Preconditioning for Bound Constrained Quadratic Programming Problems Arising from Discretization of Variational Inequalities

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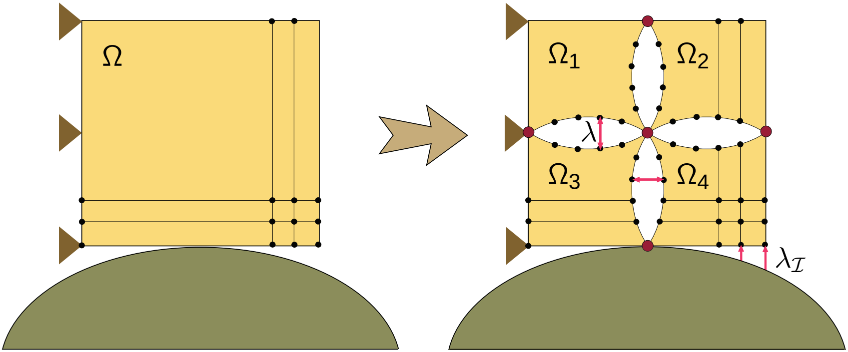
Outline

Motivation

FETI-DP Domain Decomposition



To improve rate of convergence for variational inequalities (FETI-DP, BETI-DP, . . .).

Partially Bound Constrained QP Problem

Find

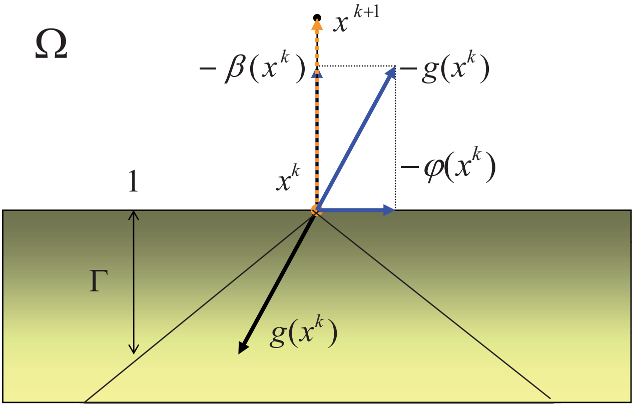
$$\min_{\mathbf{x}\in\Omega} f(\mathbf{x}), \quad \Omega = \{\mathbf{x} \in \mathbb{R}^n : \ \mathbf{x}_{\mathcal{I}} \geq \ell_{\mathcal{I}}\}, \quad \mathcal{I} = \{1, \ldots, m\},$$

where

- $f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\mathbf{A}\mathbf{x} - \mathbf{x}^T\mathbf{b}$,
- ℓ and **b** are given column *n*-vectors,
- $1 \leq m \ll n$,
- and **A** is an $n \times n$ spd matrix.

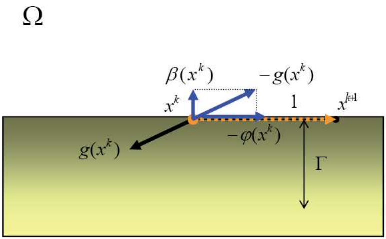
MPRGP - Proportioning

$\mathbf{x}^k$ strictly proportional $||\beta(\mathbf{x}^k)||^2 \leq \Gamma^2 \widetilde{\varphi}(\mathbf{x}^k)^T \varphi(\mathbf{x}^k)$

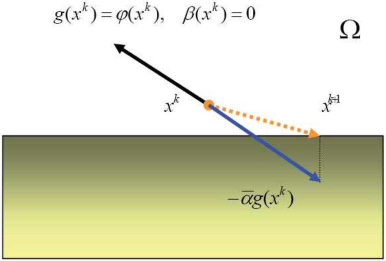


MPRGP - Proportional Iterations

Feasible CG step



Projection step:
expansion of the active set



Modified Proportioning with Reduced Gradient Projections - MPRGP

if $\mathbf{x}^k$ is *strictly proportional*

{trial conjugate gradient step}

if $\mathbf{x}^{k+1}$ is *feasible*

accept $\mathbf{x}^{k+1}$

else

{expansion step}

$x^{k+1} = P_\Omega(x^k - \overline{\alpha}\varphi(x^k))$

end

else

{proportioning step}

minimization in direction $-\beta(x^k)$

end

MPRGP Algorithm

Rate of Convergence

THEOREM

$\lambda_{\min}$ = min eigenvalue of **A**, $\Gamma > 0$, $\hat{\Gamma} = \max\{\Gamma, \Gamma^{-1}\}$

R-linear rate of convergence in energy norm

$$\|\mathbf{x}^k - \widehat{\mathbf{x}}\|_{\mathbf{A}}^2 \le 2\eta \left(f(\mathbf{x}^0) - f(\widehat{\mathbf{x}}) \right),$$

where

$$\eta = 1 - \frac{\overline{\alpha}\lambda_{\min}}{2 + 2\widehat{\Gamma}^2}.$$

Dostál and Schöberl, Computational Optimization and Applications, 2005

Conjugate Projectors

P is an **A**-*conjugate projector*

if $\mathrm{Im}\mathbf{P} \perp_{\mathbf{A}} \mathrm{Ker}\mathbf{P} \iff \mathbf{P}^T\mathbf{A}(\mathbf{I}-\mathbf{P}) = \mathbf{P}^T\mathbf{A} - \mathbf{P}^T\mathbf{A}\mathbf{P} = \mathbf{O}$

$\Downarrow$

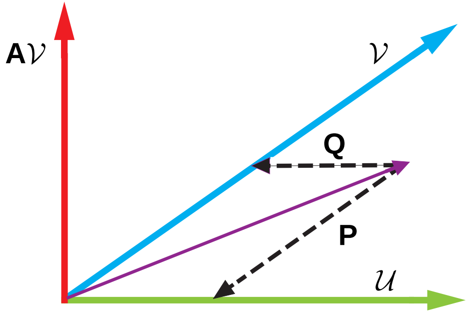
- $\mathbf{Q} = \mathbf{I} - \mathbf{P}$ is also a conjugate projector
- $\mathbf{P}^T\mathbf{A} = \mathbf{A}\mathbf{P} = \mathbf{P}^T\mathbf{A}\mathbf{P}$ and $\mathbf{Q}^T\mathbf{A} = \mathbf{A}\mathbf{Q} = \mathbf{Q}^T\mathbf{A}\mathbf{Q}$.

Conjugate Projectors

$\mathcal{U}$ = subspace spanned by columns of full rank matrix $\mathbf{U} \in \mathbb{R}^{n \times p}$

$$\mathbf{U} = \begin{bmatrix} \mathbf{O} \\ \mathbf{U}_2 \end{bmatrix}, \quad \mathbf{U}_2 \in \mathbb{R}^{n-m \times p}$$

- $\mathbf{P} = \mathbf{U}(\mathbf{U}^T\mathbf{A}\mathbf{U})^{-1}\mathbf{U}^T\mathbf{A}$ onto $\mathcal{U}$
- $\mathbf{Q} = \mathbf{I} - \mathbf{P}$ onto $\mathcal{V}$



Invariant Subspace

$\mathcal{V} = \mathrm{Im}\mathbf{Q}$. For all $\mathbf{x} \in \mathbf{A}\mathcal{V}$

$$\mathbf{Q}^T\mathbf{A}\mathbf{Q}\mathbf{x} = \mathbf{A}\mathbf{Q}\mathbf{x}$$

$$\Downarrow$$

$$\mathbf{Q}^T\mathbf{A}\mathbf{Q}(\mathbf{A}\mathcal{V}) \subseteq \mathbf{A}\mathcal{V}.$$

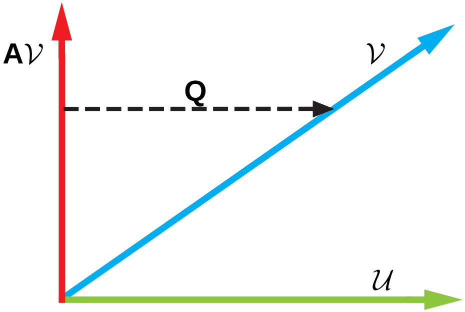
$\Rightarrow$ $\mathbf{A}\mathcal{V}$ = *invariant subspace* of $\mathbf{Q}^T\mathbf{A}\mathbf{Q}$.

Invariant Subspace

$\mathbf{Q}$ = conjugate projector on $\mathcal{V}$. Then for any $\mathbf{x} \in \mathbf{A}\mathcal{V}$

$$\|\mathbf{Qx}\| \geq \|\mathbf{x}\| \quad \text{and} \quad \mathcal{V} = \mathbf{Q}(\mathbf{A}\mathcal{V}).$$

Domorádová and Dostál, Numerical linear Algebra with Applications, 2007



Proof

- Let $\mathbf{x} \in \mathbf{A}\mathcal{V}$, so that $\exists\ \mathbf{y} \in \mathbb{R}^n : \mathbf{x} = \mathbf{AQy}$

  $$\Rightarrow \mathbf{Q}^T\mathbf{x} = \mathbf{Q}^T\mathbf{AQy} = \mathbf{AQy} = \mathbf{x}$$

- and $\mathbf{x}^T\mathbf{Qx} = \mathbf{x}^T\mathbf{Q}^T\mathbf{x} = \|\mathbf{x}\|^2$, so that

$$\begin{aligned} \|\mathbf{Qx}\|^2 &= \mathbf{x}^T\mathbf{Q}^T\mathbf{Qx} = \mathbf{x}^T\left((\mathbf{Q}^T - \mathbf{I}) + \mathbf{I}\right)\left((\mathbf{Q}^T - \mathbf{I}) + \mathbf{I}\right)\mathbf{x} \\ &= \|(\mathbf{Q} - \mathbf{I})\mathbf{x}\|^2 + \|\mathbf{x}\|^2 \geq \|\mathbf{x}\|^2. \end{aligned}$$

- $\mathcal{V} = \mathrm{Im}\mathbf{Q}$, so that $\mathcal{V} = \mathbf{Q}(\mathbb{R}^n) \supseteq \mathbf{Q}(\mathbf{A}\mathcal{V})$
- $\mathbf{A}$ is nonsingular and mapping $\mathbf{A}\mathcal{V} \ni \mathbf{x} \to \mathbf{Qx}$ is injective
- dimension argument $\Rightarrow \mathbf{Q}(\mathbb{R}^n) = \mathbf{Q}(\mathbf{A}\mathcal{V})$

□

Proof

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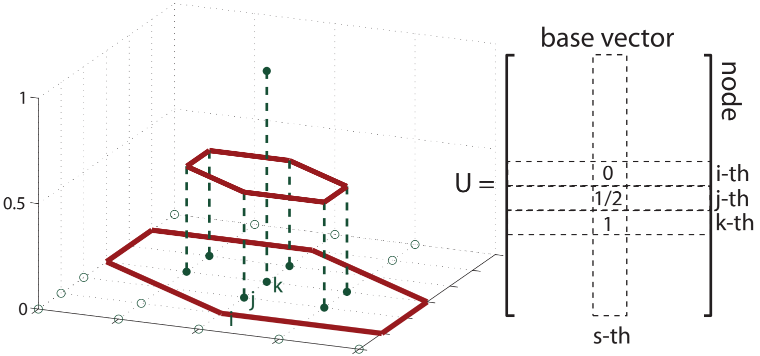
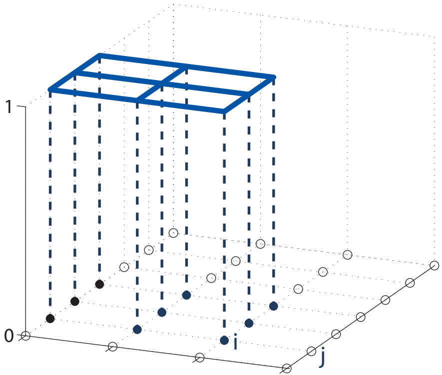
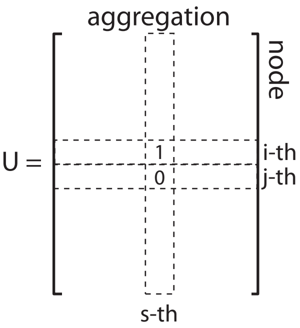
$\square$

Projector defined by traces of linear functions on coarse grid

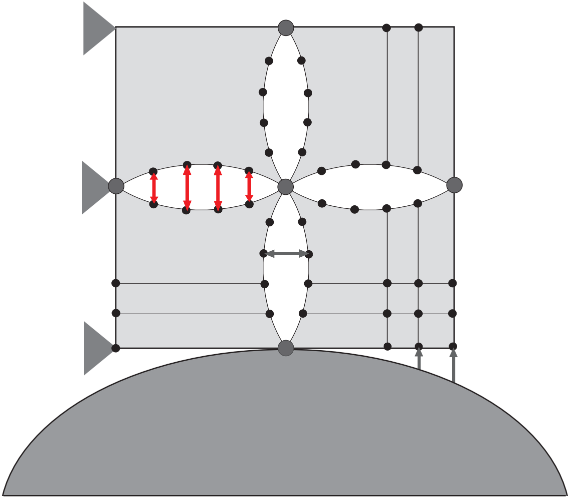


Projector defined by aggregations





Projector for FETI-DP



Preconditioning by Conjugate Projector

Decomposition by means of projectors

- $\mathbf{P} = \mathbf{U}(\mathbf{U}^T\mathbf{A}\mathbf{U})^{-1}\mathbf{U}^T\mathbf{A}$ onto $\mathcal{U}$
- $\mathbf{Q} = \mathbf{I} - \mathbf{P}$ onto $\mathcal{V} = \mathrm{Im}\mathbf{Q}$

$$\begin{aligned}
\min_{\mathbf{x}\in\Omega} f(\mathbf{x}) &= \min_{\substack{\mathbf{y}\in\mathcal{U},\mathbf{z}\in\mathcal{V}\\ \mathbf{y}+\mathbf{z}\in\Omega}} f(\mathbf{y}+\mathbf{z}) = \min_{\mathbf{y}\in\mathcal{U}} f(\mathbf{y}) + \min_{\mathbf{z}\in\mathcal{V}\cap\Omega} f(\mathbf{z})\\
&= f(\mathbf{x}^0) + \min_{\mathbf{z}\in\mathcal{V}\cap\Omega} f(\mathbf{z})\\
&= f(\mathbf{x}^0) + \min_{\substack{\mathbf{z}\in\mathbf{A}\mathcal{V}\\ \mathbf{z}_{\mathcal{I}}\geq\ell_{\mathcal{I}}}} \frac{1}{2}\mathbf{z}^T\mathbf{Q}^T\mathbf{A}\mathbf{Q}\mathbf{z} - \mathbf{b}^T\mathbf{Q}\mathbf{z}
\end{aligned}$$

Domorádová and Dostál, Numerical linear Algebra with Applications, 2007

Minimization over $\mathcal{U}$

$\mathbf{U} \in \mathbb{R}^{n\times p}$, $\mathbf{P} = \mathbf{U}(\mathbf{U}^T\mathbf{A}\mathbf{U})^{-1}\mathbf{U}^T\mathbf{A}$

$$\min_{\mathbf{x}\in\mathcal{U}} f(\mathbf{x}) = \min_{\mathbf{y}\in\mathbb{R}^p} f(\mathbf{U}\mathbf{y}) = \min_{\mathbf{y}\in\mathbb{R}^p} \frac{1}{2}\mathbf{y}^T\mathbf{U}^T\mathbf{A}\mathbf{U}\mathbf{y} - \mathbf{b}^T\mathbf{U}\mathbf{y}$$

by the gradient argument

$$\mathbf{U}^T\mathbf{A}\mathbf{U}\mathbf{y} = \mathbf{U}^T\mathbf{b}.$$

Then minimizer $\mathbf{x}^0 = \mathbf{U}\mathbf{y}^0$ of f over $\mathcal{U}$ is defined by

$$\mathbf{x}^0 = \underbrace{\mathbf{U}(\mathbf{U}^T\mathbf{A}\mathbf{U})^{-1}\mathbf{U}^T}_{\mathbf{P}\mathbf{A}^{-1}}\mathbf{b} = \mathbf{P}\mathbf{A}^{-1}\mathbf{b}.$$

Observation

$$\mathbf{P}^{\mathsf{T}}\mathbf{A} = \mathbf{A}\mathbf{P} \Rightarrow \mathbf{P}^{\mathsf{T}} = \mathbf{A}\mathbf{P}\mathbf{A}^{-1}$$

- $\mathbf{g}^0 = \mathbf{A}\mathbf{x}^0 - \mathbf{b} = \mathbf{A}\underbrace{\mathbf{P}\mathbf{A}^{-1}\mathbf{b}}_{x^0} - \mathbf{b} = (\mathbf{A}\mathbf{P}\mathbf{A}^{-1} - \mathbf{I})\mathbf{b}$
  $= (\mathbf{P}^T - \mathbf{I})\mathbf{b} = -\mathbf{Q}^T\mathbf{b} \Rightarrow \mathbf{g}^0 \in \mathrm{Im}\mathbf{Q}^{\mathrm{T}}$
- $\mathrm{Im}\mathbf{Q}^{\mathrm{T}} = \mathrm{Im}(\mathbf{Q}^{\mathrm{T}}\mathbf{A}) = \mathrm{Im}(\mathbf{A}\mathbf{Q}) = \mathbf{A}\mathcal{V}$

$\Rightarrow \mathbf{g}^0 \in \mathbf{A}\mathcal{V}$.

Lemma

Let $\mathbf{z}^1, \mathbf{z}^2, \ldots$ be generated by the MPRGP algorithm for the problem

$$\min_{\mathbf{z}_{\mathcal{I}} \geq \ell_{\mathcal{I}}} \frac{1}{2} \mathbf{z}^T \mathbf{Q}^T \mathbf{A} \mathbf{Q} \mathbf{z} + \left(\mathbf{g}^0\right)^T \mathbf{z}$$

starting from $\mathbf{z}^0 = P_\Omega\left(\mathbf{g}^0\right)$.

Then $\mathbf{z}^k \in \mathbf{A}\mathcal{V},\ k = 0, 1, 2, \ldots$.

$\Rightarrow$ $\mathbf{A}\mathcal{V}$ is invariant subspace of P_Ω

Preconditioning Effect

- $\lambda_{max} \geq \cdots \geq \lambda_{min}$ the eigenvalues of $\mathbf{A}$
- $\mathcal{E} = p$-dimensional subspace spanned by the eigenvectors corresponding to the p smallest eigenvalues of $\mathbf{A}$
- $\overline{\gamma} = \|\mathbf{R}_{\mathbf{A}\mathcal{U}} - \mathbf{R}_{\mathcal{E}}\| \ldots$ gap between $\mathbf{A}\mathcal{U}$ and $\mathcal{E}$

$$\overline{\lambda}_{min} \geq \sqrt{(1-\overline{\gamma}^2)\lambda_{min-m}^2 + \overline{\gamma}^2\lambda_{min}^2}$$

$\overline{\lambda}_{min}$ = min eigenvalue of $(\mathbf{Q}^T\mathbf{A}\mathbf{Q}|\mathbf{A}\mathcal{V})$

Dostál, International Journal of Computer Mathematics, 1988

Rate of Convergence of Reduced Problem

$\hat{\mathbf{z}}$ = unique solution, $\mathbf{g}^0 = -\mathbf{Q}^T\mathbf{b}$

$$\min_{\substack{\mathbf{z}\in\mathbf{A}\mathcal{V}\\ \mathbf{z}_\mathcal{I}\geq\ell_\mathcal{I}}} \underbrace{\frac{1}{2}\mathbf{z}^T\mathbf{Q}^T\mathbf{A}\mathbf{Q}\mathbf{z} + \left(\mathbf{g}^0\right)^T\mathbf{z}}_{f_{0,\mathbf{Q}}}$$

$$f_{0,\mathbf{Q}}(\mathbf{z}^{k+1}) - f_{0,\mathbf{Q}}(\widehat{\mathbf{z}}) \leq \overline{\eta}\left(f_{0,\mathbf{Q}}(\mathbf{z}^k) - f_{0,\mathbf{Q}}(\widehat{\mathbf{z}})\right),$$

where

$$\overline{\eta} = 1 - \frac{\overline{\alpha}\overline{\lambda}_{\min}}{2 + 2\widehat{\Gamma}^2}$$

Improved Estimate

MPRGP

$$\|\mathbf{x}^k - \widehat{\mathbf{x}}\|_{\mathbf{A}}^2 \leq 2\eta \left(f(\mathbf{x}^0) - f(\widehat{\mathbf{x}}) \right)$$

MPRGP-CP

$$f_{0,\mathbf{Q}}(\mathbf{z}^{k+1}) - f_{0,\mathbf{Q}}(\widehat{\mathbf{z}}) \leq \overline{\eta} \left(f_{0,\mathbf{Q}}(\mathbf{z}^k) - f_{0,\mathbf{Q}}(\widehat{\mathbf{z}}) \right)$$

$$\overline{\eta} < \eta$$

because for nonsingular $\mathbf{U}^T\mathbf{E}$ and $\lambda_{min} < \lambda_{min-m}$

$$\overline{\eta} = 1 - \frac{\overline{\alpha}\overline{\lambda}_{\min}}{2 + 2\widehat{\Gamma}^2} < 1 - \frac{\overline{\alpha}\lambda_{\min}}{2 + 2\widehat{\Gamma}^2} = \eta$$

Domorádová and Dostál, Numerical linear Algebra with Applications, 2007

Numerical Experiments

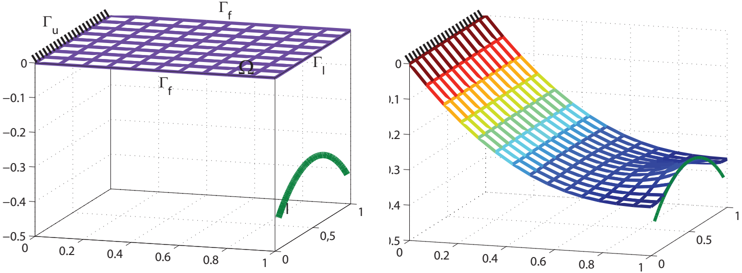
Deflection of the membrane

Find

$$\min f(u) = \frac{1}{2}\int_{\Omega} \|\nabla u(x)\|^2 \mathrm{d}\Omega + \int_{\Omega} u \,\mathrm{d}\Omega \quad \text{subject to} \quad u \in \mathcal{K},$$

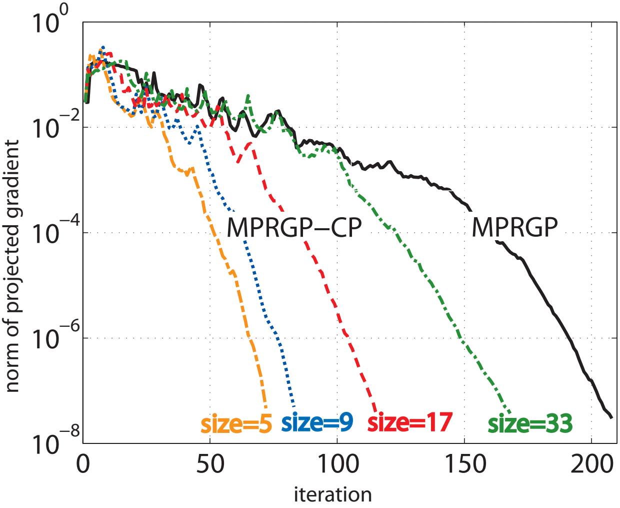
where

$$\mathcal{K} = \{u \in H^1(\Omega) : \; u = 0 \;\text{ on }\; \Gamma_u \quad \text{and} \quad c \le u \;\text{ on }\; \Gamma_c\}.$$



Numerical Experiments

Projector deffined by traces of linear functions on coarse grid



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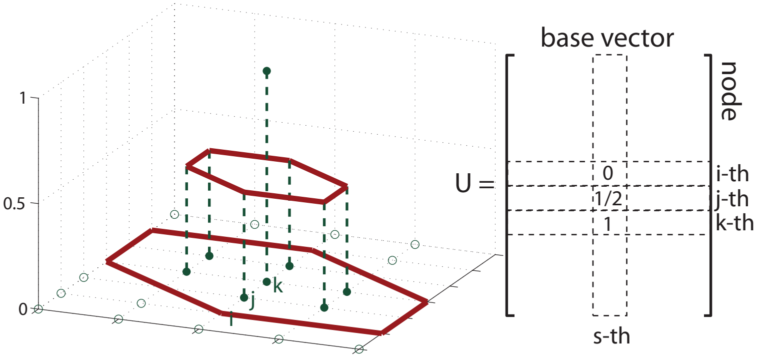
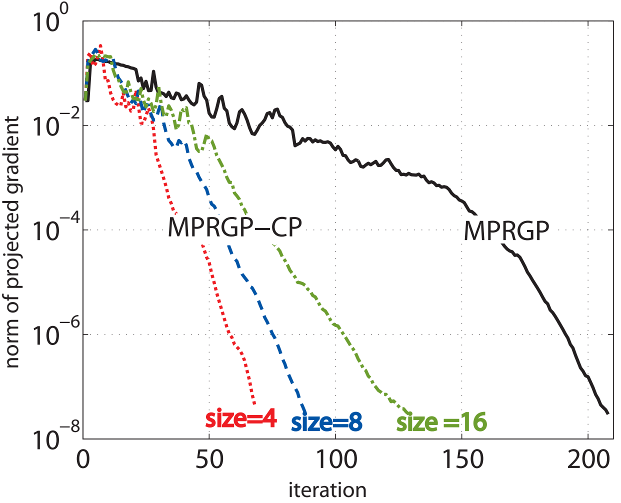


Numerical Experiments

Projector defined by aggregations



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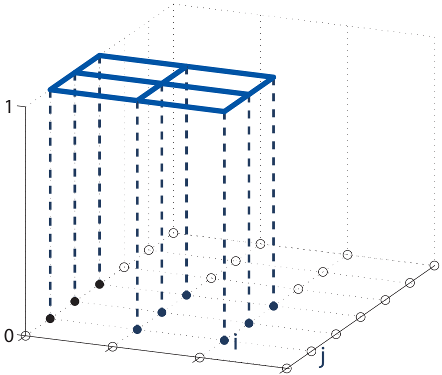
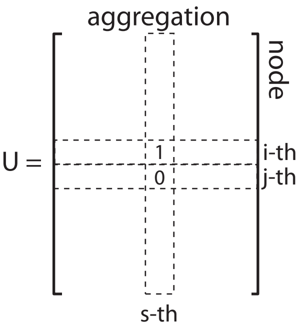
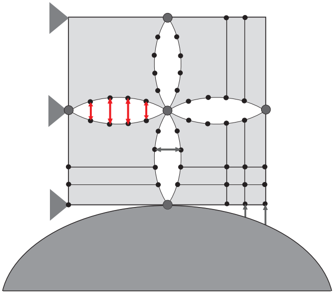




Numerical Experiments

FETI-DP



number of subdomains	number of nodes 2		4		8		16	
2	6	8	9	13	16	18	21	29
4	9	11	13	17	19	30	25	53
8	12	18	19	29	25	56	36	80
16	17	24	26	55	39	85	-	-

MPRGP-CP MPRGP

Summary

- The preconditioning effects all steps of the algorithm.
- Better rate of convergence is proved.
- It is confirmed by numerical experiments.

Our Outlook

- to examine implementation by averaging.
- to implement the algorithm into our research FETI and BETI software OOSOL.
- to consider iterative implementation of inversion in the projector.