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Nonlinear diffusions in topology optimization

M.Y. Wang, S. Zhou, and H. Ding

Abstract Filtering has been a major technique used in homogenization-based methods for topology optimization of structures. It plays a key role in regularizing the basic problem into a well-behaved setting, but it has the drawback of a smoothing effect around the boundary of the material domain. In this paper, a diffusion technique is presented as a variational approach to the regularization of the topology optimization problem. A nonlinear or anisotropic diffusion process not only leads to a suitable problem regularization but also exhibits strong "edge"-preserving characteristics. Thus, we show that the use of nonlinear diffusions brings the desirable effects of boundary preservation and even enhancement of lower-dimensional features such as flow-like structures. The proposed diffusion techniques have a close relationship with the diffusion methods and the phase-field methods from the fields of materials and digital image processing. The proposed method is described and illustrated with 2D examples of minimum compliance that have been extensively studied in recent literature of topology optimization.

Key words diffusion method, nonlinear diffusions, regularization method, topology optimization

1 Introduction

The field of topology optimization of continuum structures has been thriving in the past decades with a wide

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range of techniques having been developed by Bendsoe and Nikuchi (1988), Bendsoe (1999), Bendsoe and Sigmund (1999, 2003). In the basic problem of variable-topology optimization (Bendsoe and Nikuchi 1988) one seeks an optimal distribution of a fixed amount of material over a larger reference domain $\Omega \subseteq R^d$ ($d = 2$ or 3) through specified objective and constraint functions. The optimal design A is a part of the reference domain $A \subset \Omega$ and it can be represented by its characteristic function $\chi(x) : \Omega \to \{0, 1\}$ such that $\chi(x) = 1$ if $x \in A$ and $\chi(x) = 0$ otherwise (Bendsoe and Nikuchi 1988; Bendsoe 2003). Unfortunately, the basic topology optimization problem is often an *ill-posed* problem if without further restriction (Allaire 2001; Cheng and Olhoff 1981; Haber *et al.* 1996). Particularly for the problem of minimizing the structural compliance of an elastic body for a specified set of loads and supports, it is known that, except for some special choices of linear or anisotropic tensor corresponding to a material model, a non-convergent design sequence can be constructed such that the compliance reduces monotonically (cf. Allaire 2001; Bendsoe and Sigmund 2003). The resulting design has a configuration with an unbounded number of microscopic holes, rather than a finite number of macroscopic holes.

Well-posed problems can be generated by a relaxation procedure by allowing homogenization of the properties of the material (Bendsoe and Kikuchi 1988). Relaxation usually yields continuous design variables over the reference domain, similar to the greyscale rendering of an image, and it circumvents the numerical difficulties associated with the discrete "0–1" formulation. However, it is no longer possible to define unambiguously a point of either solid or void from the homogenized solution. Perforated microstructures are also difficult to manufacture. Thus, the "relaxed" optimal solutions may not lead directly to useful and practical designs.

Another class of methods is the explicit penalization of intermediate values of the material density. This is the type of problem formulation studied here. In this method one defines a variable of material density $\rho(x)$ at each point within the design domain $x \in \Omega$ such that the characteristic function of the structure being designed is defined by $\chi(x) : \Omega \to [0, 1]$. The model of material properties is expressed in terms of the design variable $\rho(x)$

using a simple "power-law" interpolation as an explicit means to suppress intermediate values of the bulk density (Bendsoe and Sigmund 2003, 1999). This technique becomes quite popular, especially with the "solid isotropic material with penalization" (SIMP) approach for its conceptual and practical simplicity (Rozvany 1989; Rozvany and Zhou 1991; Rozvany *et al.* 1992; Bendsoe and Sigmund 2003). In order to ensure existence of solutions for this approach, one may also introduce *a priori* restrictions on the admissible design configurations. It has been pointed out that certain configuration restrictions are equivalent to explicit penalties on intermediate densities (Bendsoe and Sigmund 1999), thus yielding similar designs. Various methods based on the concepts of homogenization and material interpolation have been extensively developed over the past decade. We shall refer the reader to the excellent books by Rozvany (1989), Allaire (2001) and Bendsoe and Sigmund (2003) for comprehensive discussions and literature coverage.

Another difficulty in topology optimization is the occurrence of checkerboard patterns in the final solutions. This is a matter of numerical instabilities, like those for the Stokes equations when two coupled fields are discretized by a discrete method (Allaire 2001; Petersson 1999). Various possibilities have been suggested, including adding perimeter controls, slope constraints and employing filters for suppressing the chattering solutions (Bendsoe 1999; Diaz and Sigmund 1995; Sigmund and Petersson 1998; Petersson 1999), and they have been widely applied to problems with multiple physics and multiple materials (Bendsoe and Sigmund 2003).

Among these approaches a filtering technique seems to be the most widely used method (Bendsoe and Sigmund 2003). A filter approach was first suggested by Sigmund by modifying the design sensitivity of a specific element and making it dependent on a weighted average over its neighbouring elements. This usually gives rise to mesh-independent and checker-pattern-free optimization results with moderate computational cost. The concept is further developed into a local gradient constraint (Sigmund and Petersson 1998), for which the existence and convergence of solutions is proven. This constraint would substantially increase the computation cost. Recently, Bourdin (2001) presented a more general filtering theory applied with a non-local relationship between the density and the material properties, for example, stiffness for minimum compliance problems. Solution existence and numerical convergence of the technique is proven, while reasonable numerical results are also provided.

As a widely observed phenomenon, the obvious disadvantage of a filtering approach is a *smoothing* effect around the boundary of the solid regions in the final optimal design, especially when the filtering range takes a relatively large value. This means that the material density variable $\rho(x)$ cannot take the value 1 at the edges of the material region. This behaviour may cause difficulties for boundary identification in a postprocessing step which is necessary for shape recovery from the optimization solution. An averaging effect is introduced into the numerical solution process by the use of filters. This is a well-known technique to ensure regularity or existence of solutions to a problem and has been used in various domains of application. The basic idea is to replace a non-regular function by its *regularization* of a smooth function.

A more general class of regularization techniques is diffusion. It is a powerful and well-founded tool in various applications, especially in multi-scale image analysis and processing (cf. Aubert and Kornprobst 2000; Sapiro 2001). Diffusion models allow the inclusion of *a priori* knowledge to ensure regularity while they can also lead simultaneously to preservation or even enhancement of important features such as edges, lines or flow-like structures, particularly with nonlinear diffusion. The concept seems to be applied to regularization of structural optimization problems first in the use of the total variation (Haber *et al.* 1996; Petersson 1999).

Nonlinear diffusion techniques are the subject of the present study. Here we present models of regularization based on diffusion theories to address the problem of shape and topology optimization of structures. The basic setting of the problem is the same with the material distribution approach (Bendsoe 1999) of a continuous variable $\rho(x) \in [0,1]$ within a fixed reference domain $x \in \Omega$. However, in contrast to the existing methods discussed above, no filter models are applied on the interpolation of the material properties; neither constraints on the microstructures of material are necessary. The ill-posed basic problem is to be regularized by introducing a diffusion in the dynamic process of optimization. This is a *posteriori* process as a feedback in adapting a diffusivity to the gradient of density variable $\rho(x)$. Therefore, this is a *variational* method. Furthermore, a diffusion may be chosen to induce a smooth solution or a solution preserving sharp transitions of the variable $\rho(x)$ across x (known as an "edge-preserving" solution), as it is often so used in image processing (Aubert and Kornprobst 2000; Charbonnier *et al.* 1997). The proposed approach is applicable to a range of problems, but the scope of this paper is to be limited to a simple 2D minimum-compliance optimization problem for a full description of the diffusion technique in this setting.

In the following, we first define the basic problem of topology optimization for minimum compliance. The conventional filtering techniques are discussed. We then describe the concept of diffusion processes and it is shown that the linear heat diffusion is equivalent to the Gaussian filtering technique. Properties of nonlinear diffusions for edge-preserving regularization are then presented. We show how a nonlinear diffusion can be incorporated in a variational framework for regularization in the problem of topology optimization. Numerical schemes are then discussed with an introduction of five different diffusivity functions commonly used in various applications. Finally, the proposed diffusion method is illustrated with 2D examples, showing its effectiveness and the effect of the diffusivity parameter on the final solutions. Some further extensions of the method are discussed in the conclusions section.

Our research work presented here is partly inspired by a recent overview of the field by Bendsoe (1999), where the current approaches of material distribution are incisively analysed and their beneficial features and some intrinsic features that are less desirable are pointed out. These fundamental issues are often the subject of argument in the literature (Ruiter and Keulen 2000; Sigmund and Petersson 1998) from investigations into alternative approaches such as the evolutionary approaches (Bendsoe and Sigmund 2003), material interpolation (Bendsoe and Sigmund 2003, 1999), and the level-set and phase-field methods being developed more recently (Osher and Santosa 2001; Sethian and Wiegmann 2000; Wang *et al.* 2003, 2004; Allaire *et al.* 2004; Bourdin and Chambolle 2003; Wang and Zhou 2003, 2004).

2 Statement of the problem

Let us consider the minimum compliance optimization problem of a statically loaded linear elastic structure under a single loading case (Bendsoe and Kikuchi 1988; Rozvany 1989). Let $\Omega \subseteq R^d$ ($d = 2$ or 3) be an open and bounded set occupied by the linear isotropic elastic structure. The boundary of Ω consists of three parts: $\Gamma = \partial\Omega = \Gamma_0 \cup \Gamma_1 \cup \Gamma_2$, with Dirichlet boundary conditions on Γ_1 and Neumann boundary conditions on Γ_2. It is assumed that the boundary segment Γ_0 is traction free. The displacement field u in Ω is the unique solution of the linear elastic system

$$\begin{aligned} &-\text{div}\,\sigma(u) = f && \text{in } \chi_\Omega(x) = 1 \\ &u = u_0 && \text{on } \Gamma_1 \\ &\sigma(u)\cdot n = h && \text{on } \Gamma_2 \end{aligned} \tag{1}$$

where the strain tensor ε and the stress tensor σ at any point $x \in \Omega$ are given in the usual form as

$$\varepsilon(u) = \frac{1}{2}\left(\nabla u + \nabla u^T\right) \qquad \sigma(u) = E\varepsilon(u) \tag{2}$$

with E as the elasticity tensor, u_0 the prescribed displacement on Γ_1, f the applied body force known for all possible configurations of Ω, h the boundary traction force applied on Γ_2 such as an external pressure load exerted by a fluid, and n the outward normal to the boundary.

The topology optimization problem of minimizing mean compliance is formulated as:

$$\inf_\rho\; l(u) = \int_\Omega f^T u \,\mathrm{d}\Omega + \int_{\Gamma_2} h^T u \,\mathrm{d}S$$

$$\text{Subject to } (u,\rho) \in S(\Omega) \tag{3}$$

The admissible space $S(\Omega)$ of the pair (u,ρ) for the problem is defined as $S(\Omega) = \{(u,\rho) \in U \times H\}$, with u and ρ satisfying

$$a(u,\rho) := \int_\Omega E(\rho)\,\varepsilon(u) : \varepsilon(v)\,\mathrm{d}\Omega =$$

$$\int_\Omega f^T v \,\mathrm{d}\Omega \;+\; \int_{\Gamma_2} h^T v \,\mathrm{d}\Gamma,\ \forall v \in U \tag{4}$$

with ‘:’ representing the second-order tensor operator. This is the weak form of the equilibrium equation of the elastic system, where the set of kinematically admissible displacements U is specified as

$$U := \left\{v \in W^{1,2}(\Omega);\ v = 0 \text{ on } \Gamma_1\right\} \tag{5}$$

and the space of feasible designs H is

$$H = \{\rho \in L^\infty(\Omega);\ 0 \le \rho \le 1 \text{ a.e. in } \Omega\} \text{ and}$$

$$\int_\Omega \rho(x)\,\mathrm{d}\Omega \le V \tag{6}$$

with a limit on the amount of material in terms of the maximum admissible volume V of the design.

A fundamental question regarding this class of structural optimization problems (3) is the existence and smoothness of the solutions. This basic problem is an ill-posed problem as explained above (cf. Cea and Malanowski 1970; Murat 1972, 1977). The conventional filtering technique replaces the dependence of the elastic properties on the density of material with a dependence on a filtered version of the density function. As explained above, this would limit the rapid variations in the material properties and thus ensure existence of solutions (Bourdin 2001).

A filter operation is achieved by means of a convolution operator on the density (Bourdin 2001)

$$(F{*}\rho)(x) = \int_\Omega F(x-y)\rho(y)\,\mathrm{d}y \tag{7}$$

This definition requires the extension of the density field ρ to the whole space Ω. Different implementation of this extension yield different versions of the filter with different smoothing effects. These filtering techniques are thoroughly examined in (Bourdin 2001). In the conventional SIMP approach for topology optimization with the so-called power-law method, it is often assumed that the Young's modulus of a material point can be written as a function of its material density as $E(\rho) = E_0\rho^p$, where E_0 is the Young's modulus of a given solid material and p is a factor of penalizing intermediate densities with $p > 1$. Thus, the equilibrium condition (4) for the filtered density field (7) becomes (Bourdin 2001)

$$\int_\Omega (F{*}\rho)^p\, E\varepsilon(u) : \varepsilon(v)\,\mathrm{d}\Omega =$$

$$\int_\Omega f^T v \,\mathrm{d}\Omega \;+\; \int_{\Gamma_2} h^T v \,\mathrm{d}\Gamma,\ \forall v \in U \tag{8}$$

Such a filtering technique is known to have a strong smoothing effect around the boundary of the material domain. Another recent scheme is to define a new stiffness-density interpolation function as (Guo and Gu 2004)

$$E(\rho(x)) = E_0\rho(x)(F*\rho(x))^p \tag{9}$$

This scheme is justified mathematically to reduce the non-local effect of a material point and thus to alleviate the undesirable boundary diffusion effect.

3
Diffusion techniques

The issue of regularization for well-posed problems has been a subject of extensive studies in a class of more general problems of domain identification with regularization (cf. Aubert and Kornprobst 2000; Sapiro 2001). Diffusions are known to be a powerful tool for the purpose (Aubert and Kornprobst 2000; Weickert 1997). In this section we introduce linear and nonlinear diffusion processes for the purpose of regularizing and solving the structural topology optimization problem (3).

3.1
Diffusion processes

Diffusion intuitively is a physical process of mass transport. Diffusion processes derive from Fick's law and the continuity condition. Fick's law expresses that a gradient concentration leads to a flow which compensates for it. If mass is only transported but can be neither created nor destroyed, the diffusion equation is obtained as

$$\partial_t\rho = \text{div}\ (D\cdot\nabla\rho) \tag{10}$$

where D is a diffusion tensor, ρ corresponds to the mass concentration or the material density in our problem setting (Weickert 1997), and t denotes the scale parameter or time. The diffusion tensor defines the diffusion process. For example, if the tensor is chosen as the identity matrix, then we have a well-known case of the diffusion process, the heat equation. If the diffusion tensor is a function of the differential structure of the mass density itself, the feedback process leads to nonlinear diffusions generally described by

$$\partial_t\rho = \text{div}\ \left(g\left(|\nabla\rho|^2\right)\nabla\rho\right) \tag{11}$$

with the diffusivity function $g\left(|\nabla\rho|^2\right)$.

In the classical variational method this nonlinear diffusion can be expressed as energy minimization. Let us consider a potential function $\varphi\left(|\nabla\rho|\right)$ whose gradient is given by

$$\nabla\varphi\ \left(|\nabla\rho|\right) = g\left(|\nabla\rho|^2\right)\nabla\rho \tag{12}$$

Then minimization of the energy functional

$$\min_\rho \int_\Omega \varphi\left(|\nabla\rho|\right)\mathrm{d}x \tag{13}$$

leads to the nonlinear diffusion equation (11) (Sapiro 2001). It is easy to show that $g(s) := \varphi'(s)/s$.

3.2
Linear diffusion filter

The oldest and most investigated diffusion equation is the linear heat equation

$$\partial_t\rho = \text{div}\ (\nabla\rho) = \Delta\rho \tag{14}$$

corresponding to $g\left(|\nabla\rho|^2\right) = 1$ and $\varphi\left(|\nabla\rho|\right) = \frac{1}{2}|\nabla\rho|^2$. Its solution is well known as the following convolution integral

$$\rho\left(x,t\right) = K_{\sqrt{2t}}*\rho(x)$$

where K_σ is the Gaussian kernel

$$K_\sigma = \frac{1}{2\pi\sigma^2}\exp\left(-\frac{|x|^2}{2\sigma^2}\right)$$

This in fact is equivalent to the linear filter models previously developed in topology optimization (Bourdin 2001). It is a low-pass filter and is isotropic. It diffuses the information equally in all directions, thus blurs important features such as edges and boundaries. In the field of variational approaches, the corresponding energy functional term $\int_\Omega |\nabla\rho|^2\,\mathrm{d}x$ is called the Thikonov regularization (Charbonnier *et al.* 1997; Tikhonov and Arsenin 1997). In our topology optimization problem, "edges" would represent the boundary of the structure. Boundaries are the most important features in our problem, and they are defined as *sharp* transitions of the density level. Thus, a more preferable regularization method should be able to yield sharp material transitions, or be "edge preserving".

3.3
Nonlinear diffusions with edge preservation

In order to achieve an "edge"-preserving effect, a nonlinear diffusion model must be used such that the following two conditions are achieved:

1. Inside a material region where $|\nabla\rho|$ is weak, the diffusion equation acts like the heat equation, resulting in isotropic filtering.
2. Near the boundary of a material region, where $|\nabla\rho|$ is large, the smoothing effect is substantially reduced and the boundary's edges are preserved.

These conditions require that the diffusivity function $g(s)$ or energy functional $\varphi(s)$ have certain unique properties in addition to being regular and continuously differentiable. Indeed, we may interpret the diffusion process as a sum of a diffusion in the tangential direction T plus a diffusion in the normal direction N. On the edges, it is preferable to diffuse the density along the tangential direction T of the boundary and not across it. It is easy to show from a simple analysis that the energy functional φ should be chosen to have at least the three following properties (Aubert and Kornprobst 2000; Samson *et al.* 2000):

1. $\varphi'(s)/s$ is strictly decreasing on $s \in [0, \infty\}$.
2. $\varphi'(0) = 0, \quad \lim_{s\to 0} \varphi'(s)/s = \varphi''(0) = \beta$, and $0 < \beta < \infty$.
3. $\lim_{s\to\infty} \varphi'(s)/s = \lim_{s\to\infty} \varphi''(s) = 0$.

The first property is to avoid numerical instabilities. The second condition requires $\varphi(s)$ to be quadratic or nearly quadratic for $s \to 0$, and its role is the regularization effect of smoothing where variations of the density are weak. The third condition requires $\varphi(s)$ to be linear or sub-linear for $s \to \infty$. This corresponds to the edge-preserving effect, where in a neighbourhood of the boundary the density presents a strong gradient. Such a typical function is $\varphi(s) = s^2/(1+s^2)$ and its behaviour is illustrated in Fig. 1, together with some other commonly used functions.

The function $\varphi(s)$ may be convex or non-convex. When φ is convex, a theoretical study of the minimizers of its energy functional can be established, such as for their existence and uniqueness. On the other hand, such a theoretical study for a non-convex function φ is often difficult. Nevertheless, in the field of image processing, non-convex functions are found to work well or even to provide better results (Guo and Gu 2004; Haber *et al.* 1996). Some widely used edge-preserving functions include $\varphi(s) = |s|$ (total variation), $\varphi(s) = s^2/(1+s^2)$, and $\varphi(s) = \log(1+s^2)$, to name a few.

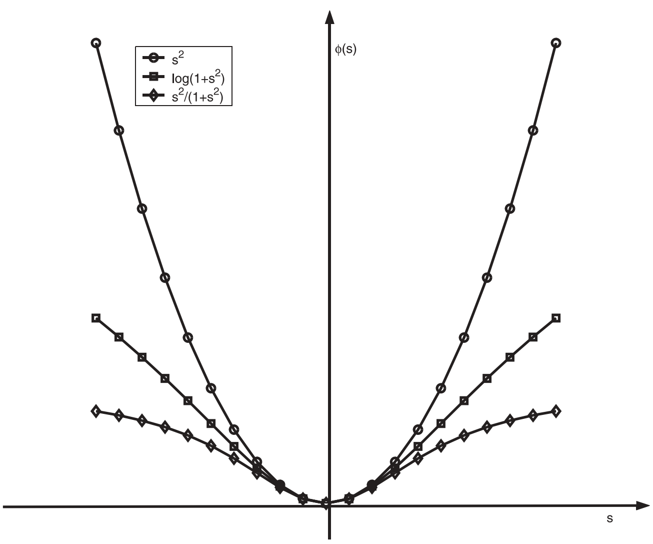

Fig. 1 Behaviour of some regularization functions

3.4
Topology optimization with edge-preserving diffusion

Following the above analysis of nonlinear diffusion, we can introduce a variational model for the continuous mean compliance minimization problem of (3), formulated with a new objective functional:

$$\inf_{\rho} \; J(u) = \int_{\Omega} f^T u \,\mathrm{d}x + \int_{\Gamma_2} h^T u \,\mathrm{d}x + \mu \int_{\Omega} \varphi(|\nabla\rho|) \,\mathrm{d}x \quad (\mu > 0)$$

$$\text{Subject to } (u,\rho) \in S(\Omega) \tag{15}$$

with u and ρ satisfying (4).

The inclusion of the energy functional term φ is for regularization. Naturally, it is not sufficient to ensure that the transitional density $0 < \rho < 1$ in the optimal design will be suppressed. As pointed out in (Haber *et al.* 1996), the elasticity tensor in the final optimal design Ω is specified by $E(\Omega) = \chi_\Omega E_0$. This constitutive model must be replaced by a continuous model consistent with the interpolation parameter ρ such that the new model defines a smooth interpolation between the elastic properties of the solid material and void. The simplest model is the "power law" used in the SIMP method (Bendsoe and Sigmund 2003),

$$E(\rho) = E_0 \rho^p \tag{16}$$

It should be emphasized that in our variational model of (15) interpolation models such as (16) are introduced here solely as continuous approximations to the basic integer problem of $\chi_\Omega(x) : \Omega \to \{0, 1\}$, similar to the case of problem formulation in (Haber *et al.* 1996). Another approach is to employ a *phase-field* model based on the theory of phase transitions from mechanics and material sciences as reported in (Cahn and Hilliard 1958; Eyre 1993; Leo *et al.* 1998; Warren 1995). In that case, the energy functional is a generalized free energy in the following form

$$\varepsilon \int_{\Omega} \varphi(|\nabla\rho(x)|) \,\mathrm{d}x + \frac{1}{\varepsilon} \int_{\Omega} W(\rho(x)) \,\mathrm{d}x \tag{17}$$

with an additional potential term W. The first term remains the same as in (15) and depends only on the gradient of $\rho(x)$. W is taken to be a double-welled potential such that $W(1) = W(0) = 0$ and is non-zero only in the transition region where $0 < \rho < 1$. The thickness of the intermediate density region is proportional to ε. As fully developed in (Bourdin and Chambolle 2003; Wang and Zhou 2003, 2004), this variational model will result in a partition of the reference domain into distinct regions, each region being characterized by the feature of being either solid ($\rho(x) = 1$) or void ($\rho(x) = 0$). Hence, the final solution will be made of homogeneous solid or void regions separated by regularized boundaries. Since our goal in this paper is to examine the role of nonlinear diffusions in topology optimization in lieu of the conventional linear filtering, we shall use the power-law model (16) for simplicity.

3.5
Non-convex diffusion functions

Strictly speaking, our continuous regularization model with diffusion of (15) may still be ill-posed, if the function $\varphi(s)$ is sub-linear with the edge-preservation properties required in Sect. 3.3. Clearly, the best regularization results are obtained for a diffusion operator which saturates when the gradient is large. This corresponds to a non-convex function $\varphi(s)$. When the potential $\varphi(s)$ is convex, then $g\left(s^2\right) s$, called the flux, is known to increase monotonously. Convex energy functional have exactly one minimum, thus a theoretical study about the minimizer can be established, such as for their existence and uniqueness. The minimizer can be found by the classical method of gradient descent (Aubert and Kornprobst 2000; Samson *et al.* 2000). Standard finite-element approximations are stable and computationally expensive methods from non-convex optimization are not necessary. On the other hand, it is often difficult to find a discrete solution for a non-convex function φ. There is no mathematical theory available which guarantees a unique or stable solution.

However, non-convex potentials are found to work well or even to provide better results in the field of image processing (Aubert and Kornprobst 2000; Samson *et al.* 2000; Sigmund and Petersson 1998). Initially reported by Perona and Malik in 1987, some non-convex potential functions have been widely employed for stronger behaviours such as edge enhancement. The non-convex effect can also be balanced by a selective smoothing scheme which acts as a tool for convexification of monotonously increasing flux (Samson *et al.* 2000). The reader is referred to the literature, for example, on image processing (Aubert and Kornprobst 2000), for the details of numerical schemes and their analyses.

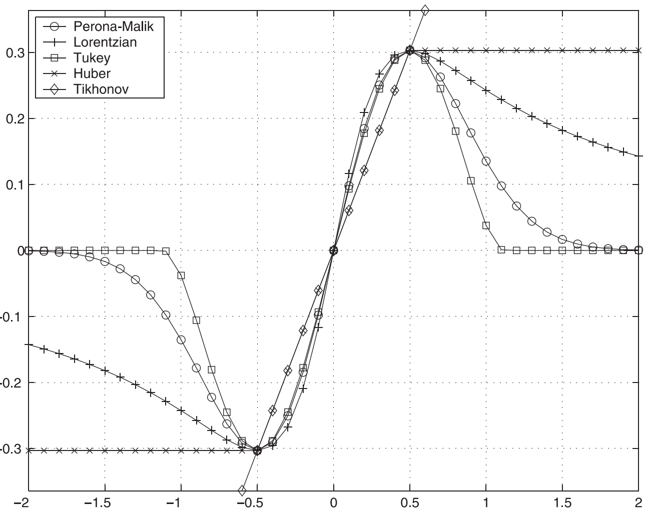

Fig. 2 Aligned and scaled flux functions (adapted from Sapiro (2001))

In this paper we use five different potential functions to examine their regularization and diffusion properties for the minimum compliance optimization of structures. They include convex and non-convex edge-preserving nonlinear functions and the conventional linear diffusion filtering (i.e. Tikhonov function) for comparison. Table 1 lists these potential functions and their diffusivities.

These five diffusion functions can be further compared in the context of robust estimation in connection to robust statistics as presented in (Sapiro 2001). With respect to a robust scale factor and range normalization, the flux functions, $g\left(s^2\right) s$, of the diffusions are plotted

Table 1 Diffusion potentials and diffusivities

Method	Diffusivity $g(s)$	Potential $\varphi(s)$	Convexity
Tikhonov	1	$\frac{s^2}{2}$	all s
Lorentzian	$\frac{1}{1+\frac{s^2}{2\sigma^2}}$	$\sigma^2 \log\left[1+\frac{1}{2}\left(\frac{s^2}{\sigma^2}\right)\right]$	$\lvert s\rvert \le \sqrt{2}\sigma$
Perona–Malik	$\mathrm{e}^{-\frac{s^2}{2\sigma^2}}$	$-\sigma^2\,\mathrm{e}^{-\frac{1}{2}\left(\frac{s}{\sigma}\right)^2}$	$\lvert s\rvert \le \sigma$
Huber	$\begin{cases} \frac{1}{\sigma} & s \le \sigma \\ \frac{sign(s)}{s} & s > \sigma \end{cases}$	$\begin{cases} \frac{s^2}{2\sigma}+\frac{\sigma}{2} & s \le \sigma \\ s & s > \sigma \end{cases}$	no
Tukey	$\begin{cases} \frac{1}{2}\left[1-\frac{s^2}{\sigma^2}\right]^2 & s \le \sigma \\ 0 & s > \sigma \end{cases}$	$\begin{cases} \frac{s^2}{\sigma^2}-\frac{s^4}{\sigma^4}+\frac{s^6}{3\sigma^6} & s \le \sigma \\ \frac{1}{3} & s > \sigma \end{cases}$	no

in Fig. 2. From the shape of the flux functions, one can conclude that diffusing with the Tukey function produces sharper boundaries than diffusing with the Lorentzian and the Perona–Malik functions, which both in turn produce shaper boundaries than the Huber function. The linear diffusion of Tikhonov is clearly shown to be isotropic without any edge-preserving effect.

4 Numerical implementations

Based on the previous discussions, we now describe the numerical aspects of our diffusion schemes. Our variational system is defined by (15), (16) and (4) together. The necessary condition required for a minimizer is the Kuhn–Tucker condition, which is derived from the Euler–Lagrange equation to compute the derivative of the functional J with respect to ρ. Then the optimal solution must satisfy the following Euler–Lagrange equation:

$$\begin{cases} a'(u,\rho) - \mu \operatorname{div}\left[g\left(|\nabla\rho|^2\right)\nabla\rho\right] = 0 & \text{for } x \in \Omega \\ \dfrac{\partial\rho(x)}{\partial n^+} = \nabla\rho\cdot n^+ = 0 & \text{on } \partial\Omega \end{cases} \tag{18}$$

where n^+ is the outward normal to the boundary of the reference domain Ω and $a'(u,\rho)$ denotes the Euler derivative of the mean compliance of the structure with respect to the density variable ρ. With the interpolation model of (4) and (16) for the elasticity tensor this derivative is well established (Bendsoe and Sigmund 1999, 2003). In the common case of a discrete solution with the finite element method, it is expressed by, for an element e,

$$a'_e(\rho) = p\rho^{p-1}K_e u_e : u_e \tag{19}$$

The optimal solution represented by the Euler–Lagrange equation (18) is in fact difficult to solve. There are two major factors behind this difficulty. First, like the homogenization-based methods in topology optimization, the number of design variables of a discrete scheme is typically very large. Thus efficiency of the numerical procedure is a strong consideration factor. This difficulty is further compounded by the complexity of the diffusion process which introduces numerical instability and nonlinearity (in the case of a nonlinear diffusion). Generally speaking, an efficient and accurate numerical solution to (18) requires a sophisticated numerical scheme (Weickert 1997). In the following we present two solution schemes based on more direct and simple ideas, followed with a discussion of other refined algorithms that appear more complex but have more appealing numerical properties.

4.1 Optimality criteria scheme with diffusion filter

Our first scheme follows the standard optimality criteria methods widely used in structural optimization, especially for the mean compliance minimization with many variables and one constraint (3). These methods are well known for their efficiency as the design variables at one point in the discrete approximation are updated independently from the updates at other points, based on the necessary conditions for an optimal solution. This updating scheme was used by many authors (cf. Bendsoe and Kikuchi 1988; Bendsoe and Sigmund 2003).

For the mean compliance problem defined by (3)–(6) with the material interpolation model of (16), the common updating formula based on the optimality condition is

$$\rho^{k+1} = -\rho^k\left(\frac{p\rho^{(p-1)}E_0\varepsilon(u):\varepsilon(u)}{\lambda}\right)^q \tag{20}$$

where λ is the Lagrange multiplier for the volume ratio constraint and q is a tuning parameter to obtain a stable convergence of the scheme and is usually set to $q = 1/2$ (cf. Bendsoe and Sigmund 2003).

With this updating formula in mind, we then take a direct approach to add the diffusion process as a feedback in the iteration procedure of optimization. Since the diffusion is a function of the differential structure of the mass density itself, we may treat it as a filter on the density itself. This means that the density variables will be modified as follows

$$\hat{\rho}^k = \rho^k + \mu \operatorname{div}\left(g\left(\left|\nabla\rho^k\right|^2\right)\nabla\rho^k\right) \tag{21}$$

In the case of the Tikhonov diffusion function, this is in fact the linear (Gaussian) filtering on the density given as

$$\hat{\rho}^k = \rho^k + \mu\,\Delta\rho^k \tag{22}$$

Here, the Laplacian is discretized in space as a sum of the second-order derivatives $\Delta\rho_{i,j}$. In two-dimensional space, the finite difference scheme is described as

$$\Delta\rho_{i,j} = \frac{1}{h^2}\left(\rho_{i+1,j} + \rho_{i-1,j} + \rho_{i,j+1} + \rho_{i,j-1} - 4\rho_{i,j}\right) \tag{23}$$

if we suppose that the point is not located on the edge of the object and the grid width is uniform in h. Alternatively, one may use the complete 3×3 neighbourhood to obtain the following approximation that has good rotation-invariance properties (cf. Aubert and Kornprobst 2000):

$$\Delta\rho_{i,j} \approx \frac{1}{3h^2}\left(\left(\rho_{i+1,j} + \rho_{i-1,j} + \rho_{i,j+1} + \rho_{i,j-1} - 4\rho_{i,j}\right) + \left(\rho_{i+1,j+1} + \rho_{i-1,j+1} + \rho_{i+1,j+1} + \rho_{i-1,j-1} - 4\rho_{i,j}\right)\right) \tag{24}$$

Of course, this is equivalent to the linear filter models previously developed in topology optimization (6). It is a low-pass filter and is isotropic. It diffuses the information equally in all directions, thus blurs important features such as edges and boundaries.

For any nonlinear diffusion potential function $\varphi(s)$, it is easy to show that the diffusion operator can be expressed as

$$\operatorname{div}\left(g\left(|\nabla\rho|^2\right)\nabla\rho\right)_{i,j}=\frac{1}{h^2}\left(\alpha_1\rho_{i+1,j}+\alpha_2\rho_{i-1,j}+\right.$$
$$\left.\alpha_3\rho_{i,j+1}+\alpha_4\rho_{i,j-1}-\left(\sum_{l=1}^{4}\alpha_l\right)\rho_{i,j}\right) \tag{25}$$

where the coefficients α_l are the weights of the Laplacian given by the diffusivity function $\varphi'(s)/s$ as (Charbonnier *et al.* 1997)

$$\begin{cases}\alpha_1=\dfrac{\varphi'\left(\rho_{i+1,j}-\rho_{i,j}\right)}{2\left(\rho_{i+1,j}-\rho_{i,j}\right)}\\ \alpha_2=\dfrac{\varphi'\left(\rho_{i-1,j}-\rho_{i,j}\right)}{2\left(\rho_{i-1,j}-\rho_{i,j}\right)}\\ \alpha_3=\dfrac{\varphi'\left(\rho_{i,j+1}-\rho_{i,j}\right)}{2\left(\rho_{i,j+1}-\rho_{i,j}\right)}\\ \alpha_4=\dfrac{\varphi'\left(\rho_{i,j-1}-\rho_{i,j}\right)}{2\left(\rho_{i,j-1}-\rho_{i,j}\right)}\end{cases} \tag{26}$$

When comparing with (22), it is clear that a nonlinear diffusion process can also be regarded as a filtering process on the density $\rho(x)$ by the position-dependent weighted filter of (24). The edge-preserving properties of the nonlinear diffusion are specified by the required conditions listed in Sect. 3.3. When the diffusivity function is such that

$$\lim_{s\to 0}\varphi'(s)/s=\varphi''(0)=\beta\,,\ \text{and } 0<\beta<\infty$$

then all weights α_l around the point are approximately equal to β and the nonlinear diffusion process behaves as the usual linear filter with diffusion (i.e. smoothing) all around the point. On the other hand, when the following condition is met

$$\lim_{s\to\infty}\varphi'(s)/s=\lim_{s\to\infty}\varphi''(s)=0$$

then the corresponding weight of the Laplacian vanishes and there is no smoothing in the direction of $s\to\infty$. This would correspond to a discontinuity of density in the neighbourhood of the point (i.e. an edge). Therefore, the nonlinear diffusion behaves in an edge-preserving manner.

4.2 Methods of gradient flow

Instead of directly solving the Euler–Lagrange equation (18) associated with the minimization problem (15), a more general technique of looking for a possible solution is to solve numerically the following partial differential equations (PDEs)

$$\begin{cases}\partial_t\rho+a'(u,\rho)-\mu\operatorname{div}\left[g\left(|\nabla\rho|^2\right)\nabla\rho\right]=0 \text{ for } x\in\Omega\\ \dfrac{\partial\rho(x)}{\partial n^+}=\nabla\rho\cdot n^+=0 \text{ on } \partial\Omega\end{cases} \tag{27}$$

with given initial condition $\rho(0,x)=\rho_0(x)$. When the steady state of this equation is obtained, a solution to the Euler–Lagrange equation is achieved. This approach is also called the gradient-descent flow (Aubert and Kornprobst 2000; Sapiro 2001). Here, the auxiliary variable t is denoted as the scale variable.

PDE-based methods have been extensively studied in the fields of digital image processing. In most applications

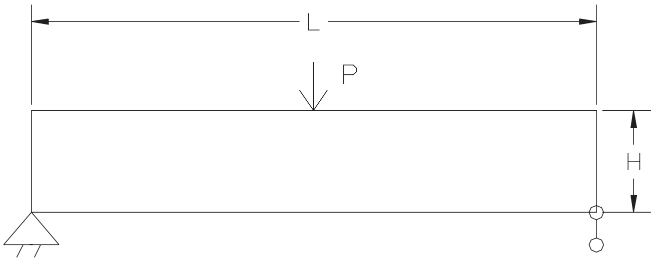

Fig. 3 The MBB structure with fixed-simple supports

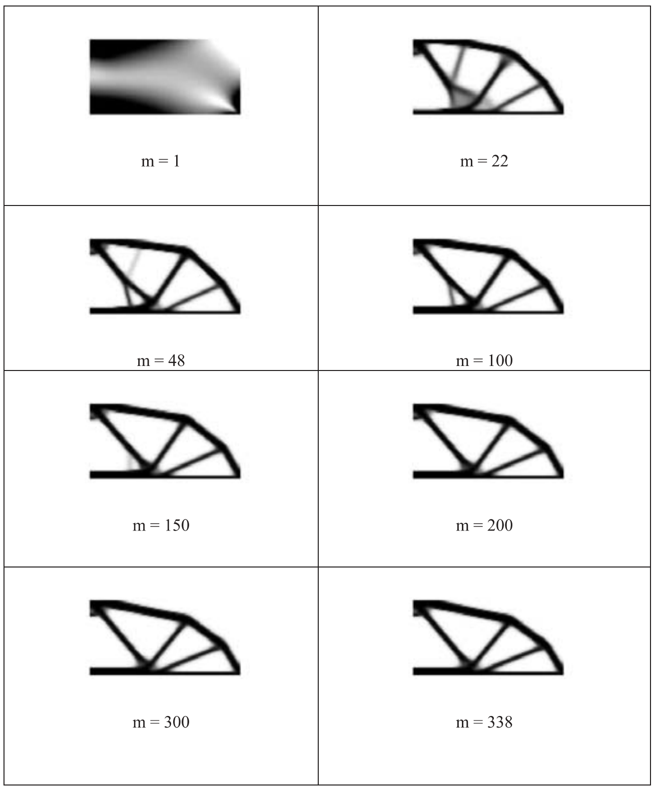

Fig. 4 The solution sequence of the MBB beam (right-half) with m being the iteration number

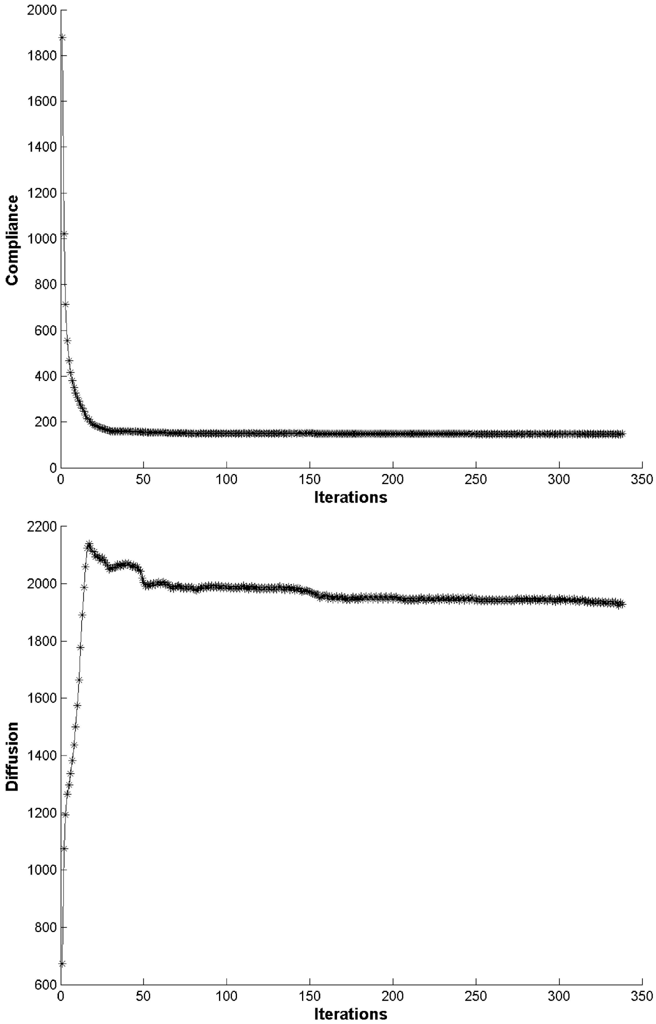

Fig. 5 The mean compliance and diffusion potential during the convergence process

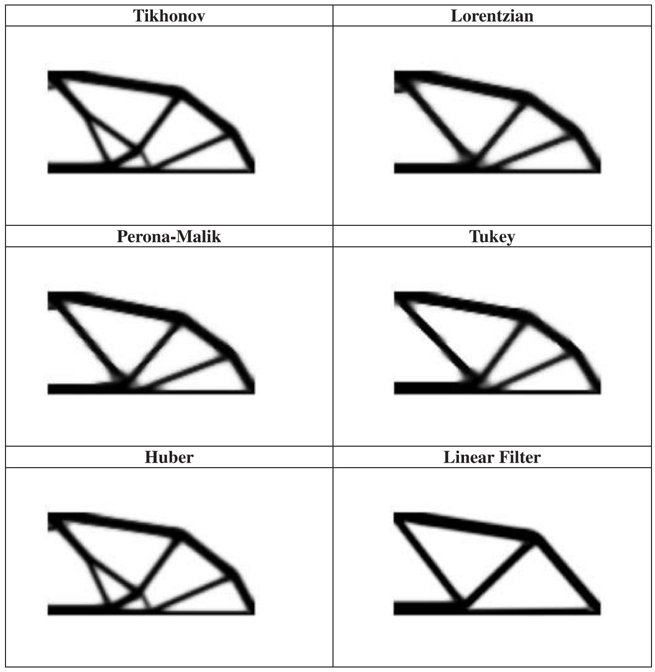

Fig. 6 Solutions for the MBB example with different diffusion functions and the linear filter

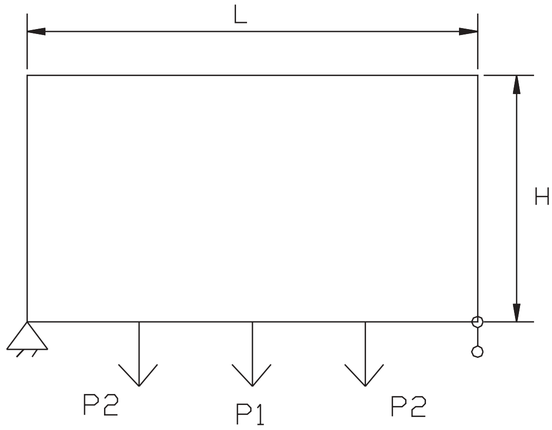

Fig. 7 A bridge-type structure with multiple loads

of nonlinear diffusions, finite difference methods are used for numerical solutions, since they are easy to handle and our fixed design domain provides a natural discretization on a fixed rectilinear grid. An explicit scheme is simple to implement and thus is used in the paper. The rotation-invariant difference scheme of (24) is also used in the implementation. However, it should be noted that conditions for numerical stability typically limit the explicit schemes to using fairly small time-step sizes. Thus, such a scheme is typically inefficient.

In the literature of digital image processing, a number of more efficient numerical methods are developed for nonlinear diffusions, including semi-implicit scheme and multi-grid techniques (cf. Aubert and Kornprobst 2000). These schemes possess much better stability and efficiency properties. Furthermore, a concept of discrete nonlinear scale space has been developed, which has led to the development of fast schemes based on adaptive operator splitting (Weickert 1997). These new schemes are found to be a few orders of magnitude more efficient under typical accuracy requirements. Moreover, another advantage of the use of PDEs is that special numerical schemes can be devised to preserve discontinuities (such as edges) in the solution, if the PDEs are modelled to describe a level-set flow as in the level-set-based modelling of topology optimization (Osher and Santosa 2001; Sapiro 2001).

5 Numerical experiments

Here we illustrate the use of the diffusion processes for mean compliance optimization problems that have been widely studied in the relevant literature (cf. Bendsoe and Sigmund 2003; Allaire 2001). For clarity in presentation, the examples are in 2D under a plane stress condition.

For the first two examples, we use the optimality criteria method with diffusion filter described in Sect. 4.1. The

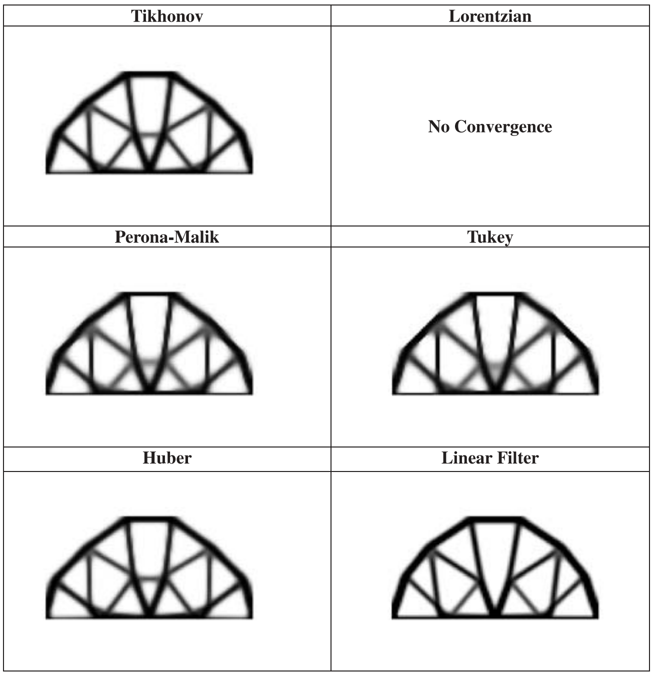

Fig. 8 A bridge structure (top) and its optimal designs with different diffusion functions and the linear filter

first example is known as MBB beams related to a problem of designing a floor panel of a passenger aeroplane in Germany. The floor panel is loaded with a unit concentrated vertical force $P = 1$ N at the centre of the top edge. It has a fixed support and a simple support at its bottom corners respectively. The design domain has a length-to-height ratio of $12 : 2$ (Fig. 3). The volume ratio is specified to be 0.3. We use 100×50 quadrilateral elements to model one half of the structure due to the geometric symmetry.

Using the Perona–Malik diffusivity function and setting $\sigma = 0.5$ and $\mu = 0.1$, we obtain a converged optimization sequence as shown in Fig. 4. Changes in the mean compliance and the potential energy during the convergence are shown in Fig. 5. Here, we deliberately kept the iteration to a high number to illustrate the convergence process of the direct numerical scheme.

For this example, other diffusivity functions are also employed. Figure 6 shows the optimal designs obtained with all of the five diffusion functions listed in Table 1. For these convex or non-convex diffusions, they all produce satisfactory results. These optimal designs are also compared with that obtained from using the SIMP method with the conventional filtering technique, also shown in the figure. It should be noted that the different diffusion process may produce different final designs with different topological configurations. It is clear that the diffusion process, just like a conventional linear filter, has a strong regularization effect that restricts the permissible space of the design.

A bridge-type structure is considered next. A rectangular design domain, L long and H high, with a ratio of $L : H = 12 : 6$ is loaded vertically at its bottom with multiple loads $P_1 = 40$ N and $P_2 = 20$ N as shown in Fig. 7. The bottom left corner of the beam is fixed, while it is simply

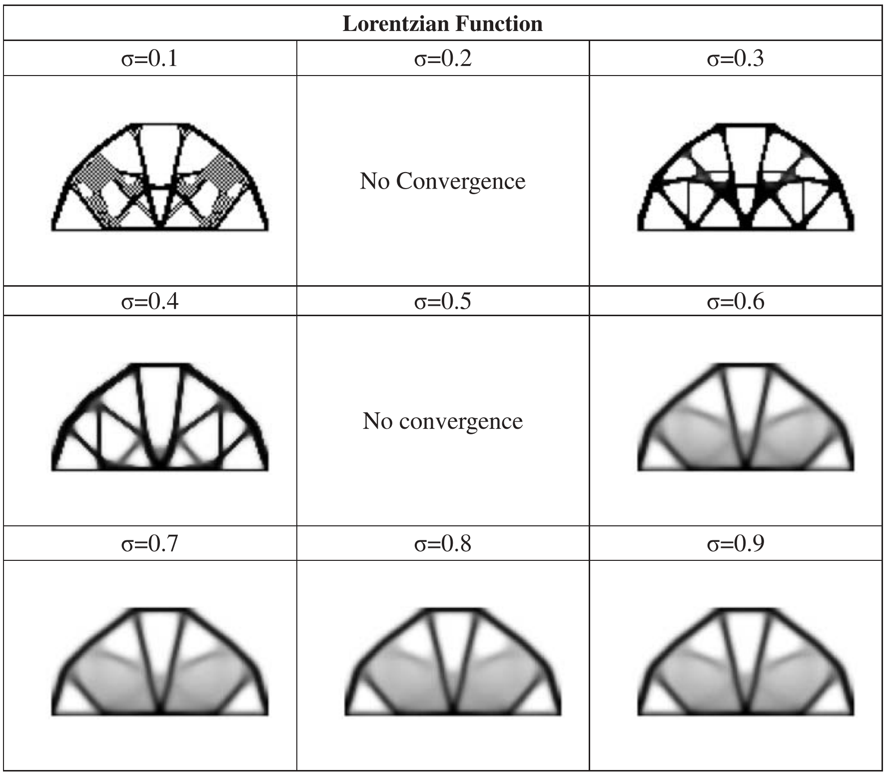

Fig. 9 Optimal designs with Lorentzian diffusion function

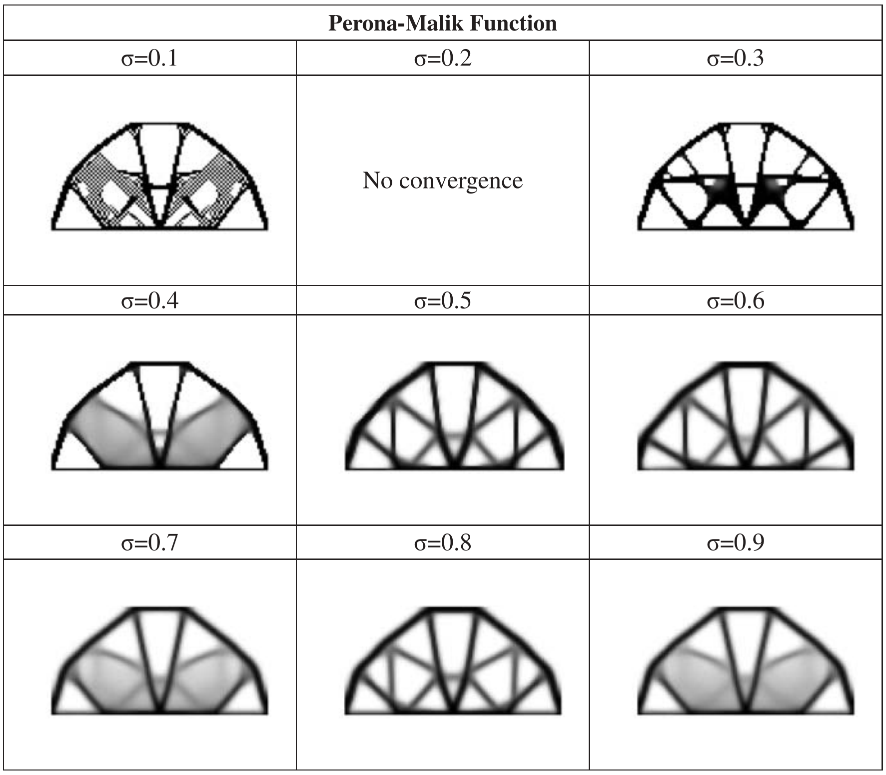

Fig. 10 Optimal designs with Perona–Malik diffusion function

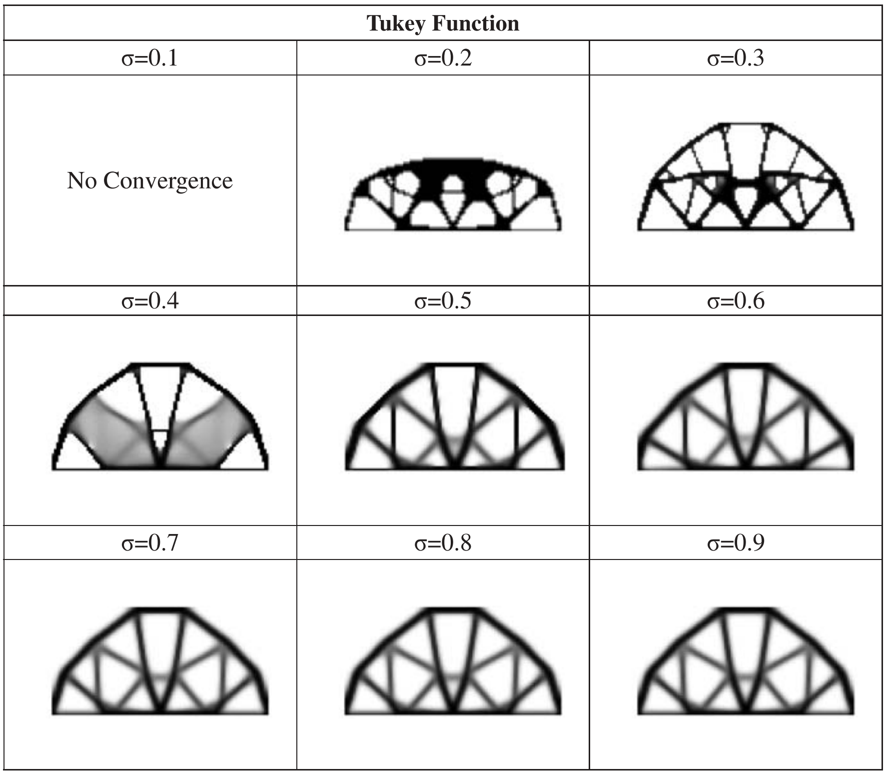

Fig. 11 Optimal designs with Tukey diffusion function

supported at the bottom right corner. The volume ratio of 0.30 is considered. A mesh of 100×50 quadrilateral elements is used for the discrete analysis and optimization, and we set $\sigma = 0.5$ and $\mu = 0.1$. Figure 8 shows the optimal designs obtained with the diffusion functions and with the SIMP method.

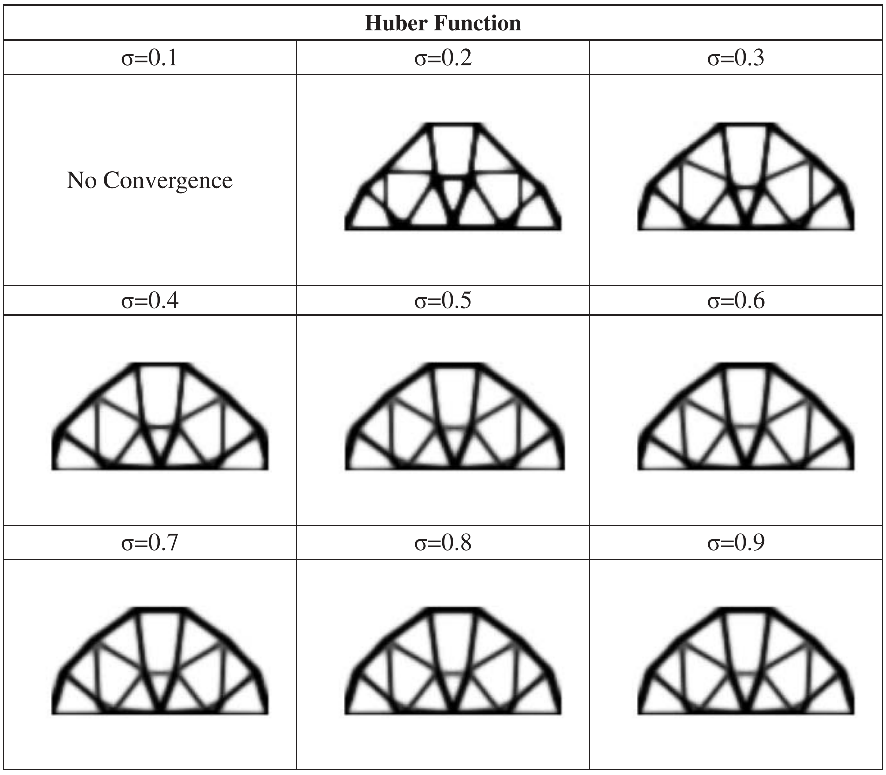

Fig. 12 Optimal designs with Huber diffusion function

From these two examples we note that our direct implementation of the diffusion process by incorporating it into the optimality-criteria-based updating of variables works as efficiently as the conventional SIMP method with a linear filter. However, the edge-preserving effects of diffusion near the edges are not well pronounced as expected for the nonlinear diffusion functions. Apparently, the direct step of (19) for variable updating has a compromising effect on the density modification for diffusion in (20). However, a detailed analysis for this effect in the use of the heuristic method is not available yet.

Note that our diffusion process did not converge for the Lorentzian diffusion process in this example. Convergence of our optimization process is determined by many factors. A key element is the scale parameter σ in the nonlinear diffusivity functions. Large values of the scale parameter will dilate the diffusivity function, and reduce its influence on the edge-preserving effect. We have examined this effect for the example of the bridge-like structure for each of the four nonlinear diffusion processes, with results given in Figs. 9–12 respectively, for σ varying from $\sigma = 0.1$ to $\sigma = 0.9$. The heuristic nature of the quick update method may also contribute to the non-convergence. These results are not meant to be comprehensive but to provide an intuitive experience for the diffusion processes proposed in the paper.

The last example is a cantilever beam with a concentrated vertical force $P = 10\,\mathrm{N}$ at the bottom of its free vertical edge. The design domain has a length-to-height ratio of $2:1$. The volume ratio is specified to be 0.3, and we use 100×50 quadrilateral.

For this example we use the method of steepest gradient flow of (26) with a fairly small time step. Since

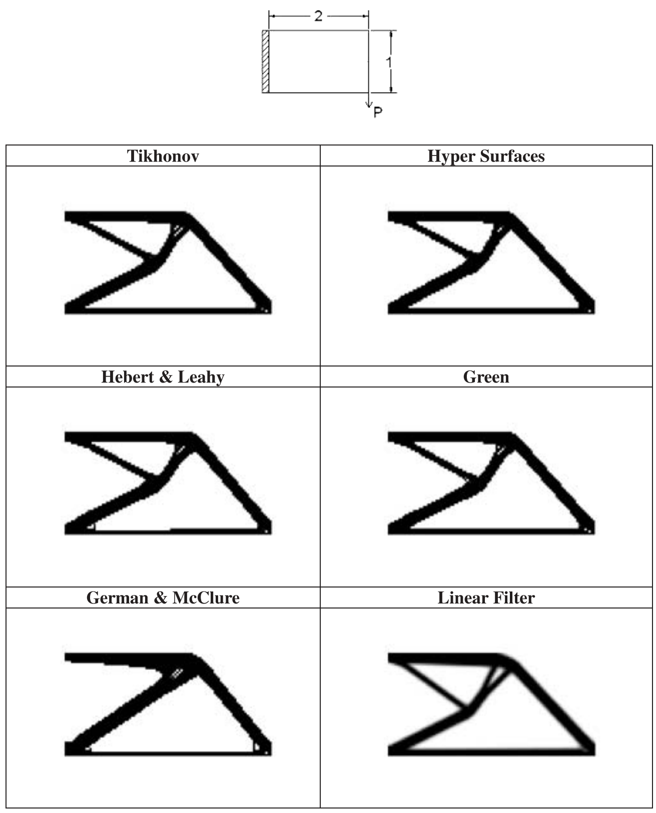

Fig. 13 The cantilever beam (top) and optimal designs with different diffusion functions and the linear filter

Table 2 Edge-preserving diffusion functions

Method	Potential $\varphi(s)$	Edge-preserving	Convexity
Tikhonov	$\dfrac{s^2}{2}$	no	yes
Hyper surface	$\dfrac{1}{2\sqrt{1+s^2}}$	yes	yes
Green	$\dfrac{\tanh(s)}{2s}$	yes	yes
Huber & Leahy	$\dfrac{2}{1+s^2}$	yes	no
German & McClure	$\dfrac{2}{(1+s^2)^2}$	yes	no

Tikhonov function does not satisfy the conditions for edge preserving specified in Sect. 3.3, we used four additional potential functions to examine their regularization and diffusion properties for the minimum compliance optimization of structures. They include convex and non-convex edge-preserving nonlinear functions and are listed in Table 2.

Figure 13 shows the optimal designs obtained with all of the five diffusion functions listed in Table 2. These optimal designs are also compared with that obtained from using the SIMP method with the conventional filtering technique, also shown in the figure. It is clearly shown that the PDE-based numerical implementation yields much crisper edges and the edge-preserving effects are highly pronounced, when comparing to the linear filter method. Smoothing across edge is virtually eliminated by the diffusions. The objective function of mean compliance is plotted in Fig. 14 for all of these cases. It should be pointed out that the PDE-based implementation has a much higher level of computational cost, by two orders of magnitude over that of the optimality criteria method of Sect. 4.1.

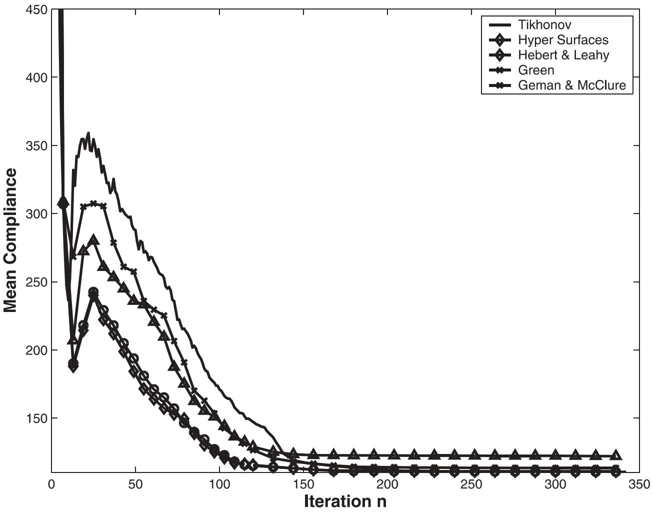

Fig. 14 The mean compliance during gradient flow for the cantilever beam example

6 Conclusions

In this paper we have presented a variational approach to using a nonlinear diffusion technique for the regularization of the topology optimization problem. The problem is formulated as a continuous problem with the density variable $0 \leq \rho(x) \leq 1$ as in the widely used material distribution approach based on homogenization. However, instead of using linear filtering in the interpolation of material properties, a potential functional is employed to induce a nonlinear diffusion process. Within this variational framework, we can incorporate an "edge"-preserving effect to lead to a well-regularized problem formulation. We show that the diffusion model has a close relationship with the phase-field methods in the fields of mechanics and materials and the variational methods used in digital image de-noising segmentation. Two different numerical implementations of the proposed approach are discussed. The proposed diffusion method is illustrated with 2D examples. While the optimality-criteria-based updating scheme is simple and easy to implement, it yields less significant edge-preserving effect. On the other hand, a general scheme based on the gradient flow concept is more accurate and virtually eliminates smoothing across edges; it is however inefficient due to severe numerical stability requirements.

All the nonlinear diffusion processes that we have investigated so far utilize a scalar-valued diffusivity function $g(\nabla\rho(x))$. They are isotropic and sub-linear. In a discrete setting, our diffusion model of (15) exhibits considerable effects of regularization and edge preserving. Strictly speaking, the effects would be weaker in the continuous domain of (15). These diffusion techniques can be further generalized to take into account possible information contained in the variations of the orientation of gradient $\nabla\rho(x)$. If we wish to smooth preferentially within each material region and to preserve or even enhance lower-dimensional features such as line-like structures, we need to use more sophisticated structure descriptors than just $\nabla\rho(x)$ to define the diffusion tensor in (10). These requirements cannot be satisfied by a scalar diffusivity anymore. A general theory of *anisotropic* structure has been introduced by Weickert (1997) and it has been well developed for edge-enhancing diffusion and coherence-enhancing diffusion in image processing (Aubert and Kornprobst 2000; Sapiro 2001). It would be a promising extension to employ such a feature-enhancing diffusion model to the variable-topology optimization problem, even though it is not variational and requires efficient well-founded algorithms for solving the problem.

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