Optimal control of non-smooth partial differential equations

Christian Clason Arnd Rösch Vu Huu Nhu[1]
Constantin Christof Christian Meyer Stephan Walther[2]

[1]Faculty of Mathematics, Universität Duisburg-Essen
[2]Faculty of Mathematics, TU Dortmund

Workshop "New Trends in PDE-constrained Optimization"
RICAM, Linz, October 14, 2019

Motivation: PDE-constrained optimization

$$\min_{u,y} F(y) + G(u) \quad \text{such that} \quad E(y,u) = 0$$

Standard questions:

1. existence of solutions
   $\rightsquigarrow$ direct method of calculus of variations
2. characterization of solutions
   $\rightsquigarrow$ (necessary) optimality conditions
3. computation of solutions
   $\rightsquigarrow$ gradient, Newton-type methods

Current research:

- F or G not differentiable (constraints, sparsity, impulse noise)
- E not differentiable

Motivation: non-smooth equations

Non-smooth equations:

- describe models with sharp phase transitions
- dual formulation of variational inequalities
- examples: free boundary problems (ice–water), contact problems with friction, non-Newtonian fluid flow, …

Two-phase Stefan problem

$$\langle -y, \varphi_t \rangle + \langle \nabla\theta(y), \nabla\varphi \rangle = \langle u, \varphi \rangle \quad \text{for all } \varphi \in H^1(Q) \text{ with } \varphi(\cdot, T) = 0$$

$$\theta(y(x,t)) = \begin{cases} y(x,t) & y(x,t) \leqslant 0 \\ 0 & y(x,t) \in [0,1] \\ y(x,t) - 1 & y(x,t) \geqslant 1 \end{cases}$$

Motivation: non-smooth equations

Model problem 1: semilinear "Saran wrap equation"

$$
\begin{aligned}
-\Delta y + \max\{0, y\} &= u \\
y|_{\partial\Omega} &= 0
\end{aligned}
$$

- superposition operator: $\max : L^2(\Omega) \to L^2(\Omega)$ pointwise a.e.
- model for membrane partially in water: y deflection, u force
- can be extended to arbitrary $f(y)$ piecewise differentiable
- well-posed (in suitable spaces)
- $u \mapsto y$ nonlinear, Lipschitz (in suitable spaces)
- $u \mapsto y$ not Gâteaux differentiable unless $|\{x : y(x) = 0\}| = 0$

Motivation: non-smooth equations

Model problem 2: quasilinear heat conduction

$$-\nabla \cdot [a(y)\nabla y] = u$$
$$y|_{\partial\Omega} = 0$$

- superposition operator: $a : L^2(\Omega) \to L^2(\Omega)$ pointwise a.e.
- $a : \mathbb{R} \to \mathbb{R}$ bounded from below, Lipschitz (or PC^1)
- nonlinear material-dependent conductivity law
  e.g., $a(y) = 1 + |y|$
- well-posed (in suitable spaces)
- $u \mapsto y$ nonlinear, continuous (in suitable spaces)
- $u \mapsto y$ not Gâteaux differentiable in general

Motivation: optimality conditions

$$F(\bar{x}) = \min_{x \in X} F(x) \quad \text{s.t.} \quad x \in C$$

Optimality conditions (F differentiable):

1. primal: directional derivative, tangent cone

$$F'(\bar{x}; h) \geqslant 0 \quad \text{for all } h \in T_C \subset X$$

2. dual: (suitable) subdifferential, indicator functional

$$0 \in \partial[F + \delta_C](\bar{x}) \subset X^*$$

3. primal-dual: calculus rules, normal cone ($\rightsquigarrow$ Lagrange multiplier)

$$F'(\bar{x}) + \bar{p} = 0, \qquad \bar{p} \in N_C(\bar{x}) \subset X^*$$

Motivation: optimality conditions

$$J(\bar{u}, \bar{y}) = \min_{u \in X, y \in Y} J(u, y) \quad \text{s.t.} \quad E(u, y) = 0$$

Unique solution $y = S(u)$ $\rightsquigarrow$ $F(u) := J(u, S(u))$ (differentiable)

1. primal: directional derivative

$$F'(\bar{u}; h) \geqslant 0 \quad \text{for all } h \in X$$

2. dual: Fréchet derivative

$$0 = F'(\bar{u}) \subset X^*$$

3. primal-dual: implicit function theorem $\rightsquigarrow$ adjoint state

$$J'_u(\bar{u}, S(\bar{u})) + \bar{p} = 0, \qquad \bar{p} = S'(\bar{u})^* J'_y(\bar{u}, S(\bar{u}))$$

Motivation: optimality conditions

$$J(\bar{u},\bar{y}) = \min_{u\in X, y\in Y} J(u,y) \quad \text{s.t.} \quad E(u,y) = 0$$

Unique solution $y = S(u)$, not Gâteaux differentiable

1. primal: directional derivative

$$F'(\bar{u};h) \geqslant 0 \quad \text{for all } h \in X$$

2. dual: (suitable) subdifferential

$$0 \in \partial F(\bar{u}) \subset X^*$$

3. primal-dual: chain rule or limit process ($\rightsquigarrow$ adjoint state)

$$J_u'(\bar{u}, S(\bar{u})) + \bar{p} = 0, \qquad \bar{p} \in \partial S(\bar{u})^* J_y'(\bar{u}, S(\bar{u}))$$

Motivation: subdifferentials

$S : X \to Y$ not Gâteaux differentiable:

- Bouligand subdifferential

$$\partial_B S(u) := \left\{ G_u \in L(X,Y) \;\middle|\; \begin{aligned} &\text{there exists } \{u_n\} \text{ with } u_n \to u \\ &\text{and } S'(u_n) \to G_u \end{aligned} \right\}$$

  (set of all limits of Gâteaux derivatives in nearby points)

- Clarke subdifferential

$$\partial_C S(u) := \operatorname{cl}\operatorname{co} \partial_B S(u)$$

  (closed convex hull)

X, Y infinite-dimensional $\rightsquigarrow$ topology matters (strong, weak(-$*$),…)

1 Overview
- Non-smooth equations
- Optimality conditions

2 Semilinear PDEs
- Optimality conditions
- Numerical solution

3 Quasilinear PDEs
- Optimality conditions
- Numerical solution

Optimal control of semilinear PDE

Semilinear "Saran wrap equation"

$$\min_{u\in L^2(\Omega), y\in H_0^1(\Omega)} J(y,u) \quad \text{s.t.} \quad -\Delta y + \max\{0,y\} = u$$

- existence of minimizer $(\bar{u},\bar{y})$ for J weakly l.s.c., coercive
- $S : u \mapsto y$ Lipschitz from $L^2(\Omega) \to H_0^1(\Omega)$
  (standard argument: max Lipschitz and monotone)
- S Gâteaux differentiable at u if and only if $S(u) \neq 0$ a.e.
- reduced functional $F(u) := J(S(u),u)$

Semilinear: primal optimality conditions

Primal optimality conditions

$$F'(\bar{u}; h) = J'_y(\bar{y}, \bar{u})S'(\bar{u}; h) + J'_u(\bar{y}, \bar{u})h \geqslant 0 \quad \text{for all } h \in L^2(\Omega)$$

- if J continuously Fréchet differentiable, partial derivatives J'_y, J'_u

  standard proof: pass to the limit in $F(\bar{u}) \leqslant F(u + th)$
- directional derivative: $w := S'(u; h) \in H^1_0(\Omega)$ satisfies

$$-\Delta w + \mathbb{1}_{\{S(u)>0\}} w + \mathbb{1}_{\{S(u)=0\}} \max\{0, w\} = h$$

- $\rightsquigarrow$ Gâteaux derivative $S'(u)h = w$ iff $S(u) \neq 0$ a.e.

Semilinear: primal-dual optimality conditions

Primal-dual optimality conditions

$$\bar{p} + J'_u(\bar{y}, \bar{u}) = 0, \qquad \bar{y} = S(\bar{u})$$
$$-\Delta\bar{p} + \xi\bar{p} = J'_y(\bar{y}, \bar{u})$$
$$\xi(x) \in \partial_C \max(\bar{y}(x)) := \begin{cases} \{1\} & \bar{y}(x) > 0 \\ \{0\} & \bar{y}(x) < 0 \\ [0,1] & \bar{y}(x) = 0 \end{cases} \quad \text{a.e.}$$

- proof: C^1 approximation $\max_\varepsilon$, localization $\rightsquigarrow$ standard conditions pass to limit $\varepsilon \to 0$, use regularity of adjoint PDE
- $G_\xi := (-\Delta + \xi)^{-1} \in \partial_B^W S(\bar{u})$ (weak limit of Gâteaux derivatives)
- $\xi(x) \in \{0,1\}$ a.e. $\rightsquigarrow$ $G_\xi \in \partial_B S(\bar{u})$
- $\rightsquigarrow$ implies dual optimality condition $0 \in \partial_B F(\bar{u}) \subset \partial_C F(\bar{u})$

Semilinear: strong optimality conditions

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Strong optimality conditions

$$\bar p + J'_u(\bar y, \bar u) = 0, \qquad \bar y = S(\bar u)$$

$$-\Delta \bar p + \xi \bar p = J'_y(\bar y, \bar u)$$

$$\xi(x) \in \partial_C \max(\bar y(x)) \quad \text{a.e.}$$

$$\bar p(x) \leqslant 0 \quad \text{a.e. where} \quad \bar y(x) = 0$$

- proof: test adjoint equation, use density
- equivalent to primal optimality condition

  proof: pointwise argument using structure of max
- overdetermined: not useful for numerical computation

Semilinear: numerical solution

$$J(y,u) = \frac{1}{2}\|y - y^d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|u\|^2_{L^2(\Omega)}$$

- finite element discretization, mass lumping for max-term
- eliminate control
- max convex $\rightsquigarrow$ proximal point reformulation of $\xi_i \in \partial_C \max(y_i)$

$$\begin{aligned} A_h y + D_h \max(y) &= -\frac{1}{\alpha} M_h p \\ A_h p + D_h\, \xi \circ p &= M_h(y - y_d) \\ y &= \operatorname{prox}_\tau(y + \tau\, \xi) \end{aligned}$$

Semilinear: numerical solution

$$
\begin{aligned}
A_h y + D_h \max(y) &= -\frac{1}{\alpha} M_h p \\
A_h p + D_h \,\xi \circ p &= M_h (y - y_d) \\
y &= \operatorname{prox}_\tau (y + \tau\,\xi)
\end{aligned}
$$

- $\rightsquigarrow$ semi-smooth Newton method
- but: Newton matrix singular for $p_i = y_i + \tau\xi = 0$
- $\rightsquigarrow$ eliminate corresponding components in iteration
- test with constructed $y^d \rightsquigarrow S$ not differentiable at solution

Semilinear: numerical example

h	α	τ	$\frac{\lVert y_h - \bar{y} \rVert_{L^2}}{\lVert \bar{y} \rVert_{L^2}}$	$\frac{\lVert p_h - \bar{p} \rVert_{L^2}}{\lVert \bar{p} \rVert_{L^2}}$	# SSN
3.030e−2	1e−4	1e−12	8.708e−1	1.606e−2	4
1.538e−2	1e−4	1e−12	2.281e−1	4.541e−3	5
7.752e−3	1e−4	1e−12	5.821e−2	1.209e−3	3
3.891e−3	1e−4	1e−12	1.469e−2	3.119e−4	3
7.752e−3	1e−4	1e−6	–	–	no conv.
7.752e−3	1e−4	1e−8	–	–	no conv.
7.752e−3	1e−4	1e−10	5.821e−2	1.209e−3	3
7.752e−3	1e−4	1e−14	5.821e−2	1.209e−3	3
7.752e−3	1e−2	1e−12	3.007e−3	1.747e−3	2
7.752e−3	1e−3	1e−12	1.659e−2	1.512e−3	2
7.752e−3	1e−5	1e−12	1.692e−1	8.659e−4	5
7.752e−3	1e−6	1e−12	–	–	no conv.

Optimal control of quasilinear PDE

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Quasilinear heat equation

$$\min_{u\in L^p(\Omega),y\in H_0^1(\Omega)} J(y,u) \quad \text{s.t.} \quad -\nabla\cdot[a(y)\nabla y] = u$$

- $a:\mathbb{R}\to\mathbb{R}$ Lipschitz continuous, directionally differentiable, bounded from below from zero
- existence of minimizer $(\bar{u},\bar{y})$ for J weakly l.s.c., coercive
- $S: u\mapsto y$ continuous from $W^{-1,p'}(\Omega)\to W_0^{1,s}(\Omega)$ for some $p', s > d$
  proof: Stampacchia trick and Schauder fixed point theorem
- $\rightsquigarrow$ S completely continuous from $L^p(\Omega)\to W_0^{1,s}(\Omega)$

Quasilinear: primal optimality conditions

Primal optimality conditions

$$F'(\bar{u};h) = J'_y(\bar{y},\bar{u})S'(\bar{u};h) + J'_u(\bar{y},\bar{u})h \geqslant 0 \quad \text{for all } h \in L^p(\Omega)$$

- if J continuously Fréchet differentiable, partial derivatives J'_y, J'_u
- directional derivative: $w := S'(u;h) \in H^1_0(\Omega)$ satisfies

$$-\nabla \cdot [a(S(u))\nabla w + a'(S(u);w)\nabla S(u)] = h$$

Quasilinear: primal-dual optimality conditions

Primal-dual optimality conditions

$$\bar p + J'_u(\bar y, \bar u) = 0, \qquad \bar y = S(\bar u)$$
$$-\nabla \cdot [a(\bar y)\nabla \bar p] + \xi \nabla \bar y \cdot \nabla \bar p = J'_y(\bar y, \bar u)$$
$$\xi(x) \in \partial_C a(\bar y(x)) \quad \text{a.e.}$$

- difficulty: non-smooth in leading term, can't pass to limit
- proof:
  1. C^1 approximation $\max_\varepsilon$, localization $\rightsquigarrow$ standard conditions
  2. pass to limit in linearized (not adjoint!) PDE, use duality
  3. boundedness, Lipschitz continuity, strong–weak-$*$ outer semicontinuity of Clarke subdifferential
- $\xi \in L^\infty(\Omega)$, not uniquely determined

Quasilinear: strong optimality conditions

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Strong optimality conditions

$$\bar{p} + J'_u(\bar{y}, \bar{u}) = 0, \quad \bar{y} = S(\bar{u})$$

$$-\nabla \cdot [a(\bar{y}) \nabla \bar{p}] + \xi \nabla \bar{y} \cdot \nabla \bar{p} = J'_y(\bar{y}, \bar{u})$$

$$\xi(x) \in \partial_C a(\bar{y}(x)) \quad \text{a.e.}$$

$$\left(a'(\bar{y}(x); t) - \xi(x) t \right) \nabla \bar{y}(x) \cdot \nabla \bar{p}(x) \geqslant 0 \quad \text{for all } t \in \mathbb{R}, \text{ a.e.}$$

- proof: test adjoint equation, use density
- not explicit: not useful for numerical computation

Quasilinear: strong optimality conditions

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Strong optimality conditions

$$\bar p + J_u'(\bar y, \bar u) = 0, \quad \bar y = S(\bar u)$$
$$-\nabla \cdot [a(\bar y)\nabla \bar p] + \xi \nabla \bar y \cdot \nabla \bar p = J_y'(\bar y, \bar u)$$
$$\xi(x) \in \partial_C a(\bar y(x)) \quad \text{a.e.}$$
$$\left(a'(\bar y(x); t) - \xi(x) t\right) \nabla \bar y(x) \cdot \nabla \bar p(x) \geqslant 0 \quad \text{for all } t \in \mathbb{R}, \text{ a.e.}$$

If a is continuous, countably piecewise differentiable (PC^1):

- $\rightsquigarrow$ S Gâteaux differentiable (but a still non-smooth!)
- $\rightsquigarrow$ strong conditions equivalent to primal-dual conditions
- $\rightsquigarrow$ primal-dual conditions hold for **any** $\chi(x) \in \partial_C a(\bar y(x))$

Semilinear: numerical solution

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$$J(y,u) = \frac{1}{2}\|y - y^d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|u\|^2_{L^2(\Omega)}$$

- $a(y) = 1 + |y|$ countably PC[1]
- eliminate control, fix $\chi = \text{sign}(\bar{y})$ single-valued (e.g., $\text{sign}(0) := 1$)
- introduce $\psi = \bar{y} + \frac{1}{2}(\bar{y}|\bar{y}|)$

$$-\Delta\psi + \frac{1}{\alpha}w = 0$$

$$-\Delta w + \frac{1 - \sqrt{1 + 2|\psi|}}{\sqrt{1 + 2|\psi|}}\,\text{sign}(\psi) + \frac{y^d}{\sqrt{1 + 2|\psi|}} = 0$$

Semilinear: numerical solution

$$-\Delta\psi + \frac{1}{\alpha} w = 0$$

$$-\Delta w + \frac{1-\sqrt{1+2|\psi|}}{\sqrt{1+2|\psi|}} \operatorname{sign}(\psi) + \frac{y^d}{\sqrt{1+2|\psi|}} = 0$$

- $\rightsquigarrow$ semi-smooth Newton method
- local superlinear convergence for $y_d \in L^\infty(\Omega)$ small or α large
- finite element discretization, mass lumping
- test with constructed $y^d \rightsquigarrow S$ not differentiable at solution

Quasilinear: numerical example

n_h	α	$\frac{\|y_h - \bar{y}\|_{H_0^1(\Omega)}}{\|\bar{y}\|_{H_0^1(\Omega)}}$	$\frac{\|w_h - \bar{w}\|_{H_0^1(\Omega)}}{\|\bar{w}\|_{H_0^1(\Omega)}}$	# SSN
100	1e-6	*3.275e–3*	*2.915e–2*	2
200	1e-6	*1.660e–3*	*1.540e–2*	4
400	1e-6	*8.357e–4*	*7.925e–3*	3
800	1e-6	*4.193e–4*	*4.027e–3*	3
1000	1e-6	*3.356e–4*	*3.237e–3*	3
800	1e-2	*6.358e–2*	*1.360e–2*	4
800	1e-4	*8.762e–3*	*7.324e–3*	3
800	1e-6	*4.193e–4*	*4.027e–3*	3
800	1e-8	*2.321e–5*	*2.192e–3*	25

Conclusion

Optimal control of non-smooth partial differential equations:

- model sharp phase transitions
- useful optimality conditions by approximation, limit
- solution by semismooth Newton method

Outlook:

- parameter identification (iterative regularization)
- application to variational inequalities
- second order optimality conditions
- discretization error estimates

Preprint, Python codes:

`http://www.uni-due.de/mathematik/agclason/clason_pub.php`