Bound-Preserving Space and Time Discretizations for Convection-Dominated Problems (Online) 21w5065

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1 Overview of the Field

The design and numerical analysis of property-preserving high-resolution schemes for convection-dominated transport problems is a research area of utmost importance to many fields of Computational Fluid Dynamics. If the exact solution of the mathematical model is known to satisfy a conservation law, a maximum principle and/or an entropy inequality, the corresponding constraints should be taken into account when it comes to discretizing the governing equations in space in time. Failure to do so may result in numerical instabilities or nonphysical side effects, especially if exact weak solutions are discontinuous or exhibit steep fronts.

2 Recent Developments and Open Problems

Recent years have witnessed significant advances in the development of bound-preserving and entropy-stable schemes for scalar conservation laws and hyperbolic systems. However, derivation of high-order methods that provably satisfy all relevant constraints remains a challenging open problem. This four-day online work-shop has greatly advanced the state of the art by bringing together participants whose fields of expertise cover a wide range of complementary fields (hyperbolic, parabolic, and elliptic problems / space and time discretizations / finite volume and finite element methods / efficient algorithms and numerical analysis).

3 Scientific Program of the Meeting

The scientific program of the workshop featured 21 talks and a discussion session. The duration of each talk (including questions) was 50 minutes. In addition to the speakers, the audience included about 20 other researchers and graduate students who were invited to attend. The talks presented at the workshop introduced a number of fundamentally new and highly promising discretization techniques such as

- positivity-preserving time integrators and bounded interpolation in time [16, 17];
- limiters and relaxation techniques for high-order Runge-Kutta methods [12, 13];

- invariant domain preserving limiters for finite element schemes [8, 5, 14];
- limiter-based entropy fixes for nonlinear hyperbolic problems [15];
- bound-preserving Arbitrary Lagrangian Eulerian (ALE) methods [6, 2];
- well-balanced treatment of source terms via flux globalization [3];
- ways to enforce conservation principles for hyperbolic problems [1];
- error estimators for algebraic flux correction schemes [11];
- well behaved methods for steady-state convection-diffusion equations [4, 8];
- efficient matrix-free algorithms and GPU acceleration [9].

Further talks focused on applications to chemotaxis problems, compressible fluid dynamics [5], shallow water [10, 7] and atmospheric models, saturated flows in porous media etc.

The presentation of new numerical approaches was followed by insightful questions and stimulating discussions. Multiple groups have expressed interest in improving their methods using the new tools presented by other groups. The discussion session was focused on open problems (bound-preserving schemes for staggered and mixed finite element approximations, radiative transport equations, well-posedness of steady-state solutions to nonlinear hyperbolic problems, matrix-free remapping via subcell residual distribution etc).

4 List of Speakers

In alphabetical order: Remi Abgrall, Martin Berzins, Jesus Bonilla, Yekaterina Epshteyn, Jean-Luc Guermond, Hennes Hajduk, Gerardo Hernandez–Dueñas, Abhinav Jha, Volker John, Chris Kees, David I. Ketcheson, Alexander Kurganov, Dmitri Kuzmin, Philipp Öffner, Manuel Quezada de Luna, Hendrik Ranocha, Andreas Rupp, Laura Saavedra, Sam Stechmann, Eric Tovar, Arturo Vargas.

5 Involvement of Students

The online format of this workshop enabled the organizers to invite more graduate students than originally expected. The students attended talks to learn about new trends in their fields of study and ask questions. The 50-minute talk given by the graduate student Hennes Hajduk (TU Dortmund) has sparkled considerable interest of leading experts working in the field (Jean-Luc Guermond, Bojan Popov). The questions they asked directly after the talk were followed by a prolonged discussion in the virtual coffee break.

6 Outcomes of the Meeting

The organizers feel that the goal of bringing together different communities to promote collaborative research has been successfully achieved, which will result in new ground-breaking contributions to the field.

References

- Remi Abgrall. A general framework to construct schemes satisfying additional conservation relations. Application to entropy conservative and entropy dissipative schemes. *Journal of Computational Physics*, 372:640–666, 2018.
- [2] Robert W Anderson, Veselin A Dobrev, Tzanio V Kolev, Robert N Rieben, and Vladimir Z Tomov. High-order multi-material ALE hydrodynamics. *SIAM Journal on Scientific Computing*, 40(1):B32–B58, 2018.

- [3] Alina Chertock, Alexander Kurganov, Xin Liu, Yongle Liu, and Tong Wu. Well-balancing via flux globalization: Applications to shallow water equations with wet/dry fronts.
- [4] Derk Frerichs and Volker John. On reducing spurious oscillations in discontinuous Galerkin (DG) methods for steady-state convection–diffusion equations. *Journal of Computational and Applied Mathematics*, 393:113487, 2021.
- [5] Jean-Luc Guermond, Matthias Maier, Bojan Popov, and Ignacio Tomas. Second-order invariant domain preserving approximation of the compressible Navier–Stokes equations. *Computer Methods in Applied Mechanics and Engineering*, 375:113608, 2021.
- [6] Jean-Luc Guermond, Bojan Popov, and Laura Saavedra. Second-order invariant domain preserving ALE approximation of hyperbolic systems. *Journal of Computational Physics*, 401:108927, 2020.
- [7] Jean-Luc Guermond, Bojan Popov, Eric Tovar, and Chris Kees. Robust explicit relaxation technique for solving the Green-Naghdi equations. *Journal of Computational Physics*, 399:108917, 2019.
- [8] Hennes Hajduk. Monolithic convex limiting in discontinuous Galerkin discretizations of hyperbolic conservation laws. *Computers & Mathematics with Applications*, 87:120–138, 2021.
- [9] Hennes Hajduk, Dmitri Kuzmin, Tzanio Kolev, and Remi Abgrall. Matrix-free subcell residual distribution for Bernstein finite element discretizations of linear advection equations. *Computer Methods in Applied Mechanics and Engineering*, 359:112658, 2020.
- [10] Gerardo Hernandez-Duenas and Jorge Balbas. A central-upwind scheme for two-layer shallow-water flows with friction and entrainment along channels. *arXiv preprint arXiv:2104.02915*, 2021.
- [11] Abhinav Jha. A residual based a posteriori error estimators for AFC schemes for convection-diffusion equations. *Computers & Mathematics with Applications*, 97:86–99, 2021.
- [12] David I Ketcheson. Relaxation Runge–Kutta methods: Conservation and stability for inner-product norms. SIAM Journal on Numerical Analysis, 57(6):2850–2870, 2019.
- [13] Dmitri Kuzmin, Manuel Quezada de Luna, David I Ketcheson, and Johanna Grüll. Bound-preserving convex limiting for high-order Runge–Kutta time discretizations of hyperbolic conservation laws. arXiv preprint arXiv:2009.01133, 2020.
- [14] Dmitri Kuzmin, Hennes Hajduk, and Andreas Rupp. Locally bound-preserving enriched Galerkin methods for the linear advection equation. *Computers & Fluids*, 205:104525, 2020.
- [15] Dmitri Kuzmin, Hennes Hajduk, and Andreas Rupp. Limiter-based entropy stabilization of semi-discrete and fully discrete schemes for nonlinear hyperbolic problems. arXiv preprint arXiv:2107.11283, 2021.
- [16] TAJ Ouermi, Robert M Kirby, and Martin Berzins. Numerical testing of a new positivity-preserving interpolation algorithm. arXiv preprint arXiv:2009.08535, 2020.
- [17] Davide Torlo, Philipp Öffner, and Hendrik Ranocha. A new stability approach for positivity-preserving Patankar-type schemes. *arXiv preprint arXiv:2108.07347*, 2021.