České vysoké učení technické v Praze
Fakulta jaderná a fyzikálně inženýrská

Hledání optimálního tvaru stěn matematického modelu proudění krve v problematice úplného kavopulmonálního cévního napojení

Optimal shape design of walls of blood flow mathematical model focusing on the total cavopulmonary connection

Master thesis

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Consultant: **MUDr. Mgr. Radomír Chabiniok, Ph.D.**

Academic year: 2024/2025

ZADÁNÍ DIPLOMOVÉ PRÁCE

I. OSOBNÍ A STUDIJNÍ ÚDAJE

Příjmení: **Bureš** Jméno: **Jan** Osobní číslo: **494688**

Fakulta/ústav: **Fakulta jaderná a fyzikálně inženýrská**

Zadávající katedra/ústav: **Katedra matematiky**

Studijní program: **Matematické inženýrství**

II. ÚDAJE K DIPLOMOVÉ PRÁCI

Název diplomové práce:

Optimální tvar stěn idealizovaného úplného kavopulmonálního spojení.

Název diplomové práce anglicky:

Optimal wall geometry of an idealized total cavopulmonary connection.

Pokyny pro vypracování:

1. S použitím dostupné literatury a konzultací s odborníky sestavte matematický model cévního proudění v problematice úplného kavopulmonálního spojení (TCPC) založený na mřížkové Boltzmannově metodě (LBM) a navrhněte vhodně parametrizovanou testovací úlohu, která aproximuje charakteristiky a funkčnost systému TCPC.
2. Formulujte optimalizační úlohu zaměřenou na hledání optimálního tvaru stěn s využitím parametricky popsané geometrie testovací úlohy z bodu 1. Pokuste se navrhnout vhodnou účelovou funkci použitelnou v rámci studované problematiky.
3. Proveďte rešerši optimalizačních metod vhodných pro řešení problémů charakterizovaných zvýšenou časovou náročností potřebnou pro vyhodnocení účelové funkce.
4. Pro simulaci proudění vhodně upravte výpočetní kód LBM vyvíjený na KM FJFI ČVUT v Praze. Navrhněte a implementujte obecný optimalizační rámec, jehož součástí bude výpočetní kód LBM. Využijte volně dostupný software nebo sám implementujte vybrané metody matematické optimalizace z bodu 3.
5. Aplikujte metody matematické optimalizace k hledání optimálního řešení pro uvažovanou optimalizační úlohu z bodu 2. Diskutujte získané výsledky a výpočetní náročnost jejich získání.

Seznam doporučené literatury:

[1] T. Krüger, et al., The lattice Boltzmann method: Principles and Practice. Springer International Publishing, 2017.
[2] Z. Guo, S. Chang, Lattice Boltzmann method and its application in engineering. World Scientific, 2013.
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Jméno a pracoviště vedoucí(ho) diplomové práce:

doc. Ing. Radek Fučík, Ph.D. katedra matematiky FJFI

Jméno a pracoviště druhé(ho) vedoucí(ho) nebo konzultanta(ky) diplomové práce:

Mudr. Mgr. Radomír Chabiniok, Ph.D. University of Texas Southwestern Medical Center, USA

Datum zadání diplomové práce: **31.10.2023** Termín odevzdání diplomové práce: **10.05.2024**

Platnost zadání diplomové práce: **31.10.2025**

doc. Ing. Radek Fučík, Ph.D. podpis vedoucí(ho) práce	prof. Ing. Zuzana Masáková, Ph.D. podpis vedoucí(ho) ústavu/katedry	doc. Ing. Václav Čuba, Ph.D. podpis děkana(ky)

III. PŘEVZETÍ ZADÁNÍ

Diplomant bere na vědomí, že je povinen vypracovat diplomovou práci samostatně, bez cizí pomoci, s výjimkou poskytnutých konzultací.
Seznam použité literatury, jiných pramenů a jmen konzultantů je třeba uvést v diplomové práci.

.	
Datum převzetí zadání	**Podpis studenta**

Acknowledgment:
I would like to thank my supervisor doc. Ing. Radek Fučík, Ph.D. for his immense care, willingness, patience, and professional background in conducting this work. I would also like to thank my expert consultant Ing. Pavel Eichler, Ph.D. for his advice, valuable comments, and above all, for his interest in the topic. Last but not least, my thanks go to MUDr. Mgr. Radomír Chabiniok, Ph.D. for his expert comments on the medical issues of this thesis.

Author's declaration:
I declare that this thesis is entirely my own work and I have listed all the used sources in the bibliography.

Prague, January 2, 2025 Jan Bureš

Kapitola 1

Mathematical optimization

1.1 Black-box Optimization

In practice, it is common to encounter cases where it is necessary to optimize an objective function f, the analytical form of which, as well as the formula for calculating its derivative, is unknown. This problem is typical, for instance, in the results of numerical simulations, where we can only evaluate the objective function at specific points and thus obtain the desired function value. Additionally, in practice, evaluating the function at a point may itself be problematic and can be, for example, very time-consuming or computationally expensive. Clearly, the standard optimization algorithms mentioned earlier are not suitable for solving problems of this nature.

The discipline that deals with problems where the objective function (or constraints) is given by a so-called black-box[1], is called black-box optimization (hereafter referred to as BBO). In BBO, it is typically not assumed that the objective function is continuous or differentiable [5, 6, 7].

It is worth noting that in the literature, black-box optimization is often confused with derivative-free optimization (DFO), which encompasses methods and techniques for objective functions whose derivatives are unknown or difficult to compute [5, 6, 8]. These two disciplines share many common characteristics, but they differ primarily in that, within DFO, the formula for calculating the derivative of the objective function may still be known. Furthermore, BBO includes heuristic methods, whereas DFO focuses mainly on methods that can be reliably analyzed mathematically in terms of convergence and stopping criteria, which is often not possible for BBO methods [5]. Therefore, although the terms BBO and DFO are often used interchangeably, in this work, we will treat them as two distinct disciplines [5].

Additionally, it should be noted that various classifications of methods within BBO can be found in the literature. In this work, we will adhere to the classification presented in [5], distinguishing between heuristic methods, direct search methods, and methods based on surrogate models. Each of these classes will be briefly described in this section.

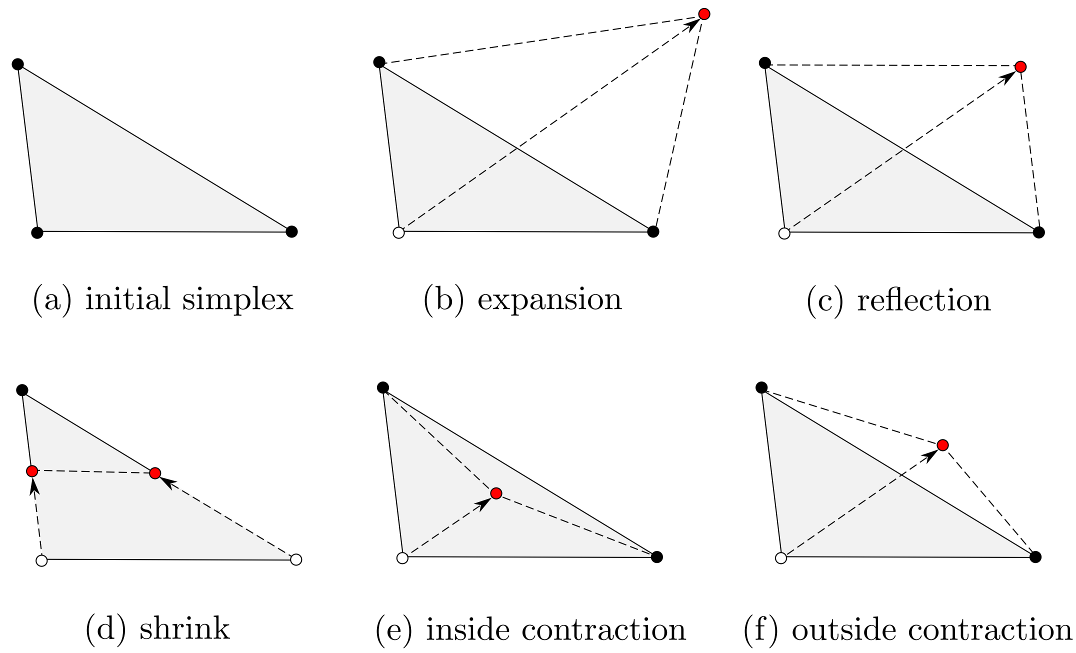
1.1.1 Heuristic Methods

Heuristic optimization methods often rely on different predefined rules or even trial and error when seeking the solution of an optimization problem. These methods usually do not guarantee optimal solutions, but they are often effective for finding near-optimal results in a reasonable amount of time. Heuristic methods include genetic algorithms, detailed in [5], along with various other heuristic approaches.

[1] In programming, a black-box refers to a system whose internal mechanisms are unknown to the user. This means that the user generally has access only to the system's input and output [5].

In this section, however, we will focus on a different widely used heuristic method, the Nelder-Mead method, also known as the simplex method[2][3] [10].

The Nelder-Mead method finds a solution to an optimization problem by iteratively constructing simplexes. The process begins by initializing a starting simplex. The objective function is then evaluated at each vertex of this simplex. In each subsequent iteration, the simplex is transformed in order to move closer to the position of the sought stationary point of the objective function. The transformation of the simplex involves manipulating its points using predefined operations – expansion, reflection, contraction (inner and outer), and shrinking, which are schematically illustrated in Figure 1.1.



Obrázek 1.1: A schematic representation of the operations used to transform simplexes in the Nelder-Mead method. The vertices generated by applying each operation are shown in red. For clarity, the operations are depicted in $\mathbb{R}^2$.

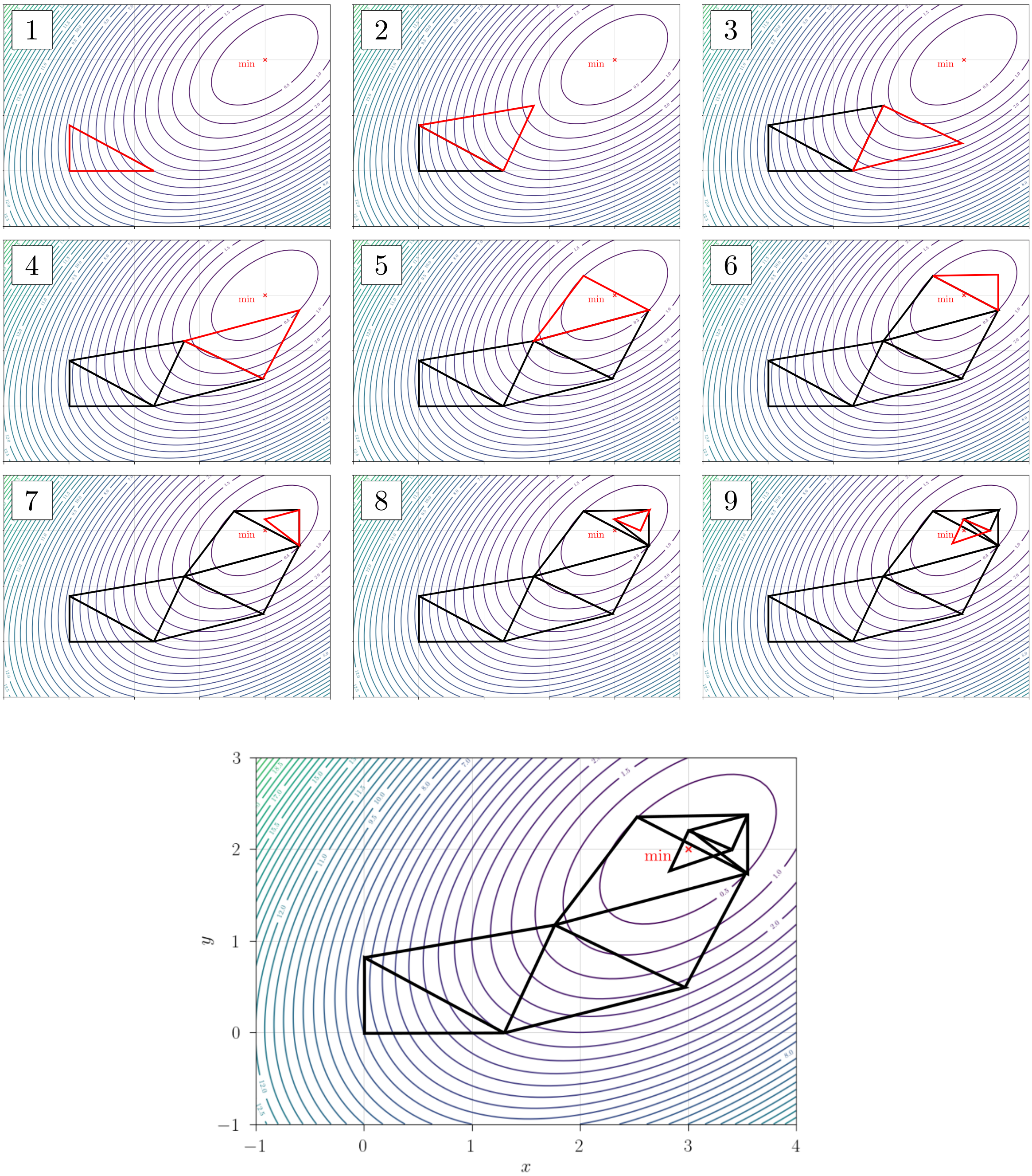
The transformations performed during each iteration are determined by comparing the function values at the vertices of the simplex. The newly formed simplex shares either exactly one vertex or exactly n vertices with the simplex from the preceding iteration. The algorithm continues to iteratively transform the simplex until a stopping condition (specified by the user) is met [5]. Details of the Nelder-Mead method, including the algorithm's description and the choice of stopping condition, are discussed in [5, 6, 10].

[2] A simplex in $\mathbb{R}^n$ is defined as a bounded convex polytope (a generalization of a polyhedron to any dimension) with a non-empty interior and exactly $n + 1$ vertices [5].

[3] The term "simplex method"more commonly refers to the algorithm used to find the optimal solution in linear programming. This algorithm was developed by George Dantzig [9].

1. **Initialise** the transformation parameters:
   - δ^{exp},
   - δ^{out},
   - δ^{ins},
   - δ^{shrink},
   - $k_{\text{iter}} = 0$
2. **Cyklus** končící splněním podmínky ukončení, která je zadána uživatelem.
   (a) **Šíření** (anglicky *streaming*) postkolizních distribučních funkcí f_k^* v příslušných směrech $\boldsymbol{\xi_k}$.
   (b) **Výpočet makroskopických veličin** pomocí vztahů (**??**).
   (c) **Kolize** (anglicky *collision*), kdy dochází k výpočtu postkolizního stavu distribuční funkce pomocí (**??**) a **vyřešení okrajových podmínek** diskutovaných v sekci **??**.
3. **Konec algoritmu.**

The heuristic nature of the Nelder-Mead method stems from the fact that its principle is based on a somewhat random search of the space using predefined rules. Several iterations of space exploration using simplexes, for a specific choice of initial simplex and a specific function, are shown in Figure 1.2. While the convergence of this method has been proven, it is not guaranteed that the method will always converge to a stationary point [5]. It should be noted that the Nelder-Mead method was primarily developed for unconstrained optimization problems, but it can be adapted for constrained optimization problems using the techniques described in section **??**.



Obrázek 1.2: Several iterations of the Nelder-Mead method for a specific choice of the initial simplex when minimizing the function $x^2 - 4x + y^2 - y - xy + 7$, with the minimum at the point (3,2) marked by a red cross.

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[1] R. Fletcher and M. J. D. Powell. A rapidly convergent descent method for minimization. *The Computer Journal*, 6(2):163–168, August 1963.

[2] C. G. BROYDEN. The convergence of a class of double-rank minimization algorithms. *IMA Journal of Applied Mathematics*, 6(3):222–231, 1970.

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[14] C. Audet, S. Le Digabel, V. Rochon Montplaisir, and C. Tribes. Algorithm 1027: NOMAD version 4: Nonlinear optimization with the MADS algorithm. *ACM Transactions on Mathematical Software*, 48(3):35:1–35:22, 2022.