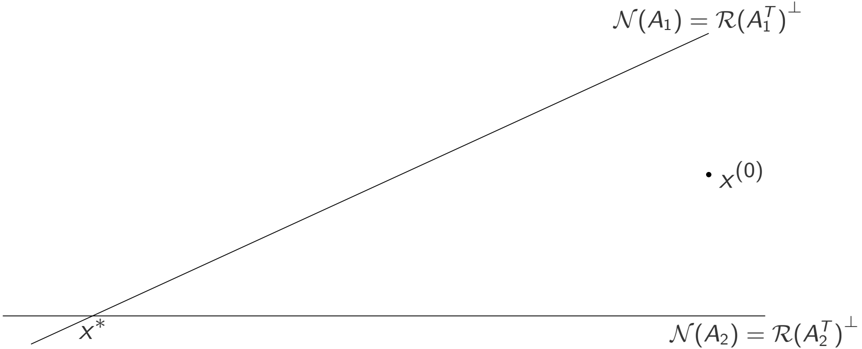



Figure: Simulation of a PDE problem leads to the solution of a sparse linear system $\mathbf{Ax} = \mathbf{b}$

# block Cimmino
## A block-iterative technique

G. Cimmino. *Estensione dell'identità di picone alla più generale equazione differenziale lineare ordinaria autoaggiunta*. Atti della Accad. Nazionanale dei Lincei, 28:354–364, 1939.



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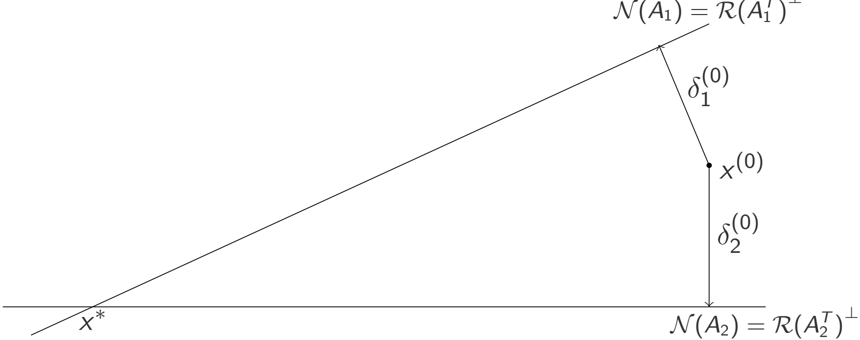

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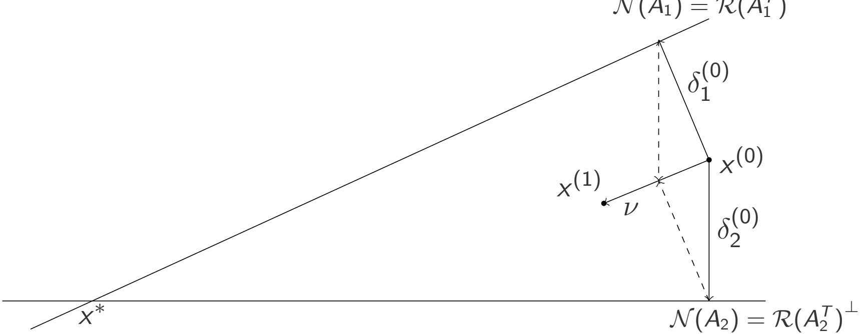
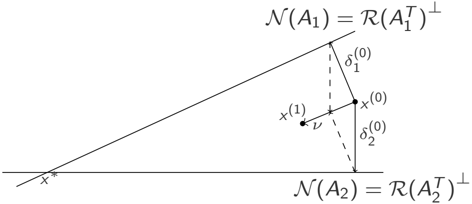


T. Elfving. *Block-iterative methods for consistent and inconsistent linear equations. Numerische Mathematik, 35(1), 1-12., 1980.*




$$Ax = b$$

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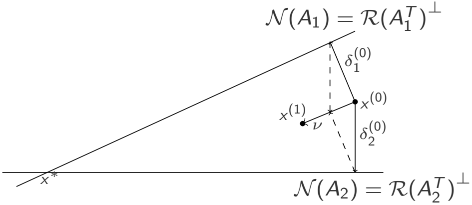


$$\begin{pmatrix} A_1 \\ A_2 \\ \vdots \\ A_p \end{pmatrix} x = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_p \end{pmatrix}$$

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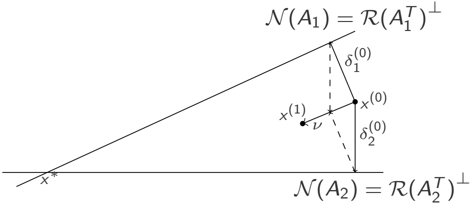


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$$\textbf{B.C:}\ x^{(k+1)} = x^{(k)} + \omega \sum_{i=1}^{p} A_i^{+}(b_i - A_i x^{(k)})$$

# block Cimmino

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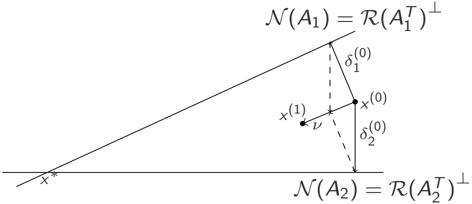
M. Arioli et al.. *Block Lanczos techniques for accelerating the block Cimmino method, CERFACS TR. PA/92/70, 1992.*

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$$\textbf{B.C:}\ x^{(k+1)} = x^{(k)} + \omega \sum_{i=1}^{p} A_i^+ (b_i - A_i x^{(k)})$$

$$\iff \mathbf{H\ x = K} \text{ with } H = \sum_{i=1}^{p} \mathcal{P}_{\mathcal{R}(A_i^T)} = \sum_{i=1}^{p} A_i^+ A_i$$

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## Proposal

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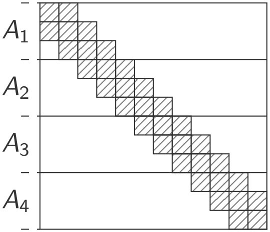
$\Rightarrow$ **A**ugmented **B**lock **C**immino **D**istributed solver (`ABCD solver`)

$$Ax = b$$

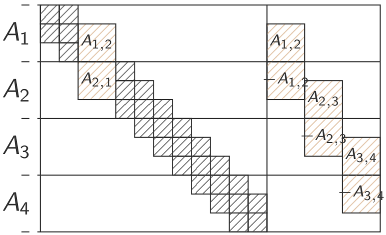



Illustrative example

I. Duff et al.. *The augmented block Cimmino distributed method. SIAM Journal on Scientific Computing, 37(3), A1248-A1269, 2015.*

## 1) Additional variables for orthogonality

$$\bar{A}\bar{x} = \begin{bmatrix} A & F(A) \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = b$$




`Illustrative example`

- $\forall\ i, j \ \in \ \{1, \ldots, p\},\ A_i A_j^T + F(A)_i F(A)_j^T = 0$

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**2) Ensure same solution with additional constraints**

$$\begin{bmatrix} \bar{A} \\ Y \end{bmatrix} \bar{x} = \begin{bmatrix} A & F(A) \\ 0 & I \end{bmatrix} \begin{bmatrix} x \\ 0 \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix}$$

- $\forall\ i, j \ \in\ \{1, \ldots, p\},\ A_i A_j^T + F(A)_i F(A)_j^T = 0$
- $y = 0$

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**3) Orthogonality of additional constraints**

$$\begin{bmatrix} \bar{A} \\ W \end{bmatrix} \bar{x} = \begin{bmatrix} A & F(A) \\ B & S \end{bmatrix} \begin{bmatrix} x \\ 0 \end{bmatrix} = \begin{bmatrix} b \\ f \end{bmatrix}$$

- $\forall\ i, j\ \in\ \{1, \ldots, p\},\ A_i A_j^T + F(A)_i F(A)_j^T = 0$
- $y = 0$ and $x$ is the original solution for $f = -Y\bar{A}^+ b$
- project $Y = \begin{bmatrix} 0 & I \end{bmatrix}$ s.t. $\bar{A} W^T = 0$ with:
  - $W^T = (I - \bar{P}) Y^T$
  - with $\bar{P} = \mathcal{P}_{\mathcal{R}(\bar{A}^T)}$

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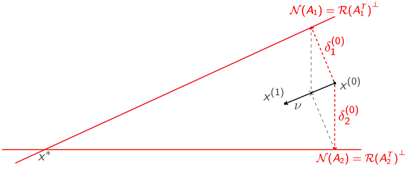


Figure: block-Cimmino

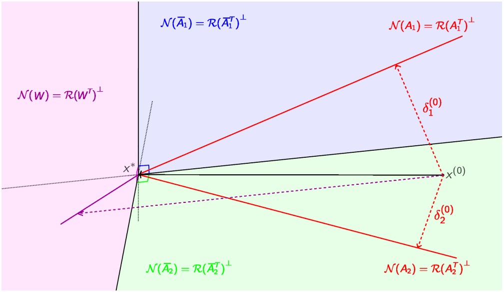


Figure: augmented block-Cimmino

# augmented block-Cimmino

## Implicit Direct Solver

The solution can be directly obtained as :

$$\begin{aligned}\begin{bmatrix} x \\ y \end{bmatrix} &= \bar{A}^{+}b + W^{+}f \\ &= \bar{A}^{+}b - \left(I - \bar{P}\right) Y^{T} S^{-1} Y \bar{A}^{+} b\end{aligned}$$

which requires only:

1. the ingredients of BC: $\sum_{i=1}^{p} \bar{A}_i^{+} b_i$,
2. S and not B,
3. to solve a system $Sz = f$ using a direct solver.

ABCD-SOLVER V1.0 available at **http://abcd.enseeiht.fr/**
Developments granted by the ANR-BARESAFE and ANR-FP3C projects, supported by the French National Agency for Research

# Augmentation on the interface

## Decoupling domains

The Augmented block Cimmino solves: $\begin{cases} 1)\ \tilde{A}\tilde{A}^T\tilde{X} = B \\ 2)\ X = \tilde{A}^T\tilde{X} \end{cases}$

$$\tilde{A} = \begin{pmatrix} A & F(A) \\ O_{q\times n} & I_q \end{pmatrix},\ B = \begin{bmatrix} b \\ 0 \end{bmatrix},\ X = \begin{bmatrix} x \\ y \end{bmatrix},\ \tilde{X} = \begin{bmatrix} \tilde{x} \\ \tilde{y} \end{bmatrix}.$$

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**1) Normal equations:** due to enforced orthogonality

$$\tilde{A}\tilde{A}^T X = B \Longleftrightarrow \begin{bmatrix} \bar{A}_1\bar{A}_1{}^T & & & F(A)1 \\ & \ddots & & \vdots \\ & & \bar{A}_p\bar{A}_p{}^T & F(A)_p \\ F(A)_1^T & \dots & F(A)_p^T & I_q \end{bmatrix} \begin{bmatrix} \tilde{x_1} \\ \vdots \\ \tilde{x_p} \\ \tilde{y} \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix} \tag{1}$$

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**2) S = Schur:** condensation on the interface between domains

$$S = Y(I - \bar{P})Y^T = I_q - \sum_{i=1}^{p} F(A)_i^T (\bar{A}_i\bar{A}_i{}^T)^{-1} F(A)_i \tag{2}$$

# A problem with the size of the augmentation

## Example on a standard 3D PDE problem

Consider a 3D Poisson problem discretized on a cube, with standard 7-point finite difference stencil. Let the cube be meshed with on each direction a number of points of $N = 2^{12} = 4.096$: the total number of nodes is then $n = N^3 \sim 68\,719\;10^6$.

Let's partition the 3D cube with $l_p = 16$ blocks in each direction, which gives $p = l_p^3 = 4096 (= N)$ partitions in total.

The interconnection between 1 partition and the rest is approximately equal to the variables in its 6 faces: $M_i = 6 \times f$ with $f = (\frac{N}{l_p})^2$ the number of variables in 1 face.

We would then end up with an augmentation of size :

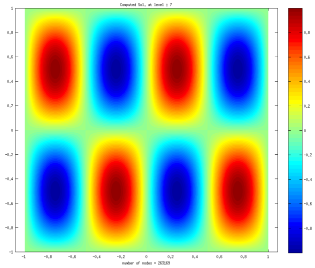
$$Total_{vars} \sim \sum_{i=1}^{p} M_i = 6p(\frac{N}{l_p})^2 = \frac{6N^3}{16^2} = \mathcal{O}(N^3) \; ! \tag{3}$$

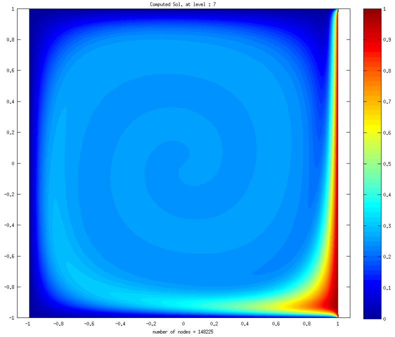
H. Elman et al.. *Finite elements and fast iterative solvers: with applications in incompressible fluid dynamics. Oxford University Press, USA. 2014.*

- Test problems on a square domain $\Omega_\square = (-1,1) \times (-1,1)$

**Helmholtz**
$\nabla^2 u + k^2 u = f$ in $\Omega_\square$ with $k = 40$
Homogeneous Dirichlet B.C.

**Convection-Diffusion with recirculating flow**
$-\epsilon \nabla^2 u + \vec{w}.\nabla u = 0$ in $\Omega_\square$
Dirichlet B.C. $\begin{cases} u = 1 \text{ on the right} \\ \text{homogeneous, else} \end{cases}$



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p=16, m=262121, nz=1 823 761

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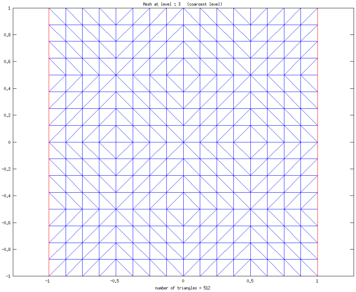
- P1 Finite Element discretization using Matlab PDE Toolbox,



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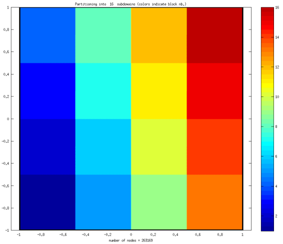

# PDE context and multigrid

## Challenging 2D PDE problems

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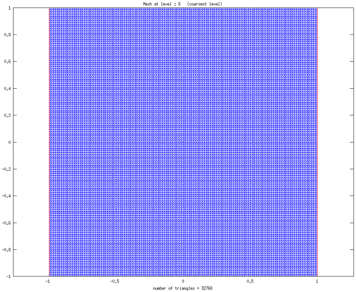
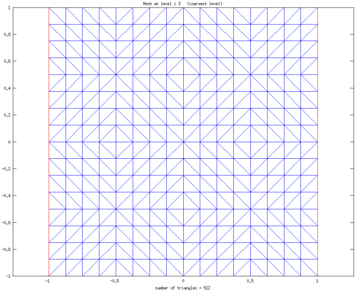
- Multiple levels of grids with prolongation operators $P_l^{l+1}$ (bilinear interpolation)



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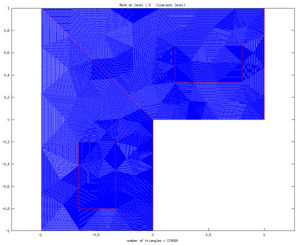
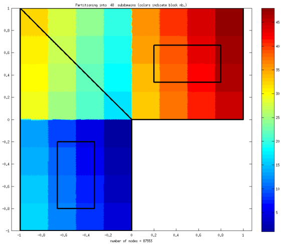
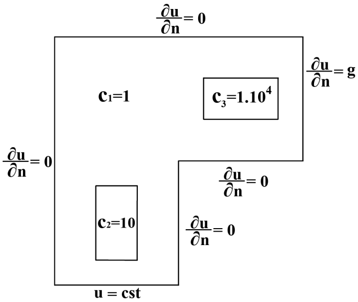
**Choice of a grid level=control of the size of S**

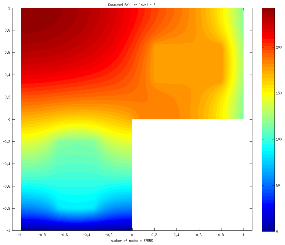
- Problem on a L-shaped domain $\Omega_{\mathbf{L}}$



- Problem on a L-shaped domain $\Omega_\mathbf{L}$
- **Heterogeneous diffusion problem:** $\nabla^2 u - k^2 u = f$ in $\Omega_\mathbf{L}$
- p=75, m=87 424, nz=606 798
- heterogeneity of the patches



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- heterogeneity of the patches
- P1 FE + Multiple levels of grids

# Partial augmentation in ABCD

## Relax the orthogonality

Looking for a good augmentation which is small and still opens the angles:

$$\forall\ i,j\ \in\ \{1,\dots,p\},\ \bar{A}_i\bar{A}_j^T \approx 0$$

Applying the same algorithm for augmentation on a matrix $V$ of size $m \times n_c$ with $n_c < n$:

$$\bar{A} = \begin{bmatrix} A & F(AV) \end{bmatrix}$$

For example, on a tridiagonal matrix

$$\bar{A} = \left[\begin{array}{ccccc|cc} A_{1,1} & A_{1,2} & & & & (AV)_{1,2} & \\ & A_{2,1} & A_{2,2} & A_{2,3} & & -(AV)_{2,1} & (AV)_{2,3} \\ & & & A_{3,2} & A_{3,3} & & -(AV)_{3,2} \end{array}\right]$$

# Partial augmentation in ABCD

## Coarse augmentation

With the augmentation:

$$\bar{A} = \begin{bmatrix} A & F(AV) \end{bmatrix}$$

Orthogonality within a subrange of A:

$$(AV)_i(AV)_j^T + F(AV)_iF(AV)_j^T = 0$$

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Orthogonality within a subrange of A:

$$(AV)_i (AV)_j^T + F(AV)_i F(AV)_j^T = 0$$

**Control on the size of the augmentation**

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<u>*Remarks:*</u>

- $P = \prod_{l=coarsest}^{finest} P_l^{l+1}$: aggressive coarsening

# Partial augmentation in ABCD

## Coarse augmentation

With the augmentation:

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**Control on the size of the augmentation**

**Natural choice: $V = P$ the prolongation operator**

<u>*Remarks:*</u>

- $P = \prod_{l=coarsest}^{finest} P_l^{l+1}$: aggressive coarsening
- 1 grid level: $F(AP) = F(A) \Longrightarrow ABCD$

# Partial augmentation in ABCD

## Control on the size

Table: Size of the augmentation depending on the grid level chosen.

| | Diffusion | | Convection-Diffusion | | Helmholtz | |
|---|---|---|---|---|---|---|
| grid levels | P | F(AP) | P | F(AP) | P | F(AP) |
| 1 (ABCD) | 87 424 | 7 011 | 146 689 | 4608 | 261 121 | 6 150 |
| 2 | 21 952 | 3 567 | 36 481 | 2 311 | 65 025 | 3 078 |
| 3 | 5 536 | 1 844 | 9 025 | 1 159 | 16 129 | 1 542 |
| 4 | 1 408 | 985 | 2 209 | 583 | 3 969 | 774 |
| 5 | 364 | 551 | 529 | 295 | 961 | 390 |

**Additional constraints and same solution**

$$\begin{bmatrix} \bar{A} \\ W \end{bmatrix} \bar{x} = \begin{bmatrix} A & F(AP) \\ B & S \end{bmatrix} \begin{bmatrix} x \\ 0 \end{bmatrix} = \begin{bmatrix} b \\ f \end{bmatrix}$$

- $\forall\ i,j\ \in\ \{1,\dots,p\},\ (AP)_i(AP)_j + F(AP)_iF(AP)_j = 0$
- $x$ is the original solution for $f = -Y\bar{A}^{+}b$
- $\bar{A}W^T = 0$ with $W^T = (I - \mathcal{P}_{\mathcal{R}(\bar{A}^T)})Y^T$
- $\begin{bmatrix} x \\ 0 \end{bmatrix} = \bar{A}^{+}b + W^{+}f$

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**Okay but...** Non-orthogonal partitions !

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   $\Longrightarrow$ Block-Cimmino iterative method on $\bar{A}$ with fast linear convergence

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   $\Longrightarrow$ Block-Cimmino iterative method on $\bar{A}$ with fast linear convergence

2. $\mathcal{P}_{\mathcal{R}(\bar{A}^T)} \neq \sum_{i=1}^{p} \mathcal{P}_{\mathcal{R}(\bar{A}_i^T)}$

   $\Longrightarrow$ How to compute $W$ and $f$ for the $W^+ f$ part ? Block Cimmino again

# Iterative solution of $A^{+}b$

## Convergence of the block-Cimmino method

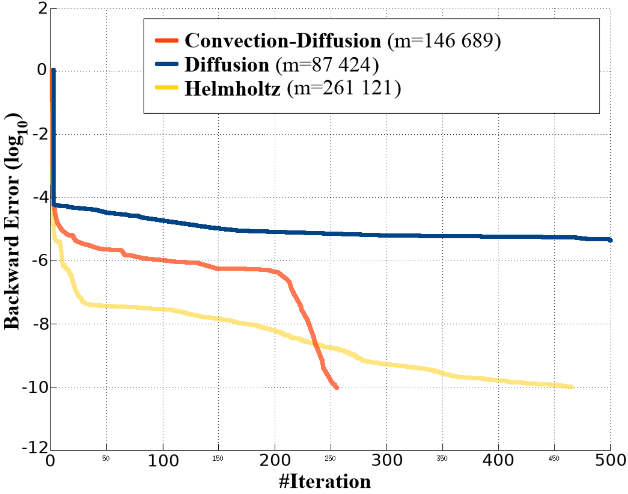



Figure: Without augmentation

# Iterative solution of $\bar{A}^{+}b$

## Convergence of the block-Cimmino method

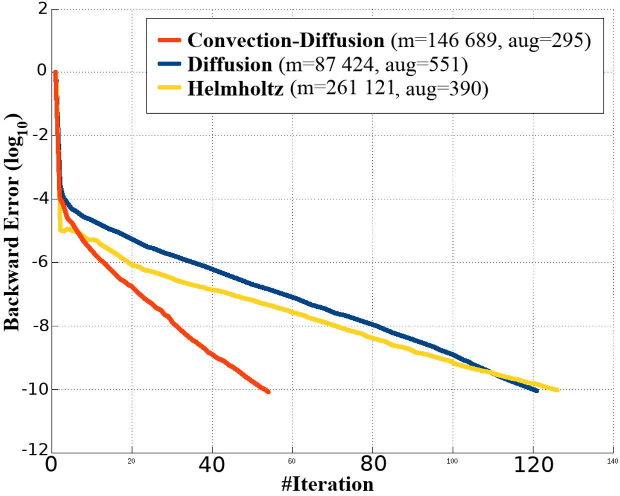
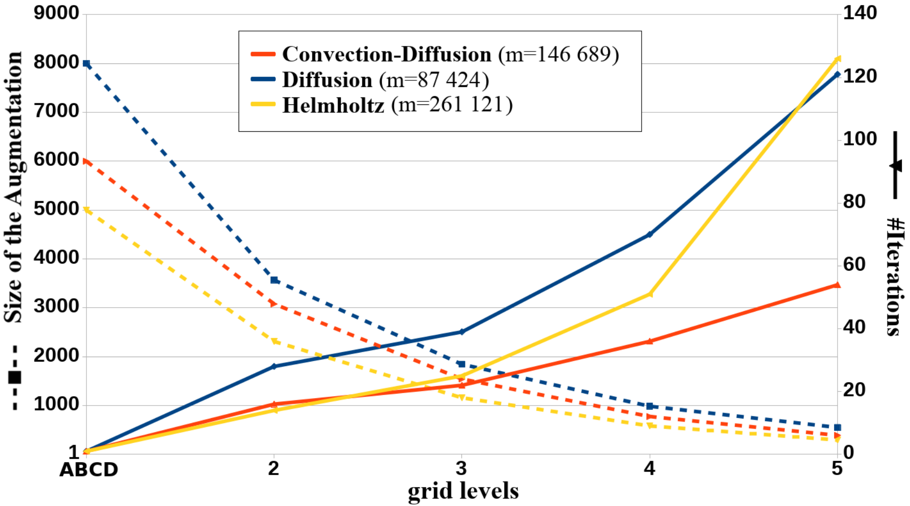



Figure: With augmentation using 5 levels of grids

# Iterative solution of $\bar{A}^+ b$

## Impact of the grid level choice



# Construction and solution of $W^+f$

## Iterative construction of $W$ and $f$

**Issue:** $W = Y(I - \mathcal{P}_{\mathcal{R}(\bar{A}^T)}) = Y - Z^T$ and $\mathcal{P}_{\mathcal{R}(\bar{A}^T)} \neq \sum_{i=1}^{p} \mathcal{P}_{\mathcal{R}(\bar{A}_i^T)}$

**Solution 1:**
$Z = \mathcal{P}_{\mathcal{R}(\bar{A}^T)} Y^T$ with $Y = \begin{bmatrix} I & 0 \end{bmatrix}$ and $f = -Y\bar{f} = -Y\bar{A}^+ b$ solution of the system:

$$\bar{A}Z = \bar{A}Y^T \text{ and } \bar{A}\bar{f} = b$$

Simultaneous stabilized Block-CG on the equivalent systems:

$$\bar{H}Z = \bar{H}Y^T \text{ and } \bar{H}\bar{f} = -b \text{ with } \bar{H} = \sum_{i=1}^{p} \bar{A}_i^+ \bar{A}_i$$

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$\Longrightarrow$ Iteratively obtained from $Y$ with CG accelerated block-Cimmino:

Technique interesting for reasonnable size of augmentation and extra costs of building $Z$ can be compensated with changing right hand sides.

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Simultaneous stabilized Block-CG on the equivalent systems:

$$\bar{H}Z = \bar{H}Y^T \text{ and } \bar{H}\bar{f} = -b \text{ with } \bar{H} = \sum_{i=1}^{p} \bar{A}_i^+ \bar{A}_i$$

$\Longrightarrow$ Iteratively obtained from $Y$ with CG accelerated block-Cimmino:

Technique interesting for reasonnable size of augmentation and extra costs of building $Z$ can be compensated with changing right hand sides.

Caution ! $W$ approximated: $\bar{A}W^T \neq 0 \Longrightarrow W$ as partition in the global BCG scheme.

# Construction and solution of $W^+f$

## Iterative construction of $S$

**Issue:** $W = Y(I - \mathcal{P}_{\mathcal{R}(\bar{A}^T)})$ and $\mathcal{P}_{\mathcal{R}(A^T)} \neq \sum_{i=1}^{p} \mathcal{P}_{\mathcal{R}(A_i^T)}$

**Solution 2:** (WIP)
Recall:

$$W^+f = \left(I - \bar{P}\right) Y^T S^{-1} Y \bar{A}^+ b$$

Construct a preconditioned CG to solve without constructing S:

$$D^{-1} Y(I - \mathcal{P}_{\mathcal{R}(\bar{A}^T)}) Y^T z = D^{-1} f$$

with:

- $\mathcal{P}_{\mathcal{R}(\bar{A}^T)} = \bar{A}^+ \bar{A}$: interior iterations of block-Cimmino,
- $D^{-1} \approx S^{-1} = I + Z^T Z$ with $Z = -A^{-1} C$
- Construct $D/Z$ with Multigrid method ?

# Conclusion

Summary:

- Controlled size of the augmentation,
- Resulting efficient block-Cimmino method with fast linear convergence,
- Problem of the construction/solution of $W$ remaining and currently the focus of our research.

A question remain: What is the interpretation in terms of PDE for this augmented approach ?

Possible extensions:

- Preprocessing: scaling of the system, use of ellipsoidal norms, multi-level augmentation, ...
- Column-oriented approach to solve least-square problems,
- Algebraic multigrid to build the prolongation operator.

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[5] ABCD-solver v1.0-beta : the Augmented Block Cimmino Distributed solver. **http://abcd.enseeiht.fr/**


Thank you, any questions?

Table: Size of the augmentation depending on the grid level chosen.

| | Diffusion | | Convection-Diffusion | | Helmholtz | |
|---|---|---|---|---|---|---|
| grid levels | Size of C | it. | Size of C | it. | Size of C | it. |
| 1 | 8000 | 1 | 5000 | 1 | 6000 | 1 |
| 2 | 3567 | 28 | 2311 | 16 | 3078 | 14 |
| 3 | 1844 | 39 | 1159 | 22 | 1542 | 25 |
| 4 | 985 | 70 | 583 | 36 | 774 | 51 |
| 5 | 551 | 121 | 295 | 54 | 390 | 126 |