Applications of topology optimization in the design of micro- and nanofluidic systems

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ABSTRACT

We present a versatile high-level programming language implementation of nonlinear topology optimization. Using this method in designing microfluidic systems may result in significant improvements in efficiency by a complete change in the geometry of the micro-channel networks used. Our implementation is based on the commercial software package Femlab. The method is general since most problems that can be formulated in the simple divergence form can be optimized, where a wide range of optimization objectives can be dealt with easily. We test the method by studying a simple steady-state Navier–Stokes flow problem. The level of complexity is then increased by optimizing micro-cooling systems with potential applications in e.g. CPU-cooling or micro heat-exchangers.

Keywords: microfluidics, topology optimization, nonlinear systems, micro-cooling

1 INTRODUCTION

The material distribution method in topology optimization was originally developed for stiffness design of mechanical structures [2] but has now been extended to a multitude of design problems in structural mechanics as well as to optics and acoustics [3]. Recently Borrvall and Petersson introduced the method for fluids in Stokes flow [1], which has now been extended to full Navier–Stokes flow by the work of Sigmund and Gersborg-Hansen [4], [5] and Olesen, Okkels and Bruus [6].

Here we use our recent versatile high-level programming-language implementation of nonlinear topology optimization for design of microsystems. Our implementation is based on the commercial finite-element package Femlab both for the solution of the flow problem and for the sensitivity analysis required by the optimization algorithm. This approach is useful for multi-field problems, where the flow problem is coupled to, e.g., heat conduction.

2 TOPOLOGY OPTIMIZATION FOR NAVIER–STOKES FLOW

We first illustrate our high-level programming-language implementation by studying a full steady-state Navier–Stokes flow problem for incompressible fluids.

Consider a given computational domain $\Omega$ with appropriate boundary conditions for the flow given on the domain boundary $\partial \Omega$. The goal of the optimization is to distribute a certain amount of solid material inside $\Omega$ such that the material layout defines a fluidic device or channel network that is optimal with respect to some objective, formulated as a function of the variables, e.g. minimization a velocity-component at a given point inside the domain.

The basic principle in the material distribution method for topology optimization is to replace the original discrete design problem with a continuous one where the material density is allowed to vary continuously between solid and void. Thus in our flow problem we assume the design domain to be filled with some idealized porous material of spatially varying permeability. Solid wall and open channels then correspond to the limits of very low and very high permeability, respectively. In the final design there should preferably be no regions at intermediate permeability since otherwise it cannot be interpreted as a solution to the original discrete problem.

2.1 Governing equations for flow in idealized porous media

We assume that the fluid flowing in the idealized porous medium is subject to a friction force $f$ which is proportional to the fluid velocity $v$, c.f. Darcy’s law. Thus $f = -\alpha v$, where $\alpha(\mathbf{r})$ is the inverse of the local permeability of the medium at position $\mathbf{r}$.

The flow problem is described in terms of the fluid velocity field $v(\mathbf{r})$ and pressure $p(\mathbf{r})$. The governing equations are the steady state Navier–Stokes equation and the incompressibility constraint

\begin{align}
\rho(\mathbf{v} \cdot \nabla)v & = \mathbf{\nabla} \cdot \sigma - \alpha \mathbf{v}, \\
\mathbf{\nabla} \cdot \mathbf{v} & = 0,
\end{align}

where $\rho$ is the mass density of the fluid. For an incompressible Newtonian fluid the components $\sigma_{ij}$ of the
Cauchy stress tensor $\sigma$ are given by

$$\sigma_{ij} = -p \delta_{ij} + \eta \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right),$$

where $\eta$ is the dynamic viscosity. The formalism is valid in three dimensions, but for simplicity we shall consider only two-dimensional problems, i.e., we assume translational invariance in the third dimension and set $r = (x_1, x_2)$ and $v = (v_1(r), v_2(r))$. The boundary conditions will typically be either Dirichlet type specifying the velocity field $v$ on the boundary or Neumann type specifying the external forces $\mathbf{n} \cdot \sigma$.

It is convenient to introduce a design variable field $\gamma(r)$ controlling the local permeability of the medium. We let $\gamma$ vary between zero and unity, with $\gamma = 0$ corresponding to solid material and $\gamma = 1$ to no material. Following Ref. [1] we then relate the local inverse permeability $\alpha(r)$ to the design field $\gamma(r)$ by the convex interpolation

$$\alpha(\gamma) \equiv \alpha_{\text{min}} + (\alpha_{\text{max}} - \alpha_{\text{min}}) \frac{q[1 - \gamma]}{q + \gamma},$$

where $q$ is a real and positive parameter used to tune the shape of $\alpha(\gamma)$. Ideally, impermeable solid walls would be obtained with $\alpha_{\text{max}} = \infty$, but for numerical reasons we need to choose a large but finite value for $\alpha_{\text{max}}$. For the minimal value we choose $\alpha_{\text{min}} = 0$.

For a given material distribution $\gamma(r)$ there are two dimensionless numbers characterizing the flow:

$$Re = \frac{\rho \ell v}{\eta}, \quad Da = \frac{\eta}{\alpha_{\text{max}} \ell^2}.$$  

The Reynolds number $Re$ describes the ratio between inertia and viscous forces, and the Darcy number $Da$ the ratio between viscous and porous friction forces. Here $\ell$ is a characteristic length scale of the system and $v$ a characteristic velocity.

### 2.2 The Optimization Problem

For a given material distribution we solve the Navier–Stokes flow problem using the commercial finite element software Femlab. Femlab provides both a graphical front-end and a library of high-level scripting tools based on the MATLAB programming language, and it allows the user to solve a wide range of physical problems by simply typing in the strong form of the governing equations as text expressions.

In order to find an optimal solution for the problem, a design objective must be defined, which is stated as the minimization of a certain objective function $\Phi(u, \gamma)$, where $u = [v_1, v_2, p]$ is the vector of all field variables of the problem. Often different constraints on the material distribution follow naturally, e.g., mass/volume constraints, or they have to be imposed in order to prevent trivial solutions like a completely full or empty design region.

The solution is optimized using the following iterative procedure: Given a guess $\gamma^{(k)}$ for the optimal material distribution we first solve physical problem $(\mathbf{u}^{(k)})$ using Femlab. Next a sensitivity analysis is performed where the gradient of the objective with respect to $\gamma (\partial \Phi / \partial \gamma)$ is evaluated by solving a related adjoint problem, also using Femlab. Finally we use the Method of Moving Asymptotes (MMA)[7] to obtain a new guess $\gamma^{(k+1)}$ for the optimal design based on the gradient information and the past iteration history. Details on the method is given in [6].

### 3 NUMERICAL EXAMPLES

Typically we have around 6000 elements in the mesh, corresponding to 30000 degrees-of-freedom. The constrained optimization problem is solved using MMA [7], and the design iterations are stopped when the maximal change in the design field is $\|\gamma^{(k+1)} - \gamma^{(k)}\|_\infty \leq 0.01$, at which point we typically have $|\Phi^{(k+1)} - \Phi^{(k)}| < 10^{-5}$.

#### 3.1 A channel with reverse flow

Our first numerical example deals with the design of a structure that at a particular point inside a long straight channel can guide the flow in the opposite direction of the given applied pressure drop. The example illustrates the importance of the choice of permeability for the porous medium.

The computational domain is shown in Fig. 1. It consists of a long straight channel of height $\ell$ and length $L = 10\ell$; the actual design domain, inside which the porous material is distributed, is limited to the central part of length $5\ell$. The boundary conditions prescribe a pressure drop of $\Delta p$ across the system, and the design objective is to reverse the flow direction at the point $r^*$ at center of the channel.
For increasing Darcy number the $S$-turn topology will cease to be optimal simply because the porous material becomes too permeable to make reversal of the flow direction possible. This is the case for the optimization at $Da = 10^{-2}$, as seen in Fig. 2(b). As a result the design domain is almost completely filled with porous material blocking the flow through the channel. Only immediately above and below the point $r^*$ we see two empty regions emerging which act to short-circuit the pressure and guide the flow away from $r^*$.

In summary, our first example has demonstrated that the implementation of topology optimization works, but that the optimal design and performance may depend strongly on the choice of the Darcy number.

### 3.2 Micro-cooling and heat-exchange

The complexity of the optimization problem is now increased by adding a steady-state temperature field $T(r)$ which is conducted through the liquid and convected by the flow-field following the equation

$$\rho C_p (v \cdot \nabla) T = k \nabla^2 T + Q,$$

where $C_p$ is the heat capacity, $k$ the heat conductivity, and $Q(r)$ a heat source.

In Fig. 3 we show an optimized microfluidic cooling system consisting of an inner and outer square (together denoted the design region) as well as inlet and outlet, see panel (a). A uniform heat-flux $Q$ is generated in the inner square, which then has to be cooled by the flow of a cooling liquid, entering through the vertical inlet in the bottom and leaves through the horizontal outlet in the top. Given a constant pressure drop between the inlet and outlet, our objective is to minimize the average temperature of the inner square by designing a fluidic network for the cooling liquid in the design region.

The design parameter $\gamma$ is shown in panel (a) together with a description of the system. The flow-speed of the cooling liquid flowing from the inlet and to the outlet at right is shown in panel (b), where dark is high speed while white is zero. The inlet/outlet have the highest flow-speed which is reduced in the finer network channels. The temperature field is shown in panel (c), where the cold liquid (white) is lead in from below and is gradually heated (darkening) during the passage. The influence of the cooling channel-network is clearly visible in temperature-field of the heating-region.

### 4 DISCUSSION

We have presented how topology optimization can be used to design microfluidic systems. The main advantages of the method is that it does not require any a priori knowledge of the channel geometry, and that the obtained design can directly be imported into lithographic CAD/CAM-systems for device fabrication. Moreover,
the method can in principle be applied to optimize a large class of lab-on-a-chip systems.

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REFERENCES


Figure 3: (a) The design parameter $\gamma$ (black) together with a description of the system. (b) The flow-speed of the cooling liquid. (c) The temperature field where the inlet is cold (white)