

Energy Minimising Coarse Spaces for Multiscale Elliptic PDEs

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in collaboration with

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Durham, Monday, July 21st 2008

Model Problem

- Elliptic PDE in 2D or 3D bounded domain Ω

$$-\nabla \cdot (\alpha \nabla u) = f \quad + \quad u = 0 \quad \text{on} \quad \partial\Omega$$

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(i.e. independent of variations in n and in $\alpha(x)$)
- Key Question: **Choice of coarse space !**

Motivation: Groundwater Flow

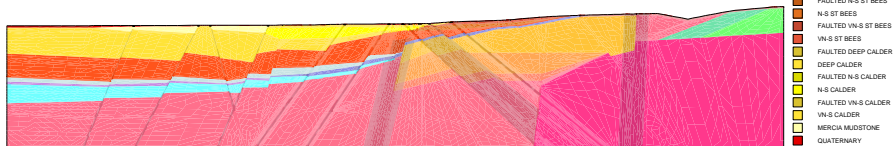
(e.g. safety assessment for radioactive waste disposal)

Darcy's Law: $q + \alpha \nabla p = f$

Incompressibility: $\nabla \cdot q = 0$

+ **Boundary Conditions**

e.g. permeability $\alpha(x)$ at Sellafield ©NIREX UK Ltd.



Relevant also for preconditioning of

- **Mixed FE discretisations** (Raviart-Thomas):

$$\begin{pmatrix} M & B^T \\ B & 0 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} g \\ 0 \end{pmatrix}$$

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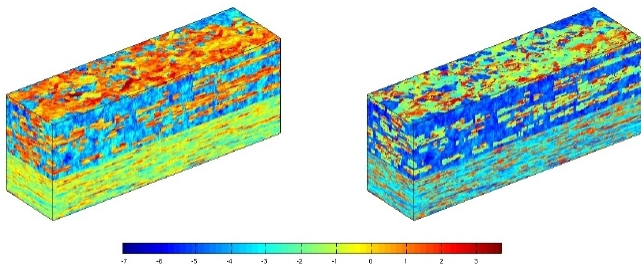
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- **Two-phase porous media flow** (e.g. oil recovery):

$$\begin{pmatrix} A_{pp} & A_{ps} \\ A_{sp} & A_{ss} \end{pmatrix} \begin{pmatrix} \delta p \\ \delta s \end{pmatrix} = \text{RHS}$$

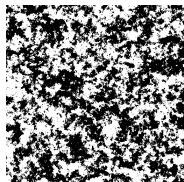
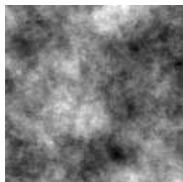
with $A_{pp} \approx -\nabla^h \cdot (\alpha \eta(s) \nabla^h) + \dots$ a diffusion-type operator.

Heterogeneous multiscale deterministic media



Society of Petroleum Engineers (SPE) Benchmark SPE10

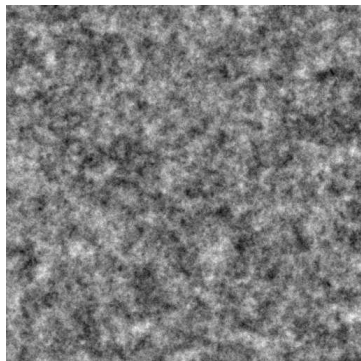
Multiscale stochastic media ($\lambda = 5h, 20h$ & clipped)



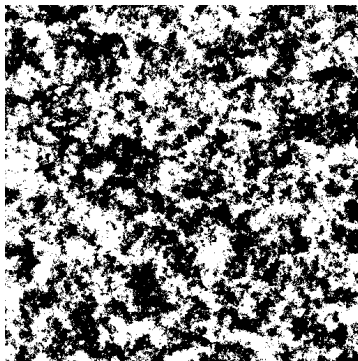
Stochastic Modelling of Heterogeneity

Log-normal random field $\alpha(x)$ (here with $n = 512^2$, $\lambda = 1/64$ and $\sigma^2 = 8$)

Log-normal Realisation



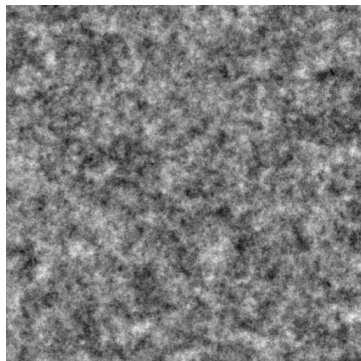
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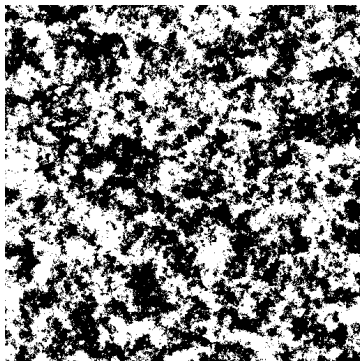
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Log-normal Realisation



$$\max_{\tau, \tau' \in \mathcal{T}^h} \left(\frac{\alpha_\tau}{\alpha_{\tau'}} \right) = O(10^{10}) \nearrow$$

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$$\max_{\tau, \tau' \in \mathcal{T}^h} \left(\frac{\alpha_\tau}{\alpha_{\tau'}} \right) = O(10^5) \nearrow$$

Variance σ^2 determines **“contrast”** !
(**Correlation length λ** determines **“roughness”**)

Difficulties

- Requires very fine mesh resolution: $h \ll L$
- Complicated variation of $\alpha(x)$ on many scales
(hard to **resolve** by (geometric) **coarse** mesh)
- A very large and very ill-conditioned, i.e.

$$\kappa(A) \lesssim \max_{\tau, \tau' \in \mathcal{T}^h} \left(\frac{\alpha_\tau}{\alpha_{\tau'}} \right) h^{-2}$$

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Meaning of \lesssim

Goals

- Solver that is efficient, scalable, parallelisable AND
 - ▶ **robust** w.r.t. problem size n and mesh resolution h
 - ▶ as well as **robust** w.r.t. coefficients α !!
- Underpinning theory \implies
“Handle” for choice of components !

Possible Methods & Existing Theory

- Standard **Domain Decomposition** and **Multigrid** robust if coarse grid(s) **resolve(s)** coefficients

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No theory explaining coefficient robustness for standard AMG!

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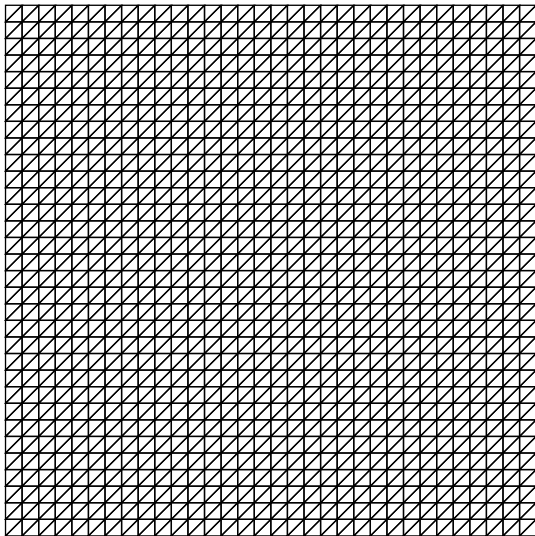
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Two-Level Overlapping Schwarz

Domain Decomposition

Two-Level Overlapping Schwarz Method

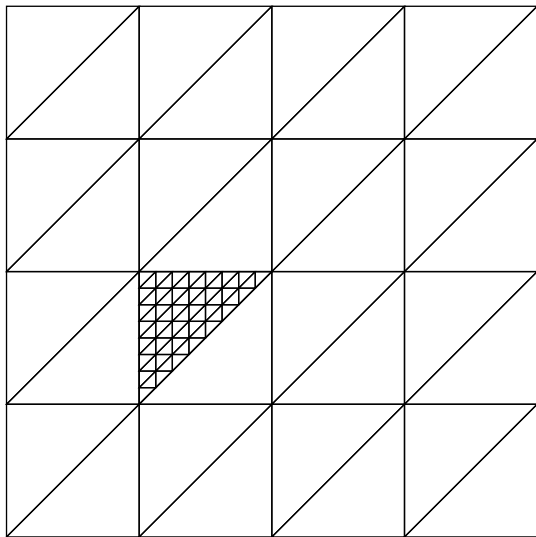
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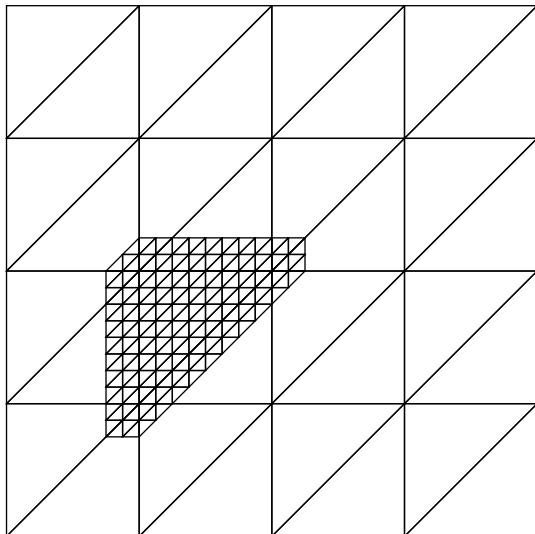
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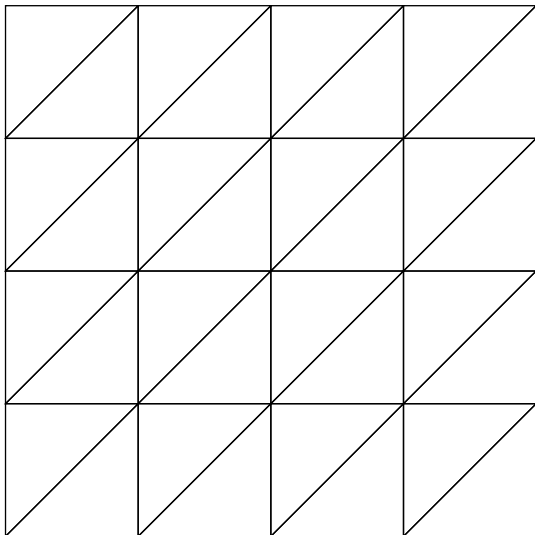
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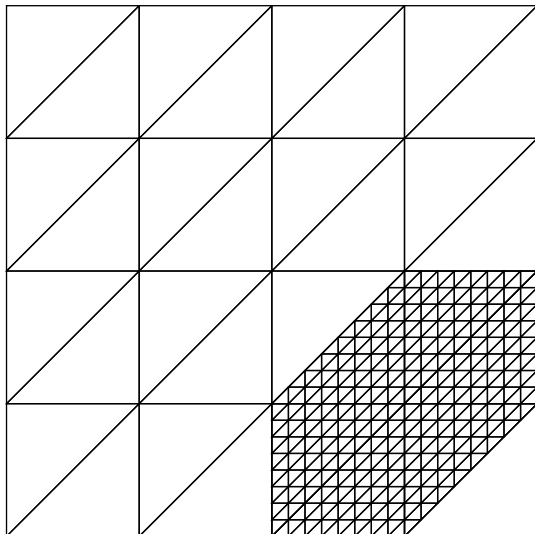
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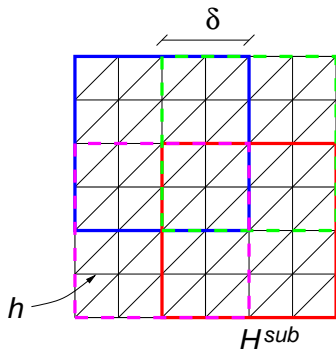
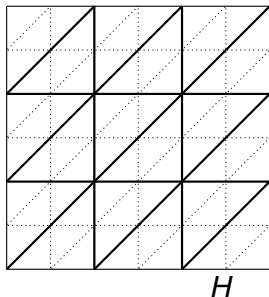
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- Coarse “grid”
- Prolongation R_0^T
(coarse space)



Two-Level Overlapping Additive Schwarz

$$M_{AS} := R_0^T A_0^{-1} R_0 + \sum_{i=1, \dots, S} R_i^T A_i^{-1} R_i$$

\uparrow **coarse solve** \uparrow **local solves**
 $(A_0 := R_0 A R_0^T)$ $(A_i := R_i A R_i^T)$

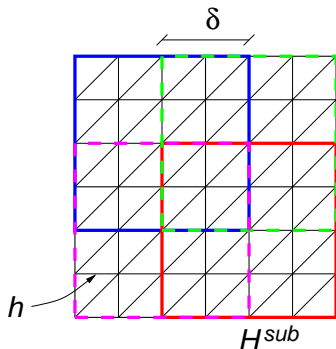
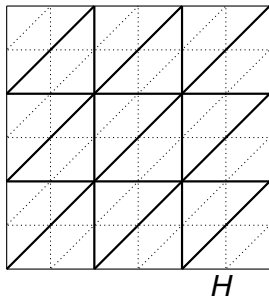


R_i simple injection into Ω_i , $i = 1, \dots, S$.

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But how to choose R_0^T ?

Choice of prolongation R_0^T (abstract)

- Select a set of linearly independent FE functions
(**coarse basis**)

$$\{\Psi_j \in V^h : j = 1, \dots, N\}$$

s.t. $\sum_j \Psi_j \equiv 1$ and $\text{supp}(\Psi_j) \subset \bar{\omega}_j$ (given)

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- **Prolongation matrix**

$$R_0^T = [\mathbf{z}_1, \dots, \mathbf{z}_N] \in \mathbb{R}^{n \times N}.$$

where \mathbf{z}_j is coefficient vector corresponding to Ψ_j .

Coefficient-explicit Conditioning Analysis

Theorem (RS, Vainikko, Computing, 2007)

Let $\omega_j = \text{supp}(\Psi_j)$. Assume that each $\omega_j \subset \Omega_i$ for some Ω_i and that $\{\omega_j\}$ is a shape regular, uniformly overlapping, finite covering of Ω .

Then

$$\kappa(M_{\text{ASA}}) \lesssim \gamma(\alpha) \left(1 + \max_j \frac{H_j}{\delta_j} \right)$$

where $H_j = \text{diam}(\omega_j)$, $\delta_j = \text{overlap}(\omega_j)$ and

$$\gamma(\alpha) = \max_j \delta_j^2 \|\alpha |\nabla \Psi_j|^2\|_{L^\infty(\Omega)},$$

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“Handle” for choosing $\{\Psi_j\}$ w.r.t. $\alpha \longrightarrow$ Energy minimisation!

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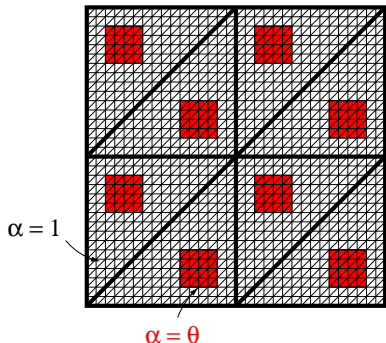
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Example: Standard pw. linear coarsening

(binary medium with $h = 1/512$ and $H = 8h$)

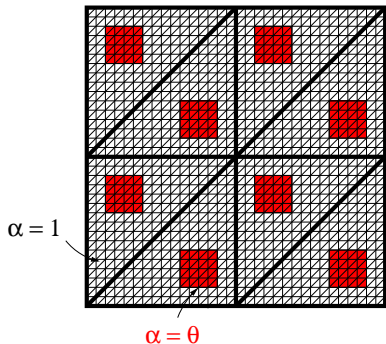


θ	$\kappa(M_{ASA})$	$\gamma(\alpha)$
10^0	5.2	2
10^1	9.1	20
10^2	58.1	200
10^3	471	2000
10^4	1821	$2.0(+4)$
10^5	2561*	$2.0(+5)$

*same as one-level method (robust!)

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→ **Coefficient-dependent Coarse Spaces**

Energy Minimising Coarse Spaces

Motivation – A bit of Linear Algebra

**For simplicity assume \mathcal{T}_h quasi-uniform, $\delta_j \sim H_j \sim H$ (generous overlap)
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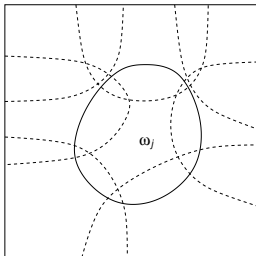
- Idea:** Replace $\|Y\|_{\max}^2$ by Frobenius norm

$$\|Y\|_F^2 = \text{tr}(Y^T Y) = \text{tr}(R_0 A R_0^T) = \sum_j \mathbf{z}_j^T A \mathbf{z}_j$$

i.e. the **energy of the coarse space basis**.

Energy Minimising Coarse Space – Method

[Wan, Chan, Smith, SISC 2000]



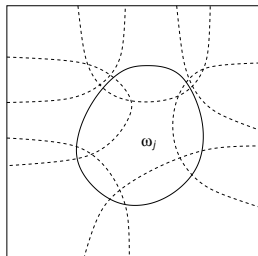
Choose **supports** $\{\omega_j\}$ for $\{\Psi_j\}$. Then solve **constrained minimisation problem** for $\{z_j\}$:

$$\min \sum_j z_j^T A z_j \quad \text{s.t.} \quad \sum_j z_j = \mathbf{1} \quad (\text{POU})$$

and $z_{j,i} \neq 0$ only if node $x_i \in \omega_j$ (**sparsity**).

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This problem has the **unique solution**

$$z_j = \mathcal{R}_j^T A_j^{-1} \mathcal{R}_j \lambda$$

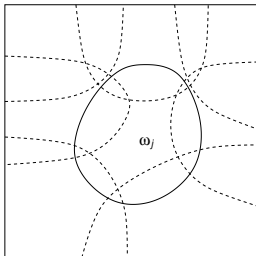
with $\mathcal{R}_j : \mathbb{R}^n \rightarrow \omega_j^h$ (**injection**) where λ is the solution of

$$B \lambda = \mathbf{1} \quad (\text{Lagrange multiplier system})$$

and $B := \sum_j \mathcal{R}_j^T A_j^{-1} \mathcal{R}_j$ (**1-level Schwarz operator w.r.t. $\{\omega_j\}$**)

Energy Minimising Coarse Space – Method

[Wan, Chan, Smith, SISC 2000]



Choose **supports** $\{\omega_j\}$ for $\{\Psi_j\}$. Then solve **constrained minimisation problem** for $\{z_j\}$:

$$\min \sum_j z_j^T A z_j \quad \text{s.t.} \quad \sum_j z_j = \mathbf{1} \quad (\text{POU})$$

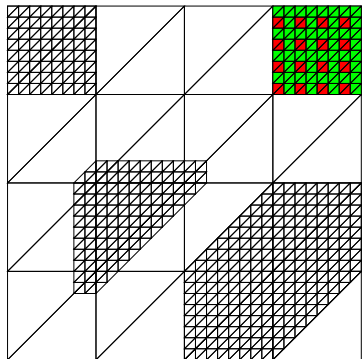
and $z_{j,i} \neq 0$ only if node $x_i \in \omega_j$ (**sparsity**).

Method/Questions

- Select a set of supports (patches) $\{\omega_j\}$. **How? Important?**
- Solve (global) problem $B\lambda = \mathbf{1}$. **How? Cost?**
- Solve (local) problems $\mathcal{A}_j \mathbf{y}_j = \mathcal{R}_j \lambda$. Set $\mathbf{z}_j = \mathcal{R}_j^T \mathbf{y}_j$. **Cheap!**

Example: Fine Scale Binary Medium

PCG-Iterations to solve $A\mathbf{u} = \mathbf{b}$ with preconditioner M_{AS} ($\varepsilon = 10^{-6}$)



$$\alpha = 1 \text{ and } \alpha = \theta$$

$$H = 8h$$

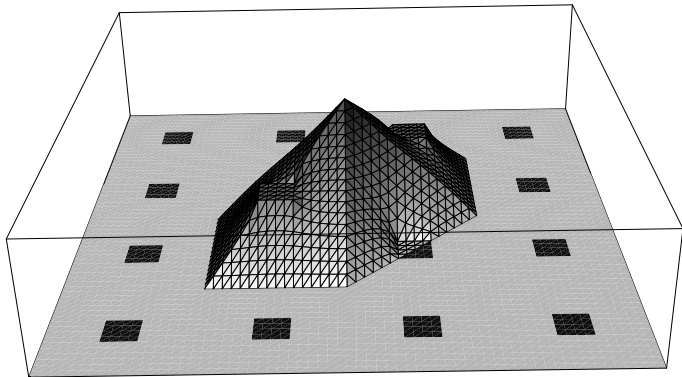
$$n = 256^2$$

θ	1-level	linear	minim.
10^0	79	13	13
10^2	80	63	14
10^4	84	113	14
10^6	87	115	14

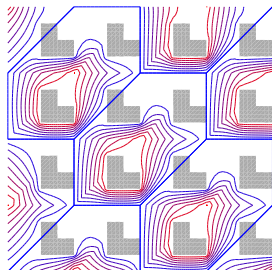
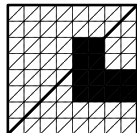
$$\theta = 10^6$$

n	1-level	linear	minim.
32^2	15	19	13
64^2	23	33	14
128^2	45	59	14
256^2	87	115	14

A Typical Basis Function



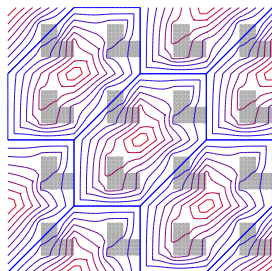
Example: L-shaped inclusion



Minimising

$n = 256^2$

θ	linear	multiFE	minim.
10^0	13	13	13
10^2	64	46	29
10^4	167	157	32
10^6	179	162	32



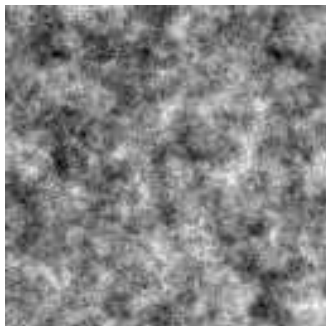
Multiscale FE

$\theta = 10^6$

n	linear	multiFE	minim.
32^2	29	26	21
64^2	48	48	26
128^2	89	88	29
256^2	179	162	32

Example: Lognormal Random Field

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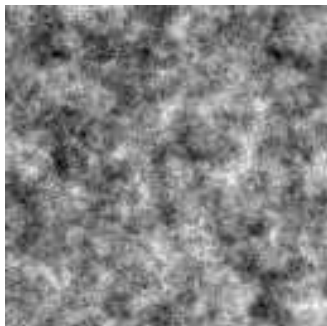
$n = 256^2$ and $\lambda = 4h$

σ^2	$\max_{\tau, \tau'} \frac{\alpha_\tau}{\alpha_{\tau'}}$	linear	multiFE	minim.
0	1.0	22	22	23
4	3.3(+7)	65	46	44
8	5.2(+10)	121	65	62
12	1.6(+13)	199	86	81

↑
Not robust!

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Need to adapt supports $\{\omega_j\}$ (see below)!

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- New Idea: **1-level** additive Schwarz preconditioner for B

$$C := \sum_j \mathcal{R}_j^T B_j^{-1} \mathcal{R}_j \quad \text{where} \quad B_j := \mathcal{R}_j B \mathcal{R}_j^T$$

Sounds impractical as B_j is **dense**.

But B_j^{-1} is **sparse(ish)**!

Implement using Linear Algebra “Trick”

- Consider ω_j overlapping only 2 neighbours ω_k & ω_l .
- **Local block**

$$B_j = A_j^{-1} + \hat{l}_{jk} A_k^{-1} \hat{l}_{jk}^T + \hat{l}_{jl} A_l^{-1} \hat{l}_{jl}^T$$

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- Invert via **Sherman-Morrison-Woodbury** formula:

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- Cost:** 1 sparse (local) solve & some sparse MatVec

Robustness of Preconditioner for B

(Preconditioned CG iterations for $B\lambda = \mathbf{1}$; tolerance $\varepsilon = 10^{-6}$)

Binary medium

θ	A	D	C
10^0	53	43	10
10^2	70	108	10
10^4	71	119	9
10^6	71	37	9

n	A	D	C
32^2	18	33	10
64^2	31	37	10
128^2	52	38	10
256^2	71	37	9

Log-normal field

σ^2	A	D	C
0	38	44	10
2	96	94	13
4	138	164	14
8	200 ⁺	200 ⁺	15
12	200 ⁺	200 ⁺	16
16	200 ⁺	200 ⁺	16

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In practice sufficient to solve $B\lambda = 1$
inaccurately!

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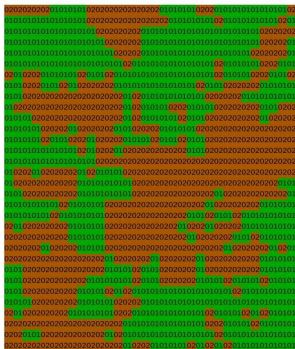
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- Also interesting for **Linear Elasticity** and **Maxwell**
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- Potential also for **numerical homogenisation & upscaling** (especially if there is **no scale separation!**)

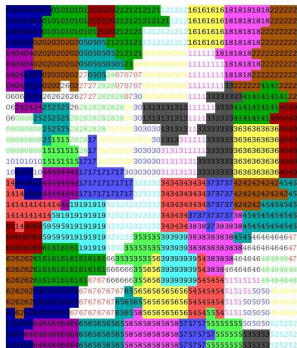
Choosing Supports via Aggregation

(based on strong connections in matrix – like in AMG)



Coefficient field (clipped)

$$(n = 32^2, \lambda = \frac{1}{8}, \max \frac{\alpha_{\tau}}{\alpha_{\tau'}} \approx 10^3)$$

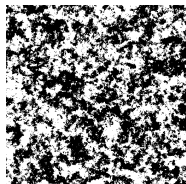


Aggregates (ADOUG)

(radius $r = 2$, threshold $\beta = 0.67$)

Example: Clipped random field

($n = 256^2$ and $\lambda = 1/64$; aggregation with radius $r = 2$ and $\beta = 0.67$)



AAMG ... Aggregation-type Algebraic Multigrid [Bastian]

DOUG ... Classical Additive Schwarz with linear coarsening

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

σ^2	$\max_{\tau, \tau'} \frac{\alpha_\tau}{\alpha_{\tau'}}$	CG-Iterations ($\varepsilon = 10^{-6}$)			CPU-time (in secs)		
		M_{AS}	AAMG	DOUG	M_{AS}	AAMG	UMFPACK
2	$1.5 * 10^1$	24	14	32	2.12	1.35	1.85
4	$2.2 * 10^2$	27	29	89	2.14	2.44	1.70
6	$3.3 * 10^3$	29	25	296	2.34	2.10	1.33
8	$4.9 * 10^4$	26	25	498	2.41	2.10	4.88

Energy minimisation for minimal overlap (no solve needed!)

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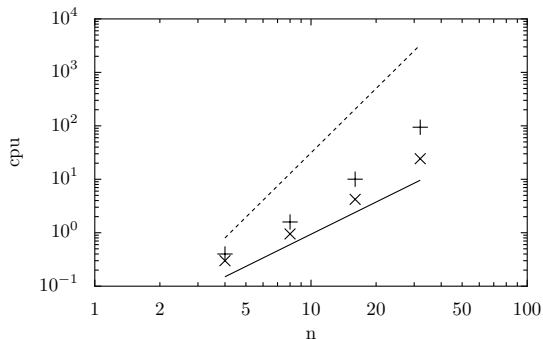
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- **Applications:** porous media flow, material science, etc...
- **Coefficient-explicit analysis** of two-level Schwarz
(when the coarse grid does **not resolve** the coefficients)
- Requirement on coarse space: **bounded/low energy** of basis
- **Explicit energy minimisation** \longrightarrow global system $B\lambda = \mathbf{1}$
- **1-Level Schwarz** Preconditioner sufficient for $B\lambda = \mathbf{1}$
- Efficient implementation via **Sherman-Morrison-Woodbury**
- **Choice of supports** crucial for random media

Thank you!

- **Mandel, Brezina, Vaněk**, Energy optimization of algebraic multigrid bases, **Computing**, 1999.
- **Wan, Chan, Smith**, An energy-minimizing interpolation for robust multigrid methods, **SISC**, 2000.
- **Xu, Zikatanov**, On an energy minimizing basis for algebraic multigrid methods, **Comput. Visual. Sci.**, 2004.
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- **Pechstein, RS**, Analysis of FETI methods for multiscale PDEs, submitted, 2008.
- **Van lent, RS, Graham**, Energy minimizing coarse spaces for two-level Schwarz methods for multiscale PDEs, submitted, 2008.

Coarse Space Construction – Timings



- + energy minimising
- × multiscale FE
- linear growth (with n^2)
- - quadr. growth (with n^2)
- $n = H/h$ ratio coarse/fine
- cpu in seconds

~2-3 times more expensive than multiscale FE (or linear) coarsening.