Review of the thesis
Mathematical modeling of two-phase compositional flow in porous media
by Ing. Jakub Solovský.

The thesis deals with its main subject - the modeling of two-phase compositional flow in porous media - from four important views presented in several chapters. Firstly, it presents a mathematical derivation and physical reasoning behind the systems of partial differential equations (PDEs) that are used in this subject. The description is mainly based on a combination of particular models into a single more general one. Secondly, it suggests numerical methods to be used to solve the model approximately with many implementation details. It exploits quite modern numerical algorithms, although in their simplest forms. Third, it suggests and successfully realizes parallel implementation of numerical solvers which is necessary to solve some larger scale problems. Finally, it confronts the numerical results with data obtained by several laboratory experiments and provides some valuable conclusions.

The topic is a natural continuation of the research realized in recent years by the group at the Department of Mathematics of FJFI at ČVUT in a valuable cooperation with an international research group. The topic is still very current with the main motivation from environmental engineering science on CO_2 geological sequestration. In my understanding the aim of the thesis is to advance the mathematical modeling of practical real field scenarios with the support of data from laboratory experiments. This aim is clearly fulfilled and the results are an important scientific contribution in related research. The author is listed as the main contributor and writer for at least two publications in the journals with the highest scientific reputation in computational physics that is a clear mark of the quality for the presented research.

From the point of view that each of these views is complex enough, it is remarkable that such compilation is provided in a single thesis. The overall text is clearly well written and structured from a formal point of view. The author has managed successfully to put together all chapters with these four different topics in an unified notation and style. I have no comments concerning the usage of English vocabulary and grammar. The methodology of presentation

Due to my main research interests, I will concentrate in my review on the one particular topic presented in the thesis, namely, the numerical methods. I understand and appreciate the approach of the author to this topic that is well justified in a large international community for which the emphasis is given on numerical modeling of nontrivial systems of PDEs as a tool to provide physical and engineering insights into important practical applications which are otherwise not available. To exaggerate, the numerical methods are a necessary evil to obtain valuable information from mathematical models. Consequently, the numerical methods are presented in a way that can be used for implementation, to some extent, in a rather straightforward and unified manner.

As a consequence of such an approach, the author presents a very formal system of PDEs (3.1) that he aims to solve numerically in a robust way. The numerical methods are chosen such that they can be applied to such a system without any specific knowledge or particular restrictions applied to (3.1). Although one can understand such an approach in general, I am missing at least some remarks and discussions in the description on numerical methods that, when missing, may mislead otherwise the readers unfamiliar with the topic. For instance, it is very formal to allow all coefficients in (3.1) to be solution-dependent (that is really considered in numerical methods) and not to mention immediately that such dependency is treated only formally and for some coefficients it shall be considered only in a very mild form, if at all. In theory, the systems (3.1) include as special cases the nonlinear hyperbolic systems in conservative or nonconservative form or nonlinear cross-diffusion systems that are very difficult problems in general. In particular, I found no discussion why the nonconservative and conservative form of advection is given separately in (3.1) and, in fact, according to my observation, the conservative one using the vectors "a" is not used in any particular models in the following sections.

Concerning the time discretization the choice of backward Euler method together with semi-implicit approach for the linearization of nonlinear coefficients is claimed to be used. It is a well justified choice, nevertheless, this is not completely right as the nonconservative advection terms are discretized in an explicit-implicit form and the discretization of the conservative advection is fully explicit. Clearly, this objection is only formal as such mixed discretizations are well justified.

I am most surprised by the fact that no discussion at all is given on the choice of time steps. It seems to me that the time step is always constant for each space grid in all presented numerical experiments. Even if advantageous variable time steps are not considered, there are at least two important reasons why some discussion on the size of constant time steps is necessary. If too small time steps are used, the efficiency of computations can be very low and the computational efficiency is one of the main topics of the chosen research. Second, if too large time steps are chosen, some instabilities can occur due to explicit parts of the time discretization in advection terms or due to (semi-) linearization of the nonlinear coefficients. In such a way, this topic has to be learned by readers themselves, but at least some warnings with references to literature shall be given. In particular, the restriction on the time step due to the so-called CFL condition for the advection can be derived for the chosen discretization, in my opinion, and that is very often useful in general. Similar objections can be stated for no discussion on conservation properties of numerical schemes, although the PDEs are based on conservation laws.

The formalism of the presentation of numerical methods is sometimes going too far, subjectively, so some facts about them are blurred. As a small illustration, the notation with superscript "upw" reserved for an upwind discretization is used on page 42 in a special case of stationary diffusion for a central (no upwind) approximation (3.42) that would be better to denote differently. The superscript "k" is used even if (purely time dependent) coefficients are evaluated at time t^{k+1}. Finally, the error coming from time discretization is excluded from the convergence test for the example with known semi-analytical solution and only the one coming from the space discretization is presented. No explanation or motivation to do so is given, and, quite likely, the experimental order of convergence of spatial-temporal discretization is lower for the chosen example.

As stated at the beginning of my comments, my objections are that the mentioned issues should be to some extent included in their description. It might be also important in a future development of the research where more specialized numerical techniques can help to provide more efficient and accurate results. Nevertheless, the given description of numerical methods in the thesis itself is valuable and of a good quality. In fact, I do not have similar objections to other parts of the thesis. The part on the mathematical derivation is nicely written and it can be offered as a very suitable introduction to the topic. The part on the parallelization of linear solvers seems to use some recent nontrivial approaches in non overlapping domain decomposition techniques. The interpretation of numerical results with respect to available measured data obtained from laboratory experiments seems to be realistic and not overvalued.

Finally, I have a few small observation of possible misprints:

- I did not find definitions of the notation for upsilon in (3.10) and x_E in (3.15)
- the index i in the step 4 of Algorithm 4 might start from 1 not 0

I suppose that the author will comment on my observations in his defense. Additionally, I would like to ask why he calls the used space discretization for scalar PDEs to be discontinuous Galerkin method as in the current form it can be viewed as a finite volume method. Is there an intention to extend the order of this discretization method?

I evaluate the thesis positively and I can clearly recommend it to be accepted for the defense and to award the title PhD. to Ing. Solovský afterwards.

Bratislava, 9.12.2022

Doc. RNDr. Peter Frolkovič, CSc.
Katedra matematiky a deskriptívnej geometrie
Stavebná fakulta, Slovenská technická Univerzita v Bratislave