

# On Hole Nucleation in Topology Optimization Using the Level Set Methods

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**Abstract:** Hole nucleation is an important issue not yet fully addressed in structural topology optimization using the level set methods. In this paper, a consistent and robust nucleation method is proposed to overcome the inconsistencies in the existing implementations and to allow for smooth hole nucleation in the conventional shape derivatives-based level set methods to avoid getting stuck at a premature local optimum. The extension velocity field is constructed to be consistent with the mutual energy density and favorable for hole nucleation. A negative extension velocity driven nucleation mechanism is established due to the physically meaningful driving force. An extension velocity filtering approach is developed to allow for nucleation of new holes at the sites where the material is ineffectively used while the ill-posed topology optimization problem can be regularized. To overcome the numerical instabilities caused by the level set evolution, the gradients of the level set function are kept bounded using a rescaling-based reinitialization scheme based on a global representation technique without moving the free boundary. Inconsistencies with the regularization and reinitialization techniques are eliminated and smooth nucleation of new holes becomes possible. The level set-based topology optimization would become more accurate and efficient. The success of the present method is demonstrated with the classical examples in minimum compliance design.

**Keyword:** Level set methods, Topology opti-

mization, Nucleation, Numerical instability, Regularization, Reinitialization

## 1 Introduction

Structural topology optimization has become an attractive design tool for obtaining more efficient structures. An optimal topology can be reached by iterative modifications of holes and connectivities in the design domain [Akin and Arjona-Baez (2001); Bendsøe and Kikuchi (1988)]. Topology optimization has the highest importance in the developing process of all structural optimization methods due to its maximum savings [Rozvany (2001); Bendsøe and Kikuchi (1988); Xie and Steven (1993); Wang, Tai, and Wang (2006); Wang and Wang (2006a)]. Further improvement due to shape or sizing optimization is only possible with greater effort with respect to time and cost. Nevertheless, structural topology optimization has been recognized as one of the most challenging tasks in structural design [Rozvany (2001); Bendsøe and Sigmund (2003)].

Recently, the level set methods, first introduced by Osher and Sethian in [Osher and Sethian (1988)], have been applied to structural shape and topology optimization problems based on the moving free boundaries (dynamic interfaces) [Sethian and Wiegmann (2000); Osher and Santosa (2001); Wang, Wang, and Guo (2003); Allaire, Jouve, and Toader (2004)]. It is well known that the level set method itself is a simple and versatile technique for computing and analyzing the motion of an interface in two or three dimensions [Sethian (1999); Osher and Fedkiw (2002); Lowengrub, Xu, and Voigt (2002); Sheen, Seo, and Cho (2003); Cheng, Kang, Osher, Shim, and Tsai (2004); Mai-Duy, Mai-Cao, and Tran-Cong (2007)]. Since these interfaces may easily develop sharp corners, break apart,

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merge together and even disappear in a stable manner [Tsai and Osher (2003)], the level set method can be quite convenient and effective to handle drastic topological changes in topology optimization. Sethian and Wiegmann (2000) [Sethian and Wiegmann (2000)] first extended the level set method of Osher and Sethian [Osher and Sethian (1988)] to capture the free boundary of a structure on a fixed Eulerian mesh. Osher and Santosa [Osher and Santosa (2001)] investigated a two-phase optimization of a membrane modeled by a linear scalar partial differential equation (PDE). More closely related works on the level set-based structural topology optimization can be found in [Wang, Wang, and Guo (2003); Allaire, Jouve, and Toader (2004)]. Wang et al. [Wang, Wang, and Guo (2003)] implemented a level set method for structural topology optimization by establishing the normal velocities in terms of the variational Frechét shape sensitivity as a physically meaningful link between the general structural topology optimization process and the universal level set methods. It was shown that using the level set methods for structural topology optimization has the potentials in flexibility of handling topological changes, fidelity of boundary representation and degree of automation. Allaire et al. [Allaire, Jouve, and Toader (2004)] proposed an implementation of the level set methods for structural topology optimization in which the classical shape derivatives [Sokolowski and Zolesio (1992)] for structural elasticity analysis were introduced in a mathematically rigorous manner. It was illustrated that drastic topological changes can be achieved during the level set evolution, but the final designs may be quite sensitive to the initial guess. Since there was no nucleation mechanism in the conventional level set methods (at least for 2D cases), it would be difficult for a level set-based topology optimization method to generate new holes to escape from a premature local optimum with fewer holes [Allaire, Jouve, and Toader (2004); Burger, Hackl, and Ring (2004)]. More recently, this important issue has been further investigated by many researchers [Allaire, Gournay, Jouve, and Toader (2004); Burger, Hackl, and Ring (2004); Wang, Mei, and Wang (2004); Allaire, de Gour-

nay, Jouve, and Toader (2005); Wang and Wei (2005); Wang and Wang (2006b); Hintermuller (2005); Amstutz and Andrä (2006); He, Kao, and Osher (2007)].

A direct method to resolve this issue is to incorporate the classical topological derivatives into the conventional shape derivatives-based level set methods, as implemented by most of the researchers in the literature [Allaire, Gournay, Jouve, and Toader (2004); Burger, Hackl, and Ring (2004); Wang, Mei, and Wang (2004); Allaire, de Gournay, Jouve, and Toader (2005); Wang and Wei (2005); Hintermuller (2005); Amstutz and Andrä (2006)]. The classical topological derivative [Sokolowski and Żochowski (2001)] is a sensitivity measure with respect to the opening of a small hole at a certain position in the design domain. Incorporating the topological derivatives into the shape derivatives-based level set methods establishes one possibility of creating new holes in the design domain, however, nucleation of new holes cannot be guaranteed due to the resulting inconsistencies with the well-established techniques such as regularization and reinitialization [Allaire, Jouve, and Toader (2004); Wang and Wang (2004a)] to overcome the numerical instabilities in the conventional level set-based topology optimization, which may prevent the occurrence of small holes. Ignoring or weakening those techniques may allow for nucleation of new holes, as shown in [Allaire, Gournay, Jouve, and Toader (2004); Burger, Hackl, and Ring (2004); Wang, Mei, and Wang (2004); Allaire, de Gournay, Jouve, and Toader (2005); Wang and Wei (2005); Wang and Wang (2006b); Hintermuller (2005); Amstutz and Andrä (2006); He, Kao, and Osher (2007)], but significant numerical instabilities may occur. Hence, further address on the inconsistencies becomes necessary to develop a robust and consistent hole nucleation method.

It is well-known that the structural topology optimization problem is ill-posed in its general continuum setting [Bendsøe (1995); Bendsøe and Sigmund (2003)] and thus existence of solutions cannot be guaranteed. To ensure existence of solutions and mesh-independent designs, a perimeter control method was usually

adopted in the level set-based topology optimization [Allaire, Jouve, and Toader (2004); Wang and Wang (2004b)] to regularize the ill-posed problem. The perimeter control method would introduce a perimeter constraint on the admissible design configurations and may thus prevent the occurrence of small holes since small holes would be taken as undesirable noises in the perimeter control method. Hence, nucleation of new holes in the design domain can be inconsistent with this popular regularization technique.

Reinitialization is a technique for the conventional level set methods [Sethian (1999); Osher and Fedkiw (2002)] to maintain stable evolution. Periodic reinitialization can avoid the development of a steep/flat level set function to destroy the numerical stability. The usual implementations of a reinitialization scheme, such as the one using the Godunov scheme to reinitialize the level set function into a signed distance function [Osher and Fedkiw (2002)], can be efficient but shift of the interface may be unavoidable, especially when drastic topological changes are involved due to nucleation of new holes. As noted in [Tsai and Osher (2003)], the usual reinitialization procedure may even take the small holes as undesirable numerical errors and thus prevent the occurrence of the small holes. Hence, nucleation of new holes can be inconsistent with the popular reinitialization schemes that may shift the free boundary. It should be noted that most of the reinitialization schemes are not robust and efficient enough to account for drastic topological changes. A reinitialization scheme that allows for significant topological changes without moving the free boundary may require prohibitive computation and might be complex to implement [Marchandise, Remacle, and Chevaugeon (2006); He, Kao, and Osher (2007)] and thus destroy the efficiency and simplicity of the conventional level set methods.

The classical topological derivative [Sokolowski and Żochowski (2001)] is with respect to the opening of a small (infinitesimal) hole. However, the sizes of new holes were not properly defined and may even be arbitrarily large [Wang, Mei, and Wang (2004)] in the current implemen-

tations using the topological derivatives for hole nucleation. This apparent inconsistency may not only weaken the theoretical basis for hole nucleation but also violate the optimality conditions. The trial and error procedure to alleviate this inconsistency recommended in [Allaire, Gournay, Jouve, and Toader (2004); Burger, Hackl, and Ring (2004); Wang, Mei, and Wang (2004); Allaire, de Gournay, Jouve, and Toader (2005); Wang and Wei (2005)] cannot be efficient in general.

The objective of the present study is to propose a robust and consistent hole nucleation method by establishing new regularization and reinitialization techniques without the significant inconsistencies in the framework of conventional shape derivatives-based level set methods without incorporating the topological derivatives. Extension velocities are constructed to be physically meaningful and favorable for hole nucleation. Nucleation of new holes is driven by the physically meaningful negative extension velocities. An extension velocity filtering approach is proposed to overcome the inconsistency in creating new holes while ensuring existence of solutions. A global support-based shift-free reinitialization scheme is proposed to avoid hampering the smooth nucleation of new holes while maintaining a well-behaved level set function. Nucleation of new holes can be achieved automatically and possible numerical instabilities can be effectively suppressed. The robustness and effectiveness of the present method can be well demonstrated by the chosen classical examples in topology optimization.

## 2 Shape Derivatives-Based Level Set Methods with Hole Nucleation Capability

### 2.1 Shape Derivatives

The level set method is a powerful and versatile numerical technique. In the standard level set method first introduced by Osher and Sethian [Osher and Sethian (1988)], the interface (or moving boundary) is embedded into a higher-order (one dimension higher) level set function  $\Phi(\mathbf{x})$  as the zero level set  $\{\mathbf{x} \in \mathbb{R}^d \mid \Phi(\mathbf{x}) = 0\}$  ( $d = 2$  or  $3$ ).

The implicit scalar level set function  $\Phi(\mathbf{x})$  has the following properties:

$$\begin{aligned}\Phi(\mathbf{x}) = 0 &\iff \forall \mathbf{x} \in \partial\Omega \cap \mathcal{D} \\ \Phi(\mathbf{x}) < 0 &\iff \forall \mathbf{x} \in \Omega \setminus \partial\Omega \\ \Phi(\mathbf{x}) > 0 &\iff \forall \mathbf{x} \in (\mathcal{D} \setminus \Omega)\end{aligned}\quad (1)$$

where  $\mathcal{D} \subset \mathbb{R}^d$  is a fixed design domain in which all admissible shapes  $\Omega$  (a smooth bounded open set) are included, i.e.  $\Omega \subset \mathcal{D}$ .

Using a level set model as defined in Eq. (1), the structural topology optimization problem with a volume constraint [Sigmund (2001); Bendsøe and Sigmund (2003)] to limit the use of material can be written as follows:

$$\begin{aligned}\min_{\Phi} \quad & J(\mathbf{u}, \Phi) = \int_{\mathcal{D}} F(\mathbf{u})H(-\Phi)d\Omega \\ \text{s. t. :} \quad & a(\mathbf{u}, \mathbf{v}, \Phi) = L(\mathbf{v}, \Phi), \mathbf{u}|_{\Gamma_D} = \mathbf{u}_0, \forall \mathbf{v} \in \mathcal{U} \\ & V(\Phi)/V_0 \leq \zeta\end{aligned}\quad (2)$$

where  $J(\mathbf{u}, \Phi)$  is the objective function,  $\mathbf{u}$  the displacement field,  $F(\mathbf{u})$  the design function,  $H(\Phi)$  the Heaviside step function,  $V(\Phi)$  the material volume,  $V_0$  the total volume of the design domain  $\mathcal{D}$ , and  $\zeta$  the prescribed volume fraction. The linearly elastic equilibrium equation is written in its weak variational form in terms of the energy bilinear form  $a(\mathbf{u}, \mathbf{v}, \Phi)$  and the load linear form  $L(\mathbf{v}, \Phi)$  [Wang and Wang (2004b)], with  $\mathbf{v}$  denoting a virtual displacement field in the space  $\mathcal{U}$  of kinematically admissible displacement fields, and  $\mathbf{u}_0$  the prescribed displacement on the admissible Dirichlet boundary  $\Gamma_D$ . Furthermore, we have

$$a(\mathbf{u}, \mathbf{v}, \Phi) = \int_{\mathcal{D}} \boldsymbol{\varepsilon}^T(\mathbf{u})\mathbf{C}\boldsymbol{\varepsilon}(\mathbf{v})H(-\Phi)d\Omega \quad (3)$$

$$\begin{aligned}L(\mathbf{v}, \Phi) &= \int_{\mathcal{D}} \mathbf{v}^T \mathbf{f} H(-\Phi) d\Omega + \int_{\mathcal{D}} \mathbf{v}^T \boldsymbol{\tau} \delta(\Phi) |\nabla \Phi| d\Omega\end{aligned}\quad (4)$$

$$V(\Phi) = \int_{\mathcal{D}} H(-\Phi) d\Omega \quad (5)$$

where  $\mathbf{C}$  is the elasticity matrix,  $\mathbf{f}$  the body force vector,  $\boldsymbol{\tau}$  the boundary traction force vector, and  $\delta(\Phi)$  the Dirac delta function.

The Lagrange multiplier method can be used to solve this optimization problem [Osher and Santosa (2001)]. By setting the constraint on the equilibrium state inactive, the Lagrangian  $\mathcal{L}(\mathbf{u}, \Phi, \ell)$  with a positive Lagrange multiplier  $\ell$  can be given by

$$\mathcal{L}(\mathbf{u}, \Phi, \ell) = J(\mathbf{u}, \Phi) + \ell G(\Phi) \quad (6)$$

where the volume constraint functional  $G(\Phi)$  can be expressed as

$$G(\Phi) = V(\Phi) - \zeta V_0 \quad (7)$$

According to the Kuhn-Tucker condition of the optimization, the necessary condition for a minimizer is

$$\begin{aligned}D_{\Phi} \mathcal{L}(\mathbf{u}, \Phi, \ell) &= 0 \\ G(\Phi) &\leq 0\end{aligned}\quad (8)$$

where  $D_{\Phi} \mathcal{L}(\mathbf{u}, \Phi, \ell)$  is the gradient of the Lagrangian with respect to  $\Phi$ . It should be noted that  $\mathbf{u}$  is also a function of  $\Phi$ , i.e.  $\mathbf{u} = \mathbf{u}(\Phi)$ .

The gradient, or shape derivative, of the Lagrangian  $D_{\Phi} \mathcal{L}(\Phi, \ell)$  may be obtained following the well-known approach of Murat and Simon of shape diffeomorphism [Haug, Choi, and Komkov (1986); Sokolowski and Zolesio (1992)]. Based on local perturbations of the moving free boundary of an admissible design [Wang and Wang (2004b)], the resulting shape derivative of the Lagrangian can be written as

$$\begin{aligned}D_{\Phi} \mathcal{L}(\mathbf{u}, \Phi, \ell) &= \int_{\mathcal{D}} (g(\mathbf{u}, \Phi) + \ell) \delta(\Phi) |\nabla \Phi| v_n d\Omega\end{aligned}\quad (9)$$

where

$$\begin{aligned}g(\mathbf{u}, \Phi) &= F(\mathbf{u}) + (\mathbf{u}^*)^T (\mathbf{f} + \kappa \boldsymbol{\tau}) + \nabla((\mathbf{u}^*)^T \boldsymbol{\tau}) \cdot \mathbf{n} \\ &\quad - \boldsymbol{\varepsilon}^T(\mathbf{u})\mathbf{C}\boldsymbol{\varepsilon}(\mathbf{u}^*)\end{aligned}\quad (10)$$

in which  $\mathbf{u}^*$  is the adjoint displacement field of  $\mathbf{u}$ , the outward normal  $\mathbf{n}$  and the curvature  $\kappa$  can be given as

$$\mathbf{n} = \frac{\nabla \Phi}{|\nabla \Phi|} \quad (11)$$

$$\kappa = \nabla \cdot (\nabla \Phi / |\nabla \Phi|) \quad (12)$$

and the relationship between the normal velocity  $v_n$  and the velocity  $v$  is:

$$v_n = v \cdot n \quad (13)$$

Furthermore, Eq. (9) can be simplified as

$$D_{\Phi} \mathcal{L}(\mathbf{u}, \Phi, \ell) = \int_{\Gamma_M} (g(\mathbf{u}, \Phi) + \ell) v_n ds \quad (14)$$

where  $\Gamma_M$  is the moving free boundary. Similarly, the resulting shape derivative of the volume constraint functional  $G(\Phi)$  (7) can be simply expressed as [Wang, Lim, Khoo, and Wang (2007b)]

$$D_{\Phi} G(\Phi) = \int_{\Gamma_M} v_n ds \quad (15)$$

## 2.2 A Consistent Extension Velocity Method

Choosing the normal velocity field  $v_n$  is of crucial importance not only for the efficiency of the level set methods as shown in [Sethian (1999); Richards, Bloomfield, Sen, and Calea (2001); Wang and Wang (2006b)] but also for the success of a hole nucleation mechanism in the shape derivatives-based level set methods as implemented in the present study. In the conventional Eulerian approach-based level set methods [Sethian (1999); Osher and Fedkiw (2002)], the normal velocity field  $v_n$  must be defined in the whole design domain  $\mathcal{D}$  or a narrow band as the extension velocity field. In the present study, a consistent extension velocity method is proposed to allow for nucleation of new holes in the shape derivatives-based level set methods.

There are many approaches to constructing the extension velocity field [Sethian (1999)]. The original level set method introduced by Osher and Sethian [Osher and Sethian (1988)] was concerned with interface problems with geometric propagation velocities and thus a natural construction of an extension velocity was obtained, in which a signed distance function was used as a level function due to its simplicity. In many fluid simulations, the fluid velocity was chosen as the extension velocity [Sussman, Smereka, and Osher (1994); Rhee, Talbot, and Sethian (1995)]. When there is no physically meaningful choice available, the extension velocity was suggested to

be constructed by extrapolating the velocity from the free boundary by some researchers [Mallad, Sethian, and Vemuri (1996)], which requires the location of the closest grid point. Adalsteinsson and Sethian [Adalsteinsson and Sethian (1999)] proposed a fast extension method which preserves the signed distance in a narrow band around the zero level set curve by assuming the normal velocity be constant along the normal. Ye et. al. [Ye, Bresler, and Moulin (2002)] developed a method to deduce the extended velocity from the value of the switching level set function without additional computation by letting the level set function convey information about the image intensity. Nevertheless, these approaches may be physically less meaningful for the present topology optimization problems.

According to the shape derivative of the Lagrangian in Eq. (9), the extension velocity  $v_n(\mathbf{x})$  based on the popular steepest gradient method [Osher and Santosa (2001); Wang, Wang, and Guo (2003); Allaire, Jouve, and Toader (2004)] can be written as

$$v_n(\mathbf{x}) = -g(\mathbf{u}, \Phi) - \ell, \quad \mathbf{x} \in \mathcal{D} \quad (16)$$

in which the extension velocity is defined in the whole design domain  $\mathcal{D}$  to cater to nucleation of new holes. The present extension velocity  $v_n(\mathbf{x})$  is consistent with the physical quantity  $g(\mathbf{u}, \Phi)$  at the point  $\mathbf{x}$  and thus different from the inconsistent extension velocity field which derives from the normal velocities at the free boundary [Adalsteinsson and Sethian (1999)]. The present consistent extension velocity field is favorable for nucleation of new holes. In case that some small new holes are created, we may still have

$$D_{\Phi} \mathcal{L}(\mathbf{u}, \Phi, \ell) = - \int_{\Gamma_M + \Gamma_h} v_n^2 ds < 0 \quad (17)$$

in which  $\Gamma_h$  is the new free boundary due to the creation of new holes. Hence, the decent direction will not be changed and nucleation of small holes without changing the total structural volume may increase the efficiency of a given structure. This is consistent with the theoretical prediction for topology optimization [Bendsøe (1995); Bendsøe and Sigmund (2003)] since the topol-

ogy optimization problem is ill-posed in its general continuum setting as shown in Eq. (2). The ill-posedness is to be overcome by a new regularization method without preventing the creation of new holes in this study. As a comparison, if the inconsistent extension velocity field is chosen, Eq. (17) becomes

$$D_{\Phi} \mathcal{L}(\mathbf{u}, \Phi, \ell) = - \int_{\Gamma_M} v_n^2 ds + \int_{\Gamma_h} (g(\mathbf{u}, \Phi) + \ell) v_n ds \quad (18)$$

and the decent direction may even be changed since the extension velocity at  $\Gamma_h$  is derived from the original free boundary  $\Gamma_M$  and thus inconsistent with the physical quantity  $(g(\mathbf{u}, \Phi) + \ell)$  at  $\Gamma_h$ . Hence, the inconsistent extension velocity field is unfavorable for hole nucleation.

Furthermore, the present extension velocities are physically meaningful. Since the physical quantity  $g(\mathbf{u}, \Phi)$  as shown in Eq. (10) can be used as a measure of mutual energy density, the sign of the extension velocity may indicate whether the material at the point is effectively used or not while  $v_n(\mathbf{x}) = 0$  is the optimality condition.

For the present topology optimization problem with a moving free boundary, without remeshing, the displacement and consistent extension velocity fields may be accurately and efficiently obtained by using several existing numerical methods such as the "ersatz material" approach [Allaire, Jouve, and Toader (2004)], the geometry projection method [Norato, Haber, Tortorelli, and Bendsøe (2004)], the extended finite element methods [Belytschko and Black (1999); Strouboulis, Copps, and Babuska (2001); Wang and Wang (2006a)], or the true meshless local Petrov-Galerkin method [Atluri and Shen (2002)]. In the present study, the moving superimposed finite element method in [Wang and Wang (2006a)] is adopted, in which a moving local mesh is superimposed onto a fixed global mesh as an adaptive local mesh refinement technique.

### 2.3 A Negative Extension Velocity Driven Nucleation Mechanism

A nucleation mechanism may be established for the conventional shape derivatives-based level set

methods without incorporating the topological derivatives due to the physically meaningful driving force generated by the present consistent extension velocity field.

The Hamilton-Jacobi equation [Osher and Sethian (1988)] for the level set evolution can be expressed as

$$\frac{\partial \Phi}{\partial t} + v_n |\nabla \Phi| = 0, \quad \Phi(\mathbf{x}, 0) = \Phi_0(\mathbf{x}), \quad \mathbf{x} \in \mathcal{D} \quad (19)$$

where  $t$  is the artificial time, and  $\Phi_0(\mathbf{x})$  embeds the initial position of the free boundary. Hence, we have

$$\frac{\partial \Phi}{\partial t} = -v_n |\nabla \Phi| \quad (20)$$

According to Eq. (20), creation of a new hole at position  $\mathbf{x} \in \Omega$  is possible if  $v_n(\mathbf{x}) < 0$  such that  $\frac{\partial \Phi(\mathbf{x})}{\partial t} > 0$ . Hence, the negative extension velocities can be used as the driving forces for hole nucleation in the conventional shape derivatives-based level set methods. Since the negative extension velocity  $v_n(\mathbf{x}) < 0$  may indicate that the material at the point  $\mathbf{x}$  is ineffectively used and can thus be removed, which is a generally accepted idea in the element removal techniques for topology optimization such as the evolutionary structural optimization approach [Xie and Steven (1993)], the present nucleation mechanism can be physically meaningful. The present nucleation mechanism has a sound theoretical basis and is thus different from the element removal techniques. It should be noted that nucleation of new holes using extension velocities was predicted by Sethian [Sethian (1999)].

Nevertheless, the present negative extension velocity driven nucleation mechanism only provides a possibility of creating new holes. Nucleation of new holes may be prevented by the popular regularization and reinitialization techniques as aforementioned. In the present study, new regularization and reinitialization techniques favorable for the present physically meaningful hole nucleation mechanism are proposed.

## 2.4 An Extension Velocity Filtering Approach

Significant numerical instabilities may occur in topology optimization due to the ill-posedness of the optimization problem [Bendsøe and Sigmund (2003); Allaire, Jouve, and Toader (2004); Wang and Wang (2006a)]. To regularize the ill-posed problem into a well-posed problem, a filtering technique is proposed to smooth the present consistent extension velocity field. Filtering has become quite popular and successful in various domains of engineering applications as a numerical method to ensure regularity or existence of solutions to an ill-posed problem and has become increasingly popular in the SIMP method continuum topology optimization [Bendsøe and Sigmund (2003); Wang and Wang (2005)].

In the present implementation, a linear smoothing filter is introduced and a linear hat kernel function [Sigmund (2001)] is used to achieve an excellent edge smoothing effect [Wang and Wang (2005)]. The filtered extension velocity  $\hat{v}_n(\mathbf{x})$  can be written as

$$\hat{v}_n(\mathbf{x}) = k^{-1}(\mathbf{x}) \sum_{\mathbf{p} \in N(\mathbf{x})} w(\|\mathbf{p} - \mathbf{x}\|) v_n(\mathbf{p}), \quad \mathbf{x} \in \mathcal{D} \quad (21)$$

where

$$w(\|\mathbf{p} - \mathbf{x}\|) = r_{\min} - \|\mathbf{p} - \mathbf{x}\| \quad (22)$$

$$k(\mathbf{x}) = \sum_{\mathbf{p} \in N(\mathbf{x})} w(\|\mathbf{p} - \mathbf{x}\|) \quad (23)$$

in which  $N(\mathbf{x})$  is the neighborhood of the point  $\mathbf{x}$  in the filter window and  $r_{\min}$  the filter window size.

Using this extension velocity filtering approach, the smoothness of the extension velocity field can be guaranteed. Furthermore, if a small hole is created at the position with negative extension velocity due to the present nucleation mechanism, the filtered extension velocities in the neighborhood of the small hole would also be negative and thus the growth of the hole in the subsequent level set evolution can be guaranteed. On the other hand, if there is a small hole in the region with positive extension velocities, this small hole cannot exist permanently with zero velocities at the boundary

since the filtered extension velocities would be positive and thus the small hole would be taken as noise and eliminated in the subsequent evolution. Hence, this regularization technique is consistent with the present nucleation mechanism.

Furthermore, according to the present consistent extension velocity method as shown in Eq. (16), there is a significant discontinuity at the free boundary. This discontinuity may cause numerical instability for the conventional level set methods. Due to the present regularization technique, the filtered extension velocities in the neighborhood of the free boundary will become smoother and thus the significant discontinuity can be eliminated. Hence, the present extension velocity filtering approach is versatile and highly indispensable.

## 2.5 A Rescaling-based Reinitialization Scheme

The present extension velocities may not allow for the development of a flat level set function in the neighborhood of the free boundary to hamper further level set evolution. According to the consistent extension velocity method as shown in Eq. (16), the extension velocities in the neighborhood of the free boundary  $\Gamma_M$  can always be significantly different due to the solid and void phases even if the optimality condition ( $v_n(\mathbf{x}) = 0, \forall \mathbf{x} \in \Gamma_M$ ) has been arrived at. The significant difference may still exist after using the present regularization technique, totally different from the constant normal extension velocities using the inconsistent extension velocity method. Therefore, a flat level set function in the neighborhood of the free boundary would not be developed. On the contrary, the level set function may become increasingly steep in the whole domain  $\mathcal{D}$ , according to the Hamilton-Jacobi equation (19). To guarantee a stable level set evolution, the gradients of the level set function must be bounded and thus a reinitialization scheme is needed.

To make the gradients of the level set function bounded, the increasingly high gradients must be evaluated accurately. Unfortunately, the commonly used finite difference methods [Osher and Fedkiw (2002)] in the level set methods may be inaccurate for estimating the increasingly high

gradients. The popular finite difference upwind ENO schemes [Osher and Fedkiw (2002); Tsai and Osher (2003)] developed under the general philosophy of the Godunov procedure and the nonlinear ENO reconstruction techniques may give a smooth reconstruction, but may still have difficulties in evaluating the increasingly high gradients both accurately and efficiently while preserving the global smoothness of the level set function due to the local representation techniques. The global smoothness is of crucial importance to maintain a stable level set evolution. The level set function must be always at least Lipschitz continuous [Osher and Fedkiw (2002)]. In this study, the evaluation of gradients is based on a global representation technique using globally supported Radial Basis Functions (RBFs) to guarantee the global smoothness. It should be noted that the applications of RBFs to achieve more accurate results in the level set methods have been at the incipient stage [Cecil, Qian, and Osher (2004); Wang and Wang (2006b,c); Wang, Lim, Khoo, and Wang (2007a,c)].

The level set function can be smoothly reconstructed from gridded data using the globally supported RBFs, which can be written as

$$\Phi = \sum_{i=1}^N \alpha_i(t) \varphi_i(\mathbf{x}) \quad (24)$$

where  $\alpha_i(t)$  is the time dependent expansion coefficient of the Multiquadric (MQ) RBF  $\varphi_i(\mathbf{x})$  positioned at the  $i$ -th grid point, or center,  $N$  the total number of RBF centers. The MQ RBF  $\varphi_i(\mathbf{x})$  can be expressed as

$$\varphi_i(\mathbf{x}) = \sqrt{(\|\mathbf{x} - \mathbf{x}_i\|)^2 + c^2} \quad (25)$$

where  $c$  ( $c > 0$ ) is a free shape parameter [Buhmann (2004); Wang and Wang (2006b)].

The RBF interpolant (24) can be obtained by solving a system of  $N$  linear equations for  $N$  unknown expansion coefficients provided that the gridded data are given:

$$\Phi(\mathbf{x}_i) = \phi_i(t), \quad i = 1, \dots, N \quad (26)$$

which can be re-written in the matrix form as

$$\mathbf{H}\boldsymbol{\alpha} = \boldsymbol{\phi}(t) \quad (27)$$

where  $\mathbf{H}$  is the multiquadric interpolation or collocation matrix [Buhmann (2004); Wang and Wang (2006b)]. It can be proven that the interpolation matrix is nonsingular [Buhmann (2004)] and thus theoretically invertible. The expansion coefficients  $\boldsymbol{\alpha}$  can be given by

$$\boldsymbol{\alpha} = \mathbf{H}^{-1}\boldsymbol{\phi}(t) \quad (28)$$

Hence, the RBF representation in Eq. (24) can be given in compact form as

$$\Phi = \boldsymbol{\varphi}^T(\mathbf{x})\mathbf{H}^{-1}\boldsymbol{\phi}(t) \quad (29)$$

where

$$\boldsymbol{\varphi}(\mathbf{x}) = [\varphi_1(\mathbf{x}) \quad \varphi_2(\mathbf{x}) \quad \dots \quad \varphi_N(\mathbf{x})]^T \quad (30)$$

After reconstructing the level set function from the gridded data, the corresponding norm of the gradient  $|\nabla\Phi|$  for a two dimensional (2D) problem can be readily obtained as follows:

$$\begin{aligned} |\nabla\Phi| &= \left[ \left( \frac{\partial\boldsymbol{\varphi}^T}{\partial x} \mathbf{H}^{-1}\boldsymbol{\phi}(t) \right)^2 + \left( \frac{\partial\boldsymbol{\varphi}^T}{\partial y} \mathbf{H}^{-1}\boldsymbol{\phi}(t) \right)^2 \right]^{1/2} \\ & \quad (31) \end{aligned}$$

where

$$\frac{\partial\boldsymbol{\varphi}}{\partial x} = \left[ \frac{\partial\varphi_1}{\partial x} \quad \frac{\partial\varphi_2}{\partial x} \quad \dots \quad \frac{\partial\varphi_N}{\partial x} \right]^T \quad (32)$$

$$\frac{\partial\boldsymbol{\varphi}}{\partial y} = \left[ \frac{\partial\varphi_1}{\partial y} \quad \frac{\partial\varphi_2}{\partial y} \quad \dots \quad \frac{\partial\varphi_N}{\partial y} \right]^T \quad (33)$$

in which

$$\frac{\partial\varphi_i}{\partial x} = \frac{x - x_i}{\sqrt{(x - x_i)^2 + (y - y_i)^2 + c^2}} \quad (34)$$

$$\frac{\partial\varphi_i}{\partial y} = \frac{y - y_i}{\sqrt{(x - x_i)^2 + (y - y_i)^2 + c^2}} \quad (35)$$

It should be noted that the MQ RBFs are infinitely smooth since they are continuously differentiable. Hence, the global smoothness of the reconstructed level set function  $\Phi$  in (29) as well as the norm of its gradient  $|\nabla\Phi|$  can be guaranteed. The present global representation technique can thus be significantly different from the commonly used finite



difference methods [Osher and Fedkiw (2002)]. Most importantly, all the gradients will become less distinct due to the global smoothness. In case that there are some extraordinarily high extension velocities in the design domain, the updated gridded data  $\phi(t)$  may also have some extraordinarily high values, but the expected development of extraordinarily higher gradients due to a local representation technique can be greatly alleviated since the present global representation technique can guarantee that the reconstructed level set function and its gradients be globally smooth. The global smoothness is the theoretical basis for the present reinitialization scheme. In [Cecil, Qian, and Osher (2004)], RBFs were used to approximate the gradients in a reconstruction stencil only and thus the global smoothness cannot be guaranteed.

Since the significant differences between high gradients and low gradients are globally smoothed, it would be easy to develop a reinitialization scheme to keep all the gradients bounded without moving the free boundary.

It is well known that the gridded data  $\phi(t)$  can be rescaled without changing the free boundary  $\Phi = 0$ . According to Eqs. (29) and (31), not only the reconstructed level set function  $\Phi$  but also the norm of its gradient  $|\nabla\Phi|$  at any point will also be equally rescaled. This rescaling may decrease all the gradients equally and thus keep the gradients bounded. Since the present extension velocity method can prevent the occurrence of a flat level set function and the gradient of the level set function is globally smooth, this rescaling will not cause the level set function to become flat. It should be noted that the local representation techniques [Osher and Fedkiw (2002)] would not help smooth the significant differences between high and low gradients and continuous rescaling would cause the low gradients independently developed in the neighborhood of the free boundary to become almost zero and thus the interface would be lost and significant numerical instability would arise. The present rescaling-based reinitialization scheme can be performed at each iteration without losing the interface and thus the difficult practical question [Gómez, Hernández, and López (2005)] that concerns the reinitialization frequency can be

clearly answered. Hence, in the present re-scaling based reinitialization scheme, the gradients of the level set function can be kept bounded, a steep/flat level set function cannot be developed while shift of the free boundary avoided.

Nevertheless, it should be stressed that the computational cost of the present scheme can become too expansive when the total number of centers is high since the interpolation matrix  $\mathbf{H}$  in (27) is dense. A sparse interpolation matrix can be achieved by using the compact support RBFs [Buhmann (2004)], but the accuracy of the RBF representation may be deteriorated because there is a trade-off between the accuracy and efficiency in using the compact support RBFs [Buhmann (2004)]. Since the accuracy is more important than efficiency for a numerical algorithm, the multiquadric RBFs are preferred in the present study. The resulting dense interpolation matrix can be efficiently handled by several existing iterative methods [Buhmann (2004)], such as the domain decomposition approach, the fast multipole method, and preconditioning techniques. It should also be noted that the present interpolation matrix  $\mathbf{H}$  is time independent and thus the computational cost due to the dense interpolation matrix would not become prohibitive during the level set evolution.

### 3 Numerical Examples and Discussion

Numerical examples in two dimensions in the framework of classical minimum compliance design are provided to illustrate the accuracy and efficiency of the present method. Unless stated otherwise, all the units are consistent and the following parameters are assumed as: the Young's elasticity modulus  $E = 1$  for solid materials and Poisson's ratio  $\nu = 0.3$ . Furthermore,  $r_{\min} = 2.4$  grid size for the filter window size. For all examples, a fixed rectilinear mesh is specified over the entire design domain as the global mesh for using the moving superimposed finite element method [Wang and Wang (2006a)]. The Euler's method is used in the temporal integration due to its simplicity. The present algorithm is terminated when the relative difference between two successive objective function values is less than  $10^{-5}$  or when

the given maximum number of iterations has been reached.

### 3.1 A Michell Type Structure

The classical Michell type structure design problem [Michell (1904)] is adopted to demonstrate the accuracy of the present method, in which a theoretical Michell's solution is available [Michell (1904); Hemp (1973)], as shown in Fig. 1. The whole design domain  $\mathcal{D}$  is a rectangle of size  $L \times H$ , the two bottom corners have the pinned supports, and a unit vertical point force  $P$  is applied at the middle point of the bottom side. As shown in Figure 1(b), the theoretical optimum topology consists of two  $45^\circ$  arms extending from the supports towards an approximately  $90^\circ$  central fan section which extends upwards from the point of application of the force. In this study, it is assumed that  $L = 2$ ,  $H = 1.2$ ,  $P = 1$ , and a volume fraction of  $\zeta = 0.3$ . The design domain  $\mathcal{D}$  is discretized with a fixed global mesh of  $100 \times 60$ . Due to the symmetry, only a half structure is used in the numerical analysis to save the computational time.

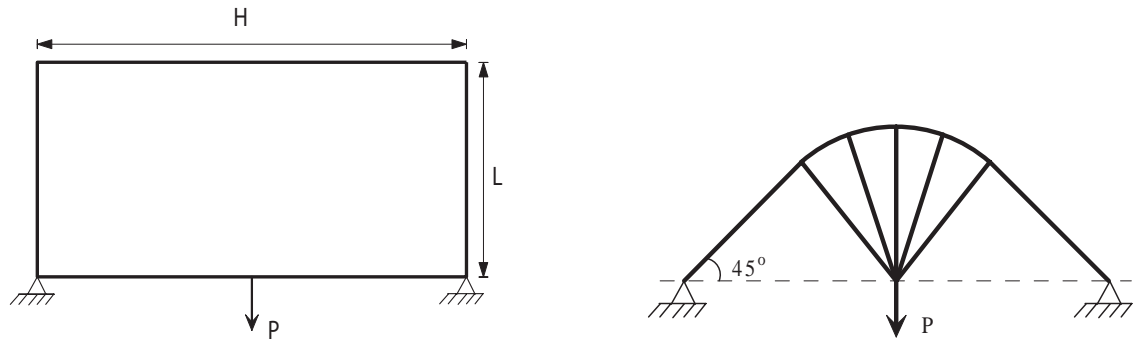
Topology optimization using an initial design without a hole is performed to demonstrate the success of the present hole nucleation mechanism. The design without a hole as shown in Fig. 2(a) is used as the initial design. A timestep size of 0.001 together with a free shape parameter of  $c = 0.001$  is used. The evolution history of the final design is shown in Fig. 2. It can be seen that topological changes due to nucleation of new holes are achieved because of the present nucleation mechanism. Figure 3 shows the scalar extension velocity field at step 8. It can be seen that the nucleation of new holes at step 9 as shown in Fig. 2(c) is in excellent agreement with the driving forces caused by the negative velocity field shown in Fig. 3. The success of the present nucleation mechanism is thus demonstrated. Hence, the conventional shape derivatives-based level set methods may possess the hole nucleation capability. The final topology shown in Fig. 2(f) is almost identical to the theoretical optimum topology as shown in Fig. 1(b). The accuracy of the present method can thus be verified. The possibility of

getting stuck at a local minimum without a hole due to the present initial guess has been overcome. Hence, the present method can be robust and less sensitive to the initial guess. Figure 4 displays a comparison between the finite element model of the final design and the corresponding scalar non-negative extension velocity field. It can be seen that the structural free boundary corresponds with the zero extension velocity curve well, as theoretically predicted. Inside the final design no regions with negative extension velocities exist, which can be greatly different from using the level set methods without a nucleation mechanism. The convergence rates of both the objective and volume functions are shown in Fig. 5. It can be seen that stable convergence can be achieved and hole nucleation may increase the efficiency of a structure due to the present consistent extension velocity method.

### 3.2 A Bridge Type Structure

The 2D bridge type structure optimal design problem [Wang, Wang, and Guo (2003)], as shown in Fig. 6, is similar to the Michell type structure problem shown in Fig. 1. In this study, it is also assumed that  $L = 2$ ,  $H = 1.2$ ,  $P = 1$ , and a volume fraction of  $\zeta = 0.3$ .

The design without any holes shown in Fig. 7(a) is taken as the initial design. A timestep size of  $\tau = 0.01$  together with a free shape parameter of  $c = 0.0001$  is adopted. Figure 7 shows the evolution history of the final design. It can be seen that drastic topological changes due to the nucleation of new holes have been achieved. The success of the present hole nucleation mechanism without incorporating the classical topological derivatives is again demonstrated. The final design shown in Fig. 7(h) is almost identical to the one in the literature [Wang, Wang, and Guo (2003)] using the conventional level set methods and an initial design with much more holes. The accuracy of the present method is again verified. Figure 8 shows that the structural free boundary corresponds with the zero extension velocity curve well and there are no regions inside the final design with negative extension velocities. The convergence rates of the objective and volume functions are shown



(a) Problem definition (b) A Michell type structure

Figure 1: Topology optimization problem for a Michell type structure.

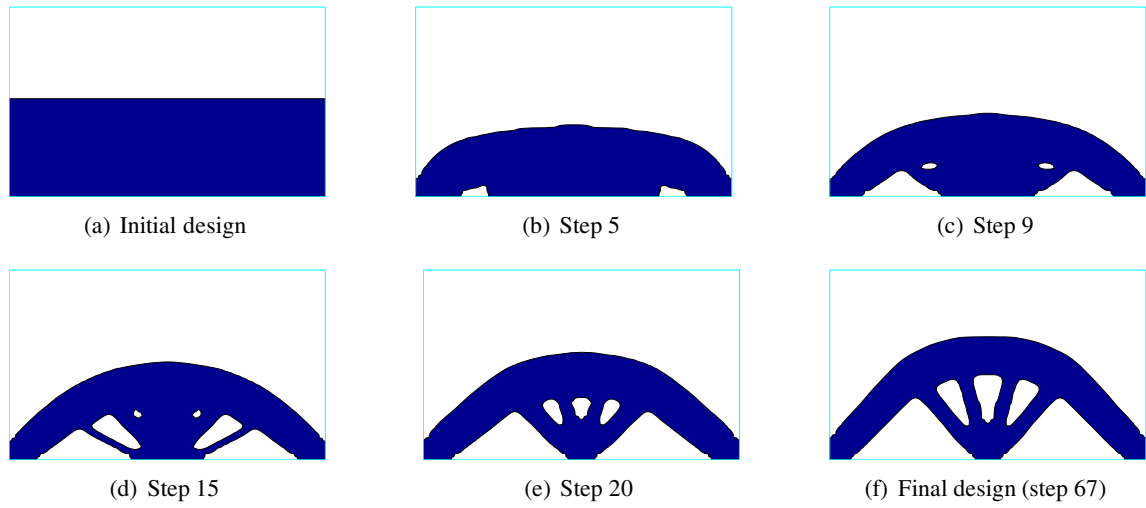


Figure 2: Evolution history of the optimal design for the Michell type structure starting with an initial design without a hole.

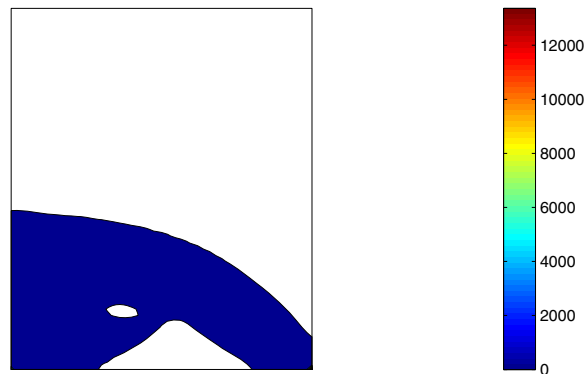


Figure 3: Scalar extension velocity field ( $v_n \geq 0$ ) of the half structure at step 8.

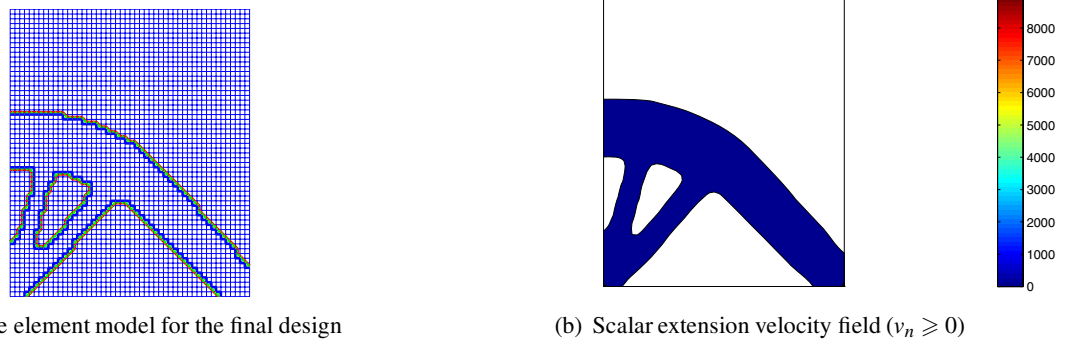


Figure 4: Final solutions (half structure) for the Michell type structure problem starting with an initial design without a hole.

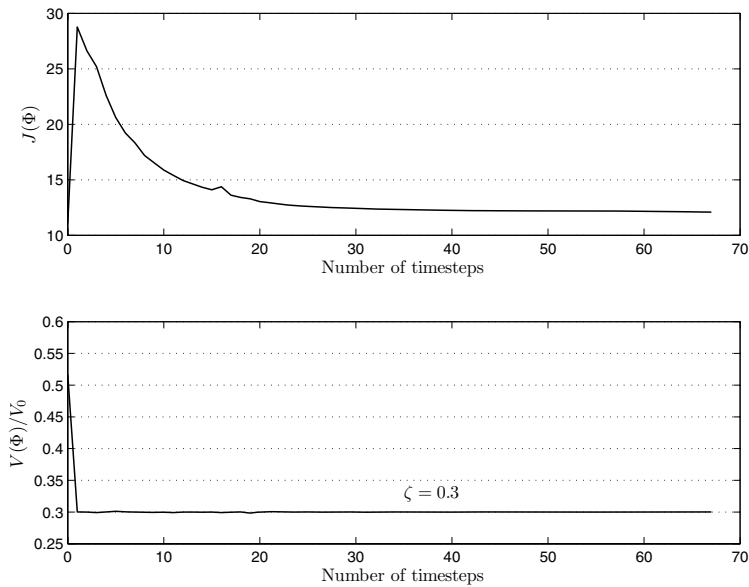


Figure 5: Convergence of the objective and volume functions for the Michell type structure starting with an initial design without a hole.

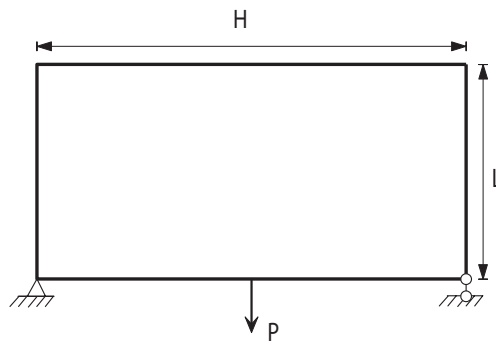


Figure 6: Optimal topology design problem for a 2D bridge type structure.

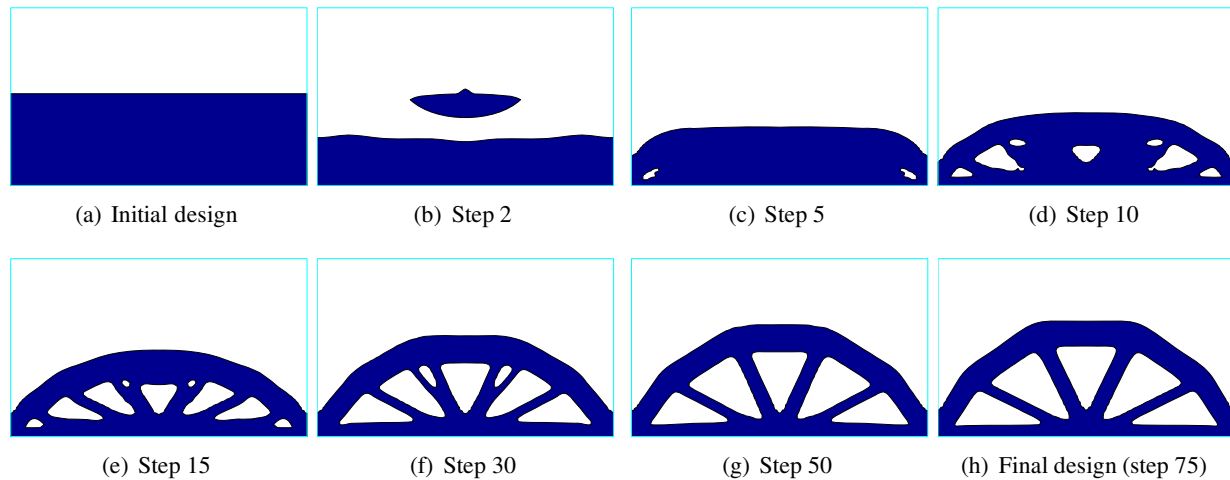


Figure 7: Evolution history of the optimal design for the 2D bridge starting with an initial design without a hole.

in Fig. 9. It can be seen that stable convergence in both the objective and volume functions has been achieved during the course of evolution since drastic topological changes due to nucleation of new holes can be favorable to obtain a more efficient structure, according to the present consistent extension velocity method.

### 3.3 A Short Cantilever Beam

The minimum compliance design problem of a short cantilever beam is shown in Fig. 10. The whole design domain is a rectangle of size  $L \times H$  with a fixed boundary (zero displacement boundary condition) on the left side and a unit vertical point load applied at the middle point of the right side. In this study, it is assumed that  $L = 2$ ,  $H = 1$ ,  $P = 1$ , and a volume fraction of  $\zeta = 0.5$ . A  $80 \times 40$  regular mesh is used as the global mesh.

The design without a hole shown in Fig. 11(a) is used as the initial design. A timestep size of  $\tau = 0.001$  together with a free shape parameter of  $c = 0.001$  is adopted. Figure 11 shows the evolution history of the optimal design. Again, it can be seen that drastic topological changes due to the nucleation of new holes have been achieved. The success of the present hole nucleation mechanism is again demonstrated. Figure 12 shows that the free boundary agrees with the zero extension velocity curve well, as theoretically predicted. The

convergence rates of the objective and volume functions are shown in Fig. 13. It can be seen that stable convergence in both the objective and volume functions has been achieved since drastic topological changes due to nucleation of new holes may be favorable to obtain a more efficient structure.

The design with some holes shown in Fig. 14(a) is used as another initial guess to further investigate the dependence of the final design on the initial guess. Figure 14 shows the corresponding evolution history of the final design. It can be seen from Fig. 14(c) that nucleation of new holes can also be achieved during the level set evolution because of the present hole nucleation mechanism. The final design as shown in Fig. 14(f) may have fewer holes than the initial design due to the optimality conditions. Figure 15 shows that the free boundary agrees with the zero extension velocity curve well. The convergence rates of the objective and volume functions are shown in Fig. 16. Again, it can be seen that stable convergence has been obtained due to the present consistent extension velocity method.

Since the final design shown in Fig. 11(f) obtained from an initial guess without a hole is different from the one shown in Fig. 14(f) obtained from another initial guess with more holes than the optimum, the dependence of the final solutions on

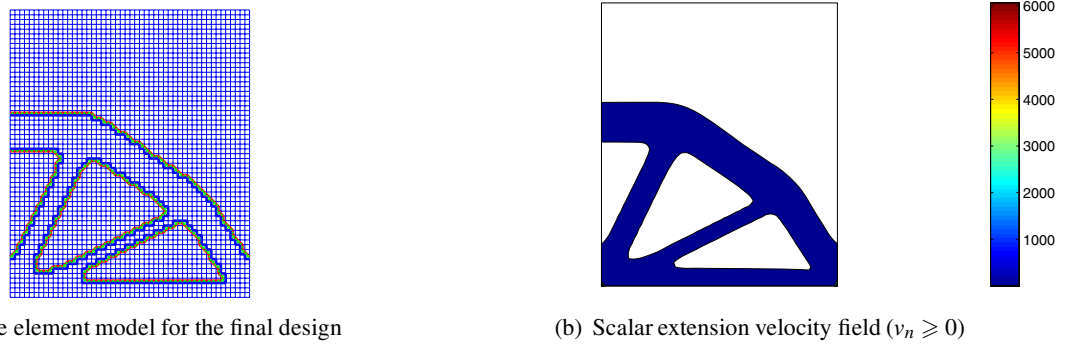


Figure 8: Final solutions (half structure) for the 2D bridge problem starting with an initial design without a hole.

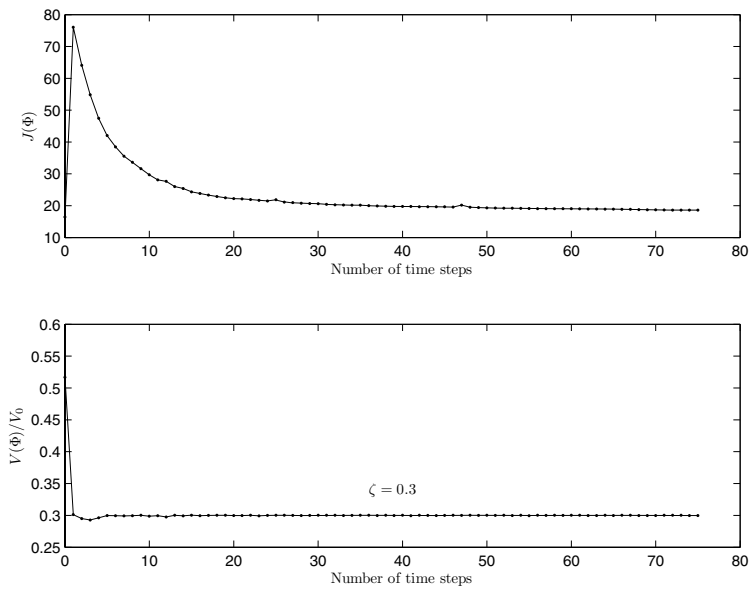


Figure 9: Convergence of the objective and volume functions for the 2D bridge starting with an initial design without a hole.

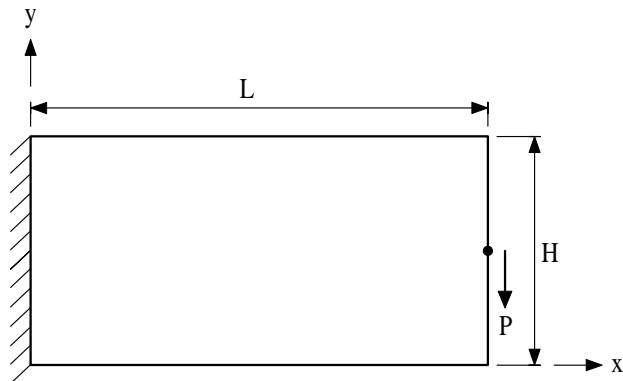


Figure 10: Minimum compliance design problem of a short cantilever beam.

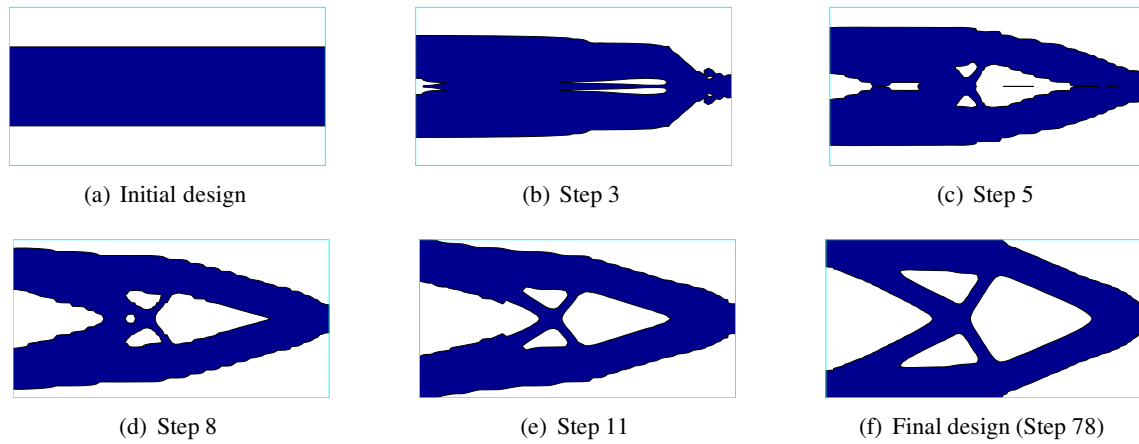


Figure 11: Evolution history of the optimal design for the cantilever beam starting with an initial design without a hole.

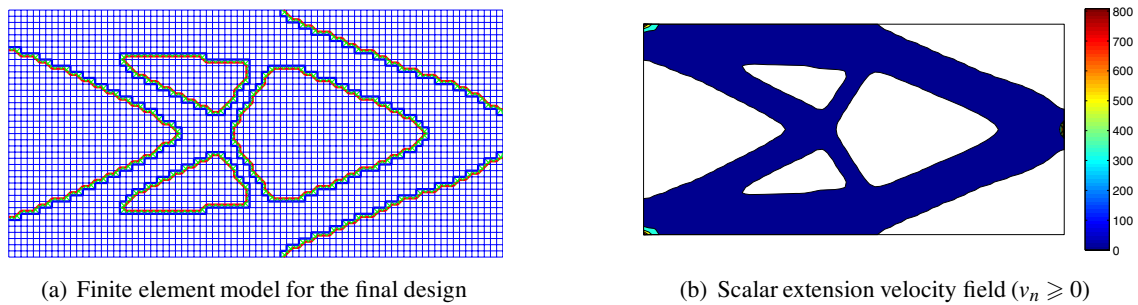


Figure 12: Final solutions for the cantilever beam starting with an initial design without a hole.

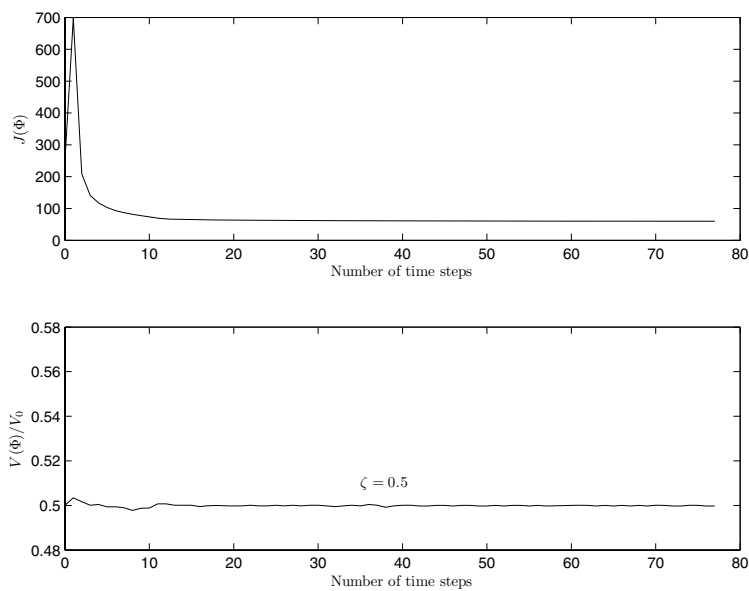


Figure 13: Convergence of the objective and volume functions for the cantilever beam starting with an initial design without a hole.

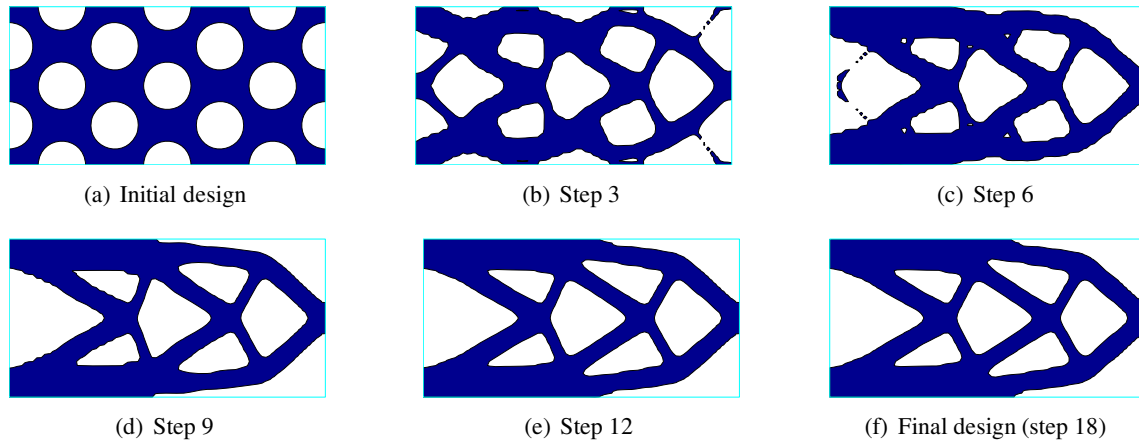
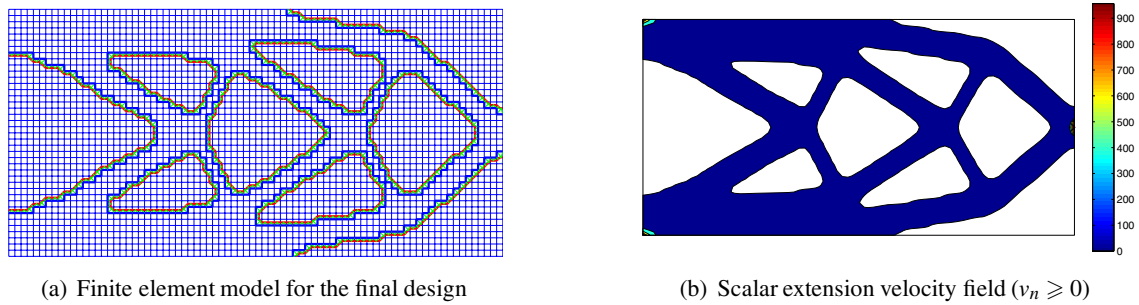


Figure 14: Evolution history of the optimal design for the cantilever beam starting with an initial design with holes.



(a) Finite element model for the final design (b) Scalar extension velocity field ( $v_n \geq 0$ )  
 Figure 15: Final solutions for the cantilever beam starting with an initial design with holes.

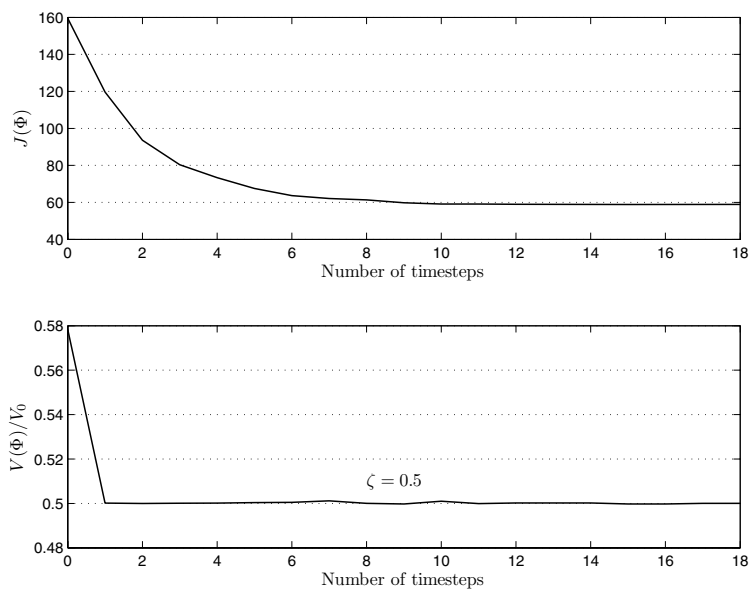


Figure 16: Convergence of the objective and volume functions for the cantilever beam starting with an initial design with holes.



the initial guess cannot be completely overcome by the present method. This is sound because the topology optimization problem is not convex and thus uniqueness of solutions cannot be guaranteed. Furthermore, the present gradient-based optimization method is only a local method, though it can effectively prevent the rapid convergence to a premature local optimum with fewer holes than the initial guess.

#### 4 Conclusions

A consistent and robust nucleation method is proposed in this study. The crucially important extension velocity field is constructed to be consistent with the mutual energy density and favorable for hole nucleation. Due to the consistent extension velocities, a negative extension velocity driven nucleation mechanism can be established and the driving forces can be physically meaningful since nucleation of new holes can be allowed for at the sites where the material is ineffectively used. An extension velocity filtering approach is developed to be consistent with the present nucleation mechanism while regularizing the ill-posed topology optimization problem to ensure existence of solutions. The smoothed extension velocities may even eliminate the discontinuity at the free boundary to favor a smooth level set evolution. To overcome the numerical instabilities caused by the level set evolution, a rescaling-based reinitialization scheme is developed to keep all the gradients bounded without moving the free boundary using a global representation technique. The globally supported multiquadric RBFs can guarantee the reconstructed level set function and its gradients to be infinitely smooth. Development of sharp differences between high and low derivatives can be prevented due to the global smoothness. Since the inconsistencies with the regularization and reinitialization techniques are eliminated, smooth nucleation of new holes becomes possible and rapid convergence to a local optimum with fewer holes than the initial guess can be avoided. The conventional level set-based topology optimization can thus become more accurate and efficient.

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