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On optimal shapes in materials and structures

P. Pedersen

Abstract In the micromechanics design of materials, as well as in the design of structural connections, the boundary shape plays an important role. The objective may be the stiffest design, the strongest design or just a design of uniform energy density along the shape. In an energy formulation it is proven that these three objectives have the same solution, at least within the limits of geometrical constraints, including the parametrization. Without involving stress/strain fields, the proof holds for 3D-problems, for power-law nonlinear elasticity and for anisotropic elasticity.

To clarify the importance of parametrization, the problem of material/hole design for maximum bulk modulus is analysed. A simple optimality criterion is derived and with a simple superelliptic parametrization, agreement with Hashin-Shtrikman bounds are found. More general examples including nonequal principal strains, nonlinear elasticity and orthotropic elasticity show the versatility of the optimality criterion approach. In spite of this, the mathematical programming approach will be used in the future study of the multiparameter and/or multipurpose problems.

Key words Shape optimization, stiffness design, stress design, uniform energy density, nonlinear elasticity

1 Introduction

Many results are available within optimal shape design, but a number of important issues still need to be addressed. The literature gives a picture of three different research directions. In mechanical and civil engineering focus has for more than 25 years been on design for minimum stress concentration, see Ding (1986). In the material and more mathematical oriented research the focus has been on design for minimum compliance, see Vigdergauz (1997). Some heuristic approaches have focussed on design for uniform stress, see Xie and Steven (1997). Not many mutual references are given among these three research directions. A goal of the present paper is to show that a unification is possible, because the three different objectives will give the same solution under certain conditions.

In order to make the background for the paper clear, some subjective points of view will be given.

– In general stress/strain fields cannot be found analytically, but the finite element method can give us a solution to almost any degree of accuracy. The aspect of stress/strain analysis will not be commented on.
– The notion of energy density concentration or energy density uniformity will be used instead of the stress/strain quantities. First of all, because extensions to nonlinear and anisotropic elasticity enforce a need for definitions alternative to, say, the von Mises stress, but also because energy densities more directly relate to the theoretical proofs.
– Design of a boundary in a material or a transition in a structure are in principle identical problems. However, for structures we mostly assume the external loads to be given, while in material design the loads are evaluated from forced displacements and they are therefore design dependent.
– General theoretical results must often be based on idealized assumptions and it is important to study the influence from violation of these assumptions. Also the influence from simple parametrization must be studied with values and graphs for specific solved problems.

In a short review of a variety of problems solved we especially concentrate on the problems setup to minimize stress concentration. We note for all the examples that the energy density along the designed boundaries is uniform, independent of model dimensions, model anisotropy, model nonlinearity, and model loads. The

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P. Pedersen

Department of Solid Mechanics, Technical University of Denmark, DK-2800 Lyngby, Denmark
e-mail: pauli@fam.dtu.dk

goal therefore has been to obtain a simple proof of this general behaviour. This proof is given in Sect. 3 with follow up comments in relation to material design. To state it briefly: the stiffest design is also the strongest design and uniform energy density will be the result under certain conditions.

A simple parametrization of the boundary shape for a hole is presented. With given relative size of the hole this only involves two parameters and still it enables a design description that agrees with the asymptotic results for relative large as well as for relative small holes. The analytical treatment of this parametrization shows that an analytical optimality criterion can be derived and a solution procedure based on this is then described.

The first example to be discussed is related to the Vigdergauz (1986) shapes that result in maximum two-dimensional "bulk" modulus. Primarily a one-parameter study shows the influence of the details of the shape. The bulk modulus is rather insensitive to the details, but the concentration of energy density is very sensitive. The maximum bulk modulus agrees with the Hashin-Shtrikman bound.

After these theoretical results, the method based on the optimality criterion derived is applied to a case of nonequal mean values of the principal strains. Stable convergence is found and again the focus is put on concentration of energy density. The formulation and the method of solution also holds for orthotropic material and for nonlinear elasticity. The final example shows an application to such a case.

2
A variety of solved problems

Studying the results of a variety of rather different shape design problems, it can be seen that very general knowledge can be obtained. The striking generality is the property of uniform energy density along the designed shapes for all the different formulations mentioned in the Introduction. Mainly from formulations with minimum stress concentration we shall here list a number of analytically and/or numerically obtained results and then the theoretical background for this will be given in Sect. 3.

2.1
The 2D-fillet problem

The 2D-fillet problem, defined with the goal of minimizing stress concentration was solved by Tvergaard (1973) using a finite difference method for stress analysis. Kristensen and Madsen (1974, 1976) and Francavilla *et al.* (1975) solved the same problem using the finite element method for stress analysis. Within the limits of the imposed geometrical constraints (length of the fillets and the parametrizations) the results of optimization give constant tangential stress along the designed shape. At this boundary we have a unidirectional state of stress and therefore constant energy density as well as constant von Mises stress. Thus these early papers point towards the importance of constant energy density.

2.2
The 3D-fillet

The 3D-fillet of an axisymmetric solid was optimized by Pedersen and Laursen (1982–83). Tension, bending and torsion were all treated as separate load cases and the length of the fillet was imposed as a geometrical constraint. The detailed stress distributions in the paper all show constant von Mises stress; until a point of the designed shape where the geometrical constraint imposes a decrease in this stress. Note that von Mises stress and energy density are only proportional for isotropic, incompressible materials (see Pedersen 1998).

2.3
The 2D-hole-problem

The 2D-hole-problem is illustrated in Fig. 1 and shown with a biaxial load case. Numerical results for this case are also contained in the paper by Kristensen and Madsen (1976) and these are compared to what is mentioned as the "analytical" results. Analytical studies of the problem are reported by Banichuk (1977) with reference to even earlier results by Cherepanov (1974). These analytical studies prove that a constant tangential stress $\sigma_t = \sigma_1 + \sigma_2$ is obtained with an elliptical shape design where the ratio of the two half axes a, b equals the ratio of the stresses, i.e. $a/b = \sigma_1/\sigma_2$, assuming equal signs for σ_1 and σ_2. More recent studies by Cherkaev *et al.* (1998) deal with nonequal signs for σ_1 and σ_2. In all these cases constant energy density is obtained but it should be remembered that the hole is assumed infinitesimally small.

2.4
The 2D-hole with orthotropic material

With the increasing use of anisotropic material, like laminated composites, there is a need for shape design also for nonistropic material. The orthotropic case was studied by Pedersen *et al.* (1992). As expected, the optimal shape design is very dependent on the level of anistropy. Results for the case illustrated in Fig. 1 are shown in Fig. 2. The important conclusion from this study is that we obtain constant strain energy density along the designed boundary. Another important conclusion is that the optimal design is not influenced much by the finite element modelling. This holds for a change in element type as well as for a change in the num-

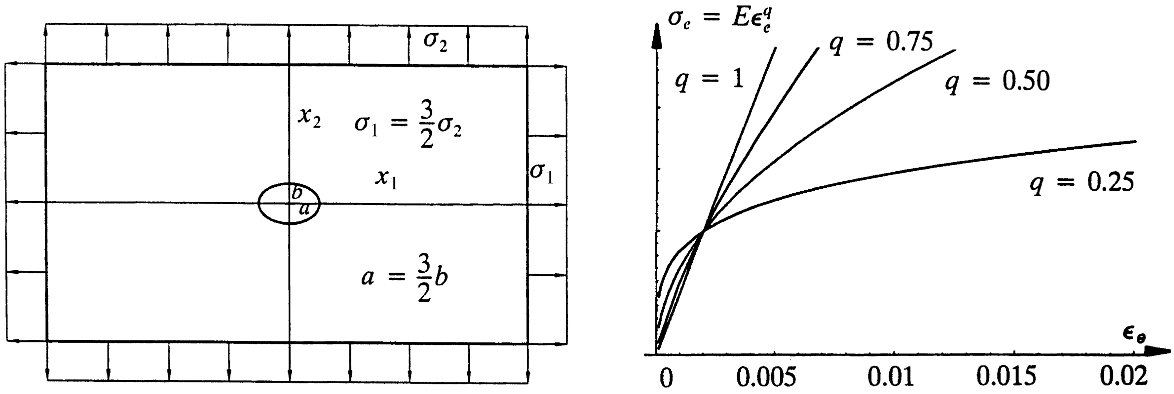

Fig. 1 Hole problem and applied materials for the discussions to follow

ber of elements (modelling refinement). Naturally, the stress/strain/energy values are sensitive to the accuracy of the finite element modelling, but the designed shape is not.

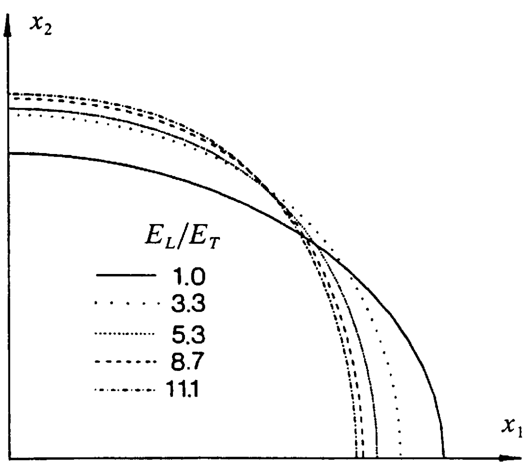

Fig. 2 Optimal boundary shapes for different "degrees" of orthotropy. For the four orthotropic materials, the resulting variation of strain energy density along these shapes are only 0.2, 0.3, 1.4 and 3.8% (from Pedersen *et al.* 1992)

2.5
The 2D-hole with nonlinear material

In a recent thesis by Stokholm (1998) we can find optimal shape designs based on a constitutive behaviour that follows from the stress energy density u^c given by $u^c = \sigma_e^{n+1}/[(n+1)E^n]$ where $n \geq 1$ and σ_e is the effective stress, as defined by Pedersen (1998). This material constitutive behaviour is illustrated in Fig. 1, noting $n = 1/q$. The results with this material constitutive model are again uniform strain energy density along the designed boundary shape for the problem in Fig. 1. In reality the optimal shape differs so little from the shapes obtained with linear elasticity that a more detailed numerical study is necessary to conclude that there is a difference. This is one of the goals of the present paper.

2.6
The cavity problem in 3-D

For the cavity problem in 3-D the shape of an inclusion with minimum stress concentration has also been studied analytically as well as numerically. As expected in an infinite model, the optimal shape is an ellipsoid, which follows from the work of Eshelby (1957). The von Mises reference stress will be constant on the surface of the cavity. Dybbro and Holm (1986) gave the optimal ellipsoidal half axis a, b and c implicitly in terms of the three principal stresses, and the ellipsoidal axes are aligned with the principal stress directions. A numerical study was also performed by Dybbro and Holm (1986) and within the accuracy of the applied finite element model, uniform energy density was found on the boundary of the shape. Also for composite materials we find three-dimensional studies, as the one by Vigdergauz (1994). However, the number of studies are limited and it is not expected that the analytical results from 2D-models (based on analytically determined stress fields) can be extended to 3D-models.

2.7
Conclusions on the basis of examples

Numerical procedures and solutions are reviewed in the surveys by Ding (1986) and Haftka and Grandhi (1986). Among the results obtained with ODESSY (see Rasmussen and Lund 1997), we find a brake arm and several 3D-models. It is interesting to note that also for these problems, with one load case and stress constraints only, we obtain uniform reference stress at least within the given geometrical limits. The general result for the examples are uniform energy density at the designed boundary shape, independent of model dimension, model anisotropy, model nonlinearity, model loads, and model objective (compliance or stress concentration). In the next section it is our goal to obtain a proof of this general behaviour.

3 Theoretical results

In this section we shall set up the conditions for obtaining the same optimal shape with the three different objectives: minimum energy concentration (strongest design), minimum compliance (stiffest design) and uniform energy density. We shall extend earlier results to cover anisotropic, nonlinear elastic behaviour for inhomogeneous structures with one arbitrary load case. As will be noted, the derivations are kept on the energy level without involving specific stress/strain calculation.

The theoretical results for *size optimization* are more developed than for shape optimization. Let us therefore start with some basic knowledge from size optimization, as can be seen in the paper by Pedersen (1998) for nonlinear elasticity and in the paper by Wasiutynski (1960) for linear elasticity. If the objective is to minimize compliance (extremize elastic energy) for given total mass, then from Pedersen (1998) we have: *for optimal stiffness design with homogeneous assumptions the ratio between subdomain energy and subdomain mass should be the same in all the design subdomains*.

Let the design parameters be h_i, then homogeneous mass relations are obtained with $M = \sum h_i^m \mathcal{M}_i$, where M is the total mass, m is a given positive value and $\mathcal{M}_i$ are independent of the design parameters. The homogeneous energy relations are obtained with $U = \sum h_i^n \mathcal{U}_i$, where U is the total strain energy, n is a given positive value and the $\mathcal{U}_i$ are *explicitly* independent of the design parameters. Then restricted to problems with constant mass density we obtain, in all design domains, the same mean energy density. Furthermore, if the model has constant energy density within a design domain, then the result u^* for the optimal design will have uniform energy density $\overline{u}$, i.e.

$$u_i^* = \overline{u} \quad \text{for all free design domains } i \,, \tag{1}$$

where lower and upper size constraints are not reached. For any other design the total energy U is larger

$$U = \sum u_i V_i > U^* = \overline{u} V = \overline{u} \sum V_i^* =$$

$$\overline{u} \sum V_i = \sum \overline{u} V_i \,, \tag{2}$$

where V is the total volume (of free domains) and V_i^* is the optimal volume of the design domain i. For an alternative design with design volumes V_i we have the same total volume $V = \sum V_i = \sum V_i^*$. From (2) we have

$$\sum (u_i - \overline{u}) \, V_i > 0 \,. \tag{3}$$

With positive volumes V_i we read from (3) that at least one u_i will not be less than $\overline{u}$. *Thus if the strongest design is defined by* $\min(\max\ u_i)$*, then the stiffest design characterized by the optimality condition (1) will also be the strongest design*. We note again that the strength may also be defined in relation to the von Mises stress or an alternative effective stress, and these measures are not always proportional to the energy density. For a detailed discussion of these aspects see Pedersen (1998).

In the following we shall use the same kind of reasoning to draw conclusions about *shape optimization*, without involving a solution to the actual stress problem. Thus the knowledge gained will be general, valuable for 3D as well as 2D problems, for nonlinear as well as for linear problems, for anisotropic as well as for isotropic problems, for any external load, for inhomogeneous as well as for homogeneous problems, and independent of the solution procedure. In order to simplify the mathematics, the design parametrization is chosen as illustrated in Fig. 3. An alternative parametrization with expansion in terms of shape design functions is formulated by Dems and Mroz (1978), a paper closely related to this one. We assume a homogeneous state for the energy density u_i within the volume V_i related to the shape parameter h_i. Let us now subject the shape to variation from only two parameters h_i and h_j. Furthermore, let the total volume V of the structure (continuum) be fixed, then

$$\Delta V = \frac{\partial V}{\partial h_i} \Delta h_i + \frac{\partial V}{\partial h_j} \Delta h_j =$$

$$\frac{\mathrm{d}V_i}{\mathrm{d}h_i} \Delta h_i + \frac{\mathrm{d}V_j}{\mathrm{d}h_j} \Delta h_j = 0 \,, \tag{4}$$

because we also assume the domain values to be dependent only on one design parameter with a positive gradient (to be used later),

$$V_i = V_i(h_i) \quad \text{and} \quad \mathrm{d}V_i / \mathrm{d}h_i > 0 \,. \tag{5}$$

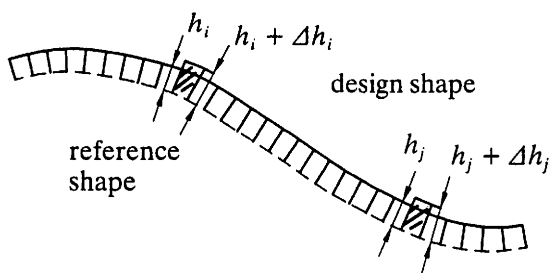

Fig. 3 Discretized design parametrization, showing two design domains i and j

In shape optimization for extremum elastic energy the increment of the objective for increments Δh_i, Δh_j

is

$$\Delta U = \frac{\partial U}{\partial h_i}\Delta h_i + \frac{\partial U}{\partial h_j}\Delta h_j \, , \tag{6}$$

which for power-law nonlinear elasticity (for 1D models: $\sigma = E\varepsilon^q$, see Fig. 1) can be written as

$$\Delta U = -\frac{1}{q}\left(\frac{\partial U}{\partial h_i}\Delta h_i + \frac{\partial U}{\partial h_j}\Delta h_j\right)_{\text{fixed strain field}} . \tag{7}$$

This is proven by Pedersen (1998) for design independent loads. Therefore only the local energies $U_i = u_i V_i$ and $U_j = u_j V_j$ are involved and the variations in the energy densities u_i, u_j need not be determined. We have

$$\Delta U = -\frac{1}{q}\left(u_i\frac{\mathrm{d}V_i}{\mathrm{d}h_i}\Delta h_i + u_j\frac{\mathrm{d}V_j}{\mathrm{d}h_j}\Delta h_j\right) . \tag{8}$$

Inserting (4) into (8) we obtain

$$\Delta U = -\frac{1}{q}(u_i - u_j)\frac{\mathrm{d}V_i}{\mathrm{d}h_i}\Delta h_i \, . \tag{9}$$

A necessary condition for optimality $\Delta U = 0$ with $\mathrm{d}V_i/\mathrm{d}h_i > 0$ is therefore $u_i = u_j$. With all design parameters, (4) and (8) are written

$$\Delta V = \sum_i \frac{\mathrm{d}V_i}{\mathrm{d}h_i}\Delta h_i \, , \quad \Delta U = -\frac{1}{q}\sum u_i\frac{\mathrm{d}V_i}{\mathrm{d}h_i}\Delta h_i \, , \tag{10}$$

and we conclude that a necessary condition for optimality $\Delta U = 0$ with constraint $\Delta V = 0$ is u_i equal to a constant. *For the stiffest design the energy density along the shape(s) to be designed* u_s *must be constant*

$$u_s = \overline{u} \, . \tag{11}$$

We now relate the stiffest design (minimum compliance) to the strongest design (minimum maximum energy density). Let us assume that the highest energy density is at the shape to be designed. With index s referring to shape design domains and index n referring to domains not subjected to design changes, this means that for the stiffest design we assume

$$\overline{u} = u_s > u_n \, . \tag{12}$$

A design domain (index s) that depends on design parameter h_s and a design domain which is not subjected to design change (index n) are shown in Fig. 4. The total elastic energy U is obtained from

$$U = U_S + U_N = \sum_s U_s + \sum_n U_n =$$

$$\sum_s u_s V_s + \sum_n u_n V_n = \overline{u}\sum_s V_s + \sum_n u_n V_n \, . \tag{13}$$

With unchanged domains n from $U > U^*$ we obtain

$$\sum_s u_s V_s + \sum_n u_n V_n > \sum_s \overline{u} V_s^* + \sum_n u_n^* V_n^* \, ,$$

$$\text{i.e.} \sum_s (u_s - \overline{u})V_s > \sum_n (u_n^* - u_n)V_n \, , \tag{14}$$

as $\sum \overline{u} V_S^* = \sum \overline{u} V_S$ and $V_n^* = V_n$.

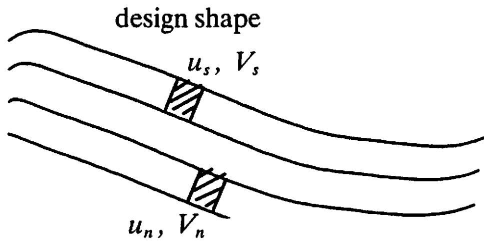

Fig. 4 Illustration of a shape related domain with energy density u_s and volume V_s. With index n a domain not connected to the boundary and thus with fixed volume V_n

The right-hand side might be negative, so we cannot conclude as from (3). However, in a complementary formulation we can prove that the right-hand side is zero and then the proof holds as from (3). The proof of increasing energy in the shape domain is as follows. We write the total stress energy U^C as the sum of stress energy in the shape domain U_S^C and stress energy in the nonshape domain U_N^C and obtain

$$U^C = U_S^C + U_N^C \Rightarrow \frac{\mathrm{d}U^C}{\mathrm{d}h} = \frac{\mathrm{d}U_S^C}{\mathrm{d}h} + \frac{\mathrm{d}U_N^C}{\mathrm{d}h} \, . \tag{15}$$

From $\mathrm{d}U^C/\mathrm{d}h = (\partial U^C/\partial h)$ in a fixed stress field (principle of complementary virtual work) we have

$$\frac{\mathrm{d}U^C}{\mathrm{d}h} = \left(\frac{\partial U_S^C}{\partial h}\right)_{\text{fixed stress field}} + \left(\frac{\partial U_N^C}{\partial h}\right)_{\text{fixed stress field}} , \tag{16}$$

where the last term will be zero when h has no direct influence on the nonshape domain. Finally for the stiffest design we have $\mathrm{d}U^C/\mathrm{d}h > 0$ and thereby conclude

$$\left(\frac{\partial U_S^C}{\partial h}\right)_{\text{fixed stress field}} = \frac{\mathrm{d}U_S^C}{\mathrm{d}h} = \frac{1}{q}\frac{\mathrm{d}U_S}{\mathrm{d}h} > 0 \, . \tag{17}$$

Summarizing the theoretical results of this section, for the general three-dimensional case with anisotropic, power law nonlinear elastic material in an inhomogeneous structure, and for any design independent load case we have that

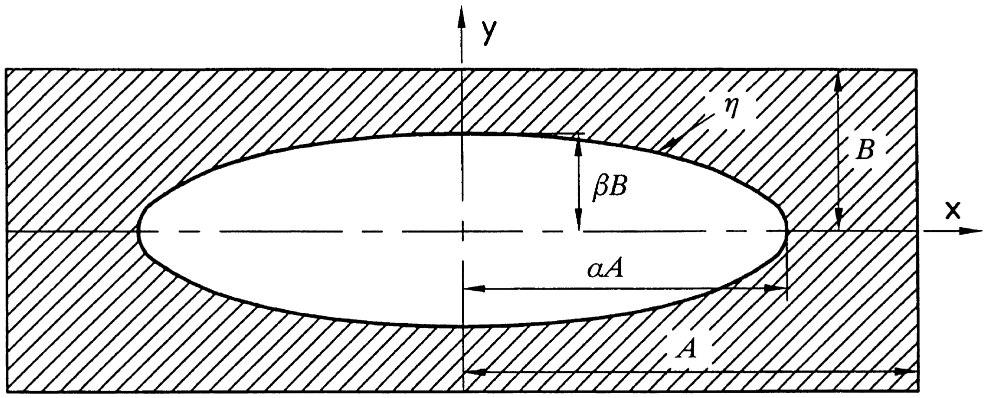

Fig. 5 A three-parameter (α, β, η) description of an internal central hole in a rectangular domain

– the minimum compliance shape design (stiffest shape design) will have uniform energy density along the designed shape, as far as the geometrical constraint makes this possible;
– if we furthermore assume that the highest energy densities are found at the designed shape, then the stiffest design will also be the strongest design, as defined by a design which minimizes the maximum energy density.

Note that these results are obtained without calculating the stress/strain fields and without specifying the constitutive behaviour. This behaviour need not be homogeneous and thus we can also include the multimaterial case. The many different problems in Sect. 2 support these results.

4
A simple parametrization and optimality criterion

In the theoretical results we have added a note "as far as the geometrical constraints makes this possible". Also it was commented that normally the shape parametrization implies such geometrical constraints. In the following two sections we shall illustrate the importance of such a shape parametrization, and at the same time present an alternative solution procedure for problems in material design.

The problem of material design for maximum bulk modulus (see the Appendix) has been studied in a number of papers by Vigdergauz, as referenced and explained by Grabovsky and Kohn (1995). Related to this we shall discuss in more detail the two-dimensional problems where the shape of an internal, central hole in a rectangular domain is designed.

The primary parameters of the problem are shown in Fig. 5 and the three-parameter shape of the hole is described by

$$\left(\frac{x}{\alpha A}\right)^{\eta} + \left(\frac{y}{\beta B}\right)^{\eta} = 1\,, \tag{18}$$

i.e. a superelliptic shape. With the known area of the hole we have two parameters and if futhermore symmetry is enforced, $\alpha = \beta$, we only have one parameter, say η. The great flexibility even for this one-parameter description is shown in Fig. 6. This parametrization naturally has its limitation, but for small as well as for large holes ($\alpha \Rightarrow 0$ or 1 and $\beta \to 0$ or 1), the parametrization gives well-known solutions. Thus we have great expectations and futhermore the extension to 3D-problems is straightforward,

$$\left(\frac{x}{\alpha A}\right)^{\eta} + \left(\frac{y}{\beta B}\right)^{\eta} + \left(\frac{z}{\gamma C}\right)^{\eta} = 1\,. \tag{19}$$

The area of the hole is

$$4\int_0^{\alpha A} \beta B \left[1 - \left(\frac{x}{\alpha A}\right)^{\eta}\right]^{1/\eta} \mathrm{d}x = 2\alpha\beta A B g(\eta)\,,$$

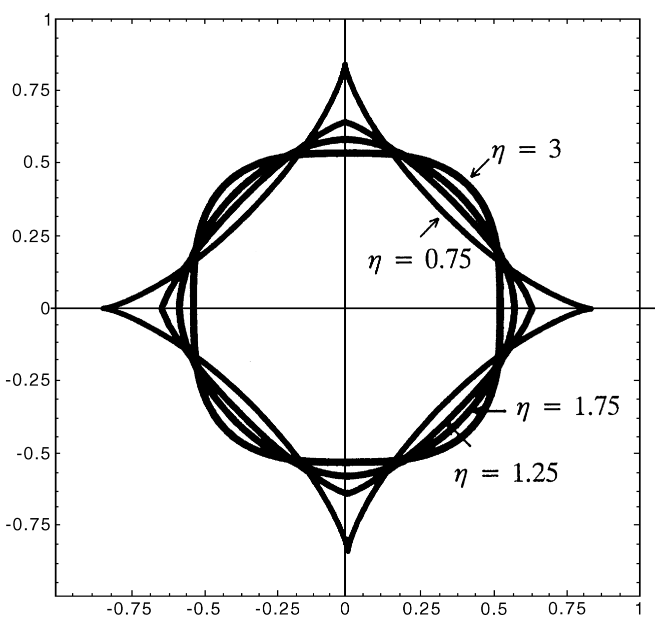

Fig. 6 Shapes giving equal relative volume density $\rho = 0.75$ corresponding to shape powers $\eta = 0.75$, 1.25, 1.75 and 3.00

with

$$g(\eta) := \Gamma\left(\frac{1}{\eta}\right)\Gamma\left(\frac{\eta+1}{\eta}\right)/\Gamma\left(\frac{2}{\eta}\right), \tag{20}$$

where Γ is the Gamma-function. With the rectangular area being $4AB$ the relative area of the hole ϕ (relative to the area $4AB$) and the relative area of the solid ρ are

$$\phi = \frac{1}{2}\alpha\beta g(\eta) = 1 - \rho\,. \tag{21}$$

An optimal design problem is formulated in order to extremize the elastic energy U for the constant relative area

$$\text{extremize } U \text{ subject to } \quad \phi(\alpha,\beta,\eta) = \overline{\phi}\,. \tag{22}$$

That this problem includes some of the Vigdergauz problems follows from the Appendix.

Within the possibilities of the three parameters α, β, η, this will also minimize energy concentration and return constant energy density along the boundary of the hole, as discussed in the previous section. Using the result (7) from sensitivity analysis we determine the differential of the elastic energy ($q = 1$ for linear elasticity)

$$dU = -\frac{1}{q}\left(\frac{\partial U}{\partial \alpha}d\alpha + \frac{\partial U}{\partial \beta}d\beta + \frac{\partial U}{\partial \eta}d\eta\right)_{\text{fixed strains}}, \tag{23}$$

and the differential of the constraint follows from (21) (with application of Mathematica to differentiate the Gamma-functions)

$$d\phi = \phi\left[d\alpha/\alpha + d\beta/\beta + p(\eta)d\eta/\eta^2\right],$$

with

$$p(\eta) := 2\Psi(2/\eta) - \Psi(1/\eta) - \Psi[(\eta+1)/\eta]\,, \tag{24}$$

where Ψ is the Psi-function. To illustrate that the functions $g(\eta)$ and $p(\eta)$ are well-behaved functions, we show in Figs. 7 and 8 these functions, available in Mathematica as well as in Fortran libraries.

The condition of $dU = 0$ when $d\phi = 0$ is a necessary condition for optimality and thus (as in general with only one constraint) from (23) and (24) we obtain the *optimality criterion* by proportional gradients, i.e.

$$\left[\alpha\partial U/\partial\alpha = \beta\partial U/\partial\beta = \eta^2(\partial U/\partial\eta)/p(\eta)\right]_{\text{fixed strains}}. \tag{25}$$

In a fixed strain field the energy densities u are constant and only the volume of domains (elements) connected to the hole boundary will change. Thus in a finite element formulation the optimality criterion (25) is written

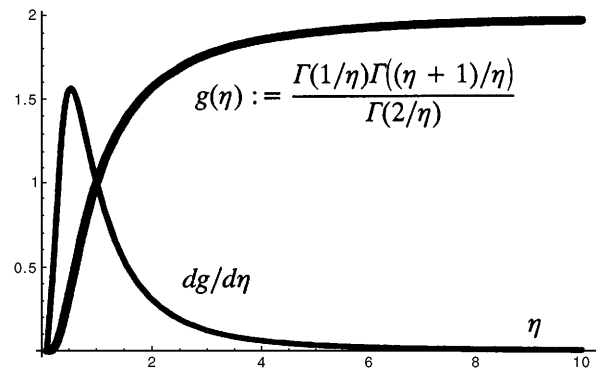

Fig. 7 The g-function and its derivative as a function of the shape power η

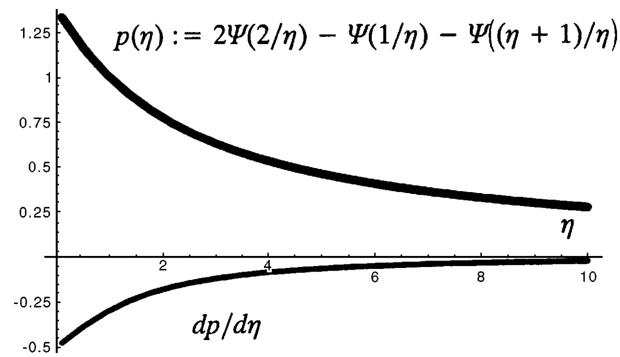

Fig. 8 The p-function and its derivative as a function of the shape power η

$$\alpha\sum_s u_s\frac{\partial V_s}{\partial\alpha} = \beta\sum_s u_s\frac{\partial V_s}{\partial\beta} = \frac{\eta^2}{p(\eta)}\sum_s u_s\frac{\partial V_s}{\partial\eta}, \tag{26}$$

where index s refers to an element connected to the hole boundary. The only information needed in addition to the results from analysis is $\partial V_s/\partial\alpha$, $\partial V_s/\partial\beta$ and $\partial V_s/\partial\eta$, i.e. only information from geometry. We note, in agreement with Sect. 3, that if u_s is constant along the hole boundary then $\sum\partial V_s/\partial\alpha = \partial V/\partial\alpha = \phi/\alpha$ etc., and the optimality criterion (25) is satisfied by $u_s\phi = u_s\phi = u_s\phi$. Thus a constant energy density along the boundary of the hole implies stationary total elastic energy. However, we can have stationary energy without constant energy density, if the possible designs are restricted. This will be illustrated in the next section.

The problem is how to find a boundary shape that satisfies (25) or in finite element formulation (26). The heuristic approach of successive iterations could be to estimate the Lagrange multiplier λ by the mean value

$$\lambda = \frac{1}{3}\left[\alpha\frac{\partial U}{\partial\alpha} + \beta\frac{\partial U}{\partial\beta} + \eta^2\frac{\partial U}{\partial\eta}/p(\eta)\right], \tag{27}$$

and then redefine α, β, and η by

$$\alpha_{\text{new}} = \lambda/(\partial U/\partial\alpha)_{\text{old}}\,, \quad \beta_{\text{new}} = \lambda/(\partial U/\partial\beta)_{\text{old}}\,,$$

$$\left[\eta^2/p(\eta)\right]_{\text{new}} = \lambda/(\partial U/\partial\eta)_{\text{old}}\,, \tag{28}$$

with iterations on λ to satisfy the constraint of (22)

$$\phi_{\text{new}} = \frac{1}{2}\alpha_{\text{new}}\beta_{\text{new}}g(\eta_{\text{new}}) = \overline{\phi}\,. \tag{29}$$

Let us assume that the three-parameter boundary shapes do not in a satisfactory way give constant energy density along the boundary shape, i.e. the energy concentration must be made smaller. We can then add modification functions $f_i(s)$ where s is the natural coordinate of the three-parameter description, and the functions f_i for $i = 1, 2, \ldots$ are chosen as described by Pedersen (1988) and used by Pedersen *et al.* (1992). The added design parameters will be the amplitudes c_i of the modification functions and gradients $\partial\phi/\partial c_i$ or $\partial V_s/\partial c_i$ must be evaluated, numerically or eventually analytically. Better solutions to problem (22) can then be obtained. Alternatively we may formulate the problem directly as a minimum energy concentration problem,

$$\min_{\alpha,\beta,\eta,c_i} \left(\max_{\text{all elements}} u_e \right),$$

$$\text{subject to } \phi(\alpha,\beta,\eta,c_i) = \overline{\phi}\,. \tag{30}$$

Solutions can be obtained with the integrated FEM-SLP approach (see Pedersen 1981). With the modification functions we also have the possibility of introducing discontinuities in the slope of the boundary shape.

5 Examples

Based on finite element modelling and the application of the optimality criterion method (25)–(29) specific examples are shown. The goal is to illustrate the versatility of the simple parametrization and the possibility of solving also problems with anisotropic and nonlinear material.

Even when we restrict ourselves to the central hole design in Fig. 5, many aspects are involved. Most of the following examples will be covered:

- quadratic domains ($A = B$)
- rectangular domains ($A \neq B$)
- different relative densities ($0 < \phi < 1$)
- forced displacements at the external boundaries (v_x at $x = A$ and v_y at $y = B$ for a model in quadrant one)
- specifically for $A = B$ the case $v_x = v_y$ (pure macro dilatation)
- prescribed stresses (loads) at the external boundaries (σ_{xx} at $x = A$ and $y = B$)
- specifically marco hydrostatic loads for $A = B$ in the case $\sigma_x = \sigma_y$
- isotropic material with influence from Poisson's ratio ν
- nonlinear power-law material behaviour
- orthotropic material behaviour

The first case is related to the problem of *optimizing the two-dimensional "bulk" modulus* κ, which is the energy density when isotropic material is subjected to pure dilatation (see the Appendix). For this case we impose

$$A = B\,, \quad \alpha = \beta\,, \quad v_x = v_y\,, \text{ linear isotropic material,} \tag{31}$$

and solutions are found in the parameter space of $\eta = \eta(\phi, \nu)$ with solution

$$\kappa = u_{\text{mean}} = U/(4tAB)\,, \tag{32}$$

where t is the constant thickness of the elements.

5.1 A one-parameter study

Without a primary interest in optimization we shall first perform a parameter study with a given relative volume density $\rho = 0.5$. Changing the shape parameter η and adjusting the relative axes $\alpha = \beta$ to satisfy $2(1-\rho) = \alpha^2 g(\eta)$ we obtain the results shown in Fig. 9 in terms of the "bulk" modulus (mean elastic energy density) and also showing the minimum and maximum energy densities along the hole boundary.

For this study we conclude that the bulk modulus is rather insensitive to the design details, but the concentration of energy density is very sensitive. This may tell us to primarily formulate the optimization as a min-max-energy density problem. The three different aspects

1. maximum bulk modulus = minimum compliance
2. minimum maximum energy density ≈ minimum maximum stress
3. minimum variation of energy density along the boundary hole

are obtained at three different, although close, shape parameters η. This is due to the one-parameter retriction and for a free parameter design, these three aspects would have been obtained simultaneously. With restricted parametrization the most important problem to solve is the min-max-energy density problem.

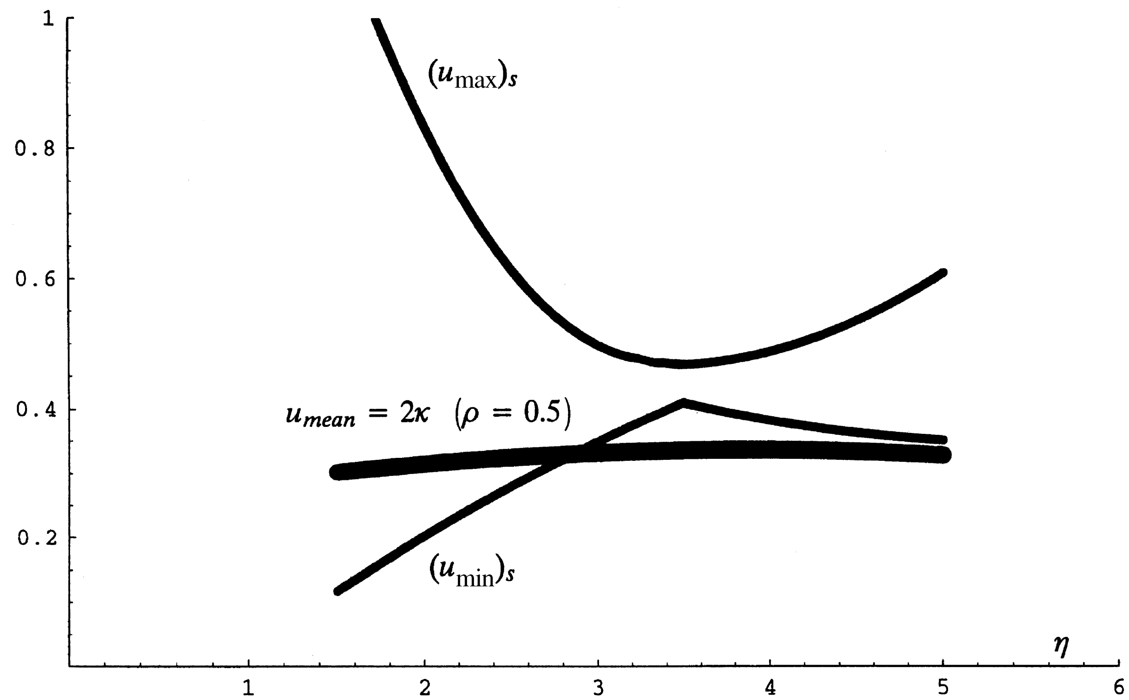

Fig. 9 Bulk modulus (thick line) as a function of the shape parameter η. Also shown are the maximum $(u_{\max})_s$ and the minimum $(u_{\min})_s$ energy densities *along the boundary shape*. Relative densities are $\rho = \phi = 0.5$ and material by $E = 1$ and $\nu = 0$

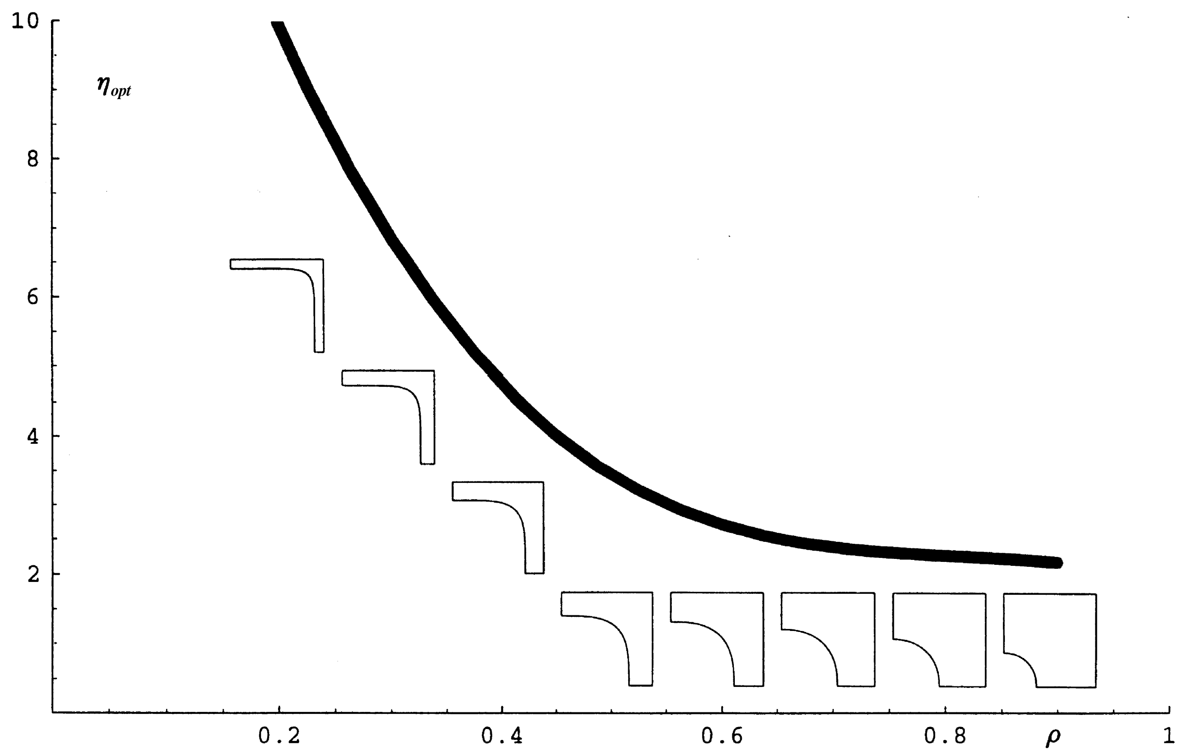

Fig. 10 Optimal shape parameter η as a function of relative volume density ρ. Based on isotropic, zero Poisson's ratio material and the Hashin-Shtrikman bound is reached

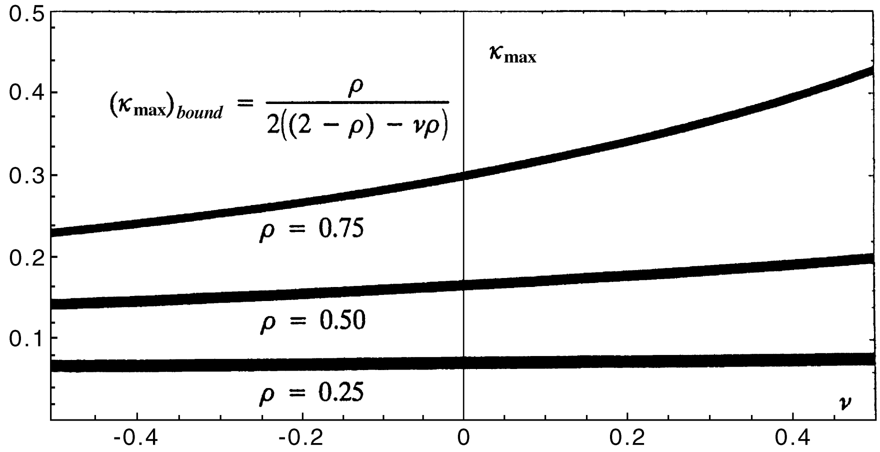

Fig. 11 Hashin-Shtrikman upper bounds on the "bulk" modulus in 2D as a function of Poisson's ratio ν (plane stress assumption), with relative mean density ρ as parameter ($E_1 = 0$, $E_2 = 1$)

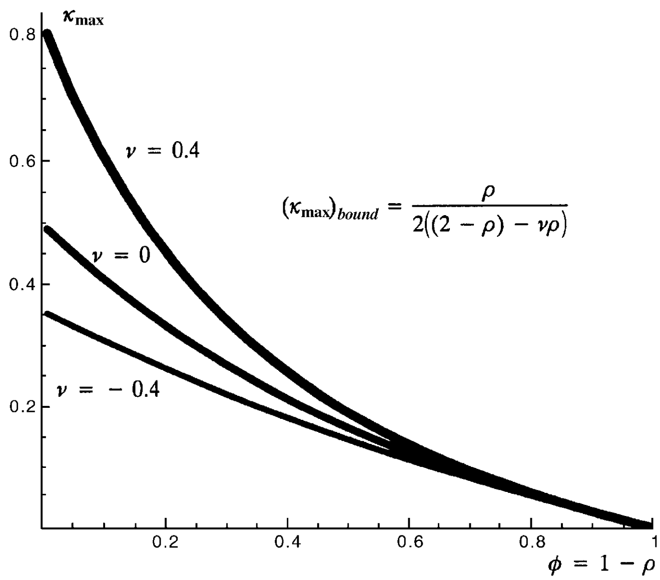

Fig. 12 Hashin-Shtrikman upper bounds on the "bulk" modulus in 2D as a function of the relative mean density ρ, with Poisson's ratio ν (plane stress assumption) as parameter ($E_1 = 0$, $E_2 = 1$)

5.2 Zero Poisson's ratio solutions

The parameter study presented above was based on zero Poisson's ratio, i.e. $\nu = 0$. We shall keep this assumption and show the optimal solutions for a variety of relative volume densities. The optimal shape parameter η_{opt} as a function of ρ is shown in Fig. 10 together with illustrations of some of the shapes. For all these solutions close agreement between the three aspects of optimization is again found. Also these solutions return the Hashin-Shtrikman upper bounds on the bulk modulus and the shapes are in agreement with the reported Vigdergauz shapes as far as it can be compared.

5.3 Hashin-Shtrikman bounds

Very close agreement (five digits) with the H-S upper bounds on the bulk modulus is found for the solutions shown in Fig. 10. With void material in the hole ($E_1 = 0$) this bound is given by

$$(\kappa_{max})_{bound} = \frac{\rho E_2}{2[(2-\rho) - \nu\rho]}, \quad (33)$$

and this function is illustrated in Figs. 11 and 12. Thus the mid-curve in Fig. 12 for $\nu = 0$ is the bulk modulus for the designs shown in Fig. 10.

5.4 Optimal design for nonzero Poisson's ratio

From a physical point of view it is to be expected that the optimal design will depend on Poisson's ratio. However, the dependence is very weak, and is only due to the incomplete uniform distribution of energy density along the hole boundary. Optimal designs for different Poisson's ratios are presented in Fig. 13 and agreement with bounds in Fig. 11 for $\rho = 0.75$ is found. Although the present results are based on the simple one-parameter (η) description, very close agreement with the bounds are found.

5.5 Optimality criterion iterations

Let us return to the optimization procedure as presented in Sect. 4. To illustrate the generality we shall treat biaxial forced displacements with displacement in the x_1-direction being twice the displacement in the x_2-direction. This means that the mean principal strains are related by $\varepsilon_1 = 2\varepsilon_2$. In Fig. 14 we show the results

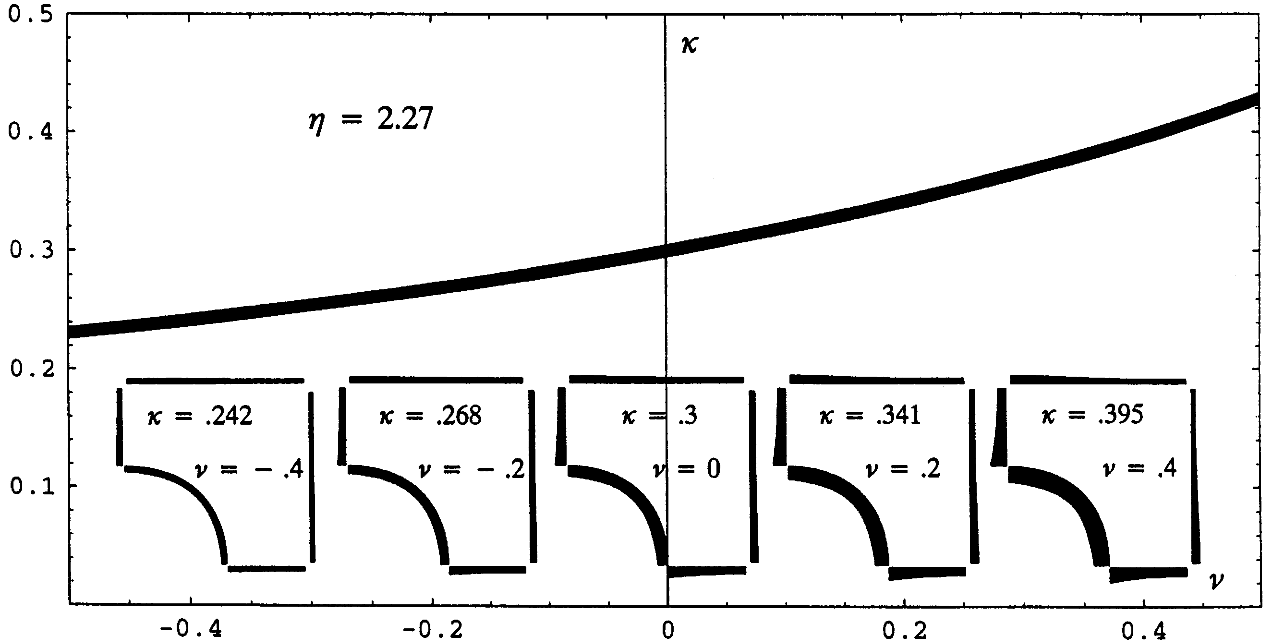

Fig. 13 Hashin-Shtrikman upper bounds on the "bulk" modulus in 2D as a function of Poisson's ratio, together with the optimal solution for a one-parameter shape with relative density 0.75

when starting from $\alpha = 2\beta$ and $\eta = 0.2$ or 0.3, assuming $\rho = 0.75$.

We again note that the total energy (compliance) is rather insensitive to design changes, in contrast to the uniformity of the energy densities along the hole boundary. Note also that the two starting designs with almost the same compliance have quite different maxima of energy densities, 2.05 and 1.66.

5.6 Optimal design with nonlinear elasticity

Next we illustrate that solutions can also be obtained with nonlinear elasticity (in 1D: $\sigma = E\varepsilon^q$). The optimal designs are close to the solution with linear elasticity, but there is a minor influence. Again this might be due to the incomplete uniform distribution of energy density. A result is illustrated in Fig. 15. Note that in designs which allow for a completely uniform energy density (say thickness design) the optimal design will be independent of the power of the nonlinearity (see Fig. 1). This is proven by Pedersen and Taylor (1993). Thus the influence of nonlinearity for shape design must come from the nonuniform energy density, when we go away from the boundary shape.

6 Conclusions

From a theoretical point of view the main conclusions are that the minimum compliance shape design (stiffest shape design) will have uniform energy density along the designed shape, as far as the geometrical constraints make this possible. If we furthermore assume that the highest energy densities are found at the designed shape, then the stiffest design will also be the strongest design, as defined by a design which minimizes the maximum energy density.

To study the influence from parametrization we have focussed on the micromechanics problem of shape design for maximum bulk modulus. With a one-parameter parametrization we can describe the optimal shape and close agreement with the Hashin-Shtrikman (H-S) upper bounds are obtained. Results directly as a function of the relative volume density are presented.

Then results for nonlinear elasticity were presented and also examples with nonequal principal mean strains were shown. In general, the approach of the present paper is also valid for anisotropic behaviour, for nonlinear elasticity, for inhomogeneous or several materials, and for general load cases. In follow up studies we will extend the examples.

In relation to load cases it should be noted that the case of bulk modulus maximization is formulated with forced displacements of the cell external boundaries, because the boundary stresses are unknown. However, even for this case the sensitivity analysis gives all the main aspects, such as the simple optimality criterion derived.

A few aspects related to the stress distribution should be mentioned. In relation to fatigue, not only the maximum stress is important but also the size of the domains where these stresses are found is important. The paper by Lund (1998) shows this aspect of optimal design formulation. Especially in optimal design with anisotropic

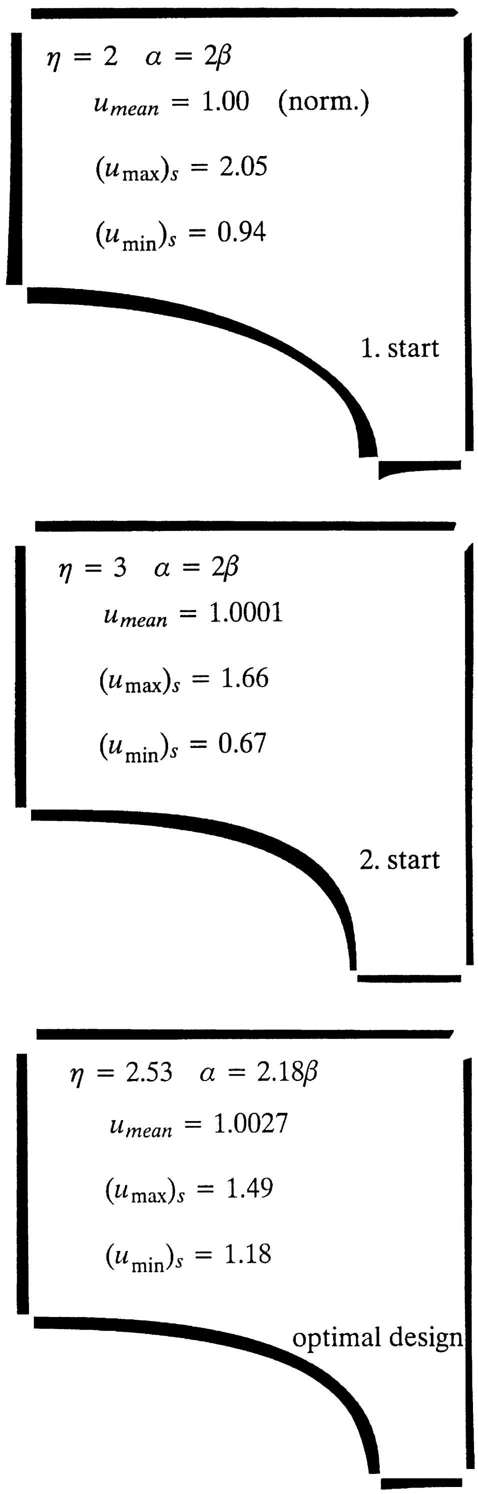

Fig. 14 Boundary strain energy density plot for a two-parameter optimal design of the case with $\varepsilon_1 = 2\varepsilon_2$. From two different starting designs and with relative volume density $\rho = 0.75$

material we have noted resulting stress fields with high stress gradients. This might also be critical and then constraints on stress gradients need to be incorporated. With the tools available this is possible from a numerical point of view, but it is outside the goal of this paper.

In a follow up paper we shall concentrate on the problem of minimum energy concentration and study the difference between solutions to given boundary stresses and to given boundary displacements.

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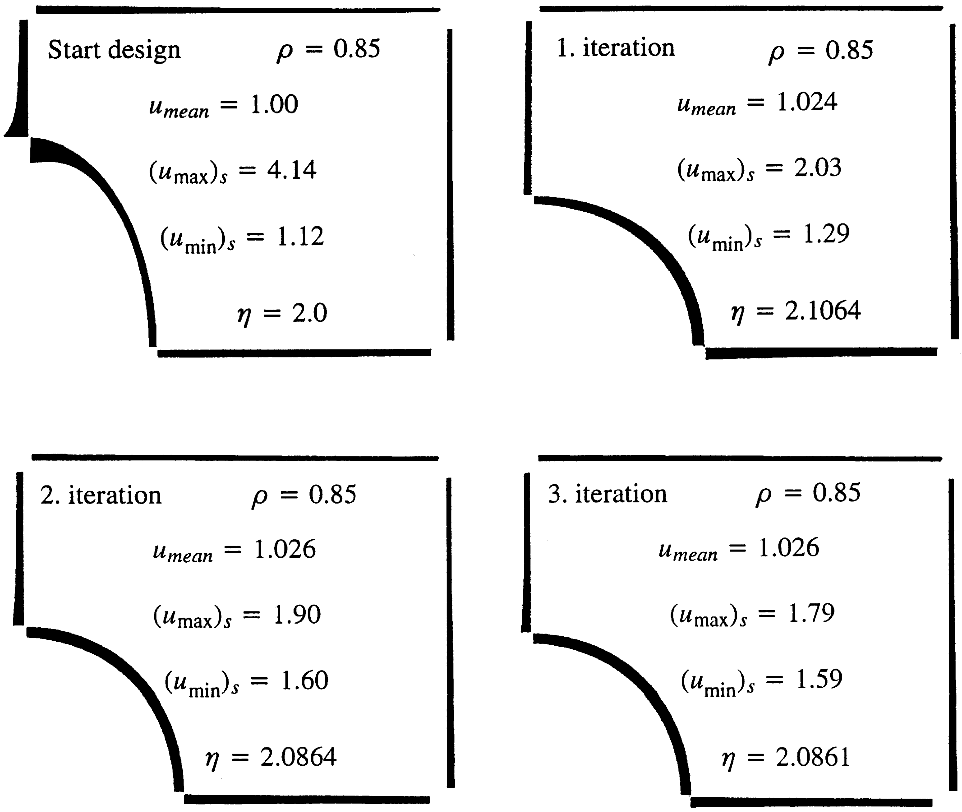

Fig. 15 Illustration of design convergence for nonequal principal mean strains, rectangular domain, orthotropic material ($C_{1111} = 1$, $C_{1122} = 0.1$, $C_{2222} = 0.3$, $C_{1212} = 0.3$) and nonlinear elasticity with $q = 0.5$

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Appendix: Bulk modulus, energy density and eigenvalues

Here we shall concentrate on *isotropic cases* and give some comments to the relations between energy density, bulk modulus and eigenvalues for consititutive matrices. In the three-dimensional case, only for the principal components we have for $\{\sigma\} = [L]\{\varepsilon\}$,

$$[L] = \frac{E(1-\nu)}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1 & \tilde{\nu} & \tilde{\nu} \\ \tilde{\nu} & 1 & \tilde{\nu} \\ \tilde{\nu} & \tilde{\nu} & 1 \end{bmatrix}, \quad \tilde{\nu} := \frac{\nu}{1-\nu}, \tag{34}$$

and for a pure hydrostatic stress state $\overline{\sigma}$ and a pure dilatational strain state

$$\{\sigma\} = \{\overline{\sigma}, \overline{\sigma}, \overline{\sigma}\}, \quad \{\varepsilon\} = \{\overline{\varepsilon}, \overline{\varepsilon}, \overline{\varepsilon}\}/3, \tag{35}$$

because dilatation $\Delta V/V$ is $(\overline{\varepsilon}+\overline{\varepsilon}+\overline{\varepsilon})/3 = \overline{\varepsilon}$.

The *bulk modulus* K is physically defined as the ratio $\overline{\sigma}/\overline{\varepsilon}$, i.e. from (34) and (35)

$$\overline{\sigma} = \frac{E(1-\nu)}{(1+\nu)(1-2\nu)}(1+2\tilde{\nu})\frac{1}{3}\overline{\varepsilon} = \frac{E}{3(1-2\nu)}\overline{\varepsilon}$$

$$\Rightarrow\; K = \frac{E}{3(1-2\nu)}\,. \tag{36}$$

The *strain energy density* u_1 for $\{\varepsilon\} = \{1\,1\,1\}/\sqrt{3}$ gives

$$u_1 = \frac{1}{2}\{\varepsilon\}^T[L]\{\varepsilon\} = \frac{E}{2(1-2\nu)}\,. \tag{37}$$

The *largest eigenvalue* $\lambda_{\max}$ of the constitutive matrix $[L]$ is $3K$, and thus for the *3D-case* we have

$$K = \frac{2}{3}u_1 = \frac{1}{3}\lambda_{\max} = \frac{E}{3(1-2\nu)}\,. \tag{38}$$

(The eigenvector corresponding to $\lambda_{\max}$ is $\{\varepsilon\} = \{1\,1\,1\}/\sqrt{3}$.)

The "bulk" modulus κ is the two-dimensional case depends on the modelling from 3D to 2D and thus has a less physical definition. With a *plane stress* assumption we have for $\{\sigma\} = [C][\varepsilon]$

$$[C] = \frac{E}{1-\nu^2}\begin{bmatrix} 1 & \nu \\ \nu & 1 \end{bmatrix},$$

$$\{\sigma\}^T = \{\overline{\sigma}\,\overline{\sigma}\}\,, \quad \{\varepsilon\}^T = \{\overline{\varepsilon}\,\overline{\varepsilon}\}/2\,, \tag{39}$$

and with the definition $\kappa = \overline{\sigma}/\overline{\varepsilon}$ we have

$$\kappa = \frac{E}{2(1-\nu)}\,. \tag{40}$$

The strain energy density u_1 for $\{\varepsilon\}^T = \{1\,1\}/\sqrt{2}$ gives

$$u_1 = \frac{1}{2}\{\varepsilon\}^T[C]\{\varepsilon\} = \frac{E}{2(1-\nu)}\,, \tag{41}$$

and the largest eigenvalue $\lambda_{\max}$ (with the eigenvector $\{\varepsilon\}^T = \{1\,1\}/\sqrt{2}$) is

$$\lambda_{\max} = \frac{E}{(1-\nu)}\,. \tag{42}$$

Thus the relation for the *2D-case* is

$$\kappa = u_1 = \frac{1}{2}\lambda_{\max} = \frac{E}{2(1-\nu)}\,. \tag{43}$$