Preconditioning semismooth Newton methods for optimal control problems with *L*<sup>1</sup>- sparsity and control constraints

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Joint work with Valeria Simoncini - Università di Bologna Martin Stoll - MPI Magdeburg

Roma - 24 Gennaio 2018

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Numerical experiments

## The Constrained Optimal Control Problem

$$\begin{array}{ll} \min & J(y,u) = \frac{1}{2} \|y - y_d\|_{L^2(\Omega)}^2 + \frac{\alpha}{2} \|u\|_{L^2(\Omega)}^2 + \beta \|u\|_{L^1(\Omega)} \leftarrow \text{ sparsity constr.} \\ & \text{over } (y,u) \in H_0^1(\Omega) \times L^2(\Omega) \\ \\ \text{s.t.} & \mathcal{L}y = u \quad \text{in } \Omega & \leftarrow \text{ state equation} \\ & \text{and} & a \leq u \leq b \text{ a.e. in } \Omega & \leftarrow \text{ box constraints} \end{array}$$

- u and y are the control and state variables
- $y_d \in L^2(\Omega)$  is the desired state,  $\Omega \subseteq \mathbb{R}^d$  with d=2,3
- $\blacktriangleright~\mathcal{L}$  is a second-order linear elliptic differential operator
- Control box constraints:  $a, b \in L^2(\Omega)$  and a < 0 < b
- ▶ Parameters: L<sup>2</sup>-norm term  $\alpha > 0$  and L<sup>1</sup>-norm term  $\beta > 0$ .

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## Sparsity constraints in optimal control problems

#### Motivation

 Optimal control applications: provide information about the optimal location of control device and actuators [Stadler, COAP 2009] [Costa et al. Comput. Struct. 2007].

#### Main references:

- ▶ L<sup>1</sup>-norm: Casas, Clacson, Kunish, Herzog, Stadler, Wachsmuth, 2009-2012
- ▶ Directional Sparsity  $\|\cdot\|_{1,2}$  Herzog, Stadler and Wachsmuth SICON 2012.

based on semismooth Newton's approach [Hintermüller, Ito, Kunish SIOPT 2002].

None of these works takes into account discretization/implementation issues for the linear algebra phase (e.g. preconditioning).

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## Box constraints: optimality conditions (simple case)

Box constrained optimization problem

$$\min f(x)$$
 s.t.  $x \ge a$ 

where  $f : \mathbb{R}^n \to \mathbb{R}$ .

The first order optimality conditions are



where the last complementarity conditions can be restated as

$$c\mu - \min(0, (x - a) + c\mu)) = 0, \quad c > 0.$$

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KKT conditions

## L<sup>1</sup> sparsity constraint: optimality conditions (simple case)

 $\ell_1$  optimization problem and a constrained problem

$$\min_{x \in \mathbb{R}^n} f(x) + \frac{\beta \|x\|_1}{n}, \quad \Leftrightarrow \quad \min_x f(x) \text{ s.t. } \|x\|_1 \le \hat{\beta},$$
  
where  $f : \mathbb{R}^n \to \mathbb{R}, \ \beta, \hat{\beta} \in \mathbb{R}^+, \ \|x\|_1 = \sum_{i=1}^n |x_i|.$ 

The first order optimality conditions are

$$\nabla f(x) = \begin{cases} = -\beta, & x > 0\\ \in [-\beta, \beta], & x = 0\\ = \beta, & x < 0 \end{cases} \Leftrightarrow \begin{cases} \nabla f(x) = -\mu\\ \mu = \beta, & x > 0\\ |\mu| \le \beta, & x = 0\\ \mu = -\beta, & x < 0 \end{cases}$$

where the last complementarity conditions can be restated as

$$x-\max(0,x+c(\mu-eta))-\min(0,x+c(\mu+eta))=0, \quad c>0.$$

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where the last complementarity conditions can be restated as

$$x - \max(0, x + c(\mu - eta)) - \min(0, x + c(\mu + eta)) = 0, \quad c > 0.$$

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## Optimality conditions

#### The KKT system [Stadler COAP 2009]

The solution  $(\bar{y}, \bar{u}) \in H_0^1(\Omega) \times L^2(\Omega)$  of the optimal control problem is characterized by the existence of  $(\bar{p}, \bar{\mu}) \in H_0^1(\Omega) \times L^2(\Omega)$  such that

$$\begin{split} \mathcal{L}y - u &= 0 \\ \mathcal{L}^* \bar{p} + \bar{y} - y_d &= 0 \\ -\bar{p} + \alpha \bar{u} + \bar{\mu} &= 0 \end{split}$$
$$F(u, \mu) &:= \bar{u} - \max(0, \bar{u} + c(\bar{\mu} - \beta)) - \min(0, \bar{u} + c(\bar{\mu} + \beta)) \\ + \max(0, (\bar{u} - b) + c(\bar{\mu} - \beta)) + \min(0, (\bar{u} - a) + c(\bar{\mu} + \beta)) = 0 \text{ a.e. in } \Omega, \end{split}$$

with c > 0.

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0

► The complementarity function F is nonlinear and semismooth ⇒ SemiSmooth Newton's method (SSN) for the KKT system, i.e. a Newton's method where the Jacobian of the system is obtained using generalized derivatives.



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## The discretized (FE) optimality system (KKT)

Let 
$$\Theta : \mathbb{R}^{4n} \to \mathbb{R}^{4n}$$
 and  $x = (y, u, p, \mu) \in \mathbb{R}^{4n}$ :

$$\Theta(x) = \begin{bmatrix} \Theta(x)^{y} \\ \Theta(x)^{u} \\ \Theta(x)^{p} \\ \Theta(x)^{\mu} \end{bmatrix} \stackrel{\text{def}}{=} \begin{bmatrix} My + L^{T}p - My_{d} \\ \alpha Mu - \bar{M}^{T}p + M\mu \\ Ly - \bar{M}u - f \\ MF(u, \mu) \end{bmatrix} = 0$$

and the complementarity function  $F : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$  is component-wise defined by

$$F(u,\mu) = u - \max(0, u + c(\mu - \beta)) - \min(0, u + c(\mu + \beta)) + \max(0, (u - b) + c(\mu - \beta)) + \min(0, (u - a) + c(\mu + \beta)), c > 0$$

- n: dimension of the discretized space.
- L: stiffness matrix (possibly unsym); M: mass matrix (lumped)
- $\overline{M}$ : discretization of the control term within the PDE-constraint (unsym).

 $\star$  Since M is diag, componentwise complementarity conditions still hold with FE.

The semismooth Newton's method

## Illustration of the Active-Set (AS) interpretation





- $u_i = 0$  for  $i \in A_0$  (sparsity);
- $u_i = a$  for  $i \in A_a$  (lower bound);
- $u_i = b$  for  $i \in A_b$  (upper bound);

- $\mu_i = -\beta$  for  $i \in \mathcal{I}_-$  (unc.); •  $\mu_i = \beta$  for  $i \in \mathcal{I}_+$  (unc.).
- ▶ Sparse control is expected at the solution (e.g. for not so small values of  $\beta$ ) ⇒ large size of  $\mathcal{A}_0$ ;

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#### Active-Set approach definition

Complementarity function:

$$F(u, \mu) = u - \max(0, u + c(\mu - \beta)) - \min(0, u + c(\mu + \beta)) + \max(0, (u - b) + c(\mu - \beta)) + \min(0, (u - a) + c(\mu + \beta))$$

• Sets of Active  $\mathcal{A} = \mathcal{A}_b \cup \mathcal{A}_a \cup \mathcal{A}_0$  and inactive  $\mathcal{I} = \mathcal{I}_+ \cup \mathcal{I}_-$  constraints

$$\begin{aligned} \mathcal{A}_{b} &= \{i \mid c(\mu_{i} - \beta) + (u_{i} - b_{i}) > 0\} \\ \mathcal{A}_{a} &= \{i \mid c(\mu_{i} + \beta) + (a_{i} - u_{i}) < 0\} \\ \mathcal{A}_{0} &= \{i \mid u_{i} + c(\mu_{i} + \beta) \ge 0\} \cup \{i \mid u_{i} + c(\mu_{i} - \beta) \le 0\} \end{aligned}$$

$$\begin{aligned} \mathcal{I}_+ &= \{i \mid u_i + c(\mu_i - \beta) > 0\} \cup i \mid c(\mu_i - \beta) + (u_i - b_i) \le 0\} \\ \mathcal{I}_- &= \{i \mid u_i + c(\mu_i + \beta) < 0\} \cup \{i \mid c(\mu_i + \beta) + (u_i - a_i) \ge 0\}. \end{aligned}$$

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#### Active-Set approach definition

Complementarity function: 

$$F(u, \mu) = u - \max(0, u + c(\mu - \beta)) - \min(0, u + c(\mu + \beta)) + \max(0, (u - b) + c(\mu - \beta)) + \min(0, (u - a) + c(\mu + \beta))$$

▶ Sets of Active  $A = A_b \cup A_a \cup A_0$  and inactive  $I = I_+ \cup I_-$  constraints

$$\begin{aligned} \mathcal{A}_{b} &= \{i \mid c(\mu_{i} - \beta) + (u_{i} - b_{i}) > 0\} \\ \mathcal{A}_{a} &= \{i \mid c(\mu_{i} + \beta) + (a_{i} - u_{i}) < 0\} \\ \mathcal{A}_{0} &= \{i \mid u_{i} + c(\mu_{i} + \beta) \ge 0\} \cup \{i \mid u_{i} + c(\mu_{i} - \beta) \le 0\} \end{aligned}$$

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 $\downarrow$ 

$$F(u,\mu) = \prod_{\mathcal{A}_0} u + \prod_{\mathcal{A}_b} (u-b) + \prod_{\mathcal{A}_a} (u-a) - c(\prod_{\mathcal{I}_+} (\mu-\beta) + \prod_{\mathcal{I}_-} (\mu+\beta))$$

 $\Pi_{\mathcal{C}}$  0-1 diagonal matrix with 1's corresponding to  $\mathcal{C}$ .

The semismooth Newton's method

#### Generalized Jacobian:

$$F(u,\mu) = \underbrace{\Pi_{\mathcal{A}_0} u + \Pi_{\mathcal{A}_b}(u-b) + \Pi_{\mathcal{A}_a}(u-a)}_{u,\mathcal{A}} \underbrace{-c(\Pi_{\mathcal{I}_+}(\mu-\beta) + \Pi_{\mathcal{I}_-}(\mu+\beta))}_{\mu,\mathcal{I}} = 0$$
  
Generalized derivative:  $F'(u,\mu) = \begin{bmatrix} \Pi_{\mathcal{A}} & -c\Pi_{\mathcal{I}} \end{bmatrix}$ 

$$\underbrace{\begin{bmatrix} M & 0 & L^{T} & 0 \\ 0 & \alpha M & -\bar{M}^{T} & M \\ L & -\bar{M} & 0 & 0 \\ 0 & \Pi_{\mathcal{A}_{k}} M & 0 & -c\Pi_{\mathcal{I}_{k}} M \end{bmatrix}}_{\Theta_{k}^{\mu}} \begin{bmatrix} \Delta_{y} \\ \Delta_{u} \\ \Delta_{p} \\ \Delta_{\mu} \end{bmatrix} = - \begin{bmatrix} \Theta_{k}^{y} \\ \Theta_{k}^{u} \\ \Theta_{k}^{\mu} \\ \Theta_{k}^{\mu} \end{bmatrix}$$



The semismooth Newton's method

#### Generalized Jacobian:

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Generalized derivative:  $F'(u,\mu) = \begin{bmatrix} \Pi_{\mathcal{A}} & -c\Pi_{\mathcal{I}} \end{bmatrix}$ 

#### SemiSmooth Newton's method (SSN)

Given the current iterate  $x_k = (y_k, u_k, p_k, \mu_k)$ , a SSN step is

$$\underbrace{\begin{bmatrix} M & 0 & L^{T} & 0 \\ 0 & \alpha M & -\bar{M}^{T} & M \\ L & -\bar{M} & 0 & 0 \\ 0 & \Pi_{\mathcal{A}_{k}} M & 0 & -c\Pi_{\mathcal{I}_{k}} M \end{bmatrix}}_{\Theta'(x_{k})} \begin{bmatrix} \Delta y \\ \Delta u \\ \Delta p \\ \Delta \mu \end{bmatrix} = - \begin{bmatrix} \Theta_{k}^{y} \\ \Theta_{k}^{u} \\ \Theta_{k}^{\mu} \\ \Theta_{k}^{\mu} \end{bmatrix}.$$

 $\Theta'(x_k)$  is unsymmetric and of dimension  $(4n \times 4n)$ .

From now on,  $P_{\mathcal{C}}$  is the projection on the subspace defined by the set  $\mathcal{C}$  and  $\Pi_{\mathcal{C}} = P_{\mathcal{C}}^T P_{\mathcal{C}}.$ 

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## Saddle-point symmetric formulations of the Newton's equation

• Augmented form  $4 \times 4 (3n + |A_k|) \times (3n + |A_k|)$ 

$$\begin{bmatrix} M & 0 & L^{T} & 0 \\ 0 & \alpha M & -\bar{M}^{T} & MP_{\mathcal{A}_{k}}^{T} \\ L & -\bar{M} & 0 & 0 \\ 0 & P_{\mathcal{A}_{k}}M & 0 & 0 \end{bmatrix} \begin{bmatrix} \Delta y \\ \Delta u \\ \Delta p \\ (\Delta \mu)_{\mathcal{A}_{k}} \end{bmatrix} = -\begin{bmatrix} \Theta_{k}^{y} \\ \tilde{\Theta}_{k}^{\mu} \\ \Theta_{k}^{\mu} \end{bmatrix} \quad \Leftrightarrow \quad J_{k}^{aug} \Delta x^{aug} = b_{k}^{aug}$$

with  $(\mu_{k+1})_{(\mathcal{I}_+)_{k+1}} = \beta$  and  $(\mu_{k+1})_{(\mathcal{I}_-)_{k+1}} = -\beta$ .

• Reduced form  $2 \times 2$   $(2n \times 2n)$ 

$$\begin{bmatrix} M & L^{T} \\ L & -\frac{1}{\alpha}\bar{M}M^{-1}\Pi_{\mathcal{I}_{k}}\bar{M}^{T} \end{bmatrix} \begin{bmatrix} \Delta y \\ \Delta p \end{bmatrix} = -\begin{bmatrix} \Theta_{k}^{Y} \\ \hat{\Theta}_{k}^{P} \end{bmatrix} \quad \Leftrightarrow \quad J_{k}^{red}\Delta x^{red} = b_{k}^{red}$$

with

$$\Delta u = \frac{1}{\alpha} (M^{-1} \bar{M}^T \Delta p - P_{\mathcal{A}_k}^T (\Delta \mu)_{\mathcal{A}_k} - M^{-1} \tilde{\Theta}_k^u),$$
  
$$(\Delta \mu)_{\mathcal{A}_k} = P_{\mathcal{A}_k} M^{-1} \Pi_{\mathcal{A}_k} \bar{M}^T \Delta p - \alpha P_{\mathcal{A}_k} M^{-1} P_{\mathcal{A}_k}^T \left( \Theta_k^\mu + \frac{1}{\alpha} P_{\mathcal{A}_k} \tilde{\Theta}_k^u \right)$$

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$$\begin{bmatrix} M & 0 & L^{T} & 0 \\ 0 & \alpha M & -\bar{M}^{T} & MP_{\mathcal{A}_{k}}^{T} \\ L & -\bar{M} & 0 & 0 \\ 0 & P_{\mathcal{A}_{k}}M & 0 & 0 \end{bmatrix} \begin{bmatrix} \Delta y \\ \Delta u \\ \Delta p \\ (\Delta \mu)_{\mathcal{A}_{k}} \end{bmatrix} = -\begin{bmatrix} \Theta_{k}^{y} \\ \tilde{\Theta}_{k}^{u} \\ \Theta_{k}^{p} \\ \tilde{\Theta}_{k}^{\mu} \end{bmatrix} \quad \Leftrightarrow \quad J_{k}^{aug} \Delta x^{aug} = b_{k}^{aug}$$

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#### Preconditioning the sequence of Newton equations

$$J_k(x_k)\Delta x = b_k$$
 (\*)

where  $J_k$  ( $J_k^{aug}$  or  $J_k^{red}$ ) is a saddle point matrix.

► Assume that Krylov subspace methods are used to solve the large and sparse Newton equations ⇒ preconditioning is mandatory.

#### Objective

Find effective optimal and robust preconditioners for the Newton equations for general box/sparsity constraints such that the number of iterations required to solve (\*) is low and (roughly) independent of the problem parameters:

- regularization parameters:  $\alpha$  ( $L^2$ ) and  $\beta$  ( $L^1$ );
- mesh size h

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#### Some background

#### Preconditioner

Given a system Ax = b, find a matrix  $P \approx A$  such that

$$P^{-1}Ax = P^{-1}b$$

is "easier" to solve than the original system by an iterative method  $\Rightarrow P^{-1}A$  has 'better" spectral properties than A.

Saddle-point matrix and its block-triangular factorization:

$$H = \begin{bmatrix} A & B^T \\ B & -C \end{bmatrix} = \begin{bmatrix} I & 0 \\ BA^{-1} & I \end{bmatrix} \begin{bmatrix} A & 0 \\ 0 & -S \end{bmatrix} \begin{bmatrix} I & A^{-1}B^T \\ 0 & I \end{bmatrix}$$

where  $S = (C + BA^{-1}B^{T})$  is the Schur complement of A in H.

- ▶ If  $A \succeq 0$ , B full rank,  $C \succ 0$   $(S \succ 0) \Rightarrow \Lambda(H) = \Lambda(A) \cup \Lambda(-S)$  (indefinite)
- ▶ If  $A \succeq 0$ , B full rank,  $C = 0 \Rightarrow S \succeq 0$ ; If  $ker(A) \cap ker(B) = \emptyset \Rightarrow H$  is nonsingular.

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Approximating the Schur complement

# Matching Schur complement approximations: the unconstrained case

$$J = \begin{bmatrix} M & 0 & -L^T \\ 0 & \alpha M & M \\ \hline -L & M & 0 \end{bmatrix}$$

• J does not depends on k (corresponds to  $A_k = \emptyset$ ).

Schur complement:

$$S = \alpha L M^{-1} L^T + M = \underbrace{(\sqrt{\alpha}L + M)M^{-1}(\sqrt{\alpha}L + M)^T}_{\hat{S}} - 2\sqrt{\alpha}L$$

• Approximation:  $S \approx (\sqrt{\alpha}L + M)M^{-1}(\sqrt{\alpha}L + M)^T$ 

Optimal bounds:

$$\lambda(\hat{S}^{-1}S) \in \left[rac{1}{2}, 1
ight]$$

independence on  $\alpha$  [Pearson and Wathen, NLAA 2012]

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Approximating the Schur complement

## The active-set Schur complement of $J^{aug}$

#### Augmented form

$$J_{k}^{aug} = \begin{bmatrix} M & 0 & L^{T} & 0 \\ 0 & \alpha M & -\bar{M}^{T} & MP_{\mathcal{A}}^{T} \\ \hline L & -\bar{M} & 0 & 0 \\ 0 & P_{\mathcal{A}}M & 0 & 0 \end{bmatrix} = \begin{bmatrix} J_{11} & J_{21}^{T} \\ J_{21} & 0 \end{bmatrix}$$

#### Matching strategy in the general case

$$\mathbf{S} = J_{21}J_{11}^{-1}J_{21}^{T} = \frac{1}{\alpha} \begin{bmatrix} I & -\bar{M}\Pi_{\mathcal{A}}M^{-1}P_{\mathcal{A}}^{T} \\ 0 & I \end{bmatrix} \begin{bmatrix} \mathbb{S} & 0 \\ 0 & P_{\mathcal{A}}MP_{\mathcal{A}}^{T} \end{bmatrix} \begin{bmatrix} I & 0 \\ -P_{\mathcal{A}}M^{-1}\Pi_{\mathcal{A}}\bar{M}^{T} & I \end{bmatrix},$$

where S is the Schur complement of S,

$$\mathbb{S} = \alpha L M^{-1} L^T + \bar{M} (I - \Pi_{\mathcal{A}}) M^{-1} \bar{M}^T$$

• If 
$$\mathcal{A} = \emptyset$$
 and  $\overline{M} = M$ ,  $\mathbb{S} = \alpha L M^{-1} L^T + M$ 

From now on the index *k* is omitted.



Preconditioning the Newton equations 0 = 0 = 0 = 0

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## The active-set Schur complement of $J^{aug}$

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#### Matching strategy in the general case

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• If 
$$\mathcal{A} = \emptyset$$
 and  $\overline{\mathcal{M}} = \mathcal{M}$ ,  $\mathbb{S} = \alpha L \mathcal{M}^{-1} L^T + \mathcal{M}$ 

From now on the index k is omitted.



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Approximating the Schur complement

## Approximating the AS Schur complement

The active-set Schur complement of  $J^{aug}$ 

$$\mathbf{S} = \frac{1}{\alpha} \begin{bmatrix} I & -\bar{M}\Pi_{\mathcal{A}}M^{-1}P_{\mathcal{A}}^{T} \\ \mathbf{0} & I \end{bmatrix} \begin{bmatrix} \mathbb{S} & \mathbf{0} \\ \mathbf{0} & P_{\mathcal{A}}MP_{\mathcal{A}}^{T} \end{bmatrix} \begin{bmatrix} I & \mathbf{0} \\ -P_{\mathcal{A}}M^{-1}\Pi_{\mathcal{A}}\bar{M}^{T} & I \end{bmatrix},$$

where S is the Schur complement of S,

$$\mathbb{S} = \alpha L M^{-1} L^T + \bar{M} (I - \Pi_{\mathcal{A}}) M^{-1} \bar{M}^T$$

The active-set Schur complement approximation

$$\widehat{\mathbf{S}} = \frac{1}{\alpha} \begin{bmatrix} I & -\bar{M}\Pi_{\mathcal{A}}M^{-1}P_{\mathcal{A}}^{\mathsf{T}} \\ 0 & I \end{bmatrix} \begin{bmatrix} \widehat{\mathbf{S}} & 0 \\ 0 & P_{\mathcal{A}}MP_{\mathcal{A}}^{\mathsf{T}} \end{bmatrix} \begin{bmatrix} I & 0 \\ -P_{\mathcal{A}}M^{-1}\Pi_{\mathcal{A}}\bar{M}^{\mathsf{T}} & I \end{bmatrix} \approx \mathbf{S}$$

with

$$\widehat{\mathbb{S}} := (\sqrt{\alpha}L + \bar{M}(I - \Pi_{\mathcal{A}}))M^{-1}(\sqrt{\alpha}L + \bar{M}(I - \Pi_{\mathcal{A}}))^{T} \approx \mathbb{S}$$

Proposed for bound-constrained optimal control problems and  $\overline{M} = M$  in [P., Simoncini, Tani, SISC 2015].

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### Active-set block-diagonal and indefinite preconditioners

#### $4\times4$ formulation

$$\mathcal{P}^{BD}_{aug} = \begin{bmatrix} J_{11} & 0 \\ 0 & \widehat{\boldsymbol{S}} \end{bmatrix},$$

and

$$\mathcal{P}_{aug}^{IP} = \begin{bmatrix} I & 0\\ J_{12}J_{11}^{-1} & I \end{bmatrix} \begin{bmatrix} J_{11} & 0\\ 0 & -\widehat{\mathbf{S}} \end{bmatrix} \begin{bmatrix} I & J_{11}^{-1}J_{12}^T\\ 0 & I \end{bmatrix},$$

where

$$J_{11} = \text{blkdiag}(M, \alpha M) \text{ and } J_{12} = \begin{bmatrix} L & -\overline{M} \\ 0 & P_A M \end{bmatrix}$$

and  $\widehat{\mathbf{S}} \approx \mathbf{S} = J_{12}J_{11}^{-1}J_{12}^{T}$ , i.e. the Schur complement of  $J^{aug}$ .

# 2 × 2 formulation $\mathcal{P}_{red}^{BD} = \begin{bmatrix} M & 0 \\ 0 & \frac{1}{\alpha} \widehat{\mathbb{S}} \end{bmatrix} \qquad \mathcal{P}_{red}^{IP} = \begin{bmatrix} I & 0 \\ LM^{-1} & I \end{bmatrix} \begin{bmatrix} M & 0 \\ 0 & -\frac{1}{\alpha} \widehat{\mathbb{S}} \end{bmatrix} \begin{bmatrix} I & M^{-1}L^T \\ 0 & I \end{bmatrix}$ and $\frac{1}{\alpha} \widehat{\mathbb{S}} \approx \frac{1}{\alpha} \mathbb{S}$ , i.e. the Schur complement of $J^{red}$ .

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#### Active-set block-diagonal and indefinite preconditioners

#### $4\times4$ formulation

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## 2 × 2 formulation $\mathcal{P}_{red}^{BD} = \begin{bmatrix} M & 0 \\ 0 & \frac{1}{\alpha} \widehat{\mathbb{S}} \end{bmatrix} \qquad \mathcal{P}_{red}^{IP} = \begin{bmatrix} I & 0 \\ LM^{-1} & I \end{bmatrix} \begin{bmatrix} M & 0 \\ 0 & -\frac{1}{\alpha} \widehat{\mathbb{S}} \end{bmatrix} \begin{bmatrix} I & M^{-1}L^T \\ 0 & I \end{bmatrix}$ and $\frac{1}{\alpha} \widehat{\mathbb{S}} \approx \frac{1}{\alpha} \mathbb{S}$ , i.e. the Schur complement of $J^{red}$ .

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#### Properties of the active-set Schur complement approximation

$$\blacktriangleright \widehat{\mathbb{S}} = \mathbb{S} + \sqrt{\alpha} (LM^{-1} \,\Pi_{\mathcal{I}} \,\overline{M}^{\mathcal{T}} + \overline{M} \,\Pi_{\mathcal{I}} \,M^{-1}L^{\mathcal{T}}).$$

► If 
$$\mathcal{A} = \{1, ..., n\}$$
  $(\mathcal{I} = \emptyset) \Rightarrow \widehat{\mathbb{S}} = \mathbb{S} \Rightarrow S = \widehat{S}$ 

▶ If 
$$\mathcal{A} = \emptyset$$
 (or unconstrained):  $\lambda(\widehat{\mathbb{S}}^{-1}\mathbb{S}) \in \begin{bmatrix} \frac{1}{2}, 1 \end{bmatrix}$  (cf. [Pearson, Wathen, 2012-2014])

#### Spectral properties of the approximation $\widehat{\mathbb{S}}$

$$\begin{array}{l} \blacktriangleright \ \lambda \in \lambda(\widehat{\mathbb{S}}^{-1}\mathbb{S}) \text{ satisfies} \\ \\ \frac{1}{2} \leq \lambda \leq \zeta^{2} + (1+\zeta)^{2} \\ \\ \text{with} \\ \\ \zeta = \|M^{\frac{1}{2}} \left(\sqrt{\alpha}L + \bar{M}\Pi_{\mathcal{I}}\right)^{-1} \sqrt{\alpha}LM^{-\frac{1}{2}}\|. \end{array}$$

\* Moreover, if  $L\bar{M}^{T} + \bar{M}L^{T} \succ 0$ , then for  $\alpha \to 0$ ,  $\zeta$  is bounded by a constant independent of  $\alpha$ .

[P., Simoncini, Tani, 2015, P., Simoncini, Stoll, 2017]



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## Spectral analysis of the preconditioner

#### Theorem (indefinite case)

Let  $\lambda$  be an eigenvalue of  $(\mathcal{P}^{IP})^{-1}J$ . Then

$$\lambda \in \{1\} \cup \left[rac{1}{2}, \zeta^2 + (1+\zeta)^2
ight].$$

- ▶ 4 × 4: there are at least 3n + |A| 2|I| eigenvalues equal to 1.
- ▶ 2 × 2: there are at least  $2n 2|\mathcal{I}|$  eigenvalues equal to 1.

#### Theorem (block-diagonal case)

Let  $\xi = \zeta^2 + (1 + \zeta)^2$ . Then  $\lambda((\mathcal{P}^{BD})^{-1}J) \subset I^- \cup I^+$  with

• 4 × 4: 
$$I^{-} = \left[\frac{1-\sqrt{1+4\xi}}{2}, \frac{1-\sqrt{3}}{2}\right]$$
 and  $I^{+} = \left[1, \frac{1+\sqrt{1+4\xi}}{2}\right]$ .  
• 2 × 2:  $I^{-} = \left[\frac{-\xi+1-\sqrt{(\xi+1)^{2}+4\zeta^{2}}}{2}, \frac{1-\sqrt{3}}{2}\right]$  and  $I^{+} = \left[1, \frac{1+\sqrt{1+4\zeta^{2}}}{2}, \frac{1-\sqrt{3}}{2}\right]$ 

using [Perugia, Simoncini, 2000

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## Spectral analysis of the preconditioner

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► 2 × 2: 
$$I^- = \left[\frac{-\xi + 1 - \sqrt{(\xi + 1)^2 + 4\zeta^2}}{2}, \frac{1 - \sqrt{3}}{2}\right]$$
 and  $I^+ = \left[1, \frac{1 + \sqrt{1 + 4\zeta^2}}{2}\right]$ 

using [Perugia, Simoncini, 2000]

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## Bounds for the block-diagonal case



Figure: Eigenvalues of the preconditioned matrices and bounds provided in the Theorem versus number of nonlinear iterations (CD problem,  $\alpha = 10^{-4}$ ,  $\beta = 10^{-4}$ ).

## Global Inexact Semismooth Newton's method

#### Algorithm [Martinez, Qi COAP 1985]

- 1. Starting  $x_0$ , parameters  $\sigma \in (0, 1]$ ,  $\gamma \in (0, 1)$ .
- 2. Until convergence do

2.1 Choose 
$$\eta_k \in (0, 1)$$
 (forcing term)

2.2 Solve

$$\Theta'(x_k)\Delta x = -\Theta(x_k) + \mathbf{r}_k,$$

with

 $\|\mathbf{r}_k\|_2 \leq \eta_k \|\Theta(\mathbf{x}_k)\|_2$ 

(inexact condition)

2.3 
$$\rho \leftarrow 1$$
;  
2.4 While  $\|\Theta(x_k + \rho\Delta x)\|_2^2 - \|\Theta(x_k)\|_2^2 > -2\sigma\gamma\rho\|\Theta(x_k)\|_2^2$   
 $\rho \leftarrow \rho/2$ .

3.  $x_{k+1} \leftarrow x_k + \rho \Delta x$ ,  $k \leftarrow k+1$ .

- ► Fast local convergence of SSN [Stadler '09] ⇒ globalization strategy is needed [Martinez and Qi '95].
- Inexactness adapted to the 4 × 4 and 2 × 2 case so that Newton's steps computed with the same accuracy.

### Experiments: implementation issues

- ▶ Preconditioners via AMG (HSL-MI20)
  - Application of  $\widehat{\mathbb{S}}$ : solving with  $(\sqrt{\alpha}L + \overline{M}(I \Pi_{\mathcal{A}_k}))$  (and its transpose)
- ► FEM matrices from the open source FE library deal.II
- Stopping test for the outer iteration:

$$\|\Theta(x_k)\| \leq 10^{-6}$$

- ► Relative residual for inner stopping criterion:
  - Exact case:

$$\eta_k = 10^{-10}$$

Inexact case:

$$\eta_k = \min \left\{ \chi \left( \|\Theta_{k+1}\| / \|\Theta_k\| \right)^2, \eta_{max} \right\}$$
with  $\chi = 0.9, \eta_0 = \eta_{max} = \{10^{-1}, 10^{-2}, 10^{-4}, 10^{-10}\}$ , [Eisenstat, Walker, SISC 1996].

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Poisson state equation

## Poisson state equation with FDs $(\mathcal{L} = -\Delta, M = \overline{M} = I)$



(a)  $\beta = 10^{-3}$  (b)  $\beta = 10^{-4}$ 

Figure: Control for two different values of the parameter  $\beta$ . Desired State  $y_d = \sin(2\pi x) \sin(2\pi y) \exp(2x)/6$ , a = -30, b = 30.

▶ 2D: 
$$n = 2^{2\ell}$$
 with  $\ell = 7, 8, 9 \Rightarrow n = 16384, 65536, 262144;$ 

▶ 3D:  $n = 2^{3\ell}$  with  $\ell = 4, 5, 6 \Rightarrow n = 4096, 32768, 262144$ .

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Poisson state equation

#### Poisson state equation with FDs (2D case, $\beta = 10^{-4}$ )

			s	SN-GMR	ES-IP	SSN-MINRES-BD					
4x4	l	$\log_{10} \alpha$	LI	CPU	TCPU	LI	CPU	TCPU	%u=0	NLI	BT
	7	-2	11	2.0	4.1	25	6.0	12.1	3.5	2	0
		-4	16	2.9	14.5	34	7.8	39.2	8.6	5	0
		-6	27	6.2	69.1	61	14.0	154.9	35.6	11	9
	9	-2	12	30.9	61.8	27	103.0	206.0	4.7	2	0
		-4	17	28.6	143.2	37	93.9	469.6	9.7	5	0
		-6	28	60.2	782.5	68	190.8	2481.5	36.4	13	11
2x2											
	7	-2	11	2.0	4.0	24	4.8	9.6	3.5	2	0
		-4	16	2.8	14.1	35	6.2	31.3	8.6	5	0
		-6	26	5.3	58.9	65	11.2	124.0	35.6	11	9
	9	-2	12	26.0	52.0	25	95.2	190.5	4.7	2	0
		-4	17	25.9	129.8	38	74.4	372.4	9.7	5	0
		-6	28	50.6	657.7	71	154.4	2007.6	36.4	13	11

- LI/NLI: average number of Linear/number of NonLinear iterations
- ▶ CPU/TCPU: average/total CPU time
- ▶ BT: total number of Back-Tracking steps in the line-search strategy

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Poisson state equation

#### Poisson state equation with FDs (3D case, $\beta = 10^{-4}$ )

			S	SN-GMR	ES-IP	SSN-MINRES-BD					
4x4	l	$\log_{10} \alpha$	LI	CPU	TCPU	LI	CPU	TCPU	%u=0	NLI	вт
	4	-2	10	0.5	1.0	21	1.9	3.8	7.4	2	0
		-4	15	0.5	2.2	31	2.3	9.1	7.6	4	0
		-6	24	0.9	7.7	51	3.8	30.6	38.6	8	5
	6	-2	11	19.1	38.2	23	82.2	164.4	11.8	2	0
		-4	16	27.5	110.1	33	121.5	486.2	17.3	4	0
		-6	31	71.3	570.5	69	261.4	2091.9	46.9	8	2
2x2											
	4	-2	10	0.3	0.7	20	1.2	2.4	7.4	2	0
		-4	14	0.5	2.1	32	1.8	7.4	7.6	4	0
		-6	23	0.8	6.7	53	2.8	22.7	38.6	8	5
	6	-2	10	17.3	34.7	22	61.4	122.9	11.8	2	0
		-4	16	26.1	104.5	34	92.8	371.5	17.3	4	0
		-6	31	59.4	475.8	74	210.0	1680.3	46.9	8	2

- LI/NLI: average number of Linear/number of NonLinear iterations
- ► CPU/TCPU: average/total CPU time
- ▶ BT: total number of Back-Tracking steps in the line-search strategy

Convection-Diffusion state equation

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#### Convection-Diffusion state equation with FE (1)

$$\mathcal{L} = -\epsilon \Delta + \mathbf{w} \cdot \nabla$$

\* 
$$w = (2y(1 - x^2), -2x(1 - y^2)), a = -20, b = 20;$$
  
\*  $\overline{M}$  and L SUPG discretization (unsym).

$$n = 4225, \qquad \beta = 10^{-2}$$

#### SSN-GMRES-IP $(2 \times 2)$

	$\epsilon = 1$		$\epsilon = 0.$	.5	$\epsilon = 0.1$		
$\log_{10} \alpha$	li (nli)	BT	LI (NLI)	BT	li (nli)	BT	
-1	10(2)	0	13(4)	2	11(2)	0	
-2	13(5)	0	17(13)	17	14(6)	3	
-3	15(7)	4	23(19)	46	17(9)	8	
-4	19(10)	11	27(23)	45	22(14)	29	
-5	22(43)	183	35(39)	127	24(36)	156	

- LI: average number of Linear Iterations ►
- NLI: total number of Nonl inear Iterations ►
- BT: total number of Back-Tracking steps in the line-search strategy

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Convection-Diffusion state equation

## Convection-Diffusion state equation with FE (2)

SSN-GMRES-IP

$$n = 16641, \beta = 10^{-4}, \epsilon = 0.1$$

	4 ×	4	2 × 2			
$\log_{10} \alpha$	li (nli)	TCPU	li (nli)	TCPU		
-1	13(4)	21.5	13(4)	20.2		
-3	23(15)	137.3	23(15)	123.6		
-5	33(56)	970.6	31(56)	864.3		

$$n = 66049, \beta = 10^{-4}, \epsilon = 0.1$$

	4 ×	< 4	$2 \times 2$		
$\log_{10} \alpha$	LI (NLI)	TCPU	LI (NLI)	TCPU	
-1	13(4)	75.9	13(4)	70.8	
-3	23(15)	502.4	23(15)	406.0	
-5	31(95)	5056.8	30(95)	4004.2	

- LS needed for convergence in 80% of the runs.
- $\blacktriangleright$  LS slow for small  $\alpha$ .



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#### Inexact solution of the Newton's equation (2)



Figure: Inexact Newton's method for different  $\eta_0$  (CD,  $\alpha = 10^{-3}, \beta = 10^{-2}, \epsilon = 1/10$ ).

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#### Inexact solution of the Newton's equation (1)



Figure: Inexact Newton's method for different  $\eta_0$  (CD,  $\alpha = 10^{-3}, \beta = 10^{-2}, \epsilon = 1/10$ ).

## Conclusions

- General SemiSmooth Newton's algorithm for control problems with bound and sparsity constraints;
- Enhancement of the linear algebra phase by:
  - reduced  $2 \times 2$  formulation of the Newton's equation;
  - preconditioners based on the active-set Schur complement approximation;
  - inexact framework;
- Spectral analysis of the Active-Set Schur complement approximation for general state equation with unsymmetric mass matrix (e.g. CD).
- ► Numerical experiments show good performance wrto different parameters

#### Current work

use alternative 2nd-order methods to accelerate convergence for limit values of the parameters

Porcelli, Simoncini, Stoll, *Preconditioning PDE-constrained optimization with*  $L^{1}$ -sparsity and control constraints, Computers and Mathematics with Applications, 74:5 (2017), pp. 1059-1075.

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## Thanks for your attention