

Evaluation of the PhD thesis submitted by the candidate Shahin Heydari entitled "*Development and analysis of monotone numerical schemes*" at Faculty of Mathematics and Physics.

The thesis focuses on investigation of several systems of nonlinear partial (or ordinary) differential equations inspired by bio-science. The considered systems are studied both from the theoretical point of view as well as from the numerical approximation - in that case the application of suitable numerical methods is discussed and numerical simulations are performed. For the considered systems of parabolic equations with cross-diffusion the existence of global classical solutions is studied for the selected cross-diffusion systems. As for such systems the analytical solution is rather difficult - or even impossible - to find, and that is why the application of numerical methods is discussed. The appearance of dominant cross-diffusion terms may lead to numerical instability of standard numerical methods and appearance of spurious oscillations. One of the standard tools in such a case is to apply a stabilized scheme. Taking into account other qualitative properties (as e.g. requirement on positivity preserving scheme) results in employment of the high-resolution nonlinear finite element flux-corrected transport (FE-FCT) methods to overcome the relevant difficulties of the problem. The proposed schemes are analyzed in terms of their solvability, positivity, and satisfaction of discrete maximum principle. The theoretical and numerical results are validated by several numerical experiments.

The thesis is composed of an introduction section, the second chapter about stabilization for convection-diffusion-reaction problems followed by 4 chapters containing 5 reprints of papers for which Shahin Heydari is an author (from this list two papers have one co-author), and conclusion. The papers are published in international scientific journals of high quality (Mathematical Modelling and Numerical Analysis (ESAIM), Mathematical Models and Methods in Applied Sciences, Journal of Computational Physics, Mathematics and Computers in Simulation - one of the included papers (paper III) was accepted for publication in proceedings of the ENUMATH conference (proceedings in Springer). Paper one focuses on the existence and positivity of the solution for the cancer invasion system. Further, also the application of the Galerkin finite element method for the time-discretized nonlinear system is discussed and numerically analyzed concerning the stability. Chapter 3 contains papers II and III interested in the modified cancer invasion model with the diffusion term omitted. In these papers only the application of finite element approximations is discussed, because leaving out the diffusion term makes the technique used in paper I not applicable. The Galerkin scheme is suggested, stabilized using the FCT technique, numerically analyzed and numerical results are presented. Paper IV focuses on approximation of partial differential equations describing "the rivaling gangs", where existence and non-negativity of the solution is proven. Further, nonlinear finite element flux-corrected transport method is applied for solution, numerically analyzed showing the positivity preserving scheme property and numerical experiments are performed. Paper V then discusses the numerical approximations of the influenza disease mathematical model consisting of a system of 4 ODEs. Positivity of the solution is shown, non-standard finite difference approximations are suggested and it is shown that this scheme preserves the conservation law and it is elementary stable. The theoretical findings are supported by numerical examples.

The papers are commented on in the Introduction section and each paper is provided with a short summary containing an explanation of what is the main result included and the description where the paper was published. The introduction section first explains what is meant by cross-diffusion systems (Section 0.1) with an attempt made to give a unified description to the problems considered in included papers and with briefly mentioning the background for analytical investigation as well as the difficulties to be overcome in the numerical approximation. Further, the second section (Section 1) focuses on a detailed description of stabilization methods applicable for convection-diffusion-reaction problems. It contains a very nice overview of the methods based on streamline upwind/Petrov-Galerkin(SUPG), Galerkin least squares method, bubble based stabilization, local projection stabilization, edge stabilization and flux corrected transport methods, etc. This overview is presented both for the stationary (Section 1.1) as well as for the transient case (Section 1.2). Section 1.3 briefly (in one paragraph of half a page) discusses the applicability of the stabilization methods for cross-diffusion systems.

The quality of the results contained in the PhD Thesis is very good due to the excellent quality of the included papers (re-prints) published in international scientific journals of high quality. It should be also emphasized that the presented papers contain not only the numerical analysis and numerical results, but also the theoretical results concerning the existence and quality of solutions. The PhD Thesis represents a very significant contribution to the field of numerical analysis with the results confirmed by numerical experiments.

However, I have several objections: The first one, the most serious one, is that the included papers have at least two authors and I am missing a detailed explanation of the contribution made by the PhD candidate - such information should be definitely included in the thesis! Second, the thesis seems to be somehow incoherent. For instance, the author in the second section mostly discusses the different stabilization methods. This is a really nice overview, but this topic does not correspond well to the content of the included papers except for the FCT technique. On the other hand the analytical results and numerical simulations from the papers are discussed only very briefly in Introduction. This structure makes the thesis very hard for someone to read and to identify the contribution of the author. Let me also mention the rather strange numbering of chapters/sections (each paper is published as a separate chapter, but paper II and III are contained in a single chapter) as well as confusing numbering of paragraphs within sections in the Introduction (starting with subsection 0.1 in the unnumbered Introduction, or the numbering of the list of stabilization methods started at page 11 followed by strange numbering of the embedded lists on pages 24 - 27).

Based on what is above the following questions should be considered by the candidate and discussed during the defense:

Q1: What is the candidate's contribution to each of the presented papers? Please provide a detailed explanation!

Q2: Did the author implement the numerical schemes? In Conclusion the author mentions MATLAB - is Matlab suitable for realization of the FCT schemes?

Q3: Numerical experiments were performed only for 1D problems or 2D problems on the unit square, probably with a cartesian type of grid. Were the numerical methods tested on a more

complex domain? Were the methods tested in the case of e.g. anisotropically refined meshes?

Q4: On page 23 in eqs. (1.50-1.51) as well as in (1.54) the author presents treatment of the Dirichlet boundary conditions. On page 25 on the last line it is mentioned that the correction factors are for the Dirichlet boundary conditions set to 1. It is rather confusing as these factors are never used in (1.54). (Same remark is valid also for the other schemes as well as for the transient one on page 37 and following).

Is this the correct description? How is the Dirichlet boundary condition treated in the FCT schemes?

Q5: On page 24 the author presents just after equation (1.58)-(1.59) that “then, the system (1.58)-(1.59) can be rewritten in **the** variational form ...” followed by an un-numbered equation. This statement is made without citation, without proof and without explanation. Can the author explain what is meant by the variational form? Please also explain the meaning of the terms in the definition of the form b_h .

Q6: Can you explain the proof of Proposition 4.1 of the 5th paper? On page 153 of the Thesis, namely how from Eq. 4.1 follows the equation before “.. thus $S_1 + I_1 + R_1 + C_1 = 1$ ”, and how from this equation follows this statement. Did you check this conservativity also for numerical experiments?

To conclude, this thesis presents material of sufficient novelty to proceed for the defense. Provided that the candidate sufficiently explains her contribution in the individual papers, I also recommend that the author should be awarded the degree of PhD.

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