dr hab. Andrzej Wyszogrodzki, prof. IMGW-PIB
Instytut Meteorologii i Gospodarki Wodnej
Państwowy Instytut Badawczy
ul. Podleśna 61, Warszawa

Warszawa, 28 stycznia 2019 r.

Review of the PhD thesis of MSc **Maciej Waruszewski**

„Genuinely third-order advection scheme for atmospheric flows : the Multidimensional Positive Definite Advection Transport Algorithm approach"

The thesis was prepared at the Institute of Geophysics, Faculty of Physics, University of Warsaw, under the supervision of Prof. **Hanna Pawłowska.**

Introduction

In his PhD thesis, Mr Maciej Waruszwski has tackled the task of construction, verification and application of a genuinely third-order variant of Multidimensional Positive Definite Advection Transport Algorithm (MPDATA), designed for variable flows in multiple dimensions. A significant part of the presented in thesis material is based on publication Waruszewski et al. (2018), extended with additional details, discussions, and simulations aimed at proving the usability of the developed algorithm for geophysical applications.

The structure of the dissertation paper.

The dissertation is written in English and contains: acknowledgement section, an abstract in two languages (Polish and English), 8 topical chapters, two appendices and a bibliography – in a total of 82 pages. The chapters are organized as follows:
Chapter 1, Introduction, contains the general overview of the research problems leading author to formulation of the presented thesis, a short description of goals, and an overview of the basic properties of MPDATA type of schemes.
Chapter 2, outlines the standard second –order-accurate, finite difference (FD) MPDATA scheme for the solution of a homogeneous, generalized transport equation, derivation of the algorithm in one- and multi-dimensions, as well as brief lists of advanced options of this scheme.
Chapter 3 derives the fully third-order accurate MPDATA with details of the construction of the third-order error compensating pseudo-velocity, both by hand and with the computer algebra.
Chapter 4 provides details of the implementation of MPDATA algorithm in an open-source library *libmpdata++*. This chapter presents highlights of the library, particularly stressing the design choices allowing easy, efficient, and maintainable implementation of the new scheme.
Chapter 5 verifies the newly developed MPDATA and assesses its merits compared to the established variants of the scheme. Three test problems are considered: bespoke 3D solution with a stationary Jacobian and a non-stationary generalized flow field (Roache, 2002) to verify the correctness of the implementation, and two established benchmarks (Nair and Jablonowski, 2008; Lauritzen et al., 2012) idealizing tracer transport on the sphere in rotating deformational flows. The first benchmark addresses a cross-polar transport in a velocity field composed of two vortices advected over the poles; whereas, the second focuses on tracer correlations in a reversible deformational flow.
Chapter 6 demonstrates the utility of the fully third-order-accurate MPDATA beyond the passive tracer advection, for simulating dry atmospheric dynamics in the nonhydrostatic regime, including in particular the ILES study of three-dimensional turbulent atmospheric boundary layer flow.
Chapter 7 presents comparison between third-order-accurate MPDATA and its second-order variants for simulating more complicated case of moist precipitating supercell dynamics.
Chapter 8 presents conclusions and final remarks.
Additional technical details of modified equation analysis of standard MPDATA and the description of warm-rain microphysics are delegated to **appendices**.
Finally, the **bibliography** section includes total of 91 items.

Evaluation of the Thesis

The thesis is written in a communicative way, an easy to read and understand English language, very well presented interdisciplinary combination of the advanced mathematical apparatus, numerical modelling and scientific analysis of the physical results. My general feeling is that manuscript is of very high quality and offers interesting analysis of the development process of a complex advection scheme, and investigation of its applicability to modeling geophysical flows at many scales and complexities. Below I list the strengths and rare weaknesses of the presentation as well as indicate additional potential areas which could be further deeper investigated.

Chapter 2 reviews the algorithmic details of the standard MPDATA scheme for integrating the homogeneous generalized transport equation, with the aim of providing the necessary background for the fully third-order-accurate scheme. This section introduces also briefly some of the advanced options of this algorithm as the "infinite-gauge" two-pass variant of the scheme extending MPDATA for transporting fields of variable sign, and the nonoscillatory option extending MPDATA to full monotonicity preservation in the framework of multidimensional Flux Corrected Transport (FCT) algorithm. Furthermore this section describes extrapolation/interpolation procedure for computing advective velocities required to maintain second-order accuracy for time dependent flows, and finally modification of the psuedo-velocities allowing for a third-order correction of MPDATA for generalized transport equation with constant coefficients. In my opinion the estimate of advective velocities at the intermediate time levels presented in subchapter 2.3.3 is really not an option but a core algorithm required to maintain the second-order accuracy and this subsection should be moved to Chapter 2.2. The additional information which fits into this Chapter could describe algorithmic details of the ILES properties of the MPDATA. While short historical overview of ILES is included in the introduction, this additional information may help to better understand outcomes from the numerical experiments presented in Chapter 6.4 (as e.g. for analysis of the organized convection at the Fig. 6.4).

Chapter 3 along with the additional information in the Appednix A is the most important chapter for this dissertation, where the third-order accurate MPDATA scheme for spatially and temporally variable flows is developed. A starting point is the derivation of a third-order error compensating pseudo-velocity based on the leading-order truncation error of standard MPDATA. Further, the unified expression for the resulting pseudo-velocity, including combined effects of various MPDATA options is discussed. The presented analysis is mathematically very advanced and contains a novel computer algebra analysis to validate and extend the modified equations of MPDATA. Two statements presented in the discussion of Chapter 3.3 are very interesting but need more elaboration. First, it is not clear how the iterations of third-order error-compressing pseudo-velocity (3.11) benefit the parallel distribution-memory communication, especially that the code is implemented in libmpdata++, which allows the shared memory parallel execution using threats (e.g. with the OpenMP library). The next statement on the possibilities of admitting larger time steps is also very intriguing. In the description of several experiments there is an information on "time step continuously adapted to keep the maximum Courant number … less than 1". It is however not clear whether this procedure describes really the continuous adaptation in the course of simulation, and how this adaptation is related to the above mentioned statement on admitting the larger time steps.

Chapter 4 overviews the open-source library of MPDATA-based solvers, *libmpdata++* , where the fully-third order MPDATA scheme was implemented. Author of this thesis is one of the core developers of this open-source free/libre library, thus the choice of this implementation was a natural for him. On the one hand the library provides a set of reusable components for building MPDATA-based numerical models, on the other hand it focuses on readability and maintainability, strictly adhering to the modern software-development practices such as automatic testing. This implementation allows for a further porting of the new MPDATA algorithm into the main branches - finite difference (FD) and finite volume (FV) - of EULAG model.

Chapters 5, 6, and 7 provide the verification of the newly developed scheme and its comparison with older variants of MPDATA for a variety of test cases and benchmarks. This analysis is very extensive and provide many useful behavioral information on scheme properties, which is summarized in the Chapter 8. The conclusion form the presented benchmarks reports general improvements of the novel third-order scheme in comparison to the established second-order and third-order constant-coefficient variants, especially for the case of tracer advection. In the presented analysis I have found however some minor discrepancies. In the case presented in Chapter 7.3 - which illustrates the evolution of the idealized superstorm – the included discussion suggest that the fully third order MPDATA has positive impact on the coarser resolution solutions. This statement is not fully supported by the Fig 7.2 and 7.3. From these figures the solution form Mg2No scheme at coarser 4km resolution is more consistent with the high 0.5km resolution comparing to the equivalent results from the Mg3No scheme. The coarse solution of new Mg3No scheme shows distinct spacing between the convective cells and additional mode in the center, which is not present at the higher resolutions. A closer analysis of the Fig 7.4 reveal that for most of the time the coarse Mg2No solutions are a bit closer to the high resolution run than for Mg3No version, except for the mentioned in the analysis small overshooting of 1km resolution run which happens between ~30-60 min. Above figures confirms the well-known property, that the standard second-order in time MPDATA is a very well-established algorithm maintaining the quality of solution across many scales. The supporting graphics may indicate however the advantage of new Mg3No scheme for cloud resolving simulations at higher resolutions, which may be investigated in the future.

The author list also some basic properties of the transport schemes important for the atmospheric flows as conservation (of mass and other quantities), sign preservation and monotonicity. The application of the nonoscillatory option (e.g. in Chapters 5.3 and 5.4) shows distinctive behavior. In the case of moving vortices, enforcing the monotonicity in the Mg3No scheme leads to a significant loss of accuracy and drop of the convergence to the second-order. For the reversing deformational flow the nonoscillatory scheme retains the third-order convergence supposedly due to scale separation between the smooth large-scale flow variations and the sharper gradients of the transported tracer. Since the convergence of new MPDATA with nonoscillatory option is not uniform but rather case dependent, this may require deeper analysis in the future. Moreover, the conservation properties of the new algorithm were not explicitly investigated in the simulations and may also be a subject of further investigation.

A several minor linguistic defects were found in the text, which overall are not diminishing the general quality of the manuscript.
P 21, FCT acronym is not defined
p 24, Chapter 3.1.2 involving -> involved
on several instances: dependant - > dependent

Summary and recommendation

The thesis provided for this review contains very interesting and difficult scientific issues related to the process of development, analysis and application of the novel third-order accurate MPDATA algorithm. The presented work is generally of high quality and proves that Maciej Waruszewski can conduct complicated scientific research on his own, especially that a significant part of this dissertation was already published in a renowned scientific journal, where Maciej Waruszewski was the first/ corresponding author. My comments formulated in this review are minor and do not diminish the positive assessment of the dissertation.

In my opinion the thesis of Maciej Waruszewski meets all customary and formal requirements of the Act on Academic Degrees and Titles, and can be allowed for the public defense to obtain the PhD degree in Physics at the University of Warsaw.

Additionally, based on my above evaluation I'm utterly impressed with this dissertation which is proving student's interdisciplinary skills in the field of mathematics, atmospheric physics, computer science and numerical modeling. I propose to distinct Mr Maciej Waruszewski with an award for this significant and valuable effort.

W. Wyszogrodzki