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Subject Evaluation of the PhD thesis Shahin Heydari

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To
Mrs. Dagmar Zádrapová
MFF UK – stud. odd.
Ke Karlovu 3
121 16 Praha 2
Czech Republic

Dear doc. RNDr. Rokyta,
Dear doc. Mgr. Kulich,

I am sending you my evaluation of the PhD thesis by Ms. Shahin Heydari entitled

Development and analysis of monotone numerical schemes

I have carefully studied the manuscript and ***recommend accepting it for presentation and defense***. In what follows I will substantiate my recommendation in more detail.

The dissertation consists of 5 chapters preceded by a brief introduction and complemented by conclusions. The 5 main chapters are based on publications by the PhD candidate that have been published in established international journals and as conference proceedings, respectively. Each chapter starts with a brief summary of the main findings in the overall context of the PhD thesis.

Chapter 1 gives a comprehensive, and well-written overview of the state of the art in numerical stabilization techniques for steady-state (Section 1.1) and time-dependent (Section 1.2) convection-diffusion-reaction problems with dominating convective term. As such, it does not provide scientifically novel content but presents the various approaches existing in the literature in a common notation. In contrast, the review of techniques to stabilize cross-diffusion problems is very brief and does not follow the style of a literature review but instead refers the reader to the 5 main chapters of the PhD thesis. Admittedly, the literature may not be as vast as for convection-dominated problems. However, it would have been of added value to the reader if the attempt had been made to give a state-of-the-art overview in the same style as in the two preceding sections. One work that should be mentioned in this context is

D. Kuzmin, M.J. Shashkov, D. Svyatskiy, A constrained finite element method satisfying the discrete maximum principle for anisotropic diffusion problems. Journal of Computational Physics, Volume 228, Issue 9, 20 May 2009, Pages 3448-3463

Chapters 2 and 3 focus on the theoretical aspects of cross-diffusion problems and on the properties of their numerically approximated solutions. In particular, Chapter 2 deals with a cancer invasion model that couples a cross-diffusion-reaction equation with two additional nonlinear ordinary differential equations for the protease and the extracellular matrix, respectively. Chapter 3 focuses on the haptotaxis counterpart of this problem that lacks the diffusion term, and hence, features different theoretical and numerical properties.

One scientific highlight of Chapter 2 (Paper I) is the existence proof of global classical solutions. The lack of the diffusion term for the haptotaxis counterpart in Chapter 3 renders the proving techniques utilized in Chapter 2 unapplicable so that the question, whether the reduced model without self-diffusion term also has a unique global classical solution, remains unanswered. The second half of Chapter 2 (Paper I) basically demonstrates, that standard numerical approaches, i.e. low-order Galerkin finite elements with semi-implicit theta-scheme, tend to yield numerical approximations that are polluted by spurious oscillations. The chapter further analyses how these oscillations depend on the haptotactic coefficient.

The main scientific result of Chapter 3 (Paper II) is the derivation of a condition on the time-step size under which the fully discretized scheme with application of nonlinear FCT limiting ensures positivity-preserving solutions as required by the underlying physics of the problem at hand. The second part of Paper II demonstrates the effectiveness of the FCT limiter scheme to suppress spurious oscillations which would be generated without appropriate stabilization techniques. The adopted Zalesak-type limiter is not per se novel, however, its application in the context of the cancer invasion model is. Section 3.2 (Paper III) extends the previous numerical study by considering different parameter settings and limiter choices. The paper is relatively short as it was published as a proceedings paper written in summary style.

Chapter 4 extends the results from the previous chapters to a cross-diffusion system in which two cross-diffusion equations are coupled with each other and with two ordinary differential equation to yield a model for describing rivaling gang interactions. The scientific highlights of this chapter are the existence proof of a unique, non-negative global solution to the model equations and the derivation of a CFL-like condition under which the flux-corrected numerical scheme ensures positivity-preserving solutions. The Chapter ends with a numerical study that investigates the model’s behavior under different parameter settings.

Chapter 5 somewhat stands out from the rest of the PhD thesis and investigates a nonstandard explicit finite difference scheme for an ODE model of the influenza disease. The numerical scheme builds on a strategy proposed by Mickens to overcome numerical instabilities. The main findings of the chapter are the theoretical proof that the influenza disease model yields positivity-preserving solutions if the initial conditions are positive and the derivation of a nonstandard explicit finite difference scheme based on Mickens' approach that ensures positivity preservation of approximate solutions under certain assumptions on the time-step function.

Overall, the different chapters of the PhD thesis are well written and nicely complement each other. While Chapter 5 stands out from the rest of the thesis in terms of its topic, it can also be seen as an alternative pathway to deriving monotone schemes. The title of the thesis, however, is somewhat unspecific since the core part of the work deals with stabilization techniques for cross-diffusion problems. In my opinion, the scientific highlights of this work are the theoretical existence proofs followed by the CFL-type criteria for choosing the time-step size to obtain positivity-preserving approximate solutions. What is somewhat uncommon for a cumulative PhD thesis are the long and varying author lists. From the five papers that form the core chapters of the PhD thesis, the PhD candidate is the lead author in only one journal paper and one conference proceedings both dealing with the cancer invasion model. However, I assume that this fact can be explained by the multiple academic stays of the PhD candidate that have led to the final PhD thesis.

In summary, I conclude that the PhD thesis has various scientific contributions both at the theoretical (e.g., existence proofs) and the methodological level (e.g., CFL-like time-step size criteria). I therefor recommend accepting it for presentation and defense.

Sincerely yours

(Dr. rer. nat. Matthias Möller)