

ODE Approach to Topology Optimization

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1. Abstract

The Ordinary Differential Equation (ODE) approach to optimization consists in replacing the optimization problem by an ODE with the property that its equilibrium points coincide with local solutions of the optimization problem. For unconstrained problems, a first order such ODE 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. For constrained problems, appropriate ODEs 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 computation, projected dynamical system approach, differential variational inequalities or ODE approach to optimization. However, it seems largely unexploited in structural optimization.

In the present contribution we show that a standard SIMP optimality criteria approach to stiffness topology optimization can be seen as an explicit time discretization of a certain ODE, representing the optimization problem in the sense indicated above. The numerical behavior of the resulting iteration formula is shown to be superior to what is found for explicit time discretization of a more straightforward ODE representation, which has been frequently used in the bone remodeling literature.

As a further illustration of the ODE approach we consider a bone remodeling formulation of Harrigan and Hamilton. This model is a priori formulated as an evolution equation for volumetric densities, but it can be shown that equilibrium points of this 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 and brittle fracture. 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 ever stating the equation that governs this evolution. In the present approach, on the other hand, evolutions towards optima are mathematically well defined.

2. Keywords: SIMP, ODE, projected dynamical system, topology optimization, optimality criteria

3. Introduction

Consider the unconstrained optimization problem of finding the value of the variable x that minimizes the objective function $f(x)$, i.e.,

$$\min_x f(x). \quad (1)$$

The following ODE (or dynamical system) can be associated to this problem:

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

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 proved that $f(x)$ is a Lyapunov function of (2), meaning that $f(x(t))$ decreases along a solution trajectory. Note that the dynamical system (2) is not the only system that has these properties: if we modify its right hand side by premultiplying by any x -dependent positive definite matrix, equilibrium and stationary points will still coincide and $f(x)$ will be a Lyapunov function.

For constrained optimization problems, which are obviously the ones of relevance for structural optimization, there are different possibilities for rewriting these as ODEs, see, e.g., [1, 2]. In the following we will

use a dynamical system based on local projections, see [3].

4. SIMP model

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

$$\mathbf{F} = \mathbf{K}(\boldsymbol{\rho})\mathbf{u}. \quad (3)$$

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 $\boldsymbol{\rho} = (\rho_1, \dots, \rho_E)^T$ of design variables in the following way:

$$\mathbf{K}(\boldsymbol{\rho}) = \sum_{i=1}^E \rho_i^q \tilde{\mathbf{K}}_i \quad (4)$$

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 $\boldsymbol{\rho} \in K$.

The efficiency or goal function f generally depends on both displacements and design variables, i.e., $f = f(\mathbf{u}, \boldsymbol{\rho})$. We can base an optimization problem on the objective function

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

where the second term represents the total mass or volume of the material, or possibly, depending on the nature of the a_i 's, a more general cost. The positive parameter μ regulates the relative importance of the two terms in f_μ . For a general function f we consider the following nested optimization problem:

$$\min_{\boldsymbol{\rho} \in K} \tilde{f}_\mu(\boldsymbol{\rho}), \quad (5)$$

where $\tilde{f}_\mu(\boldsymbol{\rho}) = f_\mu(\mathbf{u}(\boldsymbol{\rho}), \boldsymbol{\rho})$ and $\mathbf{u} = \mathbf{u}(\boldsymbol{\rho}) = \mathbf{K}(\boldsymbol{\rho})^{-1}\mathbf{F}$. When f is chosen as the compliance, problem (5) becomes

$$(C) \quad \min_{\boldsymbol{\rho} \in K} f_C(\boldsymbol{\rho}) \quad \text{where} \quad f_C(\boldsymbol{\rho}) = \frac{1}{2} \mathbf{F}^T \mathbf{u}(\boldsymbol{\rho}) + \mu \sum_{i=1}^E a_i \rho_i.$$

5. ODE Formulation

Let $\boldsymbol{\rho}$ be a function of a time-like variable t and solve, for some initial condition, the ODE

$$\dot{\boldsymbol{\rho}} = \lambda \Pi_K(\boldsymbol{\rho}, -\nabla \tilde{f}_\mu(\boldsymbol{\rho})), \quad (6)$$

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 (6) 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 (6) in an equivalent component form:

$$\dot{\rho}_i = \lambda \Pi_{K_i} \left(\rho_i, -\frac{\partial \tilde{f}_\mu(\boldsymbol{\rho})}{\partial \rho_i} \right). \quad (7)$$

Explicitly, (7) 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

$$\dot{\rho}_i = -\lambda \frac{\partial \tilde{f}_\mu(\boldsymbol{\rho})}{\partial \rho_i}. \quad (8)$$

It should be clear that (8) is a continuous version of a steepest decent algorithm.

Equilibrium points of (6) are such that $\Pi_K(\boldsymbol{\rho}, -\nabla \tilde{f}_\mu(\boldsymbol{\rho})) = \mathbf{0}$ and these points coincide with the stationary points of (5). Moreover, for a solution of (6), 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

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

where the last expression is strictly less than zero except at an equilibrium point. In other words, \tilde{f}_μ is a Lyapunov function of the ODE (6).

Now, (6) is not the only ODE for which \tilde{f}_μ is a Lyapunov function. In fact, the λ of (7) can be replaced by functions $d_i(\rho_i) > 0$ such that

$$\dot{\rho}_i = d_i(\rho_i) \Pi_{K_i} \left(\rho_i, -\frac{\partial \tilde{f}_\mu(\boldsymbol{\rho})}{\partial \rho_i} \right). \quad (9)$$

In the next section 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 (3) and (4) we find that

$$\frac{\partial f_C(\boldsymbol{\rho})}{\partial \rho_i} = \mu a_i - e_i(\boldsymbol{\rho}), \quad (10)$$

where

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

6. Algorithms

Let ρ_i^n be an approximation of $\rho_i(t)$, calculated by n previous time steps. By an explicit time discretization of equation (8) we calculate test values $\hat{\rho}_i^{n+1}$ from

$$\hat{\rho}_i^{n+1} = \rho_i^n + k[e_i(\boldsymbol{\rho}^n) - \mu a_i], \quad (11)$$

where $k = \lambda \Delta t$. After a test value is calculated by (11), we make a projection onto the constraint set K as follows:

$$\rho_i^{n+1} = \begin{cases} \bar{\rho}_i & \text{if } \hat{\rho}_i^{n+1} > \bar{\rho}_i \\ \hat{\rho}_i^{n+1} & \text{if } \underline{\rho}_i \leq \hat{\rho}_i^{n+1} \leq \bar{\rho}_i \\ \underline{\rho}_i & \text{if } \underline{\rho}_i > \hat{\rho}_i^{n+1}. \end{cases} \quad (12)$$

The new iterate ρ_i^{n+1} is taken as an approximation of $\rho_i(t + \Delta t)$. In the standard SIMP method $\bar{\rho}_i = 1$ and $\underline{\rho}_i = \epsilon$ for all i .

The optimality criteria algorithm for the optimization problem (C), see [4] or [5], 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

$$\hat{\rho}_i^{n+1} = \left(\frac{e_i(\boldsymbol{\rho}^n)}{\mu a_i} \right)^\beta \rho_i^n, \quad (13)$$

and then using the projection (12). The constant β is usually 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. 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 efficiency function as in

(5), the iteration formula is the same but μ stays constant. This is the version of the optimality criteria algorithm considered here.

Obviously the updating scheme (13) has clear resemblance to (11), but the two formulas have different logical positions in terms of underlying theory: (11) is a discretization of an ODE while (13) is supposed to solve an optimization problem. However, we will show that (13) can be seen as a time discretization of the following version of (9):

$$\mu a_i \frac{\dot{\rho}_i}{\rho_i} = \lambda_3 [e_i(\boldsymbol{\rho}) - \mu a_i] \quad (14)$$

where we do not treat the projection explicitly and where λ_3 is a constant. We first rewrite (14) as

$$\frac{d}{dt} \ln \rho_i = \lambda_3 \left(\frac{e_i(\boldsymbol{\rho})}{\mu a_i} - 1 \right). \quad (15)$$

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 (15) 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

$$\left(\frac{\hat{\rho}_i(t + \Delta t)}{\rho_i(t)} \right)^{\frac{1}{\lambda_3 \Delta t}} = \exp \left(\frac{e_i(\boldsymbol{\rho}(t))}{\mu a_i} - 1 \right) \approx \frac{e_i(\boldsymbol{\rho}(t))}{\mu a_i}, \quad (16)$$

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 (13).

7. Bone remodeling

In this section we will show in what sense the SIMP model and its formulation as an ODE relates to a simple model of bone remodeling.

Equation (4) is similar to the stiffness matrix obtained for a structure consisting of cancellous bone tissue: for such material it is found, see, e.g., [6], 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 (3) and (4) 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

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

Harrigan and Hamilton [7] assume that Ψ_i/ϕ_i^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., [8, 9]. Based on this stimuli, an evolution equation for the density is now written as

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

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 (6). Harrigan and Hamilton writes (18) without this constant, though.

Equation (18) can be rewritten as

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

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

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

Thus, (19) is an evolution equation of the same type as (9), granted that we treat upper and lower bounds of ϕ_i by a projection, and f_B is a Lyapunov function of this equation. Moreover, f_B has a clear resemblance to the objective function f_C , introduced in Section 4, in fact

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

This change of variables, from ϕ_i to ρ_i , was made also by Harrigan and Hamilton [7, 10, 11] (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 (9), with $d_i(\rho_i)$ a constant function, and f_C is a Lyapunov function of this equation. Both (19) and (21) have the same equilibrium points but different evolutions towards these are defined. In this respect Harrigan and Hamilton [7] 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.’’

8. Numerical results

We like to consider a test problem that has been used in several studies directed towards bone remodeling, see [8, 9, 12]. The geometry and load is depicted in Figure 1.

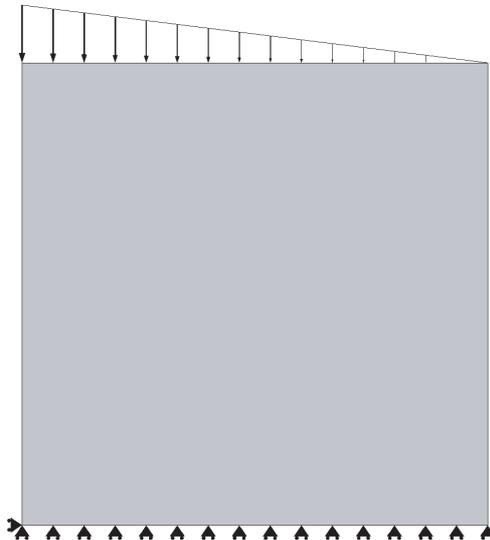


Figure 1: Geometry, loading and boundary conditions for the test problem

This problem is solved for $q = 3$ using a discretization of 120×120 elements. To avoid checkerboards and mesh dependency we have used filtering of gradients as suggested by Sigmund, see [4]. The filter function has a radius that corresponds to the width of three elements. As updating formulas for the density we have used both the Euler formula (11) and the optimality criteria formula (13). From an ODE point of view these formulas represent different differential equations, i.e., different evolutions, but they have the same stationary points, i.e., the same local minima are defined. Starting from the same uniform initial distribution of $\boldsymbol{\rho}$ it turns out that the two formulas converge towards different local minima. These local minima, together with iteration histories, are shown in Figures 2 and 3.

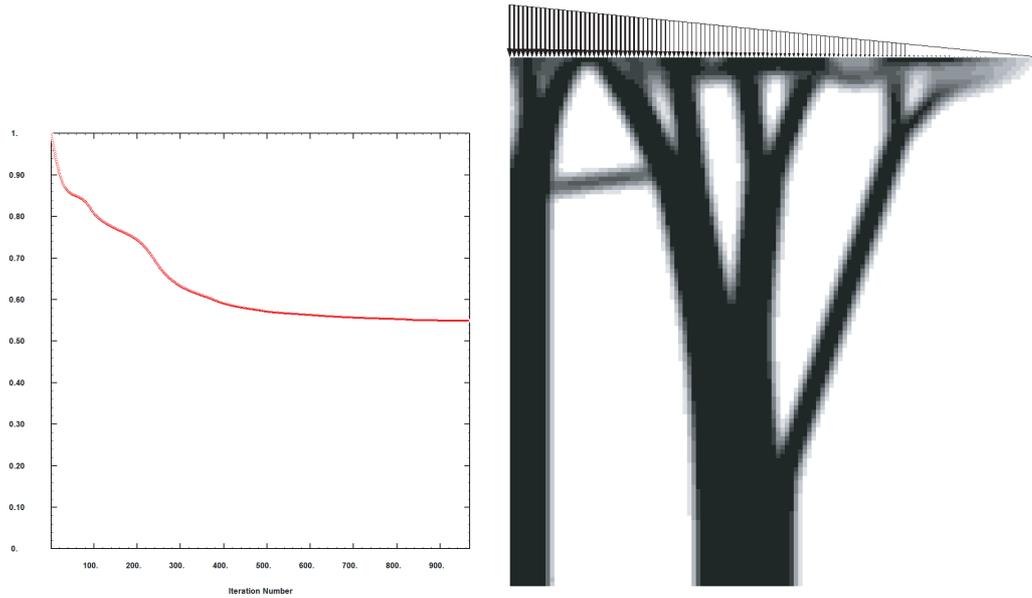


Figure 2: Solution and iteration history obtained by Euler's method, Eq. (11), $q = 3$, 120×120 elements, filter radius corresponds to 3 elements.

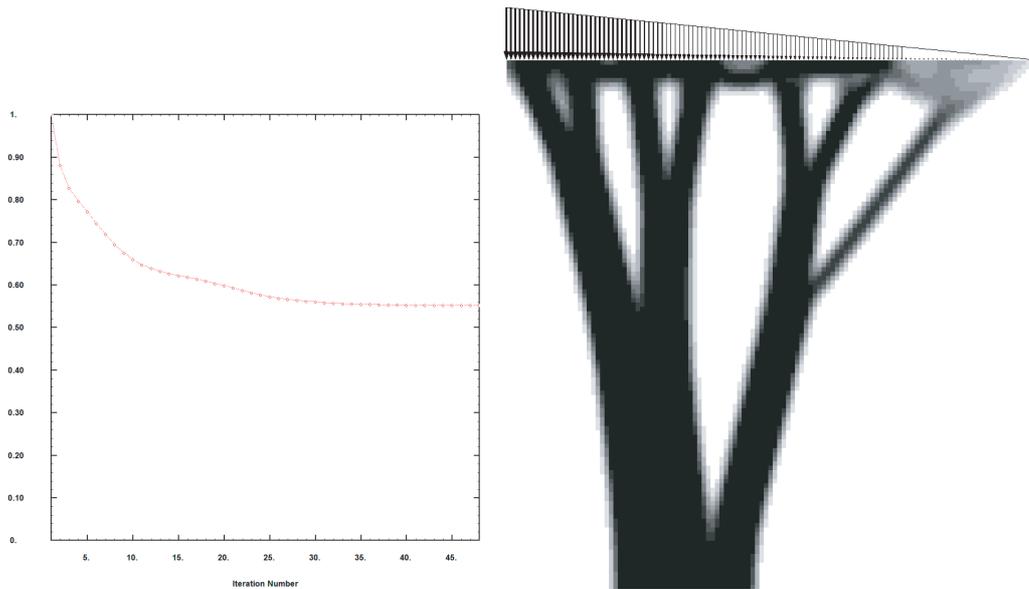


Figure 3: Solution and iteration history obtained by optimality criteria method, Eq. (13), $q = 3$, 120×120 elements, filter radius corresponds to 3 elements.

The two solutions in these figures have objective function values that are equal in the first three digits, with the one based on the optimality criteria method being slightly better. The values $k = \lambda \Delta t$ and $\beta = \lambda_3 \Delta t$, respectively, are chosen as high as possible, avoiding oscillating and non-convergent behavior. It then turns out that much fewer iterations were needed in the optimality criteria method than in the Euler method. It may be noted that in papers [8, 9, 12] Euler like methods are applied, and in all cases separate “legs” as in Figure 2 are developed.

6. References

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