Responsive optimal design with stimulus as design and state variable

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PhD Defence

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Outline

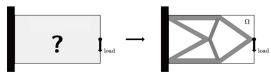
- Introduction
 - Responsive optimal design
- Responsive optimal design with stimulus as a design variable
 - Problem statement
 - The phase field approach to optimal design
 - Existence of solutions
 - Numerical implementation
 - Numerical results
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 - Stimulus governed by poisson PDE
- 4 Conclusion



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Responsive optimal design

 Optimal design deals with finding the allocation of several materials in order to enhance the performance of a structure.



- Responsive materials are those materials whose properties can changed by external stimulus.
- Examples of responsive materials
 - Shape Memory Alloy (SMA)
 - 2 Thermoelastic material
- Three design materials i.e void/holes, non-responsive and responsive
- Goal: Optimal allocation of (void/holes, non-responsive and responsive) materials and the stimulus or stimulus control that optimizes some general objective.

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- Consider a ground domain $\Omega \in \mathbb{R}^d$, d=2,3 subject to boundary force f on a part $\Gamma_N \in \partial \Omega$ of its boundary and clamped on $\Gamma_D \in \partial \Omega$.
- Let χ_v, χ_s , and χ_r be a characteristic functions such that

$$\chi_{v,s,r}(x) = \begin{cases} 1 & x \in \text{Void, Non-responsive, Responsive,} \\ 0 & x \notin \text{Void, Non-responsive, Responsive.} \end{cases}$$

We want the constraints.

$$\chi_{v}(x) + \chi_{s}(x) + \chi_{r}(x) = 1, \forall x \in \Omega,$$

$$\int_{\Omega} \chi_{v,s,r} \, dx = \theta_{v,s,r} |\Omega| \text{ such that } \theta_{v} + \theta_{s} + \theta_{r} = 1.$$

• Design variable $\Phi = [\chi_v, \chi_s, \chi_r]^T$.



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Consider the constitutive law

$$\sigma(u_j) = \sum_{i = \{v, s, r\}} \chi_i \mathbb{C}_i \left(e(u_j) - \beta_i s_j I_d \right)$$

where \mathbb{C}_i denotes the Hooke's law for material i and $e(u_i) = \frac{1}{2}(\nabla u_i + (\nabla u_i)^T)$ is the linearized strain associated to a displacement field u_i .

- β_i is a given parameter such that $\beta_v = \beta_s = 0, \beta_r = 1, s_i \in [-1, 1]$ is the stimulus associated with u_i and I_d is $d \times d$ identity matrix.
- Define the least square objective function

$$\mathcal{I}(u_1,\ldots,u_n) := \sum_{j=1}^n \frac{1}{2} \int_{\Omega_0} |u_j(x) - \bar{u}_j(x)|^2 dx, \qquad (1)$$

where $\bar{u}_1, \ldots, \bar{u}_n$ are the target displacements.

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• The displacement fields $u_j \in V$, $1 \le j \le n$, satisfy the weak form of the linearized elasticity system

$$\sum_{i=\{v,s,r\}} \int_{\Omega} \chi_i \mathbb{C}_i \left(e(u_j) - \beta_i s_j \mathbf{I}_d \right) \cdot e(v) \, dx = 0, \forall v \in V, \qquad (2)$$

where

$$V := \left\{ v \in H^1(\Omega); \ v = 0 \text{ on } \Gamma_D \right\}. \tag{3}$$

Mathematically, the responsive optimal design problem reads as

$$\begin{cases} \inf_{(\Phi,s)} \mathcal{I}(u_1, u_2, \dots, u_n) \\ u_j \text{ satisfies the state equation (2)} \end{cases}$$
 (4)

where $s := (s_1, ..., s_n)$.

- The problem (4) is ill-posed
- How to make the problem (4) well-posed?
 - Perimeter penalization

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• Let $D = (D_v, D_s, D_r)$ be a partition of the domain Ω such that $\chi_{v,s,r} = \chi_{D_{v,s,r}}$ and define

$$\mathcal{P}(\chi) := \frac{1}{2} \sum_{i,j=\{v,s,r\}, i \neq j} \mathcal{H}^{d-1} \left(\partial D_i \cap \partial D_j \cap \Omega \right), \tag{5}$$

where \mathcal{H}^{d-1} denotes the d-1 dimensional Hausdorff

ullet Given a small regularization parameter lpha > 0, we study the problem

$$\inf_{(\Phi,s)} \mathcal{I}(u_1,\ldots,u_n) + \alpha \mathcal{P}(\chi). \tag{6}$$

• Problem: It is not easy to implement (6).

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The phase field approach to optimal design

- We introduce designs of the form $\rho = (\rho_v, \rho_s, \rho_r)$, where each $\rho_v, \rho_s, \rho_r \in H^1(\Omega; [0,1])$ is a smooth continuous density function.
- For any $\varepsilon > 0$, define the vector-valued Modica-Mortola functional

$$\mathcal{P}_{\varepsilon}(\rho) = \int_{\Omega} \frac{W(\rho)}{\varepsilon} + \varepsilon |D\rho|^2 dx.$$
 (7)

• $W(\rho)$ is a non-negative multiple-well potential function vanishing only at three points (1,0,0),(0,1,0) and (0,0,1) and satisfying

$$egin{aligned} d_{ij} := \inf & \left\{ \int_0^1 W^{1/2}(\gamma(t)) |\gamma'(t)| \, dt; \gamma \in \mathit{C}^1((0,1); \mathbb{R}^m),
ight. \ & \left. \gamma(0) =
ho_i, \gamma(1) =
ho_j
ight\} = 1 \end{aligned}$$

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The phase field approach to optimal design

ullet The space of admissible designs $\mathcal{D}_
ho$ and stimuli \mathcal{S}

$$\mathcal{D}_{\rho} := \Big\{ \rho \in \big[H^1(\Omega;[0,1])\big]^3, \sum_{i=\{v,s,r\}} \rho_i = 1, \int_{\Omega} \rho_{v,s,r} \, dx = \theta_{v,s,r} |\Omega| \Big\},$$

$$\mathcal{S}:=L^1\left(\Omega,[-1,1]^n\right).$$

• The phase field regularization of (6) is then

$$\inf_{(\rho,s)\in\mathcal{D}_{\rho}\times\mathcal{S}}\mathcal{I}(u_1,\ldots,u_n)+\alpha\mathcal{P}_{\varepsilon}(\rho). \tag{8}$$

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where $u_i \in V$ satisfies the weak formulation

$$\sum_{i=\{v,s,r\}} \int_{\Omega} a(\rho_i) \mathbb{C}_i \left(e(u_j) - \beta_i s_j I_d \right) \cdot e(v) \, dx = 0 \, \forall v \in V, \, 1 \leq j \leq n$$
(9)

and a is a continuous function such that a(0) = 0 and a(1) = 1.

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Existence of solutions

- Define $\widetilde{\mathcal{I}}(\rho, \mathbf{s}) = \mathcal{I}(u_1(\rho, s_1), \dots, u_n(\rho, s_n))$.
- Consider the problem

$$\mathop{\arg\min}_{(\rho,s)\in\mathcal{D}_{\rho}\times\mathcal{S}}\,\widetilde{\mathcal{I}}(\rho,s)+\widetilde{\mathcal{P}}_{\varepsilon}(\rho,s)\stackrel{\Gamma}{\longrightarrow}\mathop{\arg\min}_{(\rho,s)\in\mathcal{D}_{\rho}\times\mathcal{S}}\,\widetilde{\mathcal{I}}(\rho,s)+\widetilde{\mathcal{P}}(\rho,s)$$

where

$$\widetilde{\mathcal{P}}_{arepsilon}(
ho, \mathrm{s}) := egin{cases} \mathcal{P}_{arepsilon}(
ho) & ext{if } (
ho, \mathrm{s}) \in \mathcal{D}_{
ho} imes \mathcal{S} \ +\infty & ext{otherwise,} \end{cases}$$

- Γ—convergence is stable under continuous perturbation.
- It is enough to prove continuity of $\widetilde{\mathcal{I}}(\rho,s)$ w.r.t to ρ and s.

Theorem (Fundamental Theorem of Γ -Convergence)

Let X be a topological space. Let (F_n) be an equi-coercive sequence of functions and let F_n Γ —converges to F in X, then the minimizers of F_n converge to a minimizer of F.

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Existence of solutions

Lemma (1)

Let $(\rho, s) \in \mathcal{D}_{\rho} \times \mathcal{S}$ and $k_1, k_2 > 0$ be such that for any $1 \leq i \leq 3$ and for any $\Psi \in \mathrm{M}^{d \times d}_{\mathrm{sym}}$, we have $k_1 \Psi \cdot \Psi \leq \mathbb{C}_i \Psi \cdot \Psi \leq k_2 \Psi \cdot \Psi$. There exists C > 0 such that if $u_j \in V$ satisfies (2), then

$$||u_j||_{H^1(\Omega)} \le C, \ 1 \le j \le n.$$

Proof.

By taking $u_j \in V$ as the test function, linearized weak form (9) becomes,

$$\sum_{i=\{v,s,r\}} \int_{\Omega} a(\rho_i) \mathbb{C}_i \mathrm{e}(u_j) \cdot \mathrm{e}(u_j) \, dx = \sum_{i=\{v,s,r\}} \int_{\Omega} a(\rho_i) \beta_i s_j \mathbb{C}_i \mathrm{I}_d \cdot \mathrm{e}(u_j) \, dx,$$

(10)

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Existence of solutions

Proof (Cont.)

We get,

$$\|k_1\|e(u_j)\|_{L^2}^2 \le \left\|\sum_{i=\{v,s,r\}} a(\rho_i)\beta_i s_j \mathbb{C}_i \mathbf{I}_d \right\|_{L^2} \|e(u_j)\|_{L^2},$$

and hence

$$||e(u_i)||_{L^2} \leq M.$$

By Korn's inequality, we have that the solution u_i is bounded

$$C||u_i||_{H^1} \le ||e(u_i)||_{L^2} \le M \implies ||u_i||_{H^1} \le M.$$

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Theorem (Continuity of displacements \implies continuity of $\widetilde{\mathcal{I}}(ho,s)$)

Consider a sequence $(\rho_{\varepsilon}, s_{\varepsilon}) \in \mathcal{D}_{\rho} \times S$ of designs and stimuli such that $\rho_{\varepsilon} \to \rho$, in $\left[L^{1}(\Omega)\right]^{3}$ and $s_{\varepsilon} \to s$ in $\left[L^{2}(\Omega)\right]^{n}$. Let $u_{\varepsilon} = (u_{1,\varepsilon}, \ldots, u_{n,\varepsilon})$ (resp. $u = (u_{1}, \ldots, u_{n})$) be the equilibrium displacements associated with $(\rho_{\varepsilon}, s_{\varepsilon})$ (resp. (ρ, s)). Then if the \mathbb{C}_{i} satisfies the hypotheses of Lemma 2, $u_{\varepsilon} \to u$ in $\left[L^{2}(\Omega)\right]^{n}$ and $\widetilde{\mathcal{I}}(\rho_{\varepsilon}, s_{\varepsilon}) \longrightarrow \widetilde{\mathcal{I}}(\rho, s)$.

Proof.

For each $(\rho_{\varepsilon}, \mathbf{s}_{\varepsilon})$ we can find sequence u_{ε} such that u_{ε} is the solution of the linearized elasticity PDE associated with $(\rho_{\varepsilon}, \mathbf{s}_{\varepsilon})$. Since u_{ε} is uniformly bounded in H^1 we can extract a convergent subsequence u_{ε_n} converging weakly to some $u \in H^1$. Recalling

$$\widetilde{\mathcal{I}}(\rho_{\varepsilon}, s_{\varepsilon}) = \mathcal{I}(u_{1,\varepsilon}(\rho_{\varepsilon}, s_{1,\varepsilon}), \dots, u_{n,\varepsilon}(\rho_{\varepsilon}, s_{n,\varepsilon})),$$

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Proof (Cont.)

and since $u_{\varepsilon_n} \to u$ strongly in L^2 we can pass the limit inside to get

$$\begin{split} \widetilde{\mathcal{I}}(\rho_{\varepsilon}, \mathbf{s}_{\varepsilon}) &= \mathcal{I}\left(u_{1,\varepsilon}(\rho_{\varepsilon}, s_{1,\varepsilon}), \dots, u_{n,\varepsilon}(\rho_{\varepsilon}, s_{n,\varepsilon})\right) \\ &\to \mathcal{I}\left(u_{1}(\rho, s_{1}), \dots, u_{n}(\rho, s_{n})\right) \\ &= \widetilde{\mathcal{I}}(\rho, \mathbf{s}). \end{split}$$

Note

The proof above assumes the minimizing sequence $(\rho_{\varepsilon}, s_{\varepsilon})$ is compact.

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Numerical implementation

- The constraint $\rho_v + \rho_s + \rho_r = 1 \implies \rho_v = 1 \rho_s \rho_r$ and introduce $\tilde{\rho} = (\rho_s, \rho_r)$.
- We add pernalties $Q(\tilde{\rho}, \mathbf{s})$ and $V_C(\tilde{\rho})$ where

$$Q(\tilde{\rho}, s) = \int_{\Omega} (\rho_{v}^{2} + \rho_{s}^{2}) s^{2} dx = \int_{\Omega} ((1 - \rho_{s} - \rho_{r})^{2} + \rho_{s}^{2}) s^{2} dx$$

and

$$V_C(\tilde{\rho}) = \nu_s \int_{\Omega} \rho_s \ dx + \nu_r \int_{\Omega} \rho_r \ dx.$$

• We consider the problem:

$$\begin{cases} \min_{(\rho,\mathbf{s}) \in \mathcal{D}_{\rho} \times \mathcal{S}} & \sum_{j=1}^{n} \frac{1}{2} \int_{\Omega_{0}} |u_{j} - \bar{u}_{j}|^{2} dx + \alpha \mathcal{P}_{\varepsilon}(\tilde{\rho},\mathbf{s}) + Q(\tilde{\rho},\mathbf{s}) + V_{C}(\tilde{\rho}) \\ u_{j} \text{ satisfies the weak form (9)} \end{cases}$$

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Numerical implementation

- We apply the adjoint method to compute the derivative of the objective function
- By collecting all terms explicitly depending on $s \implies$ closed form of an optimal stimulus.
- We tested two different numerical approaches.
 - **9 Staggered** approach \implies minimize w.r.t $\tilde{\rho}$ only and update s explicitly.
 - **2** Monolithic approach \implies minimize w.r.t $\tilde{\rho}$ and s simultaneously.
- Our numerical implementation uses Firedrake and TAO

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Numerical results

• Target displacement $\bar{u} = (0,1)$.

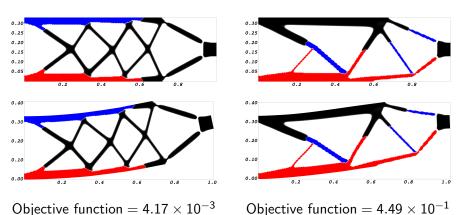


Figure: Staggered (left) vs. Monolithic (right) approach. Composite plot of both material density and the stimulus in the reference (top) and deformed (bottom) configuration for stiffness ratio $E_3/E_2=1.0$.

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Stimulus governed by poisson PDE

- Let the design variable $\tilde{\rho} = [\rho_s, \rho_r, g]^T$.
- $g \in [-1, 1]$ is the stimulus control function.
- The problem can be stated as:

$$\begin{cases} \min\limits_{(\rho,g)} \ \frac{1}{2} \int_{\Omega_0} |u - \bar{u}|^2 \ dx + \alpha \mathcal{P}_{\varepsilon}(\tilde{\rho},s) + Q(\tilde{\rho},g) + V_C(\tilde{\rho}) \\ u \text{ and } s \text{ satisfy the weak forms (12) and (13)} \end{cases}$$

$$\sum_{i=\{v,s,r\}} \int_{\Omega} a(\rho_i) \mathbb{C}_i \left(e(u) - \beta_i s \mathbf{I}_d \right) \cdot e(v) \, dx = 0 \, \forall v \in V, \qquad (12)$$

$$\sum_{i=\{v,s,r\}} \int_{\Omega} k(\rho_i) \nabla s \cdot \nabla q \, dx - \int_{\Omega} gq \, dx = 0$$
 (13)

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Stimulus governed by poisson PDE

• Target displacement $\bar{u} = (0, 1)$.

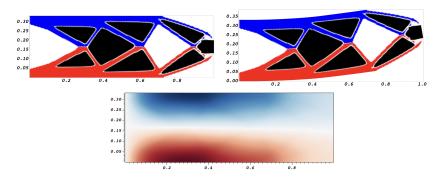


Figure: Composite plot of both material density and the heat source in the reference (top) and deformed configuration (bottom) for stiffness ratio $E_3/E_2=100$. The red and blue represent the area of the responsive material with heat source values 1 and -1 respectively.

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Conclusion

- Responsive optimal design
- Responsive optimal design with stimulus as a design variable
 - Least square objective function with *n* target displacements
 - ▶ A paper was submitted titled "Systematic design of compliant morphing structures: a phase-field approach".
- Responsive optimal design with stimulus as a state variable
 - Stimulus governed by Poisson PDE
- Stimulus governed by Transient heat PDE (Show some animations.)

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References

- S. Baldo, "Minimal interface criterion for phase transitions in mixtures of Cahn-Hilliard fluids," Annales de l'Institut Henri Poincaré C, Analyse non linéaire, vol. 7, no. 2, pp. 67–90, 1990.
- B. Bourdin and A. Chambolle, "The phase-field method in optimal design," Solid Mechanics and its Applications, pp. 207–216, Springer, June 2006.
- G. Dal Maso, An introduction to Γ-convergence. Boston: Birkhäuser. 1993.
- L. Modica and S. Mortola, "Un esempio di Γ-convergenza," Bollettino dell'Unione Matematica Italiana B (5), vol. 14, no. 1, pp. 285–299, 1977.
- J. Shabani, K. Bhattacrarya, and B. Bourdin, "Systematic design of compliant morphing structures: a phase-field approach," Applied Mathematics and Optimization, 2024 (Submitted for publication).
- A. Braides, \(\Gamma\)-convergence for beginners, vol. 22 of Oxford Lecture Series in Mathematics and its Applications. Oxford: Oxford University Press, 2002.
- G. Allaire, Shape optimization by the homogenization method. New York: Springer-Verlag, 2002.
- W. F. Simon and E. F. Patrick, "A framework for automated pde-constrained optimisation," CoRR, vol. abs/1302.3894, 2013.
- C. Andrej, Variational Methods for Structural Optimization.
 No. 140 in Applied Mathematical Sciences, Berlin: Springer Verlag, 2000.
 - A. Alexanderian and I. Sunseri. "Computing gradients and hessians using the adjoint method." North Carolina State

 A. Alexanderian and I. Sunseri. "Computing gradients and hessians using the adjoint method." North Carolina State

 Output

 Description:
- University, 2019.
- J. J. Moré and D. J. Thuente, "Line search algorithms with guaranteed sufficient decrease," ACM Transactions on Mathematical Software, vol. 20, no. 3, pp. 286–307, 1994.
- H. Rodrigue, W. Wang, B. Bhandari, and S.-H. Ahn, "Fabrication of wrist-like SMA-based actuator by double smart soft composite casting," Smart Materials and Structures, vol. 24, p. 125003, 2015.
- D. A. Ham, P. H. J. Kelly, L. Mitchell, C. J. Cotter, R. C. Kirby, K. Sagiyama, N. Bouziani, S. Vorderwuelbecke, T. J. Gregory, J. Betteridge, D. R. Shapero, R. W. Nixon-Hill, C. J. Ward, P. E. Farrell, P. D. Brubeck, I. Marsden, T. H. Gibson, M. Homolya, T. Sun, A. T. T. McRae, F. Luporini, A. Gregory, M. Lange, S. W. Funke, F. Rathgeber, G.-T. Bercea, and G. R. Markall, "Firedrake user manual," 5 2023.

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Thank You!

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