Optimal design and numerics

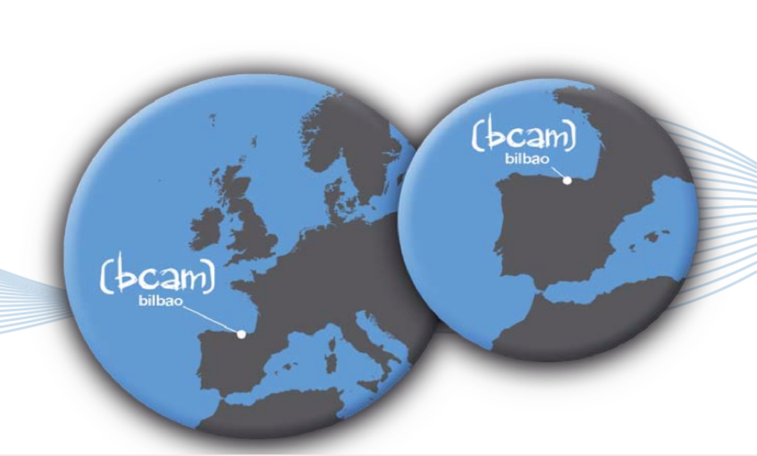
Enrique Zuazua

Ikerbasque & Basque Center for Applied Mathematics (BCAM)
Bilbao, Basque Country, Spain
zuazua@bcamath.org
http://www.bcamath.org/zuazua/

Workshop on multi-scale and high-contrast PDE: from modelling, to mathematical analysis, to inversion, Oxford, June 2011

Outline

Outline


(bcam)
bilbao
(bcam)
bilbao

Motivation

- Numerical methods for rapidly oscillating coefficients may fail to converge because of the resonance phenomena between the numerical mesh and the oscillating pattern of coefficients.
- This issue has to be taken into account carefully when dealing with numerics for homogenization problems.
- Optimal design problems often develop oscillating patterns.
- It is then natural to raise the issue of whether these resonances may also affect the convergence of numerical algorithms for optimal design.
- Generally speaking, there is a big gap between the existing theory for continuum analytical methods for optimal design and the numerical practice.

Outline

Motivation

- Numerical approximation methods for PDEs with rapidly oscillating coefficients.
- There is an extensive literature in which ideas and methods of classical Numerical Analysis (finite differences and elements) and Homogenization Theory are combined:
  Bensoussan-Lions-Papanicolaou, Sanchez-Palencia, Allaire, Cioranescu-Donato,....
  B. Engquist [1997,1998], Y. Efendiev, Th. Hou, X.Wu [1998,1999, 2002,2004], M. Matache, Babuška, Ch. Schwab [2000,2002], G. Allaire, C. Conca[1996], C. Conca, S. Natesan, M. Vanninathan [2001,2005], P. Gerard, P.A. Markowich, N. J. Mauser, F. Poupaud [1997], Kozlov [1986], Piatnitski, Remi [2001], ...

Some common facts:

- Multiscale analysis: Two scales are involved: ε for the size of the microstructure and h for that of the numerical mesh;
- As usual, three different regimes: $h << \varepsilon$, $h \sim \varepsilon$, $\varepsilon << h$;
- Slow convergence of standard approximations (finite elements, finite differences): $h << \varepsilon$.
- Resonances may occur when $\varepsilon \sim h$
- Convergence may be accelerated when the Galerkin method is built on bases adapted to the "topography" of the oscillating medium.

Two different issues:

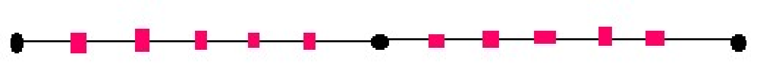
- Compute an efficient numerical approximation of the solution in the highly heterogeneous medium;
  Homogenization theory is a tool that helps doing that.
- Analyze the limit behavior as the characteristic size of the medium and the mesh-size tend to zero.

BUT A COMPLETE UNDERSTANDING OF THIS COMPLEX ISSUE NEEDS BOTH QUESTIONS TO BE ADDRESSED.

Convergence of the standard numerical methods improves when the numerical mesh samples the oscillating medium in an "ergodic way":
B. Engquist, Th. Hou [1989,1993], M.Avellaneda, Th. Hou, G. Papanicolaou [1991], Babuška, Osborn [2000].
In other words:

- According to classical homogenization theory: u^ε converges to the homogenized solution u^* as $\varepsilon \to 0$;
- This is not necessarily the case for the numerical solution u_h^ε as both $h, \varepsilon \to 0$.
- Under some ergodicity condition ($\varepsilon/h =$ irrational) $u_h^\varepsilon \to u^*$.

In [1] we explain what is going on when $\varepsilon/h =$ rational and how, using diophantine approximation, one can recover convergence for irrational ratios.



[1] R. Orive and E. Z. Finite difference approximations of homogenization problems for elliptic equations. Multiscale Modeling and Simulation: A SIAM Interdisciplinary Journal, 4 (1) (2005) pp. 36-87.

Problem formulation:

We consider the periodic elliptic equation associated to the following rapidly oscillating coefficients:

$$A^{\varepsilon} = -\frac{\partial}{\partial x_k}\left(a^{\varepsilon}_{k\ell}(x)\frac{\partial}{\partial x_\ell}\right),$$

with $a^{\varepsilon}_{k\ell}(x) = a_{k\ell}\left(x/\varepsilon\right)$, and $a_{k\ell}$ satisfying

$$\begin{cases} a_{kl} \in L^{\infty}_{\#}(Y) \text{ are } Y\text{-periodic}, \quad \text{where } Y =]0,1[^N, \\ \exists \alpha > 0 \text{ s.t.} \quad \sum_{k,\ell=1}^{N} a_{kl}(y)\eta_k\bar{\eta}_l \geq \alpha|\eta|^2, \quad \forall \eta \in \mathbf{C}^N, \\ a_{kl} = a_{lk} \quad \forall l,k = 1,\dots,N. \end{cases}$$

Homogenization: u^* limit of the solutions of $A^{\varepsilon}u^{\varepsilon} = f$, satisfies

$$A^* u^* = -\frac{\partial}{\partial x_k}\left(a^*_{k\ell}\frac{\partial u^*}{\partial x_\ell}\right) = f.$$

Discretization: Let $h = (h_1, \ldots, h_d)$ with

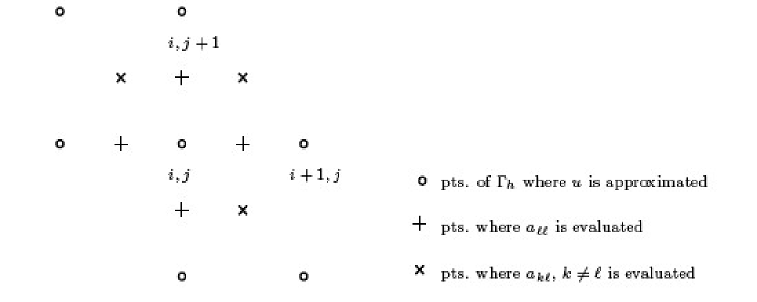
$$h_i = \frac{1}{n_i} \quad \text{with} \quad n_i \in \mathbf{N}.$$

The following is a natural numerical approximation scheme by finite-differences:

$$\sum_{i,j=1}^{d} -\nabla_i^{-h} \left[a_{ij}^{\varepsilon}(x(i,j)) \nabla_j^{+h} u_h^{\varepsilon}(x) \right] = f(x), \quad x \in \Gamma_h,$$

where Γ_h is the numerical mesh and

$$x(i,j) = x + \frac{1}{2} h_i e_i + (1 - \delta_{ij}) \frac{1}{2} h_j e_j.$$



Classical Numerical Analysis ensures

$$||u_h^\varepsilon - u^*|| \leq c\frac{h}{\varepsilon} + c'\varepsilon.$$

Note that, in particular, no convergence is guaranteed for $h \sim \varepsilon$.

Convergence under ergodicity:

In Avellaneda, Hou, Papanicolaou [1991] for the $1-d$ problem with Dirichlet conditions the following was proved:

Theorem

If f is continuous and bounded in $(0,1)$, then

$$\lim_{\epsilon,h\to 0} ||u_h^\epsilon - u^*||_\infty \to 0,$$

for sequences h,ϵ such that $h/\epsilon = r$ with r irrational.

Our goal:

- Analyze the behavior when ϵ/h=rational;
- Reprove the same result as in the Theorem above using diophantine approximation.
- Do it using explicit Bloch wave representations of solutions.

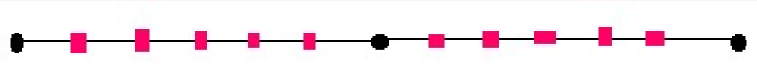
More precisely: what is the behavior of u_h^ϵ when

$$\frac{h}{\epsilon} = \frac{q}{p}, \qquad \text{with} \quad q, p \in \mathbf{N}, \quad \text{H.C.F.}(q,p) = 1,$$

and $h \to 0$????????????.

In this case the numerical mesh, despite of the fact that $h \to 0$, only samples a finite number of values in each periodicity cell of the coefficient $a(x)$. Thus, it is impossible that the numerical schemes recovers the continuous homogenized limit u^*. One rather expects a discrete homogenized limit $u^*_{q/p}$ such that

- $u^*_{q/p} \neq u^*$;
- $u^*_{q/p} \to u^*$ as $q/p \to r$, with r irrational.



Outline

Main $1-d$ result

Theorem

Assume that $a = a(x)$ *is Lipschitz, 1-periodic and* $\alpha \leq a(x) \leq \beta$. *Let* $\{u_h^\epsilon(x_i)\}_{i=0}^n$ *the approximation of* u^ϵ *with* $h/\epsilon = q/p$. *Then,*

$$||u_h^\epsilon - u_{q/p}^*||_\infty \leq c\, hp$$

Moreover, $u_{q/p}^*$ *is a discrete Fourier approximation with mesh-size* h *of the solution of*

$$\begin{cases} -a_p^* \dfrac{\partial^2 v}{\partial x^2}(x) = f(x), & 0 < x < 1, \\ v(0) = v(1) = 0, \end{cases}$$

with $a_p^* = \left(\frac{1}{p} \sum_{j=1}^{p} \frac{1}{a((j+1/2)/p)} \right)^{-1}$.

Recall that the continuous homogenized solution u^* is a solution of the same Dirichlet problem but with a continuous effective coefficient a^* defined as

$$a^* = \left(\int_0^1 (1/a(x)) dx \right)^{-1}.$$

Furthermore,

$$||u^*_{q/p} - u^*||_\infty \leq c' \frac{1}{p}.$$

In conclusion,

$$||u^\epsilon_h - u^*||_\infty \leq c\, hp + c'/p$$

where c and c' depend on α, β, $||a'||_\infty$ and $||f||_\infty$.
Note that, this estimate, together with diophantine approximation results, allows to recover convergence for h/ϵ irrational.
A similar result holds in the multi-dimensional case.

Outline

Continuous Bloch wave decomposition

Following the presentation by C. Conca & M. Vanninathan[2]:

Spectral problem family with parameter $\eta \in Y' = [-1/2, 1/2[^d$:

$$A\psi(\cdot;\eta) = \lambda(\eta)\psi(\cdot;\eta) \quad \text{in} \quad \mathbf{R}^d,$$

$\psi(\cdot;\eta)$ is (η, Y)-periodic, i.e., $\psi(y + 2\pi m;\eta) = e^{2\pi i m\cdot\eta}\psi(y;\eta)$.

$\psi(y;\eta) = e^{iy\cdot\eta}\phi(y;\eta)$, ϕ being Y-periodic in the variable y.

[2] C. Conca and M. Vanninathan, *Homogenization of periodic structures via Bloch decomposition*, SIAM J. Appl. Math., 57 (1997), pp. 1639–1659.

A discrete sequence of eigenvalues with the following properties exists:

$$\begin{cases} 0 \leq \lambda_1(\eta) \leq \cdots \leq \lambda_n(\eta) \leq \cdots \to \infty, \\ \lambda_m(\eta) \text{ is a Lipschitz function of } \eta \in Y', \forall m \geq 1. \end{cases}$$

$$\lambda_2(\eta) \geq \lambda_2^{(N)} > 0, \quad \forall \eta \in Y',$$

where $\lambda_2^{(N)} > 0$ is the second eigenvalue of A in the cell Y with Neumann boundary conditions.
The eigenfunctions $\psi_m(\cdot;\eta)$ and $\phi_m(\cdot;\eta)$, form orthonormal bases in the subspaces of $L^2_{loc}(\mathbf{R}^d)$ of (η, Y)-periodic and Y-periodic functions, respectively.

$$\lambda_m^\varepsilon(\xi) = \varepsilon^{-2}\lambda_m(\varepsilon\xi), \qquad \phi_m^\varepsilon(x;\xi) = \phi_m(\frac{x}{\varepsilon};\varepsilon\xi).$$

Given f, the mth Bloch coefficient of f at the ϵ scale:

$$\widehat{f}_m^\epsilon(k) = \int_Y f(x)e^{-ik\cdot x}\overline{\phi_m^\epsilon}(x;k)dx \quad \forall m \geq 1,\ k \in \Lambda_\epsilon,$$

$$\Lambda_\epsilon = \{k = (k_1,\dots,k_d) \in \mathbb{Z}^d : [-1/2\epsilon] + 1 \leq k_i \leq [1/2\epsilon]\}.$$

$$f(x) = \sum_{k\in\Lambda_\epsilon}\sum_{m\geq 1}\widehat{f}_m^\epsilon(k)e^{ik\cdot x}\phi_m^\epsilon(x;k).$$

$$\int_Y |f(x)|^2 dx = \sum_{k\in\Lambda_\epsilon}\sum_{m\geq 1}|\widehat{f}_m^\epsilon(k)|^2.$$

$$\lambda_m^\epsilon(k)\widehat{u}_m^\epsilon(k) = \widehat{f}_m^\epsilon(k), \quad \forall\, m \geq 1,\ k \in \Lambda_\epsilon.$$

$$u^{\varepsilon}(x) = \sum_{k\in\Lambda_\epsilon} \sum_{m=1}^{\infty} \frac{\widehat{f}_m^{\epsilon}(k)}{\lambda_m(\epsilon k)/\epsilon^{-2}} e^{ik\cdot x} \phi_m^{\varepsilon}(x;k).$$

$$u^{\varepsilon}(x) \sim \epsilon^2 \sum_{k\in\Lambda_\epsilon} \frac{\widehat{f}_1^{\epsilon}(k)}{\lambda_1(\epsilon k)} e^{ik\cdot x} \phi_1^{\varepsilon}(x;k).$$

$$c_1|\eta|^2 \leq \lambda_1(\eta) \leq c_2|\eta|^2, \quad \forall \eta \in Y',$$
$$\lambda_1(0) = \partial_k \lambda_1(0) = 0, k = 1, \ldots, N,$$
$$\partial^2_{k\ell}\lambda_1(0) = 2a^*_{k\ell}, k, \ell = 1, \ldots, N,$$

where $a^*_{k\ell}$ are the homogenized coefficients.

$$\eta \in B_\delta \to \phi_1(y;\eta) \in L^\infty \cap L^2_\#(Y) \text{ is analytic},$$
$$\phi_1(y;0) = (2\pi)^{-\frac{d}{2}}.$$
$$\widehat{f}_1^\varepsilon(k) \sim \widehat{f}_k$$
$$\widehat{u}_1^\varepsilon(k) \sim \widehat{u}_k^* \qquad \text{as } \epsilon \to 0,$$
$$u^\varepsilon(x) \sim \sum_{k\in\Lambda_\epsilon} \frac{\widehat{f}_1^\epsilon(k)}{\lambda_1(\epsilon k)/\epsilon^{-2}} e^{ik\cdot x}\phi_1^\varepsilon(x;k) \sim \sum_{k\in\mathbb{Z}^d} \frac{\widehat{f}^k}{a^*_{ij}k_ik_j} e^{ik\cdot x}$$

which is the solution of the homogenized problem in its Fourier representation.

Outline

Discrete Bloch waves

- In $1-d$ one can use the explicit representation formula for discrete solutions. But, of course, this is impossible for multi-dimensional problems.
- In $1-d$ the homogenized coefficient a^* can be computed explicitly as above. But in several space dimensions, the homogenized coefficients depend on test functions χ_k that are defined by solving elliptic problems on the unit cell.
- In several space dimensions Bloch wave expansions can be used to derive explicit representation formulas and to prove homogenization. This is the method we shall employ to derive our results.

Explicit $1-d$ computations.

$$\begin{cases} -a_i^\epsilon u_{i+1}^\epsilon + (a_i^\epsilon + a_{i-1}^\epsilon) u_i^\epsilon - a_{i-1}^\epsilon u_{i-1}^\epsilon = h^2 f_i, \quad 1 \le i \le n-1, \\ u_0^\epsilon = b, \quad u_n^\epsilon = c. \end{cases}$$

Therefore,

$$u_i^\epsilon = b + U_0^{\epsilon,h} \sum_{j=1}^{i} \frac{h}{a_j^\epsilon} - \sum_{j=1}^{i} \frac{h}{a_j^\epsilon} \sum_{k=1}^{j} h f_k \quad 1 \le i \le n-1,$$

with $$U_0^{\epsilon,h} = a_h^{\epsilon,*}(c-b) + a_h^{\epsilon,*} \sum_{j=1}^{n-1} \left(\frac{1}{a_j^\epsilon} \sum_{k=1}^{j} h^2 f_k \right),$$

and $$a_h^{\epsilon,*} = \left(\sum_{j=0}^{n-1} \frac{h}{a_j^\epsilon} \right)^{-1}.$$

Using that $a_{p+i}^\epsilon = a_i^\epsilon$, $a_h^{\epsilon,*} \to a_p^*$ (with explicit estimates).

DISCRETE BLOCH WAVE METHOD: $1-d$

Since $h/\epsilon = q/p$, $a^\epsilon(x+ph) = a^\epsilon(x)$, $\quad x \in \Gamma_h$

$$\Gamma_h^p = \{x = zh : \quad 0 \leq z < p, \quad z \in \mathbb{Z}\}$$

$$f(x,k) = hp^{\frac{1}{2}} \sum_{z \in \Gamma_{hp}} f(x+z) e^{-i2\pi k\cdot(x+z)}, \quad k \in \Lambda_{q\epsilon},$$

$$\Lambda_{q\epsilon} = \left\{ k \in \mathbb{Z}^d, \text{ such that } \left[\frac{-1}{2q\epsilon}\right] + 1 \leq k \leq \left[\frac{1}{2q\epsilon}\right] \right\}.$$

The discrete Bloch waves are defined by the family of eigenvalue problems:

$$-\nabla^{-h}\left[a^\epsilon(x)\nabla^{+h}(e^{i2\pi x\cdot\xi}\phi_h^\epsilon(x,\xi))\right] = \lambda(\xi)e^{ix\cdot\xi}\phi_h^\epsilon(x,\xi), \quad x \in \Gamma_h^p,$$
$$\phi_h^\epsilon(x,\xi) \text{ is } ph\text{-periodic in } x, \text{ i.e.,} \quad \phi_h^\epsilon(x+ph,\xi) = \phi_h^\epsilon(x,\xi).$$

There exist a sequence $\lambda_1(\xi), ..., \lambda_p(\xi) \geq 0$ and their eigenfunctions $\{\phi^{\epsilon}_{h,m}(x,\xi)\}_{m=1}^{p}$.

$$\lambda_m(\xi) \geq \frac{c}{\epsilon^2 q^2} > 0, \quad m \geq 2$$

$$\xi \in B_\delta \mapsto (\lambda_1(\xi), \phi_1(\cdot,\xi)) \in \mathbf{R} \times \mathbf{C}^p \text{ is analytic.}$$

$$\phi_1(y,0) = p^{-1/2}$$

$$\lambda_1(0) = \partial\lambda_1(0) = 0, \partial^2\lambda_1(0) = \left(\frac{1}{p}\sum_{i=1}^{p}\frac{1}{a\left(\left(i+0.5\right)/p\right)}\right)^{-1}.$$

This method allows obtaining sharp estimates on both $||u_h^\epsilon - u_{q/p}^*||$ and $||u^* - u_{q/p}^*||$.
Indeed,

- All solutions involved can be represented in a similar form by means of Bloch wave expansions;
- The contribution of Bloch components $m \geq 2$ is uniformly negligible;
- The dependence of the first Bloch component, both in what concerns the eigenvalue and eigenfunction, can be estimated very precisely in terms of the various parameters.

Outline

1. Motivation
2. Numerics for Homogenization
   - Motivation
   - The $1-d$ case
   - The continuous Bloch wave decomposition
   - The Discrete Bloch wave decomposition
   - Conclusion
3. Numerics for some (toy) optimal design problems
   - An example
   - A $1-d$ model for mixtures
   - $1-d$ relaxation
   - Finite element approximation
4. Concluding remarks

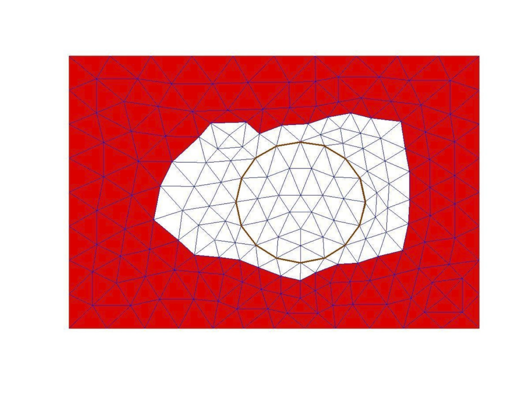
Conclusion

- Discrete Bloch waves allow getting a complete representation formula for the numerical approximations when h/ϵ is rational.
- This allows deriving the discrete homogenized solution with convergence rates.
- The discrete homogenized problem has the same structure as the continuous one but with different effective coefficients.
- The distance between the discrete and continuous effective coefficients can be estimated as well.
- This allows recovering, with convergence rates, results on numerical homogenization under ergodicity conditions.

Outline

An example

The finite element approximation to $2-d$ optimal design problems for the Dirichlet Laplacian. [3] [4]



[3] V. Šveràk, *On optimal shape design*, JMPA, 72, 1993, pp. 537-551.

[4] D. Chenais and E. Z. *Finite Element Approximation of 2D Elliptic Optimal Design*, JMPA, 85 (2006), 225-249.

Outline

A model for mixtures

For a given bounded open set Ω of $\mathbb{R}^N$, $N \geq 1$, consider the optimization problem [5]

$$(P) \begin{cases} \text{Find } \omega_0 \in \mathcal{U} \text{ such that} \\ \mathcal{J}(\omega_0) = \min_{\omega \in \mathcal{U}} \mathcal{J}(\omega), \end{cases}$$

with

$$\mathcal{U} = \{\omega \subset \Omega : \ \omega \text{ measurable }, \quad |\omega| \leq \kappa\},$$

$$\mathcal{J}(\omega) = \int_\omega F_1(x, u_\omega, \nabla u_\omega)\, dx + \int_{\Omega \setminus \omega} F_2(x, u_\omega, \nabla u_\omega)\, dx,$$

where $F_1, F_2 : \Omega \times \mathbb{R} \times \mathbb{R}^N \to \mathbb{R}$, the source term $f : \Omega \to \mathbb{R}$ and the material constants α and β are given, and

$$u_\omega \in H_0^1(\Omega); \quad -\mathrm{div}\Big((\alpha\chi_\omega + \beta(1-\chi_\omega))\, \nabla u_\omega \Big) = f \quad \text{in } \Omega. \quad (1)$$

[5] J. Casado-Díaz, C. Castro, M. Luna-Laynez and E. Z., Numerical approximation of a one-dimensional elliptic optimal design problem, SIAM J. Multiscale Analysis, to appear.

(P) has not a solution in general $\rightarrow$ Relaxation. [6] [7]

- Replace the characteristic function χ_ω by a measurable function θ with values in $[0,1]$.
- Replace the function $(\alpha\chi_\omega + \beta(1-\chi_\omega))$ in the elliptic PDE by a matrix function A in the set $\mathcal{K}(\theta)$ of matrices constructed by homogenization mixing the materials α and β with respective proportions θ and $1-\theta$.
- The corresponding state is denoted by $u_{\theta,A}$.
- Replace the cost functional $\mathcal{J}$ by another one of the form

$$\hat{\mathcal{J}}(\theta, A) = \int_\Omega H(x, u_{\theta,A}, \nabla u_{\theta,A}, A\nabla u_{\theta,A}, \theta)\, dx,$$

where H is a function known explicitly only in a few cases $(N=1,\ F_i(x,s,\xi) = |\xi|^2, \ldots)$.

[6] F. Murat. *Un contre-example pour le problème du contrôle dans les coefficients.* C.R.A.S Sci. Paris A 273 (1971), 708-711.

[7] F. Murat, L. Tartar. *H-convergence.* In *Topics in the Mathematical Modelling of Composite Materials*, ed. by L. Cherkaev, R.V. Kohn. Progress in Nonlinear Diff. Equ. and their Appl., 31, Birkaüser, Boston, 1998, 21-43.

In practice it would be very natural to:

- Discretize (by FEM, for instance) the problem using finite element approximations of the PDE and the functional under consideration.
- Search for the discrete optimal shape design (finite-dimensional problem).
- "Hope" that, as the mesh-size tends to zero, the discrete optimal shape will converge to the continuous one.

CONTINUOUS SOLUTION OF THE OPTIMAL DESIGN PROBLEM

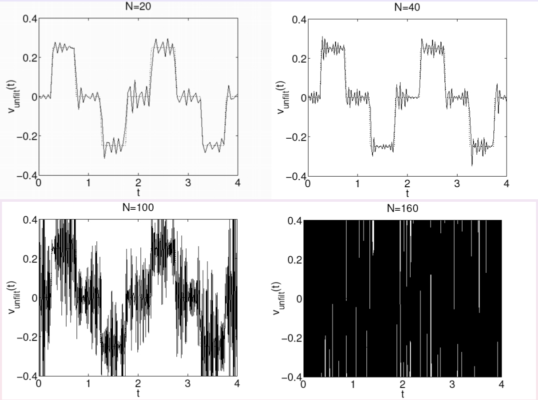
$+$

CONVERGENT ALGORITHM FOR SOLVING THE PDE

$=$

CONVERGENT ALGORITHM FOR OPTIMAL SHAPES?????

NOT NECESSARILY !!!!



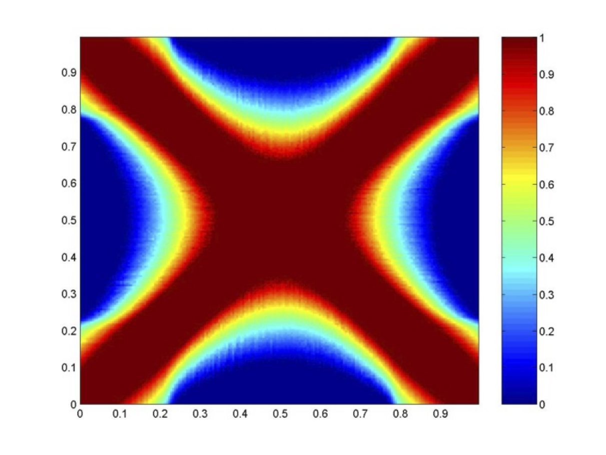
E. Z., SIAM Review, 47 (2) (2005), 197-243.

Two (main) strategies for discretization:

- **Discrete approach:** Discretize directly the original problem.
- **Continuous approach:** Discretize the relaxed formulation.

We analyze the $1-d$ problem $N=1$ showing that the continuous approach provides a better approximation and a faster convergence rate with a lower computational cost.

Both approaches, discrete and continuous, were successfully developed in [8] but no convergence rates were obtained.



[8] J. Casado-Díaz, J. Couce-Calvo, M. Luna-Laynez, J.D. Martín-Gómez. *Optimal design problems for a non-linear cost in the gradient: numerical results*. Applicable Anal. 87 (2008), 1461-1487.

Outline

Theorem

A relaxation of problem (P) is given by

$$(\hat{P}) \qquad \text{Find } \theta_0 \in \hat{\mathcal{U}} \text{ such that } \hat{\mathcal{J}}(\theta_0) = \min_{\theta \in \hat{\mathcal{U}}} \hat{\mathcal{J}}(\theta),$$

$$\hat{\mathcal{U}} = \left\{ \theta \in L^\infty(0,1;[0,1]) \ : \ \int_0^1 \theta dx \le \kappa \right\},$$

and $\hat{\mathcal{J}} : \hat{\mathcal{U}} \longrightarrow \mathbb{R}$ *is defined by*

$$\hat{\mathcal{J}}(\theta) = \int_0^1 \left(\theta F_1 \left(x, u_\theta, \frac{M_\theta}{\alpha} \frac{du_\theta}{dx} \right) + (1-\theta) F_2 \left(x, u_\theta, \frac{M_\theta}{\beta} \frac{du_\theta}{dx} \right) \right) dx,$$

for every $\theta \in \hat{\mathcal{U}}$, *with* $M_\theta = \left(\frac{\theta}{\alpha} + \frac{1-\theta}{\beta} \right)^{-1}$ *and* $u_\theta \in H_0^1(0,1)$ *the solution of*

$$-\frac{d}{dx} \left(M_\theta \frac{du_\theta}{dx} \right) = f \quad \text{in } (0,1).$$

For $r > 0$, we consider a partition $\mathcal{Q}^r = \{y_k\}_{k=0}^{m_r}$ of $[0,1]$, with

$$r = \max_{1 \leq k \leq m_r} \left(y_k - y_{k-1} \right).$$

We now approximate both optimal design problems, the original and the relaxed one, but we do it in a stratified manner, in two levels, increasing complexity and making the method better adapted to simulation practices.

- **Approximation level #1:** Continuous PDE but discrete control sets or coefficients.
- **Approximation level #2:** Discrete approximation of PDE and also discrete control sets or coefficients.

Discrete Approach, Level #1:

$$(P^r) \qquad \text{Find } \omega_0^r \in \mathcal{U}^r \text{ such that } \mathcal{J}(\omega_0^r) = \min_{\omega \in \mathcal{U}^r} \mathcal{J}(\omega)$$

where

$$\mathcal{U}^r = \left\{ \omega \in \mathcal{U} \,:\, \exists J \subset \{1 \ldots, m_r\} \text{ such that } \omega = \cup_{k \in J} (y_{k-1}, y_k) \right\}.$$

Continuous Approach, Level #1:

$$(\hat{P}^r) \qquad \text{Find } \theta_0^r \in \hat{\mathcal{U}}^r \text{ such that } \hat{\mathcal{J}}(\theta_0^r) = \min_{\theta \in \hat{\mathcal{U}}^r} \hat{\mathcal{J}}(\theta)$$

where

$$\hat{\mathcal{U}}^r = \left\{ \theta \in \hat{\mathcal{U}} \,:\, \theta \text{ constant in every } (y_{k-1}, y_k) \right\}.$$

Theorem

[Discrete Approach, Level #1]

Problem (P^r) has a solution for every $r > 0$, and we have

$$0 \leq \min_{\omega \in \mathcal{U}^r} \mathcal{J}(\omega) - \inf_{\omega \in \mathcal{U}} \mathcal{J}(\omega) \leq C r^{\frac{1}{2}}.$$

Moreover, if for some integer $\ell \geq 1$, we have that f belongs to $W^{\ell,1}(0,1)$ and $F_i(x,s,\xi)$ is independent of s and belong to $C^{\ell,1}_{loc}([0,1] \times \mathbb{R})$, then we have

$$0 \leq \min_{\omega \in \mathcal{U}^r} \mathcal{J}(\omega) - \inf_{\omega \in \mathcal{U}} \mathcal{J}(\omega) \leq C r^{\frac{\ell+1}{\ell+2}}.$$

Theorem

[Continuous Approach, Level #1]

Problem $(\hat{P}^r)$ *has a solution for every* $r > 0$*, and we have*

$$0 \leq \min_{\theta \in \hat{\mathcal{U}}^r} \hat{\mathcal{J}}(\theta) - \inf_{\omega \in \mathcal{U}} \mathcal{J}(\omega) = o(r).$$

Moreover, if problem $(\hat{P})$ *has a solution* θ_0 *in* $BV(0,1)$*, then*

$$0 \leq \min_{\theta \in \hat{\mathcal{U}}^r} \hat{\mathcal{J}}(\theta) - \inf_{\omega \in \mathcal{U}} \mathcal{J}(\omega) \leq Cr^2.$$

Remark

- The convergence rate for $(\hat{P}^r)$ is better than the one for (P^r).
- These convergence rates are sharp.
- Problem $(\hat{P}^r)$ is simpler to solve because the set of controls $\hat{\mathcal{U}}^r$ is convex.
- This is true even in those cases where problem (P) has a classical solution, and therefore a relaxation is not necessary.

Outline

Now we consider a full discretization of problem (P), where not only we discretize the set of controls but we also approximate the state equation and the cost functional.

For $h>0$, we set $r=\sqrt{h}$ and take two partitions $\mathcal{Q}^h=\{x_i\}_{i=0}^{n_h}$, $\mathcal{Q}^r=\{y_k\}_{k=0}^{m_r}$ of $[0,1]$, with $\mathcal{Q}^r\subset\mathcal{Q}^h$ and

$$h=\max_{1\le i\le n_h}(x_i-x_{i-1}),\quad r=\max_{1\le k\le m_r}(y_k-y_{k-1}),$$

and we define

$$W^h=\{v\in C_0^0([0,1])\,:\,v \text{ is affine on every } (x_{i-1},x_i)\}.$$

For $\theta \in \hat{\mathcal{U}}$, constant in every (x_{i-1}, x_i), we define $\tilde{u}_\theta \in W^h$ by

$$\int_0^1 M_\theta \frac{d\tilde{u}_\theta}{dx}\frac{dv}{dx}dx = \int_0^1 fvdx, \quad \forall v \in W^h$$

and

$$\hat{\mathcal{J}}^h(\theta) = \int_0^1 \left(\theta F_1\left(x, \tilde{u}_\theta, \frac{M_\theta}{\alpha}\frac{d\tilde{u}_\theta}{dx}\right) + (1-\theta)F_2\left(x, \tilde{u}_\theta, \frac{M_\theta}{\beta}\frac{d\tilde{u}_\theta}{dx}\right)\right) dx$$

For $\omega \in \mathcal{U}$, with $\omega = \cup_{i\in J}(x_{i-1}, x_i)$, $J \subset \{1 \ldots, n_h\}$, we denote $\tilde{u}_\omega = \tilde{u}_{\chi_\omega}$ and define

$$\mathcal{J}^h(\omega) = \int_\omega F_1\left(x, \tilde{u}_\omega, \frac{d\tilde{u}_\omega}{dx}\right) dx + \int_{(0,1)\backslash\omega} F_2\left(x, \tilde{u}_\omega, \frac{d\tilde{u}_\omega}{dx}\right) dx$$

Discrete Approach – Full Discretization:

(P_c^h) Find $\omega_0^h \in \mathcal{U}^h$ such that $\mathcal{J}^h(\omega_0^h) = \min_{\omega \in \mathcal{U}^h} \mathcal{J}^h(\omega)$

where

$$\mathcal{U}^h = \{\omega \in \mathcal{U} \,:\, \exists J \subset \{1\ldots, n_h\} \text{ such that } \omega = \cup_{i \in J}(x_{i-1}, x_i)\}$$

Continuous Approach – Full Discretization:

$(\hat{P}_c^h)$ Find $\theta_0 \in \hat{\mathcal{U}}^{\sqrt{h}}$ such that $\hat{\mathcal{J}}^h(\theta_0) = \min_{\theta \in \hat{\mathcal{U}}^r} \hat{\mathcal{J}}^h(\theta)$

where

$$\hat{\mathcal{U}}^r = \{\theta \in \hat{\mathcal{U}} \,:\, \theta \text{ constant in every } (y_{k-1}, y_k)\}$$

Theorem

[Discrete approach]

Problem (P_c^h) *has a solution for every* $h > 0$. *Moreover, every solution* ω_0 *satisfies*

$$0 \leq \mathcal{J}(\omega_0) - \inf_{\omega \in \mathcal{U}} \mathcal{J}(\omega) \leq C h^{\frac{1}{2}}.$$

Moreover, if for some nonnegative integer ℓ, *we have that* f *belongs to* $W^{\ell,1}(0,1)$ *and* $F(x,s,\xi)$ *is independent of* s *and belong to* $C^{\ell,1}_{loc}([0,1]\times\mathbb{R})$, *then we have*

$$0 \leq \mathcal{J}(\omega_0) - \inf_{\omega \in \mathcal{U}} \mathcal{J}(\omega) \leq C h^{\frac{\ell+1}{\ell+2}}.$$

Theorem

[Continuous approach]

Problem $(\hat{P}_c^h)$ has a solution for every $h > 0$. Moreover, if we assume that exists an optimal control of bounded variation for $(\hat{P})$, then every θ_0 solution of $(\hat{P}_c^h)$ satisfies

$$0 \leq \mathcal{J}(\theta_0) - \inf_{\omega \in \mathcal{U}} \mathcal{J}(\omega) \leq C h.$$

Remark

- In the discrete approach, based on the unrelaxed formulation, the PDE and the control are discretized in the same fine grid of size h.
- The continuous full discretization, implemented on the relaxed version, constitutes a bigrid strategy: The PDE is discretized in the fine grid of size h while the control is discretized in the coarse one of size $\sqrt{h}$. And it gives a faster convergence with a lower computational cost !

The methods of proof combine:

- Fine properties on the dependence of the $1-d$ elliptic problem on its coefficients.
- Convergence properties of the FEM.
- Oscillatory constructions of bang-bang oscillating functions towards relaxation.

Bang-bang postprocessing of relaxed numerical shapes

Relaxed numerical coefficient profiles can be approximated by classical piecewise constant bang-bang functions, repredsenting pure mixtures.

Assume $f \in L^{\infty}(0,1)$ and

$$\theta = \sum_{k=1}^{m_r} t_k \chi_{(y_{k-1}, y_k)} \in \hat{\mathcal{U}}^r,$$

with $t_k \in [0,1]$ for every $k \in \{1, \ldots, m_r\}$. Set

$$j_k = \left[\frac{y_k - y_{k-1}}{r^2} \right] + 1, \; s_k = \frac{y_k - y_{k-1}}{j_k}, \quad \forall\, k \in \{1, \ldots, m_r\},$$

$$\omega = \bigcup_{k=1}^{m_r} \bigcup_{i=1}^{j_k} (y_{k-1} + (i-1)s_k, y_{k-1} + (i-1+t_k)s_k). \tag{2}$$

Then, we have

$$\left| \hat{\mathcal{J}}(\theta) - \mathcal{J}(\omega) \right| = \left| \hat{\mathcal{J}}(\theta) - \hat{\mathcal{J}}(\chi_\omega) \right| \leq Cr^2. \tag{3}$$

Concluding remarks

- There is a big gap between the existing theory for continuum analytical methods for optimal design and the numerical practice.
- We have shown that numerics and oscillating coefficients easily produce resonances.
- Optimal design problems are often better behaved since numerics is capable of finding the microstructure that minimization sequences develop.
- There are several ways of discretizing the optimal design problems and the convergence rate may differ from one to another.
- The use of relaxed formulations may help in improving the convergence rates..
- A LOT is still to be done....