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Turbulence structure and particle transport in particle loaded non-Newtonian Fluids

Thesis for the degree of Philosophiae doctor

Trondheim, October 2018

Norwegian University of Science and Technology
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ISBN 978-82-326-2638-0 (printed version)
ISBN 978-82-326-2639-7 (electronic version)
ISSN 1503-8181

Doctoral theses at NTNU, 2019:285

Printed by Skipnes Kommunikasjon AS

Abstract

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Preface

The work presented in this thesis was carried out in the period from September 2014 to July 2017, at the Department of Energy and Process Engineering at the Norwegian University of Science and Technology. The project has been funded through the SIMCOFLOW project, carried out by the SINTEF Materials and Chemistry. I gratefully acknowledge the financial support from the Research Council of Norway (project no. 234126/30).

I wish to thank my supervisor, Professor Bernhard Müller, for allowing and encouraging me to pursue my own ideas, while ensuring that I stay on planned schedule and agreed deadlines. I am especially thankful for a lot of patience during the beginning of my PhD when I had a lot to learn and catch up with. I would like to thank my co-supervisor Tore Flåtten for all our scientific and nonscientific discussions. I am especially thankful for teaching me countless mathematical concepts and tools and for having endless faith in our work even when I didn't. I wish to thank my co-supervisor Marica Pelanti for arranging my stay at ENSTA ParisTech and for being a great host during my six months stay in Paris. My stay in Paris has been a valuable experience both professionally and personally. Further, Marica's knowledge on HLL(C) schemes has been an invaluable asset when I first started to work with this schemes. I also wish to thank my co-supervisor Ernst Arne Meese. We did not collaborate closely, but I appreciated our discussions and interest in my work.

These three years would have been much less fun without all my co-workers from the Department of Energy and Process Engineering. I am very thankful for all Green Room breaks, movie nights, dinners and skiing trips, but most of all, thank you for sharing with me the joys and excitement of doing sweet science. There are too many people to name them all, and I will point out Øyvind, Ehsan, Eskil and Anna who had a misfortune of sharing an office and an apartment with me.

Lastly, I wish to thank all my friends back home in German for not forgetting me during my long absences, and I wish to thank Martina for her endless support in all my endeavors.

Trondheim, December 2018
Alexander Busch

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Nomenclature

x	Description
y	Description

Contents

1 Introduction

1.1. Motivation

phenomena [5] phenomena [3] phenomena [2] phenomena [1] phenomena [4]

phenomena [1] phenomena [4] phenomena [3] phenomena [2] phenomena [5]

Hyperbolic conservation laws are widely used to model a variety of physical phenomena, such as fluid dynamics, geophysics, biomechanics, electrodynamics, magnetohydrodynamics, astrophysics, etc. They are also heavily used in modeling multiphase flow phenomena [1], which is of particular interest for the SIMCOFLOW project [**wallis1969**][1]. In this thesis, we consider already existing models and focus on numerical methods for hyperbolic conservation laws rather than on physical modeling. To simplify the analysis, we mostly use simpler models (such as the Euler equations) instead of more complicated multiphase flow models. However, we believe that the numerical tools developed here should be applicable to a wide class of hyperbolic problems.

1.2. State of the art

1.3. Goals and thesis outline

In particular, our goals are:

[1] The PhD project is a part of the research project *SIMCOFLOW – a framework for complex 3D multiphase and multi physics flows* carried out by SINTEF Materials and Chemistry from July 2014 until June 2017 and funded by the Research Council of Norway.

- Develop LTS extensions of the HLL and HLLC schemes.
- Study entropy stability of the LTS-HLL(C) schemes.
- Study positivity preservation of the LTS-HLL(C) schemes.
- Study boundary and source term treatment in the LTS methods.

The thesis outline and contributions can be summarized as follows: in chapter **??** we present the mathematical models we solve, we outline the framework of the numerical methods we will consider, and we present the existing LTS methods. In chapter **??** we present the main results:

- In **??** we develop LTS extensions of the HLL and HLLC schemes. We develop the LTS-HLL-type schemes, we determine their numerical viscosity and flux-difference splitting coefficients, and we investigate their convergence. This new class of schemes allows us to deduce some already existing LTS methods such as the LTS-Roe and LTS-Lax-Friedrichs, and it allows us to deduce LTS extensions of other methods, such as the Rusanov and Engquist-Osher schemes. Parts of this section are adapted from our second journal paper *Large Time Step HLL and HLLC Schemes* **[jp2]**.
- In **??** we study entropy stability of LTS-HLL-type schemes. We use modified equation analysis to investigate how entropy violations occur in the LTS-HLL-type schemes and how can they be avoided. Parts of this section are adapted from our second conference paper *Numerical Viscosity in Large Time Step HLL-type Schemes* **[cp2]**.
- In **??** we study monotonicity and positivity preservation of LTS-HLL(C) schemes. We determine monotonicity conditions on numerical flux function of an LTS method, and we show that positivity preserving conditions in LTS methods are stronger than in standard methods. We investigate different ways how is positivity lost in the LTS-HLL scheme, and we propose a simple way to increase robustness of the scheme by adding numerical diffusion. This section closely follows our third journal paper *Monotonicity and Positivity Preservation in Large Time Step Methods* **[jp3]**.

In addition to the work on the LTS-HLL(C) schemes, we applied the LTS-Roe scheme to a one-dimensional two-fluid model and focused on the treatment of the source terms and the boundary conditions. By introducing a new type of boundary conditions and by treating source terms in a similar way as

, we are able to notably improve accuracy of the solution. These results are presented in **??**. Content of **??** corresponds to our first journal paper *Large Time Step Roe Scheme for a Common 1D Two-Fluid Model* [**jp1**], and our first conference paper *Boundary and Source Term Treatment in the Large Time Step Method for a Common Two-Fluid Model* [**cp1**]. Finally, chapter 2 closes with conclusions and comments regarding possible further research directions.

In the presentation of the thesis results, we aimed to give a structured overview of our findings, but also tried to depict the order in which our work was done and how it was motivated.

2 Conclusions and Outlook

2.1. Conclusions

We developed and investigated Large Time Step HLL-type finite volume methods for hyperbolic conservation laws. Our major contributions are presented in **????** and they can be summarized as follows:

- **??**: We developed the LTS-HLL-type schemes.
- **??**: We investigated entropy stability of LTS methods by using the modified equation analysis.
- **??**: We investigated monotonicity and positivity preservation of LTS methods.
- **??**: We investigated the treatment of boundary conditions and source terms in LTS methods.

In **??** we interpreted the HLL scheme as a numerical scheme for scalar conservation laws. We developed a two-parameter HLL-type schemes, and determined the TVD conditions on the wave velocity estimates. We showed that the HLLE scheme is consistent, TVD and entropy stable, i.e. it converges to the entropy solution. We then developed the LTS-HLL-type schemes. We described these new schemes in the numerical viscosity, flux-difference splitting and wave propagation form, and we determined the TVD conditions on the wave velocity estimates. We showed that the LTS-HLLE scheme is consistent and TVD. However, a rigorous proof of entropy stability remains unresolved.

This new class of schemes provided greater flexibility in constructing new schemes because it has two free parameters, while at the same time it allows us to simply deduce LTS extensions of standard one-parameter methods, such as the Roe, Lax-Friedrichs, Rusanov, Godunov and Engquist-Osher schemes. Working along the lines of the approach above, we extended the standard HLL and HLLC schemes for systems of conservation laws to the LTS-HLL(C) schemes.

In **??** we investigated the question of entropy stability by using the modified equation analysis. First, we used the modified equation to quantify the amount of numerical diffusion in the LTS-HLL-type schemes. We performed numerical experiments to gain better insight into how entropy violations happen in LTS methods, and to conjecture how are they avoided in certain LTS-HLL-type schemes. In particular, we conjecture that the LTS-HLLE and LTS-Rusanov schemes are entropy stable. Numerical results for both scalar conservation laws and the Euler equations are in agreement with theoretical results obtained with the modified equation analysis.

In **??** we investigated questions of monotonicity and positivity preservation. First, we determined the monotonicity conditions on the numerical flux function of an LTS method, and we showed that the LTS-Lax-Friedrichs scheme is monotone. Then, we moved to systems of equations and showed that the positivity preserving conditions in LTS methods are stronger than in standard methods. For some special cases of initial data, we described how loss of positivity preserving occurs in the LTS-HLLE scheme, we showed that the LTS-Lax-Friedrichs scheme is positivity preserving, and we numerical demonstrated that robustness of the LTS-HLLE scheme can be increased by adding numerical diffusion.

Lastly, in **??** we applied the LTS-Roe scheme to a one-dimensional two-fluid model and focused on the difficulties related to the boundary conditions and the source terms. We proposed a new way to define the boundary conditions in the LTS framework, and we handled the source terms by following Morales-Hernández and co-workers [**mur06**, **mor12a**, **mor12b**, **mor14**, **mor17**]. It is shown that the accuracy of the solution can be greatly improved by appropriate treatment of boundary conditions and source terms.

2.2. Future outlook

Large Time Step methods have been around for more than thirty years, but they never really became a part of the mainstream in the finite volume methods/hyperbolic conservation laws community. Nevertheless, there seems to be an unfailing appeal in their increased stability and explicitness, and it seems that throughout their history there was always someone trying to exploit their full potential.

I am not convinced that my humble contributions will change this trend. But in case time proves me wrong, and for those who will be interested in further exploring LTS methods I will consider some possible directions and possibilities.

- *Numerical diffusion:* The majority of the numerical investigations performed by us and other authors suggest that most errors in LTS methods appear in form of oscillations around shocks and contact discontinuities. These errors can be reduced by introducing numerical diffusion, as it was successfully done by Lindqvist et al. [**lin16**], Solberg [**sol16**] and Nygaard [**nyg17**]. Therein, the amount of the numerical diffusion being added is partially automated and partially tuned manually. We showed that manually adding numerical diffusion increases the robustness of LTS methods. Any LTS method aiming for generality and robustness will need to have a sophisticated and fully automatized mechanism to add numerical diffusion.

  One idea on how to do this might be along the lines of how higher order TVD methods are designed: use second-order scheme where the data is smooth, and reduce it to a first-order schemes around discontinuities. We believe that is possible to construct an LTS method which will automatically introduce appropriate amount of numerical diffusion around discontinuities or when loss of positivity is likely to happen.

- *Computational efficiency and convergence rates:* Even though the computational efficiency is one of the most attractive features of LTS methods, it was not the main objective of our investigations. However, any strong argument in favor of LTS methods must be supported by evidence of increased computational efficiency.

  Our preliminary investigations suggest that the decrease in computational time is greatest immediately after going from $\bar{C} = 1 \rightarrow \bar{C} = 2$. A further increase in Courant number yielded smaller and smaller gains in computational time (see for instance our papers [**jp1**, **jp2**, **cp1**]). This suggests that in terms of computational time, it might be optimal to use a relatively small Courant number. A better criterion for choosing the Courant number would be computational efficiency, which was also investigated in our papers [**jp1**, **jp2**]. Therein, computational efficiency and convergence rates are studied, and it is observed that LTS methods generally have higher convergence rates than their first-order counterparts. We note that our numerical codes were build to be simple and modular, and we believe that by optimizing the code we could further improve the gains in computational time and computational efficiency.

Since a significant increase in Courant number leads to oscillations and inevitable decrease in accuracy, it might not be fruitful to push the Courant number above a single digit numbers. Another attractive feature of keeping the Courant number relatively low is that it might result in increased computational efficiency while applying the LTS method only on acoustic waves, which brings us to the next point.

- *Low Mach number flows:* LTS methods might be an attractive candidate for low Mach number flows, where it would be possible to use very high Courant numbers for the acoustic waves, and standard methods for the slow waves. We obtained some preliminary results in this direction in our paper [**jp1**], where we considered the water faucet test case. Therein, slow waves are not strongly affected by acoustic waves and it was possible to use an LTS method for the acoustic waves in a straightforward way, which led to a notable decrease in computational time and increase in accuracy of slow waves.

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A
Research papers

A.1. Main contributions

[1] A. Busch, A. Islam, D. Martins, F. P. Iversen, M. Khatibi, S. T. Johansen, R. W. Time, and E. A. Meese. "Cuttings Transport Modeling - Part 1: Specification of Benchmark Parameters with a Norwegian Continental Shelf Perspective". In: *SPE Drilling & Completion* preprint (preprint 2018). Main. URL: https://www.onepetro.org/journal-paper/SPE-180007-PA.

[2] Alexander Busch and Stein T. Johansen. "An Eulerian-Lagrangian CFD Study of a Particle Settling in an Orthogonal GNF Shear Flow". In: *Journal of Non-Newtonian Mechanics* In Review (tbd 2018). Main.

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Main, pp. 1–16. URL: http://www.ar.ethz.ch/cgi-bin/AR/view?DOI=10.3933/ApplRheol-28-25154.

My contributions to manuscripts:

All manuscripts were written by me. Flåtten proposed the *Steady-state boundary conditions* (SSBC) used in papers [**cp1**, **jp1**], and determined the flux-difference splitting coefficients of the LTS-HLL scheme [**jp2**], and TVD conditions for the LTS-HLL scheme [**jp2**]. Flåtten contributed to all articles by discussing the manuscripts and reported results. Müller contributed to all articles by discussing the manuscripts and reported results.

Journal paper 1 (jp1)

Large Time Step Roe scheme for a common 1D two-fluid model

Marin Prebeg, Tore Flåtten and Bernhard Müller

Applied Mathematical Modelling, Vol. 44, pp. 124–142, 2017.

Conference paper 1 (cp1)

Boundary and source term treatment in the Large Time Step method for a common two-fluid model

Marin Prebeg, Tore Flåtten and Bernhard Müller

In: Proceedings of the 11th International Conference on CFD in the Minerals and Process Industries. Melbourne, Australia, 2015.

A.4. Additional contributions

[1] Ulf Jakob F. Aarsnes and Alexander Busch. “Transient Modeling of One-Dimensional Solid-Liquid Flow in Conduits”. In: *International Journal of Multiphase Flow* 105 (2018). Additional, pp. 102–111.

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A.6. Other works

Curriculum vitae