Proposal Report

IMPLEMENTATION OF FINITE ELEMENTS METHOD ON A DIFFUSION-ADVECTION PROBLEM

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1 PROBLEM DESCRIPTION

In nature, advection, diffusion and other underlying processes deal with the transportation of a given chemical species in the medium. Now, taking advection and diffusion only in count and letting c be the concentration of the specie as a function of position (x_1, x_2, x_3) and time t, the partial differential equation (1) describing the convection-diffusion phenomena on a physical system is found over any bounded domain D whose boundary conditions are defined on the boundary of D denoted by ∂D:

$$\frac{\partial C}{\partial t} + \nabla.(\mathbf{u}C) = D\nabla^2 C \tag{1}$$

where $\mathbf{u}$ is the chemical crossflow velocity and D the diffusion coefficient. Now, if we wanted to present Equation (1) on a more realistic way, for example, on not rectangular domains such as steady surfaces then our problem would be defined as follows.

Let Ω be an open domain in $\mathbb{R}^3$ and Γ be a connected C^2 compact surface contained in Ω. Assuming the advection velocity is everywhere tangential to the surface and having $\mathbf{w} : \Omega \rightarrow \mathbb{R}^3$ as a divergence-free velocity field in Ω then the surface advection-diffusion equation, analogous to Equation (1), takes the form:

$$u_t + \mathbf{w}. \bigtriangledown_\Gamma u - \epsilon \bigtriangleup_\Gamma u = 0 \tag{2}$$

where $\bigtriangleup_\Gamma$ denotes the *Laplace-Beltrami* operator on Γ defined as the Laplace operator extension on surfaces, i.e., the divergent of the gradient.

Now, Equation (2) has been studied by Olshanskii [1] applying one only numerical method, the finite elements method, which under the given conditions would provide a stabilized discretization method for the surface equation, letting apply numerical experiments and get consistent results with those expected from other similar approaches like the one proposed by Bochev [2].

Our problem is then, using the finite elements technique, be able to find discretizations on other kind of domains such as not regular surfaces.

2 OBJECTIVES

2.1 General objective

Study the application of the finite elements method to the advection-diffusion equation defined on not regular surfaces/domain, being able to propose discretized equations and therefore perform a computational implementation of such equations.

2.2 Specific objectives

- Understand and, if possible, modify the classical advection-diffusion problem, more precisely its domain, in order to pose a more realistic and complex one.
- Implement the theorical discretizations on a computer using *Matlab*, *Mathematica* or *Python*, being able to present the results on a graphical and numerical way.

3 JUSTIFICATION

The problem we want to study is based on the transportation of a pollutant in the enviroment under certain conditions. Such kind of problem is usually treated from the partial differential equation scheme and exact methods such as separation of variables, change of variables and transformations are usually used in order to look for exact solutions in a given domain; however, these methods cannot be applied when we treat with non-linear equations, non-homogeneous initial or boundary conditions, irregular domains or when the resources are not enough. For this reason, several numerical methods are being used in order to achieve approximate results of equations whose importance laids on the problems they represent or model. In this work we focus on two proccesses, advection and diffusion, which would allow us to build a theorical model, letting us predict, for example, how peak concentrations will change in response to prescribed changes in the domain and in the nature and source of pollution.

We think that using more accurate methods, such as the finite elements one, we can build more realistic cases applying real conditions and therefore get better results describing a problem that by today has became into a societal issue. We do not seek to add literature on a classical problem, but to contribute on the development of new theory aiming to understand and apply knowledge coming from our daily work.

4 Background

The development of the Finite Elements Method has increased widely since its presentation at 1943 by *Richard Courant*. Nowadays it is used to approximate solutions of partial differential equations governing mechanical systems and it is also commonly used in the thermodicamical and engineering area. Now, dealing with the advection-diffusion equation it has been only a few studies concerning on the numerical but also new theorical approach with the method, i.e, Olshanskii [1] and Bochev [2] have been able to work from the theorical aspect of this application but without going further on the stability criteria. Nevertheless it was shown that such application is possible and has the posibility of been improved by adding computacional perfomances or changing/mixing the classical problem and its characteristics, such as domain or initial-boundary conditions.

The galerkin formulation and finite differences method have been also used to study the problem described above by Roig [3] and Friedman [4] respectively, both of which present the Finite Element Method as a further work. From here that several authors had made so many contributions to the subject over the years, specially mixing methods with the finite elements one. Ewing [5], for example, in his remarkable work *"A summary of numerical methods for time-dependent advection-dominated partial differential equations"*, shows a general prospect on how the methods and techniques have been applied on the advection-diffusion problem and also presents a light discussion on the incoming methods, all of them related with the finite elements scheme.

5 Scope

Having the complexity and theorical and computational costs of represent Equation (1) or Equation (2) in mind, we make this work only as a first insight into the treatment of the approximations displayed as results from the Finite Element Method since a more global goal would require much more time and knowledge on the theory underlying our problem. Our scope would be then build a general presentation of the psysical problem along with a good description of its properties in order to give initiation to the pre-process step, where we could define our geometry and boundary conditions, generalize the mesh, preconditionate the problem, among others. If possible, we would give way to the calculation/pos-process stage where we assign a series of functions on the nodes so we develop the discretization needed for further computational implementations.

6 METHODOLOGY

In order to achive the objective of this work we will employ five hours per week which would be distributed in short sessions with the tutor and individual research. In such meeting both student and tutor would discuss the progress on the achivement of the objectives mentioned on Section [2] as well questions arising from the provided theory or the incoming one. The student will attend, as many times as possible, to the seminar instructed by Professor Jairo Alberto Villegas, which would ensure him known theory and would let him acquire new theory related to differential equations.

7 RESOURCES

We expect, according to our scope (Section 5), to focus our work on the theorical aspect of the problem and therefore we will be using most of the time the bibliographical databases provided by the University. It is clear that if we succeed with the first modellation stage then licenced softwares such as *MATLAB*, *Mathematica* or similar will be needed in order to develop numerical approximations to our problem.

8 INTELLECTUAL PROPERTY

According to the EAFIT's University internal intellectual property reglamentation, the patrimonial rights over the academic products resulting from this project will belong to the authors, Obed Ríos-Ruiz and Jairo Villegas-Gutiérrez in a *30%*, to the *Functional Analisys Research Group* in a *15%* and to the University in a *55%*.

9 Activity schedule

Activities schedulling		
Activity	**Description**	**Week range**
Proposal report		3 - 4
Proposal presentation		4
Literature review	Search on bibliographical databases	3 - 6
Theorical model construction	Definition of the problem geometric aspect, formulation of general model	6 - 10
Oral progress report		10
Finite elements method application	Model discretization to finite elements, simplification on the discreet problem transformation	10 - 16
Project report		16
Project presentation		19

We propose the following schedule letting the student use a good amount of time to develop, together and closely with his tutor, a good understanding on the activity in order to achieve, slowly but safely, the project specific objectives and therefore the geneal one (Section [2]).

References

[1] M. A. Olshanskii, A. Reusken, and X. Xu, "A stabilized finite element method for advection–diffusion equations on surfaces," *IMA Journal of Numerical Analysis*, 2013.

[2] P. B. Bochev, M. D. Gunzburger, and J. N. Shadid, "Stability of the SUPG finite element method for transient advection–diffusion problems," *Computer Methods in Applied Mechanics and Engineering*, vol. 193, no. 23–26, pp. 2301 – 2323, 2004.

[3] B. Roig, "One-step Taylor–Galerkin methods for convection–diffusion problems," *Journal of Computational and Applied Mathematics*, vol. 204, no. 1, pp. 95 – 101, 2007.

[4] A. Friedman and W. Littman, *Industrial Mathematics: A Course in Solving Real-World Problems*. Philadelphia, Pennsylvania: SIAM: Society for Industrial and Applied Mathematics, 1994.

[5] R. E. Ewing and H. Wang, "A summary of numerical methods for time-dependent advection-dominated partial differential equations," *Journal of Computational and Applied Mathematics*, vol. 128, no. 1–2, pp. 423 – 445, 2001.