HOMOGENIZATION

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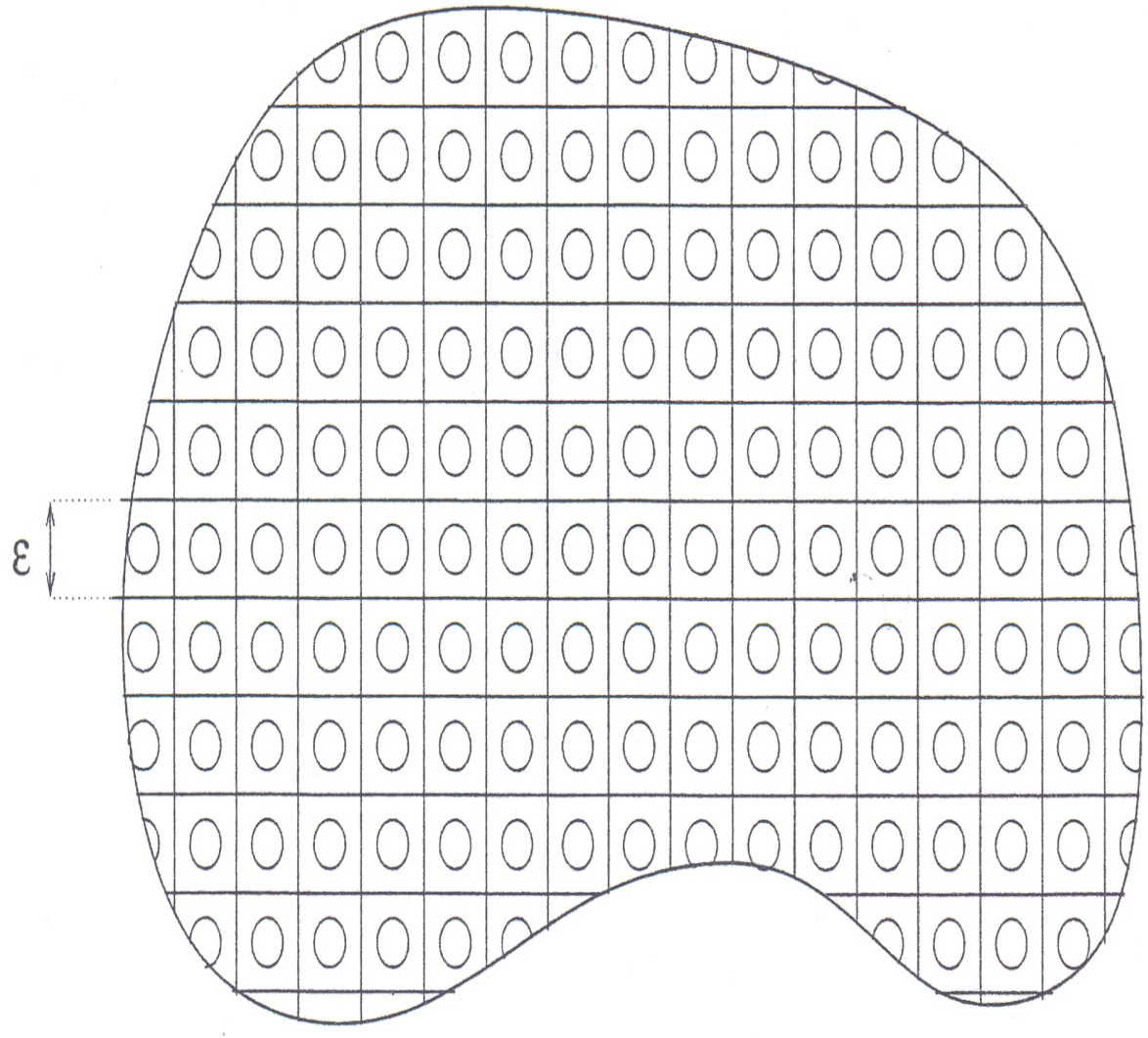
I wish to talk to you about **complex systems (inhomogeneous media)** and optimization problems with them.Complexity enters the picture through inhomogeneities in the media (e-g:composite materials).
Goal: Approximation of such media. These media have microstructures defined by the location of inhomogeneities and they influence the behaviour. How to design them suitably to achieve the desired behaviour of the medium.More generally, we wish to know all possibilities of design available by varying microstructurs.

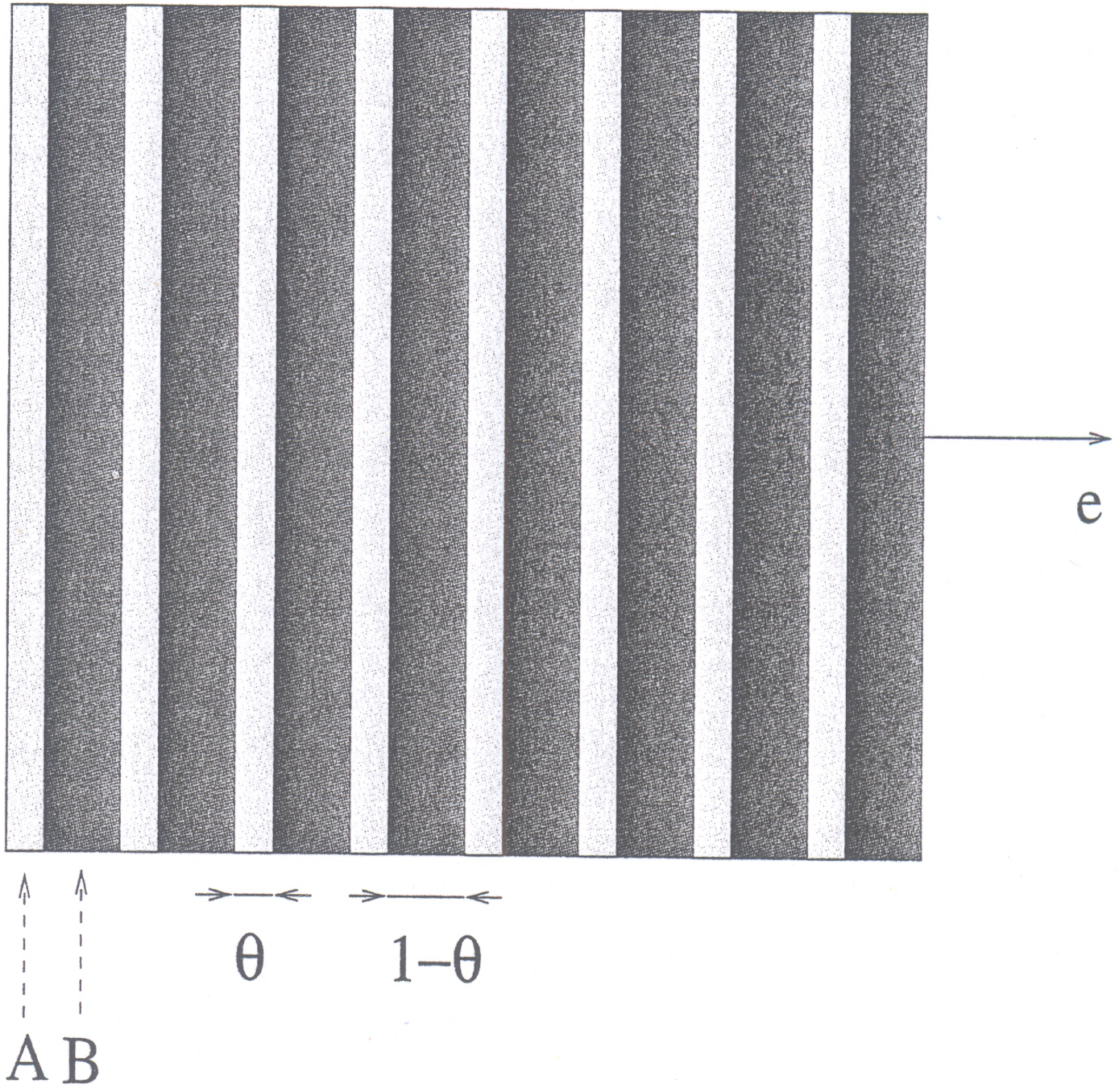
This classical problem calls for certain new mathematical notions and some progress has been achieved.My aim is to present some of these ideas and also recent developments.

Examples of complex media/microstructures (Mixing process): Laminates, Periodic structures, Hashin-Shtrikman structures, etc. with two phases:

$$A^\epsilon(x) = a_1 \chi_{\omega_{A^\epsilon}}(x) + a_2 \left(1 - \chi_{\omega_{A^\epsilon}}(x)\right)$$

In pictures, we can easily see the set ω_{A^ϵ} and its complement.


ε
Ω


e
θ
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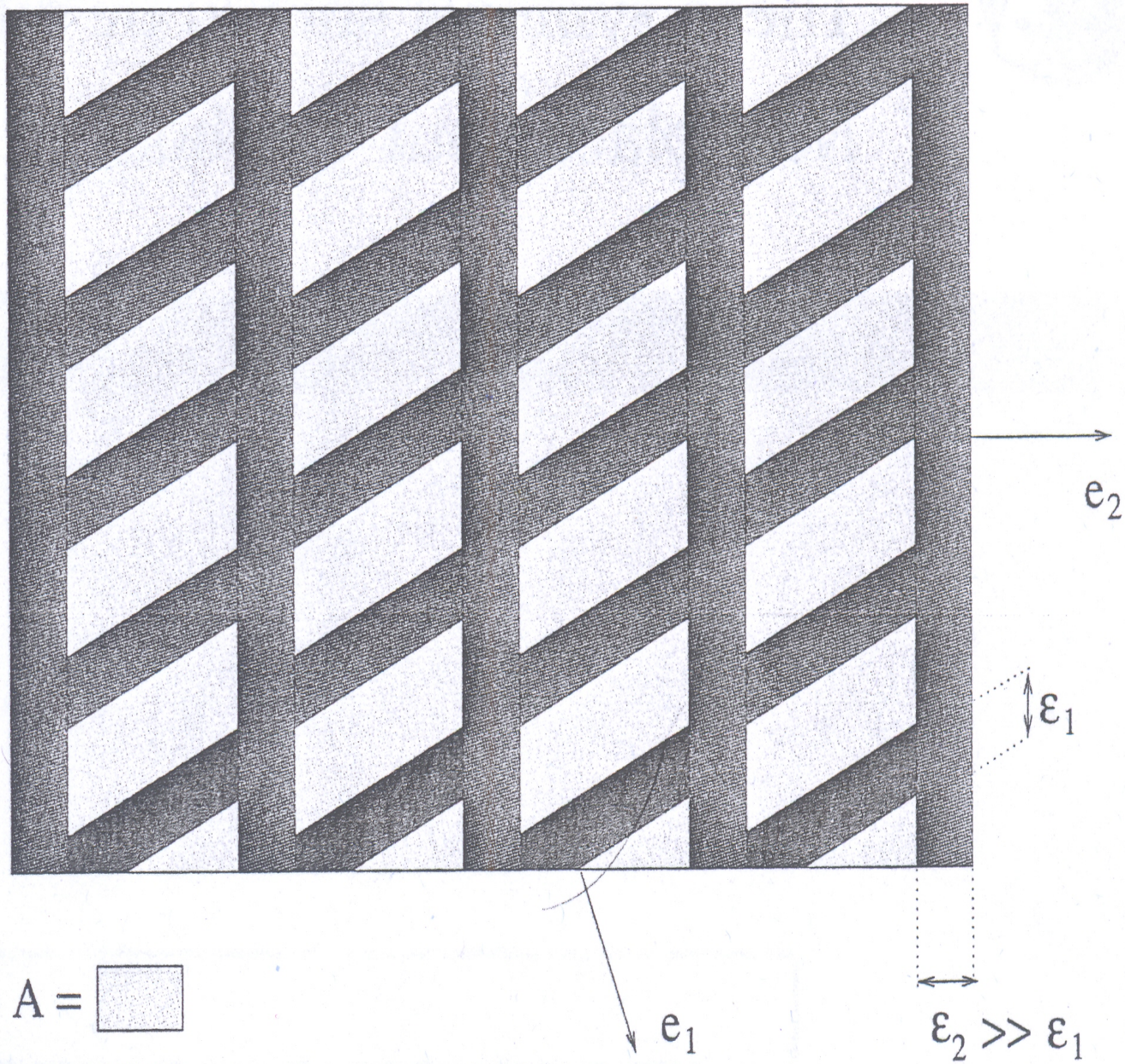
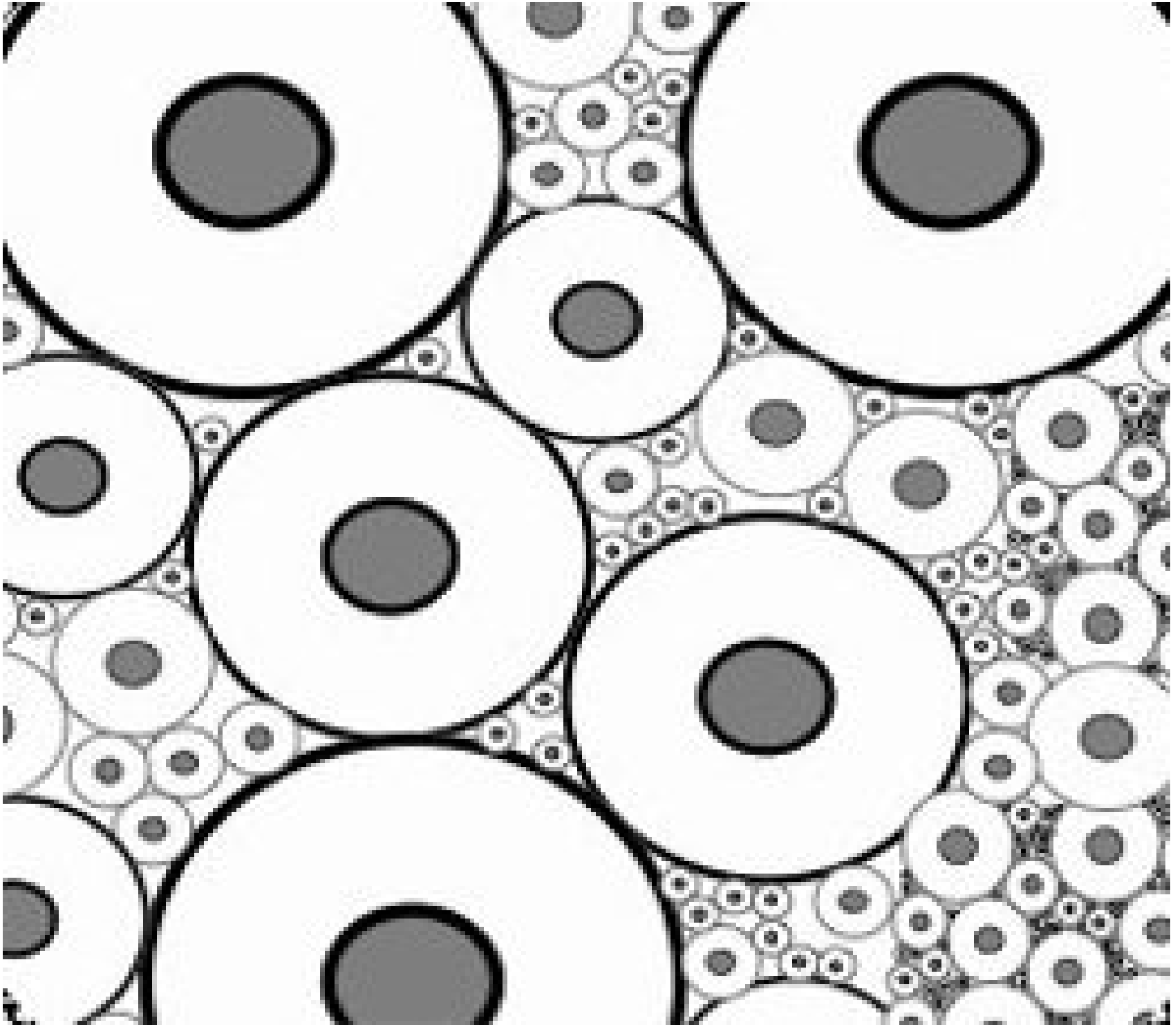
A B


e_2
ε_1
e_1
$\varepsilon_2 >> \varepsilon_1$
A =
B =



Direct Numerical Simulations (DNS) is very difficult in such media. Solutions develop "horns", across inhomogeneities and which are more pronounced as the strength of inhomogeneities increases.

So we need to approximate complex media by simpler ones. What is the right concept of approximation? **Convergence of materials** , Topology among the family of materials. This is different from convergence of functions.

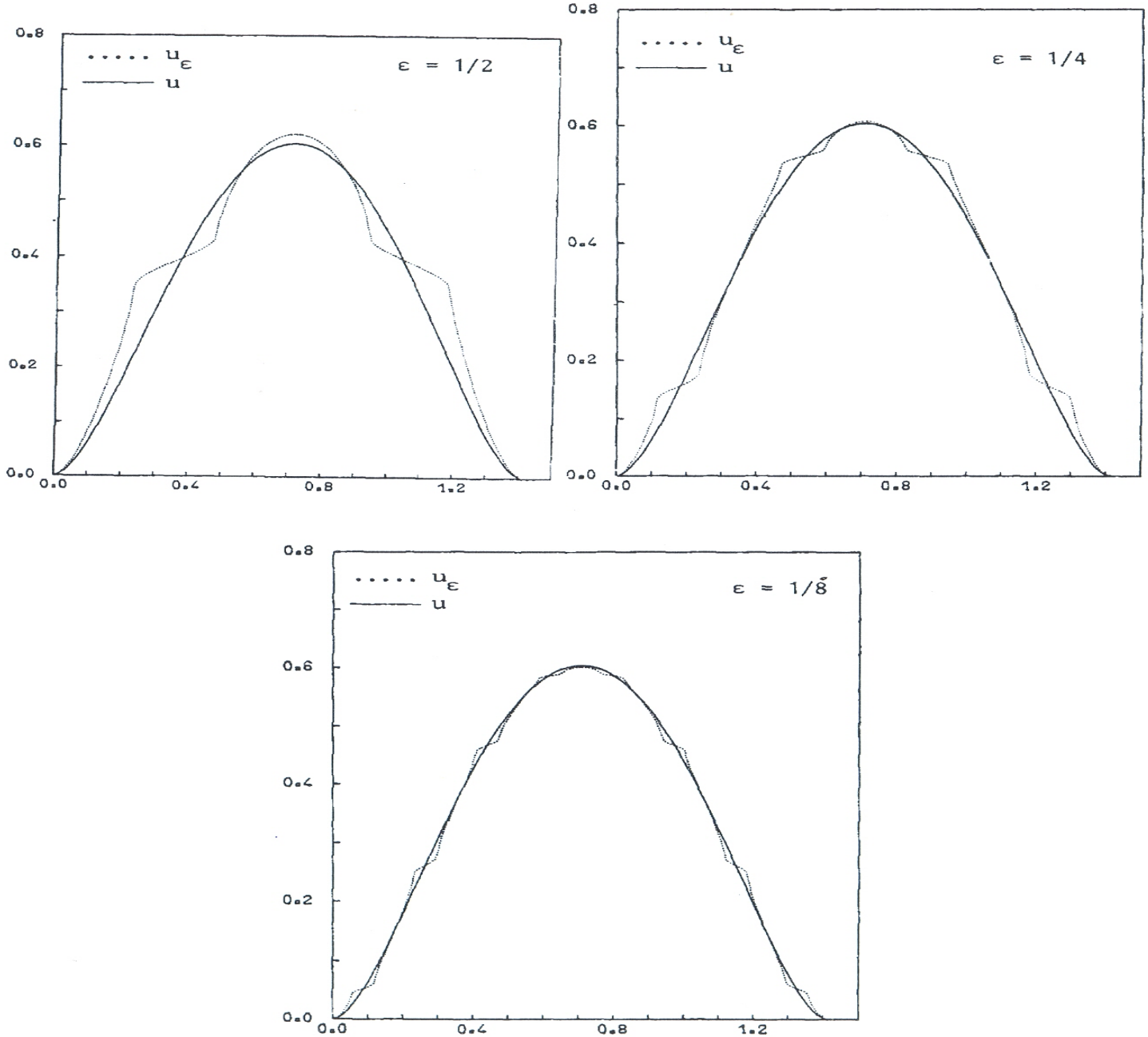


Figure 12 - Comparison of u_ε with u for λ = 10.

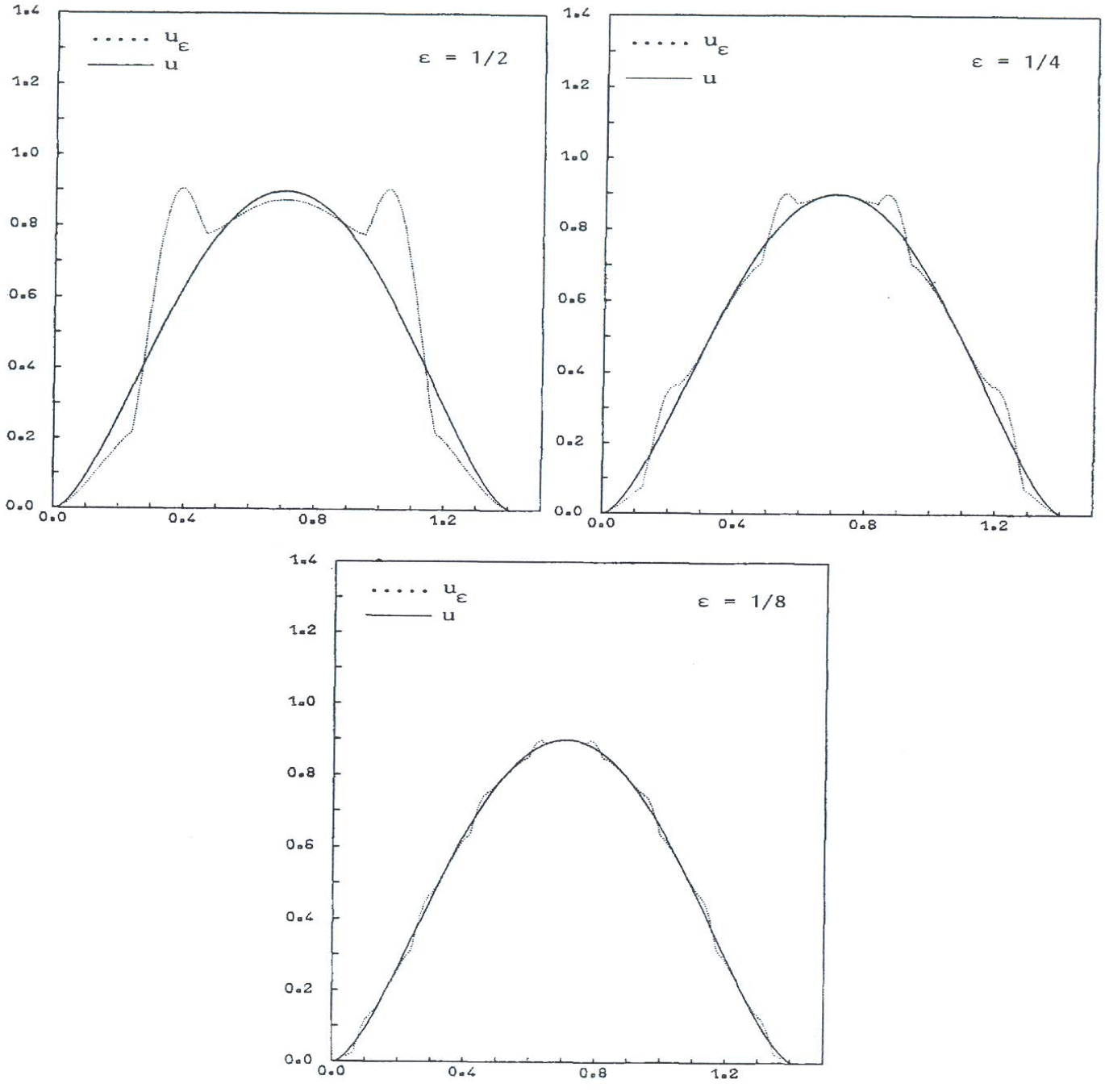
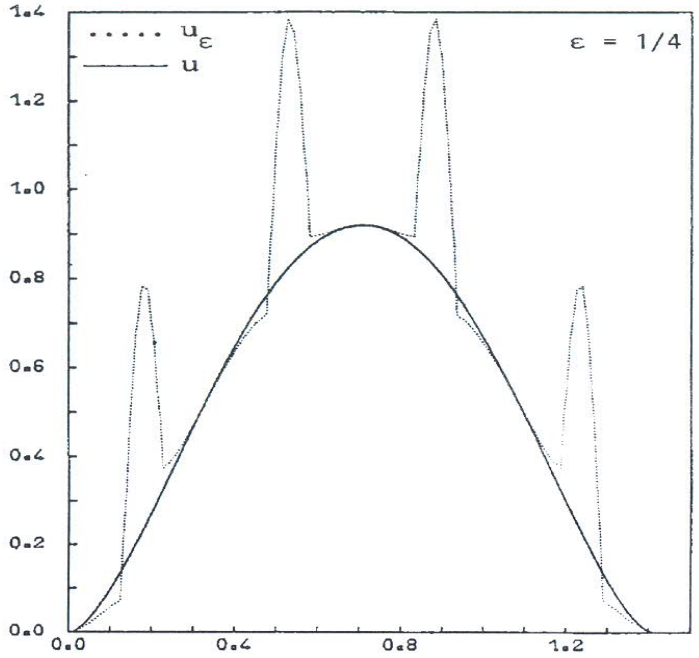


Figure 13 - Comparison of u_ε with u for $\lambda = 1/18$.



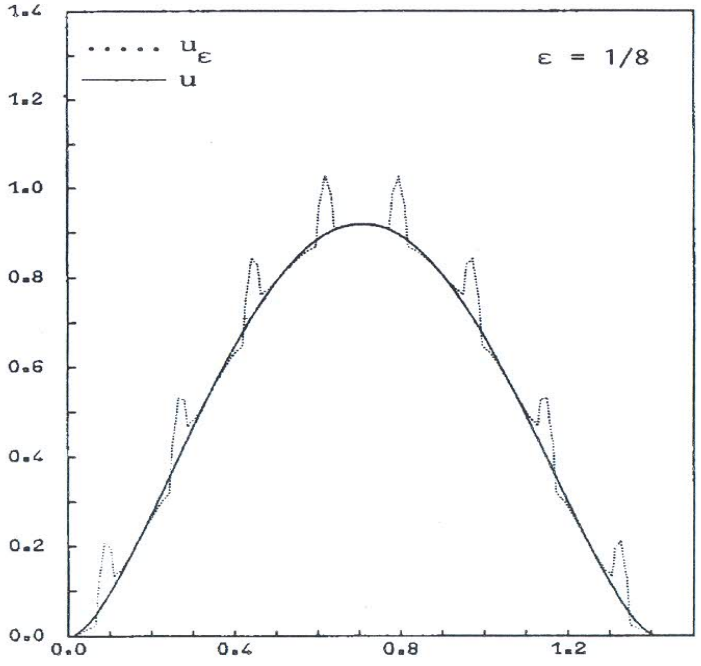


Figure 14 - Comparison of u_ε with u for $\lambda = 1/114$.

For convergence of materials, the hint comes from design optimization process which produces fine mixtures of materials. Mixing means that there is a **convergence process** hidden behind.At the limit,the medium looks very complex. Understanding this convergence requires an insight into the mixing process. Mixing of conducting materials is well-understood. We wish to introduce the corresponding mathematical concept.

Idea: Approximation is based on method of averaging.There are various types:
Ensemble averaging:Assuming probabilistic information on the distribution of heterogeneities,we can talk about convergence in law.
Drawback: In situations where microstructures are generated automatically by the system itself (hence unknown), there is no clear way in general to guess the correct probability distribution governing them.
Mixing of material is a physical deterministic process. Apriori there is no probability involved.If probabilistic tools are used in its description,it is because of our choice for simplification purposes. Avoiding it is desirable.
There are some issues that one can settle without probability.This includes basic concepts.
We follow a deterministic approach.It may be more difficult but worthwhile to explore. For periodic structures, there is a well-defined notion of (deterministic) averages. We wish to generalize it.

Concept of **weak convergence** from Functional Analysis:

E is Banach. E' is its dual (Continuous linear functionals on E).
E' is also Banach. E' acts on E linearly and continuously.
Similarly, E acts on E' in the same way.

Definition:Let $x(n)$ be a sequence in E. x is an element in E. We have then **norm/strong convergence:** $x(n) \to x$ in E.

$$\|x(n) - x\| \to 0.$$

We have **weak convergence** on E induced by E':

$\langle l, x(n) \rangle \to \langle l, x \rangle$ for all l in E'.

Similarly we have weak* convergence on E' induced by E:

$$\langle l(n), x \rangle \to \langle l, x \rangle \text{ for all } x \in E.$$

Weak Convergence of functions = Generalized convergence of averages of functions (against suitable test functions) :

$$\int f_n g \to \int fg$$

for a class of test functions g. (Spatial Averages converge).
Example: For periodic functions, weak limit is given by the average:

$$g\left(\frac{x}{\epsilon}\right) \rightharpoonup \frac{1}{|Y|}\int_Y g(y)dy.$$

Advantage: It enjoys compactness properties,as if we are in finite dimension.
Disadvantage: Bad behaviour with respect to nonlinearities.
Example: sin nx converges weakly to zero. But $(\sin nx)^2$ converges weakly to 1/2. This is the effect of oscillations as n becomes large.

Since optimization process generates minimizing/maximizing sequence of materials, we consider such sequences indexed by ϵ, which is a small parameter destined to tend to zero.

ϵ represents scale of variation of the medium/the size of heterogeneities. Smaller the ϵ, the more heterogeneities are present, more complex the medium is (**mixing process**).

We are interested in weak limit as ϵ tends to zero.This will give an approximation.It gives a macroscopic approximation to the microscopic details of heterogeneities, by means of averaging process based on weak convergence.

Model Problem: Consider heat conduction problem.Notion of H-convergence among materials.
Based on weak convergence using State space.

Local volume proportion of components $\{a_1, a_2\}$ in a mixture is $\{\theta_A, 1 - \theta_A\}$ where

$$\omega_{A^\epsilon}(x) \rightharpoonup \theta_A(x) \text{ in } L^\infty(\Omega) \text{ weak*}$$

Notion of weak limit is adequate.

Heat Conductivity of a mixture:
$A^\epsilon \rightharpoonup \overline{A}$ in $L^\infty(\Omega)$ weak*
This weak limit is not appropriate.

We need the notion of **Homogenization, H-convergence, H-limit:**
We say that A^ϵ is $H-$convergent to $A^\star$

$$A^\epsilon \overset{H}{\rightharpoonup} A^\star \text{ if}$$

$$A^\epsilon \nabla u^\epsilon \rightharpoonup A^\star \nabla u \text{ in } L^2(\Omega) \text{ weak},$$

for all test sequences $\{u^\epsilon\}$ such that

$$\begin{aligned} u^\epsilon &\rightharpoonup u \text{ weakly in } L^2(\Omega), \\ \nabla u^\epsilon &\rightharpoonup \nabla u \text{ weakly in } L^2(\Omega), \\ \text{div } (A^\epsilon \nabla u^\epsilon) &\quad \text{is strongly convergent in } H^{-1}(\Omega). \end{aligned}$$

(Oscillating system with differential constraints).

It follows that not only we have convergence of heat flux, but also canonical energy densities converge:

$$A^\epsilon \nabla u^\epsilon \rightharpoonup A^\star \nabla u \text{ in } L^2(\Omega)$$

$$A^\epsilon \nabla u^\epsilon \cdot \nabla u^\epsilon \rightharpoonup A^\star \nabla u \cdot \nabla u \text{ in } D'(\Omega).$$

About A^*:

A^* is a macro quantity depending on conductivities of individual components of the mixture,their volume proportions and more importantly on the microstructure. We are interested in getting estimates on A^* independent of microstructures,using only macro quantities.
A^* is local quantity.

Problems that can be treated: Heat conduction problem.More complicated systems can also be treated using similar ideas.(e-g: Stokes system for creeping fluids, Lame system of elasticity, Maxwell system of Electromagnetism etc). But results are less complete.

First Task: Compactness Theorem showing the existence of mixtures:
Theorem: Given A^ϵ, there is a subsequence which H-converges to some A^* which represents the mixture.

Compactness means some sort of stability. Secondly, H-limit of Fourier materials is again Fourier. This means that the mixture is a Fourier material. However, H-limit of isotropic materials need not be isotropic.
These results provide confirmation of correctness of the topology for the mixing process.

Second Task: Initial engineering problem is Optimal Design according to specific criterion (modeled by ODP).Mathematicians aimed at more ambitious goal of characterizing all possible designs (called **G-closure problem**) and then ODP resolution amounts to making a choice among them. The surprise is that the harder problem of G-closure can be solved in certain cases.

G-closure problem:

Given a finite set of heat conducting materials with prescribed volumes, mix them in all possible ways. Describe the heat conducting coefficients of all such mixtures.

Analogous statement for other physical attributes:Elasticity, electric conduction, magnetic properties, viscosities of mixtures of fluids etc.

It is a fundamental question.
In some cases this has been resolved:e-g:two-phase materials in a conductivity problem.

Theorem (Murat-Tartar, Lurie-Cherkaev): Conductivities of various mixtures that can be formed by varying microstructures are characterized by a set of **bounds/inequalities** in the space of conductivities. These define a convex lens shaped region. They are **optimal** in the whole physical domain. Theorem also constructs the microstructures/ mixing process corresponding to these bounds. In other words, the result describes full details of all possible materials obtained.

Once we have such a result, it is then easy to choose the desired material behaviour via optimization.

Celebrated Theorem (Murat-Tartar, Lurie-Cherkaev)
H-limits $A^\star$ are charcterized by the following inequalities:

$$\underline{A}(x) \leq A^*(x) \leq \overline{A}(x),$$

$$Tr\{(A^* - a_1 I)^{-1}\} \leq \frac{1}{N} Tr\{(\underline{A} - a_1 I)^{-1}\} + \frac{N-1}{N} Tr\{(\overline{A} - a_1 I)^{-1}\}$$

$$Tr\{(a_2 I - A^*)^{-1}\} \leq \frac{1}{N} Tr\{(a_2 I - \underline{A})^{-1}\} + \frac{N-1}{N} Tr\{(a_2 - \overline{A})^{-1}\}$$

Here $\overline{A}$ and $\underline{A}$ are respectively arithmetic and harmonic means of $\{A^\varepsilon\}$

$$A^\varepsilon \rightharpoonup \overline{A} \text{ in } L^\infty(\Omega) \text{ weak } *$$

$$(A^\varepsilon)^{-1} \rightharpoonup (\underline{A})^{-1} \text{ in } L^\infty(\Omega) \text{ weak } *$$

$$
\begin{aligned}
\overline{a}(x) &= a_1\theta_A(x) + a_2(1-\theta_A(x)) \\
\underline{a}(x) &= \left(a_1^{-1}\theta_A(x) + a_2^{-1}(1-\theta_A(x)\right)^{-1} \\
\sum_{i=1}^{N} \frac{1}{\lambda_i(x)-a_1} &\leq \frac{1}{\underline{a}(x)-a_1} + \frac{N-1}{\overline{a}(x)-a_1} \\
\sum_{i=1}^{N} \frac{1}{a_2-\lambda_1(x)} &\leq \frac{1}{a_2-\underline{a}(x)} + \frac{N-1}{a_2-\overline{a}(x)} \\
\underline{a}(x) &\leq \lambda_i(x) \leq \overline{a}(x)
\end{aligned}
$$

Above bounds are in terms of eigenvalues of $A^\star$ which represent conductivity of the mixture in the eigenvector directions. They are **optimal** in the following sense : Any $A^\star$ satisfying above bounds is a H-limit of two-phase mixtures with some microstructures.

Phase diagram in the space of macro parameters $A^\star$ is depicted in the following picture: convex lens shaped region.

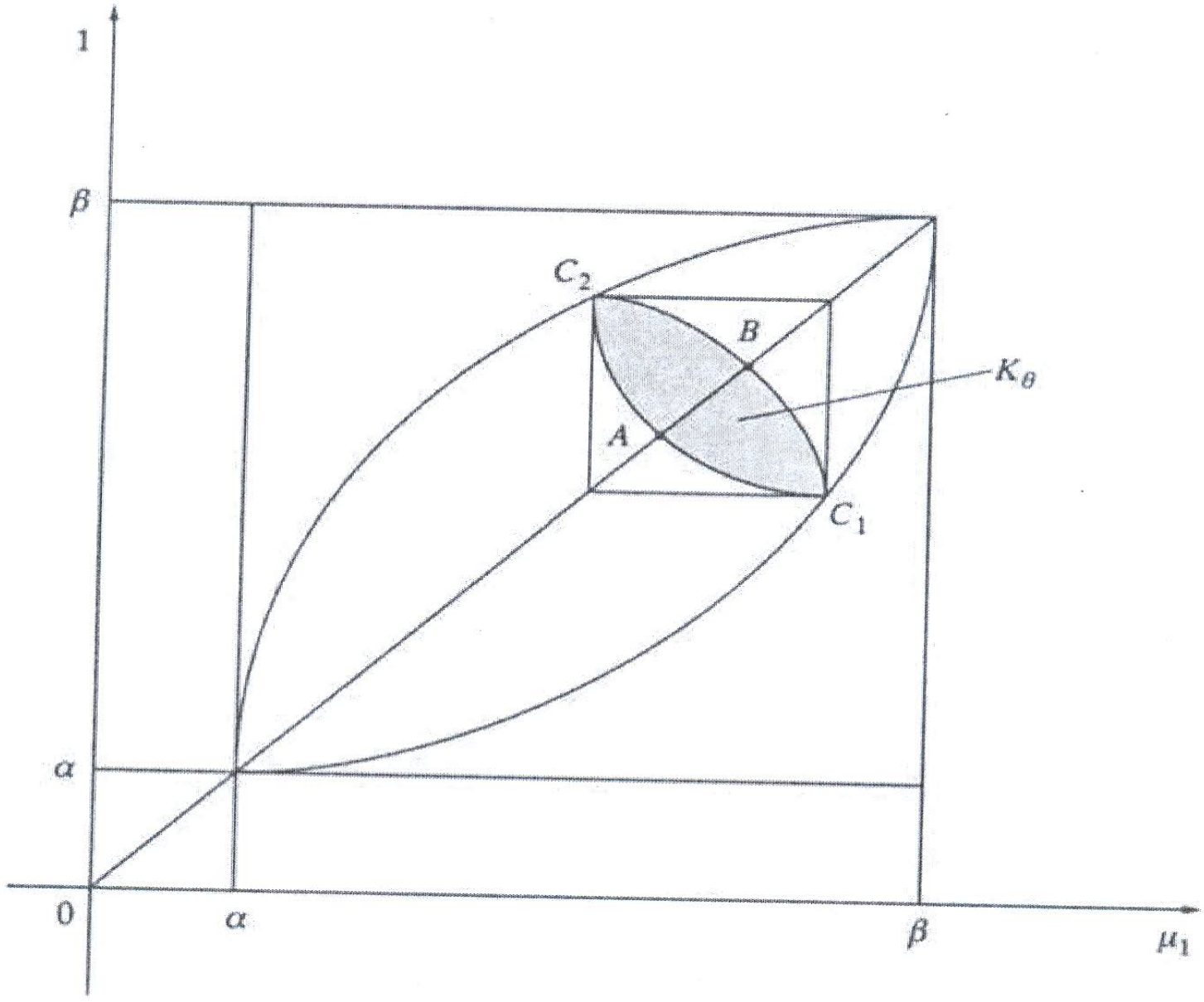


Figure 1.

Mathematical ideas behind proving these results:
Div-Curl Lemma, Compensated Compactness,H-measures, Wave cone etc.

At a fundamental level, the central problem of Homogenization is to find the (weak) limit of quadratic quantities of oscillating sequences satisfying certain differential constraints.In fact, the very definition of the homogenized matrix is based on the following framework:
Gradient of the temperature field oscillate satisfying differential constraint defined by balance equations.Also curl-free condition. The corresponding energy density is a quadratic quantity incorporating the interaction between the heat flux and the gradient of the temperature field. We are interested in the (weak) limit of this quantity and the homogenized matrix appears in the limiting energy density.

Thus we consider an **oscillating sequence** (with zero mean) satisfying certain differential constraints.We view them as waves.They have well-defined **location** in the physical space and well-defined **directions** of propagation and also well-defined **amplitudes**. Such bad amplitudes constitute the **wave cone** of the system. Squaring these amplitudes, we get the **intensity** of these waves.
The significance is that using the above ingredients, we can constuct waves whose presence is an obstruction to the compactness (strong convergence, stability) of the sequence.

H-measure, denoted by μ is a measure on the phase space,associated to such an oscillating sequence.It is a weak limit constructed from all the above pointwise ingredients. It quantifies the non-compactness of the given oscillating sequence.Indeed, if μ is zero, then the sequence is compact (and conversely).

Compensation Condition: It is intuitively clear that a good quadratic quantity Q is the one which annihilates all bad amplitudes of the wave cone. Such quadratic quantities are (weakly) continuous and hence its limit is zero.We note here how the bad behaviour of the sequence is compensated by the good behaviour of the nonlinearity. Hence the name **Compensated Compactness.**

If the above compensation condition is not satisfied,then the above bad amplitudes of the wave cone are expected to contribute to the weak limit.Indeed, the weak limit is $Q(\mu)$.

Optimal bounds on homogenized matrix are deduced by applying above ideas with judicious choice of quadratic quantities.This part is technical.

Application to Optimal Design Problem (ODP):
Control, State Equation,Objective functional, Minimization problem.
Typically, this class of problems do not admit classical solutions with two-phases.Optimizers are genuine mixtures; that is, optimizing sequences H-converge to a genuine composite material in which individual phases cannot be distinguished.

Application to Calculus of Variations:

Optimal Design Problem (ODP):

Control : Characteristic function: χ_{ω_A}

State equation:

$$u_{\omega_A} \in H_0^1(\Omega)$$

$$-\operatorname{div}\left(A_{\omega_A}\nabla u_{w_A}\right) = g \in H^{-1}(\Omega)$$

$$\text{where } A_{\omega_A} = a_1\chi_{\omega_A} + a_2(1-\chi_{\omega_A}).$$

Cost functional :

$$J(\chi_{\omega_A}) := \int_\Omega A_{\omega_A}(x)\nabla u_{\omega_A}\cdot\nabla u_{\omega_A}dx = \int_\Omega g u_{\omega_A}dx.$$

Minimization problem:

$$\inf\{J(\chi_{\omega_A});\, |\omega_A| = \delta_A|\Omega|\}$$

Minimization over characteristic functions.
Difficulties:Non-existence of minimizers,
lack of convexity,
not-so-rich variations among characteristic functions to deduce optimality conditions. (e-g:Hadamard variations).
Remedy:Relaxation.
Roughly speaking, add limit points of all minimizing sequences.
In our model ODP, this requires H-limits and the resolution of the G-closure problem.
Fortunately, both issues are solved for two-phase media.
Minimizers to ODP are found among $N-$rank laminates.

Numerics of ODP: Exact optimum solution is of course a genuine microstructure/composite. But in practice, we need a two-phase material. (one of them is void in case of shape optimization). Since ODP is a relaxed version of the corresponding ODP with classical materials, there is one classical microstructure lying near (w.r.t H-**topology**) our optimal relaxed microstructure for which the objective functional value is close to the optimal one.There are many techniques to implement this idea in Numerics.

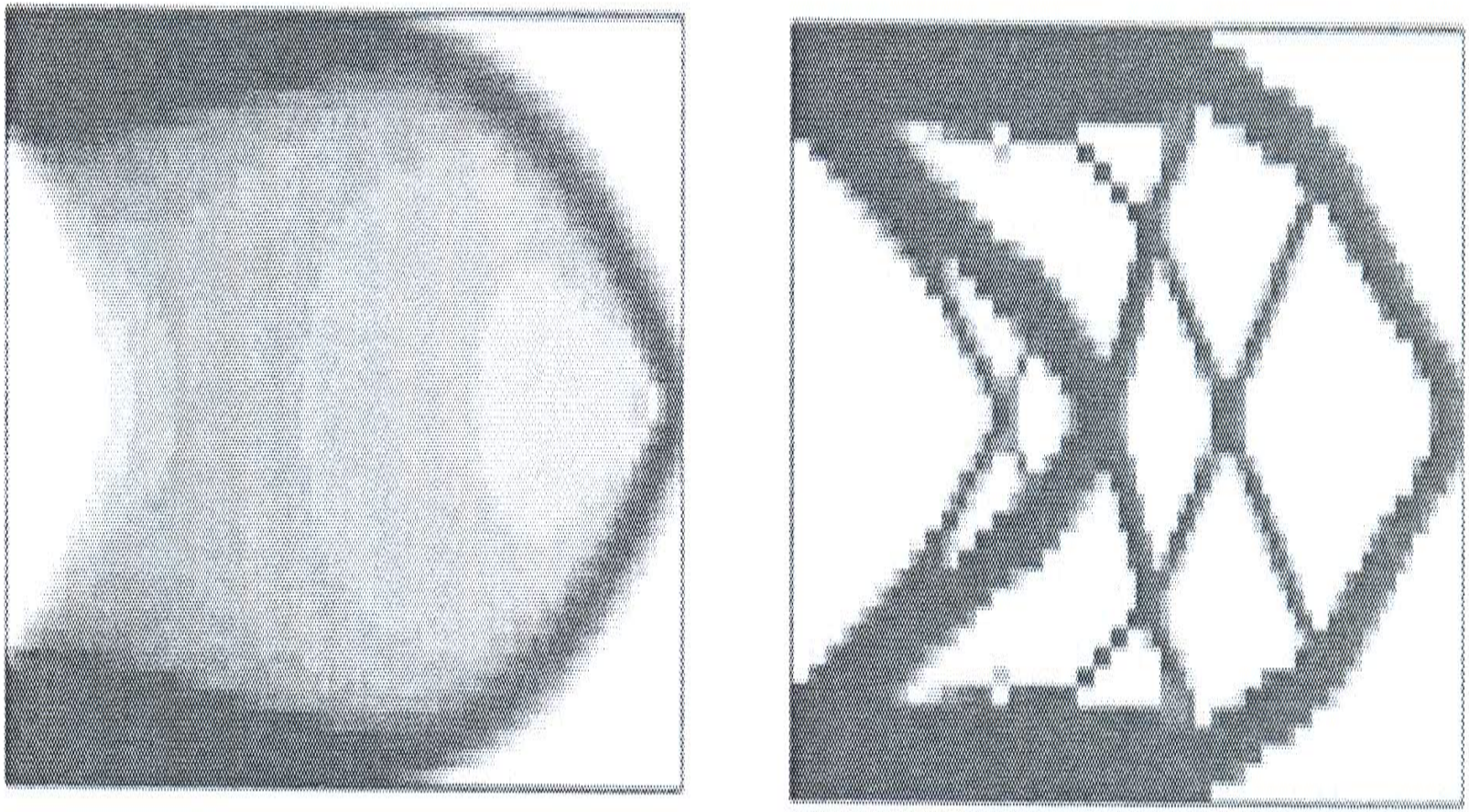


Figure 5.8: Optimal shape of the cantilever: composite (left) and penalized (right).

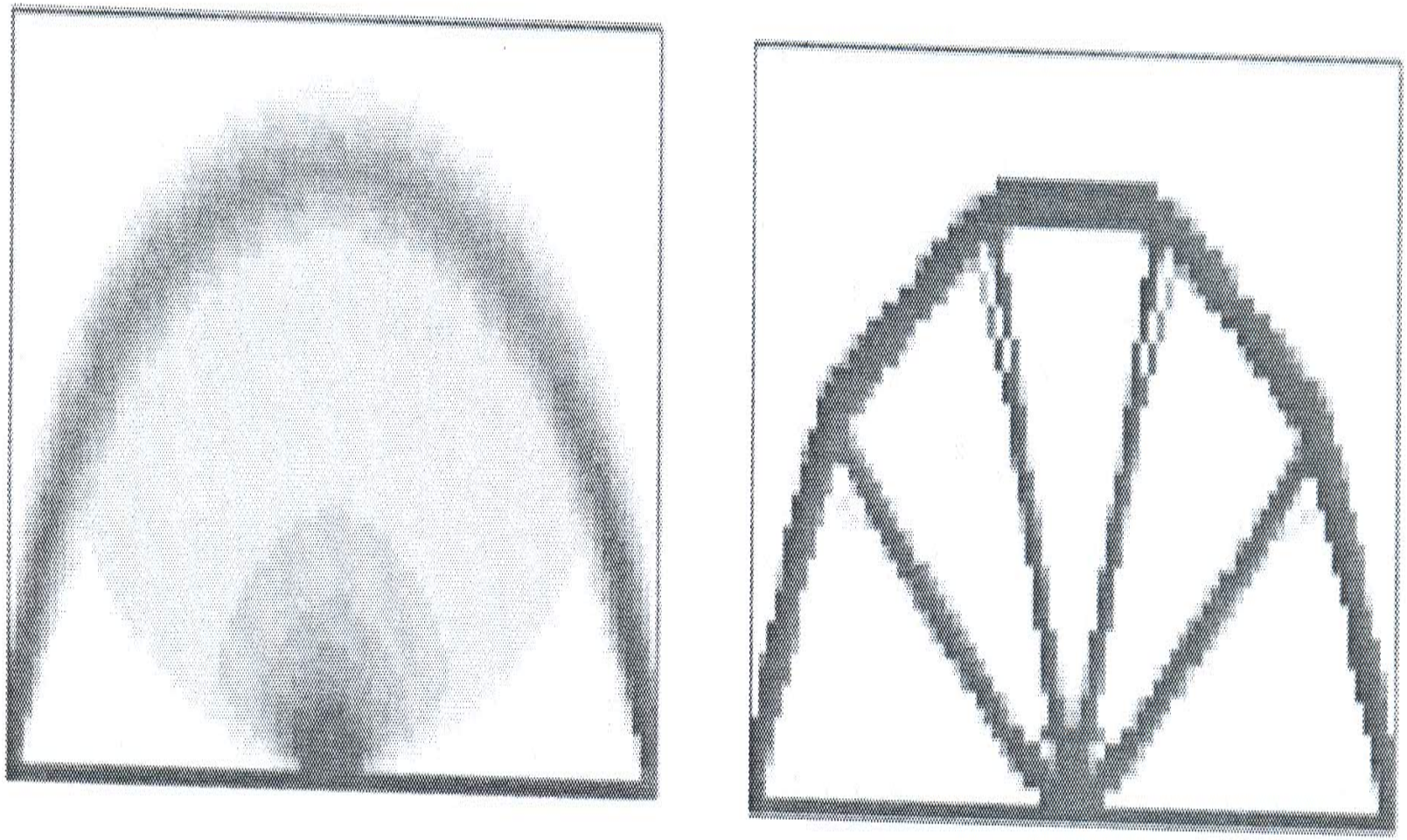


Figure 5.11: Optimal shape of the bridge: composite (left) and penalized (right).

More complicated than ODP:
Objective Functional depends on gradient of the state.
OODP: Optimal Oscillation-Dissipation Problems:

Optimal Oscillation-Dissipation Problem (OODP):
Controls : Two characteristic functions: $(\chi_{\omega_A}, \chi_{\omega_B})$
State equation:

$$u_{\omega_A} \in H_0^1(\Omega)$$

$$-\text{ div } (A_{\omega_A} \nabla u_{w_A}) = g \in H^{-1}(\Omega)$$

where $A_{\omega_A} = a_1 \chi_{\omega_A} + a_2(1 - \chi_{\omega_A})$ (with two phases).

Cost functional :

$$J(\chi_{\omega_A}, \chi_{\omega_B}) := \int_\Omega B_{\omega_B}(x) \nabla u_{\omega_A} \cdot \nabla u_{\omega_A} dx.$$

with $B_{\omega_B} = b_1 \chi_{\omega_B} + b_2(1 - \chi_{\omega_B})$ (with two phases).
Minimization problem:

$$\inf \{ J(\chi_{\omega_A}, \chi_{\omega_B}); |\omega_A| = \delta_A |\Omega|, |\omega_B| = \delta_B |\Omega| \}.$$

Motivation/Interpretation for OODP:
In our context, the state equation defines a complex system. If $B = Id$, then we are trying to minimize the energy of the oscillations of the state in a uniform way in space.This is against the natural behaviour of inhomogeneous media. We introduce therefore non-uniformity via a variable $B(x)$.
Example: Energy Dissipation is not uniform in fluids.

Secondly, by allowing minimization wrt B, we let the system to choose its own **dissipation field** and its structure is captured by minimizer $B^{\#}$.Roughly, large energy of oscillations would require small values of B and viceversa.

Interpretation of Solution to OODP:

Basic idea is that the total energy of the oscillations after appropriate dissipation in the whole domain is minimized.This is captured by minimization wrt both (A, B) of the cost/objective functional.
Let $(A^*, B^{\#})$ be optimal solution.
The minimizer $(A^*, B^{\#})$ is a macro representation of Oscillation-Dissipation processes which co-exist in the system.

One is reminded of inertial range in turbulent fluids in which oscillation and dissipation co-exist.Following picture is classical:Kinetic energy injected at big wavelengths of the velocity field is cascading down to small wavelengths creating oscillations of the field.At small wavelengths, dissipation of kinetic energy takes place, which is not uniform in spacetime (intermittency).These two processes co-exist and sustain the turbulent state of the fluid.

We can thus guess that there are macro quantities behind turbulent flows and that there is a need to estimate them.Formulation and resolution of this problem constitutes **Homogenization Problem of Turbulence.**

Why OODP is not trivial?

Ideally speaking, we would like to put minimum value of B in regions of large gradient of the state u .The difficulty is that such regions are not known apriori. It is part of the minimization problem. Moreover, these regions can be large whereas minimum value material of B can have small volume.
Secondly, there is an interaction between microstructures ω_A, ω_B.
Thirdly, when A =B, the OODP coincides with ODP and so non-trivial.

As before, there are three tasks in the resolution of OODP.

1) New Notion of Convergence is required: Notion of convergence relative to a microstructure:
2) Compactness Theorem
3) Optimal Bounds on emerging new Macro Parameters.

Main feature of the problem which is present here but not in previous ODP:Interaction between microstructures.

Notion of Convergence relative to a microstructure:

A^ϵ, B^ϵ are given.
We say $\{B^\epsilon\}$ converges to $B^\#$ relative to A^ϵ if

$$B^\epsilon \nabla u^\epsilon \cdot \nabla u^\epsilon \rightharpoonup B^\# \nabla u \cdot \nabla u \text{ in } D'(\Omega),$$

for all test sequences $\{u^\varepsilon\}$ such that

$$\begin{aligned} u^\epsilon &\rightharpoonup u \text{ in } H^1(\Omega) \text{ weak} \\ -\operatorname{div}(A^\epsilon \nabla u^\epsilon) &\to H^{-1}(\Omega) \text{ strong.} \end{aligned}$$

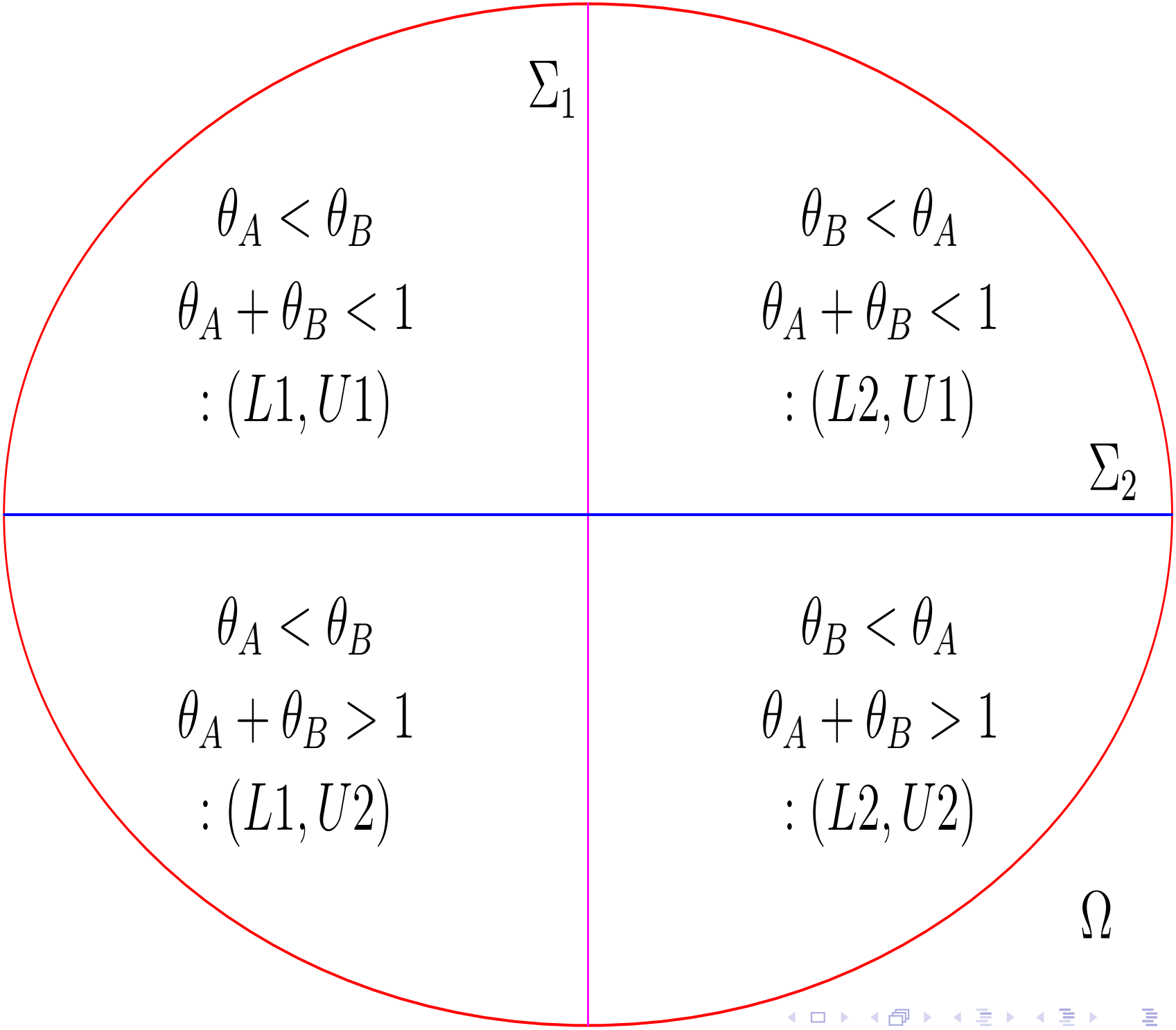
Notation: $B^\epsilon \overset{A^\epsilon}{\rightharpoonup} B^\#$.
$B^\#$ is a new macro matrix apart from A^*.

$B^{\#}$ is an outcome of interaction between microstructures $\{A^{\epsilon}, B^{\epsilon}\}$. The case $B^{\epsilon} = A^{\epsilon}$ is called **self-interacting case**. In this case, $B^{\#} = A^{\star}$ and so there are no new macro parameters. This case coincides with the previously treated case. Thus we are dealing with a genuine extension of the old problem. In the extended problem, there are new macro parameters $B^{\#}$ apart from $A^{\star}$.

The two lower bounds $(L1), (L2)$ reduce to the two known bounds for A^{*}. The two upper bounds $(U1), (U2)$ define certain regions in the phase space of A^{*} which are not of any importance.

New Results:

The original physical domain Omega is divided into four sub-domains with interfaces between them. There are four optimal regions in the phase space of macro parameters $(A^{\star}, B^{\#})$, corresponding to four sub-domains.(See Picture). These four regions are defined by four inequalities labeled as $\{L1, L2, U1, U2\}$. Because of these structural changes, minimizers for OODP are found among N-rank laminates with an interface across which core-matrix values get switched.
In the classical case, there was only one region and consequently, ODP solutions did not have interfaces.


Σ_1
$\theta_A < \theta_B$
$\theta_A + \theta_B < 1$
$: (L1, U1)$
$\theta_B < \theta_A$
$\theta_A + \theta_B < 1$
$: (L2, U1)$
Σ_2
$\theta_A < \theta_B$
$\theta_A + \theta_B > 1$
$: (L1, U2)$
$\theta_B < \theta_A$
$\theta_A + \theta_B > 1$
$: (L2, U2)$
Ω

Lower Trace Bound (L1)

There exists a unique $\theta(x) \leq \theta_A(x)$ such that

$$Tr(A^\star(x) - a_1 I)^{-1} = Tr(\overline{A}_\theta(x) - a_1 I)^{-1} + \frac{\theta(x)}{(1-\theta(x))a_1}$$

where $\overline{A}_\theta(x) = \{a_1\theta(x) + a_2(1-\theta(x))\} I$.
Then we have

$$Tr\left\{(B^\#(x) - b_1 I)(\overline{A}_\theta(x) - a_1 I)^2 (A^\star(x) - a_1 I)^{-2}\right\}$$

$$\geq N(b_2 - b_1)(1 - \theta_B(x) + \frac{b_1(a_2 - a_1)^2}{a_1^2}\theta(x)(1-\theta(x)).$$

This is optimal in the sub-domain $\{x : \theta_A(x) \leq \theta_B(x)\}$.

L1 Bound

$A^\star$ and $B\#$ commute

$$\sum_{i=1}^{N} \frac{(\mu_i(x) - b_1)}{(\lambda_i(x) - a_1)^2} \geq \frac{N(b_2 - b_1)(1 - \theta_B(x))(a_1 \sum_{i=1}^{N} (\lambda_i(x) - a_1)^{-1} + 1)^2}{(a_2 + a_1(N-1))^2}$$

$$+ \frac{b_1}{a_1} \frac{((a_2 - a_1) \sum_{i=1}^{N} (\lambda_i(x) - a_1)^{-1} - N)}{(a_2 + a_1(N-1))}$$

Upper Trace Bound (U1)

$$Tr\left\{\left(\frac{b_2}{a_1}A^*(x) - B^{\#}(x)\right)(\overline{A}_\theta(x) - a_1 I)^2 (A^*(x) - a_1 I)^{-2}\right\}$$
$$\geq N(b_2 - b_1)\theta_B(x) + N\frac{b_2}{a_1}(a_2 - a_1)(1 - \theta(x)).$$

This is optimal in the sub-domain $\{x : \theta_A(x) + \theta_B(x) \leq 1\}$.

To prove these results, we make use of previous notions and also a sharp compactness to deal with the interaction of microstructures. Differential relations with constant coefficients (homogeneous situations)can be equivalently transformed into algebraic relations using **Fourier transform.** On the other hand, for periodic coefficients,we have **Bloch waves** doing the job.
What about arbitrary variable coefficients? (inhomogeneous situations).

For arbitrary structures, *H*-**measure** is the right tool. **Differential Relations** with variable coefficients expressing compactness (so crucial in the theory) can be equivalently transformed to **algebraic relations** involving H-measures. In a sharp sophisticated way, the above algebraic relation ensures the decay of short waves in the system and thereby implies compactness. Such a sharp result is needed to study interaction between two microstructures.

Conclusions:

We have seen the need for different kinds of averaging.For approximating materials,strong convergence is not appropriate. Even weak convergence (spatial averaging) is not good enough.We need H-convergence,which is not weak convergence,but based on weak convergence.H-convergence is not a simple-minded spatial averaging;it is somewhat sophisticated.Simple minded averaging simply leads to wrong results in oscillating systems. H-convergence is adequate for classical ODP. For OODP,we need another convergence concept (still more sophisticated spatial averaging) is required, because of interaction of microstructures.

If you find this talk too abstract, here is one practical message:It is with regard to design in the homogenized region where there is a genuine mixture of two materials.(See picture). Here we need to put individual phases.For this,we need a design principle.Here is where H-topology comes into the picture.If your intuition for design is not consistent with H-topology then you may expect trouble.

Conclusions:

Why weak convergence for certain quantities?
Why H-convergence and relative H-convergence are used for some other quantities? Is weak convergence alone not enough?

Weak convergence is appropriate for quantities modeled by differential forms.Material conductivity tensor/dielectric conductivity tensor are not modeled by differential forms.They are linear transforms between differential forms.Weak convergence on differential forms naturally induces H-convergence on such linear transforms.

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