

Finite Element Method Simulations of Composite Materials

Abner J. Ortiz, Greichaly Cabrera
Department of Mathematics
University of Puerto Rico at Humacao
Humacao, PR 00791-4300

Faculty Advisor: Pablo V. Negrón-Marrero

Abstract

A *composite* material consists of a mixture of a base material called the *matrix*, with grains of other materials called the *inclusions*. These materials are very common in engineering applications like the construction industry. Composite materials have also been used for the production of capacitors with different military applications, yet the role of the composite in the efficiency of such device is not well understood. Modeling composite materials is difficult due to the random nature of such mixtures. However if some controls are established during the production process, it is reasonable to assume homogeneity and isotropy. Models for composite materials have been proposed in the literature, for example by Hill (1972), and can be either random or periodic. The main goal of the present work is to study numerical methods based on the finite element method to determine the mechanical properties of periodic composite materials. We present some preliminary computations for a model of a composite material based on the equations of nonlinear elasticity. The constitutive equations that we used are those usually employed to model rubbery materials. We study a composite of two materials: a matrix with inclusions of a given (nonlinear) material, and determine numerically how the stress distribution depends on the different constitutive and geometric parameters.

Keywords: Composite Materials, Finite Element Method, Elasticity

1. Introduction:

A *composite material* consists of a mixture of a base material called the *matrix*, with grains of other materials called the *inclusions*. These materials are very common in engineering applications like the construction industry. Composite materials have also been used for the production of capacitors with different type of military applications. The mathematical modeling of composite materials is difficult due to the random nature of such mixtures. If some controls are established during the production process, the resulting mixtures are essentially homogeneous and isotropic in the sense that their mechanical behavior is unchanged under rigid rotations. Typical models of composite materials fall within two categories: either *random* or *periodic* in the sense that some basic matrix-inclusion arrangement repeats periodically. In this paper some numerical schemes are developed that are suitable to study homogenous, isotropic, and periodic composite materials. The literature for composite materials is extensive but we refer to ⁵ for the elements of the theory, and to ^{8, 2} for methods for estimating the overall properties of the mixture.

The main goal of the present work is to study numerical methods based on the finite element method ^{6, 9} to determine the mechanical properties of periodic composite materials. Our model of a composite material is based on the equations of nonlinear elasticity (see e.g. ¹). The constitutive equations that we used are those usually employed in the engineering literature to model rubbery materials⁷. We study a composite of two materials: a matrix with inclusions of a given (nonlinear) material, and determine numerically how the computed deformations depend on different constitutive and geometric parameters. In particular we concentrate on the computation of jump discontinuities on the deformation gradient across the internal material interfaces. To compute these jumps it is

necessary to work in suitable finite element spaces. We use the so called Crouzeix-Raviart elements³ which are continuous only at the barycenters of faces in the FEM triangulation.

Notation: For any set $\Omega \subset \mathfrak{R}^n$ and integer $k \geq 0$, we denote by $C^k(\Omega)$ the set of all the functions $u : \Omega \rightarrow \mathfrak{R}$ for which all of its partial derivatives up to order k are continuous over Ω . For $1 \leq p < \infty$, let

$$L^p(\Omega) = \{u : \Omega \rightarrow \mathfrak{R} : \int_{\Omega} |u|^p dx < \infty\}.$$

The set $W^{k,p}(\Omega)$ consists of functions $u \in L^p(\Omega)$ with its (distributional) partial derivatives up to order k also belonging to $L^p(\Omega)$. $W_0^{1,p}(\Omega)$ is the subspace of functions of $W^{1,p}(\Omega)$ that are zero (in the sense of trace) on $\partial\Omega$.

2. The model problem:

The region occupied by the body in its *reference configuration* is denoted by $\Omega \subset \mathfrak{R}^2$. Let $\mathbf{f} : \Omega \rightarrow \mathfrak{R}^2$ denote a deformation of the body and let its *deformation gradient* be

$$\nabla \mathbf{f}(\mathbf{x}) = \frac{d\mathbf{f}}{d\mathbf{x}}(\mathbf{x}).$$

For smooth deformations, the requirement that $\mathbf{f}(\mathbf{x})$ is locally *invertible and preserves orientation* takes the form

$$\det \nabla \mathbf{f}(\mathbf{x}) > 0, \quad \mathbf{x} \in \Omega. \quad (1)$$

Let $W : \Omega \times \text{Lin}^+ \rightarrow \mathfrak{R}$ be the *stored energy function* of the material of the body where $M^{2 \times 2}$ denotes the space of real 2×2 matrices and $\text{Lin}^+ = \{\mathbf{F} \in M^{2 \times 2} : \det \mathbf{F} > 0\}$. The total energy stored in the body due to the deformation \mathbf{f} is given by

$$I(\mathbf{f}) = \int_{\Omega} W(\mathbf{x}, \nabla \mathbf{f}(\mathbf{x})) d\mathbf{x}. \quad (2)$$

The derivatives

$$\mathbf{S}(\mathbf{x}, \mathbf{F}) = \frac{d}{d\mathbf{F}} W(\mathbf{x}, \mathbf{F}), \quad \mathbf{C}(\mathbf{x}, \mathbf{F}) = \frac{d^2}{d\mathbf{F}^2} W(\mathbf{x}, \mathbf{F}), \quad (3)$$

are the usual (Piola-Kirchhoff) *stress* and *elasticity* tensors, respectively.

It is assumed that the body Ω is composed of two phases in the sense that $\Omega = \Omega_0 \cup \Omega_1$. The *matrix* is Ω_0 and Ω_1 is the set of *inclusions*. The stored energy function for the composed material is given by:

$$W(\mathbf{x}, \mathbf{F}) = \chi_0(\mathbf{x})W_0(\mathbf{F}) + (1 - \chi_0(\mathbf{x}))W_1(\mathbf{F}), \quad (4)$$

where χ_0 is the characteristic function of Ω_0 , and W_i describes the mechanical properties of the material that composes Ω_i , $i = 0, 1$. The material of each phase is *isotropic* if there exist functions $\sigma^{(i)} : (0, \infty) \times (0, \infty) \rightarrow \mathfrak{R}$ such that:

$$W_i(\mathbf{F}) = \sigma^{(i)} \left(\frac{1}{2} \mathbf{F} \cdot \mathbf{F}, \det \mathbf{F} \right), \quad i = 0, 1. \quad (5)$$

One can show that for any $\mathbf{F} \in \text{Lin}^+$, $\mathbf{H} \in M^{2 \times 2}$:

$$\mathbf{S}^{(i)}(\mathbf{F}) = \frac{d}{d\mathbf{F}} W_i(\mathbf{x}, \mathbf{F}) = \sigma_{,1}^{(i)} \mathbf{F} + \sigma_{,2}^{(i)} \mathbf{F} (\text{adj} \mathbf{F})^t, \quad (6a)$$

$$\begin{aligned} \mathbf{C}^{(i)}(\mathbf{F})[\mathbf{H}] &= \frac{d^2}{d\mathbf{F}^2} W_i(\mathbf{x}, \mathbf{F}) = \sigma_{,1}^{(i)} \mathbf{H} + (\sigma_{,11}^{(i)} (\mathbf{H} \cdot \mathbf{F}) + \sigma_{,12}^{(i)} (\mathbf{H} \cdot (\text{adj} \mathbf{F})^t)) \mathbf{F} \\ &\quad + \sigma_{,2}^{(i)} (\text{adj} \mathbf{H})^t + (\sigma_{,21}^{(i)} (\mathbf{H} \cdot \mathbf{F}) + \sigma_{,22}^{(i)} (\mathbf{H} \cdot (\text{adj} \mathbf{F})^t)) (\text{adj} \mathbf{F})^t, \end{aligned} \quad (6b)$$

$i = 0, 1$, where $\sigma_{,k}^{(i)}$, $\sigma_{,kj}^{(i)}$ denote partial derivatives of $\sigma^{(i)}$ evaluated at $((1/2)\mathbf{F} \cdot \mathbf{F}, \det \mathbf{F})$, and $\text{adj} \mathbf{F} = (\det \mathbf{F}) \mathbf{F}^{-1}$. It follows now from (3) and (4) that

$$\mathbf{S}(\mathbf{x}, \mathbf{F}) = \chi_0(\mathbf{x}) \mathbf{S}^{(0)}(\mathbf{F}) + (1 - \chi_0(\mathbf{x})) \mathbf{S}^{(1)}(\mathbf{F}), \quad (7a)$$

$$\mathbf{C}(\mathbf{x}, \mathbf{F}) = \chi_0(\mathbf{x}) \mathbf{C}^{(0)}(\mathbf{F}) + (1 - \chi_0(\mathbf{x})) \mathbf{C}^{(1)}(\mathbf{F}). \quad (7b)$$

Let $\partial\Omega = \Gamma_1 \cup \Gamma_2$ with $\Gamma_1 \cap \Gamma_2 \neq \emptyset$, so that $\partial\Omega_0 = \Gamma_1 \cup \Gamma_2 \cup \partial\Omega_1$. For any given \mathbf{f}_0 consider the problem of minimizing (2) over the set

$$A = \{ \mathbf{f} \in W^{1,1}(\Omega) : \det \nabla \mathbf{f} > 0 \text{ a.e. in } \Omega, \mathbf{f} = \mathbf{f}_0 \text{ on } \Gamma_1 \}.$$

The Euler-Lagrange equations for this problem are formally given by:

$$\text{div} \mathbf{S}(\mathbf{x}, \nabla \mathbf{f}(\mathbf{x})) = 0 \quad \text{in } \Omega, \quad (8a)$$

$$\mathbf{f} = \mathbf{f}_0 \quad \text{on } \Gamma_1, \quad \mathbf{S}(\mathbf{x}, \nabla \mathbf{f}(\mathbf{x})) \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_2, \quad (8b)$$

$$[\mathbf{S}(\mathbf{x}, \nabla \mathbf{f}(\mathbf{x}))] \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega_1. \quad (8c)$$

where \mathbf{n} is the unit normal vector to the given boundary and

$$[\mathbf{S}(\mathbf{x}, \nabla \mathbf{f}(\mathbf{x}))] = \lim_{\varepsilon \rightarrow 0} \mathbf{S}(\mathbf{y}, \nabla \mathbf{f}(\mathbf{y})) \Big|_{\mathbf{y}=\mathbf{x}-\varepsilon \mathbf{n}(\mathbf{x})}^{\mathbf{y}=\mathbf{x}+\varepsilon \mathbf{n}(\mathbf{x})}, \quad \mathbf{x} \in \partial\Omega_1,$$

is the jump in $\mathbf{S}(\cdot, \nabla \mathbf{f}(\cdot))$ across the matrix-inclusion interface $\partial\Omega_1$. If $\nabla \mathbf{f}$ is continuous across $\partial\Omega_1$, which would happen if the matrix and inclusion materials are equal, then this jump is clearly zero. However, for different matrix-inclusion materials, $\nabla \mathbf{f}$ can be discontinuous across $\partial\Omega_1$, with the zero jump boundary condition (8c) still holding. Note that (8c) is just a consequence of the fact that at a minimum configuration of (2), the internal forces within the body must be in equilibrium.

3. The finite element method and the Newton iteration:

This section contains the specifics of a finite element method (FEM) to approximate solutions of the problem (8). As this problem is nonlinear, the FEM formulation leads to a nonlinear set of equations, which are solved, using the Newton iteration. The Newton iteration solves at each step a linear problem using the FEM.

Let $T = \{T_k\}$ be a triangulation or mesh over Ω . Let $E = \{e_k\}$ denote the set of all edges of the triangles in T . The space of all piecewise affine functions relative to the partition T is defined by:

$$P_1(T) = \{ \mathbf{v} \in L^1(\Omega) : \mathbf{v}|_{T_k} \text{ is affine } \forall T_k \in T \}.$$

Let N_{nc} be the set of barycenters of edges, that is

$$N_{nc} = \left\{ \frac{1}{|e|} \int_e \mathbf{x} \, ds : e \in E \right\}.$$

The first-order Crouzeix–Raviart finite element space $\text{CR}(T)$ is given now by

$$\text{CR}(T) = \{ \mathbf{v} \in P_1(T) : \mathbf{v} \text{ is continuous at each } \mathbf{x} \in N_{nc} \}.$$

For any given $\mathbf{f} \in \text{CR}(T)$, we define the linear functional:

$$L(\mathbf{f})[\mathbf{v}] = \int_{\Omega} \mathbf{S}(\nabla \mathbf{f}) : \nabla \mathbf{v} \, d\mathbf{x}, \quad \mathbf{v} \in H, \quad (9)$$

Where

$$H = \{ \mathbf{v} \in \text{CR}(T) : \mathbf{v} = \mathbf{0} \text{ on } \Gamma_1 \}. \quad (10)$$

The FEM formulation of the problem (8) is to find $\mathbf{f} \in \text{CR}(T)$ satisfying $\mathbf{f} = \mathbf{f}_0$ on Γ_1 and such that

$$L(\mathbf{f})[\mathbf{v}] = 0, \quad \forall \mathbf{v} \in H. \quad (11)$$

A Newton type iteration to solve (11) can be described as follows. To this end we will need the bilinear form:

$$B(\mathbf{f})[\mathbf{w}, \mathbf{v}] = \int_{\Omega} \mathbf{C}(\nabla \mathbf{f})[\nabla \mathbf{w}] : \nabla \mathbf{v} \, d\mathbf{x}, \quad \mathbf{w}, \mathbf{v} \in H. \quad (12)$$

Newton's method for the solution of (11) (or to minimize (2)) takes the form:

1. Let \mathbf{f}_0 be an initial approximation of the minimizer of (2).
2. For $n = 0, 1, 2, \dots$,
 - i. Compute $\mathbf{w}_n \in H$ such that,

$$B(\mathbf{f}_n)[\mathbf{w}_n, \mathbf{v}] = L(\mathbf{f}_n)[\mathbf{v}], \quad \mathbf{v} \in H. \quad (13)$$

- ii. Set $\mathbf{f}_{n+1} = \mathbf{f}_n - (1 - \rho^{n+1})\mathbf{w}_n$.

3. Repeat step (2) until the norm of \mathbf{w}_n is sufficiently small.

Here $\rho \in (0,1)$ is a parameter used to slowdown the method on the initial steps.

4. Implementation of the Numerical Scheme and results:

For the numerical simulations the package FreeFem++⁴ was used for the solution of the problem (13) using the finite element method with piecewise linear non-conforming elements³. The coding with FreeFem++ resembles very much the underline mathematics of the problem. This package includes high level constructs to define domains, meshes, finite element spaces, and variational forms. It includes as well basic flow controls like loops and conditionals. Of particular importance for our simulation is the command **region** which allows for identifying regions in the domain and the command **jump** to compute the jump of the deformation gradient across the internal interfaces of the mixture.

For the stored energy function $\sigma^{(i)}$ in (5), the following function was used which is a good model for rubber-like materials⁷:

$$\sigma^{(i)}(v_1, v_2) = v_1^{\alpha_i/2} + b_i v_2^{\beta_i} + c_i v_2^{-\gamma_i}, \quad i = 0,1, \quad (14)$$

where $\alpha_i, \beta_i, \gamma_i, b_i, c_i$ are nonnegative constants. From the expressions (6a) and (7a), is obtained that the reference configuration is stress-free, i.e., $\mathbf{S}(\mathbf{I}) = \mathbf{0}$, if and only if

$$c_i = \frac{b_i \beta_i + 0.5 \alpha_i}{\gamma_i}, \quad i = 0,1. \quad (15)$$

For the set Ω the unit square $[0,1] \times [0,1]$ minus a disk of radius $r=0.1$ with center at $(0.25, 0.75)$ is used. For the boundary conditions, Γ_2 is taken to be the boundary of this disk, Γ_1 the outer boundary of the square, and

$$\mathbf{f}_0(x, y) = (x, 1.2y), \quad (x, y) \in \Gamma_1. \quad (16)$$

(When extended to all of Ω , this function is used as well as the initial approximation in Newton's method.) Ω_1 consists of the union of three disks of radius $r=0.1$ each, with centers at $(0.25, 0.25)$, $(0.75, 0.25)$, and $(0.75, 0.75)$. It follows that $\Omega_0 = \Omega \setminus \Omega_1$. Figure (1) shows the geometry of Ω with the inclusions given by Ω_1 . The same figure also shows the finite element mesh generated with FreeFem++ which is the one used for the computations.

For the first simulation the following coefficients were used in (14):

Table 1. coefficients of the matrix and inclusion for the first simulation.

i	α_i	b_i	β_i	γ_i
0	1.5	0.5	2.5	2.0
1	1.5	0.1	1.5	2.0

Note that these numbers make the material of the matrix Ω_0 to be stronger or harder to deform than that of the inclusions Ω_1 . Figure (2) shows a sketch of the final computed deformation corresponding to the boundary condition (16). Both $\mathbf{S}(\mathbf{x}, \nabla \mathbf{f}(\mathbf{x})) \cdot \mathbf{n}$ and the jump of this quantity across $\partial\Omega_1$, are zero over Γ_2 and $\partial\Omega_1$ respectively to within the mesh precision. In Figure (3) a contour plot of the $\det \nabla \mathbf{f}$ is shown which clearly

shows a jump discontinuity in $\nabla \mathbf{f}$ across $\partial\Omega_1$. Note also that the material within the inclusions is more deformed, as measured by the determinant, in comparison to that outside the inclusions. This is consistent with the material of the matrix being stronger than that of the inclusions.

In the second simulation the material of the inclusions remained fixed and the one corresponding to the matrix is varied. The parameters for the inclusions are:

Table 2. parameters for the inclusions for the second simulation.

α_1	b_1	β_1	γ_1
1.5	0.4	2.1	2.0

The parameters for the matrix have $\alpha_0 = \alpha_1$, $\gamma_0 = \gamma_1$, with $0.1 \leq b_0 \leq 0.65$ and $1.5 \leq \beta_0 \leq 1.6$. Figure (4) shows a plot of the total jump across $\partial\Omega_1$ as given by the expression

$$\left[\int_{\partial\Omega_1} \|\llbracket \nabla \mathbf{f} \rrbracket \cdot \mathbf{n} \|^2 ds \right]^{\frac{1}{2}}.$$

Here $\llbracket \nabla \mathbf{f} \rrbracket$ represents the jump in $\nabla \mathbf{f}$ across $\partial\Omega_1$ at the given point. The “valley” in the figure corresponds to values of b_0, β_0 for which the materials of the matrix and inclusions are very similar. From this figure it follows as well that the jump across $\partial\Omega_1$ increases as the difference in the mechanical behavior between the phases becomes more pronounced.

5. Closing remarks:

Using a finite element method with a Newton type iteration is possible to perform simulations of composite materials for a wide range of nonlinearly elastic materials and which in principle can have very general matrix-inclusion arrangements. The use of non-conforming finite elements allowed us to detect and compute jump discontinuities in the deformation gradient across the material interfaces. As a future project, it is planned to use the techniques in this paper to study periodic composite materials, that is, where the basic matrix-inclusions arrangements (like the one in Figure 1) is at the nano scale and repeats periodically.

6. Acknowledgements:

This research was supported in part by the PREM and RISE programs of the University of Puerto Rico at Humacao.

7. References:

1. Antman, S. S., *Nonlinear Problems of Elasticity*, Springer Verlag, New York, 1995.
2. Brun, M., Lopez-Pamies, O., Ponte Castañeda, P., “Homogenization estimates for fiber-reinforced elastomers with periodic microstructures”, *International Journal of Solids and Structures*, 44, 5953-5979, 2007.
3. Crouzeix, M. and Raviart, P. A., “Conforming and nonconforming finite element methods for solving the stationary Stokes equation”, *RAIRO Sér. Rouge* 7, 33–75, 1973.
4. Hecht, F., Pironneau, O., Le Hyaric, A., and Ohtsuka, K., *FreeFem++ Manual*, <http://www.freefem.org>.
5. Hill, R., “On constitutive macro-variables for heterogeneous solids at finite strain”, *Proceedings Royal Society of London*, A. 326, 131-147, 1972.
6. Mitchell, A. R. and Wait, R., *The Finite Element Method in Partial Differential Equations*, John Wiley & Son, New York, 1977.
7. Ogden, R. W., “Large deformation isotropic elasticity”, *Proc. Roy. Soc. London*, A326:565-584 and A328:567-583, 1972.

8. Ponte-Castañeda, P., "The Overall Constitutive Behavior of Nonlinearly Elastic Composites", *Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences*, Vol. 422, No. 1862, pp. 147-171, 1989.
9. Zienkiewicz, O. C., Taylor, R. L., and Zhu, J. Z., *The Finite Element Method: Its Basis and Fundamentals*, Six Edition, Elsevier, New York, 2005.

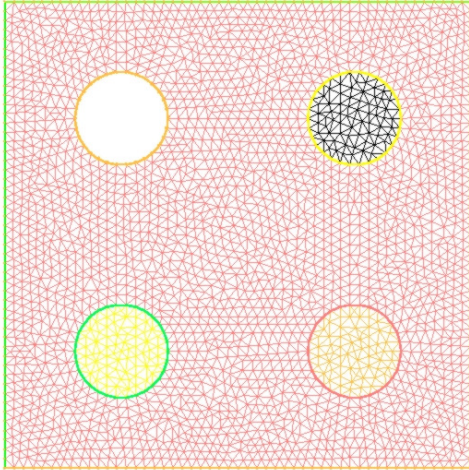


Figure 1. Geometry of Ω with the inclusions given by Ω_1 (the three filled circles) and the finite element mesh.

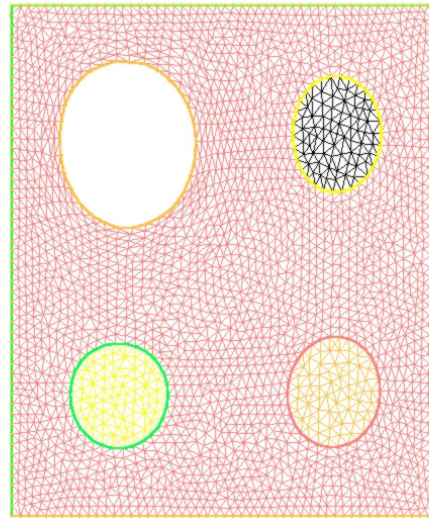


Figure 2. Final computed deformation.

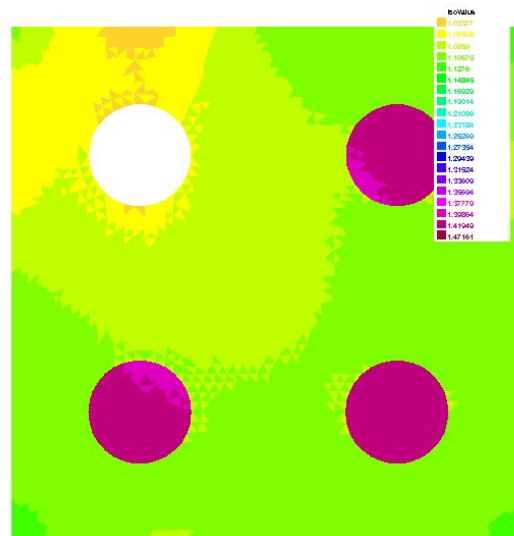


Figure 3. Graph of $\det \nabla \mathbf{f}$ showing the jump discontinuity in $\nabla \mathbf{f}$ across $\partial\Omega_1$.

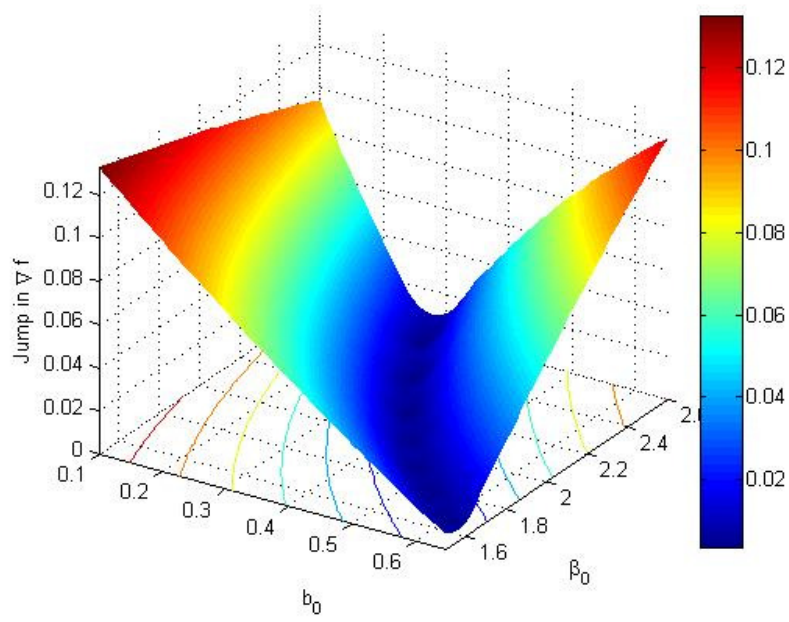


Figure 4. Jump in $\nabla \mathbf{f}$ across $\partial\Omega_1$ as a function of the parameters b_0, β_0 .