PROGRAMUL CERCETARE DE EXCELENTA 2005 - 2008

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MATHEMATICAL MODELLING IN DIFFUSION PROCESSES

Presentation of the project

The general objective of this project was the mathematical modelling of diffusion processes, the functional approach and numerical methods developed for the proposed models. The realization of the project included both the fundamental research concerning general models of diffusion and the analysis of some particular models of great importance in sciences and engineering. The research within this project comported the qualitative study of each type of model (existence, uniqueness, properties of the solutions) and the development of numerical methods for solving the equations. Especially, one focused on the various types of nonlinearities which due to their complexity lead to new significant results. We consider that the results of our research constitute a support for applications in biology, medicine and the management of natural resources.

The research was carried out by four partners and had three main targets:

1.Modelling and qualitative study of diffusion models

2.Numerical techniques, algorithms, numerical simulation and validation

3.A comparative analysis of the diffusion processes discrete and continuous.

The preoccupation of the Coordinator (Institute of Mathematical Statistics and Applied Mathematics) was mainly for the pure mathematical aspects of the project. Thus, a functional study of diffusion models in nonhomogeneous porous media was developed. First, the diffusive models of water flow in saturated-unsaturated media, characterized by a space variation of the porosity were introduced in a functional form. Then, a representative model with mixed boundary conditions involving a nonhomogeneous Neumann boundary condition on a part of the boundary and a Robin condition on the other part of the boundary was analyzed for the fast diffusion model which refers to a singular situation (i.e., the blowing up diffusion coefficient). The analysis was extended to degenerate models and resided in the study of a degenerate nonlinear variational inequality which can be reduced to a multivalued inclusion by an appropriate change of the unknown function. Also, a hysteretic model applied to the process of water infiltration in soils was investigated. Existence, uniqueness and some properties of the solutions for each type of models were established and numerical simulations have been run.

The numerical integration technique previously developed within the partnership framework was assessed, by the Coordinator and Partner 1, against numerical simulations conducted on the FEM multiphysics implementation of the mathematical model, based on COMSOL Galerkin formulation. The tests that were performed refer to water infiltration and evaporation in an unsaturated porous medium by considering both types of boundary conditions: Dirichlet and Robin. The results that were obtained proved the efficiency of the proposed numerical schemes.

Another task of the Coordinator was the study of numerical methods, for a class of nonlinear diffusion processes that includes the unsaturated water flow through porous media and fast diffusion. Specifically an approximation method consists in the discretization of space derivative operators using the finite volume scheme and keeping the continuum time differentiation was developed. As result, the solution to the partial differential equations is approximated by the solution of a system of ordinary differential equations. A scheme for approximating the diffusion term and the convective term such that to obtain a quasi-monotone ODE system was defined. It was proved that there exists a discrete comparison principle and it was showed that the solutions of the discrete model are bounded and its upper and lower bounds are independent of the mesh size of triangulation. To perform the time numerical integration a class of implicit backward differentiation formulae with adaptive time step was used. As the implicit schemes require a nonlinear solver it was built up a method that mixes Broyden method and an inexact Newton method. The performances of the new method are illustrated by some numerical results concerning fast diffusion equation and water infiltration through layered soil.

Partner 1 (University Politehnica of Bucharest) studied the following models:

1. Post-synaptic nicotinic currents triggered by the acetylcholine distribution within the synaptic cleft

A mathematical model that describes the postsynaptic nicotinic currents out of the acetylcholine distribution within the synaptic cleft is proposed. The model describes the most important steps of synaptic transmission: neurotransmitter release from pre-synaptic vesicles, its diffusion in the synaptic cleft, receptor-neurotransmitter coupling, and the induced post-synaptic current inflow. Relying on previous results on acetylcholine distribution in the synaptic space, the current work is concerned with the postsynaptic currents that convect through open nicotinic acetylcholine receptors, which act as ionic channels. The nicotinic currents are the outcome of a deterministic model that is based on the intra-synaptic cleft acetylcholine space-time distribution, and on the nicotinic receptors opening dynamics. The mathematical model is solved numerically, using the Femlab 3.1 software package by a Galerkin finite element method.

2. Diffusion processes in the electrical activity of the heart – numerical simulation of the normal and arythmic cardiac rhythms

The cardiac electrical activity is macroscopically manifested as action potentials that travel through atria and ventricles in a synchronized fashion. Cardiac arrhythmias are disorders of the normal electrical rhythm. At high heart rate, the action potential duration follows a long-short-long pattern. This oscillatory electrical rhythm is called alternans and it is believed to be a precursor to the development of severe ventricular arrhythmias. In this computational study we analyze the initiation of alternans in paced one-dimensional strand of cardiac cells governed by the Beeler-Reuter model. We present results from numerical experiments and a qualitative description of the observed patterns of cardiac activation.

3. Transport Effects on DNA Hybridization On Flow-Through Microarrays

Considering the complex interactions between different physico-chemical phenomena in flow-through microarrays it becomes apparent that experimental approaches must be complemented with mathematical models in order to understand the effects of flow on the hybridization kinetics. This study aims at developing a theoretical framework for the analysis of transport effects on DNA hybridization reaction on flow-through microarrays. We present a simple yet efficient mathematical model of coupled convection, diffusion and reaction in porous media.

4. The numerical analysis of a PEM fuel cell with interdigitated flow

The physical model consists of Darcy’s flow for the transversal flow in the electrodes and electrolyte, an electro-kinetic model for the electrical field in the electrodes and membrane, and Maxwell – Stephen convection and diffusion for mass transport in the electrodes. In the analysis we propose, the primitive variables are the electrical potential, pressure and velocity fields, and the species concentration for hydrogen, oxygen, nitrogen and water. The model is isothermal therefore the properties are temperature independent. Using the maximum electrical power as the figure of merit, an optimal channel width size was identified by numerical simulations.

According to the scheduled Project Realization Plan, Partner 2 – UOC (University Ovidius Constanta) had as main research activity the elaboration, conceptual analysis and software implementation of some classes of numerical algorithms to efficiently solve some categories of diffusion problems. In this purpose an algorithm of nonlinear alternating direction Gauss-Seidel type was built (ALGS) and a nonlinear multigrid algorithm of type Full Approximation Storage type (MG-FAS). The idea of the algorithm ALGS is to consider succesive columns of the discretization. In each of these columns we find the values of the unknown solution in the points of the fixed column as a function of the values already modified from the columns previously considered and the values which are not yet modified from the other columns. For each column a tridiagonal system is solved. The MG-FAS algorithm uses maximum 4 levels of succesive discretization and has the following structure: (i) a V type cycle; (ii) alternating line Gauss-Seidel relaxation (before correction 2 steps of relaxation are made, and after correction only one step); (iii) bilinear interpolation (for corrections); (iv) “full weighting” restriction operator for the residuals. Implementation of these solvers was done in the FORTRAN language and for the graphical analysis and presentation of the results some components of the MATLAB software were used. In this way, a development and interactive software was produced, which gives the possibility of comparative analysis to the different problems and boundary conditions considered.

The classes of diffusion problems analysed are the following:

1. A simplified variant of the dimensionless porous media transport problem (where $g(x,y) \le 1$ is of Dirac type, and Pe is Peclet number), with the general form

$$-\Delta u(x,y) + Pe\frac{\partial u}{\partial x} + \beta(x,y)u(x,y) = 0, \quad \beta(x,y) = \begin{cases} Da, (Damkholer\ number) \\ Da \cdot g(x,y) \end{cases}$$

2. A problem which models an infiltration process in an anisotropic porous media, homogeneous, unsaturated and with constant porosity of a general form given by

$$\frac{\partial u}{\partial t} - \nabla \bullet \left(\beta(u) \nabla u \right) + \frac{\partial K(u)}{\partial y} = f(x,y)$$

where u (x, y) is the fluid content (dimensionless), hydraulic diffusivity and conductivity

$$\beta(u) = \frac{c(c-1)}{(c-u)^2},\ c \in (1,\infty) \qquad K(u) = \frac{(c-1)u^2}{c-u},\ c \in (1,\infty)$$

Boundary conditions are of Dirichlet or Robin type, and problem 2 was analysed also in the case of heterogenous porous media. In order to validate these 2 algorithms and interactive software media established, the obtained results (values and graphical representations) were compared with those of Partner 1, who used for the same experiments the software product COMSOL. This proves the precision and robustness of the algorithms established by Partner 2 – UOC. Efficiency and originality of these algorithms are certified by the published papers (in ISI quoted journals or CNCSIS recognized) and papers presented at international and national scientific meetings, along project’s development (pointed in each Intermediate Activity Report).

The research of Partner 3 (University of Pitesti) was oriented towards the applications of the notion of approximate inertial manifold in the construction of approximate solutions for semilinear parabolic problems, and in particular, for equations modelling diffusion problems. Partner 3 elaborated a new variant of “the nonlinear Galerkin method”, a variant that has some advantages towards the classical one: the computations are better structured, a smaller amount of memory is used, a smaller computational cost is payed. In what concerns the approximation order, this is the same as in the “classical” nonlinear Galerkin method.As a starting point, the Navier-Stokes model, for which a lot of scientific literature concerning the approximate inertial manifolds and the so-called "non-linear Galerkin method" exists, was considered. The method was implemented for the two-dimensional Navier-Stokes equations. Next, the method was applied to a simple diffusion problem, that is the diffusion of a substance in a Newtonian fluid, under a nonsteady flow, in the framework of the Fickean model. The new method was applied to this problem and the error was estimated for every level of approximation. Besides these studies, Partner 3 also collaborated with the Coordinator to a research concerning the nonFickean diffusion and to a study regarding some numeric methods for evolution equations.

The scientific production obtained during this project contains 3 books, 27 articles, 47 communications, a web page, soft.

Economical development elements

Economical and social impact:

- maintaining and extending European collaborations and involving the Romanian research in high international standards
- new areas of education for the students allowing them face new challenges of labour market
- making use of computational mechanics to reducing design, testing and execution cycles
- improving teaching and instruction
- diminishing the Romanian intelligence emigration by engaging in project-work master and PhD students
- the management of groundwater resources and protection