SAND2015-5137C

Robust Constraint Selection in BDDC Algorithms for Three-Dimensional Problems

Clark Dohrmann[1] & Clemens Pechstein[2]

23rd International Conference on Domain Decomposition Methods
Jeju Island, Korea
July 6-10, 2015

[1] Sandia National Laboratories, Albuquerque, New Mexico, USA
[2] CST Computer Simulation Technology AG, Darmstadt, Germany

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Outline

- **Goals:**
  - Automated BDDC for challenging problems
  - Reasonably sized coarse spaces
  - Efficient implementations for 3D problems
- **Background:**
  - Problem setting and BDDC preconditioner
- **Theory:**
  - Localization of BDDC estimate
- **Implementation**
- **Examples**
- **Conclusions**

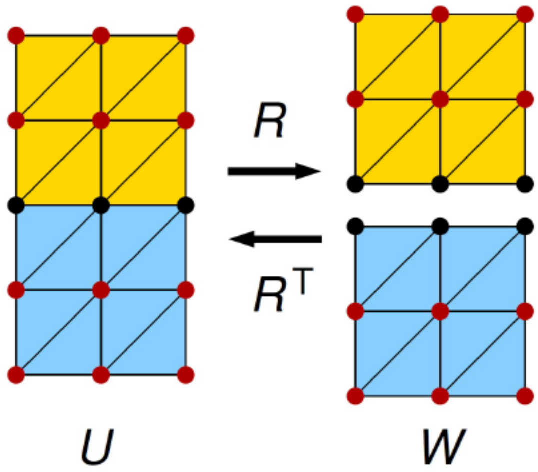
Problem Setting

Find $u \in U$: $\quad \underbrace{(R^T S R)}_{=:\bar{S}} \bar{u} = \underbrace{R^T g}_{=:\bar{g}}$ (global, assembled system)

$$\underbrace{S = \begin{bmatrix} S_1 & & 0 \\ & \ddots & \\ 0 & & S_N \end{bmatrix}}_{W \to W := \bigotimes_{i=1}^{N} W_i} \qquad \underbrace{g = \begin{bmatrix} g_1 \\ \vdots \\ g_N \end{bmatrix}}_{\in W} \qquad \underbrace{R = \begin{bmatrix} R_1 \\ \vdots \\ R_N \end{bmatrix}}_{U \to W}$$

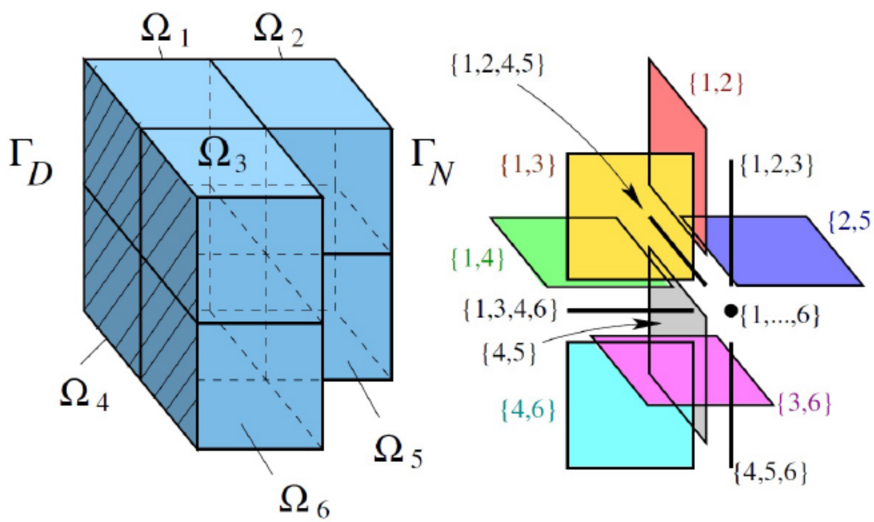
Assumptions:

- R_i zero-one matrix, $R_i R_i^T = I$
- R full column rank
- each dof has multiplicity ≥ 2
- each S_i is SPSD
- assembled matrix $\overline{S} = R^T S R$ is SPD



Equivalence Classes (Globs)

Partition global dofs (algebraically) into equivalence classes (globs): dofs within a glob are shared by the same set of substructures



Notation:

- $\mathcal{G}_i$ globs of subdomain i
- $\mathcal{N}_G$ subdomains sharing glob G
- R_{iG} restriction matrix from W_i to space of dofs on glob G

BDDC Preconditioner

Averaging operator

$$E_D : W \to U, \qquad E_D R = I \quad \text{partition of unity}$$

Our Assumption:

$$E_D w = \sum_{i=1}^{N} R_i^T D_i w_i$$

$$D_i = \sum_{G \in \mathcal{G}_i} R_{iG}^T D_{iG} R_{iG}$$

(each D_i is **block-diagonal** with respect to the globs)

$$\sum_{j \in \mathcal{N}_G} D_{jG} = I$$

Note: This allows for **deluxe scaling**

BDDC Preconditioner

Primal dofs (here based on globs)

For each glob G, have matrix Q_G *evaluating* primal dofs

Intermediate space $\widehat{W} \subset \widetilde{W} \subset W$:

$$\widetilde{W} := \{w \in W : \forall G \in \mathcal{G} \forall i, j \in \mathcal{N}_G : Q_G R_{iG} w_i = Q_G R_{jG} w_j\}$$

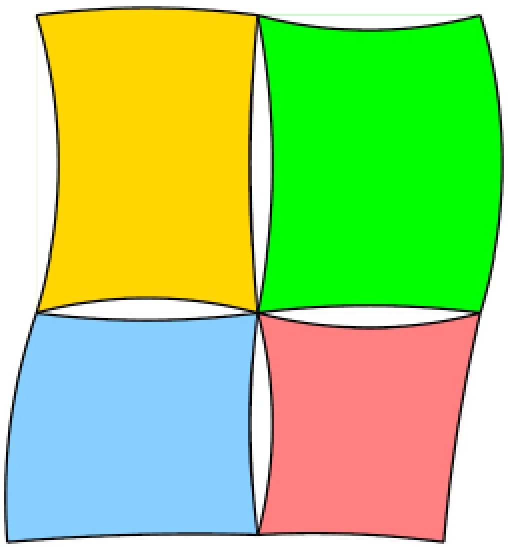
Condition needed:

- S is definite on $\widetilde{W}$ (primal dofs 'fix' local kernels)

BDDC preconditioner

$$M_{\text{BDDC}}^{-1} = E_D \underbrace{\tilde{I}(\tilde{I}^T S \tilde{I})^{-1} \tilde{I}^T}_{\substack{\text{partially} \\ \text{subassembled model}}} E_D^T$$

$\tilde{I} : \widetilde{W} \rightarrow W$ natural embedding



Well Known Theory

If S is definite on $\widetilde{W}$ and if

$$|P_D w|_S^2 \;\le\; \omega\, |w|_S^2 \qquad \forall w \in \widetilde{W}$$

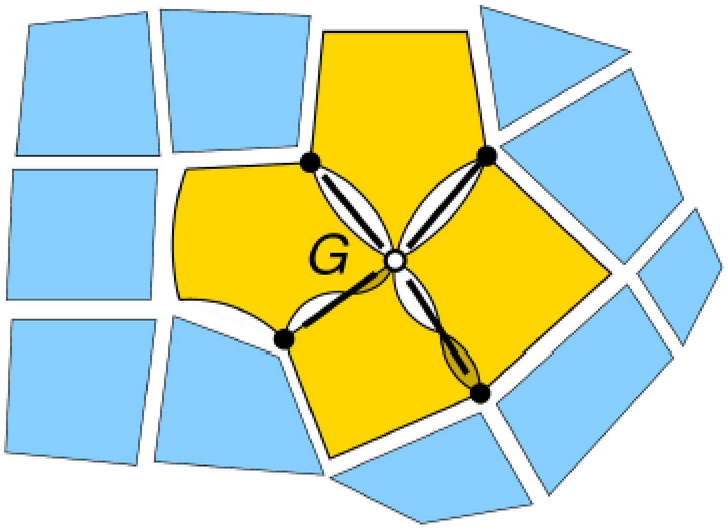
where $P_D := I - RE_D$, then

$$\kappa(M_{\mathrm{BDDC}}^{-1}\bar{S}) \;\le\; \omega$$

---

see, e.g., Mandel, et al. (2005)

Localization of BDDC Estimate



For fixed glob G, define

$\widetilde{W}_{\mathcal{N}_G}$:= restriction of $\widetilde{W}$ to neighboring subdomains of G

For $w \in \widetilde{W}_{\mathcal{N}_G}$ define

$$\underbrace{(P_{D,G}\, w)_i}_{\text{jump after averaging}} := R_{iG}^T \sum_{j \in \mathcal{N}_G} D_{jG}\left(R_{iG}\, w_i - R_{jG}\, w_j\right)$$

(local version of P_D, only acting on G)

Note: This particular choice of the space $\widetilde{W}_{\mathcal{N}_G}$ is essential: **all** possible constraints on the *glob patch* are enforced – very important later on

Localization of BDDC Estimate

Theorem

If for each glob $G \in \mathcal{G}^*$ we have

$$\sum_{i \in \mathcal{N}_G} |(P_{D,G} w)_i|^2_{S_i} \;\leq\; \omega_G \sum_{i \in \mathcal{N}_G} |w_i|^2_{S_i} \qquad \forall w \in \widetilde{W}_{\mathcal{N}_G}$$

then the P_D-estimate holds with

$$\omega \;=\; \max_{i=1,\dots,N} |\mathcal{G}_i^*| \sum_{G \in \mathcal{G}_i^*} \omega_G \;\leq\; C \max_{G \in \mathcal{G}^*} \omega_G$$

Remark: This shows that for 2D problems with all vertices totally primal, the *condition number indicator* by Sousedík & Mandel (2007/2012) is rigorous (up to harmless factor C)

$\mathcal{G}^*$ ... set of globs that are not *totally primal*

Generalized Eigenproblems

Spectral theory tells us:

$$\sum_{i\in\mathcal{N}_G} |(P_{D,G}w)_i|_{S_i}^2 \;\le\; \frac{1}{\lambda_{G,\min}} \sum_{i\in\mathcal{N}_G} |w_i|_{S_i}^2 \qquad \forall w \in \widetilde{W}_{\mathcal{N}_G}$$

if $\lambda_{G,\min} > 0$ minimal eigenvalue of (case $\lambda_{G,\min} = 0$ treated later on)

$$\sum_{i\in\mathcal{N}_G} z_i^T S_i w_i \;=\; \lambda \sum_{i\in\mathcal{N}_G} (P_{D,G}z)_i^T S_i (P_{D,G}w)_i \qquad \forall w, z \in \widetilde{W}_{\mathcal{N}_G}$$

in short

$$\mathcal{A}_G w \;=\; \lambda\, \mathcal{B}_G w \qquad \lambda \in [0, \infty]$$

Similar approaches:

Mandel, Sousedík & Šístek (BDDC, 3D) Galvis & Efendiev, Spillane & Co (Schwarz)

Kim & Chung '15 (BDDC, 2D)
Klawonn, Radtke & Rheinbach '15 (FETI-DP, 2D)

Adaptive Enrichment of Coarse Space

The spectral information $\omega_G = \frac{1}{\lambda_{G,\min}}$ can be used for

1. **condition number indicator** (rigorous up to harmless factor)
2. **adaptive selection of primal dofs** (following Mandel & Sousedík) for m smallest eigenvectors $y_{G,1}, \ldots, y_{G,m}$:

$$w^T \mathcal{B}_G w \;\leq\; \frac{1}{\lambda_{G,m+1}} w^T \mathcal{A}_G w \qquad \forall w \perp_{\mathcal{B}_G} \operatorname{span}\{y_{G,k}\}_{k=1}^{m}$$

Challenge: turn $y_{G,k}^T \mathcal{B}_G w = 0$ into **new primal constraints**

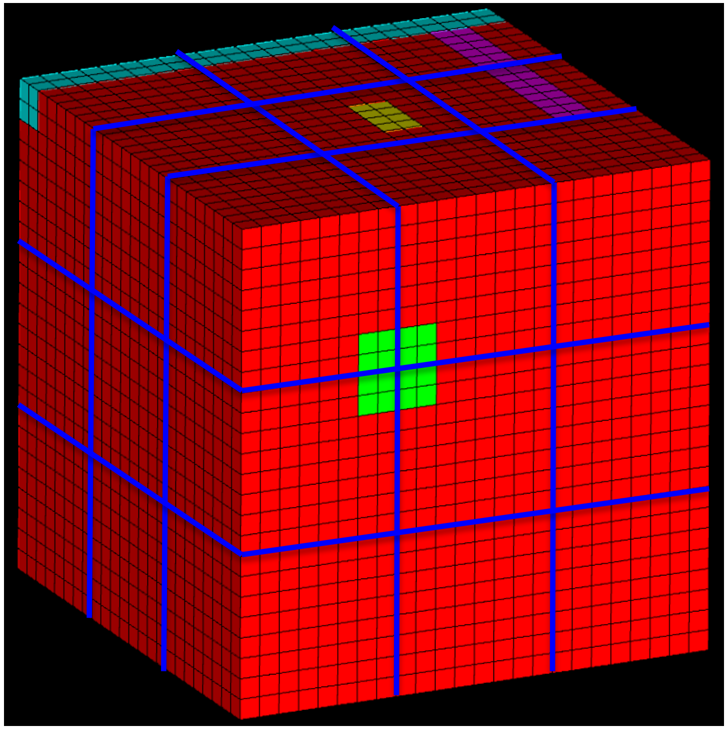
Current Implementation

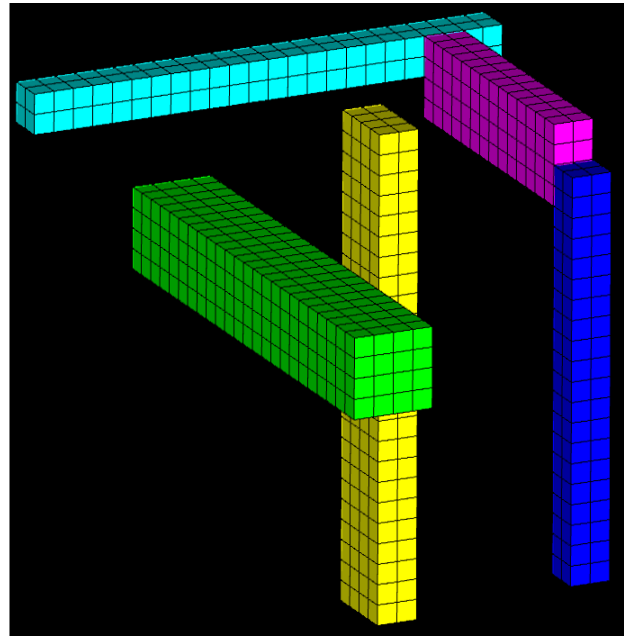
1. For $\mathcal{A}$, eliminate unknowns not in G via energy minimization. Likewise, remove corresponding zero blocks from $\mathcal{B}$.
2. Introduce change of variables involving jumps to remove null space of $\mathcal{B}_G$. Trailing blocks of rows and columns of $\mathcal{B}$ are then zero and removed. Same blocks of $\mathcal{A}$ eliminated via energy minimization.
3. For edges in 2D or faces in 3D, we can now solve eigenproblem to determine additional constraints.
4. For edges in three dimensions, the dimension of $\mathcal{A}$ and $\mathcal{B}$ is $(|\mathcal{N}_G| - 1)n_G$, where n_G is the number of rows in R_{iG}. This is too large to directly obtain constraints from eigenproblems. Details for this case appear in Extra Slides.

Current Implementation

- **Parallel C++ code:**
  - Code complexity increased by need for parallel communications when processing equivalence classes (coloring used)
  - Same local factorizations needed in conventional BDDC algorithms can be reused to avoid new ones
  - Plans to migrate to Trilinos when code more mature

Diffusion Example

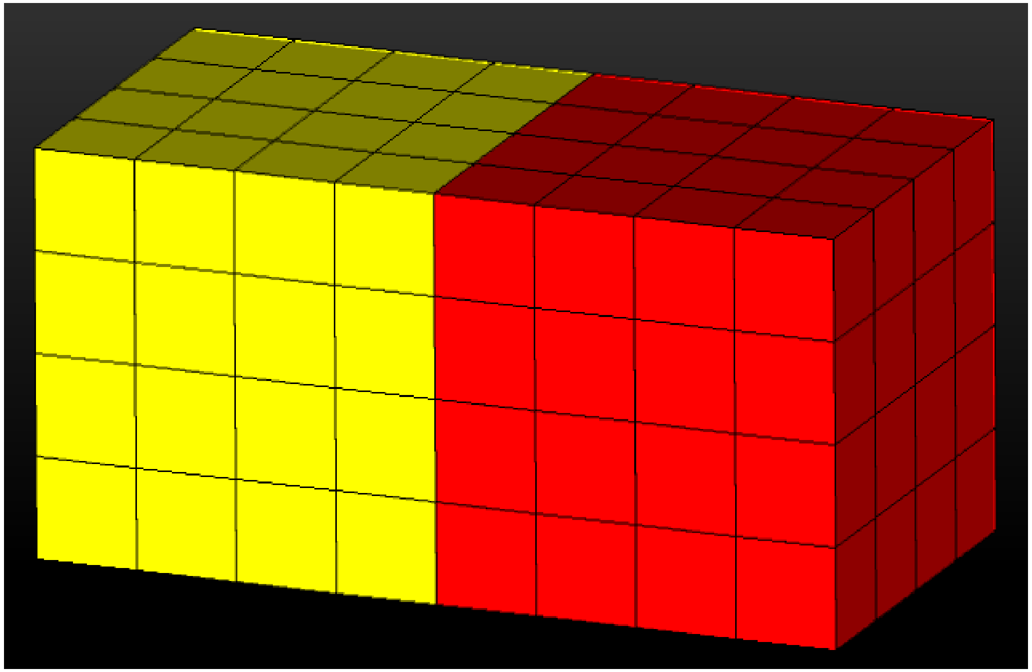




Q1 elements
27 subdomains
initial coarse space
dimension 28 (corners)
left boundary fixed
red: $\rho = 1$
other colors: $\rho = 10^4$

	stiffness weights			deluxe weights		
Threshold	+face	+edge	cond	+face	+edge	Cond
	0	0	2.7×10^4	0	0	2.4×10^4
0.001	6	2	296	10	2	297
0.01	8	2	24	21	2	23
0.10	43	2	9.3	81	2	9.3

Elasticity Example 1



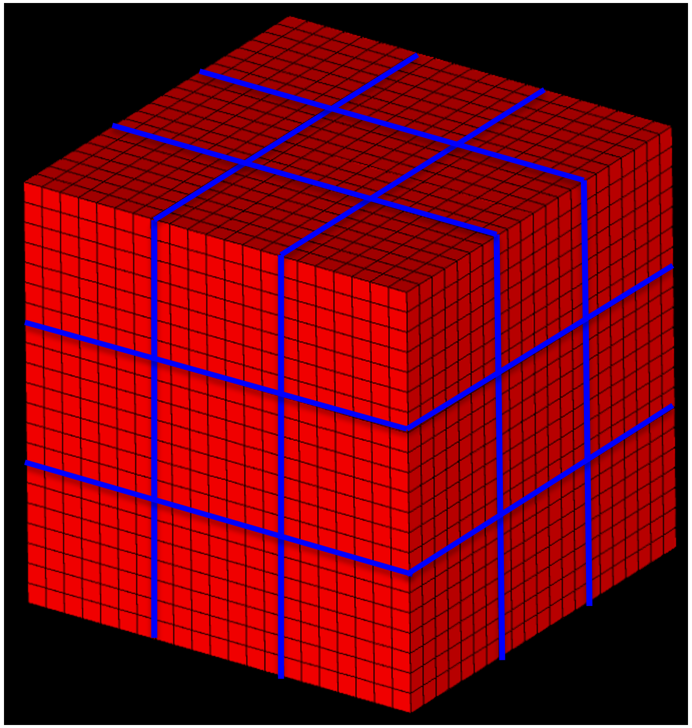
Q2P0 elements, 2 subdomains
initial coarse space dimension 0
entire boundary fixed
yellow: $E = 10^3$, $\nu = 0.3$
red: $E = 1$, $\nu = 0.49999$

Note: existing theory applies, but rho scaling not directly available from matrix

	stiffness weights		deluxe weights	
threshold	additional constraints	condition number	additional constraints	condition number
	0	797	0	1
0.05	90	1.44	1	1
0.035	87	28.4		
0.0015	8	665		

weights matter!

Elasticity Example 2



Q2P0 elements, 27 subdomains
initial coarse space dimension 24
exterior boundary fixed
E = 1, ν = 0.4999
stiffness-based weights

H/h	# add face	# add edge	cond #
4	84	84	3.5
5	108	84	3.8
6	108	84	4.3
7	108	84	4.7

Note: Use of deluxe weights was problematic and currently being investigated

Conclusions

- **Summary:**
  - Algebraic theory for very general SPD problems
  - Eigenproblems include constraints on neighboring globs
    - Helps limit number of additional constraints
  - Numerical results encouraging, but work remains
    - More efficient implementations (e.g. solutions of eigenproblems)
    - Weight selection remains open
  - Theory holds as well for corresponding FETI-DP method

Extra Slides

Present Implementation

1. Eliminate rows and columns of $\mathcal{A}_G$ not directly associated with G via energy minimization while enforcing existing constraints.
2. The dimension of the resulting matrices $\hat{\mathcal{A}}_G$ and $\hat{\mathcal{B}}_G$ is $|\mathcal{N}_G| n_G$, where n_G the number of dofs for G.
3. $\hat{\mathcal{B}}_G$ still has a null space associated with continuous values in G. To remove this, first introduce transformation of variables $\tilde{w}_G = T w_G$, where, e.g., for an edge with $|\mathcal{N}_G| = 3$,

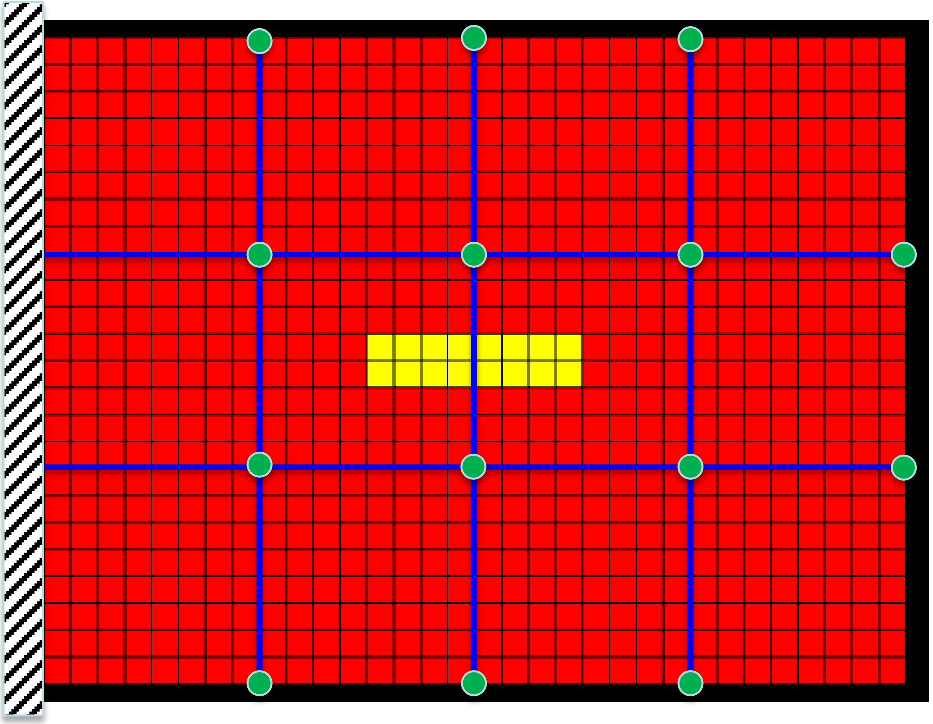
$$T = \begin{bmatrix} I & 0 & -I \\ 0 & I & -I \\ 0 & 0 & I \end{bmatrix}, \quad T^{-1} = \begin{bmatrix} I & 0 & I \\ 0 & I & I \\ 0 & 0 & I \end{bmatrix}$$

4. With $\tilde{\mathcal{A}} := T^{-T} \hat{\mathcal{A}}_G T^{-1}$ and $\tilde{\mathcal{B}} := T^{-T} \hat{\mathcal{B}}_G T^{-1}$, we observe the trailing block of rows and columns of $\tilde{\mathcal{B}}_G$ vanishes.
5. The eigenproblem of interest is $\bar{\mathcal{A}}_G y_G = \lambda \bar{\mathcal{B}}_G$, where $\bar{\mathcal{A}}_G$ is obtained my removing the trailing blocks of $\tilde{\mathcal{A}}_G$ via energy minimization and $\bar{\mathcal{B}}$ is simply the non-vanishing blocks of $\tilde{\mathcal{B}}_G$.

Present Implementation

6. If $|\mathcal{N}_G| = 2$, constraints for G can be obtained by solving the eigenproblem $\bar{\mathcal{A}}_G x_G = \lambda \bar{\mathcal{B}}_G x_G$.
7. If $|\mathcal{N}_G| > 2$, then we can consider $|\mathcal{N}_G| - 1$ different eigenproblems and introduce a constraint associated with the smallest eigenvalue from all these problems. Again, energy minimization is used to obtain these independent problems.
8. By enforcing the new constraint, the dimension of each of the different eigenproblems is reduced by one.
9. Constraints continue to be added until the smallest eigenvalue exceeds a specified threshold.

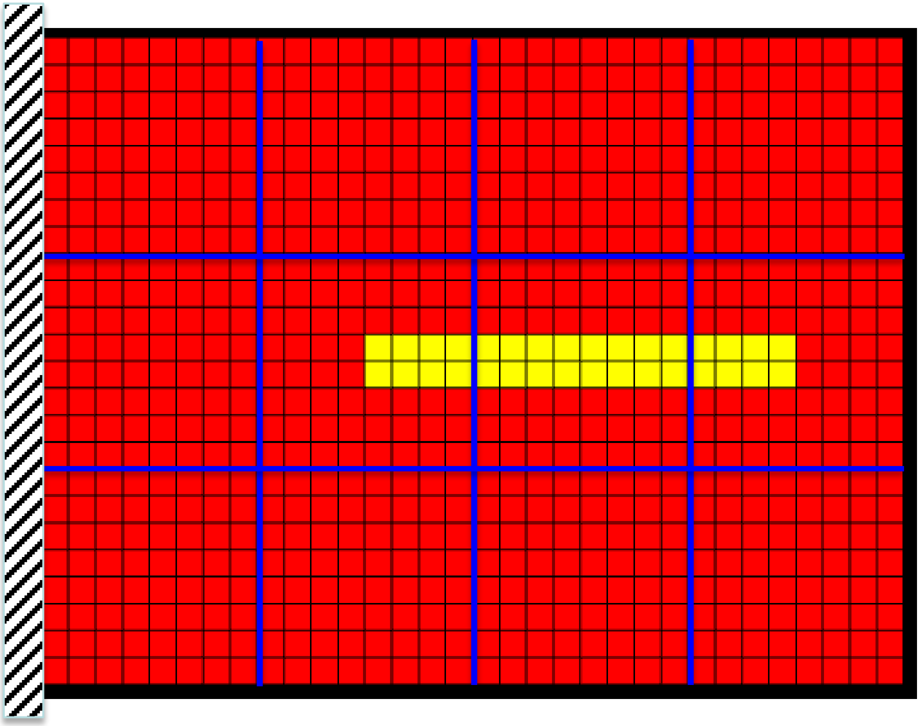
2D Diffusion Example 1



standard Q1 elements
14 corner constraints
eigen threshold = 0.01
red: $\rho = 1$
yellow: $\rho = 10^3$

stiffness weights		deluxe weights	
# additional constraints	condition number	# additional constraints	condition number
0	3.71	0	3.76

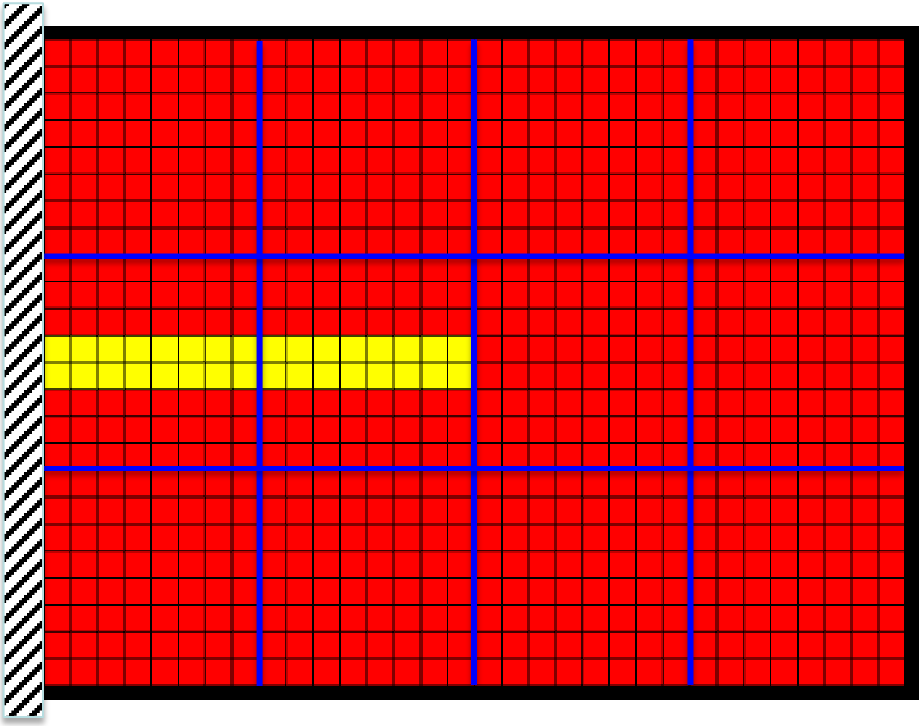
2D Diffusion Example 2



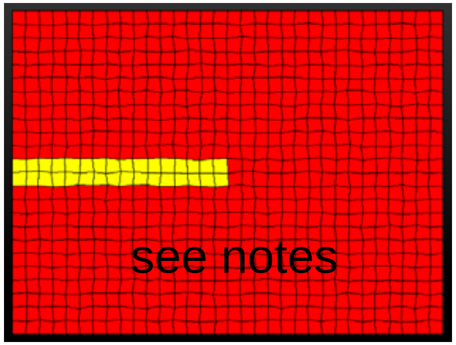
standard Q1 elements
14 corner constraints
eigen threshold = 0.01
red: $\rho = 1$
yellow: $\rho = 10^4$

stiffness weights		deluxe weights	
# additional constraints	condition number	# additional constraints	condition number
0	1.6×10^3	0	8.8
2	3.0		

2D Diffusion Example 3



standard Q1 elements
14 corner constraints
eigen threshold = 0.05
red: $\rho = 1$
yellow: $\rho = 10^4$



stiffness weights		deluxe weights	
# additional constraints	condition number	# additional constraints	condition number
0	1.6×10^3	0	1.6×10^3
1	4.2	3	2.8

Notes: similar results for H/h = 16 and perturbed nodal positions