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Dynamical systems and topology optimization

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Abstract

This paper uses a dynamical systems approach for studying the material distribution (density or SIMP) formulation of topology optimization of structures. Such an approach means that an ordinary differential equation, such that the objective function is decreasing along a solution trajectory of this equation, is constructed. For stiffness optimization two differential equations with this property are considered. By simple explicit Euler approximations of these equations, together with projection techniques to satisfy box constraints, we obtain different iteration formulas. One of these formulas turns out to be the classical optimality criteria algorithm, which, thus, is receiving a new interpretation and framework. Based on this finding we suggest extensions of the optimality criteria algorithm.

A second important feature of the dynamical systems approach, besides the purely algorithmic one, is that it points at a connection between optimization problems and natural evolution problems such as bone remodeling and damage evolution. This connection has been hinted at previously but, in the opinion of the authors, not been clearly stated since the dynamical systems concept was missing. To give an explicit example of an evolution problem that is in this way connected to an optimization problem, we study a model of bone remodeling.

Numerical examples, related to both the algorithmic issue and the issue of natural evolution represented as bone remodeling, are presented.

1 Introduction

In the dynamical systems approach to optimization the optimization problem is replaced by an Ordinary Differential Equation (ODE) with the property that its equilibrium points coincide with local optima. For unconstrained minimization problems, a first order such dynamical system is obtained by simply taking its right hand side to be equal to the negative of the gradient of the objective function, but it is obvious that this is not the only possible choice. Moreover, for constrained problems, appropriate dynamical systems can be obtained by using projections. By this procedure algorithms for solving the original optimization problem can be obtained by utilizing standard discretization schemes for ODEs.

This approach to optimization is known in wide circuits as neurodynamical optimization [15], projected dynamical system approach [17], differential variational inequalities [19], gradient flow or ODE approach to optimization. However, it seems largely unexploited in structural optimization.

To be more specific, consider the unconstrained optimization problem of finding the value of the variable x that minimizes the objective function $f(x)$, i.e.,

$$\min_x f(x). \tag{1}$$

The following dynamical system can be associated to this problem:

$$\frac{dx(t)}{dt} = -\nabla f(x(t)), \tag{2}$$

where t is a time-like variable and $x(t)$ is a solution trajectory. Clearly, the stationary points of (1) coincide with the equilibrium points of (2), and it is easily proven that

$$\frac{d}{dt}f(x(t)) \leq 0, \tag{3}$$

meaning that $f(x(t))$ decreases along a solution trajectory of (2). We call (3) the Lyapunov property, since it is the essential property that is required from a Lyapunov function, the existence of which guarantees the stability of equilibrium points of dynamical systems.

Note that the dynamical system (2) is not the only system that has equilibrium points that coincide with the stationary points of (1) and for which (3) holds: any system that is obtained from (2) by premultiplying its right hand side by an x -dependent positive definite matrix has these properties.

For constrained optimization problems, which are obviously the ones of relevance for structural optimization, there are different possibilities for rewriting these as dynamical systems, see, e.g., [20, 26, 27]. In the following we will use a dynamical system based on local projections, see [17].

As indicated in the abstract, the purpose of a dynamical systems approach in structural optimization is at least twofold. There is the algorithmic issue but also the issue of modeling problems such as bone remodeling and damage that have been seen both as evolution problems and optimization problems in the past. Concerning the first issue, new methods can be obtained by simply utilizing well known algorithms for numerical solutions of ODEs. In this paper we show that a standard SIMP optimality criteria approach to stiffness topology optimization can be seen as a result of an explicit time discretization of a certain ODE, representing the optimization problem in the sense indicated above. This result opens the possibility of refining the SIMP optimality criteria approach by utilizing other explicit time discretizations such as Adams-Bashforth. We also find a natural modification of the OC-method where an exponential updating formula is used. As a further comment on the OC method we like to mention that the interpretation given here complements two other interpretations of this method, as recently reviewed in [14]: the traditional interpretation of the OC formula is that it represents a fixed point iteration for satisfying optimality conditions, but it can also be seen as a special case of a sequential explicit approximation method; in fact, for classical stiffness optimization it is

a generalization of the CONLIN approximation and a special case of the MMA approximation. A further remark on the algorithmic issue is that although ODE methods for optimization have sometimes been viewed as ineffective, there are also reports to the opposite [5].

Concerning the second issue of modeling natural evolution problems we use as an example a bone remodeling formulation of Harrigan and Hamilton [10, 11, 12]. This model is *a priori* formulated as an evolution equation for volumetric densities, but it can be shown that equilibrium points of the ODE are local solutions of an optimization statement. Thus, the sequence of problems indicated above – from optimization problem to evolution problem – is naturally reversed in this case. This can be taken to illustrate that many problems have a dual character as both optimization problems and as evolution problems: examples of this, previously treated in the literature, are damage evolution [1], fracture [9] and optimal flow patterns such as those of Bejan [2], see also [13]. Another comment in this respect is that several structural optimization algorithms (e.g., ESO) are intuitively thought of as producing an “evolution” of designs, without explicitly stating the mathematical problem that governs this evolution: the evolutions are only algorithmically defined. In the present approach, on the other hand, evolutions towards optima are well defined mathematically and choices of discretizations and algorithms are seen as separate steps.

In Section 2 we formulate the SIMP model of structural optimization and in Section 3 a dynamical systems formulation utilizing this model is given. Section 4 presents the bone remodeling formulation of Harrigan and Hamilton which exemplifies how optimality and evolution are connected. Section 5 presents different algorithms for integrating the dynamical systems and among them we identify the classical optimality criteria formula of structural optimization. Section 6 introduces two restriction methods needed to make the non-convex case of the formulation well-posed. Section 7 presents numerical solutions of both convex and non-convex problems. In particular, we study a problem that has been popular as a test example for bone remodeling algorithms. Finally, in an appendix we give equations relevant to higher order explicit integration schemes.

2 The SIMP model

The quasi-static equilibrium equation for linear discrete structures, where the stiffness depends on design variables, reads

$$\mathbf{F} = \mathbf{K}(\boldsymbol{\rho})\mathbf{u}. \quad (4)$$

Here \mathbf{u} is the vector of nodal displacements and \mathbf{F} is the corresponding force vector. The symmetric positive semi-definite stiffness matrix $\mathbf{K}(\boldsymbol{\rho})$ depends on a vector $\boldsymbol{\rho} = (\rho_1, \dots, \rho_n)^T$ of design variables in the following way:

$$\mathbf{K}(\boldsymbol{\rho}) = \sum_{i=1}^E \rho_i^q \tilde{\mathbf{K}}_i \quad (5)$$

where E is the number of elements in the structure and $\tilde{\mathbf{K}}_i$ is an element stiffness matrix for a unit value of the design variable ρ_i . In topology optimization we seek methods that returns values (close to) 0 or 1 for ρ_i , and these values are

interpreted as presence of material or holes in the structure. In the SIMP method this is achieved by letting the design variables be constricted to the set

$$K = \{\boldsymbol{\rho} \mid \epsilon \leq \rho_i \leq 1, i = 1, \dots, E\}$$

and by letting the penalty parameter $q > 1$ (in practise, say, $q = 3$). Here, $\epsilon > 0$ is a small value that, by being non-zero, has the effect of making $\mathbf{K}(\boldsymbol{\rho})$ non-singular for $\boldsymbol{\rho} \in K$.

When formulating an optimization problem that determines optimal design variables it is natural to introduce the following constraint set:

$$K_V = \{\boldsymbol{\rho} \in K \mid \sum_{i=1}^E a_i \rho_i \leq V\},$$

for positive constants a_i and a bound V . The condition $\boldsymbol{\rho} \in K_V$ is a constraint on the total mass or volume of the material, or possibly, depending on the nature of the a_i 's, a more general cost.

The objective or goal function f generally depends on both displacements and design variables, i.e., $f = f(\mathbf{u}, \boldsymbol{\rho})$. Moreover, we consider a nested formulation, where $\mathbf{K}(\boldsymbol{\rho})$ is assumed nonsingular for all $\boldsymbol{\rho} \in K$, so that the displacement can be seen as a function of the design variables, i.e.,

$$\mathbf{u} = \mathbf{u}(\boldsymbol{\rho}) = \mathbf{K}(\boldsymbol{\rho})^{-1} \mathbf{F}.$$

An optimization problem for a general objective function can then be formulated as

$$\min_{\boldsymbol{\rho} \in K_V} \tilde{f}(\boldsymbol{\rho}), \tag{6}$$

where $\tilde{f}(\boldsymbol{\rho}) = f(\mathbf{u}(\boldsymbol{\rho}), \boldsymbol{\rho})$.

As an alternative to (6) we can base an optimization problem on the objective function

$$f_\mu = f_\mu(\mathbf{u}, \boldsymbol{\rho}) = f(\mathbf{u}, \boldsymbol{\rho}) + \mu \sum_{i=1}^E a_i \rho_i$$

and consider

$$\min_{\boldsymbol{\rho} \in K} \tilde{f}_\mu(\boldsymbol{\rho}), \tag{7}$$

where $\tilde{f}_\mu(\boldsymbol{\rho}) = f_\mu(\mathbf{u}(\boldsymbol{\rho}), \boldsymbol{\rho})$. The positive parameter μ regulates the relative importance of the two terms in f_μ .

Problems (6) and (7) are strongly related: If for all $\boldsymbol{\rho} \in K$,

$$\frac{\partial \tilde{f}}{\partial \rho_i} < 0 \text{ for at least one } i, \tag{8}$$

then $\sum_{i=1}^E a_i \rho_i \leq V$ will always be satisfied as an equality at optimal points of (6). Therefore, if $\boldsymbol{\rho}^*$ is an optimal solution to (7) for some fixed μ , then $\boldsymbol{\rho}^*$ is an optimal solution also to (6) for the constant $V = \sum_{i=1}^E a_i \rho_i^*$. Moreover,

since the second term in f_μ is linear, properties of convexity or non-convexity of problem (7) will be the same as for the corresponding problem (6). In the following we will be mainly concerned with problem (7), see the note below.

A specific classical example of an objective function, used widely in sizing and topology optimization problems, is compliance C , which is defined as $1/2\mathbf{F}^T\mathbf{u}$. Note that, due to (4), compliance is equivalent to strain energy, i.e.,

$$C = \frac{1}{2}\mathbf{F}^T\mathbf{u} = \frac{1}{2}\mathbf{u}^T\mathbf{K}(\boldsymbol{\rho})\mathbf{u}. \quad (9)$$

Of special interest is the following case of the general optimization problem (7):

$$(C) \quad \min_{\boldsymbol{\rho} \in K} f_C(\boldsymbol{\rho}),$$

where

$$f_C(\boldsymbol{\rho}) = \frac{1}{2}\mathbf{F}^T\mathbf{u}(\boldsymbol{\rho}) + \mu \sum_{i=1}^E a_i \rho_i.$$

As will be seen below, (8) holds for the compliance objective, which motivates handling the volume (or cost) as a term in the objective function.

It follows from a result by Stolpe and Svanberg [22] (see also Svanberg [23]) that (C) is a convex problem for $q \leq 1$. However, such values of q do not penalize intermediate values of $\boldsymbol{\rho}$ and are not useful from the point of view of topology optimization. Nevertheless, as will be seen in Section 4, they play a role in a similar problem related to bone remodeling.

Note that we will base the developments in the rest of the paper on problem (7), instead of (6), even though the latter is the standard choice in the topology optimization literature. One reason for this may be simplicity, but the main reason is that we want a model that is close to physical evolution processes. As an example of such a process, in strong analogy with the the SIMP model, we will study bone remodeling in Section 4. As another example we have mentioned damage evolution that was studied in a structural optimization framework in [1]. It is not natural to have a limit on the total amount of material that is included in a growing bone structure, and in the same way total damage cannot be controlled in advance. This being said, one should also note, as indicated in the remark of the next section, that there are dynamical systems, associated with both problems (6) and (7), and from a purely algorithmic or mathematical point a view, a study of the first problem by a dynamical systems approach is possible.

3 Dynamical systems approach

A necessary condition for $\boldsymbol{\rho} \in K$ to be a solution of (7) is that it satisfies the stationarity condition

$$(\boldsymbol{\rho}^* - \boldsymbol{\rho})^T \nabla \tilde{f}_\mu(\boldsymbol{\rho}) \geq 0 \quad \forall \boldsymbol{\rho}^* \in K. \quad (10)$$

An analogous condition holds for (6).

An indirect but from several point of views very useful approach to finding a $\boldsymbol{\rho}$ that satisfies (10) is to consider a dynamical system (gradient flow, dynamical

system, ODE, neurodynamical) reformulation of the problem. Here we give the most direct such formulation for (7), see, e.g., Nagurney and Zhang [17], based on local projections. Let $\boldsymbol{\rho}$ be a function of a time-like variable t and solve, for some initial condition, the ODE

$$\dot{\boldsymbol{\rho}} = \lambda \Pi_K(\boldsymbol{\rho}, -\nabla \tilde{f}_\mu(\boldsymbol{\rho})), \quad (11)$$

where a superposed dot indicates a derivative with respect to t , λ is a positive constant that has a physical dimension that depends on the choice of objective function and it also represents different time scales, and $\Pi_K(\boldsymbol{\rho}, -\nabla \tilde{f}_\mu(\boldsymbol{\rho}))$ is the Euclidean projection of $-\nabla \tilde{f}_\mu(\boldsymbol{\rho})$ on the tangent cone of K at $\boldsymbol{\rho}$. Equation (11) is a formulation that applies to any convex set K . When this set has the present structure of the cartesian product of the sets

$$K_i = \{\rho_i \mid \epsilon \leq \rho_i \leq 1\},$$

we can write (11) in an equivalent component form:

$$\dot{\rho}_i = \lambda \Pi_{K_i} \left(\rho_i, -\frac{\partial \tilde{f}_\mu(\boldsymbol{\rho})}{\partial \rho_i} \right), \quad (12)$$

Explicitly, (12) means that $\dot{\rho}_i = 0$ if $\rho_i = 1$ and $\partial \tilde{f}_\mu / \partial \rho_i < 0$ or $\rho_i = \epsilon$ and $\partial \tilde{f}_\mu / \partial \rho_i > 0$, and otherwise

$$\dot{\rho}_i = -\lambda \frac{\partial \tilde{f}_\mu(\boldsymbol{\rho})}{\partial \rho_i}. \quad (13)$$

It should be clear that (13) is a continuous version of a steepest decent algorithm.

Equilibrium points of (11) are such that $\Pi_K(\boldsymbol{\rho}, -\nabla \tilde{f}_\mu(\boldsymbol{\rho})) = \mathbf{0}$ and these points coincide with the stationary points of (7), defined by (10). Moreover, for a solution of (11), the function $\tilde{f}_\mu(\boldsymbol{\rho})$ is strictly decreasing with respect to t unless $\boldsymbol{\rho}$ is an equilibrium point. This fact follows from

$$\begin{aligned} \frac{d\tilde{f}_\mu(\boldsymbol{\rho})}{dt} &= \nabla \tilde{f}_\mu(\boldsymbol{\rho})^T \dot{\boldsymbol{\rho}} = \lambda \nabla \tilde{f}_\mu(\boldsymbol{\rho})^T \Pi_K(\boldsymbol{\rho}, -\nabla \tilde{f}_\mu(\boldsymbol{\rho})) \\ &= -\lambda \Pi_K(\boldsymbol{\rho}, -\nabla \tilde{f}_\mu(\boldsymbol{\rho}))^T \Pi_K(\boldsymbol{\rho}, -\nabla \tilde{f}_\mu(\boldsymbol{\rho})), \end{aligned}$$

where the last expression is strictly less than zero except at an equilibrium point. On other words, \tilde{f}_μ has a Lyapunov property in relation to the ODE (11). Even more to the point concerning the connection between the minimization problem (7) and the dynamical system (11), Theorem 2.5 in [20] shows that a solution path of (11) that starts sufficiently close to a stationary point of (7) will converge exponentially towards that point, if the Hessian of \tilde{f}_μ is positive definite at the point.

Now, (11) is not the only ODE for which \tilde{f}_μ has the Lyapunov property. In fact, the λ of (12) can be replaced by functions $d_i(\rho_i) > 0$ such that

$$\dot{\rho}_i = d_i(\rho_i) \Pi_{K_i} \left(\rho_i, -\frac{\partial \tilde{f}_\mu(\boldsymbol{\rho})}{\partial \rho_i} \right). \quad (14)$$

In Section 5 we will see that the case when $d_i(\rho_i)$ is linear is related to the classical optimality criteria algorithm of topology optimization.

We like to calculate the gradient of the objective function for the compliance optimization problem (C). Using (4) and (5) we find that

$$\frac{\partial f_C(\boldsymbol{\rho})}{\partial \rho_i} = \mu a_i - e_i(\boldsymbol{\rho}), \quad (15)$$

where

$$e_i(\boldsymbol{\rho}) = q\rho_i^{(q-1)}\frac{1}{2}\mathbf{u}^T\tilde{\mathbf{K}}_i\mathbf{u} \quad \text{and} \quad \mathbf{u} = \mathbf{u}(\boldsymbol{\rho}) = \mathbf{K}(\boldsymbol{\rho})^{-1}\mathbf{F}.$$

Since $\tilde{\mathbf{K}}_i$ is positive semi-definite one concludes that $e_i(\boldsymbol{\rho}) \geq 0$, and since $\mathbf{K}(\boldsymbol{\rho})$ is non-singular, at least one of the e_i :s will be strictly positive when $\mathbf{F} \neq \mathbf{0}$. This implies that (8) is satisfied. Equation (13), when specialized to problem (C), becomes

$$\dot{\rho}_i = \lambda(e_i(\boldsymbol{\rho}) - \mu a_i). \quad (16)$$

Remark: Note that the idea of reformulating an optimization problem as a dynamical system, presented in this section, is by no means restricted to problem (7), where the constraint on total volume is removed and added to the objective function. As was pointed out above, equation (11) is not restricted to a particular convex set and by changing K to K_V and \tilde{f}_μ to \tilde{f} we have a dynamical systems reformulation that applies to problem (6). However, an alternative such reformulation of problem (6), which directly generalizes the developments of this paper, is the following:

$$\begin{aligned} \dot{\boldsymbol{\rho}} &= \lambda \Pi_K(\boldsymbol{\rho}, -\nabla \tilde{f}(\boldsymbol{\rho}) - \mathbf{a}\Lambda), \\ \Lambda &\geq 0, \quad \Lambda \left(\sum_{i=1}^E a_i \rho_i - V \right) = 0, \quad \sum_{i=1}^E a_i \rho_i \leq V, \end{aligned}$$

where $\mathbf{a} = (a_1, \dots, a_E)^T$ and Λ is the Lagrangian multiplier that replaces μ . Using this formulation the optimality criteria algorithm, that is derived in Section 5.2, would be modified to include an updating formula for the Lagrangian multiplier, which is the traditional way of presenting this algorithm.

4 Bone remodeling

Equation (5) has some similarity with the stiffness matrix obtained for a structure consisting of cancellous bone tissue: for such material it is found, see, e.g., [18], that the elasticity modulus E depends on the bone volumetric density ϕ such that

$$E = E_0 \phi^N,$$

where N is a material parameter the value of which is in the range of 2 or 3, E_0 is the elasticity modulus for unit volumetric density, and Poisson's ratio can be considered independent of ϕ . When doing a finite element discretization and taking the density to be a constant ϕ_i for each element i , this material behavior gives equations (4) and (5) if ρ_i is changed for ϕ_i , q is changed for N and the vector $\boldsymbol{\rho}$ is changed for $\boldsymbol{\phi} = (\phi_1, \dots, \phi_E)^T$.

If the constants a_i represents the volumes of finite elements, the strain energy volumetric density of element i can be written as

$$\Psi_i = \frac{\phi_i^N \mathbf{u}^T \tilde{\mathbf{K}}_i \mathbf{u}}{2a_i} \quad \text{where} \quad \mathbf{u} = \mathbf{u}(\phi) = \mathbf{K}(\phi)^{-1} \mathbf{F}. \quad (17)$$

Harrigan and Hamilton [10] assume that Ψ_i/ϕ^m , where m is an adjustable parameter, acts as a tissue stimulus for bone remodeling. This is a generalization of the special case when $m = 1$, which has been used in a large number of papers, e.g., [16, 24, 6]. Based on this stimuli, an evolution equation for the density is now written as

$$\dot{\phi}_i = \lambda_1 \left(\frac{\Psi_i}{\phi_i^m} - \tilde{\mu} \right) = \lambda_1 \left(\phi_i^{(N-m)} \frac{\mathbf{u}^T \tilde{\mathbf{K}}_i \mathbf{u}}{2a_i} - \tilde{\mu} \right), \quad (18)$$

where $\tilde{\mu}$ is a target value for the stimulus, and λ_1 is a positive constant of physical dimension, similar to λ in equation (11). Harrigan and Hamilton writes (18) without this constant, though.

Equation (18) can be rewritten as

$$N a_i \dot{\phi}_i = \lambda \phi_i^{(1-m)} \left[N \phi_i^{(N-1)} \frac{\mathbf{u}^T \tilde{\mathbf{K}}_i \mathbf{u}}{2} - N \tilde{\mu} a_i \phi_i^{(m-1)} \right]. \quad (19)$$

It turns out that the function within the brackets equals the negative of the partial derivative of

$$f_B(\phi) = \frac{1}{2} \mathbf{F}^T \mathbf{u}(\phi) + \frac{N}{m} \tilde{\mu} \sum_{i=1}^N a_i \phi_i^m.$$

Thus, (19) is an evolution equation of the same type as (14), granted that we treat upper and lower bounds of ϕ_i by a projection, and f_B has the Lyapunov property with respect to this equation. Moreover, f_B has a clear resemblance to the objective function f_C , introduced in Section 2; in fact

$$f_B(\phi) = f_C(\boldsymbol{\rho}) \quad \text{if} \quad \rho_i = \phi_i^m, \quad \mu = \tilde{\mu} \frac{N}{m} \quad \text{and} \quad q = \frac{N}{m}. \quad (20)$$

This change of variables, from ϕ_i to ρ_i , was made also by Harrigan and Hamilton [11, 12, 10] (however, not for the reason of identification with f_C) and they also suggested (save the physical constant λ_2) to replace the evolution equation (18) by

$$a_i \dot{\rho}_i = -\lambda_2 \frac{m}{N} \frac{\partial f_C(\boldsymbol{\rho})}{\partial \rho_i}. \quad (21)$$

This is again an evolution equation of the same type as (14), with $d_i(\rho_i)$ a constant function, and f_C has the Lyapunov property with respect to this equation. Both (19) and (21) have the same equilibrium points but different evolutions towards these are defined. In this respect Harrigan and Hamilton [10] states that ‘‘Since no current bone remodeling rule purports to closely mimic transient remodeling processes, we do not consider our modification to be a serious problem for the theoretical development.’’

Furthermore, Harrigan and Hamilton [12] showed that f_C is a convex function for $N \leq m$, which is the condition found also by applying the result in Stolpe and Svanberg [22] as indicated in Section 2. In fact, Harrigan and Hamilton found that this condition is necessary for convexity. They interpret the convexity condition as one of stability for the corresponding evolution equation.

5 Algorithms

In this section we will develop numerical algorithms for two dynamical system formulations. The first one is defined by equation (11) when the objective function is f_C , i.e., equation (16) when appropriate projections are introduced to treat upper and lower bounds for ρ_i . The second formulation is defined by (14), when $d_i(\rho_i)$ is a certain linear function and when the objective function is f_C . This second dynamical system will turn out to be connected to the classical optimality criteria method of SIMP topology optimization. We do not discuss convergence of algorithms but refer to [17, 8].

5.1 Projected Euler method

We first suggest a simple projected Euler method, see [17], for the solution of equation (12). Given a solution $\boldsymbol{\rho}(t)$ at time t , we calculate an approximation of the solution at time $t + \Delta t$. By an explicit time discretization of equation (13) we calculate test values $\hat{\rho}_i(t + \Delta t)$ from

$$\frac{\hat{\rho}_i(t + \Delta t) - \rho_i(t)}{\Delta t} = -\lambda \frac{\partial \tilde{f}_\mu(\boldsymbol{\rho}(t))}{\partial \rho_i}. \quad (22)$$

When applied to problem (C), this gives the following iteration formula:

$$\hat{\rho}_i^{n+1} = \rho_i^n + k[e_i(\boldsymbol{\rho}^n) - \mu a_i], \quad (23)$$

where $k = \lambda \Delta t$, and $\hat{\rho}_i^{n+1}$ and ρ_i^n are algorithmic versions of $\hat{\rho}_i(t + \Delta t)$ and $\rho_i(t)$, respectively. After a test value is calculated by (23), we make a projection onto the constraint set K as follows:

$$\rho_i^{n+1} = \begin{cases} \bar{\rho}_i & \text{if } \hat{\rho}_i^{n+1} > \bar{\rho}_i \\ \hat{\rho}_i^{n+1} & \text{if } \underline{\rho}_i \leq \hat{\rho}_i^{n+1} \leq \bar{\rho}_i \\ \underline{\rho}_i & \text{if } \underline{\rho}_i > \hat{\rho}_i^{n+1}. \end{cases} \quad (24)$$

The new iterate ρ_i^{n+1} is taken as an approximation of $\rho_i(t + \Delta t)$. In the present problem $\bar{\rho}_i = 1$ and $\underline{\rho}_i = \epsilon$ for all i . Note that this method is essentially a steepest descent method. It can therefore be expected to show slow convergence, which is confirmed by the numerical experiments.

5.2 Optimality criteria method

The optimality criteria algorithm for the optimization problem (C), see [3] or [7], consists of a simple updating formula which defines a sequence of iterates

that should converge to an optimum: when an iterate $\boldsymbol{\rho}^n$ is known, the next iterate is calculated by first calculating the test value

$$\hat{\rho}_i^{n+1} = \left(\frac{e_i(\boldsymbol{\rho}^n)}{\mu a_i} \right)^\beta \rho_i^n, \quad (25)$$

and then using the projection (24). The constant β is referred to as a damping coefficient. Note that the optimality criteria algorithm is usually defined for a structural optimization problem where the cost of design variables is a constraint as in problem (6). The constant μ then becomes a Lagrangian multiplier that has to be iteratively calculated. On the other hand, when the cost is added to the objective function as in (7), the iteration formula is the same but μ stays constant. This is the version of the optimality criteria algorithm considered here, but as pointed out in the remark of Section 3, an alternative dynamical systems formulation would introduce the Lagrangian multiplier that has to be iteratively adjusted so as to satisfy a volume constraint.

Obviously the updating scheme (25) has clear resemblance to (23), but the two formulas have different logical positions in terms of underlying theory: (23) is a discretization of an ODE while (25) is supposed to solve an optimization problem. However, we will show that (25) can be seen as a time discretization of the following version of (14):

$$\mu a_i \frac{\dot{\rho}_i}{\rho_i} = \lambda_3 [e_i(\boldsymbol{\rho}) - \mu a_i], \quad (26)$$

where we do not write the projection explicitly and where λ_3 is a constant. We first rewrite (26) as

$$\frac{d}{dt} \ln \rho_i = \lambda_3 \left(\frac{e_i(\boldsymbol{\rho})}{\mu a_i} - 1 \right). \quad (27)$$

Given a solution $\boldsymbol{\rho}(t)$ at time t , we like to calculate an approximation of the solution at time $t + \Delta t$. By an explicit time discretization of the left hand side of equation (27) we calculate test values $\hat{\rho}_i(t + \Delta t)$ from

$$\frac{\ln \hat{\rho}_i(t + \Delta t) - \ln \rho_i(t)}{\Delta t} = \lambda_3 \left(\frac{e_i(\boldsymbol{\rho}(t))}{\mu a_i} - 1 \right),$$

which we rewrite, using standard formulas for logarithms, as

$$\left(\frac{\hat{\rho}_i(t + \Delta t)}{\rho_i(t)} \right)^{\frac{1}{\lambda_3 \Delta t}} = \exp \left(\frac{e_i(\boldsymbol{\rho}(t))}{\mu a_i} - 1 \right) \approx \frac{e_i(\boldsymbol{\rho}(t))}{\mu a_i}, \quad (28)$$

and where the approximation comes from using the first two terms in the Taylor expansion for the exponential. By letting $\beta = \lambda_3 \Delta t$ and by doing other appropriate identifications we obtain the iteration formula (25).

Remark: By doing a slightly different time discretization, (25) can be derived from (26) without the need to approximate the exponent as above: We rewrite the quotient of the left hand side of (26) as follows:

$$\frac{\dot{\rho}_i}{\rho_i} = \beta \frac{\frac{d}{dt} \rho_i^{1/\beta}}{\rho_i^{1/\beta}}$$

for a positive constant β . Thus, (26) reads

$$\frac{d}{dt}\rho_i^{1/\beta} = \rho_i^{1/\beta} \frac{\lambda_3}{\beta} \left(\frac{e_i(\boldsymbol{\rho})}{\mu a_i} \right) - \rho_i^{1/\beta} \frac{\lambda_3}{\beta}.$$

An explicit time discretization of this equation reads

$$\frac{\hat{\rho}_i(t + \Delta t)^{1/\beta} - \rho_i(t)^{1/\beta}}{\Delta t} = \rho_i(t)^{1/\beta} \frac{\lambda_3}{\beta} \left(\frac{e_i(\boldsymbol{\rho}(t))}{\mu a_i} \right) - \rho_i(t)^{1/\beta} \frac{\lambda_3}{\beta}.$$

Taking $\beta = \Delta t \lambda_3$ results in

$$\hat{\rho}_i(t + \Delta t)^{1/\beta} = \rho_i(t)^{1/\beta} \left(\frac{e_i(\boldsymbol{\rho}(t))}{\mu a_i} \right),$$

which, again, can be identified with (25).

6 Restriction methods

When $q > 1$. i.e., when problem (\mathcal{C}) is non-convex, it is well known that the underlying continuum problem that results in (\mathcal{C}) is not well-posed in the sense that it in general lacks solutions: a minimizing sequence tends to structures consisting of infinitely thin structural parts. In the discretized problem this turns up as solutions with strut-like members of typically one to two element thickness, resulting in artificial stiffness. There are also presence of mesh dependency and so-called checkerboard patterns. Several amendments to the problem formulation that results in existence of solutions and well behaved discrete approximations are possible, see Bendsøe and Sigmund [3]. One such possibility is filtering of design variables. This means that the design variable ρ (the continues version of $\boldsymbol{\rho}$) is changed for a filtered design variable $\tilde{\rho}$ everywhere in the problem formulation. The filtered design is calculated from an essentially non-physical “unfiltered” design variable ξ that becomes the independent variable of the optimization problem. Note that while ρ is defined on the potential structural domain only, the variable ξ may be defined on the whole space, see [4]. However, a simplified treatment, discussed, e.g., in [21], is to use a ξ -variable that is defined in the structural domain only and that is what is used in the sequel. The discretized version of the relation between the ξ and $\tilde{\rho}$ variables is

$$\tilde{\rho}_j = \sum_{i=1}^E \Psi_{ji} \xi_i, \quad j = 1, \dots, E. \quad (29)$$

Here

$$\Psi_{ij} = \frac{\psi_{ij} a_j}{\sum_{k=1}^E \psi_{ik} a_k}, \quad \psi_{ij} = \max \left(0, 1 - \frac{|\mathbf{e}_i - \mathbf{e}_j|}{R} \right),$$

where \mathbf{e}_i denotes the position vector of the geometric centroid of element i and R is the filter radius. Note that Ψ_{ij} is zero unless the centroids of elements i and j are within distance R .

Substituting $\tilde{\boldsymbol{\rho}} = (\tilde{\rho}_1, \dots, \tilde{\rho}_E)^T$ for $\boldsymbol{\rho}$ in (\mathcal{C}) results in the filtered problem $(\tilde{\mathcal{C}})$, where we search for an optimal $\boldsymbol{\xi} = (\xi_1, \dots, \xi_E)^T \in K$, by solving

$$(\tilde{\mathcal{C}}) \quad \min_{\boldsymbol{\xi} \in K} f_C(\tilde{\boldsymbol{\rho}}(\boldsymbol{\xi})).$$

Note that $\boldsymbol{\xi} \in K$ implies $\tilde{\boldsymbol{\rho}} \in K$. The gradient of the objective function, that will replace (15), becomes

$$\frac{\partial f_C(\tilde{\boldsymbol{\rho}}(\boldsymbol{\xi}))}{\partial \xi_j} = \sum_{i=1}^E \Psi_{ij} \frac{\partial f_C(\tilde{\boldsymbol{\rho}}(\boldsymbol{\xi}))}{\partial \tilde{\rho}_i} = \sum_{i=1}^E \Psi_{ij} (\mu a_i - e_i(\tilde{\boldsymbol{\rho}}(\boldsymbol{\xi}))). \quad (30)$$

Modifications of the dynamical systems formulations in Section 3 using this gradient are obvious.

Equation (30) shows that filtering has essentially two implications for the algorithms of Section 5. Firstly, the displacement solution of equation (4) that is needed for calculating $e_i(\tilde{\boldsymbol{\rho}}(\boldsymbol{\xi}))$ should be obtained using the filtered designs. Secondly, an averaging of gradients from elements within a radius R of each element needs to be done. An heuristic method which essentially makes only the second of these steps has been suggested by Sigmund, see [21]. In that approach a modification of the gradient is introduced directly without the need for an additional variable $\boldsymbol{\xi}$. The gradients in the algorithms of Section 5 is changed for

$$\frac{\widetilde{\partial f_C}}{\partial \rho_i} = \frac{\sum_{j=1}^E \psi_{ij} \rho_j \frac{\partial f_C(\boldsymbol{\rho})}{\partial \rho_j}}{\rho_i \sum_{j=1}^E \psi_{ij}}. \quad (31)$$

Clearly, this resembles the summation in (30) but there are some differences that are motivated in Sigmund [21].

7 Numerical results

Results will be presented for two problems:

1. Convergence studies for the convex problem with $q = 1$.
2. Non-convex problem with $q = 3$, showing several equilibrium points (local optima).

All calculations are made using the in-house FE program TRINITAS, [25].

7.1 Convex problem

We first study the properties of the projected Euler method of subsection 5.1 and the optimality criteria algorithm of subsection 5.2 for the convex case ($q = 1$). The design domain and load are defined in Figure 1. The solution is shown in Figure 2.

Iteration histories are studied in two different ways. Firstly, we generate graphs of objective function values versus the iteration number for different values of $\beta = \lambda_3 \Delta t$ and $k = \lambda \Delta t$, in the optimality criteria algorithm and in the projected Euler method, respectively. Secondly, we are interested in objective function values versus time, which gives an indication of how well the iteration methods represent solutions of ordinary differential methods. In Figure 3 these

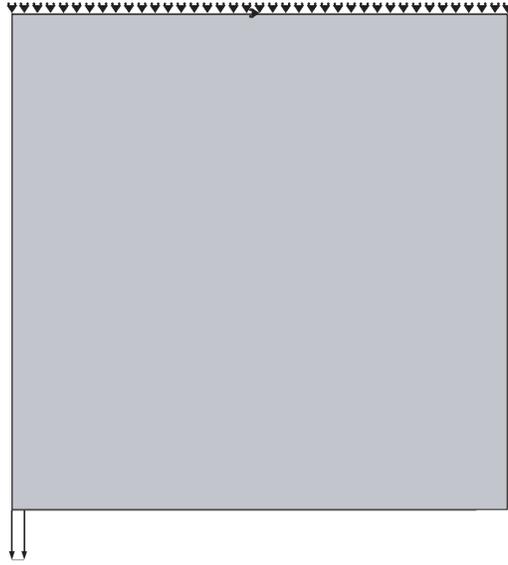


Figure 1: Definition of design domain, loads and boundary conditions.

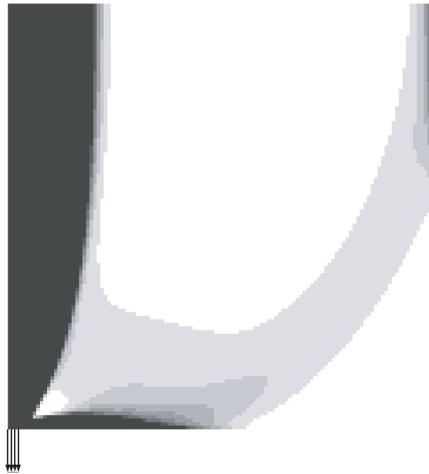


Figure 2: Solution, i.e., the optimal distribution of ρ , for the problem in Figure 1. The convex case ($q = 1$) is treated and 120×120 elements are used.

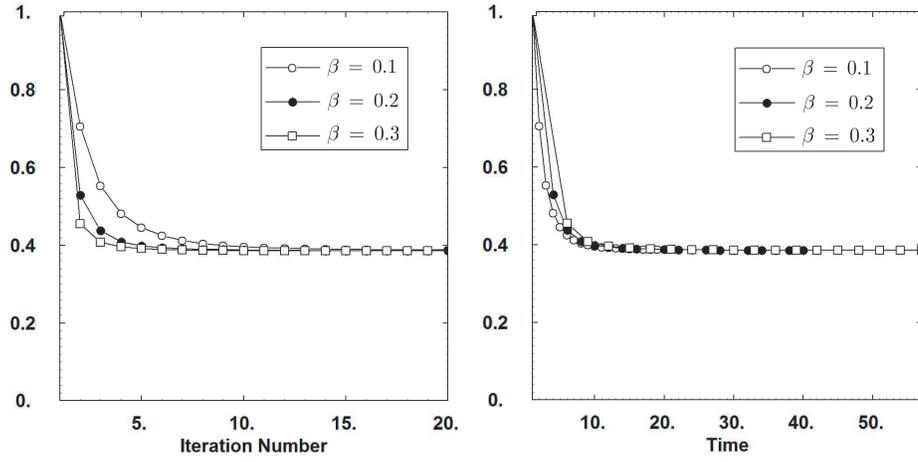


Figure 3: Iteration and time histories for the optimality criteria method applied to the problem in Figure 1. The converge solution is shown in Figure 2. The left hand figure shows objective function values versus iterations for different damping coefficients $\beta = \lambda_3 \Delta t$. To the right the same iteration histories are shown, but scaled so that the x -axis represents time.

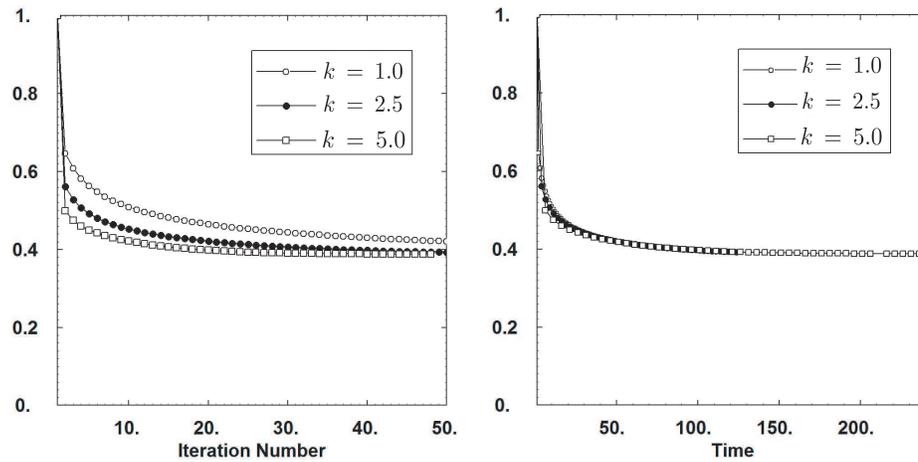


Figure 4: Similar results as in Figure 3, but for the the projected Euler method

plots are shown for the optimality criteria algorithm and in Figure 4 the same results for the projected Euler method are shown. What is seen from these graphs is that both methods well represent solutions of the ordinary differential equations, since the curves of the right hand plots essentially coincide. We also conclude from the number of iterations needed for convergence, and since k is chosen as large as possible without occurrence of oscillatory behavior, that the optimality criteria method is significantly more efficient than the projected Euler method. In order to investigate convergence rates, we have plotted $|\rho^{n+1} - \rho^*|$ versus $|\rho^n - \rho^*|$, where ρ^* is the converged design, in a log-log diagram. As may be expected from first order methods, both the Euler method and the optimality criteria method show linear convergence. The superior behavior of the optimality criteria methods comes from it being able to make larger design changes, i.e., larger values of the norm $|\rho^{n+1} - \rho^n|$ generally occurs.

7.2 Non-convex problem with several equilibrium points

We consider a test problem that has been used in several studies directed towards bone remodeling, see [6, 16, 28]. It seems as if this problem has several local optima with different topologies, but with very similar objective function values. The geometry and load is depicted in Figure 5.

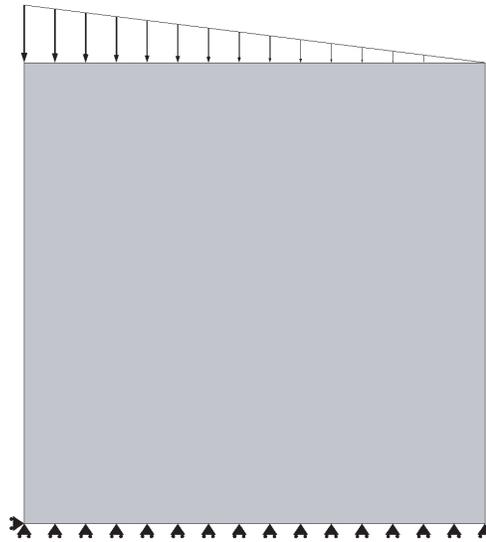


Figure 5: Geometry, loading and boundary conditions for the second test problem

The problem setting uses the exponent $q = 3$ and a discretization of 120×120 elements. Both Sigmund's filtering of gradients and filtered designs have been used, but the former is used when not mentioned otherwise. Except for one figure, where the influence of filter radius is tested, the filter function has a radius that corresponds to the width of three elements. The start solution in all calculations is a uniform distribution of the design variable with $\rho_i = 0.33$. In Figure 6, the objective function iteration history and the optimal topology is shown for a calculation using the projected Euler method. In Figure 7 similar

results are shown for the optimality criteria method. The objective function value is 0.128131 for the former method and 0.128664 for the latter. It should be noted that the number of iterations required for convergence of the projected Euler method is much larger than the number required for the optimality criteria method. It should also be noted that these two topologies are typical for the respective methods, i.e., in case of convergence, changing parameters does not produce a different topology.

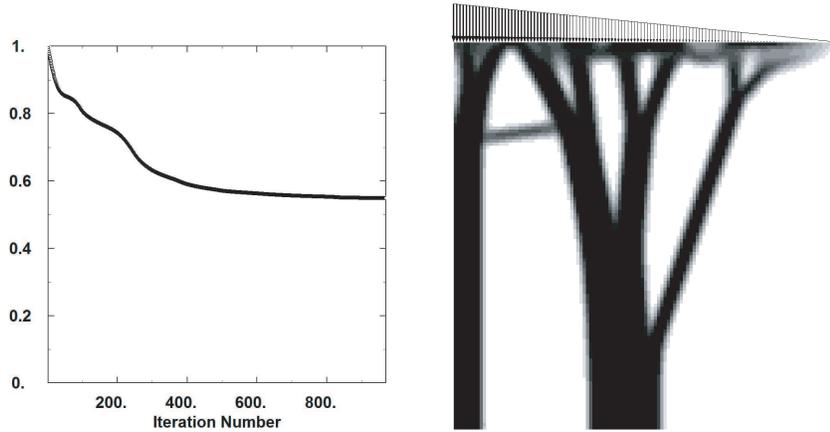


Figure 6: Solution and iteration history obtained by the projected Euler method for the problem in Figure 5.

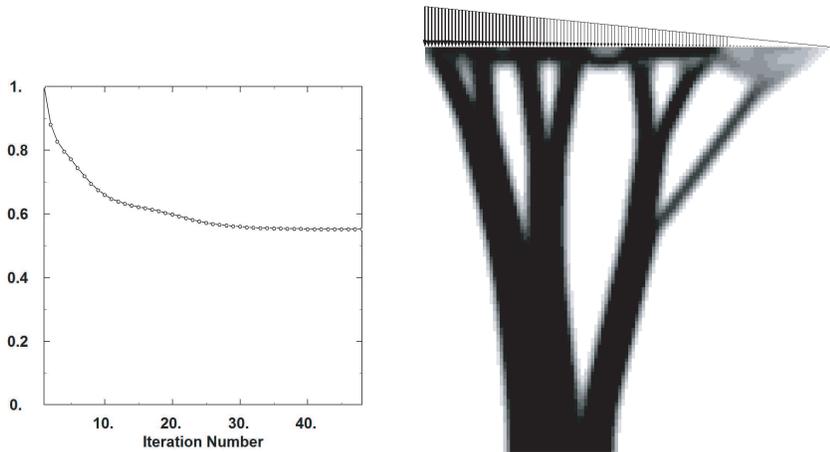


Figure 7: Solution and iteration history obtained by optimality criteria method for the problem in Figure 5.

Moreover, the overall topology is also insensitive to the choice of filtering method. In Figures 8 and 9 the two filter methods are compared and only local changes in topology are observed.

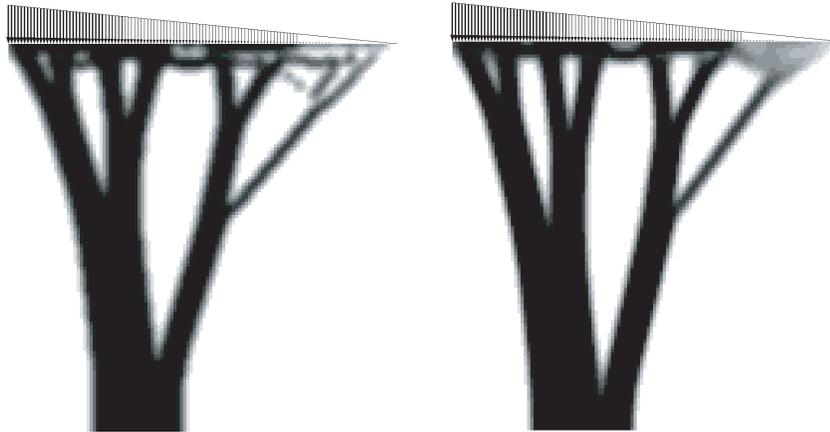


Figure 8: Solution obtain by the optimality criteria method. To the left density filtering is used and to the right Sigmund's derivative filter is used.

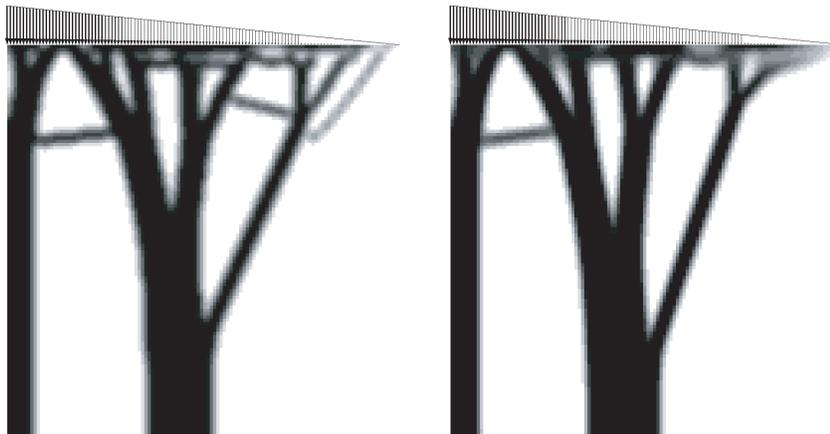


Figure 9: Solution obtain by the projected Euler method. To the left density filtering is used and to the right Sigmund's derivative filter is used.

In Figure 10 we have investigated the influence of changing filter radius. It is concluded that the overall topology is stable with respect to this parameter, although we clearly see widespread checkerboard patterns when the filter is removed.



Figure 10: Solution obtain by the optimality criteria method. The filter radius from left two right is 3, 2 and 1 (zero) elements in Sigmund’s filter.

Finally, in Figure 11 we compare the modified optimality criteria method, when the exponent is left exact in equation (28), to the standard optimality criteria algorithm. Again the topology is different and a third local solution in addition to the ones in Figures 6 and 7 is found. The objective function value for this new topology is 0.128177, which is in between the projected Euler method (best) and the standard optimality criteria method (worst). It may also be noted that in other papers where Euler-like methods are applied to this problem, [6, 16, 28], the solutions presented show separate “legs”, as in Figure 6 and in the right hand plot of Figure 11. It may also be notes, in relation to all three topologies generated by different iteration formulas, that the solution is very much determined by the very first iterations in the sequence.

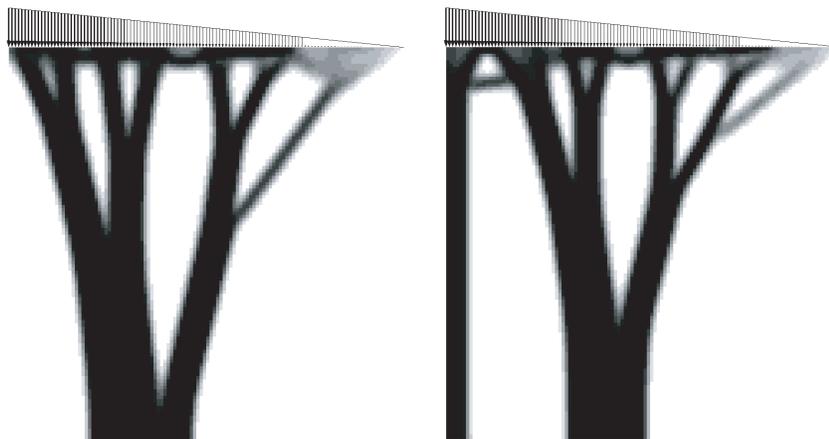


Figure 11: Solution obtain by the standard optimality criteria method (left) and by a modified method where the exponent function is not approximated (right).

8 Discussion and conclusions

We have applied a dynamical systems approach to a standard model of topology optimization. We find as a first result of such an approach that the classical optimality criteria method can be seen as an outcome of an explicit time discretization of a certain ODE. This knowledge may possibly be used to refine the optimality criteria method. One such refinement used here is an exponential updating formula, which for small updates coincide with the standard updating formula. Another modification is to use higher order explicit discretizations of the underlying ODE. However, an initial effort in this direction did not give positive results and the relevant equations are reported in the appendix.

A further interest in the dynamical systems approach to optimization is the dual view on design problems – on the one hand as the choice of best (i.e., optimization) and on the other hand as the evolution towards best (i.e., the dynamical systems approach) – may be beneficial in understanding certain problems like damage evolution and bone remodeling. As an exemplification of the latter we present a model of Harrigan and Hamilton and show that the initially formulated evolution problem actually describes an evolution towards an optimum of a certain function.

We have performed numerical tests which indicate convergence of the numerical solutions as the time discretizations of the dynamical systems are refined. Moreover, a non-convex problem, that has been studied in several papers directed towards bone remodeling, has been solved using several different methods and formulations. We find that the problem has several local minima with very similar objective function values, but convergence toward these are stable with respect to time step length and regularization methods.

A Appendix: Projected Adams-Bashforth algorithms

We have treated the two ODEs (16) and (27) by using the simplest type of explicit time discretization. It turned out that the optimality criteria method of structural optimization could be seen as a result of such a discretization. A crucial feature of the resulting computational schemes is that no extra evaluations of functions values, i.e., of $e_i(\boldsymbol{\rho})$, during a time step, need to be done, as would be the case when applying, say, a Runge-Kutta method. However, an extension of the simplest explicit method that also avoids extra function evaluations is the Adams-Bashforth method: it uses function values of previous time steps to produce an approximation that at least for smooth trajectories should be better than the Euler approximation. Because of this appealing property we chose to investigate the Adams-Bashforth method for both (16) and (27), the latter resulting in an extension of the optimality criteria method. However, since no improved numerical performance was found, we chose to place this development as a note in an appendix.

We write the ODE (16) in the following form

$$\rho_i(t + \Delta t) = \rho_i(t) + \lambda \int_t^{t+\Delta t} e_i(\boldsymbol{\rho}) dt - \lambda \Delta t \mu a_i. \quad (32)$$

Let the n :th point in the integration scheme correspond to time t and point $n+1$ to time $t + \Delta t$. In Adams-Bashforth's method of order ℓ we approximate the function value, in this case $e_i(\boldsymbol{\rho})$, in the interval t to $t+\Delta t$, by using a polynomial of degree $\ell + 1$ that interpolates computed function values at ℓ previous time steps. One then obtains, for the test function $\hat{\rho}_i^{n+1}$,

$$\hat{\rho}_i^{n+1} = \rho_i^n + \Delta t \sum_{j=1}^{\ell} \gamma_{j-1} \nabla^{j-1} e_i(\boldsymbol{\rho}^n) - \lambda \Delta t \mu a_i, \quad (33)$$

where the backward differences ∇^i of a function f^n are given by $\nabla^0 f^n = f^n$, $\nabla^1 f^n = f^n - f^{n-1}$, $\nabla^2 f^n = \nabla^1 f^n - \nabla^1 f^{n-1}$, etc., and γ_i are the Adams-Bashforth coefficients¹. After $\hat{\rho}_i^{n+1}$ has been calculated from (33), we obtain ρ_i^{n+1} from the projection (24).

Equation (27) can be integrated to give

$$\ln \rho_i(t + \Delta t) - \ln \rho_i(t) = \lambda_3 \int_t^{t+\Delta t} \left[\left(\frac{e_i(\boldsymbol{\rho})}{\mu a_i} \right) - 1 \right] dt. \quad (34)$$

Applying the polynomial approximation of the Adams-Bashforth method to this equation gives the following relation for iterates

$$\ln \rho_i^n - \ln \rho_i^{n-1} = \lambda_3 \Delta t \left[\sum_{i=1}^{\ell} \gamma_{i-1} \nabla^{i-1} \left(\frac{e_i(\boldsymbol{\rho}^n)}{\mu a_i} \right) - 1 \right],$$

which can be rewritten, similarly to (28), as

$$\begin{aligned} \left(\frac{\hat{\rho}_i(t + \Delta t)}{\rho_i(t)} \right)^{\frac{1}{\lambda_3 \Delta t}} &= \exp \left[\sum_{i=1}^{\ell} \gamma_{i-1} \nabla^{i-1} \left(\frac{e_i(\boldsymbol{\rho}^n)}{\mu a_i} \right) - 1 \right] \\ &\approx \sum_{i=1}^{\ell} \gamma_{i-1} \nabla^{i-1} \left(\frac{e_i(\boldsymbol{\rho}^n)}{\mu a_i} \right). \end{aligned} \quad (35)$$

Again, the next iterate is obtained by projecting $\hat{\rho}_i(t + \Delta t)$ according to (24).

As indicated above, no improved numerical performance could be seen by using these methods. In the iteration formula (33), of order $\ell = 3$, the time step had to be as small as in the Euler version, and, in fact, the first initial steps had to be done using $\ell = 1$ to avoid oscillations. Our interpretation of these results is that the projection makes the solution path non-smooth and therefore nothing is gained by using a method that approximates higher order derivatives.

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¹The first five Adams-Bashforth coefficients are 1, 1/2, 5/12, 3/8, 251/720 and 95/298.

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