Algebraic Domain Decomposition Preconditioners for the Solution of Linear Systems

Tyrone Rees

UKRI-STFC Rutherford Appleton Laboratory

Joint work with Hussam Al Daas (RAL) and Pierre Jolivet (CNRS)


Culham Centre for Fusion Energy
Rutherford Appleton Laboratory
ATLANTIC OCEAN
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IRISH SEA
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SCOTLAND
NORTHERN IRELAND
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Arbroath
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Glasgow
Motherwell
Kilmarnock
Belfast
Dundalk
DUBLIN
Waterford
Newcastle
Sunderland
Middlesbrough
Blackpool
Bradford
Leeds
Preston
Liverpool
Manchester
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Notthingham
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Norwich
Peterborough
Northampton
Cambridge
Oxford
Cardiff
Bristol
Swansea
Exeter
Southampton
Portsmouth
Brighton
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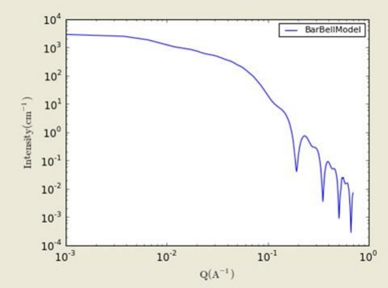
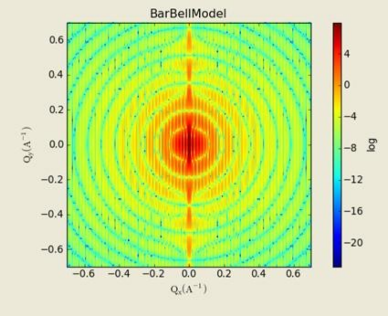
Optimization



SasView



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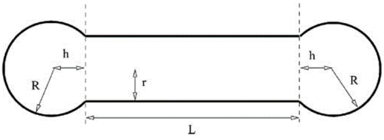
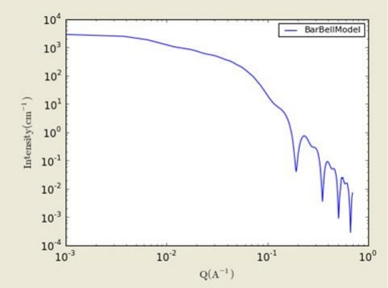
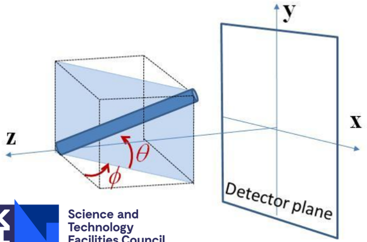
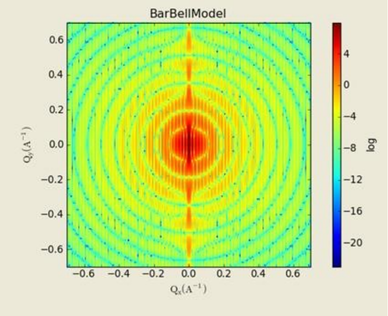
Optimization





SasView





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Description of problem

Given m raw data points, (t_i, y_i), we want to fit a curve of the form $f(\mathbf{x}, t)$ through these points so that we find

$$\min_{\mathbf{x}} \frac{1}{2} \underbrace{\sum_{i=1}^{m} (y_i - f(\mathbf{x}, t_i))^2}_{:=\|\mathbf{r}(\mathbf{x})\|^2}$$

Pick an initial point $\mathbf{x}^{(0)}$ and iterate.

Given $\mathbf{x}^{(k)}$ we look for $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \mathbf{s}^{(k)}$.

How to choose $\mathbf{s}^{(k)}$?

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Levenberg-Marquardt

We need to find

$$\min_{x} \frac{1}{2}\|\mathbf{r}(\mathbf{x})\|^2.$$

Levenberg-Marquardt (L-M) is one of the most widely used methods for these problems.

Approximate $\mathbf{r}(\mathbf{x}^{(k)} + \mathbf{s}^{(k)})$ by its first-order Taylor approximation

$$\mathbf{r}(\mathbf{x}^{(k)} + \mathbf{s}^{(k)}) \approx \mathbf{r}(\mathbf{x}^{(k)}) + J_k\mathbf{s}^{(k)},$$

and then add a regularization term

$$\mathbf{s}^{(k)} = \arg\min_{\mathbf{s}} \frac{1}{2}\|\mathbf{r}(\mathbf{x}^{(k)}) + J_k\mathbf{s}\|^2 + \frac{\sigma_k}{2}\|\mathbf{s}\|^2$$

σ_k is shrunk or grown between steps.

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$$(J_k^T J_k + \sigma_k I)\mathbf{s}^{(k)} = -J_k^T\mathbf{r}(\mathbf{x}^{(k)})$$

σ_k is shrunk or grown between steps.

Levenberg-M

We need to fi

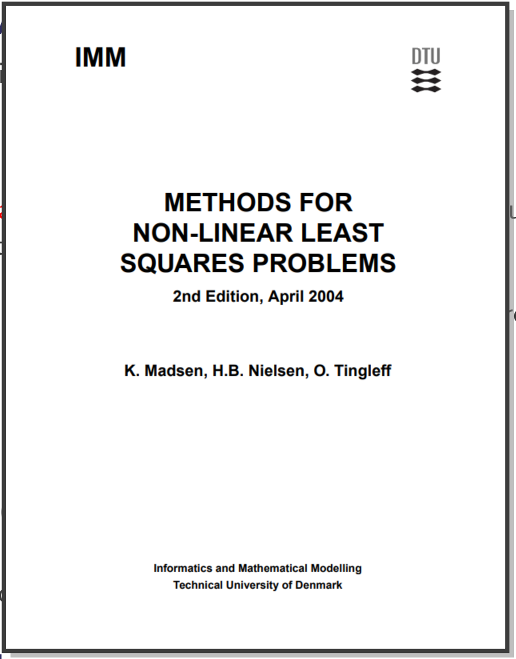
Levenberg-Ma used
methods for t

Approximate roximation

and then add

s

σ_k is shrunk


IMM

DTU

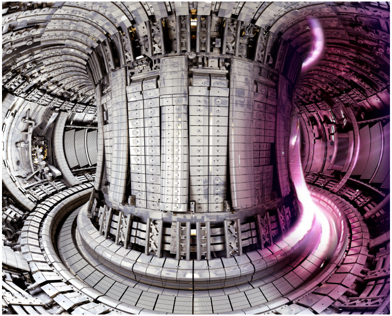
METHODS FOR
NON-LINEAR LEAST
SQUARES PROBLEMS

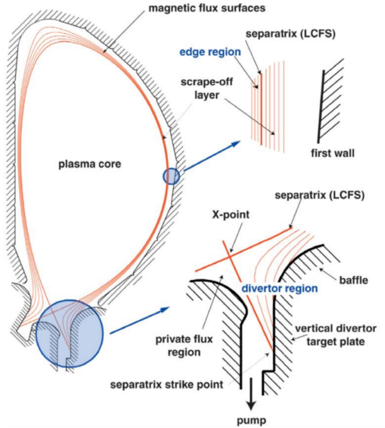
2nd Edition, April 2004

K. Madsen, H.B. Nielsen, O. Tingleff

Informatics and Mathematical Modelling
Technical University of Denmark

NEPTUNE (NEutrals and Plasma TUrbulence Numerics)





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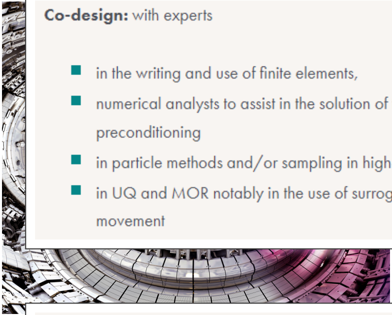
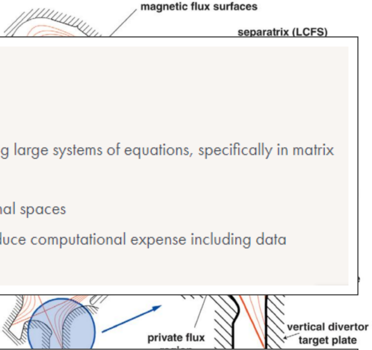
ExCALIBUR

NEPTUNE (NEutrals and Plasma TUrbulence Numerics)





Co-design: with experts

- in the writing and use of finite elements,
- numerical analysts to assist in the solution of the resulting large systems of equations, specifically in matrix preconditioning
- in particle methods and/or sampling in high-dimensional spaces
- in UQ and MOR notably in the use of surrogates to reduce computational expense including data movement

Co-design: with theoretical plasma physicists constructing high-dimensional plasma models, and experts in the use of particle codes on pre-Exascale hardware.

https://excalibur.ac.uk/themes/high-priority-use-cases/

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ExCALIBUR

Given a sparse matrix, $A \in \mathbb{R}^{n \times n}$, and vector $\mathbf{b} \in \mathbb{R}^n$, find $\mathbf{x}$ such that

$$A\mathbf{x} = \mathbf{b}.$$

Our ideal algorithm would

- only use algebraic properties of A
- be able to take advantage of modern architectures
- be able to solve large problems with modest memory requirements

Krylov subspace methods

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Krylov subspace methods

Suppose we wish to solve

$$\mathcal{A}\mathbf{x} = \mathbf{b}.$$

Look for an approximation $\mathbf{x}^{(k)}$ such that

$$\mathbf{x}^{(k)} - \mathbf{x}^{(0)} \in span\left\{\mathbf{r}^{(0)}, \mathcal{A}\mathbf{r}^{(0)}, \ldots, \mathcal{A}^{k-1}\mathbf{r}^{(0)}\right\},$$

where $\mathbf{r}^{(0)} = \mathbf{b} - \mathcal{A}\mathbf{x}^{(0)}$.

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A zoo of Krylov methods

TFQMR

MINRES

BiCGStab

Conjugate Gradients

QMR

BiCG

GMRES

GCR

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A zoo of Krylov methods

TFQMR

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GCR

Methods which minimize *something* over the entire Krylov space

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A zoo of Krylov methods

TFQMR

MINRES

BiCGStab

Conjugate Gradients

QMR

BiCG

GMRES

GCR

Methods which minimize *something* over the entire Krylov space

Methods based on short term recurrences

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GMRES

- suitable for all linear systems
- minimizes $\|\mathbf{b} - \mathcal{A}\mathbf{x}_k\|_2$

Finds $\mathbf{x}_k$ in the Krylov subspace

$$\mathbf{x}_0 + \mathrm{span}\{\mathbf{r}^{(0)}, \mathcal{A}\mathbf{r}^{(0)}, \ldots, \mathcal{A}^{k-1}\mathbf{r}^{(0)}\}$$

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Preconditioning

$$\mathcal{A}\mathbf{x} = \mathbf{b}$$

While any eigenvalues do not fully determine convergence for GMRES [Greenbaum, Ptak, Strakos (1996)] , GMRES tends to work well if $\mathcal{A}$ has a small condition number.

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Preconditioning

$$\mathcal{A}\mathbf{x} = \mathbf{b}$$

While any eigenvalues do not fully determine convergence for GMRES [Greenbaum, Ptak, Strakos (1996)] , GMRES tends to work well if $\mathcal{A}$ has a small condition number.

Preconditioning: solve the equivalent problem

$$\mathcal{M}_L^{-1}\mathcal{A}\mathcal{M}_R^{-T}(\mathcal{M}_R^T\mathbf{x}) = \mathcal{M}_L^{-1}\mathbf{b}.$$

Let $\mathcal{P} = \mathcal{M}_L\mathcal{M}_R^T$.

Competing aims:

- Need eigenvalues of $\mathcal{M}_L^{-1}\mathcal{A}\mathcal{M}_R^{-1}$ to be clustered
- Need a solve with $\mathcal{M}_L$ or $\mathcal{M}_R$ to be cheap

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Preconditioning

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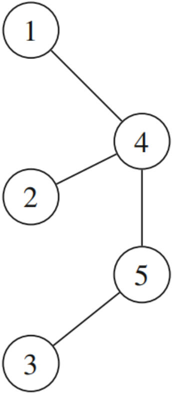
Sparse Matrices and Graphs

	1	2	3	4	5
1	*			*	
2		*		*	
3			*		*
4	*	*		*	*
5			*	*	*



[Scott and Tuma, Algorithms for Sparse Linear Systems, 2023]

Partitioning

1	*	*	*	*									
2	*	*		*	*								
3	*		*	*		*	*						
4	*	*	*	*	*		*	*					
5		*		*	*			*					
6			*			*	*		*	*			
7			*	*		*	*	*		*	*		
8				*	*		*	*			*		
9						*			*	*		*	
10						*	*		*	*	*	*	*
11							*	*		*	*		*
12									*	*		*	*
13										*	*	*	*

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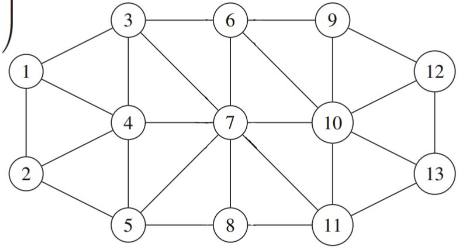
[Scott and Tuma, Algorithms for Sparse Linear Systems, 2023]

Partitioning

1	*	*	*	*									
2	*	*		*	*								
3	*		*	*		*	*						
4	*	*	*	*	*		*	*					
5		*		*	*			*					
6			*			*	*		*	*			
7			*	*		*	*	*		*	*		
8				*	*		*	*			*		
9						*			*	*		*	
10						*	*		*	*	*	*	*
11							*	*		*	*		*
12									*	*		*	*
13										*	*	*	*



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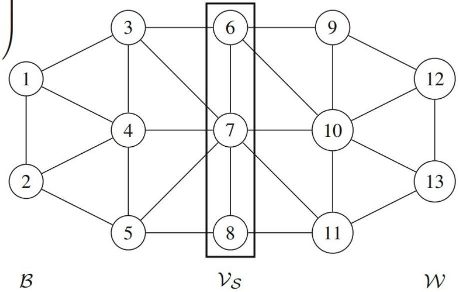
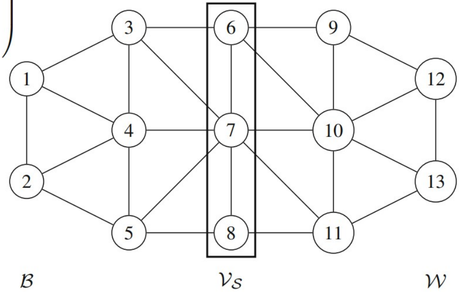
Partitioning

1	*	*	*	*									
2	*	*		*	*								
3	*		*	*		*	*						
4	*	*	*	*	*		*	*					
5		*		*	*			*					
6			*			*	*		*	*			
7			*	*		*	*	*		*	*		
8				*	*		*	*			*		
9						*			*	*		*	
10						*	*		*	*	*	*	*
11							*	*		*	*		*
12									*	*		*	*
13										*	*	*	*



Partitioning

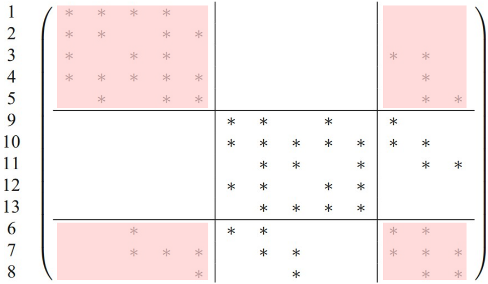
$$
\begin{array}{r}
1\\2\\3\\4\\5\\9\\10\\11\\12\\13\\6\\7\\8
\end{array}
\left(\begin{array}{ccccc|ccccc|ccc}
* & * & * & * &   &   &   &   &   &   &   &   &   \\
* & * &   & * & * &   &   &   &   &   &   &   &   \\
* &   & * & * &   &   &   &   &   &   & * & * &   \\
* & * & * & * & * &   &   &   &   &   &   & * &   \\
  & * &   & * & * &   &   &   &   &   &   & * & * \\
\hline
  &   &   &   &   & * & * &   & * &   & * &   &   \\
  &   &   &   &   & * & * & * & * & * & * & * &   \\
  &   &   &   &   &   & * & * &   & * &   & * & * \\
  &   &   &   &   & * & * &   & * & * &   &   &   \\
  &   &   &   &   &   & * & * & * & * &   &   &   \\
\hline
  &   & * &   &   & * & * &   &   &   & * & * &   \\
  &   & * & * & * &   & * & * &   &   & * & * & * \\
  &   &   &   & * &   &   & * &   &   &   & * & *
\end{array}\right)
$$



One-level Additive Schwarz

1	*	*	*	*									
2	*	*		*	*								
3	*		*	*							*	*	
4	*	*	*	*	*							*	
5		*		*	*							*	*
9						*	*		*		*		
10						*	*	*	*	*	*	*	
11							*	*		*		*	*
12						*	*		*	*			
13							*	*	*	*			
6			*			*	*				*	*	
7			*	*	*		*	*			*	*	*
8					*			*				*	*

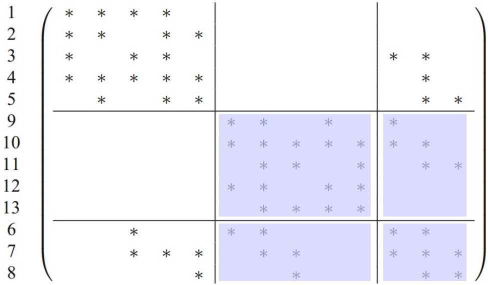
One-level Additive Schwarz



$$M_{ASM}^{-1} = R_1^T \, {A_{11}}^{-1} R_1 +$$

[Scott and Tuma, Algorithms for Sparse Linear Systems, 2023]

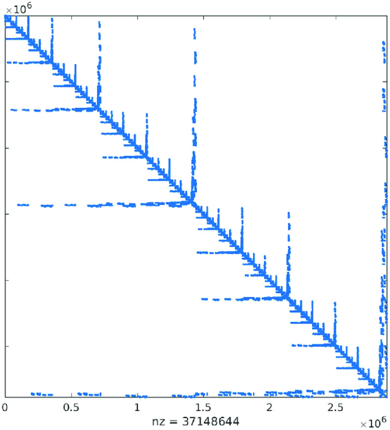
One-level Additive Schwarz



$$M_{ASM}^{-1} = R_1^T {\color{red}A_{11}}^{-1} R_1 + R_2^T {\color{blue}A_{22}}^{-1} R_2$$

[Scott and Tuma, Algorithms for Sparse Linear Systems, 2023]

One-level Additive Schwarz



$$M_{ASM}^{-1} = \sum_{i=1}^{N} R_i^T A_{ii}^{-1} R_i$$

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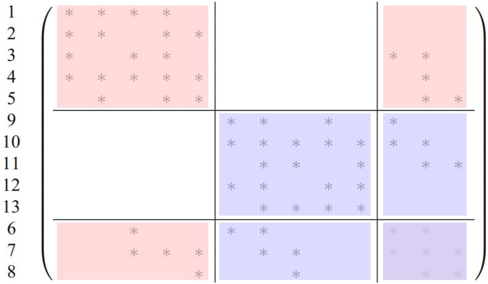
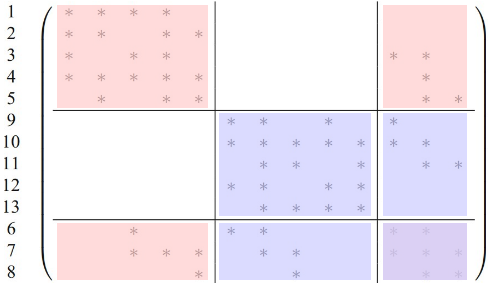
[Amestoy et al., Computational Geosciences, 2019]

One-level Restricted Additive Schwarz



$$M_{ASM}^{-1} = R_1^T {\color{red}A_{11}}^{-1} R_1 + R_2^T {\color{blue}A_{22}}^{-1} R_2$$

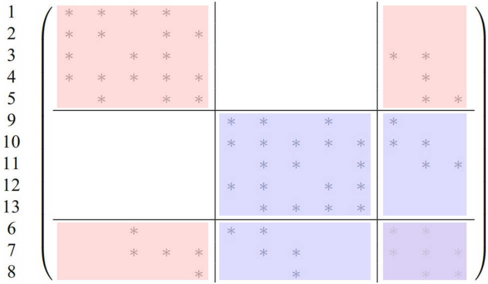
One-level Restricted Additive Schwarz



Partition of unity: $D_i \in \mathbb{R}^{n_i \times n_i}$ non-negative, diagonal so that

$$\sum R_i^T D_i R_i = I$$

One-level Restricted Additive Schwarz



Partition of unity: $D_i \in \mathbb{R}^{n_i \times n_i}$ non-negative, diagonal so that

$$\sum R_i^T D_i R_i = I$$

$$\text{e.g., } R_1^T D_1 R_1 = \begin{bmatrix} I & 0 & 0 \\ 0 & 0 & 0 \\ & & \begin{matrix} 1 & 0 & 0 \end{matrix} \\ 0 & 0 & \begin{matrix} 0 & 0 & 0 \end{matrix} \\ & & \begin{matrix} 0 & 0 & 0 \end{matrix} \end{bmatrix}, \quad R_2^T D_2 R_2 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & I & 0 \\ & & \begin{matrix} 0 & 0 & 0 \end{matrix} \\ 0 & 0 & \begin{matrix} 0 & 1 & 0 \end{matrix} \\ & & \begin{matrix} 0 & 0 & 1 \end{matrix} \end{bmatrix}$$

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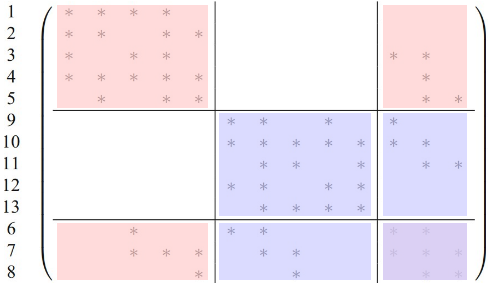
One-level Restricted Additive Schwarz



Partition of unity: $D_i \in \mathbb{R}^{n_i \times n_i}$ non-negative, diagonal so that

$$\sum R_i^T D_i R_i = I$$

$$\text{e.g., } R_1^T D_1 R_1 = \begin{bmatrix} I & 0 & & 0 & \\ 0 & 0 & & 0 & \\ & & 0.5 & 0 & 0 \\ 0 & 0 & 0 & 0.5 & 0 \\ & & 0 & 0 & 0.5 \end{bmatrix}, \quad R_2^T D_2 R_2 = \begin{bmatrix} 0 & 0 & & 0 & \\ 0 & I & & 0 & \\ & & 0.5 & 0 & 0 \\ 0 & 0 & 0 & 0.5 & 0 \\ & & 0 & 0 & 0.5 \end{bmatrix}$$

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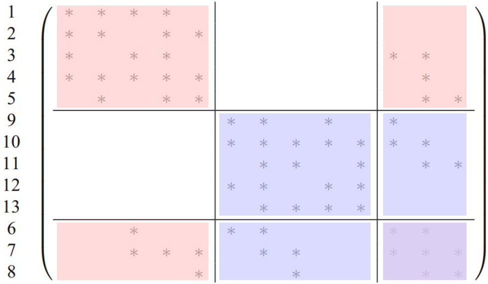
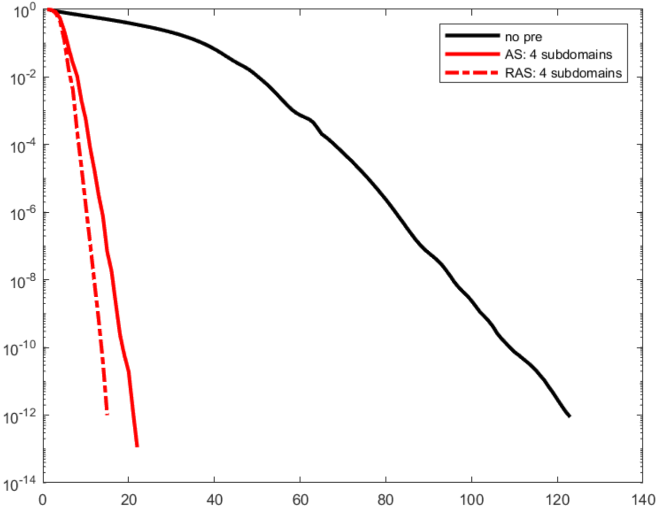
One-level Restricted Additive Schwarz



$$M_{RAS}^{-1} = \sum_{i=1}^{N} R_i^T D_i A_{ii}^{-1} R_i$$

Comparison



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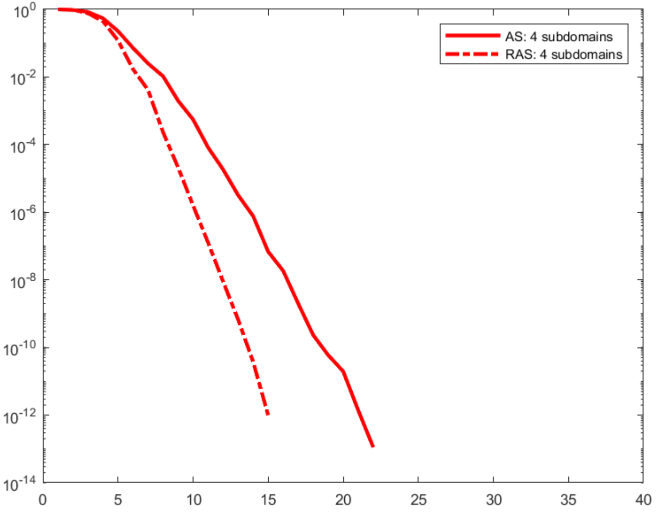
Comparison



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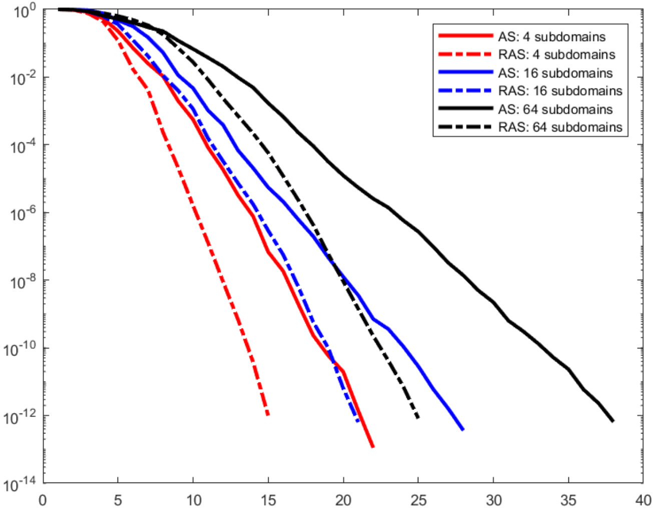
Comparison



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Solution: Coarse spaces

$$M_{\star,AD}^{-1} = R_0^T A_{00}^{-1} R_0 + M_{\star}^{-1}$$

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$$M_{\star,AD}^{-1} = R_0^T A_{00}^{-1} R_0 + M_{\star}^{-1}$$

or

$$M_{\star,DEF}^{-1} = R_0^T A_{00}^{-1} R_0 + M_{\star}^{-1}(I - AR_0^T A_{00}^{-1} R_0)$$

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Solution: Coarse spaces

$$M_{\star,AD}^{-1} = R_0^T A_{00}^{-1} R_0 + M_{\star}^{-1}$$

or

$$M_{\star,DEF}^{-1} = R_0^T A_{00}^{-1} R_0 + M_{\star}^{-1}(I - AR_0^T A_{00}^{-1} R_0)$$

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Spectral Coarse Spaces

Multigrid Brezina, Heberton *et al.* (1999), Charier, Falgout *et al.* (2003), Kolev, Vassilevski, (2006), Efendiev, Galvis, Vassilevski (2011)
DD Nataf, Xiang, Dolean, Spillane (2011), Spillane, Rixen (2013), Spillane, Dolean *et al.* (2014), Klawonn, Radtke, Rheinbach (2015), Klawonn, Kühn, Rheinbach (2016), Al Daas, Grigori (2019), Al Daas, Grigori, Jolivet, Tournier (2021), Al Daas, Jolivet (2021)
Indefinite/non-self-adjoint systems Manteuffel, Ruge, Soutworth (2018), Manteuffel, Müzenmaier, Ruge, Soutworth (2019), Bootland, Dolean *et al.* (2019, 2020, 2021, 2021, 2021, 2021), Dolean, Jolivet *et al.* (2021)

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Fictitious Subspace Lemma

Let H and H_D be two Hilbert spaces, with scalar products $(\cdot,\cdot)$ and $(\cdot,\cdot)_D$. Let $A : H \to H$ and $B : H_D \to H_D$, and consider the spd bilinear forms generated by these operators $a(u,v) = (Au,v)$, $b(u_D, v_D) = (Bu_D, v_D)$. Let $\mathcal{R}$ be an operator such that $H_D \to H$, and $\mathcal{R}^*$ be its adjoint. Suppose that:

- The operator $\mathcal{R}$ is surjective
- There exists $c_u > 0$ such that

$$a(\mathcal{R}v, \mathcal{R}v) \leq c_u b(v,v), \ \forall v \in H_D$$

- There exists $c_l > 0$ such that for all $u \in H$, there exists $v \in H_D$ such that $u = \mathcal{R}v$ and

$$c_l b(v,v) \leq a(\mathcal{R}v, \mathcal{R}v) = a(u,u)$$

Then $\lambda(\mathcal{R}B^{-1}\mathcal{R}^*A) \in [c_l, c_u]$.

Fictitious Subspace Lemma

$$\mathcal{R} : \prod_{i=0}^{N} \mathbb{R}^{n_i} \to \mathbb{R}^n$$

$$(u_i)_{0\le i\le N} \longmapsto \sum_{i=0}^{N} R_i^T u_i$$

ert ... / an ... ed b ... et $\mathcal{R}$ ... ppos

$$\mathcal{B} : \prod_{i=0}^{N} \mathbb{R}^{n_i} \to \mathbb{R}^{n_i}$$

$$(u_i)_{0\le i\le N} \longmapsto \Big((R_i^T A R_i) u_i\Big)_{0\le i\le N}$$

- The operator $\mathcal{R}$ is surjective
- There exists $c_u > 0$ such that

$$a(\mathcal{R}v, \mathcal{R}v) \le c_u b(v, v), \ \forall v \in H_D$$

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$$c_l b(v, v) \le a(\mathcal{R}v, \mathcal{R}v) = a(u, u)$$

$M_{\star,AD}^{-1}$

Then $\lambda(\mathcal{R}B^{-1}\mathcal{R}^* A) \in [c_l, c_u]$.

Block Splitting Matrices

A local Symmetric positive semi-definite (SPSD) splitting of a sparse SPD matrix is any SPSD matrix of the form:

$$P_i \widetilde{A}_i P_i^T = \begin{bmatrix} A_{Ii} & A_{I\Gamma,i} \\ A_{\Gamma I,i} & \widetilde{A}_{\Gamma,i} \\ & \end{bmatrix},$$

where $\widetilde{A}_{\Gamma,i}$ is any SPSD matrix such that

$$0 \leq u^T \widetilde{A}_i u \leq u^T A u, \;\; u \in \mathbb{R}^n.$$

[Al Daas, Grigori (2019)]

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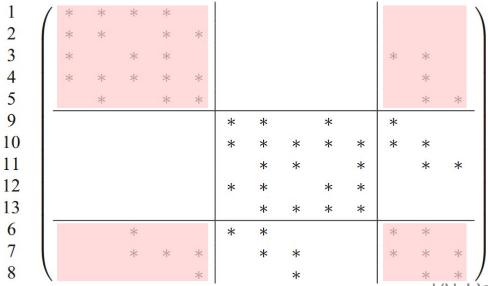

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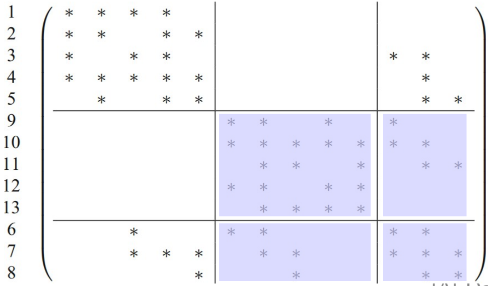

[Al Daas, Grigori (2019)]

Block Splitting Matrices

A local Symmetric positive semi-definite (SPSD) splitting of a sparse SPD matrix is any SPSD matrix of the form:

$$P_i \widetilde{A}_i P_i^T = \begin{bmatrix} \boxed{\widetilde{A}_{ii}} & \\ & \end{bmatrix},$$

where $\widetilde{A}_{\Gamma,i}$ is any SPSD matrix such that

$$0 \leq u^T \widetilde{A}_i u \leq u^T A u, \; u \in \mathbb{R}^n.$$

[Al Daas, Grigori (2019)]

Building a coarse space

Given the local non-singular matrix $A_{ii} = R_i A R_i^T$, the local splitting matrix $\widetilde{A}_{ii} = R_i \widetilde{A}_{ii} R_i^T$, and the partition of unity matrix, D_i, let $L_i = ker(D_i A_{ii} D_i)$ and $K_i = ker(\widetilde{A}_{ii})$.

Consider the generalized eigenvalue problem: find (λ, u) such that

$$\Pi_i D_i A_{ii} D_i \Pi_i u = \lambda \widetilde{A}_{ii} u,$$

where Π_i is the projection on $range(\widetilde{A}_{ii})$.

Given $\tau > 0$, let Z_i be the matrix whose columns form a basis of the subspace

$$(L_i \cap K_i)^{\perp_{K_i}} \oplus span\{u \ : \ |\lambda| > 1/\tau\}$$

Consider the coarse space defined as

$$R_0^T = [R_1^T D_1 Z_1 \ \dots \ R_N^T D_N Z_N]$$

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How effective is this?

Theorem [Al Daas and Grigori, 2019]
If we build a spectral coarse space using local SPSD splitting matrices, as described, then

$$\frac{1}{2 + (2k_c + 1)k_m \tau} \leq \lambda(M^{-1}_{ASM,additive} A) \leq (k_c + 1),$$

where

- τ is the parameter chosen in the construction of the coarse space
- k_c is the number of colours required to colour the graph of A such that two neighbouring subdomains have different colours, and
- k_m is the maximum number of overlapping subdomains sharing a row of A.

Proof Show that this construction satisfies the fictitious subspace lemma.

Choice of splitting matrices?

GenEO (*'Generalized Eigenvalue Problems in the Overlap'*) [Spillane, Nataf, *et al.* (2014)] fits into this framework.

Here

$$P_i \widetilde{A}_i P_i^T = \begin{bmatrix} A_{Ii} & A_{I\Gamma,i} \\ A_{\Gamma I,i} & \widetilde{A}_{\Gamma,i} \end{bmatrix}.$$

Note that the upper bound in GenEO is algebraic, but the lower bound requires properties from the discretization of the underlying PDE.

The integral of the operator in the overlapping region with its neighbouring subdomains .

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A fully algebraic choice?

Suppose that A is diagonally dominant, and for each i we have

$$P_i A P_i^\top = \begin{pmatrix} A_{Ii} & A_{I\Gamma i} & \\ A_{\Gamma Ii} & A_{\Gamma i} & A_{\Gamma ci} \\ & A_{c\Gamma i} & A_{ci} \end{pmatrix}$$

Let $s_i(j) = \sum_k |A_{\Gamma ci}(j,k)|$, and define

$$\widetilde{A}_{ii} = \begin{bmatrix} A_{Ii} & A_{I\Gamma i} \\ A_{\Gamma Ii} & \widetilde{A}_{\Gamma i} \end{bmatrix},$$

where $\widetilde{A}_{\Gamma i} = A_{\Gamma i} - diag(s_i)$.

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SPSD splitting matrix

Lemma [Al Daas, Jolivet, R. (2023)]
This local block splitting defines a local SPSD splitting matrix of A with respect to subdomain i.

Proof
First, note that

$$\widetilde{A}_i(j,j) = \begin{cases} A(j,j) & \text{if } j \in \Omega_{Ii}, \\ A(j,j) - s_i(j) & \text{if } j \in \Omega_{\Gamma i}, \\ 0 & \text{if } j \in \Omega_{ci}, \end{cases}$$

- $\widetilde{A}_i$ is symmetric and diagonally dominant, by construction, hence SPSD
- $A - \widetilde{A}_i$ is symmetric and diagonally dominant, hence SPSD

Therefore, by the local structure of $\widetilde{A}_i$, it is a SPSD splitting of A wrt subdomain i.

Numerical results: Set Up

- Used as a preconditioner for right-preconditioned GMRES: restart parameter of 30, with relative tolerance of 10^{-8}.
- Use the implementation as `-pc_hpddm_block_splitting` (part of PCHPDDM) in PETSc (from 3.17) to compute local splitting matrices
- Uses 256 MPI processes
- Matrix reordered by applying ParMETIS to $A + A^T$.
- At most 60 eigenpairs are computed, and $\tau = 0.3$.

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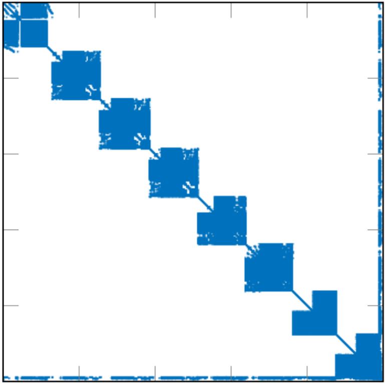
Numerical results: SuiteSparse

Identifier	n	nnz(A)	AGMG	BoomerAMG	GAMG	M^{-1}_{deflated}	n_0
light_in_tissue	29,282	406,084	15	‡	53	**6**	7,230
finan512	74,752	596,992	9	7	8	**6**	2,591
consph	83,334	6,010,480				**93**	31,136
Dubcova3	146,689	3,636,643		72	71	**7**	21,047
CO	221,119	7,666,057		**25**		26	56,135
nxp1	414,604	2,655,880	†	†	†	**20**	19,707
CoupCons3D	416,800	17,277,420		†	26	**20**	28,925
parabolic_fem	525,825	3,674,625	12	8	16	**5**	24,741
Chevron4	711,450	6,376,412		‡	†	**5**	22,785
apache2	715,176	4,817,870	14	11	35	**8**	45,966
tmt_sym	726,713	5,080,961	14	10	17	**5**	28,253
tmt_unsym	917,825	4,584,801	23	13	18	**6**	32,947
ecology2	999,999	4,995,991	18	12	18	**6**	34,080
thermal2	1,228,045	8,580,313	18	**14**	20	26	40,098
atmosmodj	1,270,432	8,814,880	†	8	17	**7**	76,368
G3_circuit	1,585,478	7,660,826	25	12	35	**8**	71,385
Transport	1,602,111	23,487,281	18	10	98	**9**	76,800
memchip	2,707,524	13,343,948	†	**15**	†	36	57,942
circuit5M_dc	3,523,317	14,865,409	†	**5**		7	8,629

Numerical results



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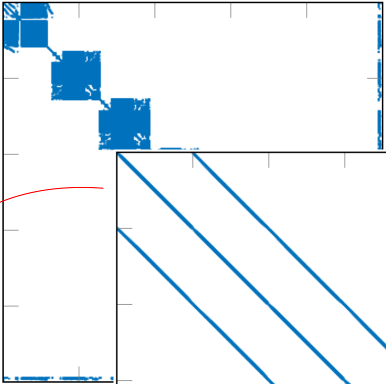

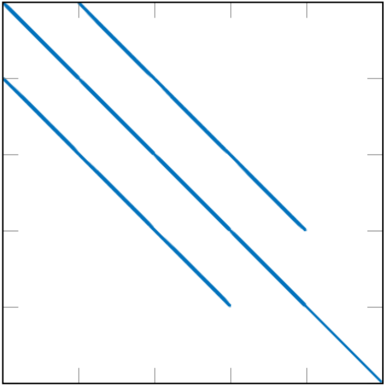

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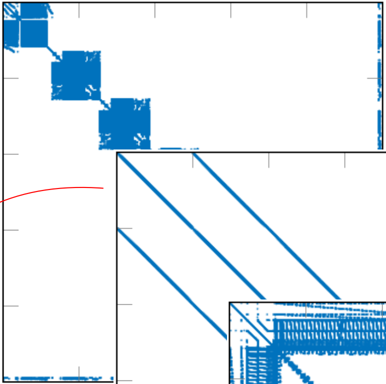

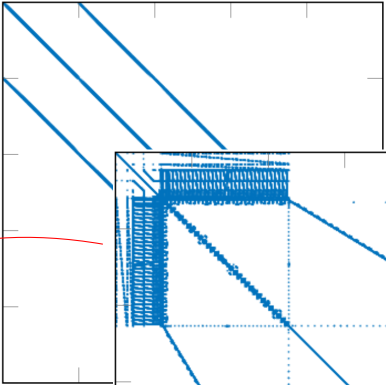

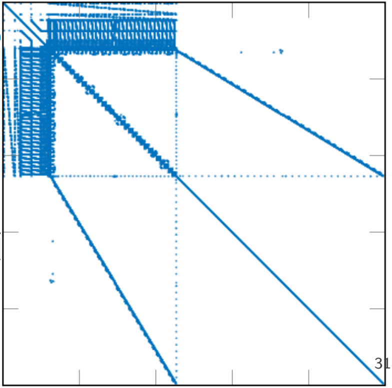

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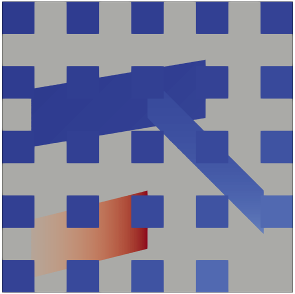
Numerical results: Convection Diffusion

$$\nabla \cdot (Vu) - \nu \nabla \cdot (\kappa \nabla u) = 0 \text{ in } \Omega$$
$$u = 0 \text{ in } \Gamma_0$$
$$u = 1 \text{ in } \Gamma_1$$



Discretized using SUPG stabilization in FreeFEM.

The value of the velocity field V is either:

$$V(x,y) = \begin{pmatrix} x(1-x)(2y-1) \\ -y(1-y)(2x-1) \end{pmatrix} \quad \text{or} \quad V(x,y,z) = \begin{pmatrix} 2x(1-x)(2y-1)z \\ -y(1-y)(2x-1) \\ -z(1-z)(2x-1)(2y-1) \end{pmatrix},$$

in 2D and 3D, respectively.

[Notay (2012)]

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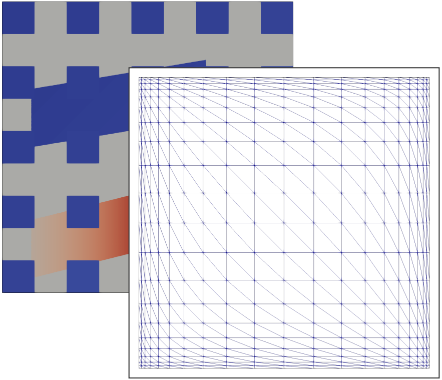

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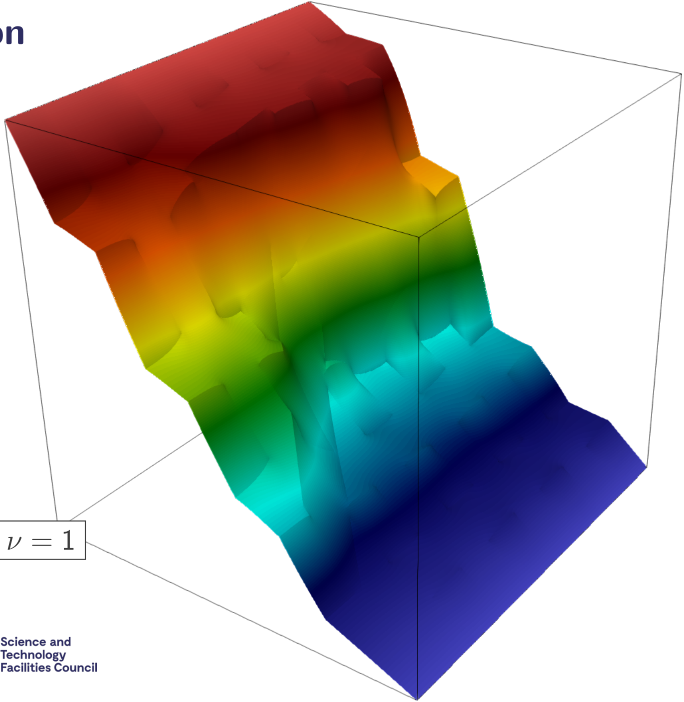
Solution



$\nu = 1$

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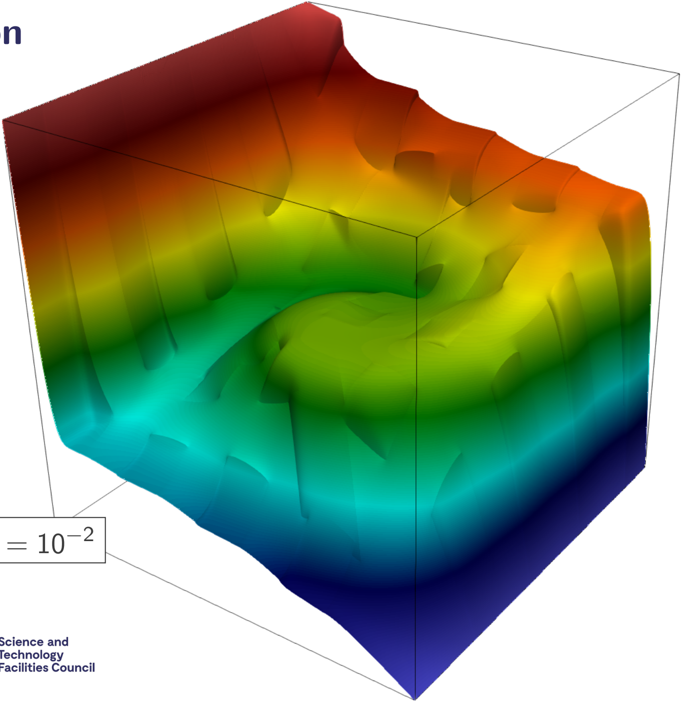
Solution



$\nu = 10^{-2}$

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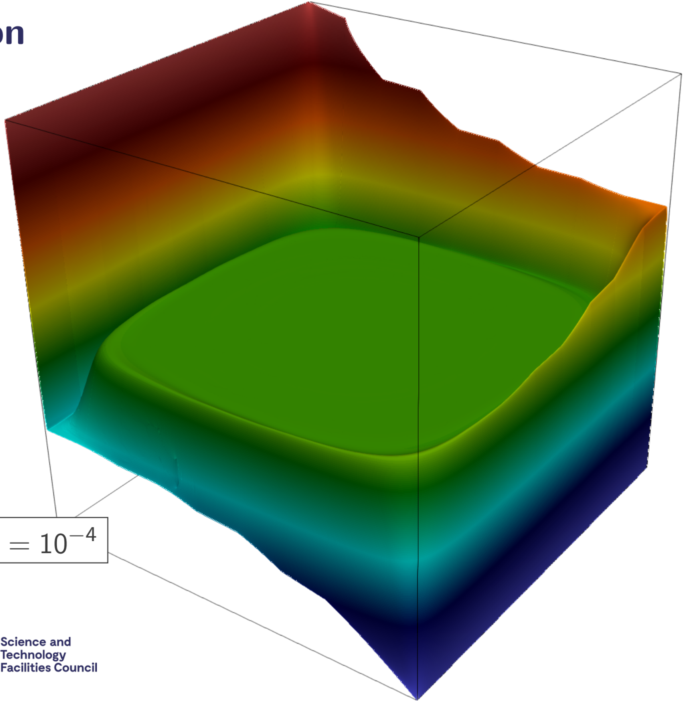
Solution



$\nu = 10^{-4}$

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Numerical results

Dimension	k	N	n	ν: 1	10^{-1}	10^{-2}	10^{-3}	10^{-4}
2	1	1,024	$6.3 \cdot 10^6$	23 (52,875)	20 (52,872)	19 (52,759)	20 (47,497)	21 (28,235)
3	2	4,096	$8.1 \cdot 10^6$	18 ($1.8 \cdot 10^5$)	14 ($1.8 \cdot 10^5$)	11 ($1.6 \cdot 10^5$)	16 (97,657)	29 (76,853)

2-level Additive Schwarz

Dimension	n	ν: 1	10^{-1}	10^{-2}	10^{-3}	10^{-4}
2	$6.3 \cdot 10^6$	42	48	88	†	†
3	$8.1 \cdot 10^6$	40	38	65	†	†

GAMG

Dimension	n	ν: 1	10^{-1}	10^{-2}	10^{-3}	10^{-4}
2	$6.3 \cdot 10^6$	50	49	19	7	†
3	$8.1 \cdot 10^6$	12	9	7	†	†

BoomerAMG

Saddle point systems?

What about systems of the form

$$\begin{bmatrix} A & B^T \\ B & -C \end{bmatrix}$$

Not symmetric positive definite – do not fit in this framework

Saddle point systems

We have the block factorization

$$\begin{bmatrix} A & B^T \\ B & -C \end{bmatrix} = \begin{bmatrix} I & 0 \\ BA^{-1} & I \end{bmatrix} \begin{bmatrix} A & 0 \\ 0 & -(C + BA^{-1}B^T) \end{bmatrix} \begin{bmatrix} I & A^{-1}B^T \\ 0 & I \end{bmatrix}$$

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Saddle point systems

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It's enough to be able to solve with A and $S = C + BA^{-1}B^T$.

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It's enough to be able to solve with A and $S = C + BA^{-1}B^T$.

If $A \approx D$, a diagonal matrix, then we can apply the ideas earlier to A and S (see [Al Daas, Jolivet, Scott (2022)])

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Helmholtz optimal control

$$\min_{u \in U, z \in Z} \frac{1}{2} \|\mathcal{W}(u) - w\|_W^2 + \frac{\beta}{2} \|z\|_Z^2$$

subject to

$$\begin{aligned} -\nabla^2 u - \kappa^2 u &= \mathcal{F}(z) \ in \ \Omega \\ \partial_\nu u &= \mathcal{B}_1(z) \ on \ \Gamma_1 \\ \partial_\nu u - i\delta\kappa u &= \mathcal{B}_2(z) \ on \ \Gamma_2 \\ u &= 0 \ on \ \Gamma_3. \end{aligned}$$

See [Kouri, Ridzal, Tuminaro (2021)]

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Discretized problem

$$\begin{bmatrix} C & 0 & K^* \\ 0 & \beta R & L^* \\ K & L & 0 \end{bmatrix} \begin{bmatrix} u \\ z \\ \lambda \end{bmatrix} = \begin{bmatrix} w \\ 0 \\ 0 \end{bmatrix}$$

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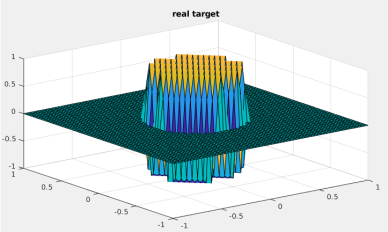

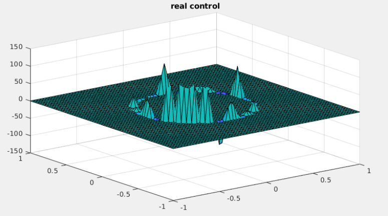

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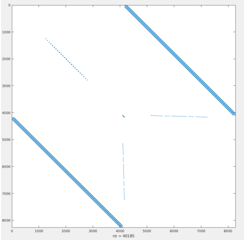
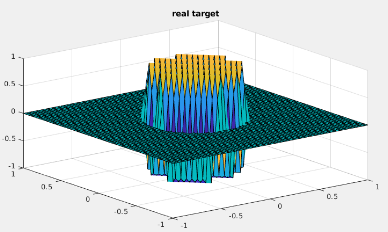
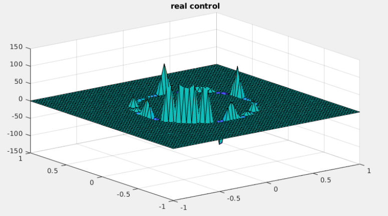


$$\begin{bmatrix} u \\ z \\ \lambda \end{bmatrix} = \begin{bmatrix} w \\ 0 \\ 0 \end{bmatrix}$$





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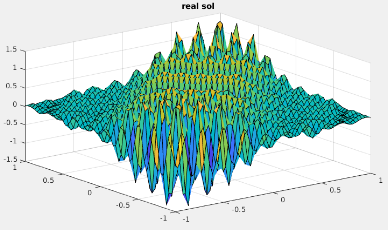

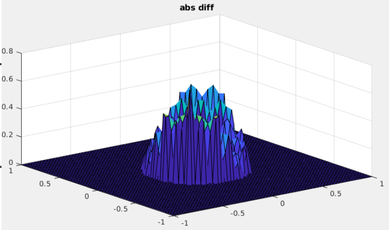

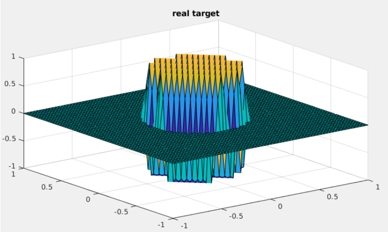

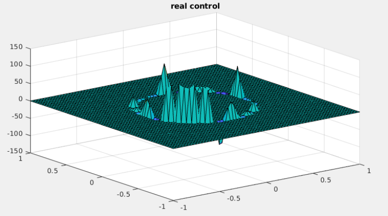

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Results

2 dimensions, $2^6 \times 2^6$ uniform mesh, $\beta = 10^{-4}$.
DD uses 128 subdomains, $\kappa(M^{-1}S) \leq 100$.

Preconditioner	ω 0	1	2	4	6
DD	54 (2,653)	64 (2,724)	63 (2,729)	62 (2,773)	66 (2,781)
Kouri et al.	12	10	12	15	15

Conclusions

- We have presented a fully algebraic DD preconditioner for diagonally dominant matrices
- Although we have proved convergence for diagonally dominant matrices, the construction is algebraic and can be applied to any systems
- By breaking down more complex systems into SPD subproblems, this can be applied more widely, e.g., to certain saddle point systems.

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References

- Al Daas and Grigori, 'A Class of Efficient Locally Constructed Preconditioners Based on Coarse Spaces' SIMAX (2019)
- Al Daas, Jolivet and Rees, 'Efficient Algebraic Two-Level Schwarz Preconditioner for Sparse Matrices' SISC (2023)
- Jolivet et al., 'HPPDM - high performance unified framework for domain decomposition methods' `https://github.com/hpddm/hpddm`