On a Multigrid Preconditioned Augmented Lagrangians Applied to the Stokes and Optimization Problems

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Outline

- Motivation: Large–scale discretized topology optimization
- Setting of the saddle–point problem
- Optimal Uzawa–type methods
- Semi–monotonic augmented Lagrangian method
- Multigrid preconditioning
- An application to the Stokes problem, numerical results
- Outlook: Applications in topology optimization

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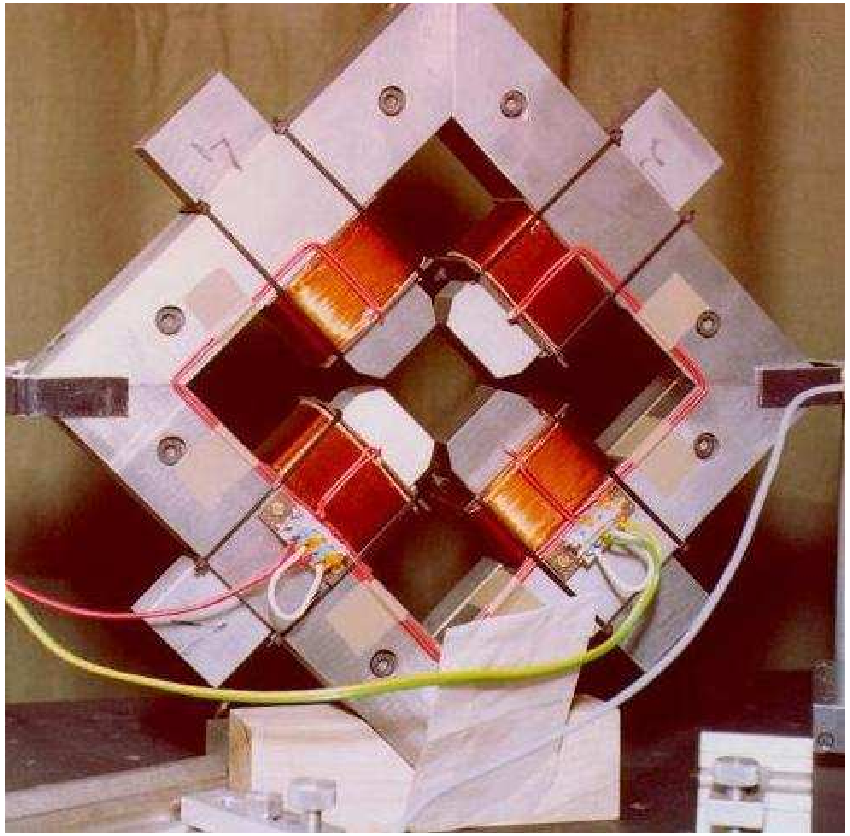
Motivation: Large–scale discretized topology optimization

Topology optimization of an electromagnet



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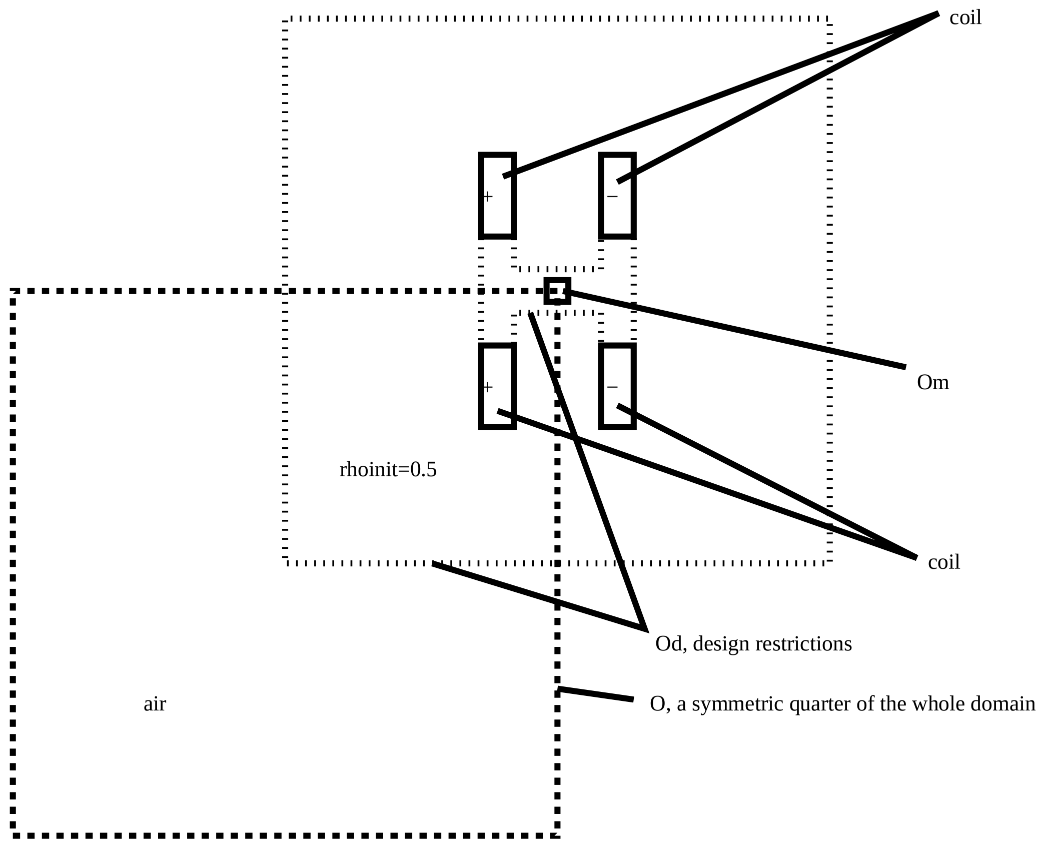

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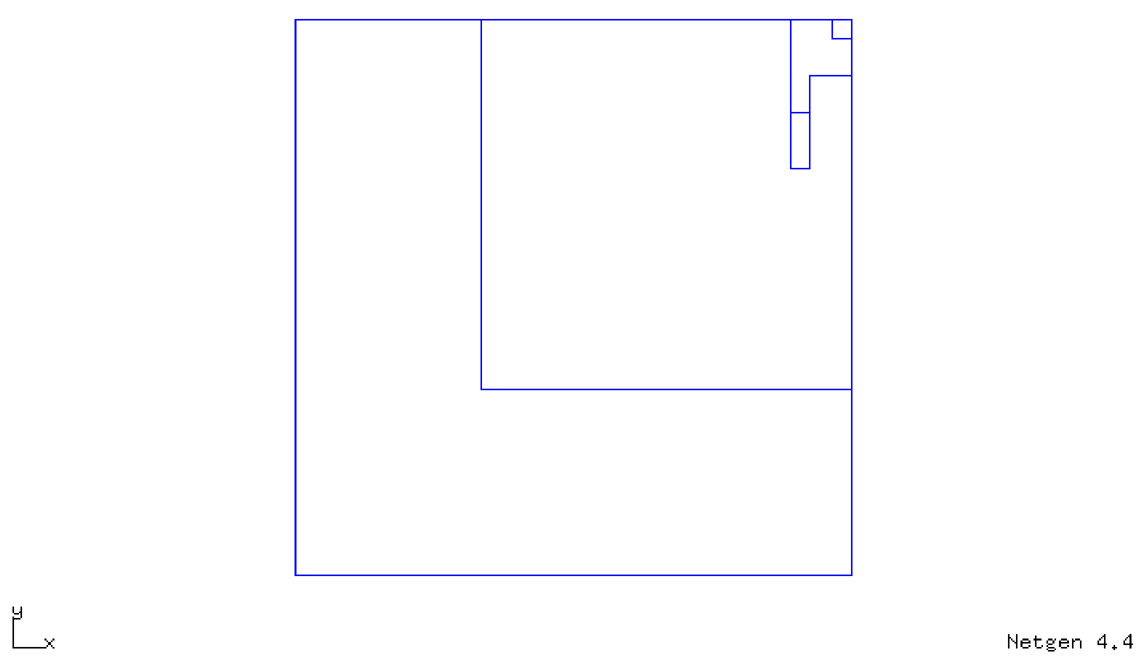

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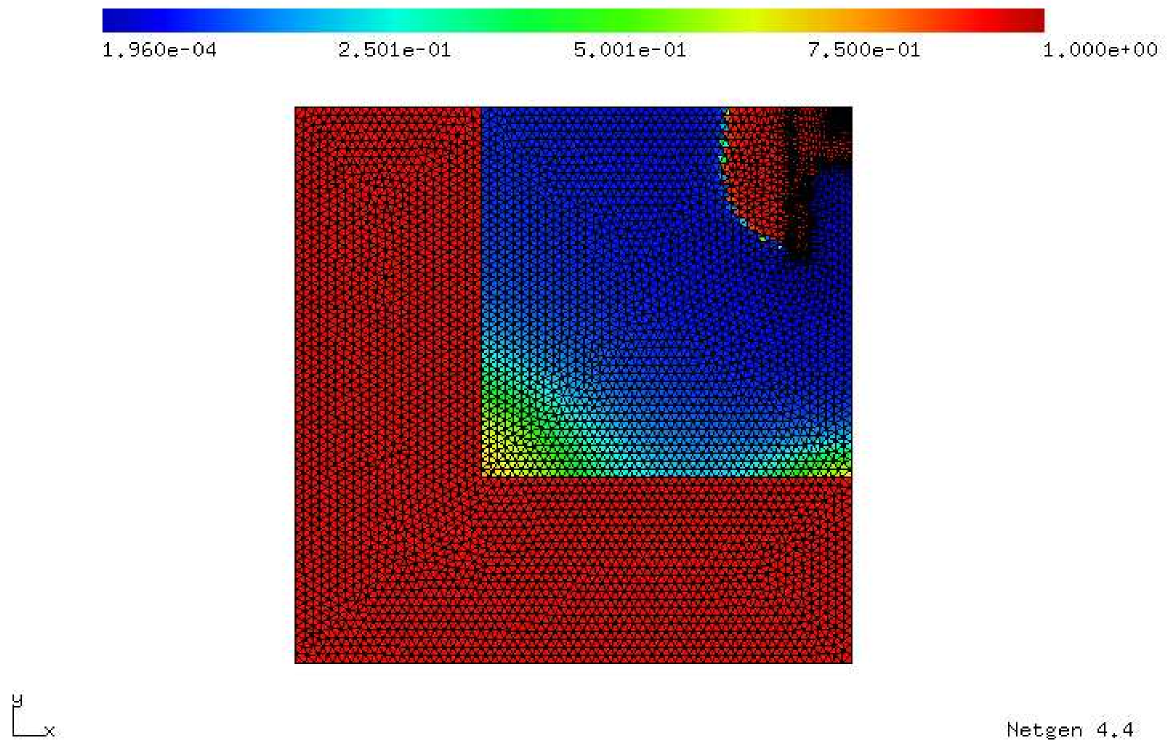

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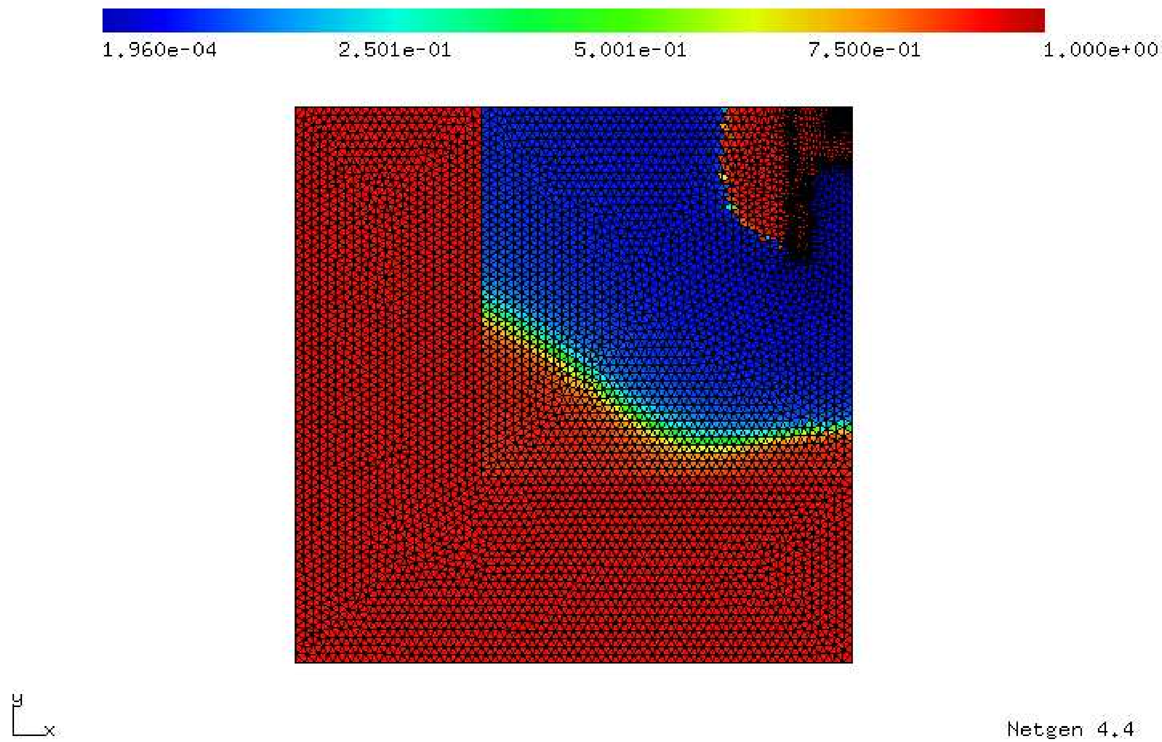

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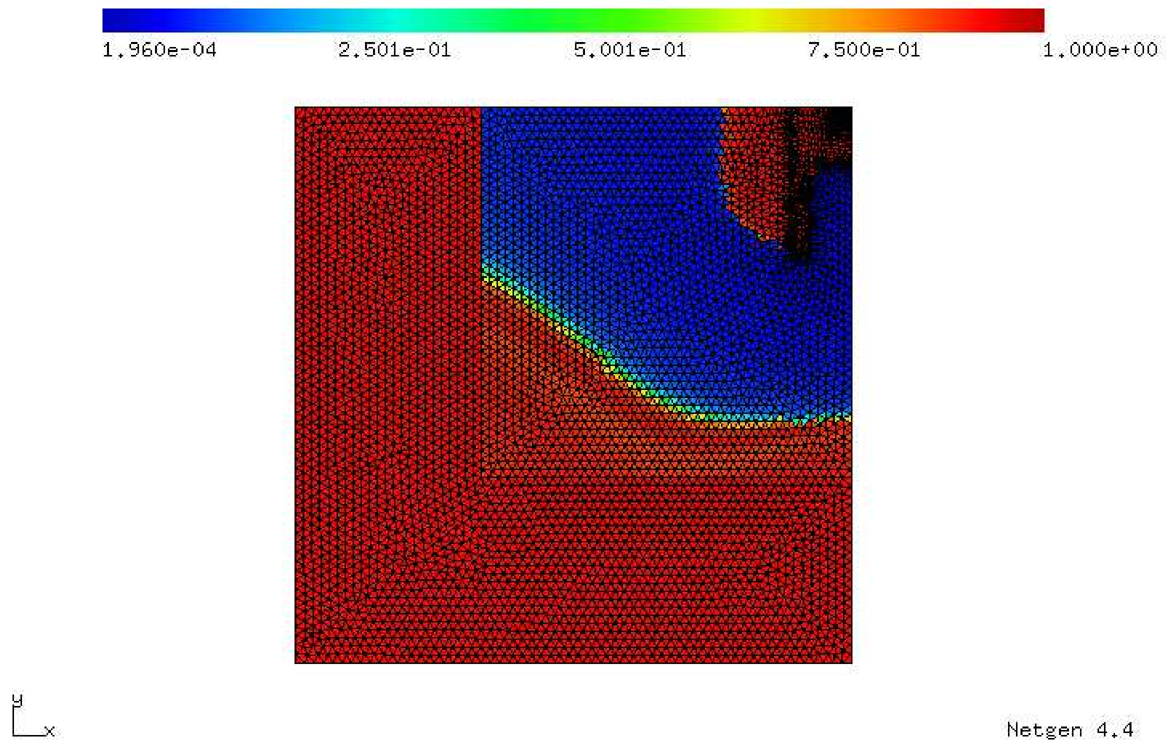

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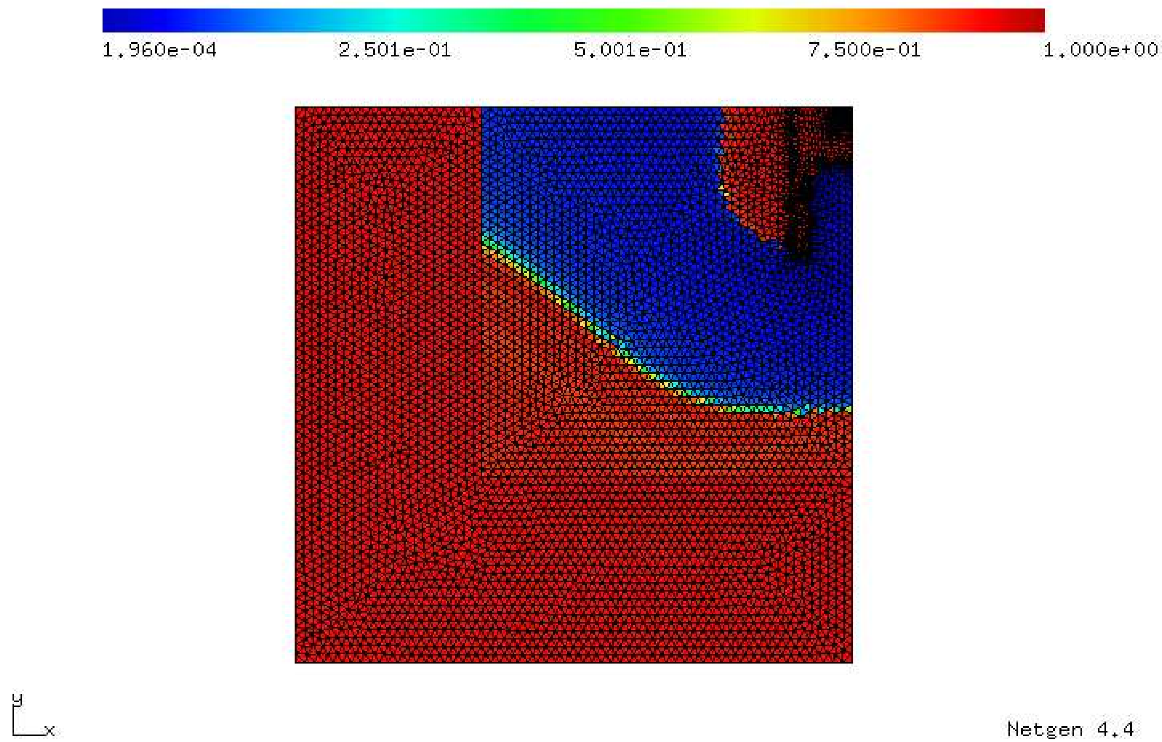

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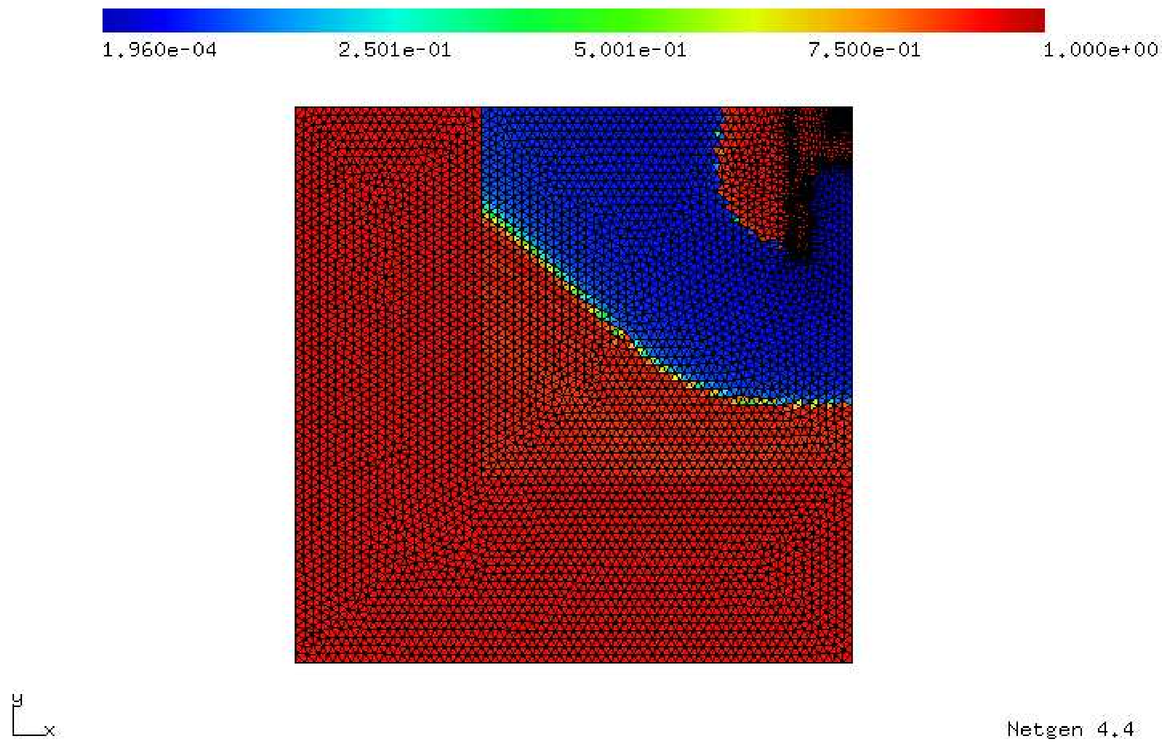

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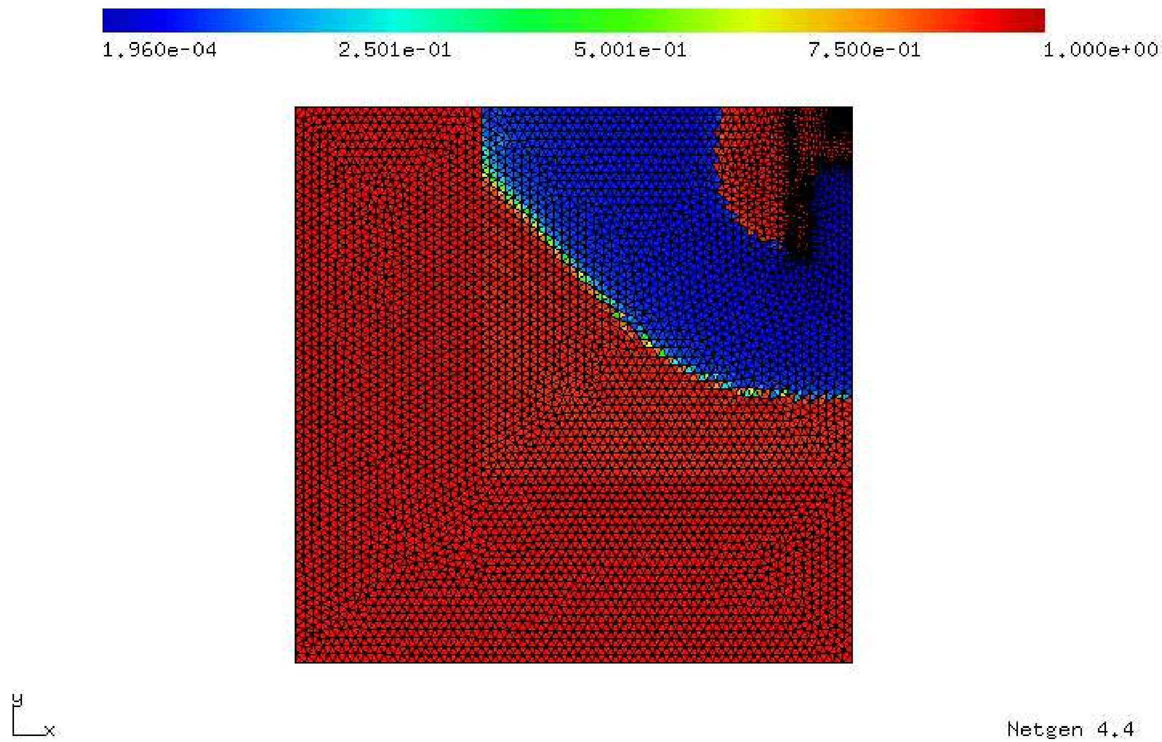

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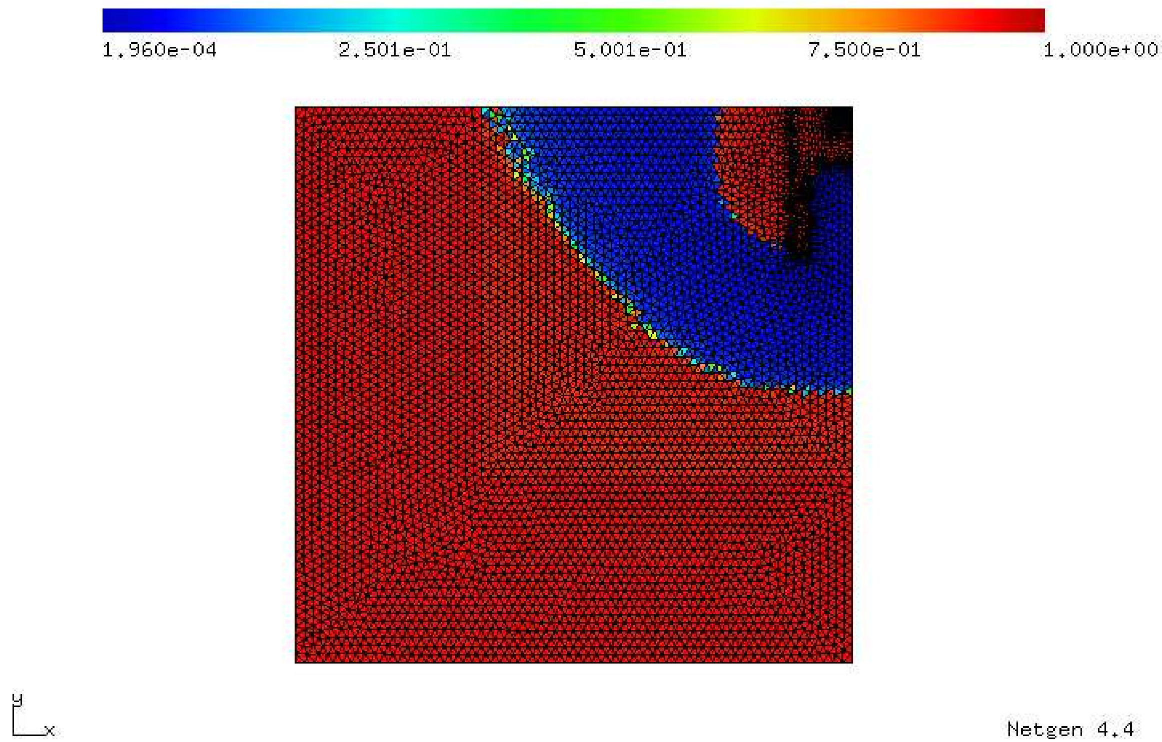

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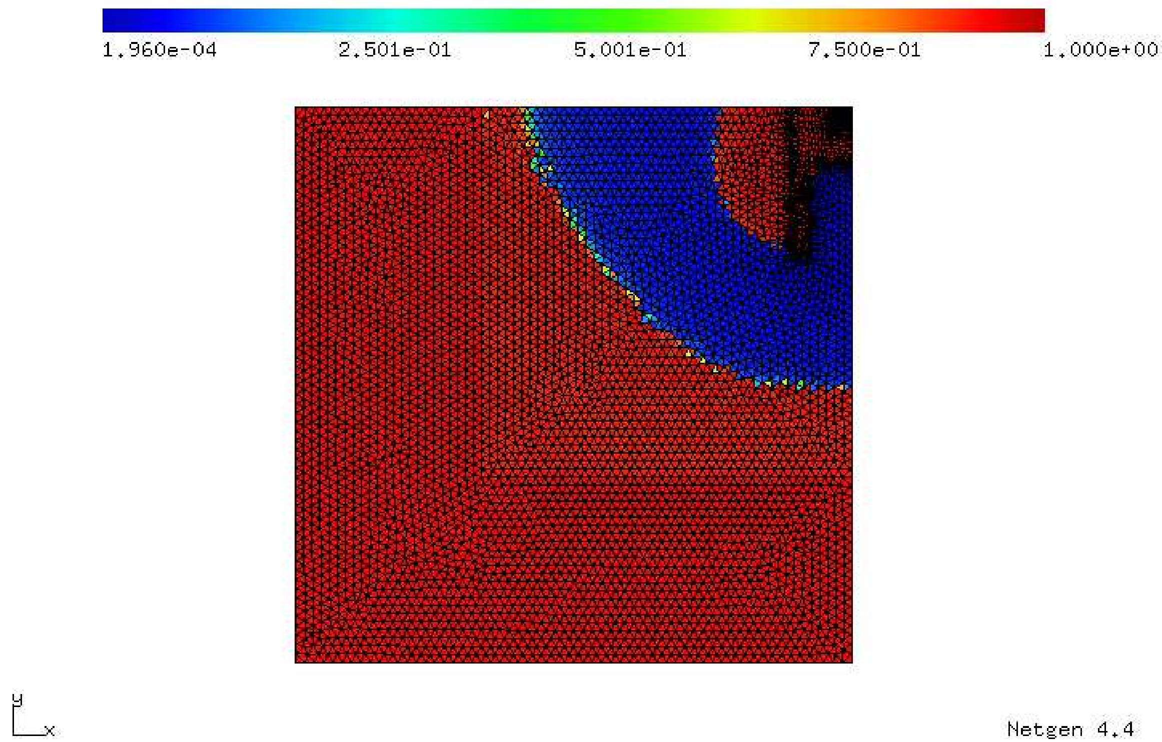

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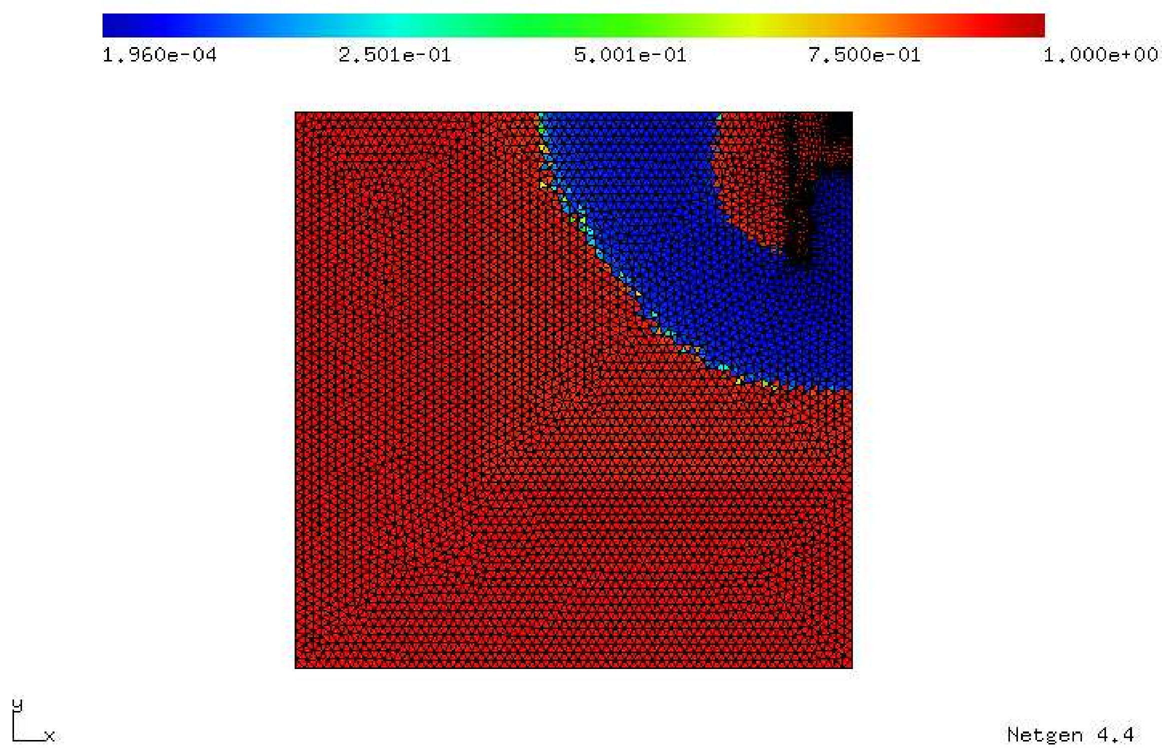

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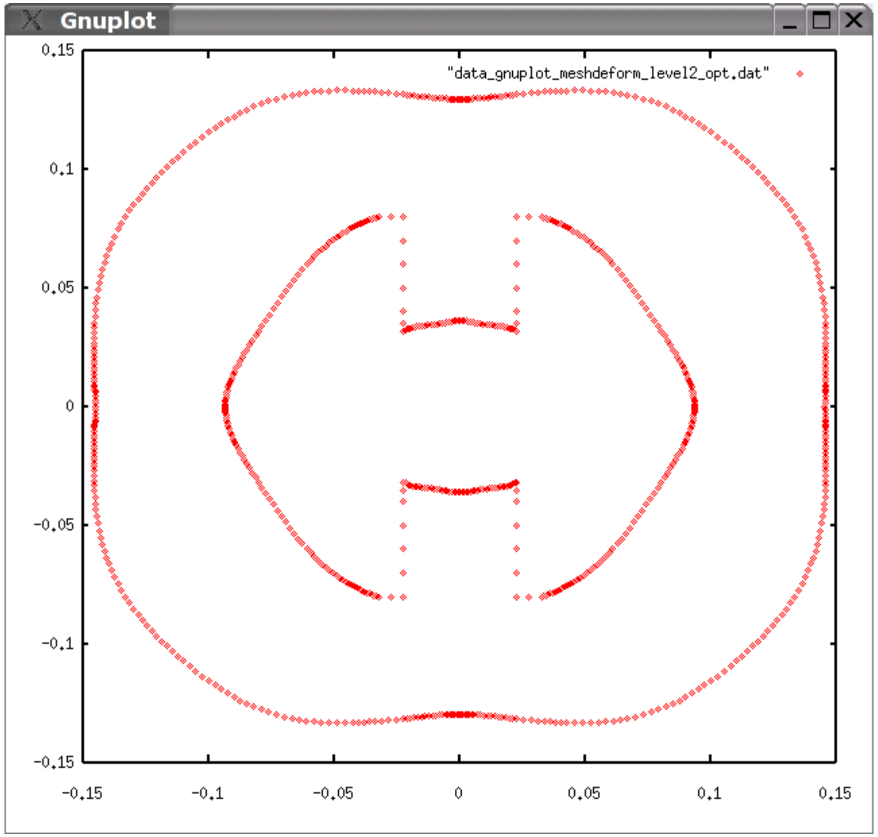

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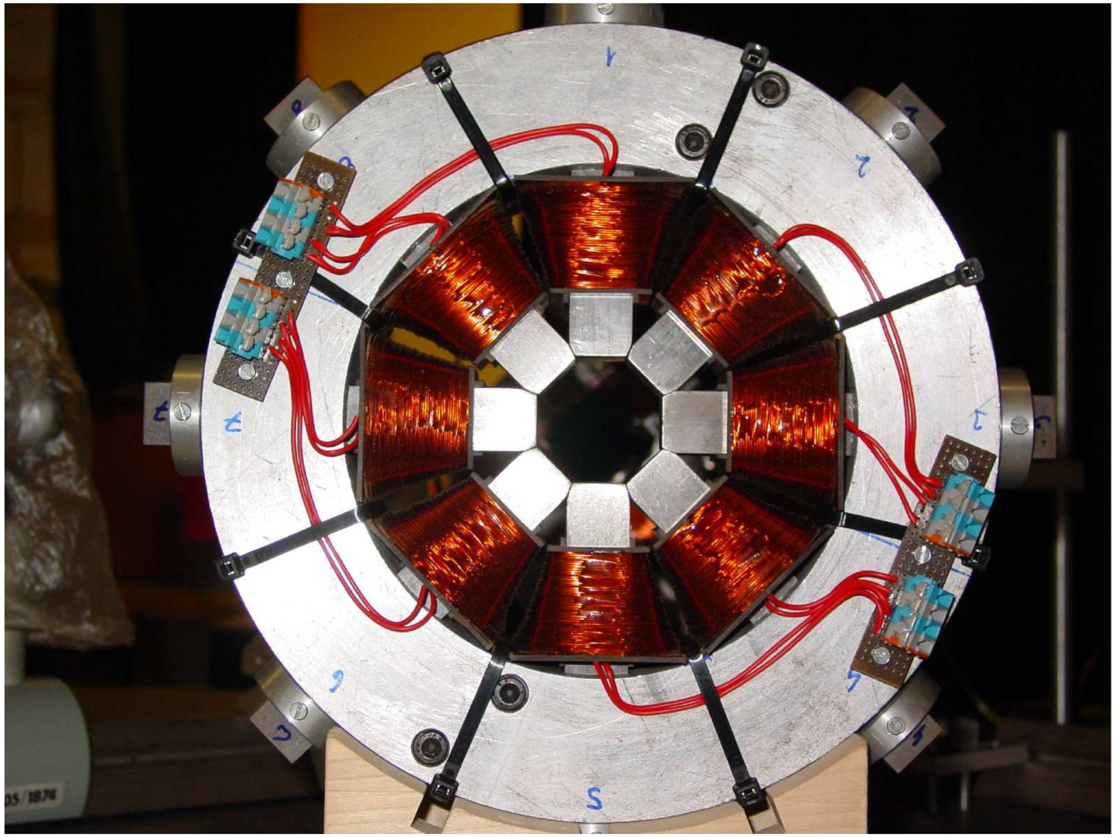

Motivation: Large–scale discretized topology optimization

Topology optimization

$$\min_{q\in Q} J(q,u) \quad \text{subject to} \quad B(q)u = g \text{ na } V'$$

In order to use sequential quadratic programming, we need the Hessian linearization of the functional J.

State elimination

$$\min_{q\in Q}\; J(q, B(q)^{-1}g)$$

Discretizations of the linearized Hessian is large–scale and dense!

Simultaneous (all–at–once) method

$$\min_{(q,u)\in Q\times V}\;\max_{\lambda\in V}\{J(q,u) + \langle B(q)u - g, \lambda\rangle_V\}$$

Discretizations of the linearized Hessian are even bigger, but sparse and well–structured!

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Setting of the Saddle–Point Problem

Saddle–point problem

V, Z …Hilbert spaces,
$(.,.)_V$, $(.,.)_Z$ …inner products, $\langle .,. \rangle_V$, $\langle .,. \rangle_Z$ …duality pairings:

$$\min_{u \in V} h(u) \quad \text{s.t. } Bu = g,$$

where $h(u) := \frac{1}{2}\langle Au, u\rangle_V - \langle f, u\rangle_V$, $A : V \to V'$ linear bounded self–adjoint and positive definite, $B : V \to Z'$ linear and bounded, $f \in V'$, $g \in \text{Range}(B)$.

Lagrange formalism

$p \in Z$ …Lagrange multiplier

$$\min_{u \in V} \max_{p \in Z} \{h(u) + \langle Bu - g, p\rangle_Z\} \quad \text{equivalent to} \quad \begin{pmatrix} A & B^T \\ B & 0 \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix},$$

where $B^T : Z \to V'$ adjoint to B, i.e. $\langle B^T z, v\rangle_V = \langle Bv, z\rangle_Z$.
$\exists! u^* \in V$, $\exists p^* \in Z$. Moreover, if $\text{Kernel}(B^T) = \{0\}$, then $\exists! p^* \in Z$.

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Optimal Uzawa–Type Methods

Symmetric Uzawa methods

$\widehat{A}^{-1}$ ... preconditioner to A, $\widehat{S}^{-1}$ ... preconditioner to Schur complement $S := BA^{-1}B^T$,
α_V, α_Z ... small enough positive damping parameters.

The outer k–th iteration:

$$\begin{aligned} u^{(k+1/2)} &:= u^{(k)} + \alpha_V \widehat{A}^{-1}\left[f - \left(Au^{(k)} + B^T p^{(k)}\right)\right], \\ p^{(k+1)} &:= p^{(k)} + \alpha_Z \widehat{S}^{-1}\left[Bu^{(k+1/2)} - g\right], \\ u^{(k+1)} &:= u^{(k)} + \alpha_V \widehat{A}^{-1}\left[f - \left(Au^{(k)} + B^T p^{(k+1)}\right)\right]. \end{aligned}$$

α_V a α_Z often difficult to find!

The Uzawa method is the outher loop and the inner loop is preconditioning using multigrid and/or PCG.

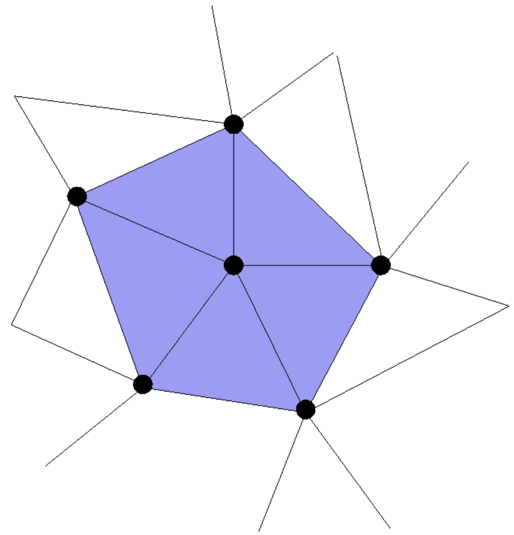
Optimal Uzawa–Type Methods

Schöberl & Zulehner, 2003: Additive multigrid smoother

(V_i), (Z_i) …sequences of FE-subspaces of V and Z, respectively; (P_i), (Q_i) …the corresponding prolongations, i.e. $P_i : V_i \to V$, $Q_i : Z_i \to Z$:

$$u^{(k+1)} := u^{(k)} + \alpha_V \sum_{i=1}^{N} P_i w_i^{(k)},$$

$$p^{(k+1)} := p^{(k)} + \alpha_Z \sum_{i=1}^{N} Q_i r_i^{(k)},$$



where $(w_i^{(k)}, r_i^{(k)})$ is a solution to a local saddle–point subproblem, typically defined around a discret. node:

$$\begin{pmatrix} P_i^T A P_i & P_i^T B^T Q_i \\ Q_i^T B P_i & 0 \end{pmatrix} \begin{pmatrix} w^{(k+1)} \\ r^{(k+1)} \end{pmatrix} = \begin{pmatrix} P_i^T \left[f - A u^{(k)} \right] \\ Q_i^T \left[g - B u^{(k)} \right] \end{pmatrix}.$$

Equivalent to a symmetric Uzawa method.

Multigrid methods

Vanka, 1986: Multiplicative smoother

(V_i), (Z_i) …sequences of FE-subspaces of V and Z; (P_i), (Q_i) …the corresponding prolongations, i.e. $P_i : V_i \to V$, $Q_i : Z_i \to Z$:

$$u^{(k+\frac{i}{N})} := u^{(k+\frac{i-1}{N})} + P_i w_i^{(k+\frac{i}{N})},$$
$$p^{(k+\frac{i}{N})} := p^{(k+\frac{i-1}{N})} + Q_i r_i^{(k+\frac{i}{N})},$$

where

$$\begin{pmatrix} P_i^T A P_i & P_i^T B^T Q_i \\ Q_i^T B P_i & 0 \end{pmatrix} \begin{pmatrix} w^{(k+\frac{i}{N})} \\ r^{(k+\frac{i}{N})} \end{pmatrix} = \begin{pmatrix} P_i^T \left[f - A u^{(k+\frac{i-1}{N})} - B^T p^{(k+\frac{i-1}{N})} \right] \\ Q_i^T \left[g - B u^{(k+\frac{i-1}{N})} \right] \end{pmatrix}.$$

The multiplicative smoother is numerically more efficient than additive, no damping parameters needed, but for saddle–point problems there is no convergence theory!

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Augmented Lagrangians Methods

$h(u) := (1/2)\langle Au, u\rangle_V - \langle f, u\rangle_V$, $\rho \ldots$ positive augmented Lagrange penalty, $\iota_Z : Z \to Z'$ inner product on Z (Riesz isomorphism).

The outer k-th iteration:

Step 1. $u^{(k+1)}$ solves $\min\limits_{u \in V} \left\{ h(u) + \langle Bu - g, p^{(k)}\rangle_Z + \frac{\rho^{(k)}}{2} \|Bu - g\|_{Z'}^2 \right\}$,

Step 2. $p^{(k+1)} := p^{(k)} + \rho^{(k)} \iota_Z^{-1} \left(Bu^{(k+1)} - g \right)$,

Step 3. Increase $\rho^{(k)}$.

Denote:
$L(u, p, \rho) := h(u) + \langle Bu - g, p\rangle_Z + \frac{\rho}{2}\|Bu - g\|_{Z'}^2$ Lagrange functional, $F(u, p, \rho) := \nabla_u L(u, p, \rho) = Au - f + B^T p + \rho B^T \iota_Z^{-1}(Bu - g)$ its Fréchet derivative.

Then, Step 1 is equivalent to

$$\left[A + \rho^{(k)} B^T \iota_Z^{-1} B \right] u^{(k+1)} = f - B^T (p^{(k)} - \iota_Z^{-1} g).$$

Semi–Monotonic Augmented Lagrangians Method

Dostál, 2005: The algorithm

The k-th iteration:

Find $u^{(k+1)} : \|F(u^{(k+1)}, p^{(k)}, \rho^{(k)})\|_{V'} \leq \min\left\{\nu \|Bu^{(k+1)} - g\|_{Z'}, \eta\right\}$ %PCG◯◯MG

if $\|F(u^{(k+1)}, p^{(k)}, \rho^{(k)})\|_{V'} \leq \varepsilon$ and $\|Bu^{(k+1)} - g\|_{Z'} \leq \varepsilon_{\text{feas}}$ **then**

  break

end if

$p^{(k+1)} := p^{(k)} + \rho^{(k)} \iota_Z^{-1}(Bu^{(k+1)} - g)$

if $L(u^{(k+1)}, p^{(k+1)}, \rho^{(k)}) < L(u^{(k)}, p^{(k)}, \rho^{(k)}) + \frac{\rho^{(k)}}{2}\|Bu^{(k+1)} - g\|_{Z'}$ **then**

  $\rho^{(k+1)} := \beta \rho^{(k)}$

else

  $\rho^{(k+1)} := \rho^{(k)}$

end if

$\nu > 0$, $\eta > 0$, $\beta > 1$, $\varepsilon > 0$, $\varepsilon_{\text{feas}} > 0$ and where $\|Bu - g\|_{Z'} := \sqrt{\left\langle Bu - g, \iota_Z^{-1}(Bu - g)\right\rangle_Z}$ a $\|F(u,p,\rho)\|_{V'} := \sqrt{\left\langle F(u,p,\rho), \iota_V^{-1} F(u,p,\rho)\right\rangle_V}$.

Semi–Monotonic Augmented Lagrangians Method

Dostál, 2005: Analysis

1. The number of the outer iterations is bounded:

$$k \leq \left(\frac{(1+s)\eta^2 + \|f\|_{V'}^2}{\lambda \rho^{(0)}} + \rho^{(0)} \|g\|_{Z'}^2 \right) / \min{}^2 \{\nu\varepsilon, \varepsilon_{\text{feas}}\} =: k_{\max},$$

where $\lambda > 0$ is the smallest eigenvalue of A, $s > 0$ is the smallest integer so that $\beta^s \rho^{(0)} \geq \frac{\nu^2}{\lambda}$.

2. The augmented Lagrange parameter is bounded

$$\rho^{(k)} \leq \beta^s \rho^{(0)} < \frac{\beta \nu^2}{\lambda} =: \rho_{\max}.$$

Consequently, we have the uniform spectral equivalence

$$\forall k : A + \rho^{(k)} B^T M^{-1} B \approx A,$$

since $\forall v \in V : \lambda(v,v)_V \leq \left(\|A\|_{V'}^2 + \rho_{\max} \|B^T M^{-1} B\|_{V'}^2 \| \right) (v,v)_V$ and $\|v\|_A \approx \|v\|_V$.

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Multigrid Preconditioned Augmented Lagrangians Method

Implementation

requires only the following changes:

- In PCG (step 1) we use the preconditioner $\widehat{A}^{-1}$.
- Each occurences of ι_V^{-1} and ι_Z^{-1} are replaced by $\widehat{A}^{-1}$ a $\widehat{M}^{-1}$, respectively.
- The norms are calculated as follows:

$$\|Bu-g\|_{\widehat{Z}'} := \sqrt{(Bu-g)^T \cdot \widehat{M}^{-1} \cdot (Bu-g)}$$

and

$$\|\widetilde{F}(u,p,\widehat{\rho})\|_{\widehat{V}'} := \sqrt{\widetilde{F}(u,p,\widehat{\rho})^T \cdot \widehat{A}^{-1} \cdot \widetilde{F}(u,p,\widehat{\rho})}.$$

Then, $\lambda_{\min}\left(\widehat{A}_{\frac{1}{2}}^{-1} A \widehat{A}_{\frac{1}{2}}^{-T}\right) \approx 1$, $\operatorname{cond}\left(\widehat{A}_{\frac{1}{2}}^{-1} A \widehat{A}_{\frac{1}{2}}^{-T}\right) \approx 1$ yields an optimal method.

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An Application to the Stokes Problem

The Stokes problem

$\Omega \subset \mathbb{R}^2$ ... bounded polygonal computational domain, $\mathbf{f} \in [L^2(\Omega)]^2$

$$\begin{aligned} -\triangle \mathbf{u} + \boldsymbol{\nabla} p = \mathbf{f} &\quad \text{in } \Omega, \\ \operatorname{div} \mathbf{u} = 0 &\quad \text{in } \Omega, \\ \mathbf{u} = \mathbf{0} &\quad \text{on } \partial\Omega. \end{aligned}$$

Fitting to our framework

$$V := [H_0^1(\Omega)]^2, \quad Z := L^2(\Omega), \quad \langle A\mathbf{u}, \mathbf{v}\rangle_V := \int_\Omega \sum_{i=1}^{2} \boldsymbol{\nabla} u_i \cdot \boldsymbol{\nabla} v_i \, d\mathbf{x},$$

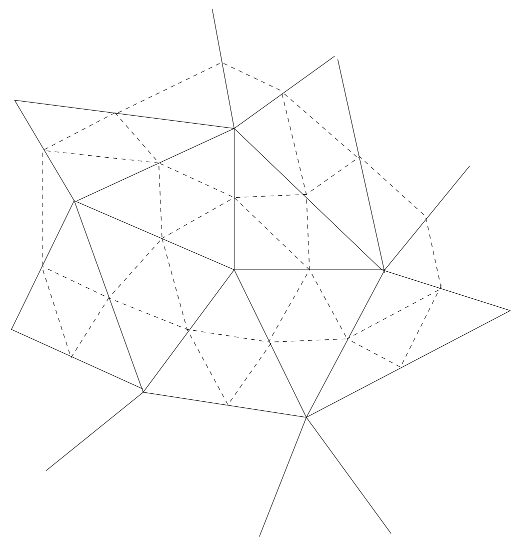
$$\langle b, \mathbf{v}\rangle_V := \int_\Omega \mathbf{f} \cdot \mathbf{v} d\mathbf{x}, \quad \langle B\mathbf{u}, z\rangle_Z := \int_\Omega \operatorname{div} \mathbf{u} \, z \, d\mathbf{x}.$$

Thus, A is a tensor product Laplacian and M is the L^2–inner product.

An Application to the Stokes Problem

FE–multigrid discretization

$(\mathcal{T}_l)$ . . . a nested sequence of triangulations of Ω



Crouzeix–Raviart elements

A nonnested sequence of FE–spaces:

$$V_l := \Big\{ v \in \left[L^2(\Omega)\right]^2 : v|_T \text{ is linear for all } T \in \mathcal{T}_l,$$
$$v \text{ is continuous at the midpoints of interelement boundaries}$$
$$\text{and } v = 0 \text{ along } \partial\Omega \Big\},$$
$$Z_l := \left\{ z \in L^2(\Omega) : z|_T \text{ is constant for all } T \in \mathcal{T}_l \right\}.$$

An Application to the Stokes Problem

Brenner, 1993: Multigrid preconditioning

Smoothers: multilevel diagonal scaling for $\widehat{A_l^{-1}}$, $M_l^{-1} = [\mathrm{diag}(M_l)]^{-1}$

Prolongations: $I_{l-1}^l : V_{l-1} \times Z_{l-1} \to V_l \times Z_l$ given by

$$I_{l-1}^l(v, z) := (J_{l-1}^l v, z)$$

with

$$J_{l-1}^l v(m_e) := \begin{cases} v(m_e) & \text{if } m_e \in \operatorname{int} T \text{ for some } T \in \mathcal{T}_{l-1} \\ \frac{1}{2}\left[v|_{T_1} + v|_{T_2}\right] & \text{if } e \subset T_1 \cap T_2 \text{ for some } T_1, T_2 \in \mathcal{T}_{l-1} \end{cases}$$

at midpoints m_e of internal edges e in $\mathcal{T}_l$.

An Application to the Stokes Problem

Numerical results

$\Omega := (-1,1)\times(-1,1)$, $\mathbf{f}(x_1,x_2) := \operatorname{sign}(x_1)\operatorname{sign}(x_2)\,(1,1)$, $\mathbf{u}^{(0)} := \mathbf{0}$, $p^{(0)} := 0$
3 pre– and 3 post–smoothing steps, $\varepsilon/\varepsilon^{(0)} = \varepsilon_{\text{feas}}/\varepsilon_{\text{feas}}^{(0)} = 10^{-3}$:

level l	$\dim V_l$	$\dim Z_l$	point additive smoother		block multiplicative smoother	
			outer/PCG **iterations**	**total PCG iterations**	**outer**/PCG **iterations**	**total PCG iterations**
1	56	32	**6**/1,0,1,2,4,8	**16**	**6**/1,0,1,2,4,8	**16**
2	208	128	**6**/1,0,1,4,16,30	**52**	**6**/1,0,1,2,5,13	**22**
3	800	512	**5**/1,1,4,20,41	**67**	**6**/1,0,1,2,5,14	**23**
4	3136	2048	**5**/1,1,3,16,47	**68**	**6**/1,0,1,2,6,14	**24**
5	12416	8192	**5**/1,1,3,17,50	**72**	**6**/1,0,1,2,6,15	**25**
6	49408	32768	**5**/1,1,3,19,54	**77**	**6**/1,0,1,2,6,16	**26**

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Outlook: Applications in Topology Optimization

$$\min_{q \in Q} J(q,u) \quad \text{s.t.} \quad A(q,u) = b \text{ on } V'$$

Nested approach

$$q^* := \arg\min_{q \in Q} J(q, u(q)), \text{ where } A(q, u(q)) = b \text{ on } V'$$

The Hessian is dense!

All–at–once approach

$$\min_{(q,u) \in Q \times V} \max_{\lambda \in V} \{ J(q,u) + \langle \lambda, A(q,u) - b \rangle \}$$

The Hessian is bigger, but sparse and well–structured!

Outlook: Applications in Topology Optimization

Burger & Mühlhuber, 2002: All–at–once parameter identification

$$\min_{q \in L^2(\Omega)} \frac{1}{2}\|\nabla u - \mathbf{B}_{\text{given}}\|^2_{L^2(\Omega)} + \frac{1}{2}\|q\|^2_{L^2(\Omega)} \quad \text{s.t.} \quad -\operatorname{div}(q\nabla u) = f \text{ in } H^1_0(\Omega)'$$

Leads to a sequence of

$$\begin{pmatrix} I & 0 & \text{sym.} \\ 0 & -\triangle & \text{sym.} \\ -\operatorname{div}(\cdot\nabla u^{(k)}) & -\operatorname{div}(q^{(k)}\nabla\cdot) & 0 \end{pmatrix} \begin{pmatrix} \delta q^{(k)} \\ \delta u^{(k)} \\ \delta\lambda^{(k)} \end{pmatrix} = \begin{pmatrix} \cdot \\ \cdot \\ \cdot \end{pmatrix}$$

$$\begin{aligned} q^{(k+1)} &:= q^{(k)} + \delta q^{(k)} \\ u^{(k+1)} &:= u^{(k)} + \delta u^{(k)} \\ \lambda^{(k+1)} &:= \lambda^{(k)} + \delta\lambda^{(k)} \end{aligned}$$

Outlook: Applications in Topology Optimization

All–at–once topology optimization

$$\min_{q\in L^2(\Omega)} \frac{1}{2}\|\nabla u - \mathbf{B}_{\text{given}}\|^2_{L^2(\Omega)} + \frac{1}{2}\|q\|^2_{L^2(\Omega)} \quad \text{s.t.} \quad -\operatorname{div}(\nu(q)\nabla u) = f \text{ in } H^1_0(\Omega)'$$

Leads to a sequence of

$$\begin{pmatrix} I + \langle \lambda^{(k)}, A''_{qq}(q^{(k)}, u^{(k)})(\cdot)\rangle & \text{sym.} & \text{sym.} \\ \langle \lambda^{(k)}, A''_{uq}(q^{(k)}, u^{(k)})(\cdot)\rangle & -\triangle + \langle \lambda^{(k)}, A''_{uu}(q^{(k)}, u^{(k)})(\cdot)\rangle & \text{sym.} \\ -\operatorname{div}(\nu'_q(q^{(k)})(\cdot)\nabla u^{(k)}) & -\operatorname{div}(\nu(q^{(k)})\nabla\cdot) & 0 \end{pmatrix} \begin{pmatrix} \delta q^{(k)} \\ \delta u^{(k)} \\ \delta\lambda^{(k)} \end{pmatrix} = \begin{pmatrix} \cdot \\ \cdot \\ \cdot \end{pmatrix}$$

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