A semi-deterministic optimization method: multi-level shooting algorithm

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2 AUTHORS, INCLUDING:

Benjamin Ivorra
Complutense University of Madrid

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By Ivorra Benjamin, Mohammadi Bijan

Optimization method

Most deterministic algorithms which perform the minimization of a function $J : \Omega \mapsto \mathbb{R}$ can be seen as discretizations of the following dynamical system :

$$\begin{cases} M(\zeta)x_\zeta = -d(x(\zeta)) \\ x(\zeta = 0) = x_0 \end{cases} \quad (1)$$

For example if $d = \nabla J$ and $M = Id$, we recover the classical steepest descent method.

We make here the following assumptions on J : $J \in C^1(\Omega, \mathbb{R})$, is coercive (i.e. $J(x) \to \infty$ when $|x| \to \infty$) and the infimum J_m is known. The problem is also admissible, that is the infimum is reached inside the admissible domain: $\exists x_m \in \Omega, s.t. J(x_m) = J_m$

We consider that system (1) has a solution if for a given $x_0 \in \Omega$, we can find a finite Z_{x_0} such that $J(x(Z_{x_0})) = J_m$:

$$\begin{cases} M(\zeta)x_\zeta = -d(x(\zeta)) \\ x(0) = x_0 \\ J(x(Z_{x_0})) = J_m \end{cases} \quad (2)$$

This is an over-determined boundary value problem (BVP) which can be solved using classical techniques for BVPs (e.g. shooting, finite differences,...). This over determination can be removed, for instance, by considering $x_0 = v$ for (1) as a new variable to be found by the minimization of $h(v) = J(x_v(Z_v)) - J_m$, where $x_v(Z_v)$ is the solution of (1) found at $\zeta = Z_v$ starting from v.

The algorithm $A_1(v_1, v_2)$ reads:

- *(v_1, v_2) given,*
- *Find $v \in argmin_{w \in \mathcal{O}(v_2)} h(w)$ where $h(w) = J(x_w(Z_w)) - J_m$, with $x_w(Z_w)$ solution of system (1) found at $\zeta = Z_w$ starting from w, and $\mathcal{O}(v_2) = \{t\overrightarrow{v_1 v_2}, t \in \mathbb{R}\} \cap \Omega$.*
- *return v*

The line search minimization might fail. For instance, a secant method degenerates on plateaus and critical points. In that case, we add an external level to the algorithm A_1, keeping v_1 unchanged, and looking for v_2 by minimizing a new functional h^2 defined by $h^2(v_2^2) = \min_{v_2^2} h(v_2^2)$ by algorithm $A_1(v_1, v_2^2)$.

This leads to the following two-level semi-deterministic algorithm (SDA) $A_2(v_1, v_2^2)$:

- *(v_1, v_2^2) given,*
- *Find $v_2 \in argmin_{w \in \mathcal{O}(v_2^2)} h^2(w)$ where $h^2(w) = h(A_1(v_1, w))$ and $\mathcal{O}(v_2^2) = \{t\overrightarrow{v_1 v_2^2}, t \in \mathbb{R}\} \cap \Omega$.*
- *return v_2*

The choice of initial conditions in this algorithm contains the non-deterministic feature of the algorithm. The construction can be pursued building recursively $h^i(v_2^i) = \min_{v_2^i} h^{i-1}(v_2^i)$ using $A_{i-1}(v_1, v_2^i)$, with $h^1(v) = h(v)$ where i denotes the external level.

In practice, if J_m is unknown, we set $J_m = -\infty$ and look for the best solution for a given complexity and computational effort. This is the approach adopted here where we predefine the effort we would like to make in each level of the algorithm .

Applications

The previous method is used to solve three complex industrial problems:

- **Shape optimization of a Fast-Microfluidic-Mixer:**

  We focus on the shape optimization of a pressure driven microfluidic mixer designed for fast mixing of protein solutions (See Figure 1). To improve the efficiency of the device based on the reduction of the mixing time (i.e time for which the center inlet solution concentration in the mixing region is go from 90% to 30%) we would like to modify the shape of the channel at given functioning conditions (i.e. given side and central injection velocities). For the device to be realizable we need to control both the maximum curvature of the shape and minimum thickness of the channel. To control the curvature we introduce a CAD-based parameterization using segments and cubic splines. Only half the mixer was simulated, since it is symmetric. This parameterization is suitable and permits to reach non-intuitive shapes (see Figure 2). Optimization has led to a reduction by a factor of 8 of the mixing time (see Figure 3).

- **Design of multichannel filters based on optical fibers:**

  We focus on the realization of particular designs corresponding to multichannel filters that consist of 16 totally reflective identical channels spaced by 100 GHz. The efficiency of the SDA is compared with a classical design method based on a Sinus cardinal (Sinc) fiber core apodization (equivalents to refractive index modulation) profile. SDA has led to better solutions in terms of reflection characteristics than the Sinc profile (see Figure 4), parasite side peaks are diminished. In addition, the SDA-optimized apodization profile (see Figure 5) is also more suitable for industrial realization as the number of necessary π-phase shifts (or equivalently sign changes in the profile), that requiring to master the writing process, is reduced. Moreover, the index modulation is more homogeneously distributed along the pattern, does not exhibit any predominant lobe and the maximum amplitude of the profile which has been reduced.

- **Temperature and pollution control in bunsen flames:**

  We focus on a simple bunsen laminar flame . We concentrate on the reduction of the thermal N_O. This is the major source in formation of N_O in a bunsen flame. We also study the control of temperature distribution in flames which is of importance in combustion engine design. This permits also to use the link between thermal N_O and temperature to give recommendations on the design of burners and thermal engine concerning environmental issues. The N_O flux (through a surface Γ inside the flame) has been reduced (see Figure 6). Furthermore the maximal temperature value has been controlled (see Figure 7).

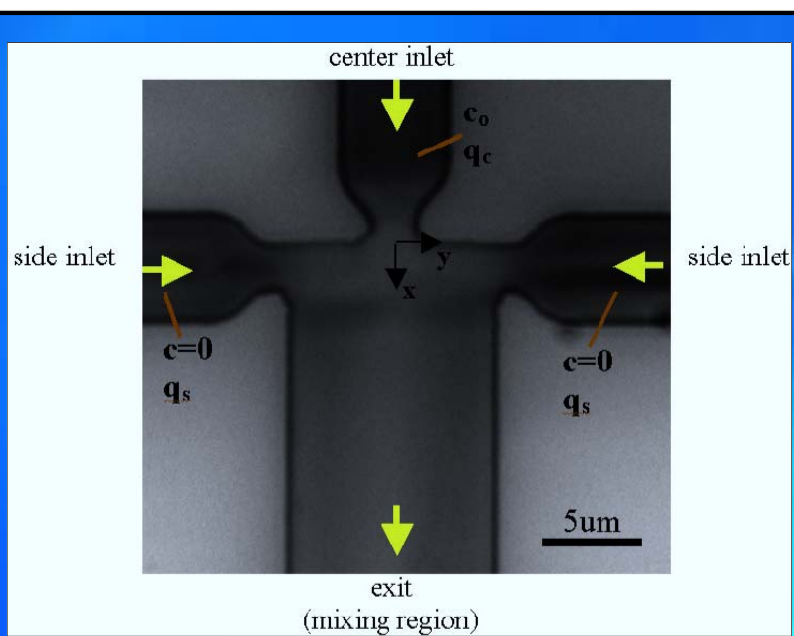

Fig.1 Typical microfluidic mixer geometry.

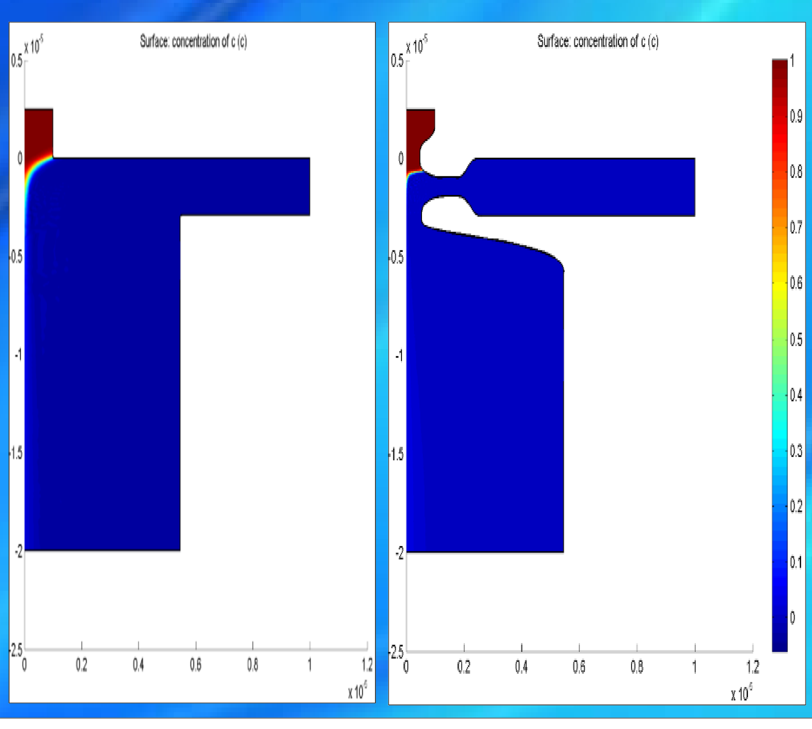

Fig.2 -Left: Initial shape and its impact on the transport.
-Right: Optimized shape and its impact on the transport.

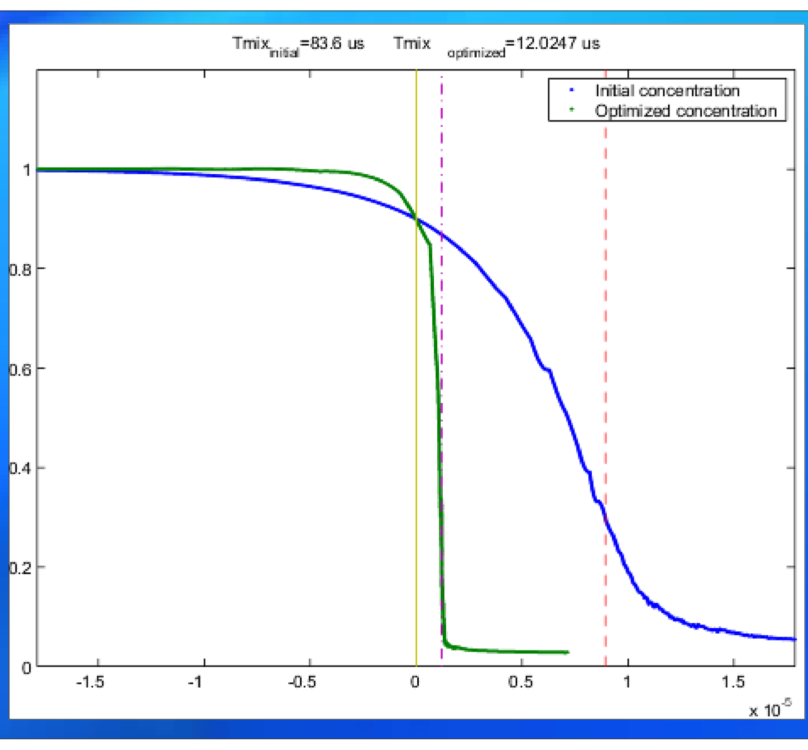

Fig.3 Center inlet solution concentration evolution vs. Time for the initial and optimized shapes.

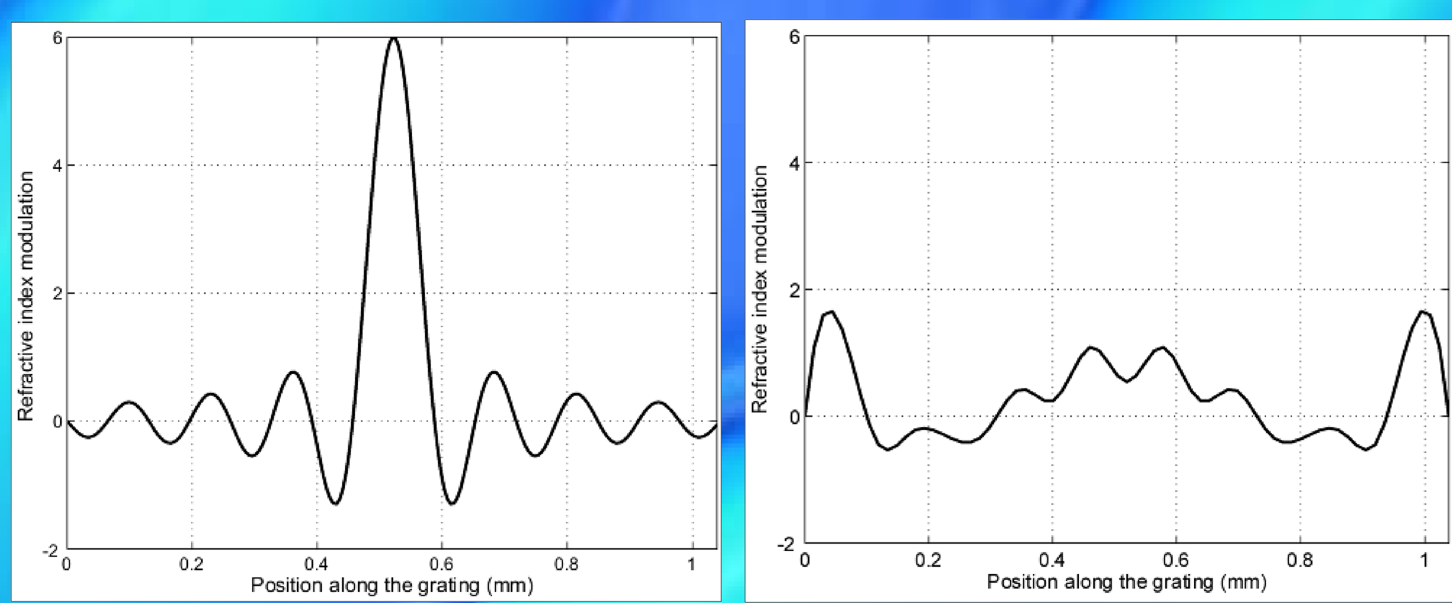

Fig.4 -Left: Apodization profile of the Sinc-based design.
-Right: Apodization profile of the optimized design.

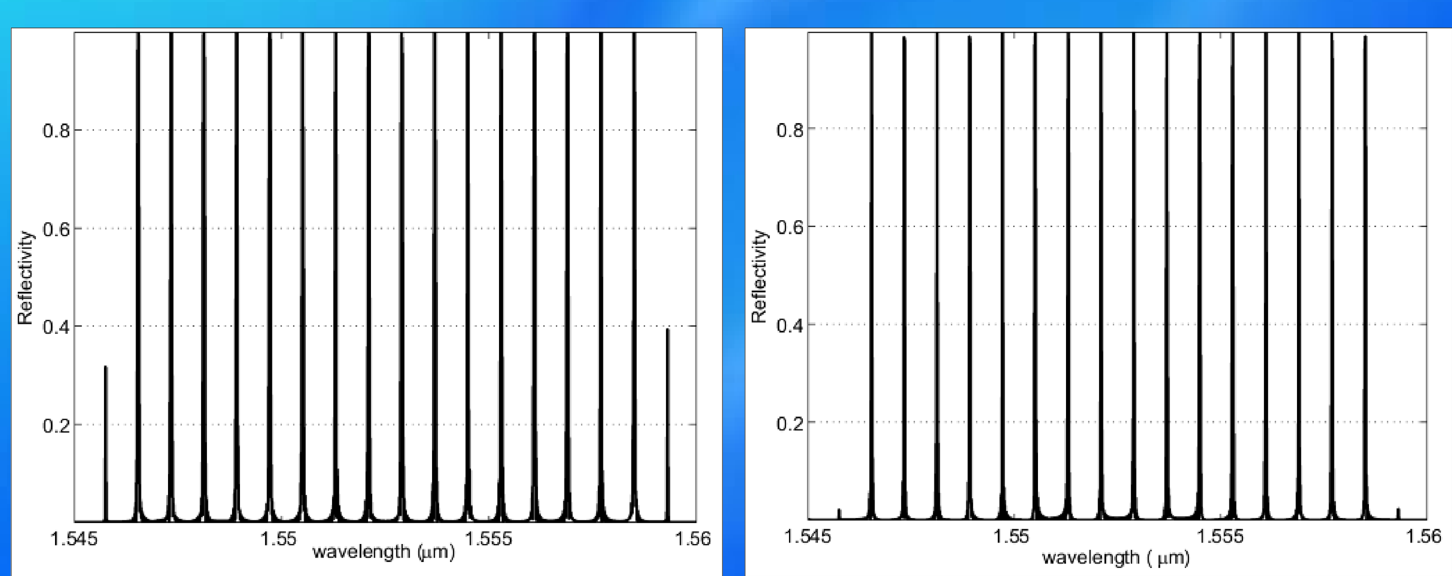

Fig.5 -Left: Linear reflectivity obtained with the sinc-based design.
-Right: Linear reflectivity obtained with the optimized design.

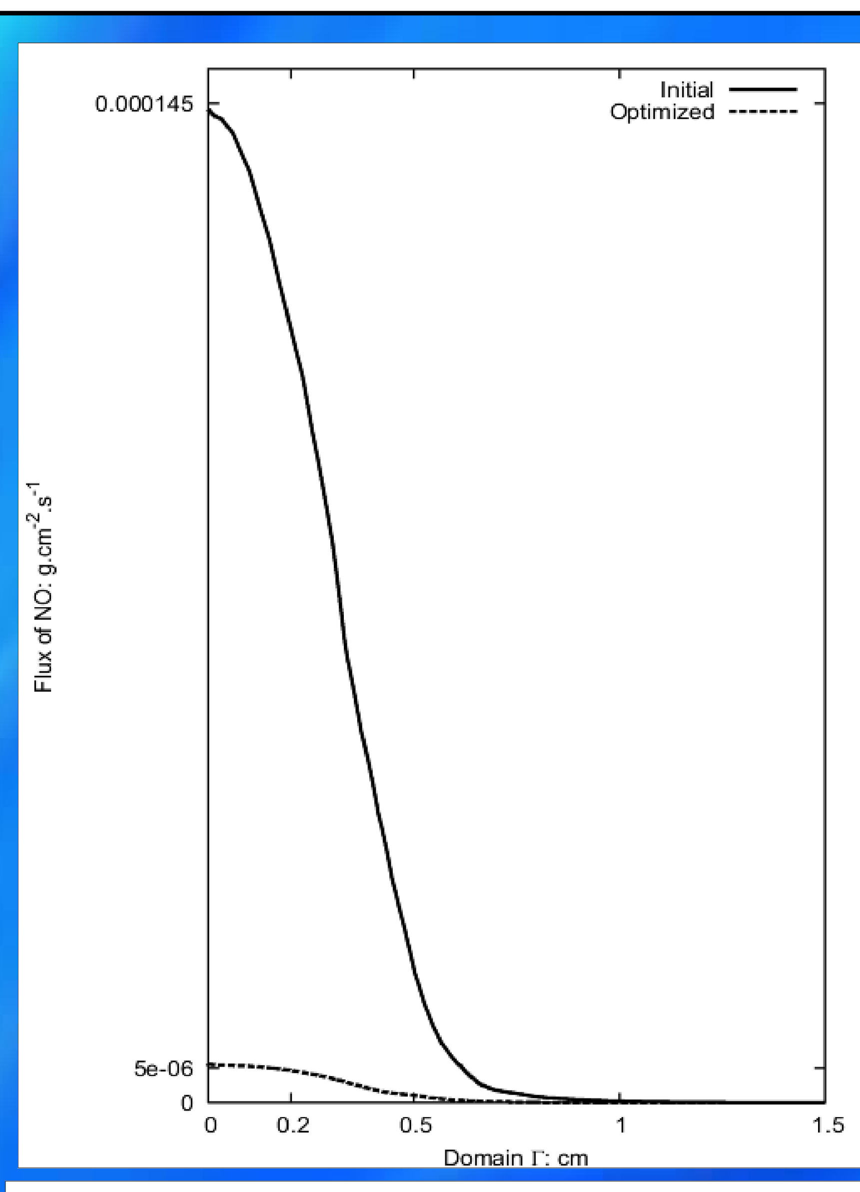

Fig.6 *No* Flux through the surface Γ before and after optimization.

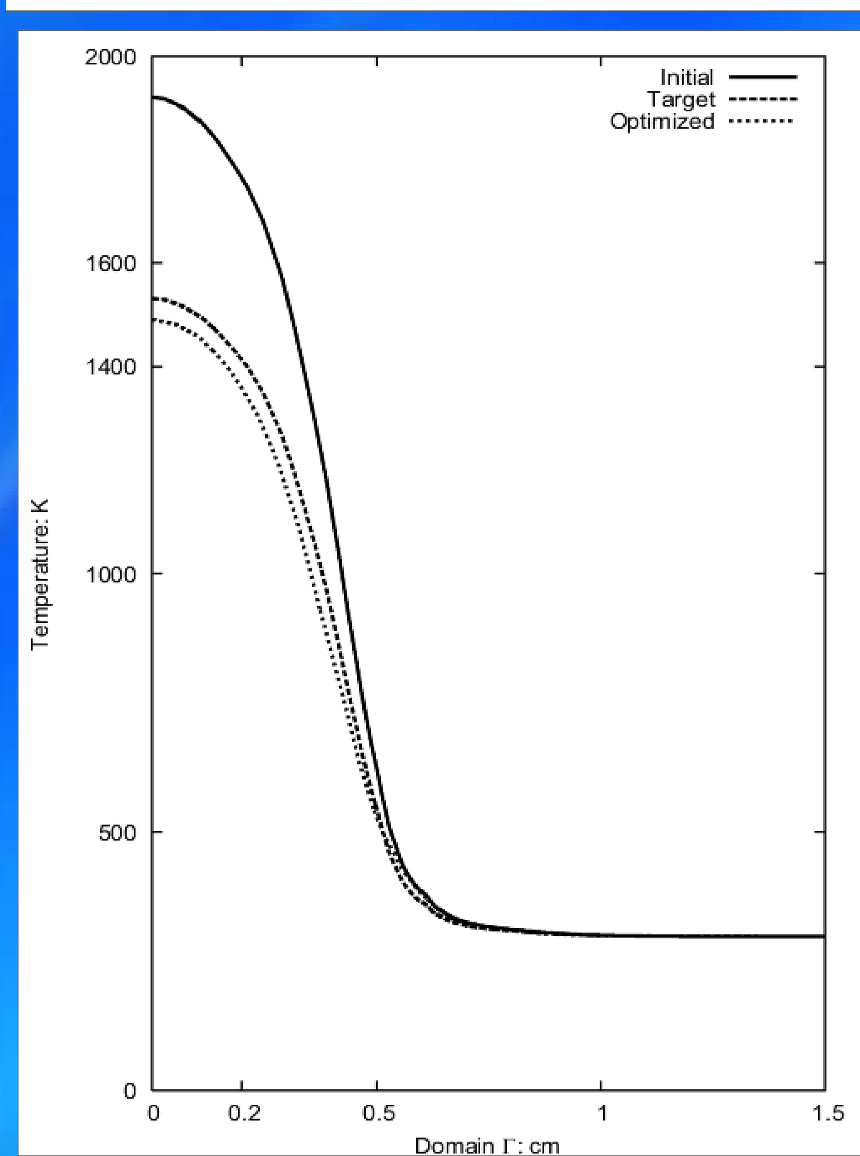

Fig.7 Initial, target and optimized tempera-

This work has been performed in partnership with :