Convex relaxation of hybrid discrete-continuous control problems

Christian Clason

Faculty of Mathematics, Universität Duisburg-Essen

joint work with Florian Kruse and Karl Kunisch

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Motivation: hybrid discrete optimization

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$$\min_{u \in U} \mathcal{F}(u) + \frac{\alpha}{2}\|u\|^2$$

- $\mathcal{F}$ discrepancy term (involving PDEs)
- U discrete set

$$U = \left\{ u \in L^p(\Omega) : u(x) \in \{u_1, \dots, u_d\} \text{ a.e.} \right\}$$

- $u_1, \dots, u_d$ given voltages, velocities, materials, …
  (assumed here: ranking by magnitude possible!)
- motivation: topology optimization, medical imaging

Motivation: penalty

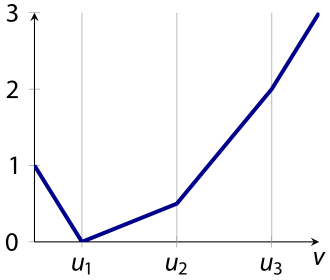
- convex relaxation: replace U by convex hull $u(x) \in [u_1, u_d]$
- works only for $d = 2$, cf. bang-bang control ($\alpha = 0$)
- $\rightsquigarrow$ promote $u(x) \in \{u_1, \dots, u_d\}$ by convex pointwise penalty

$$\mathcal{G}(u) = \int_\Omega g(u(x))\,dx$$

- generalize L^1 norm: polyhedral epigraph with vertices $u_1, \dots, u_d$
- not exact relaxation/penalization (in general)!

Motivation: penalty

- generalize L^1 norm: polyhedral epigraph with vertices $u_1, \dots, u_d$



- motivation: convex envelope of $\frac{1}{2}\|u\|^2 + \delta_U$
- multi-bang (generalized bang-bang) control
- $\rightsquigarrow$ non-smooth optimization in function spaces

- pointwise penalty $\rightsquigarrow$ add total variation regularization

Convex analysis approach

$$\mathcal{F}(\bar{u}) + \mathcal{G}(\bar{u}) = \min_u \mathcal{F}(u) + \mathcal{G}(u)$$

1. Fermat principle: $0 \in \partial\left(\mathcal{F}(\bar{u}) + \mathcal{G}(\bar{u})\right)$
2. sum rule: $0 \in \partial\mathcal{F}(\bar{u}) + \partial\mathcal{G}(\bar{u})$, i.e., there is $\bar{p} \in V^*$ with

$$\begin{cases} -\bar{p} \in \partial\mathcal{F}(\bar{u}) \\ \bar{p} \in \partial\mathcal{G}(\bar{u}) \end{cases}$$

3. Fenchel duality:

$$\begin{cases} -\bar{p} \in \partial\mathcal{F}(\bar{u}) \\ \bar{u} \in \partial\mathcal{G}^*(\bar{p}) \end{cases}$$

Convex analysis approach

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For $\min_u \mathcal{F}(u) + \mathcal{G}(u), \quad \mathcal{G}(u) = \int_\Omega g(u(x))\,dx$ convex

Approach: pointwise

1. compute subdifferential ∂g (or Fenchel conjugate g^*)
2. compute conjugate subdifferential ∂g^*
3. compute proximal mapping $\text{prox}_{\gamma g^*}$
4. compute Moreau–Yosida regularization ∂g_γ^*
5. compute Newton derivative $D_N \partial g_\gamma^*$

⇝ semismooth Newton method, continuation in γ for

superposition operator $\quad [\partial \mathcal{G}_\gamma^*(p)](x) = \partial g_\gamma^*(p(x))$

Multi-bang penalty

$$g : \mathbb{R} \to \overline{\mathbb{R}}, \qquad v \mapsto \begin{cases} \frac{1}{2}\left((u_i + u_{i+1})v - u_i u_{i+1}\right) & v \in [u_i, u_{i+1}] \\ \infty & \text{else} \end{cases}$$

piecewise differentiable $\rightsquigarrow$ subdifferential convex hull of derivatives

$$\partial g(v) = \begin{cases} \left(-\infty, \frac{1}{2}(u_1 + u_2)\right] & v = u_1 \\ \left\{\frac{1}{2}(u_i + u_{i+1})\right\} & v \in (u_i, u_{i+1}) \quad 1 \leqslant i < d \\ \left[\frac{1}{2}(u_{i-1} + u_i), \frac{1}{2}(u_i + u_{i+1})\right] & v = u_i \quad 1 < i < d \\ \left[\frac{1}{2}(u_{d-1} + u_d), \infty\right) & v = u_d \end{cases}$$

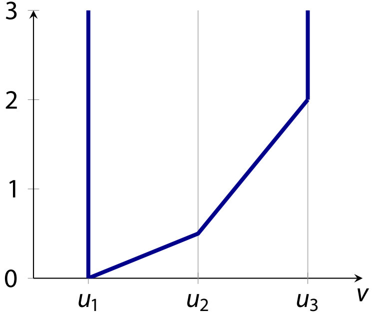
Multi-bang penalty

$$\partial g(v) = \begin{cases} \left(-\infty, \frac{1}{2}(u_1 + u_2)\right] & v = u_1 \\ \left\{\frac{1}{2}(u_i + u_{i+1})\right\} & v \in (u_i, u_{i+1}) \quad 1 \leqslant i < d \\ \left[\frac{1}{2}(u_{i-1} + u_i), \frac{1}{2}(u_i + u_{i+1})\right] & v = u_i \quad 1 < i < d \\ \left[\frac{1}{2}(u_{d-1} + u_d), \infty\right) & v = u_d \end{cases}$$

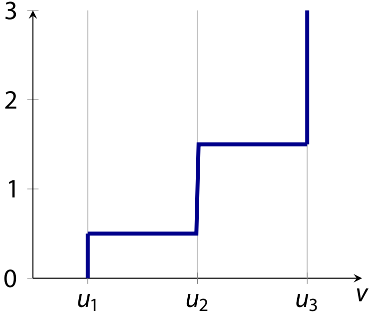
convex inverse function theorem:

$$\partial g^*(q) \in \begin{cases} \{u_1\} & q \in \left(-\infty, \frac{1}{2}(u_1 + u_2)\right) \\ [u_i, u_{i+1}] & q = \frac{1}{2}(u_i + u_{i+1}), \quad 1 \leqslant i < d \\ \{u_i\} & q \in \left(\frac{1}{2}(u_{i-1} + u_i), \frac{1}{2}(u_i + u_{i+1})\right) \quad 1 < i < d, \\ \{u_d\} & q \in \left(\frac{1}{2}(u_{d-1} + u_d), \infty\right) \end{cases}$$

Multi-bang penalty: sketch

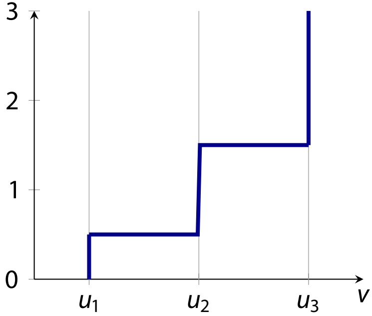


(a) g $(u_1 = 0, u_2 = 1, u_3 = 2)$

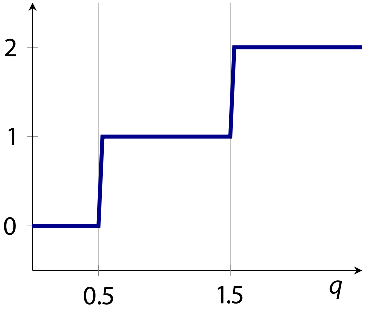


(b) ∂g $(u_1 = 0, u_2 = 1, u_3 = 2)$

Multi-bang penalty: sketch



(c) ∂g $(u_1 = 0, u_2 = 1, u_3 = 2)$



(d) ∂g^* $(u_1 = 0, u_2 = 1, u_3 = 2)$

Optimality conditions (linear)

$$\min_{u,y\in L^2(\Omega)} \frac{1}{2}\|y-z\|^2 + \alpha\,\mathcal{G}(u)$$

$$\bar p = \tfrac{1}{\alpha}A^{-*}(z - A^{-1}\bar u)$$

$$\bar u \in \partial\mathcal{G}^*(\bar p) = \begin{cases} \{u_i\} & \bar p(x) \in Q_i \\ [u_i, u_{i+1}] & \bar p(x) \in \overline{Q}_i \cap \overline{Q}_{i+1} \end{cases}$$

- singular arc $\mathcal{S} = \left\{x : \bar u(x) \neq u_i\right\} \subset \left\{x : \bar p(x) = \tfrac{1}{2}(u_i + u_{i+1})\right\}$
- for suitable K, $\bar p(x)$ constant implies $[z - A^{-1}\bar u](x) = 0$ (e.g., A pure second-order elliptic)

$\rightsquigarrow$ $\left|\{x : A^{-1}\bar u(x) = z(x)\}\right| = 0 \;\Rightarrow\; \bar u \in \{u_1, \dots u_d\}$ a. e. (true multi-bang)

Moreau–Yosida regularization

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Proximal mapping $\quad \text{prox}_{\gamma g^*}(q) = w \text{ iff } q \in \{w\} + \gamma \partial g^*(w)$

case-wise inspection of subdifferential:

$$\partial g_\gamma^*(q) = \frac{1}{\gamma}\left(q - \text{prox}_{\gamma g^*}(q)\right) = \begin{cases} u_i & q \in Q_i^\gamma \\ \frac{1}{\gamma}\left(q - \frac{1}{2}(u_i + u_{i+1})\right) & q \in Q_{i,i+1}^\gamma \end{cases}$$

$$Q_i^\gamma = \left(\tfrac{1}{2}(u_{i-1} + u_i) + \gamma u_i, \tfrac{1}{2}(u_i + u_{i+1}) + \gamma u_i\right)$$
$$Q_{i,i+1}^\gamma = \left[\tfrac{1}{2}(u_i + u_{i+1}) + \gamma u_i, \tfrac{1}{2}(u_i + u_{i+1}) + \gamma u_{i+1}\right]$$

Regularized optimality system (linear)

$$\begin{cases} p_\gamma = \frac{1}{\alpha} A^{-*}(z - A^{-1}u_\gamma) \\ u_\gamma = \partial \mathcal{G}_\gamma^*(p_\gamma) \end{cases}$$

- optimality conditions for $\mathcal{F}(u) + \alpha\, \mathcal{G}(u) + \frac{\gamma}{2}\|u\|^2$ (non-smooth)
- $\rightsquigarrow$ unique solution (u_γ, p_γ)
- $(u_\gamma, p_\gamma) \rightharpoonup (\bar{u}, \bar{p})$ as $\gamma \to 0$
- ∂g_γ^* Lipschitz continuous, piecewise C^1, norm gap $V \hookrightarrow L^2(\Omega)$
- $\rightsquigarrow$ semismooth Newton method

Regularized optimality system (linear)

$$\begin{cases} A^* p_\gamma = \frac{1}{\alpha}(z - y_\gamma) \\ A y_\gamma = \mathcal{G}_\gamma^*(p_\gamma) \end{cases}$$

- optimality conditions for $\mathcal{F}(u) + \alpha\,\mathcal{G}(u) + \frac{\gamma}{2}\|u\|^2$ (non-smooth)
- $\rightsquigarrow$ unique solution (u_γ, p_γ)
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- ∂g_γ^* Lipschitz continuous, piecewise C^1, norm gap $V \hookrightarrow L^2(\Omega)$
- $\rightsquigarrow$ semismooth Newton method

Semismooth Newton method (linear)

$$\begin{pmatrix} \frac{1}{\alpha}\operatorname{Id} & A^* \\ A & -D_N\mathcal{G}_\gamma^*(p^k) \end{pmatrix} \begin{pmatrix} \delta y \\ \delta p \end{pmatrix} = -\begin{pmatrix} A^*p^k + \frac{1}{\alpha}(y^k - z) \\ Ay^k - \mathcal{G}_\gamma^*(p^k) \end{pmatrix}$$

$$[D_N\mathcal{G}_\gamma^*(p)\delta p](x) = \begin{cases} \frac{1}{\gamma}\delta p(x) & p(x) \in Q_{i,i+1}^\gamma \\ 0 & \text{else} \end{cases}$$

- symmetric, but: local convergence
- $\rightsquigarrow$ continuation in $\gamma \to 0$
- $\rightsquigarrow$ backtracking line search based on residual norm
- only number of sets Q_i^γ depends on d $\rightsquigarrow$ linear complexity

1 Overview

2 Multi-bang penalty

3 Total variation regularization

Nonlinear forward mapping

Goal: application to EIT

- $S : u \mapsto y$ solving
$$-\nabla \cdot (u \nabla y) = f$$
- difficulty: $\bar{u} \in L^\infty(\Omega) \quad \rightsquigarrow \quad S$ not weakly-$*$ closed
  1. lack of existence of minimizer ($\bar{y} \neq S(\bar{u})$, cf. homogenization)
  2. lack of convergence $\gamma \to 0$
  3. lack of Newton differentiability of $\partial \mathcal{G}_\gamma^*$ (no norm gap)
- remedies: higher regularity of y or u by
  1. local smoothing: consider $\quad -\nabla \cdot \left(\int_{B_\varepsilon(x)} u(s)\, ds \nabla y \right)$
  2. TV regularization: add $\|Du\|_{\mathcal{M}} \quad \rightsquigarrow u \in BV(\Omega) \cap L^\infty(\Omega) \hookrightarrow_c L^p(\Omega)$

Difficulty:

- existence requires box constraints $\rightsquigarrow$ use penalty

$$\big(G(u) + \delta_{[u_1,u_d]}(u)\big) + TV(u)$$

(here: G multi-bang penalty with dom $G = L^1(\Omega)$)

- but: $TV(u) + \delta_{[u_1,u_d]}(u)$ not continuous on $L^p(\Omega)$, $p < \infty$
- but: multipliers $\xi \in \partial TV(u)$, $q \in \partial G(u)$ not pointwise on BV, L^∞

- $\rightsquigarrow$ replace box constraints by ($C^{1,1}$) projection of $u \in L^1(\Omega)$

$$[\Phi_\varepsilon(u)](x) = \mathrm{proj}^{\varepsilon}_{[u_1,u_d]}(u(x)) \qquad \text{a.e. } x \in \Omega$$

TV regularization: existence

$$\begin{cases} \min_{u\in BV(\Omega)} \frac{1}{2}\|y-z\|^2_{L^2(\Omega)} + \alpha\, G(u) + \beta\, TV(u) \\ \text{s.t.} \quad -\nabla\cdot(\Phi_\varepsilon(u)\nabla y) = f \text{ in } \Omega \\ \qquad\qquad\qquad\qquad y = 0 \text{ on } \partial\Omega \end{cases}$$

- existence of optimal $\bar{u} \in BV(\Omega) \cap L^\infty(\Omega)$ for $\varepsilon \geqslant 0$
- tracking term Fréchet differentiable in $\Phi_\varepsilon(u) \in L^\infty$ for $\varepsilon > 0$
- regularity of state, adjoint $\rightsquigarrow$ derivative in $L^r(\Omega)$, $r > 1$ (instead of $L^\infty(\Omega)^*$)
- $\rightsquigarrow$ sum rule applicable, subgradients in $L^r(\Omega)$, $r > 1$

TV regularization: optimality conditions

$$\begin{cases} 0 = F'(\Phi_\varepsilon(\bar{u}))\Phi'_\varepsilon(\bar{u}) + \alpha\bar{q} + \beta\bar{\xi} \\ \bar{u} \in \partial G^*(\bar{q}) \\ \bar{\xi} \in \partial TV(\bar{u}) \end{cases}$$

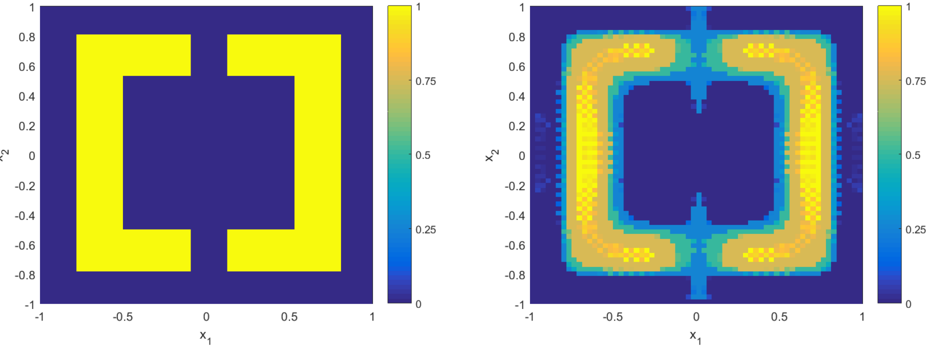
- $F'(\Phi_\varepsilon(\bar{u})) = (\nabla\bar{y} \cdot \nabla\bar{p}) \in L^r(\Omega)$ (optimal state, adjoint)
- $\bar{q} \in L^r(\Omega)$, $r > 1 \rightsquigarrow$ pointwise multi-bang
- $\bar{\xi} \in L^r(\Omega)$, $r > 1 \rightsquigarrow$ characterization via *full trace* [Bredies/Holler '12]
- $\rightsquigarrow$ pointwise optimality conditions
- semi-smooth Newton (after discretization, regularization)

TV regularization: numerical solution

Approach: discretize before optimize

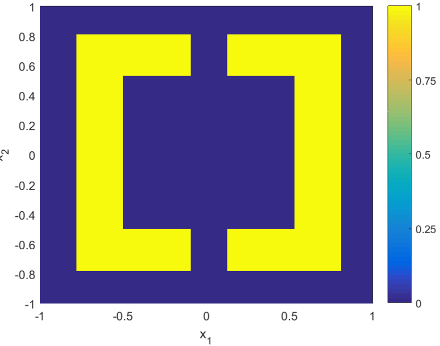
- consider finite element discretization of problem (p.w. linear)
- include projection in multi-bang penalty, eliminate Φ_ε
- apply sum rule, chain rule for $\partial TV(u_h) = -\mathrm{div}_h \partial(\|\cdot\|_1)(\nabla_h u_h)$
- apply Moreau–Yosida regularization to $\partial \mathcal{G}^*$, $\partial(\|\cdot\|_1)^*$
- $\rightsquigarrow$ semi-smooth Newton-type method (modified Newton step to avoid kernel of div_h; line search)
- local convergence: path-following with extrapolation

Numerical example: topology optimization

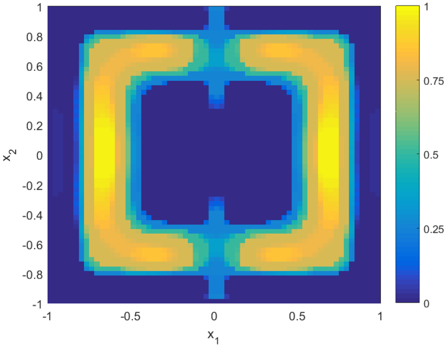


(a) $u^\dagger$ (b) $\alpha = 10^{-3}, \beta = 0$

Numerical example: topology optimization

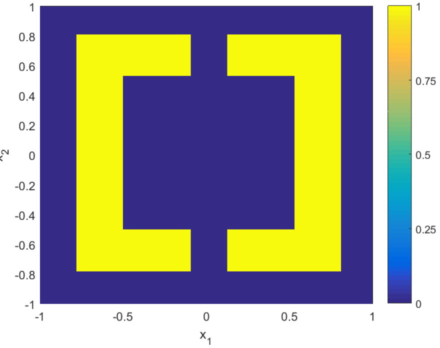


(c) $u^{\dagger}$

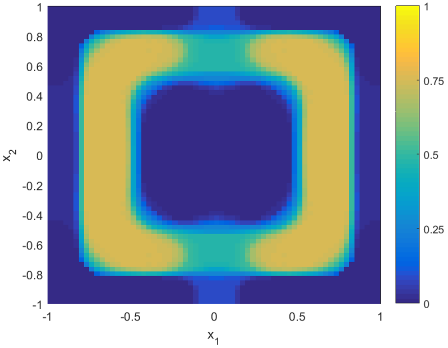


(d) $\alpha = 10^{-3}, \beta = 10^{-6}$

Numerical example: topology optimization



(e) $u^\dagger$



(f) $\alpha = 10^{-3}, \beta = 5 \cdot 10^{-5}$

Numerical example: inverse problem

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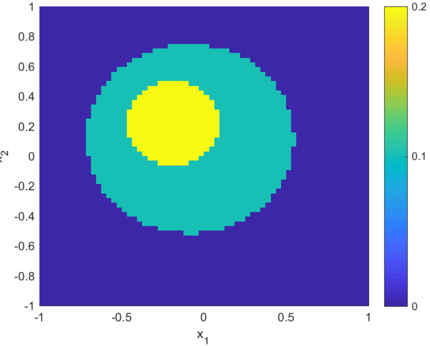
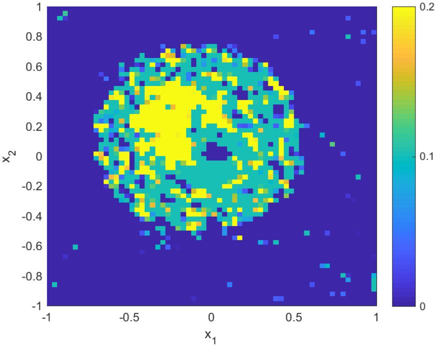
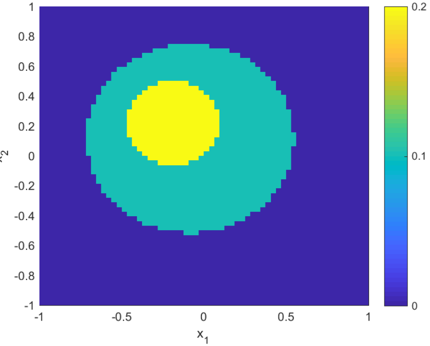


(a) $u^\dagger$

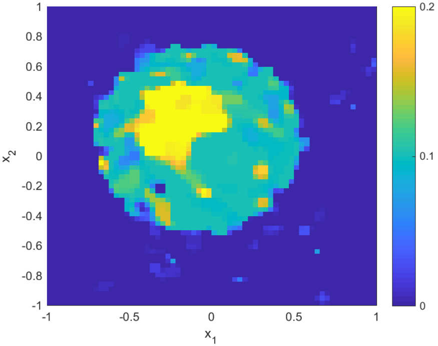


(b) $\alpha = 5 \cdot 10^{-4}, \beta = 0$

Numerical example: inverse problem

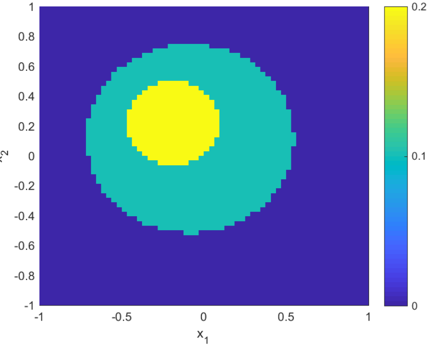


(c) $u^\dagger$

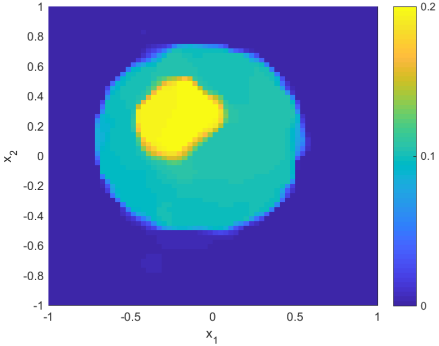


(d) $\alpha = 5 \cdot 10^{-4}, \beta = 10^{-5}$

Numerical example: inverse problem



(e) $u^\dagger$



(f) $\alpha = 5 \cdot 10^{-4}, \beta = 10^{-5}$

Conclusion

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Convex relaxation of discrete–continuous control problems

- well-posed pointwise primal-dual optimality conditions
- strong structural properties
- efficient numerical solution (superlinear convergence)
- can be combined with *total variation regularization*

Outlook:

- nonlinear inverse problems: EIT
- (heuristic) parameter choice
- vector-valued multi-bang
- other hybrid discrete–continuous problems

Preprint:

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