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Report on the doctoral thesis

"Numerical solution of degenerate parabolic problems"

by Sunčica Sakić

Introduction:

The Richards equation is a mathematical model for unsaturated flow in a porous medium. It models many real-life applications, like the flow in the vadose zone, through hygiene products, or fuel cells. From a mathematical point of view, Richards' equation is nonlinear and parabolic, but also doubly degenerate, featuring both fast and slow diffusion. Its solution often lacks regularity, which makes the development of efficient discretization schemes, or of linear iterative approaches and their analysis a challenging task.

Although the Richards equation has been studied for almost one century, the development of efficient numerical schemes is far from being established, which makes the topic of the thesis a very timely one. The thesis of Sunčica Sakić, which I studied with much interest, is a step forward in this direction. It proposes a discontinuous Galerkin (DG) approach, for which the convergence is proved rigorously by providing error estimates. Further, it addresses aspects like the adaptive discretization, or linearization, which makes this thesis relevant also from a practical point of view.

Thesis:

This thesis is addressing various aspects related to the numerical discretization for the Richards equation, written in the pressure-head formulation. The numerical scheme is involving a DG method. In my view, the following aspects constitute the main outcome of this research:

- The development of a numerical discretization scheme (in both time and space);
- The mathematically rigorous convergence analysis, and the error estimates;
- The adaptive strategy in both time and space;
- The convergence study of a Newton-like method, and the effect of the Anderson acceleration.

The effectiveness of the algorithms developed here is proved not only theoretically, but also by applying it to problems involving realistic parameters.

The thesis is well structured. After a brief introduction, it starts with a presentation of the Richards equation, which I find very useful. It includes the mathematical model, its various possible formulations, and different types of boundary conditions. Also, the main challenges and ideas are discussed in a few pages, providing a kind of guideline to the content. This helps to understand better the results obtained here.

The original contribution is contained in the following chapters. The second states the mathematical framework, including the abstract spaces for the weak solution, as well as for the spatial discretization. Also, the spatial discretization is introduced, involving an interior penalty DG scheme. This scheme is analyzed in Chapter 3, for the semi-discrete case. Specifically, in the absence of gravity, the stability of the scheme is proved and a priori error estimates are obtained. These results are provided under certain assumptions on the parameter functions, some of them being restrictive from the application point of view. Particularly, the permeability is uniformly strictly positive definite, which rules out the slow diffusion case if induced by a vanishing relative permeability. Also, the pressure and the flux are assumed to have a high regularity in space (H^s) for some $s \geq 2$, while the time derivative of the pressure is essentially bounded. For degenerate situations, these assumptions may only hold true locally but not globally, so extending the proofs for the error estimates so that such assumptions are avoided would be a further step forward.

The theoretical estimates are verified practically in the numerical experiments given in Chapter 4. First, one academic example is discussed. Depending on the choice of the parameters, one either ends up with a fast diffusion problem, or with the porous medium equation. This test case is well chosen, since an exact solution is known, also for degenerate situations. The numerical tests show that the proposed scheme behaves at least as good as predicted theoretically in the fast diffusion case, in agreement with the order of the polynomials. For the slow diffusion case, the convergence is still good, but does not follow the order of the method. This can be explained by the fact that, in this case, the regularity assumptions are not fulfilled globally.

Chapter 5 is discussing the discretization in time, starting from the spatial discretization introduced in Chapter 3. This extends the spatial DG scheme to a space-time one, STDG. The scheme is clearly formulated, and, in my view, extending the stability analysis and the error estimates from Chapter 4 to the fully discrete case would be a very good publication. This part is then continued in Chapter 6, where the fully discrete problems are considered as nonlinear algebraic systems, and for which a damped Newton iterative scheme is proposed. Since the Newton scheme may fail to converge if the initial guess is not close enough to the solution, and this in particular in degenerate cases, an Anderson acceleration technique is adopted. The iterative schemes with and without Anderson acceleration are tested, showing the superiority of the latter for the price of a very inexpensive postprocessing step. This approach is tested on a problem involving realistic parameters, namely a heterogeneous dam problem. This features all challenges presented until now, and, additionally, includes an outflow boundary condition describing seepage. This chapter ends with the presentation of an hp-adaptive strategy, tested again on a realistic example. In my view, this chapter can be the basis of another publication in a scientific computing journal.

Evaluation:
This contribution in this thesis is in the development and the analysis of efficient numerical schemes for the Richards equation. The key ingredient is an interior penalty DG approach, which is analyzed rigorously. Also, the adaptive discretization, as well as the linear iterative solution to the emerging nonlinear, fully discrete problems are studied. The results are relevant and correct, and have led to a publication in one of the leading journals in the numerical analysis, and one in the proceedings of an important conference in the field. I am convinced that this work can lead to other publications in journals focusing on scientific computing or porous media flows.

This thesis, which is well written, leaves room for further discussion, which, in my view, is a good point. Specifically, I think the following aspects can be addressed in the defense:

1. As a general observation, solutions to degenerate parabolic problems, and in particular to the Richards equation, lack regularity. On the other hand, at least from a theoretical point of view higher order methods are truly efficient when approximation solutions with sufficient regularity (in both, space and time). How can we see that the DG scheme used here (in space, resp. space-time) performs better than others, particularly when the solution features free boundaries?

2. What are the advantages of the hydraulic head formulation used here, compared to the pressure-based one?
3. How to deal with situations when the Kirchhoff transformation (or equivalent, see (1.8) – needed for the hydraulic head formulation) cannot be computed explicitly?
4. What is the meaning of the first boundary condition in (1.16)? Is there any way to reduce it to a standard (e.g. Robin-type) boundary condition?
5. Assuming that the pressure head is H^2 in space, which allows rewriting (2.11) as (2.14), is quite strong, at least globally. For the Richards equation, this assumption may not hold true globally. Can the proposed DG scheme be adapted to deal with situations where the solution lacks regularity?
6. Why was the arithmetic average of the permeability functions chosen in (2.23). Wouldn't it be more suitable to use e.g. a weighted harmonic mean, as the permeability is not vanishing and, at the same time, this is the outcome of a mass-conservative averaging?
7. How does the analysis in Chapter 3 change when gravity effects are included?
8. Can one extend the analysis in Chapter 3 to remove the strong assumptions ($\boldsymbol{K}$ – nondegenerate, regularity for u and the flux, in both space – H^s with $s \geq 2$, and time – that $\partial_t u$ in L^∞ and in L^2 lies)?
9. What time discretization is used in Chapter 4, and how is the time step chosen?
10. Does the convergence behavior of the iterations in Chapter 6 change w.r.t. the regularization parameter, or with the spatial mesh? Are there any rigorous convergence proofs?

To conclude, I think that the work of Sunčica Sakić demonstrates a good understanding of the numerical analysis for partial differential equations, particularly degenerate parabolic equations. Through this thesis, she has proved the ability to carry out creative scientific research of excellent quality. The cited literature shows an extensive documentation. The results are presented in a very clear manner. I have no doubt that this work has the expected level of a Ph.D. and, therefore, I recommend this thesis to be defended.

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