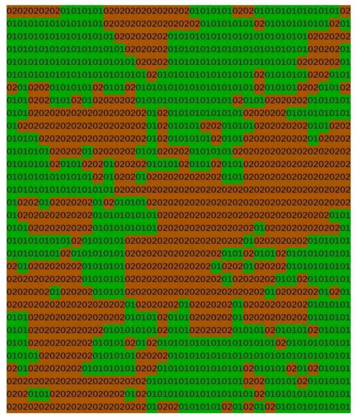
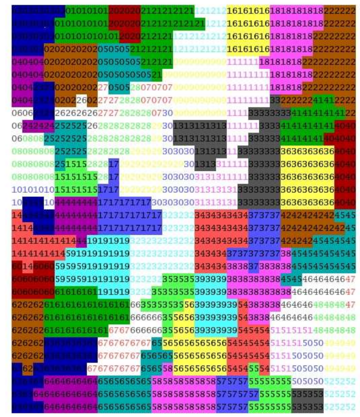
Robust Aggregation–Based Coarsening for Multiscale PDEs





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in collaboration with **Eero Vainikko** (Tartu, Estonia)

DD17, Strobl, Austria, July 2006

Model Problem:

$$\begin{aligned} -\nabla \cdot \Big(\mathcal{A}(\boldsymbol{x}) \nabla u(\boldsymbol{x}) \Big) &= f(\boldsymbol{x}) && \text{in } \Omega \subset \mathbb{R}^d \ (d = 1,2,3) \\ u &= g && \text{on } \Gamma_D \subset \partial\Omega \\ \mathcal{A} \nabla u \cdot \boldsymbol{n} &= 0 && \text{on } \Gamma_N = \partial\Omega \backslash \Gamma_D \end{aligned}$$

- Modelling **flow in heterogeneous porous media** (u fluid pressure)
- **Emergent properties of materials with microstructures** (thermal, electrical, mechanical)
- **In today's talk** we will only consider $\Gamma_N = \emptyset$, $g \equiv 0$ and $\boxed{\mathcal{A}(\boldsymbol{x}) = \alpha(\boldsymbol{x}) I}$
- **Main difficulty:** **highly variable (discontinuous) coefficient function** $\alpha(\boldsymbol{x})$

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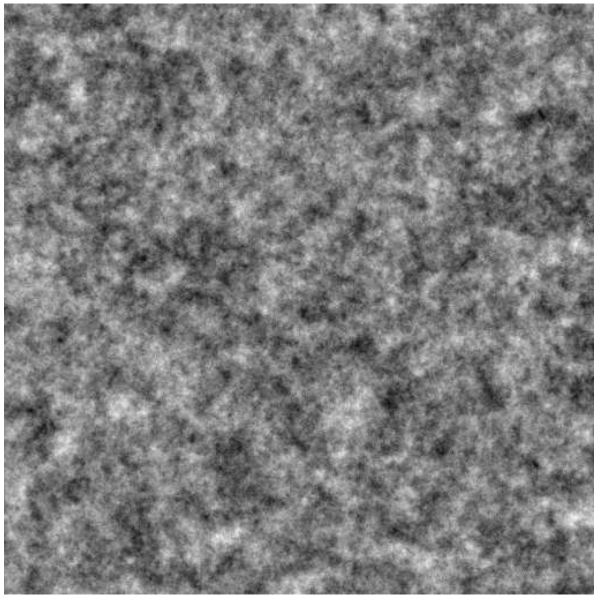
- Main difficulty: **highly variable (discontinuous) coefficient function** $\alpha(\boldsymbol{x})$

Provides **important insight** for more complicated problems (e.g. oil reservoir simulation)!

Stochastic Model: $\log \alpha(\boldsymbol{x}) =$ (homogeneous, isotropic) Gaussian random field with
(i.e. log-normal $\alpha(\boldsymbol{x})$) **mean** 0, **variance** σ^2, **correlation length scale** λ

Typical Realisation of log-normal $\alpha(\boldsymbol{x})$

($n = 512^2$, $\sigma^2 = 8$ and $\lambda = \frac{1}{64}$)



"Clipped" Realisation ("two-phase" media)

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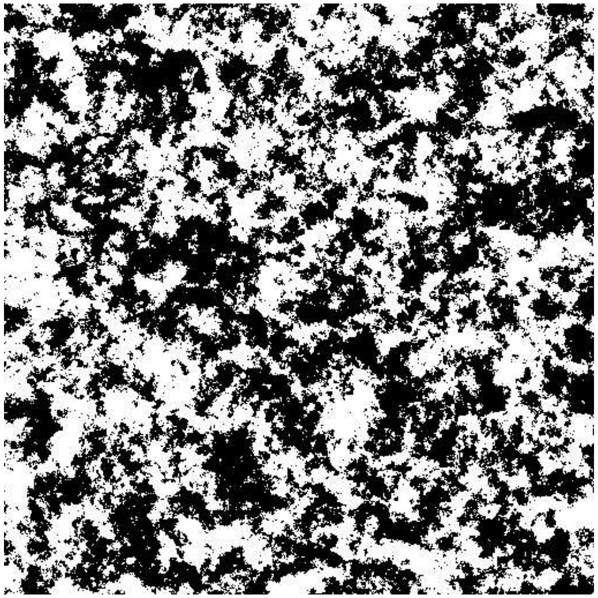

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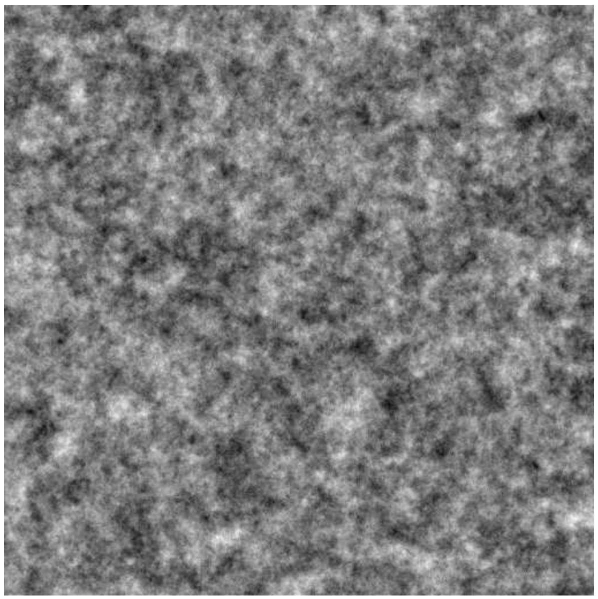

$$\sup_{\mathbf{x},\mathbf{y}\in\Omega} \frac{\alpha(\mathbf{x})}{\alpha(\mathbf{y})} = O(10^{10}) \nearrow$$

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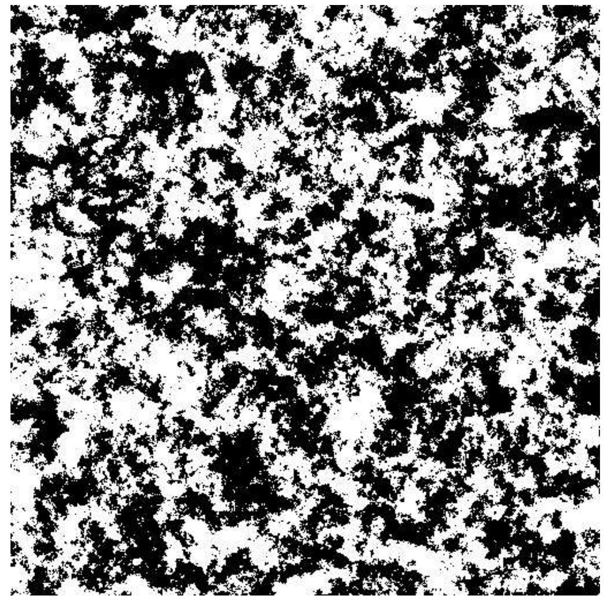
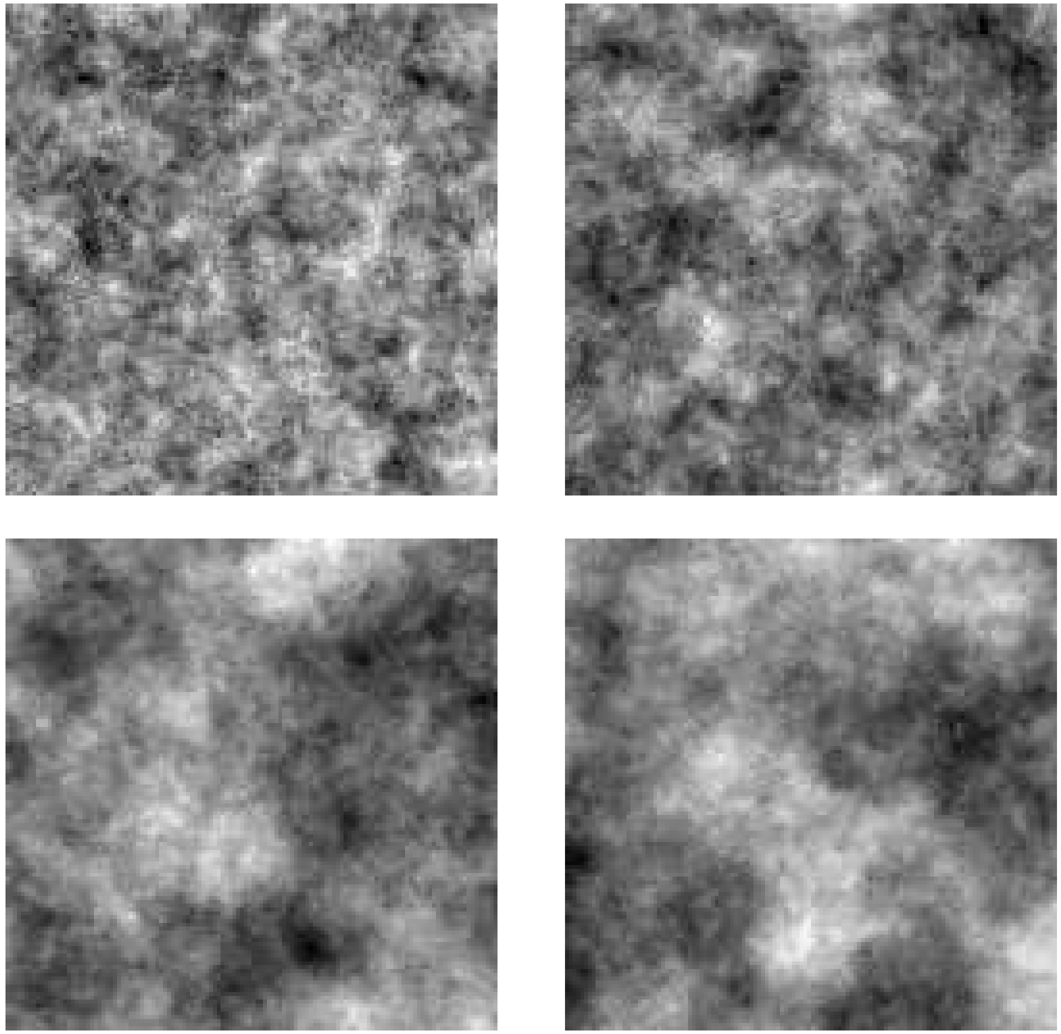


$$\sup_{\mathbf{x},\mathbf{y}\in\Omega} \frac{\alpha(\mathbf{x})}{\alpha(\mathbf{y})} = O(10^{5}) \nearrow$$

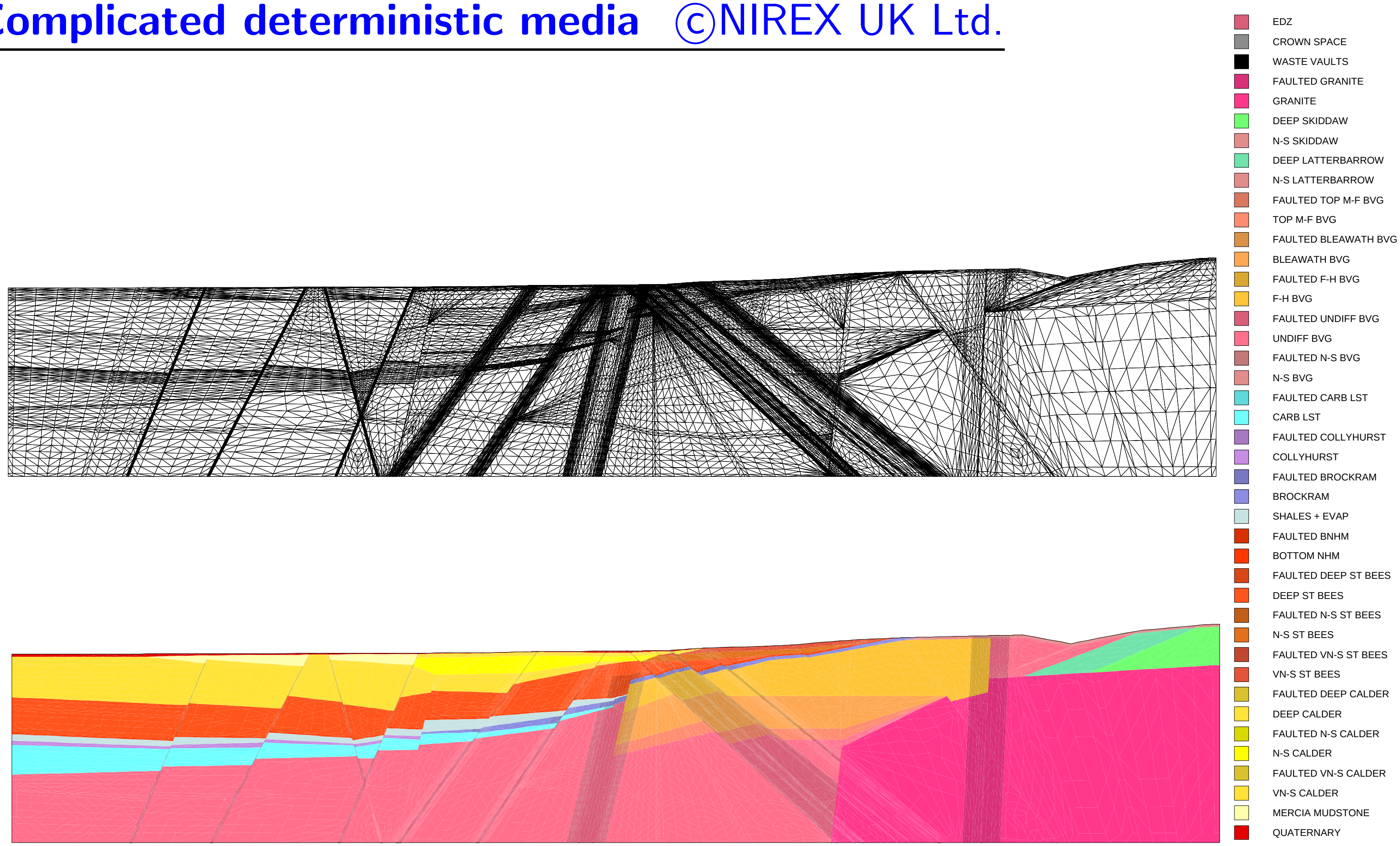
Variance σ^2 determines **"contrast"** !



Correlation length scale λ determines **"roughness"** **!**

Typical multiscale coefficient functions

Complicated deterministic media ©NIREX UK Ltd.



Finite Element Method:

$a(u,v) := \int_\Omega \alpha \nabla u \cdot \nabla v$ ... bilinear form on $(\,H_0^1(\Omega)\,)^2$ corresponding to model problem

$\mathcal{V}^h \subset H^1(\Omega)$ ... FE space of continuous, piecewise linear functions on $\tau \in \mathcal{T}^h$

$\{\varphi_p\} \subset \mathcal{V}^h \cap H_0^1(\Omega)$ ... "hat" functions corresponding to the nodes $\boldsymbol{x}_p^h$ of $\mathcal{T}^h$

Then the FE approximation $u_h = \sum_{p=1}^{n} U_p \varphi_p \in \mathcal{V}^h \cap H_0^1(\Omega)$ where $\mathbf{U} = (U_p)_{p=1,\ldots,n}$ satisfies

$$\boxed{A\,\mathbf{U} = \mathbf{b}}$$

with $A_{p,q} = \sum_\tau \alpha_\tau \int_\tau \nabla\varphi_p \cdot \nabla\varphi_q$ and $\alpha_\tau := \frac{1}{|\tau|}\int_\tau \alpha$.

$$\boxed{\kappa(A) \lesssim \max_{\tau,\tau' \in \mathcal{T}^h} \left(\frac{\alpha_\tau}{\alpha_{\tau'}}\right) h^{-2}} \quad = O(10^{16}) \quad \text{for} \quad h = \frac{1}{512},\ \sigma^2 = 8 \text{ !!}$$

Assume w.l.o.g. that α is piecewise constant and $\min_{\tau \in \mathcal{T}^h} \alpha_\tau = 1$ (otherwise rescale!).

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Conjugate Gradients:

$\#\text{Its} = O\left(\sqrt{\kappa(A)}\right)$

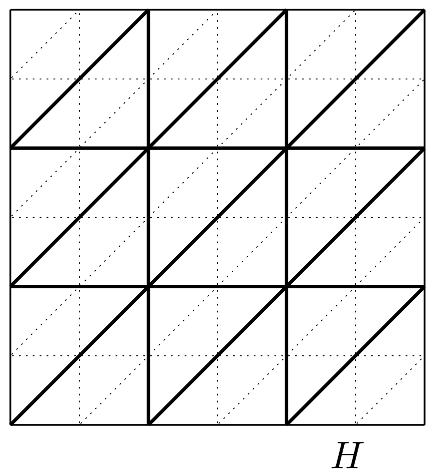
Meaning of $\lesssim$ **!**

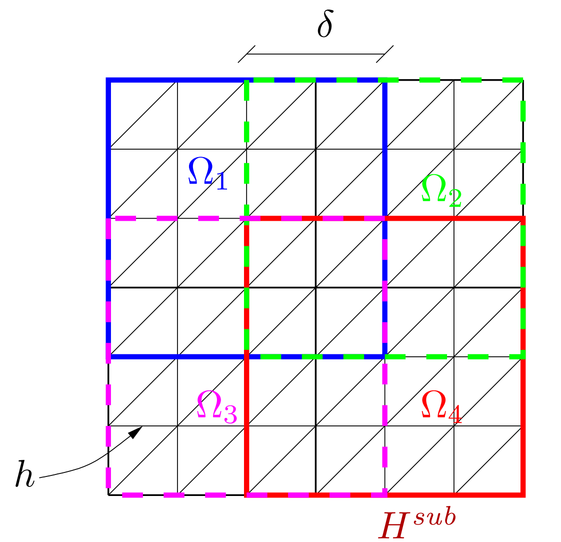
Assume w.l.o.g. that α is piecewise constant and $\min_{\tau \in \mathcal{T}^h} \alpha_\tau = 1$ (otherwise rescale!).

Two-Level Additive Schwarz:

$$\mathcal{P}_{\mathrm{AS}}^{-1} \quad = \quad \underset{\substack{\uparrow}}{R_0^T\, A_0^{-1}\, R_0} \quad + \quad \sum_{i=1}^{s} \underset{\substack{\uparrow}}{R_i^T\, A_i^{-1}\, R_i}$$

coarse solve with $A_0 := R_0\, A\, R_0^T$ **local solves** with $A_i := R_i\, A\, R_i^T$





$\{\Omega_i : i = 1, \ldots, s\}$ ... overlapping covering of Ω (**Note.** $H^{sub} \gg H$ for best efficiency)

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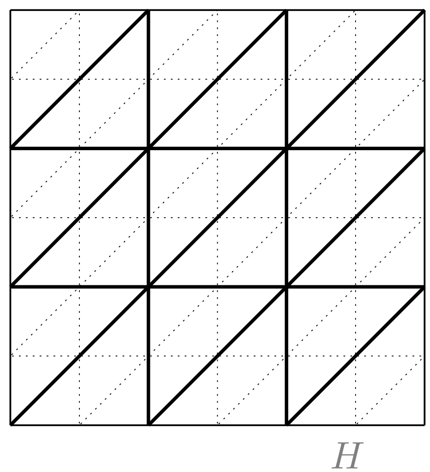

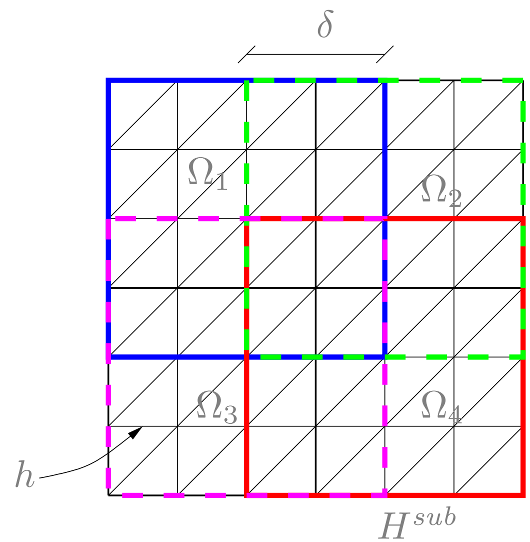

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IMPORTANT: **choice of** **covering** $\{\Omega_i\}$, **coarse space** $\mathcal{V}_0$ and **operator** R_0 **!**

Coarsening via Aggregation

Linear Coarse Space (classical):

Dryja, Widlund, Bramble, Pasciak, Schatz, . . . , Sarkis **[Toselli & Widlund, 2005]**

Assume: coarse mesh $\mathcal{T}^H$, for $K \in \mathcal{T}^H$: $\Omega_K \sim K$, $H_K = \mathrm{diam}(K)$ and $\delta_K =$ overlap of Ω_K.
Then:

$$\kappa(\mathcal{P}_{\mathrm{AS}}^{-1} A) \lesssim \max_{K \in \mathcal{T}^H} \max_{\tau, \tau' \subset \omega_K} \left(\frac{\alpha_\tau}{\alpha_{\tau'}}\right) \left(1 + \frac{H_K}{\delta_K}\right)$$

$$\kappa(\mathcal{P}_{\mathrm{AS}}^{-1} A) \lesssim \mathbf{C}\,(\mathbf{H}/\mathbf{h}) \max_{K \in \mathcal{T}^H} \max_{\tau, \tau' \subset K} \left(\frac{\alpha_\tau}{\alpha_{\tau'}}\right) \left(1 + \frac{H_K}{\delta_K}\right)$$

where $\omega_K := \bigcup_{\{K' : K \cap K' \neq \emptyset\}} K'$ and $\mathbf{C}\,(\mathbf{H}/\mathbf{h}) = \log(\mathbf{H}/\mathbf{h})$ in **2D** and $\mathbf{H}/\mathbf{h}$ in **3D**.

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i.e. "jump-independence" by resolving discontinuities with the coarse mesh!

- Results extend to **non-standard (partition of unity) coarse spaces** **[Sarkis, 1993–]**
- **Unresolved layers** $\Rightarrow$ **spectral clustering** **[Graham & Hagger, 1999]**

BUT what about case of large variation of α inside coarse elements/subdomains?

Abstract Coarse Space:

$$\mathcal{V}_0 = \mathrm{span}\{\Phi_j : j = 1, \ldots, N\}$$

where $\{\Phi_j : j = 1, \ldots, N_H\} \subset \mathcal{V}^h$ are **linearly independent coarse space basis functions** such that $\Phi_j \in H_0^1(\Omega)$ for all $j \leq N$ and

(C1) $\displaystyle\sum_{j=1}^{N_H} \Phi_j(x) = 1$ for all $x \in \bar{\Omega}$

(C2) $\|\Phi_j\|_{L_\infty(\Omega)} \lesssim 1$ for all $j = 1, \ldots, N_H$

(C3) $\forall j = 1, \ldots, N_H \quad \exists\, i \in \{1, \ldots, s\}$ such that $\omega_j := \mathrm{supp}\{\Phi_j\} \subset \Omega_i$

Important Parameters: $H_j := \mathrm{diam}\{\omega_j\}$, $H := \max_j H_j$, $\delta_j :=$ overlap for ω_j, $\delta := \min_j \delta_j$.

Definition. (Coarse Space Robustness Indicator)

$$\gamma(\alpha) := \max_{j=1}^{N_H} \delta_j^2 \left\| \alpha |\nabla \Phi_j|^2 \right\|_{L_\infty(\Omega)}$$

Note. For the theory we need also **shape regularity**, **uniform overlap**, **finite covering** of the $\{\omega_j\}$.

Theorem (S., 2006).
$$\kappa(P_{\mathrm{AS}}^{-1}A) \lesssim \gamma(\alpha)\left(1 + \max_{j=1}^{N_H} \frac{H_j}{\delta_j}\right)$$

Remarks:

- **Previous results** had extra assumption $\|\nabla\Phi_j\|^2_{L_\infty(\Omega)} \lesssim \delta_j^{-2}$ (or a weaker L_2–version):

  Here, **interplay** between coarse space basis functions and α is made **explicit** in $\gamma(\alpha)$!

- **No dependency** on the subdomain sizes (even for $H^{sub} \gg H$) !

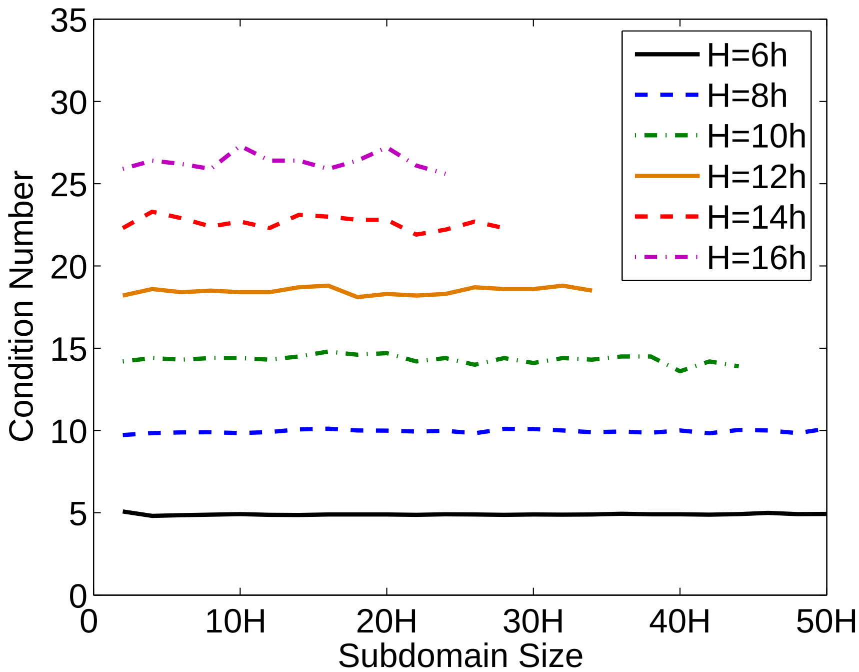
- The dependency on the "mesh" parameters is **sharp**, i.e. linear in H/δ.

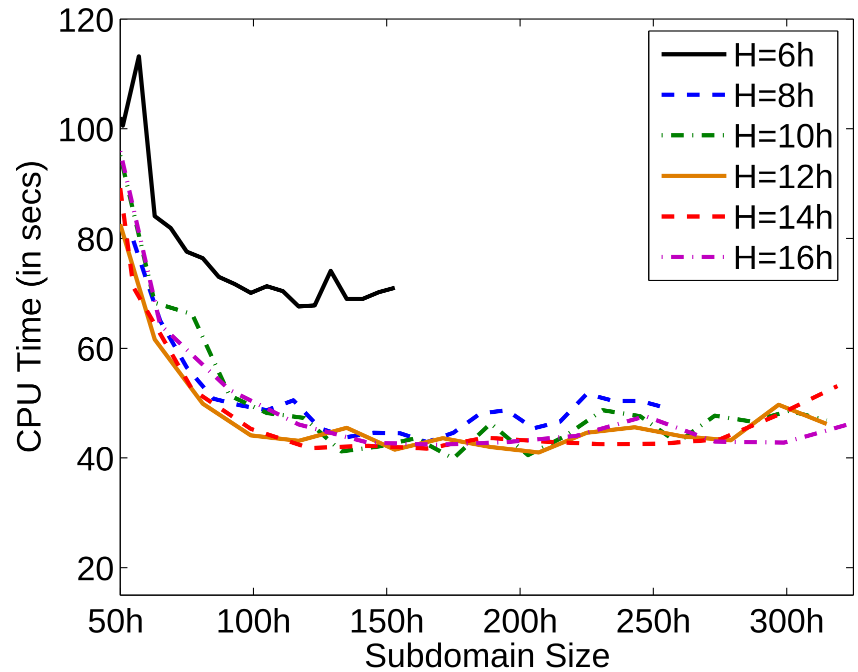
- Previously best theoretical result for smoothed aggregation coarse spaces (for $\alpha \equiv 1$):

$$\kappa(P_{\mathrm{AS}}^{-1}A) \lesssim 1 + \frac{H}{\delta} + \frac{H^{sub}}{\delta}$$

[Sala, Shadid & Tuminaro, SIMAX 2006]

Example (Laplacian): $\alpha \equiv 1 \quad \Longrightarrow \quad \gamma(\alpha) \sim 1$



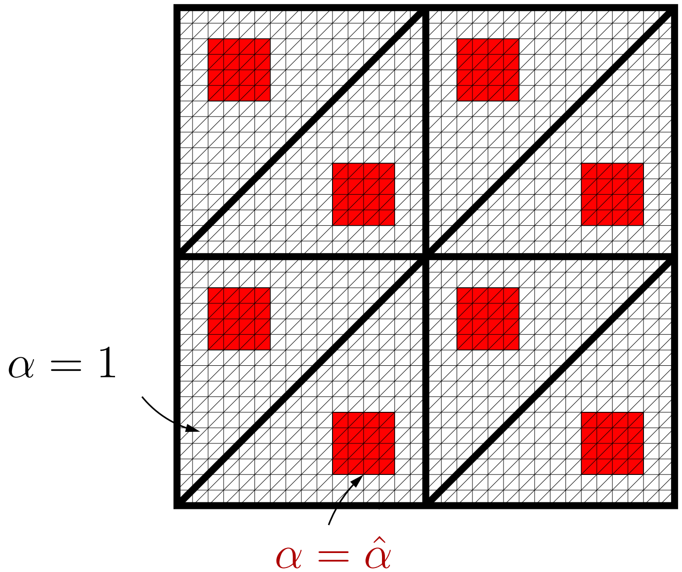


$n = 1024 \times 1024$, minimal overlap (i.e. $\delta = 3h$), $1\times$smoothed aggregation

Note. All CPU times were obtained on a 3GHz INTEL Pentium 4 processor.

Example (two media) – Linear Coarsening

- $\mathcal{T}^h$ and $\mathcal{T}^H$ uniform.
- Square subdomains Ω_i (consisting of 8 coarse elements $K \in \mathcal{T}^H$), i.e. overlap $\delta = H$.



For $h = \frac{1}{256}$ and $H = 8h$:

$\hat{\alpha}$	$\kappa(P_{AS}^{-1}A)$	$\gamma(\alpha)$
10^0	5.2	**4**
10^1	9.1	**40**
10^2	58.1	**400**
10^3	471	**4000**
10^4	1821	**4.0(+4)**
10^5	2561*	**4.0(+5)**

$*$ **same as 1-level method (i.e. no coarse grid)**

Idea of Proof. ($\gamma(\alpha)$ **crucial !** Then use classical Schwarz theory introducing "weight" α**!**)

- To bound $\lambda_{\max}(P_{\mathrm{AS}}^{-1}A)$ use a **colouring argument**.

- To bound $\lambda_{\min}(P_{\mathrm{AS}}^{-1}A)$ find **stable splitting** for each $u \in \mathcal{V}^h$: $v_0 \in \mathcal{V}_0$ and $v_j \in \mathcal{V}^h(\omega_j)$ s.t.

$$u = \sum_{j=0}^{N_H} v_j \quad \text{and} \quad \sum_{j=0}^{N_H} a(v_j, v_j) \lesssim \gamma(\alpha) \left(1 + \max_j \tfrac{H_j}{\delta_j}\right) a(u,u)$$

i.e. $v_0 := \sum_{j=0}^{N} \bar{u}_j \Phi_j$ with $\bar{u}_j := |\omega_j|^{-1} \int_{\omega_j} u$ and (**quasi-interpolant**)

$$v_j := \begin{cases} I_h(\Phi_j(u - \bar{u}_j)), & j \le N, \\ I_h(\Phi_j u), & j > N. \end{cases}$$

Now, $a(v_0, v_0) \lesssim \gamma(\alpha) \left(\max_j \tfrac{H_j}{\delta_j}\right) a(u,u)$ and

$$a(v_j, v_j) \lesssim \| \alpha |\nabla \Phi_j|^2 \|_{L_\infty(\omega_j)} \|u - \bar{u}_j\|^2_{L_2(\omega_{j,\delta_j})} + |u - \bar{u}_j|^2_{H^1(\omega_j),\alpha} \lesssim \gamma(\alpha) \left(1 + \frac{H_j}{\delta_j}\right) a(u,u)$$

- To find stable splitting in $\mathcal{V}^h(\Omega_i)$ set $u_i := \sum_{j \in \mathcal{I}_i} v_j$ where $\mathcal{I}_i := \{j : \omega_j \subset \Omega_i\}$ and use again a **colouring argument**.

Geometric Multigrid Idea: Relaxation schemes (like ω-Jacobi or SOR) **smooth** the error

$\Longrightarrow$ restrict to a (geometrically) **coarser** grid. Breaks down for large variation in $\alpha(\boldsymbol{x})$!

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Algebraic Multigrid Idea: Relaxation schemes smooth error along **strong connections** in A:

Use **graph** $\mathcal{G}$ associated with A: node x_q^h is **strongly connected** to x_p^h if $|A_{p,q}|$ is **large**,

e.g. $\boxed{|\tilde{A}_{p,q}| \;\geq\; \varepsilon \max_{k\neq p} |\tilde{A}_{p,k}|}$ where $\tilde{A} := D^{-1/2}\, A\, D^{-1/2}$ **[Bastian, 1996]**

$\Longrightarrow$

- (a) Select **"well-connected"** coarse nodes, and interpolate to strongly connected neighbours based on **heuristic** $A\mathbf{e} = \mathbf{r} \approx 0$ **[Ruge & Stueben, 1985]**.
- (b) **Aggregate** strongly connected neighbours, and use p.w. constant prolongation, smoothed along the strong connections **[Vanek, Mandel & Brezina, 1995]**.

Main Idea:

Extend the notion of **strong connections** to **any** pair of nodes by considering **paths** in $\mathcal{G}$!

Define the **strongly-connected graph-r neighbourhood** of x_p^h by the set of all nodes x_q^h s.t. there exists a path $\gamma_{pq} := [x_p^h = x_{p_0}, x_{p_1}, \ldots, x_{p_k} = x_q^h]$ of length $k \le r$ from x_p^h to x_q^h, and x_{p_i} is strongly connected to $x_{p_{i-1}}$ for all $i = 1, \ldots, k$.

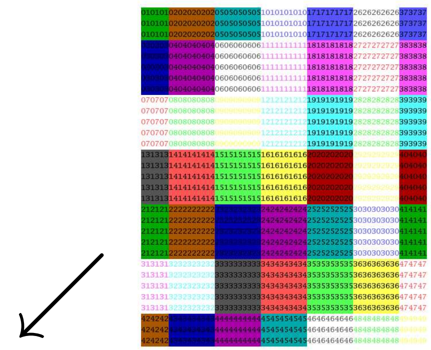
- This is readily available from compressed row storage of so-called **"filtered" matrix**

$$A^{\varepsilon}_{p,q} := \begin{cases} A_{p,p} + \displaystyle\sum_{x_k^h \overset{\text{not str. con.}}{\longrightarrow} x_p^h} A_{p,k} & \text{if } x_q^h = x_p^h \\ A_{p,q} & \text{if } x_q^h \text{ strongly connected to } x_p^h \\ 0 & \text{otherwise} \end{cases}$$

  (i.e. graph $\mathcal{G}$ not needed !)

- To find good **seed nodes** x_p^h for the **aggregates** we use an advancing front **[Raw, 1996]**
- Related to **"aggressive" coarsening** in algebraic multigrid, e.g. **[Papadopoulos, 2004]**

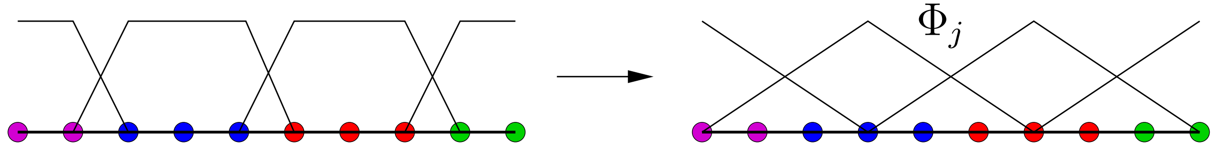
Algorithm:[1]



(Laplacian, i.e. $\alpha \equiv 1$)

1. Select aggregation radius r and threshold ε.
2. Find strong connections in A.
3. Aggregate strongly-connected graph-r neighbourhoods.
   (**IMPORTANT:** choice of seed nodes & shape regularity where possible.)
4. Set $R_0^T = SP$ where $P =$ p.w. constant prolongation and $S =$ simple smoother (ω-Jacobi)

   e.g. for $\alpha \equiv 1$ in 1D with $\omega = \frac{2}{3}$:



5. Subdomains are aggregated using same algorithm on A_0 (Overlap comes from smoothing!)

[1] see also **[Vanek & Brezina, 1999]** , **[Jenkins et al., 2001]**, **[Lasser & Toselli, 2002]**

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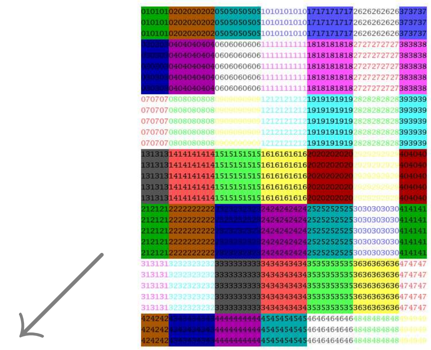

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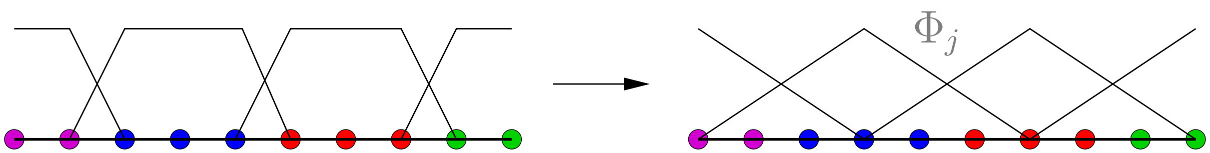

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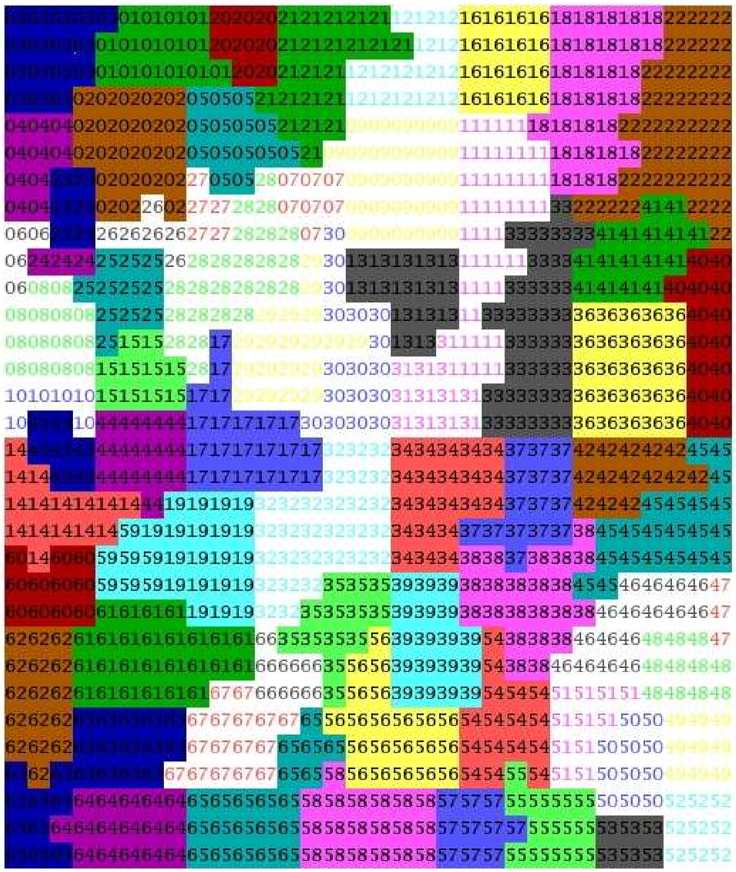
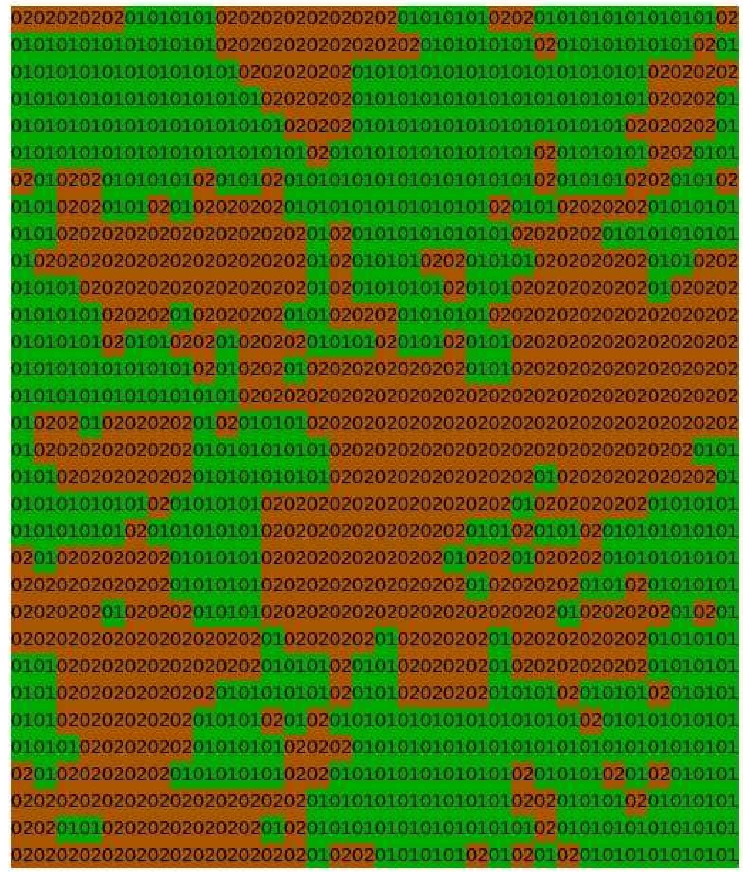
Novel Aspects (apart from new theory)

- Making use of strong connections in a **domain decomposition method**
- Second aggregation for **subdomains** $\longrightarrow$ $H^{\text{sub}} \gg H$

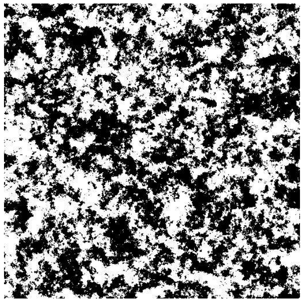
[1] see also **[Vanek & Brezina, 1999]** , **[Jenkins et al., 2001]**, **[Lasser & Toselli, 2002]**





Obtained with $r = 2$ and $\varepsilon = 0.67$ for typical realisation $\left(n = 32^2,\ \lambda = \frac{1}{8},\ \max_{\tau,\tau'} \frac{\alpha_\tau}{\alpha_{\tau'}} \approx 10^3\right)$

Example (clipped random fields):



with $n = 256 \times 256$ and $\lambda = 1/64$

CG–Iterations ($\mathbf{b = 1}$, $\mathrm{tol} = 10^{-6}$)

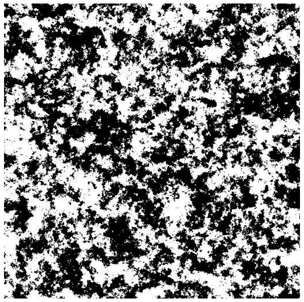
σ^2	$\max_{\tau,\tau'} \frac{\alpha_\tau}{\alpha_{\tau'}}$	**New**	AMG	DOUG
2	$\mathbf{1.5 * 10^1}$	**24**		
4	$\mathbf{2.2 * 10^2}$	**27**		
6	$\mathbf{3.3 * 10^3}$	**29**		
8	$\mathbf{4.9 * 10^4}$	**26**		

CPU–Time (in secs)

σ^2	**New**	AMG	UMFPACK
2	**2.12**		
4	**2.14**		
6	**2.34**		
8	**2.41**		

All numerical results with $r = 2$ and $\varepsilon = 0.67$ and no smoothing!

Example (clipped random fields):



AMG ... Aggregation–type Algebraic Multigrid [Bastian]
(no smoothing – piecewise constant prolongation)

DOUG ... Classical Additive Schwarz with linear coarsening
(parallel run on slow network – CPU-times pessimistic)

UMFPACK ... Sparse direct solver [Davies & Duff]

with $n = 256 \times 256$ and $\lambda = 1/64$

CG–Iterations ($\mathbf{b} = \mathbf{1}$, $\mathrm{tol} = 10^{-6}$)

σ^2	$\max_{\tau,\tau'} \frac{\alpha_\tau}{\alpha_{\tau'}}$	New	AMG	DOUG
2	$1.5 * 10^1$	24	14	32
4	$2.2 * 10^2$	27	27	89
6	$3.3 * 10^3$	29	40	296
8	$4.9 * 10^4$	26	77	498

CPU–Time (in secs)

σ^2	New	AMG	UMFPACK
2	2.12	1.35	1.85
4	2.14	2.27	1.70
6	2.34	3.31	1.33
8	2.41	6.23	4.88

All numerical results with $r = 2$ and $\varepsilon = 0.67$ and no smoothing!

CG–Iterations ($\mathrm{b} = \mathbf{1}$, $\mathrm{tol} = 10^{-6}$)

λ	**New**	AMG	DOUG
1/16	**26**		
1/32	**27**		
1/64	**26**		
1/128	**33**		
1/256	**48**		

CPU–Time (in secs)

λ	**New**	AMG	UMFPACK
1/16	**2.20**		
1/32	**2.24**		
1/64	**2.41**		
1/128	**2.71**		
1/256	**3.84**		

Clipped random fields with $n = 256 \times 256$ and $\sigma^2 = 8$.

CG–Iterations ($\mathrm{b} = \mathbf{1}$, $\mathrm{tol} = 10^{-6}$)

n	**New**	AMG	DOUG
128^2	**25**		
256^2	**26**		
512^2	**34**		
1024^2	**74**		

CPU–Time (in secs)

n	**New**	AMG	UMFPACK
128^2	**0.46**		
256^2	**2.41**		
512^2	**16.8**		
1024^2	**105.9**		

Clipped random fields with $\sigma^2 = 8$ and $\lambda = 4h$.

Numerical Results with Aggregation – Clipped Fields

CG–Iterations ($\mathbf{b} = \mathbf{1}$, $\mathrm{tol} = 10^{-6}$)

λ	New	AMG	DOUG
1/16	26	18	355
1/32	27	64	430
1/64	26	77	498
1/128	33	70	655
1/256	48	166	858

CPU–Time (in secs)

λ	New	AMG	UMFPACK
1/16	2.20	1.67	4.52
1/32	2.24	5.14	4.77
1/64	2.41	6.23	4.88
1/128	2.71	5.77	7.48
1/256	3.84	13.5	10.2

Clipped random fields with $n = 256 \times 256$ and $\sigma^2 = 8$.

CG–Iterations ($\mathbf{b} = \mathbf{1}$, $\mathrm{tol} = 10^{-6}$)

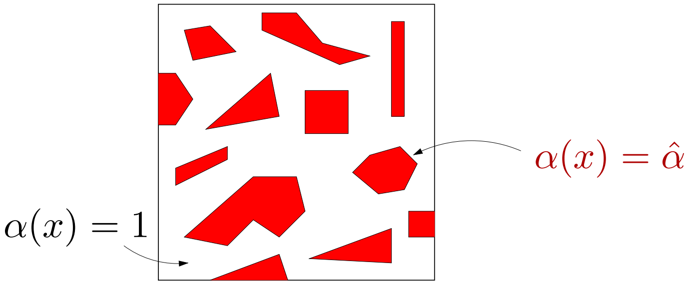
n	New	AMG	DOUG
128^2	25	35	136
256^2	26	77	498
512^2	34	100	1111
1024^2	74	422	***

CPU–Time (in secs)

n	New	AMG	UMFPACK
128^2	0.46	0.68	0.52
256^2	2.41	6.23	4.88
512^2	16.8	33.8	88.8
1024^2	105.9	540	***

Clipped random fields with $\sigma^2 = 8$ and $\lambda = 4h$.

Example ("Islands"):



with $\hat{\alpha} \gg 1$ and $\boxed{\text{diam(islands)} \lesssim h}$

> **Theorem.** For r appropriately chosen, the aggregation algorithm with $R_0^T = P$ (i.e. no smoothing) produces **coarse space basis functions** $\{\Phi_j : j = 1, \ldots, N_H\}$ that satisfy the **Assumptions** (C1)–(C3) and
>
> $$\gamma(\alpha) \;\le\; 1$$
>
> Moreover
>
> $$\kappa(P_{\text{AS}}^{-1} A) \;\le\; C$$

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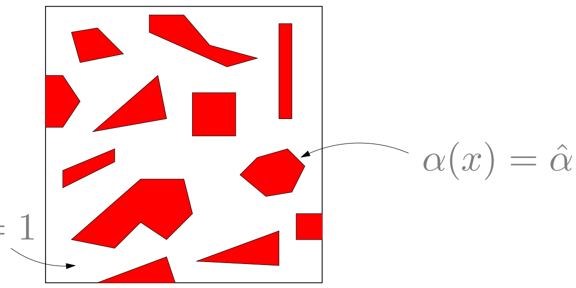

with $\hat{\alpha} \gg 1$ and $\boxed{\mathrm{diam(islands)} \lesssim h}$

> **Theorem.** For r appropriately chosen, the aggregation algorithm with $R_0^T = P$ (i.e. no smoothing) produces **coarse space basis functions** $\{\Phi_j : j = 1, \ldots, N_H\}$ that satisfy the **Assumptions** (C1)–(C3) and
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> Moreover
>
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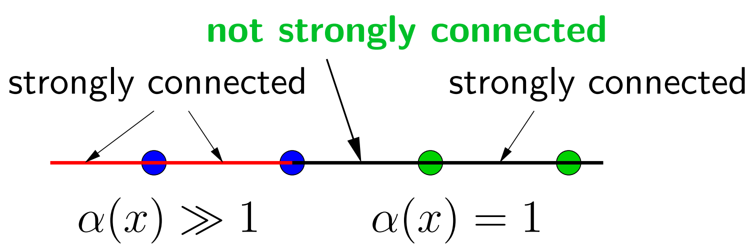
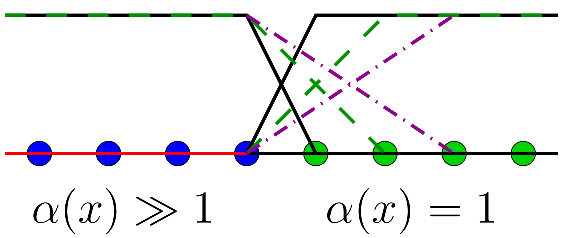
Idea of Proof. In the case $R_0^T = P$ assumptions (C1)–(C3) are satisfied by construction, we have uniform overlap, and finite covering. Also $|\nabla \Phi_j(x)| \le \delta_j^{-1} \;\; \forall\, x \in \Omega$.

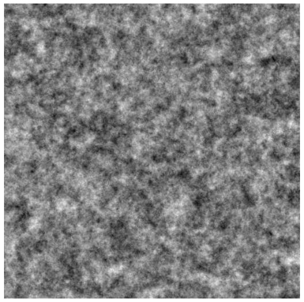




$\Longrightarrow$ (for r sufficiently large) $\alpha(x) = 1$ wherever $\nabla \Phi_j(x) \neq 0$ $\quad\Longrightarrow\quad$ $\gamma(\alpha) \le 1$

Moreover $\delta_j = O(h)$ and since $\mathrm{diam(islands)} \lesssim h$ we can choose r s.t. $H_j \lesssim h \implies \kappa(P_{\mathrm{AS}}^{-1} A) \;\le\; C$ where C is independent of h, r and α but may depend on the shape of the islands.

Example (log-normal $\alpha(\mathbf{x})$):



	New	AMG	DOUG	UMFPACK
Iterations	**19**	38	62	
CPU-time	**8.3s**	13.1s	29.7s	10.3s

Note. Simpler than clipped fields !!

with $n = 512 \times 512$, $\sigma^2 = 8$ and $\lambda = 1/64$

Current/Future Work:

- **Parallelisation**
- **Multiplicative Schwarz**
- Extension of **theory for discontinuous coefficients** to **Algebraic Multigrid**
- **Combination** with **multiscale FE interpolation**

Two preprints available at

http://www.bath.ac.uk/math-sci/BICS